Full wwPDB EM Validation Report

Feb 26, 2024 – 01:00 PM JST

PDB ID	:	8X19
EMDB ID	:	EMD-37988
Title	:	Structure of nucleosome-bound SRCAP-C in the ADP-BeFx-bound state
Authors	:	Yu, J.; Wang, Q.; Yu, Z.; Li, W.; Wang, L.; Xu, Y.
Deposited on	:	2023-11-06
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

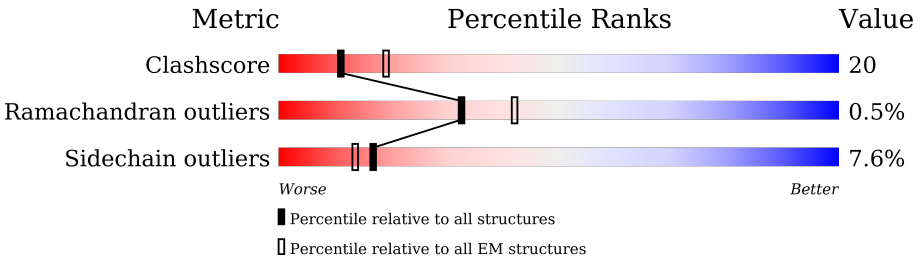
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	130	13% 24% 50% 9% 17%
1	E	130	6% 26% 43% 12% 19%
2	B	126	10% 31% 37% 8% 24%
2	F	126	37% 33% 5% 25%
3	C	136	12% 36% 28% 6% 30%
3	G	136	37% 32% 29%
4	D	103	5% 57% 21% 21%
4	H	103	41% 28% 9% 22%

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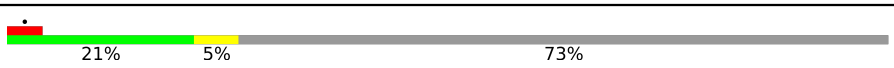
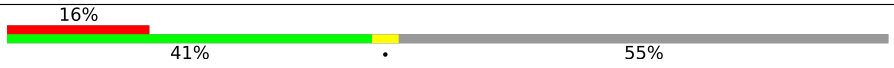
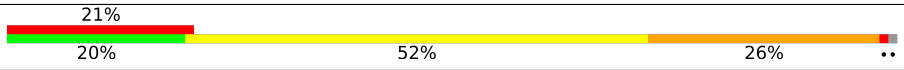
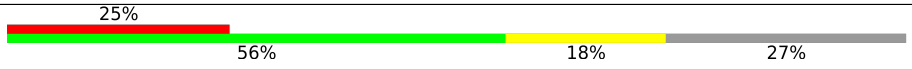
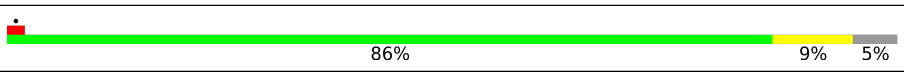
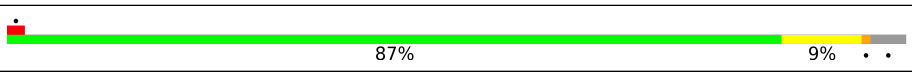
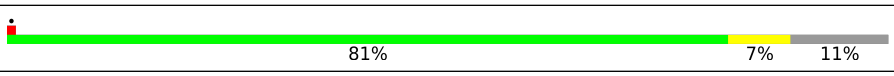
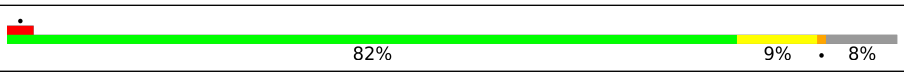
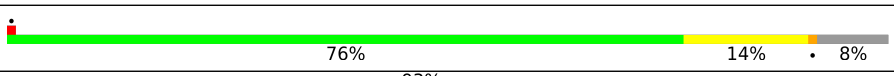
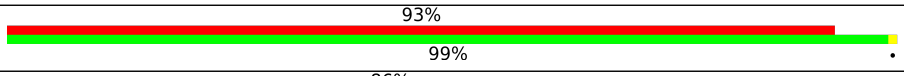
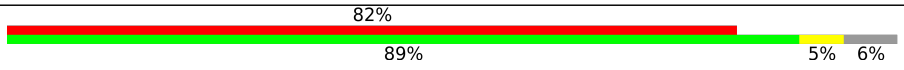
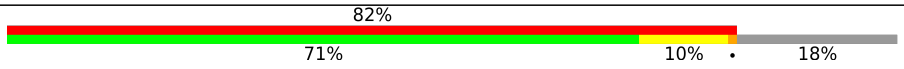
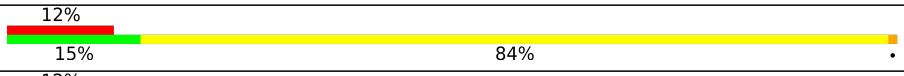
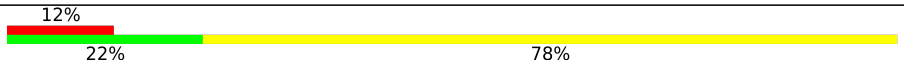
Mol	Chain	Length	Quality of chain
5	I	3230	
6	J	364	
7	K	396	
8	L	154	
9	M	456	
9	O	456	
9	Q	456	
10	N	463	
10	P	463	
10	R	463	
11	S	375	
11	U	375	
12	T	429	
13	V	467	
14	W	227	
15	X	147	
16	Y	147	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	BEF	I	3303	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 56704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	108	Total 833	C 525	N 165	O 143	0	0
1	E	105	Total 808	C 510	N 158	O 140	0	0

- Molecule 2 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	96	Total 755	C 473	N 138	O 142	S 2	0	0
2	F	94	Total 736	C 461	N 134	O 139	S 2	0	0

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total 779	C 491	N 148	O 136	S 4	0	0
3	G	97	Total 801	C 505	N 155	O 137	S 4	0	0

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	81	Total 646	C 407	N 126	O 112	S 1	0	0
4	H	80	Total 638	C 401	N 125	O 111	S 1	0	0

- Molecule 5 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	864	Total	C	N	O	S	0	0
			7122	4533	1314	1236	39		

- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	162	Total	C	N	O	S	0	0
			1350	846	260	239	5		

- Molecule 7 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	394	Total	C	N	O	S	0	0
			3209	2054	526	611	18		

- Molecule 8 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	113	Total	C	N	O	S	0	0
			893	546	173	165	9		

- Molecule 9 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	418	Total	C	N	O	S	0	0
			3213	2026	557	614	16		
9	O	435	Total	C	N	O	S	0	0
			3339	2105	571	646	17		
9	Q	440	Total	C	N	O	S	0	0
			3368	2121	579	651	17		

- Molecule 10 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	411	Total	C	N	O	S	0	0
			3185	1988	560	622	15		
10	P	427	Total	C	N	O	S	0	0
			3287	2054	576	642	15		
10	R	424	Total	C	N	O	S	0	0
			3293	2057	578	642	16		

- Molecule 11 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	375	Total	C	N	O	S	0	0
			2925	1850	491	561	23		
11	U	359	Total	C	N	O	S	0	0
			2802	1775	468	540	19		

- Molecule 12 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	403	Total	C	N	O	S	0	0
			3146	1988	535	599	24		

- Molecule 13 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	204	Total	C	N	O	S	0	0
			1757	1117	327	309	4		

- Molecule 14 is a protein called YEATS domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	187	Total	C	N	O	S	0	0
			1542	998	255	284	5		

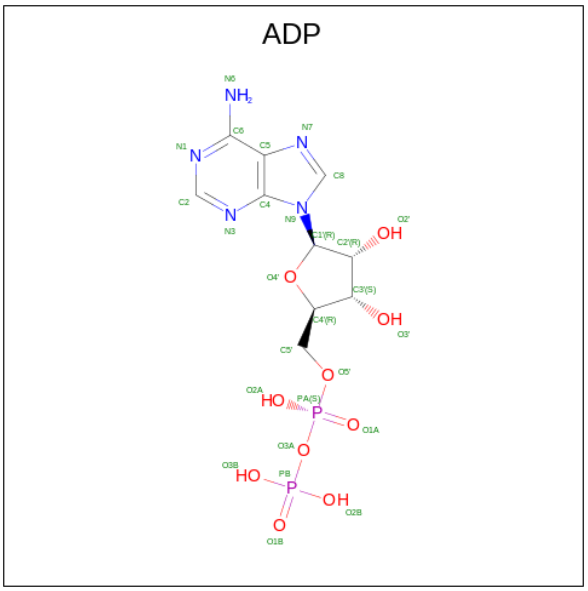
- Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	147	Total	C	N	O	P	0	0
			3031	1435	572	878	146		

- Molecule 16 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	147	Total	C	N	O	P	0	0
			2990	1422	540	882	146		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

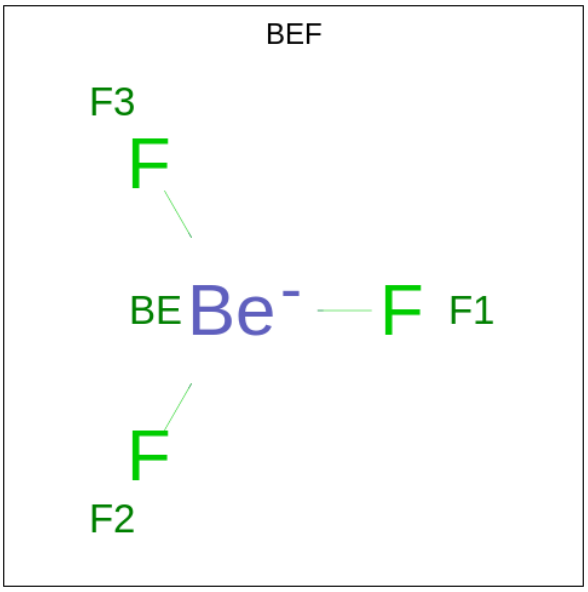


Mol	Chain	Residues	Atoms					AltConf
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	R	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

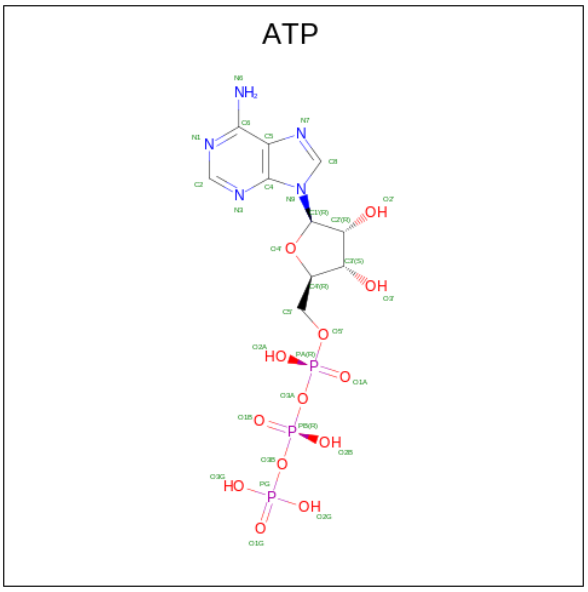
Mol	Chain	Residues	Atoms		AltConf
18	I	1	Total	Mg	0
			1	1	

- Molecule 19 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	I	1	Total	Be	F	0
			4	1	3	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

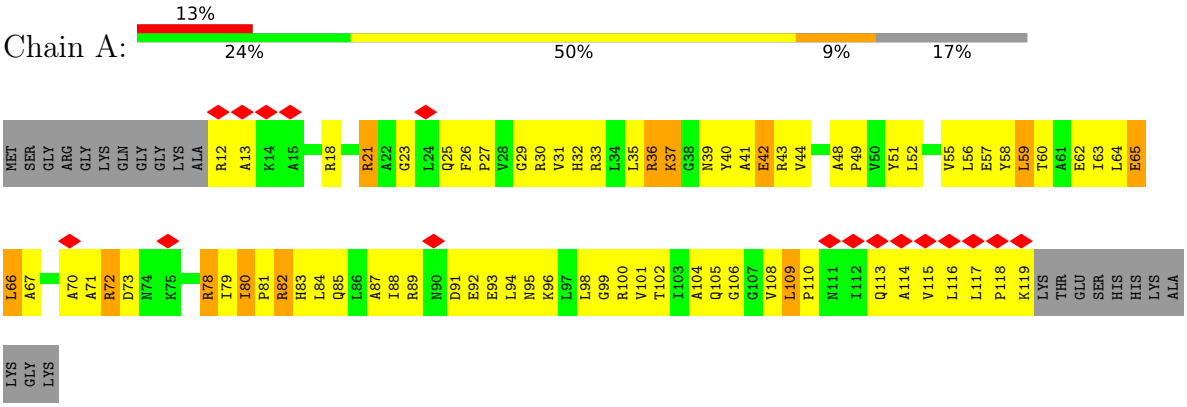


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	

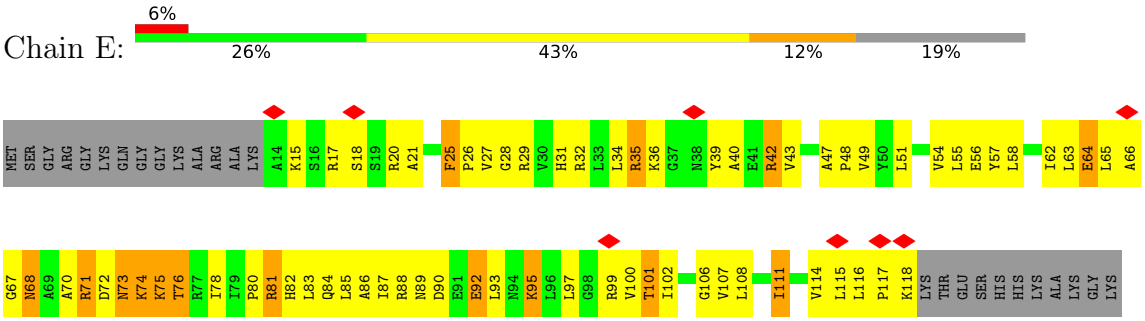
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

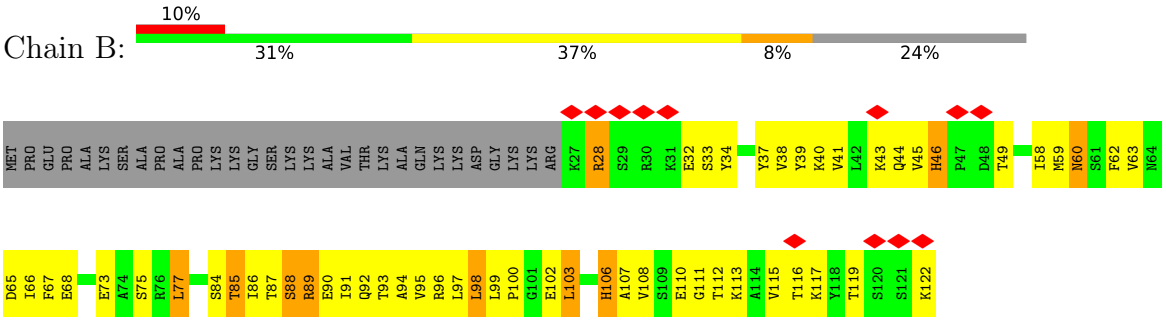
• Molecule 1: Histone H2A type 1-C



• Molecule 1: Histone H2A type 1-C

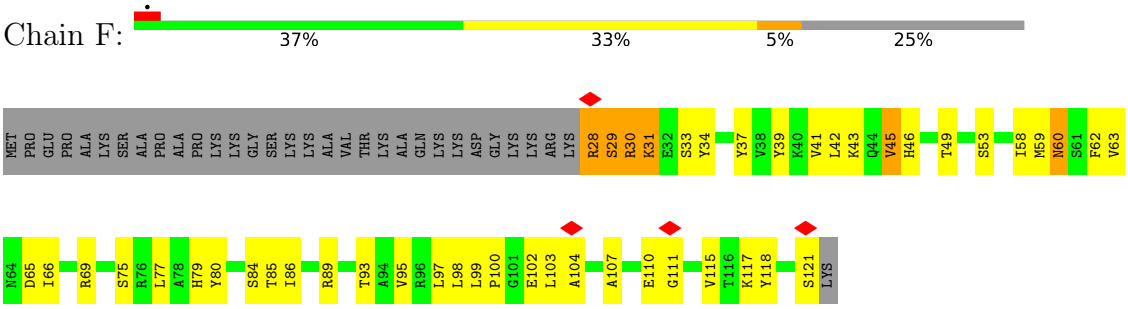


• Molecule 2: Histone H2B type 1-C/E/F/G/I



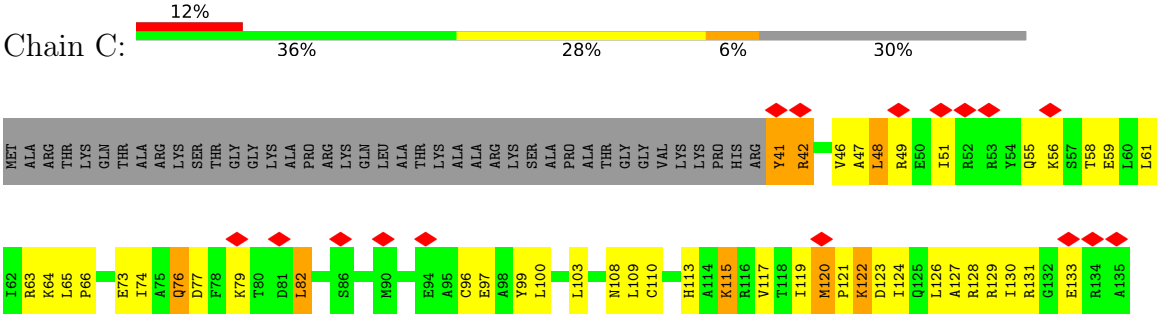
• Molecule 2: Histone H2B type 1-C/E/F/G/I

Chain F:



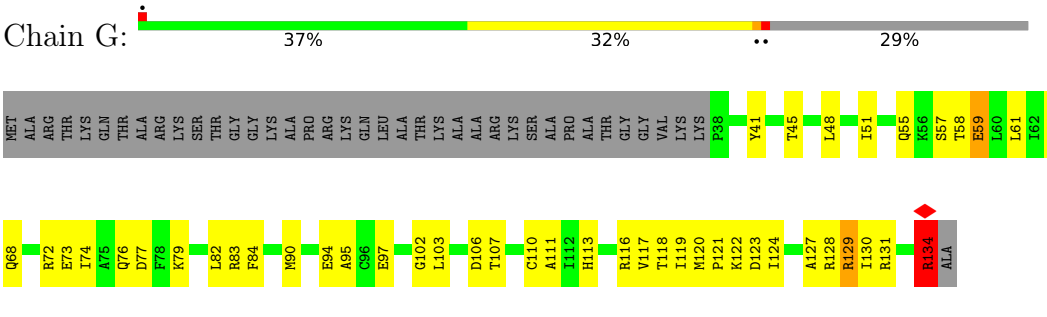
• Molecule 3: Histone H3.1

Chain C:



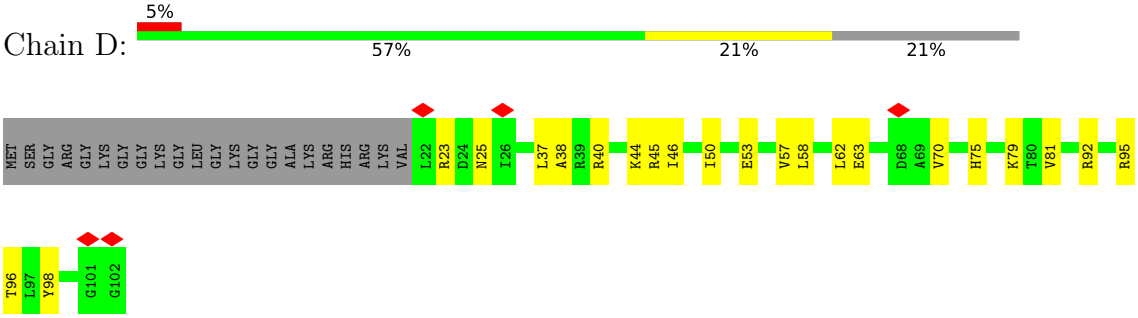
• Molecule 3: Histone H3.1

Chain G:



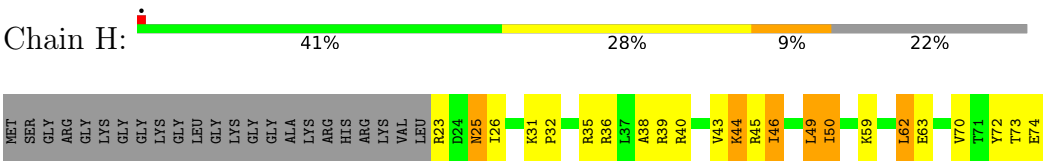
• Molecule 4: Histone H4

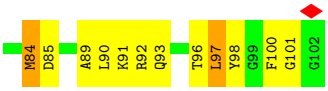
Chain D:



• Molecule 4: Histone H4

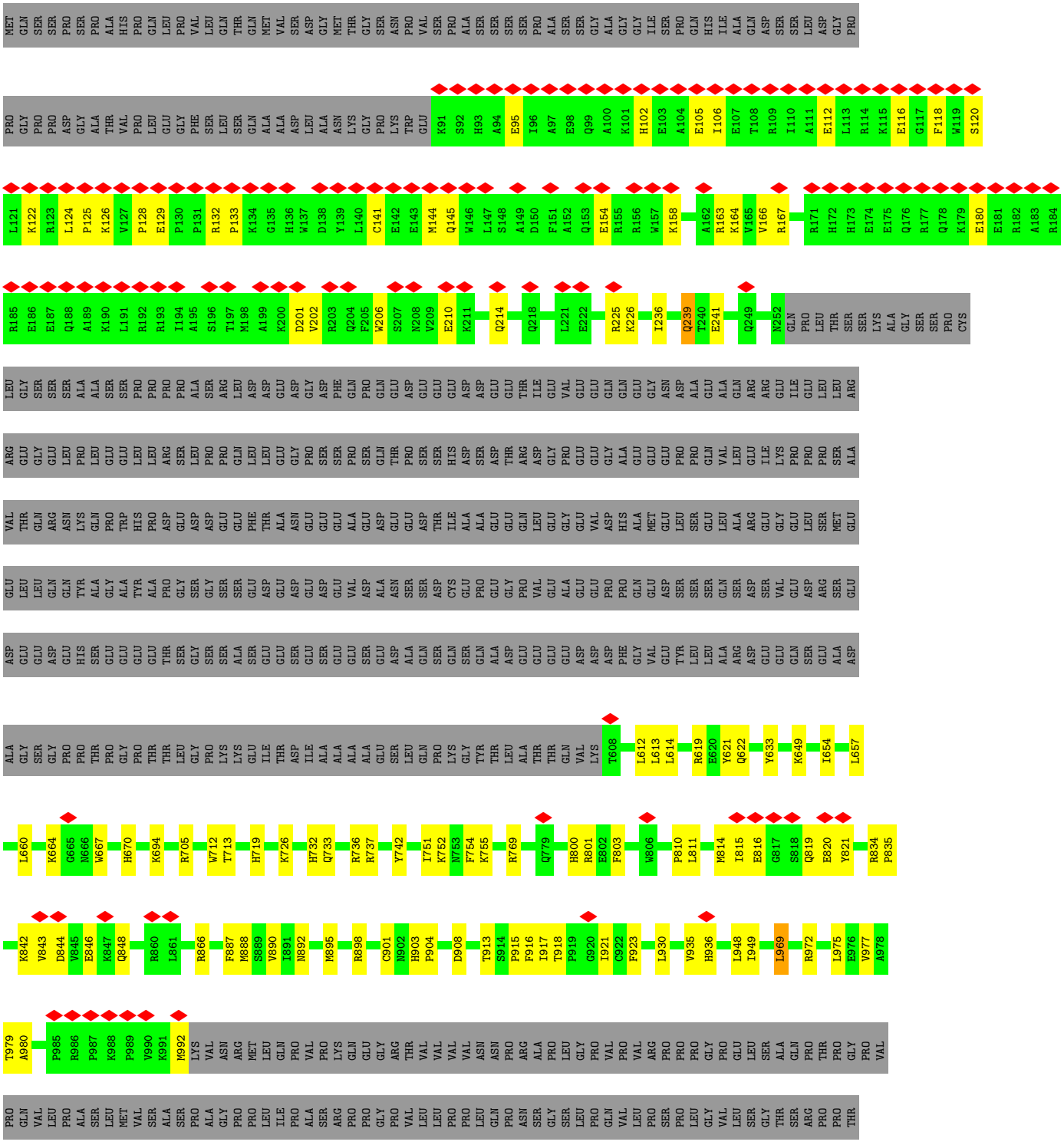
Chain H:

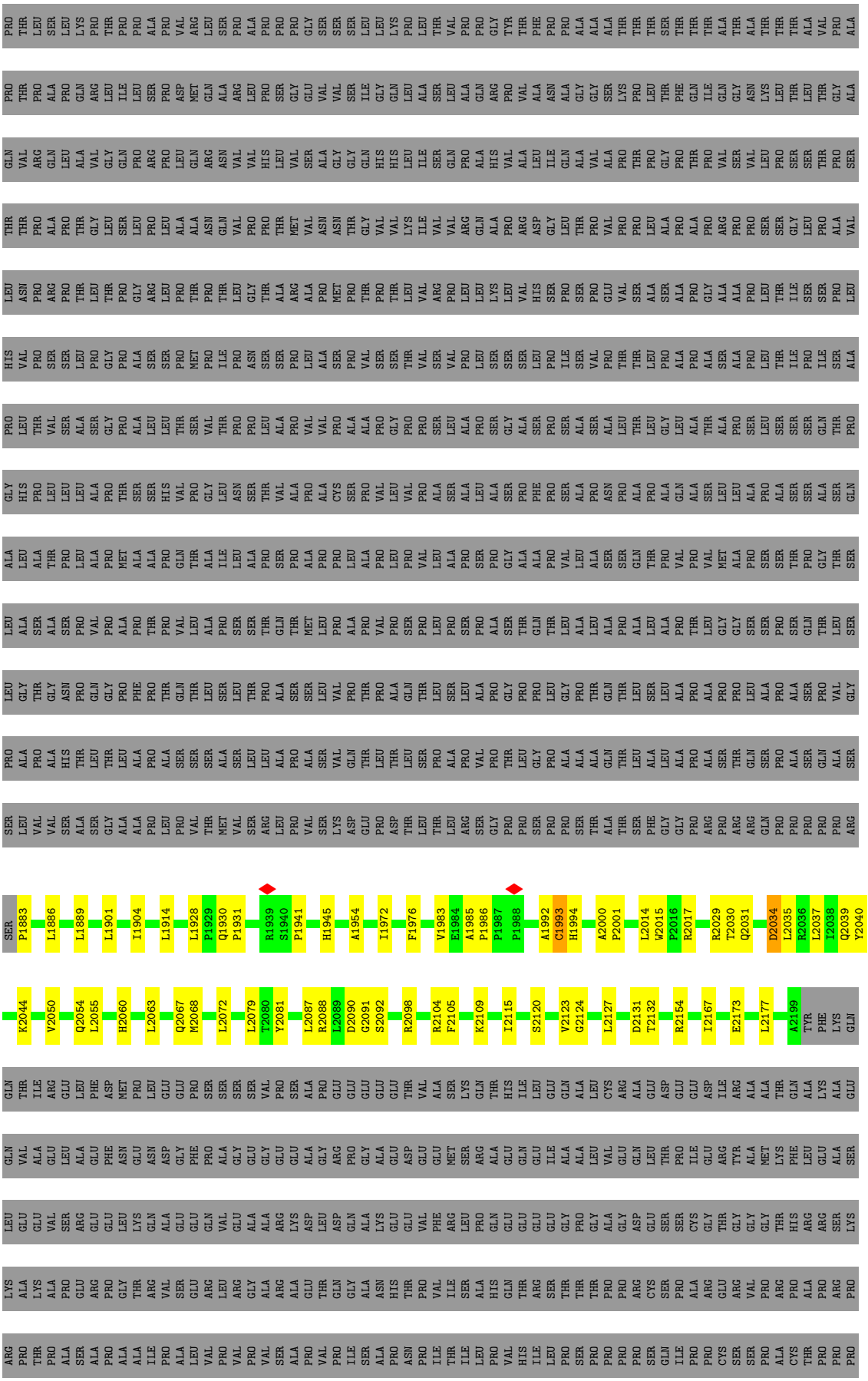




• Molecule 5: Helicase SRCAP

Chain I:




SER P1883 L1886 L1889 L1901 I1904 L1914 L1928 P1929 Q1930 P1931 R1939 S1940 P1941 H1945 A1954 I1972 F1976 V1983 E1984 A1985 P1986 P1987 P1988 A1992 C1993 H1994 A2000 P2001 L2014 W2015 P2016 R2017 R2029 T2030 Q2031 D2034 L2035 R2036 L2037 I2038 Q2039 Y2040
K2044 V2050 Q2054 L2055 H2060 L2063 Q2067 M2068 L2072 L2079 T2080 Y2081 L2087 R2088 L2089 D2090 G2091 S2092 R2098 R2104 F2105 K2109 I2115 S2120 V2123 G2124 L2127 D2131 T2132 R2154 I2167 E2173 L2177 A2199 TYR PHE LYS GLN

ALA CYS THR PRO PRO PRO ALA HIS THR PRO PRO PRO ALA GLN THR CYS LEU VAL THR PRO SER SER PRO LEU LEU LEU GLY PRO PRO SER VAL PRO ILE SER ALA SER VAL THR ASN LEU PRO LEU GLY LEU ARG PRO GLU ALA GLU LEU CYS ALA GLN ALA LEU ALA SER PRO GLU SER

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ALA PRO ASP SER ALA GLU GLY THR THR LEU THR VAL LEU PRO GLU GLY GLU GLU LEU PRO LEU CYS VAL SER GLU SER ASN GLY LEU GLU LEU PRO PRO SER ALA ALA SER ASP GLU PRO LEU GLN GLU PRO LEU GLU ALA ASP ARG THR SER GLU GLU LEU THR GLU ALA LYS THR PRO

THR SER SER PRO GLU LYS PRO GLN GLU LEU VAL THR ALA GLU VAL ALA ALA PRO SER THR SER SER ALA THR SER SER PRO GLU GLY PRO SER PRO ALA ARG PRO PRO ARG ARG THR SER ALA ASP VAL GLU ILE ARG GLY GLN GLY THR GLY ARG PRO GLY GLN PRO PRO GLY

PRO LYS VAL LEU ARG LYS LEU PRO GLY ARG LEU VAL THR VAL VAL GLU GLU LYS GLU LEU VAL ARG ARG ARG ARG GLN GLN ARG GLY ALA ALA SER THR LEU VAL PRO GLY VAL SER GLU THR SER ALA SER PRO GLY SER PRO SER VAL ARG SER MET SER GLY PRO GLU SER SER PRO

PRO ILE GLY GLY PRO CYS GLU ALA ALA PRO SER SER SER LEU PRO THR PRO PRO GLN GLN PRO PHE ILE ALA ARG ARG HIS ILE GLU LEU GLY VAL THR GLY GLY GLY SER PRO GLU ASN GLY ASP GLY ALA LEU LEU ALA ILE THR PRO PRO ALA VAL LYS ARG ARG ARG GLY ARG PRO

PRO LYS LYS ASN ARG SER PRO ALA ASP ALA GLY ARG GLY VAL ASP GLU ALA PRO SER SER THR LEU LYS GLY LYS THR ASN GLY ALA ASP PRO VAL PRO GLY PRO GLU THR LEU ILE VAL ALA ASP PRO VAL LEU GLU PRO GLN LEU ILE PRO GLY PRO GLN PRO LEU GLY PRO GLN PRO

VAL HIS ARG PRO ASN PRO LEU LEU SER PRO VAL GLU LYS ARG ARG GLY ARG PRO PRO LYS ALA ARG ASP LEU PRO ILE PRO GLY THR ILE SER SER ALA GLY ASP GLY ASN SER GLU SER ARG THR GLN PRO PRO HIS PRO SER PRO LEU THR PRO LEU PRO PRO LEU LEU VAL

CYS PRO THR ALA THR VAL ALA ASN THR VAL THR THR VAL THR ILE SER THR SER PRO PRO LYS ARG LYS ARG GLY ARG PRO PRO LYS ASN PRO PRO SER PRO ARG PRO SER GLN LEU PRO VAL LEU ASP ARG ASP SER THR SER VAL LEU GLU SER CYS GLY LEU GLY ARG ARG GLN

PRO GLN GLY GLN GLY GLU SER GLU GLY SER SER SER ASP GLU ASP GLY SER ARG PRO LEU THR ARG LEU ALA ARG LEU ARG LEU GLU ALA GLU GLY MET ARG GLY ARG LYS SER GLY GLY SER MET VAL VAL ALA VAL ILE GLN ASP ASP LEU ASP LEU ALA ASP SER GLY PRO GLY GLY

LEU GLU LEU THR PRO PRO VAL VAL SER LEU THR PRO LYS LEU ARG SER THR ARG LEU ARG PRO GLY SER LEU VAL PRO PRO LEU GLU THR GLU LYS LEU PRO ARG LYS ARG ALA GLY ALA PRO VAL GLY GLY SER PRO GLY LEU ALA LYS ARG GLY ARG LEU GLN PRO PRO SER PRO LEU

GLY PRO GLU GLY SER VAL GLU GLU SER GLU ALA GLU ALA SER GLY GLU GLU GLU GLY ASP GLY THR PRO ARG ARG ARG PRO GLY PRO ARG ARG LEU VAL GLY THR THR ASN GLN GLY ASP GLN ARG ILE LEU ARG SER SER ALA PRO PRO SER LEU ALA GLY PRO ALA VAL SER HIS

ARG GLY ARG LYS ALA LYS THR

- Molecule 6: Vacuolar protein sorting-associated protein 72 homolog

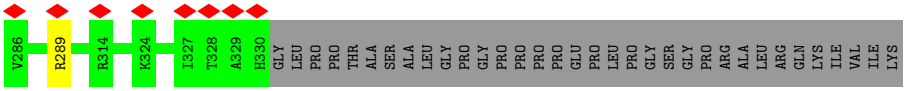
Chain J: 16% 41% • 55%

MET SER LEU ALA GLY GLY ARG ALA PRO ARG LYS THR ALA GLY ASN ARG LEU SER GLY LEU LEU GLU ALA GLU GLU GLU ASP GLU PHE TYR GLN THR THR TYR GLY GLY PHE THR GLU GLU SER GLY ASP ASP GLU TYR GLN GLY ASP GLN SER ASP THR GLU ASP GLU VAL ASP SER ASP

PHE ASP ILE ASP GLU GLY ASP GLU PRO SER SER ASP GLY GLU ALA GLU GLU PRO ARG ARG LYS ARG ARG VAL VAL THR LYS ALA TYR LYS GLU PRO LEU LYS SER LEU ARG PRO ARG LYS VAL ASN THR PRO ALA GLY SER SER GLN LYS ALA ARG GLU GLU LYS ALA LEU LEU PRO LEU

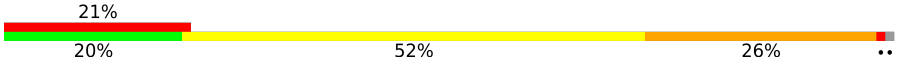
GLU LEU GLN ASP ASP GLY SER ASP SER R130 H140 T141 R142 Q143 T144 F145 L146 R147 V148 Q149 E150 R151 Q152 G153 Q154 S155 R156 R157 R158 K159 G160 P161 H162 C163 E164 R165 P166 L167 T168 Q169 K177 I178 T179 E180 T189 Y190 E191 R192 L193 E194 A195 D196 K197 K198 K199 Q200 V201

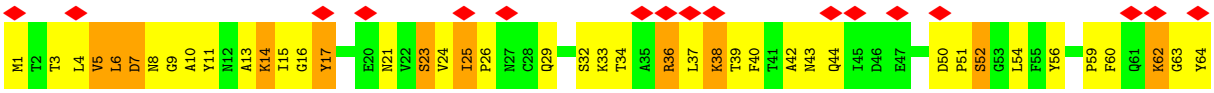
H202 K203 K204 R205 K206 C207 P210 P220 LEU VAL GLY GLU PRO GLY PRO LYS GLU GLU ASN VAL ASP ILE GLU GLY LEU ASP PRO ALA PRO SER VAL SER ALA LEU THR PRO HIS ALA GLY THR GLY PRO VAL ASN PRO PRO ALA R260 S269 E276 Q280 G281 R282 K285

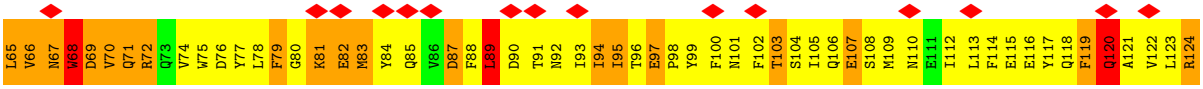


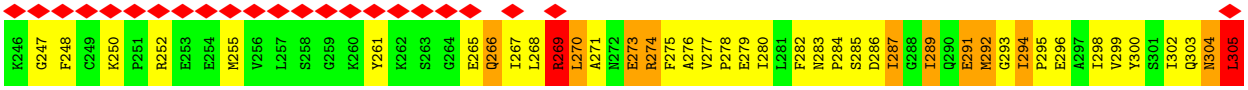
• Molecule 7: Actin-related protein 6

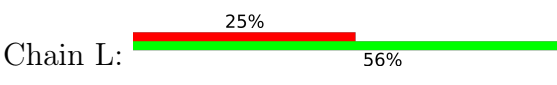
Chain K:





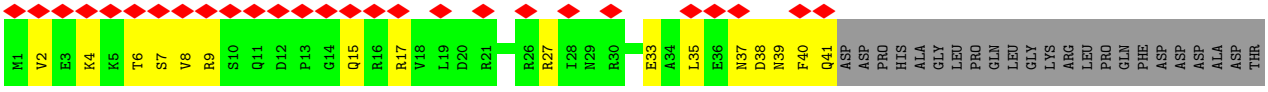


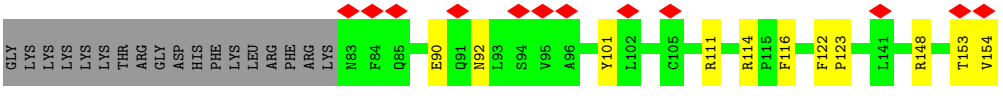




• Molecule 8: Zinc finger HIT domain-containing protein 1

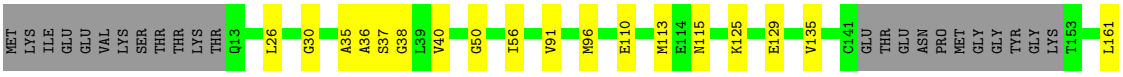
Chain L:

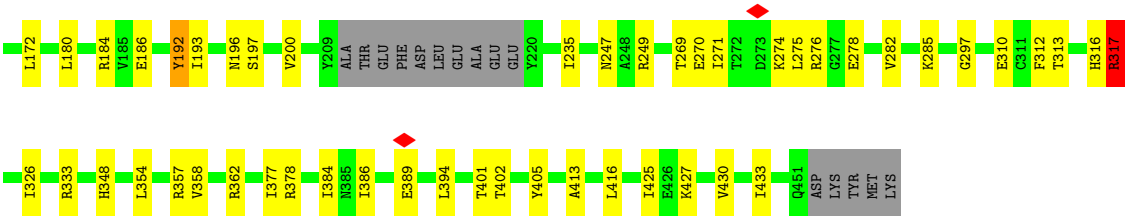




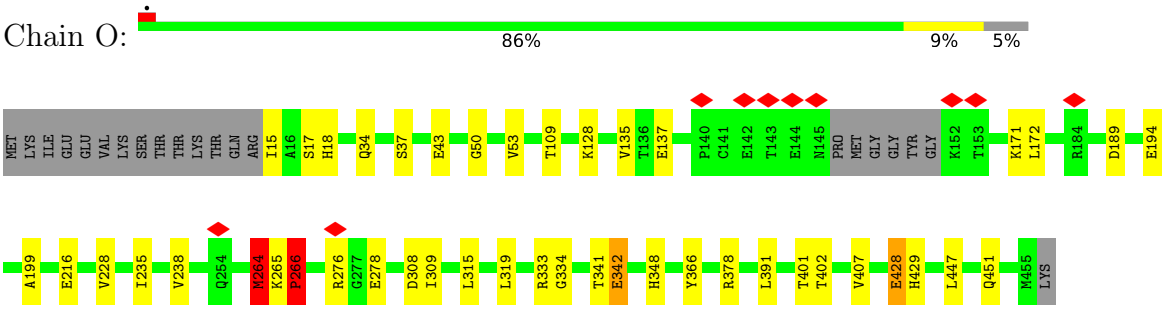
• Molecule 9: RuvB-like 1

Chain M:

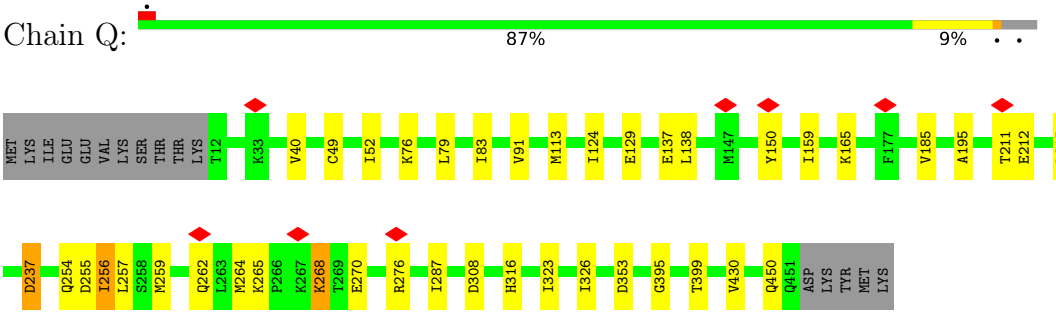




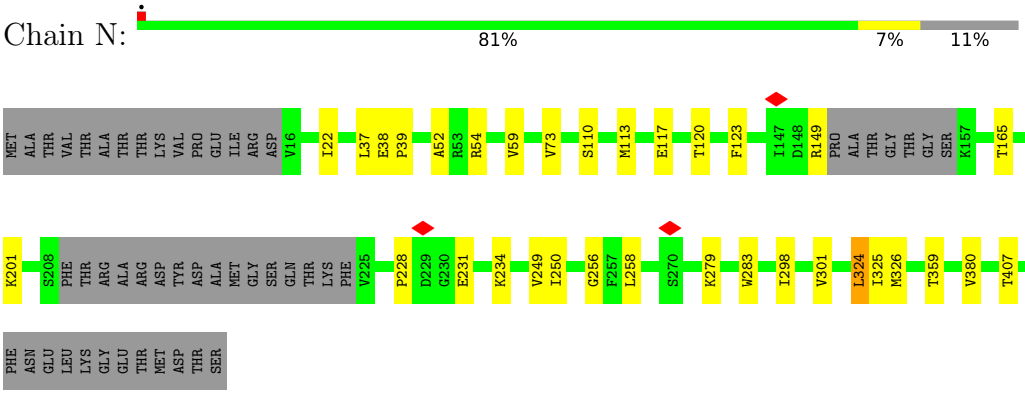
• Molecule 9: RuvB-like 1



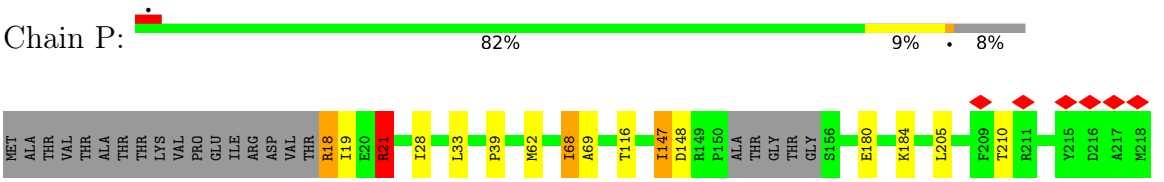
• Molecule 9: RuvB-like 1

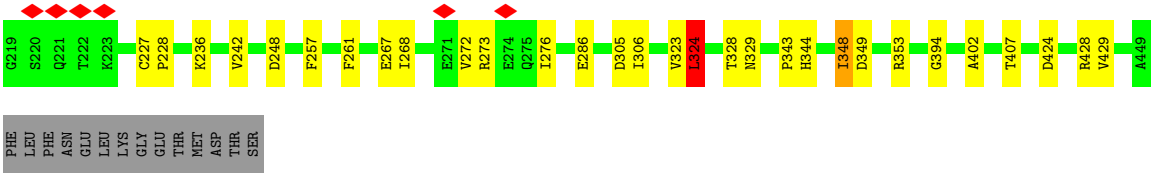


• Molecule 10: RuvB-like 2



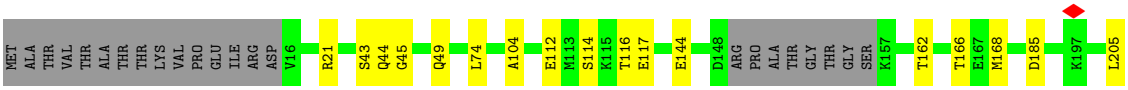
• Molecule 10: RuvB-like 2

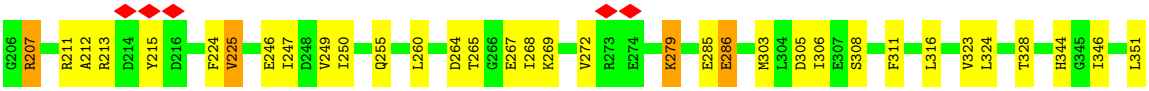




• Molecule 10: RuvB-like 2

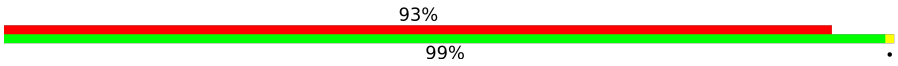
Chain R:

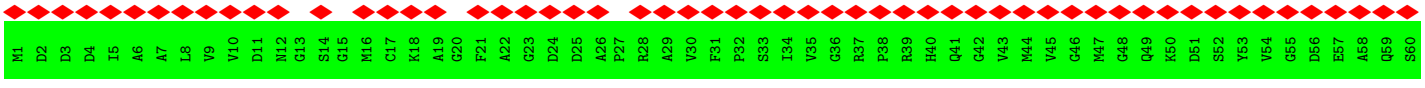


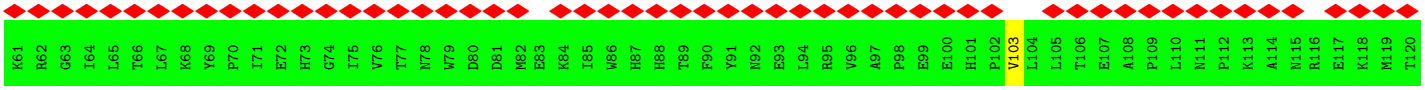


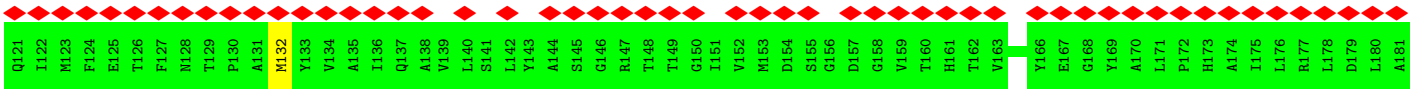
• Molecule 11: Actin, cytoplasmic 1

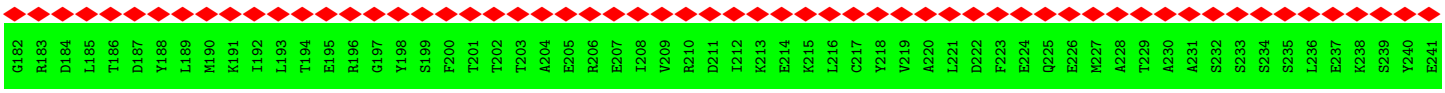
Chain S:

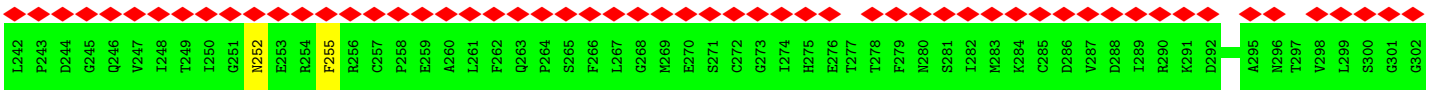


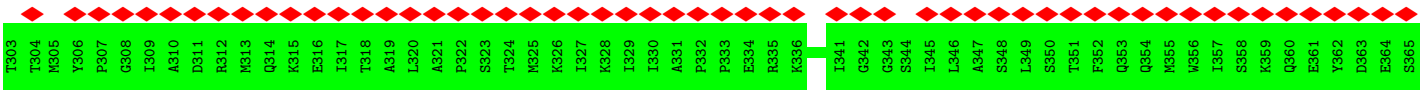


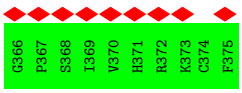






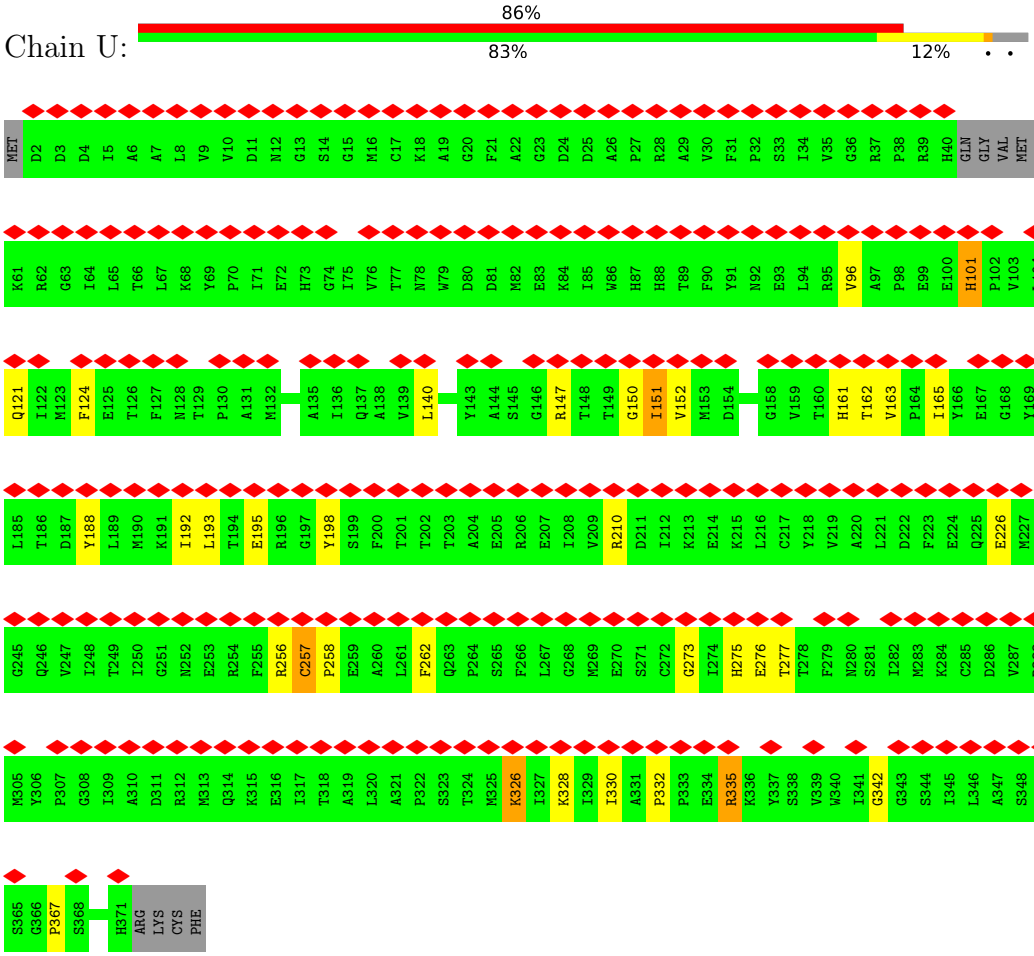






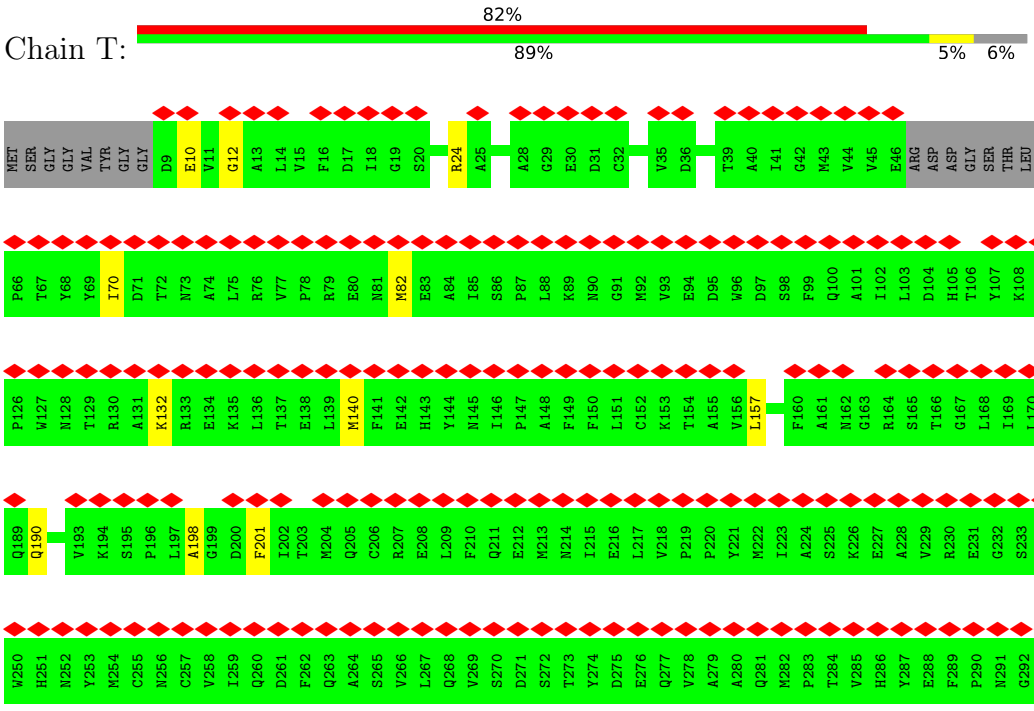
• Molecule 11: Actin, cytoplasmic 1

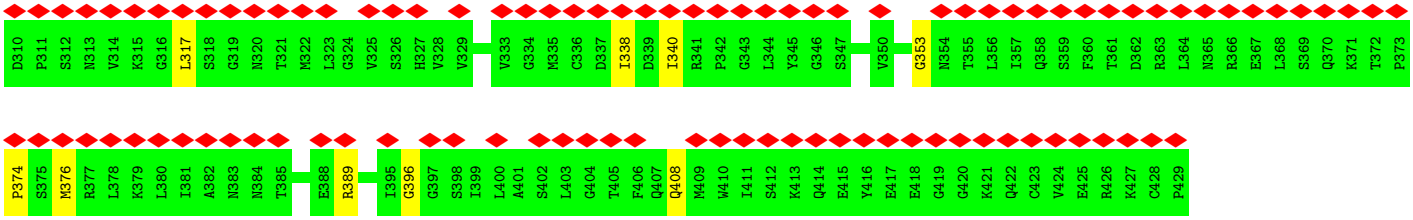
Chain U:



• Molecule 12: Actin-like protein 6A

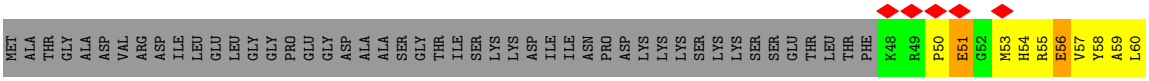
Chain T:

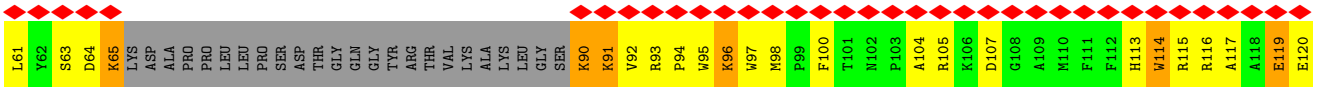


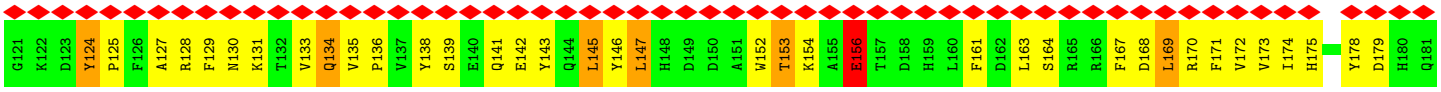


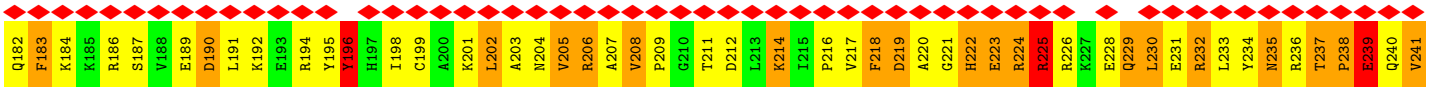
• Molecule 13: DNA methyltransferase 1-associated protein 1

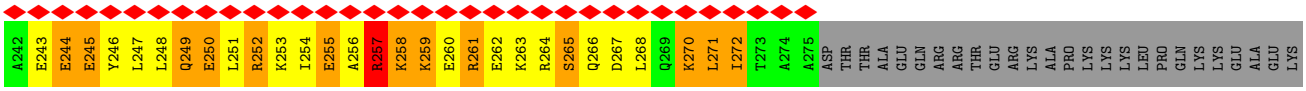
Chain V:





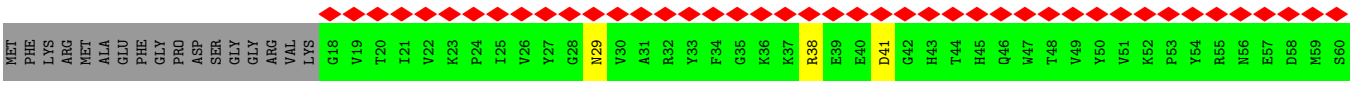


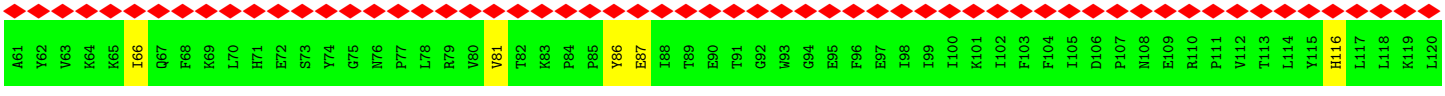


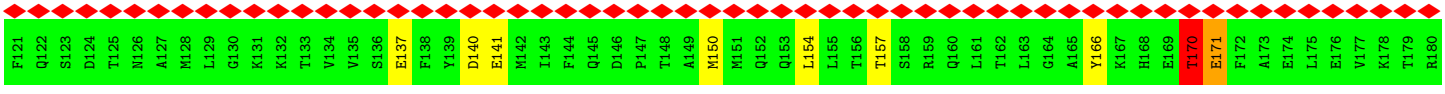


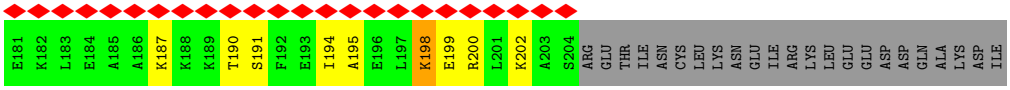
• Molecule 14: YEATS domain-containing protein 4

Chain W:



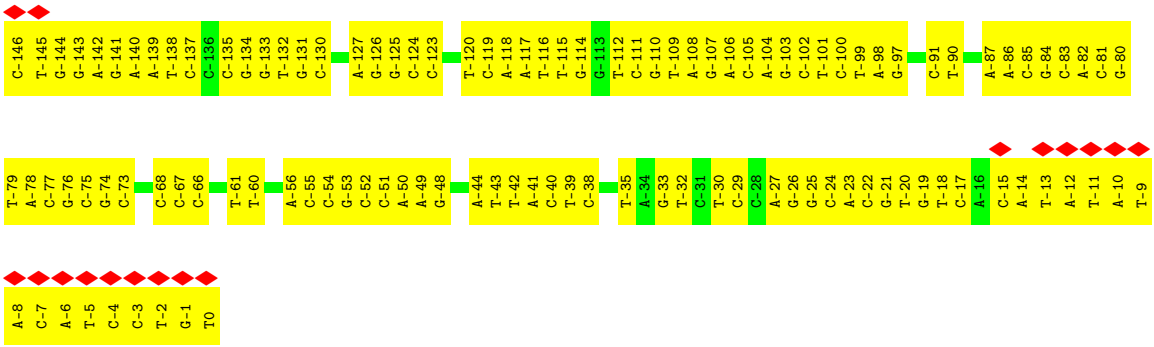






• Molecule 15: DNA (147-MER)

• Molecule 16: DNA (147-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	475617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.115	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	533.6, 533.6, 533.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ATP, ADP, MG

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	0.31	0/843	0.58	0/1136
1	E	0.26	0/818	0.54	0/1104
2	B	0.27	0/766	0.50	0/1026
2	F	0.27	0/747	0.50	0/1004
3	C	0.28	0/789	0.56	0/1057
3	G	0.27	0/813	0.56	0/1090
4	D	0.30	0/653	0.58	0/873
4	H	0.25	0/645	0.56	0/862
5	I	0.32	0/7296	0.62	1/9855 (0.0%)
6	J	0.34	0/1381	0.62	0/1861
7	K	0.31	0/3283	0.55	2/4445 (0.0%)
8	L	0.35	0/909	0.63	0/1227
9	M	0.31	0/3253	0.58	0/4382
9	O	0.32	0/3382	0.57	0/4559
9	Q	0.31	0/3413	0.56	1/4603 (0.0%)
10	N	0.30	0/3217	0.60	1/4328 (0.0%)
10	P	0.30	0/3324	0.60	1/4477 (0.0%)
10	R	0.30	0/3329	0.60	0/4479
11	S	0.29	0/2988	0.50	0/4045
11	U	0.31	0/2863	0.56	0/3882
12	T	0.29	0/3217	0.50	0/4362
13	V	0.57	5/1801 (0.3%)	0.67	2/2419 (0.1%)
14	W	0.37	1/1578 (0.1%)	0.53	0/2128
15	X	0.58	0/3405	0.95	2/5259 (0.0%)
16	Y	0.56	0/3349	0.93	0/5162
All	All	0.36	6/58062 (0.0%)	0.64	10/79625 (0.0%)

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	G	0	1
5	I	0	1
9	M	0	1
10	P	0	2
10	R	0	1
13	V	0	3
14	W	0	1
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	156	GLU	CD-OE1	8.47	1.34	1.25
13	V	183	PHE	CD1-CE1	8.17	1.55	1.39
13	V	183	PHE	CE2-CZ	6.55	1.49	1.37
14	W	198	LYS	CD-CE	6.44	1.67	1.51
13	V	196	TYR	CD1-CE1	-5.59	1.30	1.39
13	V	156	GLU	CD-OE2	-5.16	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	89	LEU	CB-CG-CD2	-7.39	98.43	111.00
7	K	89	LEU	CA-CB-CG	6.25	129.68	115.30
15	X	89	DA	O4'-C1'-N9	6.19	112.33	108.00
13	V	156	GLU	CG-CD-OE2	-6.15	106.01	118.30
9	Q	79	LEU	CA-CB-CG	5.68	128.36	115.30
13	V	156	GLU	CG-CD-OE1	5.67	129.63	118.30
10	P	324	LEU	CA-CB-CG	5.65	128.30	115.30
10	N	324	LEU	CA-CB-CG	5.34	127.59	115.30
5	I	969	LEU	CA-CB-CG	5.32	127.54	115.30
15	X	91	DG	O4'-C4'-C3'	-5.04	102.49	104.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	134	ARG	Sidechain
5	I	2029	ARG	Sidechain
9	M	317	ARG	Sidechain
10	P	18	ARG	Sidechain
10	P	21	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	R	213	ARG	Sidechain
13	V	225	ARG	Sidechain
13	V	257	ARG	Sidechain
13	V	261	ARG	Mainchain
14	W	170	THR	Peptide

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	833	0	895	184	0
1	E	808	0	864	118	0
2	B	755	0	782	136	0
2	F	736	0	756	68	0
3	C	779	0	816	72	0
3	G	801	0	839	93	0
4	D	646	0	687	36	0
4	H	638	0	676	63	0
5	I	7122	0	7212	309	0
6	J	1350	0	1370	28	0
7	K	3209	0	3132	518	0
8	L	893	0	880	52	0
9	M	3213	0	3331	90	0
9	O	3339	0	3425	28	0
9	Q	3368	0	3453	33	0
10	N	3185	0	3269	44	0
10	P	3287	0	3335	22	0
10	R	3293	0	3373	41	0
11	S	2925	0	2891	2	0
11	U	2802	0	2760	34	0
12	T	3146	0	3086	20	0
13	V	1757	0	1736	326	0
14	W	1542	0	1556	70	0
15	X	3031	0	1650	241	0
16	Y	2990	0	1652	182	0
17	I	27	0	12	6	0
17	M	27	0	12	0	0
17	N	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	27	0	12	1	0
17	P	27	0	12	0	0
17	Q	27	0	12	1	0
17	R	27	0	12	0	0
18	I	1	0	0	0	0
19	I	4	0	0	3	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
All	All	56704	0	54534	2263	0

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 20.

All (2263) 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)
9:M:313:THR:HA	9:M:316:HIS:CE1	1.28	1.63
1:A:13:ALA:HB2	5:I:164:LYS:CD	1.25	1.61
9:M:413:ALA:HA	9:M:433:ILE:CD1	1.35	1.53
5:I:936:HIS:CE1	10:N:279:LYS:HZ3	1.29	1.48
5:I:936:HIS:HE1	10:N:279:LYS:NZ	1.08	1.47
5:I:2063:LEU:HD21	5:I:2127:LEU:CD2	1.44	1.46
5:I:732:HIS:HD2	5:I:736:ARG:NH1	1.17	1.41
5:I:2014:LEU:HD12	9:Q:259:MET:SD	1.62	1.39
6:J:269:SER:HB2	9:Q:150:TYR:CD1	1.55	1.39
5:I:936:HIS:CE1	10:N:279:LYS:NZ	1.87	1.35
5:I:732:HIS:CD2	5:I:736:ARG:HH12	1.45	1.33
1:A:13:ALA:CB	5:I:164:LYS:HD2	1.60	1.31
5:I:921:ILE:CG2	5:I:1986:PRO:HD2	1.62	1.28
1:A:13:ALA:CB	5:I:164:LYS:CD	2.14	1.25
5:I:969:LEU:HD22	10:R:224:PHE:O	1.31	1.25
5:I:921:ILE:HG21	5:I:1986:PRO:CD	1.66	1.24
5:I:949:ILE:HG21	9:M:247:ASN:O	1.11	1.23
9:M:26:LEU:HD22	9:M:30:GLY:O	1.37	1.23
5:I:949:ILE:CG2	9:M:247:ASN:O	1.87	1.22
9:M:313:THR:CA	9:M:316:HIS:CE1	2.21	1.22
6:J:269:SER:HB2	9:Q:150:TYR:CG	1.73	1.22
6:J:269:SER:CB	9:Q:150:TYR:HB3	1.73	1.19
5:I:1983:VAL:CG2	9:O:238:VAL:HG11	1.76	1.16
1:E:20:ARG:CG	2:F:121:SER:OG	1.92	1.16
5:I:1972:ILE:HG23	5:I:1976:PHE:CD2	1.80	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2063:LEU:HD21	5:I:2127:LEU:HD21	1.27	1.15
9:M:413:ALA:CA	9:M:433:ILE:CD1	2.26	1.15
5:I:660:LEU:HD23	5:I:742:TYR:CZ	1.82	1.14
5:I:2014:LEU:CD1	9:Q:259:MET:SD	2.34	1.14
5:I:2060:HIS:NE2	5:I:2132:THR:HG21	1.59	1.14
8:L:27:ARG:HE	8:L:153:THR:CG2	1.61	1.13
9:O:34:GLN:OE1	9:O:43:GLU:OE2	1.65	1.12
5:I:732:HIS:CD2	5:I:736:ARG:NH1	2.10	1.12
5:I:667:TRP:NE1	5:I:719:HIS:ND1	1.98	1.11
6:J:269:SER:CA	9:Q:150:TYR:HB3	1.81	1.11
13:V:239:GLU:HA	13:V:243:GLU:HB2	1.33	1.11
5:I:921:ILE:HG22	5:I:1985:ALA:HB1	1.29	1.11
9:M:113:MET:HG3	9:M:276:ARG:NH1	1.65	1.10
1:E:67:GLY:HA2	1:E:78:ILE:HG12	1.32	1.10
8:L:27:ARG:HE	8:L:153:THR:HG22	1.17	1.10
13:V:136:PRO:HB2	13:V:202:LEU:HD12	1.31	1.09
5:I:969:LEU:CD2	10:R:224:PHE:O	2.01	1.08
15:X:22:DG:H2"	15:X:23:DT:H5"	1.23	1.08
5:I:2060:HIS:NE2	5:I:2132:THR:CG2	2.14	1.08
16:Y:-140:DA:H2"	16:Y:-139:DA:H5"	1.36	1.07
5:I:667:TRP:HE1	5:I:719:HIS:CE1	1.72	1.06
5:I:810:PRO:O	5:I:814:MET:HG2	1.53	1.06
9:M:413:ALA:HA	9:M:433:ILE:HD12	1.32	1.06
6:J:269:SER:CB	9:Q:150:TYR:CB	2.34	1.06
7:K:56:TYR:HB2	8:L:39:ASN:ND2	1.70	1.06
13:V:153:THR:HG23	13:V:156:GLU:HB2	1.36	1.05
5:I:667:TRP:NE1	5:I:719:HIS:CE1	2.24	1.05
1:A:13:ALA:HB2	5:I:164:LYS:HD2	1.07	1.05
5:I:670:HIS:NE2	5:I:742:TYR:HD2	1.53	1.05
9:M:413:ALA:HA	9:M:433:ILE:HD13	1.36	1.04
9:M:110:GLU:OE2	9:M:276:ARG:NH2	1.89	1.04
8:L:27:ARG:NE	8:L:153:THR:HG22	1.73	1.03
5:I:621:TYR:CE2	5:I:846:GLU:OE1	2.11	1.03
13:V:96:LYS:HD2	13:V:98:MET:HG2	1.38	1.02
5:I:949:ILE:HG22	10:R:260:LEU:HD22	1.36	1.02
5:I:163:ARG:O	5:I:166:VAL:HG22	1.58	1.02
7:K:6:LEU:HD12	7:K:93:ILE:HD11	1.41	1.02
6:J:269:SER:CB	9:Q:150:TYR:CG	2.42	1.02
1:E:20:ARG:HG3	2:F:121:SER:OG	1.59	1.01
5:I:921:ILE:HD13	5:I:1986:PRO:HG2	1.38	1.01
5:I:2063:LEU:HD21	5:I:2127:LEU:HD23	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2063:LEU:CD2	5:I:2127:LEU:CD2	2.39	1.00
9:M:313:THR:HA	9:M:316:HIS:ND1	1.76	1.00
13:V:264:ARG:HH12	14:W:194:ILE:HD13	1.23	0.99
7:K:81:LYS:HA	7:K:85:GLN:HA	1.42	0.99
13:V:233:LEU:HA	13:V:236:ARG:HD3	1.38	0.99
5:I:660:LEU:HD23	5:I:742:TYR:OH	1.62	0.99
5:I:660:LEU:CD2	5:I:742:TYR:OH	2.10	0.99
5:I:901:CYS:O	5:I:2044:LYS:CE	2.11	0.99
5:I:670:HIS:CE1	5:I:742:TYR:CD2	2.51	0.99
1:A:13:ALA:HB2	5:I:164:LYS:HD3	1.02	0.98
5:I:670:HIS:NE2	5:I:742:TYR:CD2	2.31	0.98
6:J:269:SER:HA	9:Q:150:TYR:HB3	1.40	0.98
7:K:56:TYR:CB	8:L:39:ASN:HD21	1.75	0.98
15:X:48:DC:H2"	15:X:49:DT:H71	1.45	0.98
7:K:146:ILE:HD11	7:K:317:ILE:HG12	1.44	0.97
1:A:59:LEU:HD11	2:B:66:ILE:HG21	1.44	0.97
4:D:23:ARG:HH21	14:W:81:VAL:HG11	1.28	0.97
5:I:2087:LEU:HD11	5:I:2104:ARG:NH1	1.79	0.97
3:C:127:ALA:HA	3:G:130:ILE:HD13	1.42	0.97
9:M:413:ALA:HA	9:M:433:ILE:HD11	1.45	0.96
13:V:237:THR:HG23	13:V:238:PRO:HD3	1.46	0.96
5:I:2072:LEU:HB3	5:I:2088:ARG:HD2	1.45	0.96
11:U:121:GLN:NE2	13:V:95:TRP:O	1.98	0.96
9:M:110:GLU:HG2	9:M:269:THR:HG22	1.48	0.96
10:N:38:GLU:OE1	10:N:54:ARG:NH1	1.98	0.96
15:X:51:DG:H1'	15:X:52:DG:H5'	1.46	0.96
6:J:269:SER:CB	9:Q:150:TYR:CD1	2.48	0.95
16:Y:-50:DA:H2"	16:Y:-49:DA:H5"	1.48	0.95
9:M:313:THR:HA	9:M:316:HIS:HE1	1.17	0.94
16:Y:-14:DA:H2"	16:Y:-13:DT:C7	1.97	0.94
3:G:73:GLU:HA	4:H:23:ARG:HH22	1.32	0.94
10:N:73:VAL:HB	10:N:325:ILE:HG12	1.50	0.94
13:V:264:ARG:HB3	14:W:198:LYS:CE	1.95	0.94
16:Y:-52:DC:H1'	16:Y:-51:DC:H5'	1.47	0.94
2:F:29:SER:HB3	16:Y:-119:DC:H4'	1.47	0.94
5:I:163:ARG:O	5:I:166:VAL:CG2	2.15	0.93
13:V:264:ARG:HB3	14:W:198:LYS:HE2	1.47	0.93
16:Y:-145:DT:H2"	16:Y:-144:DG:H5"	1.46	0.93
7:K:234:ILE:HD12	7:K:271:ALA:HA	1.47	0.93
15:X:73:DG:O6	16:Y:-73:DC:N4	2.01	0.93
1:A:21:ARG:HH11	1:A:21:ARG:HB2	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HB2	2:B:62:PHE:HZ	1.30	0.93
5:I:921:ILE:HD13	5:I:1986:PRO:CG	1.98	0.93
9:M:193:ILE:HG12	9:M:200:VAL:HG22	1.49	0.93
5:I:2120:SER:OG	15:X:55:DG:O5'	1.85	0.92
13:V:98:MET:SD	13:V:115:ARG:HB2	2.09	0.92
7:K:128:GLY:HA2	7:K:147:ILE:HG21	1.48	0.92
4:D:23:ARG:HH21	14:W:81:VAL:CG1	1.82	0.92
5:I:1972:ILE:HG23	5:I:1976:PHE:HD2	1.24	0.92
5:I:936:HIS:HE1	10:N:279:LYS:HZ1	0.95	0.92
5:I:921:ILE:HG21	5:I:1986:PRO:HD2	0.92	0.91
4:D:75:HIS:O	2:F:89:ARG:NH1	2.03	0.90
15:X:48:DC:H2"	15:X:49:DT:C7	2.01	0.90
7:K:56:TYR:O	8:L:39:ASN:ND2	2.03	0.90
7:K:165:LYS:HG2	7:K:167:LYS:HD2	1.52	0.90
1:A:116:LEU:HD11	3:C:108:ASN:HD21	1.35	0.90
5:I:901:CYS:O	5:I:2044:LYS:HE2	1.71	0.90
13:V:261:ARG:HD2	14:W:198:LYS:CG	2.01	0.90
16:Y:-116:DT:C6	16:Y:-115:DT:H72	2.06	0.90
6:J:162:HIS:CE1	15:X:137:DG:H4'	2.07	0.90
16:Y:-131:DG:H2"	16:Y:-130:DC:C5	2.06	0.90
3:G:79:LYS:HG2	3:G:82:LEU:HG	1.53	0.90
13:V:250:GLU:O	13:V:254:ILE:HG23	1.72	0.89
1:E:102:ILE:HG23	2:F:58:ILE:HD13	1.53	0.89
15:X:3:DG:H2"	15:X:4:DG:H5'	1.52	0.89
15:X:136:DG:H5"	15:X:136:DG:H8	1.35	0.89
1:E:64:GLU:HB2	2:F:45:VAL:HG11	1.54	0.89
9:M:125:LYS:HG2	9:M:235:ILE:HG12	1.54	0.89
5:I:2044:LYS:NZ	5:I:2173:GLU:OE1	2.04	0.89
16:Y:-102:DC:H2"	16:Y:-101:DT:H72	1.55	0.89
1:A:25:GLN:NE2	8:L:7:SER:O	2.06	0.89
5:I:713:THR:OG1	15:X:135:DG:O3'	1.89	0.89
16:Y:-5:DT:H2"	16:Y:-4:DC:H5'	1.52	0.89
7:K:56:TYR:CB	8:L:39:ASN:ND2	2.35	0.88
1:A:59:LEU:CD1	2:B:66:ILE:HG21	2.04	0.88
5:I:660:LEU:CD2	5:I:742:TYR:CZ	2.56	0.88
1:A:82:ARG:HB2	3:C:58:THR:HG21	1.54	0.88
1:A:42:GLU:HG2	2:B:84:SER:HB2	1.56	0.88
7:K:211:TYR:HE1	7:K:274:ARG:HD3	1.36	0.88
3:C:109:LEU:HD13	3:G:129:ARG:HG2	1.54	0.88
13:V:187:SER:OG	13:V:190:ASP:OD1	1.91	0.87
1:A:23:GLY:O	8:L:9:ARG:NH1	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH2	1:A:108:VAL:O	2.06	0.87
5:I:621:TYR:HE2	5:I:846:GLU:OE1	1.53	0.87
7:K:106:GLN:HB3	7:K:124:ARG:HH22	1.40	0.87
7:K:106:GLN:HB3	7:K:124:ARG:NH2	1.90	0.87
15:X:48:DC:OP2	15:X:48:DC:H2'	1.75	0.87
1:E:63:LEU:HD13	2:F:42:LEU:HB2	1.56	0.86
7:K:236:TYR:HB3	7:K:269:ARG:HG3	1.57	0.86
13:V:164:SER:HA	13:V:174:ILE:HD11	1.56	0.86
5:I:2014:LEU:HG	5:I:2017:ARG:HD2	1.57	0.86
16:Y:-21:DG:H2'	16:Y:-20:DT:H71	1.57	0.86
15:X:22:DG:C2'	15:X:23:DT:H5"	2.05	0.86
7:K:5:VAL:HA	7:K:94:ILE:HG23	1.55	0.86
7:K:26:PRO:HG2	7:K:42:ALA:HA	1.56	0.86
15:X:45:DC:H2"	15:X:46:DC:H5"	1.58	0.85
5:I:657:LEU:CD2	5:I:670:HIS:ND1	2.40	0.85
5:I:2037:LEU:CD1	5:I:2039:GLN:HG2	2.06	0.85
1:A:59:LEU:HB2	2:B:62:PHE:CZ	2.10	0.85
6:J:269:SER:HB2	9:Q:150:TYR:CB	1.99	0.85
5:I:1983:VAL:HG23	9:O:238:VAL:HG11	1.58	0.85
9:M:113:MET:HG3	9:M:276:ARG:HH12	1.37	0.85
3:C:110:CYS:SG	3:G:130:ILE:HD11	2.16	0.85
13:V:261:ARG:HD2	14:W:198:LYS:HG3	1.56	0.85
1:E:57:TYR:HA	6:J:130:ARG:HH12	1.40	0.85
1:E:106:GLY:HA3	3:G:58:THR:HG22	1.59	0.85
7:K:146:ILE:HG22	7:K:158:VAL:H	1.41	0.85
6:J:269:SER:HB2	9:Q:150:TYR:HD1	1.42	0.85
9:M:413:ALA:CA	9:M:433:ILE:HD12	2.02	0.85
5:I:2060:HIS:CD2	5:I:2132:THR:HG23	2.12	0.84
16:Y:-146:DC:H6	16:Y:-146:DC:H5'	1.42	0.84
15:X:116:DA:H2"	15:X:117:DT:H5'	1.59	0.84
13:V:264:ARG:HG2	13:V:264:ARG:HH11	1.41	0.84
7:K:56:TYR:HB2	8:L:39:ASN:HD21	1.35	0.83
9:M:26:LEU:HD11	9:M:50:GLY:HA3	1.58	0.83
4:D:92:ARG:NH2	2:F:97:LEU:O	2.12	0.83
16:Y:-14:DA:H2"	16:Y:-13:DT:H73	1.59	0.83
16:Y:-125:DG:H2"	16:Y:-124:DC:H5"	1.60	0.83
13:V:244:GLU:O	13:V:247:LEU:HG	1.77	0.83
13:V:116:ARG:N	13:V:119:GLU:OE2	2.12	0.83
4:D:23:ARG:NH2	14:W:87:GLU:O	2.12	0.82
9:M:413:ALA:CA	9:M:433:ILE:HD13	2.00	0.82
13:V:156:GLU:OE1	13:V:183:PHE:CG	2.31	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:73:DG:N1	16:Y:-73:DC:N3	2.27	0.82
1:A:32:HIS:O	1:A:36:ARG:HG2	1.80	0.82
7:K:196:MET:O	8:L:41:GLN:NE2	2.13	0.81
1:E:92:GLU:HG3	2:F:100:PRO:HB2	1.62	0.81
5:I:2060:HIS:HD2	5:I:2131:ASP:OD2	1.63	0.81
15:X:2:DA:H2"	15:X:3:DG:N7	1.96	0.81
1:A:89:ARG:HB2	1:A:109:LEU:HD21	1.60	0.81
5:I:118:PHE:CE1	13:V:247:LEU:HD22	2.16	0.81
5:I:622:GLN:OE1	17:I:3301:ADP:N6	2.12	0.81
10:N:231:GLU:HB2	10:N:234:LYS:CE	2.10	0.81
15:X:43:DA:H2"	15:X:44:DT:H5"	1.60	0.81
2:B:28:ARG:NE	2:B:28:ARG:HA	1.96	0.81
7:K:221:ASP:HA	7:K:224:LYS:HZ2	1.46	0.81
13:V:201:LYS:HD2	13:V:204:ASN:HD22	1.45	0.81
1:A:27:PRO:HD3	2:B:37:TYR:CD2	2.15	0.81
3:G:106:ASP:HB3	3:G:127:ALA:HB1	1.63	0.80
15:X:46:DC:H4'	15:X:46:DC:OP1	1.77	0.80
3:C:65:LEU:HB2	15:X:91:DG:OP2	1.80	0.80
10:N:301:VAL:HG21	10:N:326:MET:HB2	1.61	0.80
16:Y:-82:DA:H1'	16:Y:-81:DC:H5'	1.62	0.80
3:G:106:ASP:OD2	3:G:131:ARG:NE	2.12	0.80
5:I:949:ILE:HD12	9:M:249:ARG:O	1.82	0.80
8:L:27:ARG:NE	8:L:153:THR:CG2	2.37	0.80
13:V:136:PRO:HB2	13:V:202:LEU:CD1	2.08	0.80
13:V:264:ARG:NH1	14:W:194:ILE:HD13	1.96	0.80
1:A:26:PHE:CD1	1:A:57:GLU:HB2	2.16	0.80
7:K:159:PRO:HB2	7:K:166:LYS:HB2	1.63	0.80
7:K:139:ASN:HB3	7:K:142:GLU:HG2	1.62	0.80
13:V:239:GLU:CA	13:V:243:GLU:HB2	2.11	0.80
5:I:2060:HIS:CD2	5:I:2132:THR:CG2	2.65	0.80
16:Y:-107:DG:H1'	16:Y:-106:DA:C8	2.16	0.80
16:Y:-133:DG:C8	16:Y:-132:DT:H72	2.17	0.79
5:I:846:GLU:HG2	5:I:848:GLN:HG2	1.63	0.79
5:I:1983:VAL:HG21	9:O:238:VAL:HG11	1.62	0.79
5:I:2014:LEU:O	5:I:2014:LEU:HD23	1.82	0.79
7:K:352:PRO:HB3	7:K:358:TYR:CD1	2.18	0.79
7:K:376:VAL:HG13	7:K:377:VAL:N	1.96	0.79
5:I:694:LYS:HB2	5:I:719:HIS:CD2	2.18	0.79
7:K:5:VAL:O	7:K:15:ILE:HA	1.83	0.79
7:K:379:ARG:HA	7:K:382:TYR:HB3	1.65	0.79
6:J:269:SER:HB3	9:Q:150:TYR:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:222:ILE:O	7:K:230:ASN:HB2	1.82	0.79
7:K:374:ASP:OD1	7:K:374:ASP:N	2.15	0.79
13:V:262:GLU:HG3	14:W:202:LYS:NZ	1.97	0.79
13:V:239:GLU:HA	13:V:243:GLU:CB	2.12	0.79
1:E:81:ARG:HG2	3:G:58:THR:CG2	2.13	0.79
13:V:261:ARG:O	14:W:198:LYS:HE3	1.83	0.79
5:I:126:LYS:HE3	13:V:216:PRO:HB2	1.63	0.79
9:O:34:GLN:CD	9:O:43:GLU:OE2	2.20	0.79
9:M:235:ILE:HG22	9:M:235:ILE:O	1.83	0.79
1:E:81:ARG:HG2	3:G:58:THR:HG21	1.63	0.78
4:H:46:ILE:HG22	4:H:50:ILE:HG21	1.65	0.78
5:I:116:GLU:O	13:V:232:ARG:NH2	2.16	0.78
7:K:224:LYS:HB3	8:L:122:PHE:CE2	2.17	0.78
1:A:56:LEU:O	1:A:60:THR:HG23	1.84	0.78
1:A:56:LEU:HD21	2:B:67:PHE:N	1.97	0.78
3:G:73:GLU:HA	4:H:23:ARG:NH2	1.99	0.78
13:V:133:VAL:HG21	13:V:168:ASP:HA	1.63	0.78
7:K:110:ASN:OD1	7:K:124:ARG:NH1	2.17	0.78
7:K:378:THR:HG22	7:K:379:ARG:H	1.48	0.78
1:E:64:GLU:HB2	2:F:45:VAL:CG1	2.13	0.78
1:A:13:ALA:HB3	5:I:164:LYS:HD2	1.64	0.77
7:K:193:LEU:HB2	7:K:268:LEU:HD22	1.65	0.77
10:N:37:LEU:O	10:N:54:ARG:HG3	1.83	0.77
15:X:136:DG:H5"	15:X:136:DG:C8	2.19	0.77
5:I:118:PHE:CD2	13:V:247:LEU:HD13	2.19	0.77
15:X:57:DT:H6	15:X:57:DT:H5'	1.50	0.77
15:X:126:DC:H1'	15:X:127:DT:H5'	1.67	0.77
5:I:1983:VAL:HG23	9:O:238:VAL:CG1	2.14	0.77
1:A:55:VAL:HG13	2:B:107:ALA:HB1	1.67	0.77
1:A:84:LEU:HD13	2:B:58:ILE:HG21	1.64	0.77
13:V:190:ASP:OD1	13:V:190:ASP:N	2.14	0.77
15:X:75:DG:H1	16:Y:-75:DC:H42	1.29	0.77
15:X:141:DC:H2"	15:X:142:DT:H5'	1.67	0.77
1:A:13:ALA:CB	5:I:164:LYS:HD3	1.96	0.77
2:B:34:TYR:H	2:B:60:ASN:HD21	1.33	0.77
7:K:92:ASN:HB3	7:K:120:GLN:HB3	1.67	0.77
7:K:220:MET:HE2	8:L:123:PRO:HD3	1.67	0.77
1:A:55:VAL:O	1:A:59:LEU:HG	1.85	0.77
7:K:238:LEU:HG	7:K:266:GLN:HB2	1.67	0.77
7:K:277:VAL:HB	7:K:278:PRO:HD3	1.65	0.77
7:K:332:ARG:O	7:K:336:GLU:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG13	2:B:67:PHE:CE2	2.20	0.77
5:I:923:PHE:CE1	10:N:201:LYS:NZ	2.52	0.77
16:Y:-53:DG:H4'	16:Y:-52:DC:OP1	1.82	0.77
3:C:127:ALA:O	3:C:131:ARG:HG3	1.84	0.76
9:M:113:MET:HG3	9:M:276:ARG:HH11	1.49	0.76
5:I:2037:LEU:HD11	5:I:2039:GLN:HG2	1.66	0.76
13:V:237:THR:CG2	13:V:238:PRO:HD3	2.13	0.76
15:X:7:DG:H1'	15:X:8:DT:H5"	1.67	0.76
5:I:915:PRO:O	9:O:128:LYS:NZ	2.18	0.76
15:X:136:DG:H2"	15:X:137:DG:O4'	1.85	0.76
1:E:20:ARG:CD	2:F:121:SER:OG	2.32	0.76
13:V:208:VAL:HG13	13:V:209:PRO:HD3	1.68	0.76
7:K:155:THR:HG23	7:K:173:ILE:HB	1.68	0.76
5:I:120:SER:HB2	13:V:233:LEU:HD12	1.66	0.76
1:A:33:ARG:HA	1:A:36:ARG:CG	2.15	0.76
7:K:121:ALA:HB2	7:K:376:VAL:HG22	1.66	0.76
7:K:224:LYS:HB3	8:L:122:PHE:CZ	2.21	0.76
10:N:123:PHE:CE1	10:N:324:LEU:HD23	2.21	0.76
15:X:139:DT:H2"	15:X:140:DT:H5'	1.66	0.76
15:X:53:DC:H2"	15:X:54:DG:C8	2.19	0.75
7:K:70:VAL:O	7:K:74:VAL:HG23	1.86	0.75
1:A:35:LEU:HD21	2:B:67:PHE:CE1	2.21	0.75
1:A:58:TYR:OH	2:B:106:HIS:ND1	2.18	0.75
1:E:57:TYR:HA	6:J:130:ARG:NH1	2.00	0.75
15:X:59:DA:H2"	15:X:60:DA:H5"	1.65	0.75
5:I:660:LEU:HD23	5:I:742:TYR:CE2	2.22	0.75
5:I:930:LEU:HD21	10:N:250:ILE:HD12	1.66	0.75
15:X:99:DA:H1'	15:X:100:DG:H5'	1.67	0.75
7:K:175:VAL:HA	7:K:179:LEU:HD22	1.69	0.75
13:V:94:PRO:O	13:V:117:ALA:HB2	1.86	0.75
1:A:51:TYR:HB3	2:B:91:ILE:HG21	1.69	0.75
7:K:375:MET:O	7:K:376:VAL:HG12	1.86	0.75
1:A:55:VAL:HG12	1:A:59:LEU:HD21	1.67	0.75
7:K:212:VAL:HG12	7:K:332:ARG:HG3	1.69	0.75
13:V:119:GLU:OE1	13:V:119:GLU:N	2.19	0.75
5:I:2014:LEU:HD11	9:Q:256:ILE:HG13	1.68	0.74
5:I:2088:ARG:HG3	5:I:2115:ILE:O	1.87	0.74
10:N:231:GLU:HB2	10:N:234:LYS:HE3	1.67	0.74
13:V:169:LEU:HD21	13:V:195:TYR:CZ	2.22	0.74
16:Y:-14:DA:H2"	16:Y:-13:DT:C5	2.22	0.74
13:V:156:GLU:OE1	13:V:183:PHE:CD1	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:205:LEU:HG	10:R:225:VAL:HG22	1.70	0.74
3:C:51:ILE:HD11	4:D:44:LYS:HA	1.70	0.74
5:I:754:PHE:CD1	5:I:755:LYS:HG3	2.22	0.74
7:K:216:PHE:O	7:K:220:MET:HG2	1.87	0.74
7:K:99:TYR:OH	7:K:158:VAL:HG21	1.88	0.74
9:M:172:LEU:HD21	9:M:193:ILE:HD13	1.70	0.74
15:X:3:DG:C2'	15:X:4:DG:H5'	2.18	0.74
16:Y:-26:DG:H2"	16:Y:-25:DG:C8	2.23	0.74
7:K:144:CYS:HA	7:K:160:TYR:O	1.87	0.74
1:E:68:ASN:ND2	1:E:71:ARG:HB3	2.03	0.74
2:B:87:THR:OG1	2:B:90:GLU:OE1	2.05	0.73
7:K:304:ASN:ND2	7:K:306:PRO:HD2	2.03	0.73
9:M:313:THR:HG21	10:R:303:MET:HG3	1.68	0.73
3:G:107:THR:CG2	3:G:124:ILE:HG12	2.18	0.73
5:I:95:GLU:OE2	13:V:261:ARG:NH2	2.20	0.73
5:I:1886:LEU:HD21	7:K:315:LYS:HE2	1.69	0.73
1:A:27:PRO:HD2	2:B:34:TYR:HE1	1.52	0.73
15:X:54:DG:H2'	15:X:54:DG:OP2	1.89	0.73
1:E:39:TYR:O	2:F:75:SER:HB2	1.88	0.73
16:Y:-23:DA:H2'	16:Y:-22:DC:C6	2.23	0.73
4:H:39:ARG:NH1	4:H:46:ILE:HD11	2.04	0.73
7:K:298:ILE:O	7:K:302:ILE:HG12	1.88	0.73
10:R:114:SER:OG	10:R:117:GLU:OE1	2.06	0.73
13:V:222:HIS:HA	13:V:225:ARG:HD3	1.71	0.73
7:K:88:PHE:HB3	7:K:119:PHE:HD2	1.54	0.73
7:K:123:LEU:HA	7:K:394:PHE:CZ	2.24	0.73
7:K:237:VAL:HG11	7:K:250:LYS:HE2	1.71	0.73
7:K:302:ILE:HG22	7:K:310:GLN:HB3	1.69	0.73
15:X:55:DG:H2"	15:X:56:DT:H5"	1.70	0.73
15:X:97:DC:H6	15:X:97:DC:H5"	1.54	0.73
3:C:130:ILE:HD13	3:G:127:ALA:HA	1.71	0.72
1:E:20:ARG:HG2	2:F:121:SER:OG	1.87	0.72
5:I:128:PRO:HB3	13:V:216:PRO:HG2	1.71	0.72
7:K:302:ILE:HG21	7:K:314:PHE:CD1	2.23	0.72
7:K:377:VAL:CG2	7:K:393:LYS:HG3	2.19	0.72
15:X:10:DT:H1'	15:X:11:DA:H5'	1.72	0.72
1:A:32:HIS:ND1	1:A:49:PRO:HG3	2.05	0.72
15:X:114:DC:H1'	15:X:115:DA:C8	2.25	0.72
1:A:81:PRO:HB2	1:A:105:GLN:O	1.89	0.72
3:G:103:LEU:HD21	3:G:128:ARG:HD2	1.71	0.72
9:M:35:ALA:CB	9:M:40:VAL:HG22	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:96:LYS:CD	13:V:98:MET:HG2	2.18	0.72
13:V:169:LEU:HD11	13:V:195:TYR:OH	1.89	0.72
4:D:92:ARG:HH21	2:F:98:LEU:HD23	1.55	0.72
5:I:116:GLU:OE1	13:V:240:GLN:HG3	1.89	0.72
5:I:2063:LEU:HD11	5:I:2127:LEU:HD23	1.70	0.72
13:V:139:SER:HB3	13:V:142:GLU:HG3	1.72	0.72
15:X:87:DT:H1'	15:X:88:DT:C6	2.25	0.72
1:E:65:LEU:HB3	1:E:86:ALA:HB1	1.72	0.72
10:N:301:VAL:HG21	10:N:326:MET:CB	2.18	0.72
7:K:36:ARG:NE	7:K:36:ARG:HA	2.04	0.72
1:A:41:ALA:HB2	2:B:86:ILE:HG13	1.70	0.71
2:F:99:LEU:HB2	2:F:104:ALA:HB2	1.70	0.71
5:I:2037:LEU:HD13	5:I:2081:TYR:CE2	2.24	0.71
5:I:667:TRP:CE2	5:I:719:HIS:CE1	2.78	0.71
13:V:262:GLU:HG3	14:W:202:LYS:HZ2	1.54	0.71
16:Y:-22:DC:H2"	16:Y:-21:DG:H8	1.54	0.71
1:A:32:HIS:HB2	1:A:49:PRO:CB	2.20	0.71
1:A:116:LEU:CD1	3:C:108:ASN:HD21	2.03	0.71
16:Y:-52:DC:H2"	16:Y:-51:DC:O5'	1.89	0.71
5:I:163:ARG:C	5:I:166:VAL:HG22	2.11	0.71
7:K:302:ILE:HG21	7:K:314:PHE:CE1	2.26	0.71
5:I:901:CYS:O	5:I:2044:LYS:HE3	1.90	0.71
16:Y:-101:DT:H2"	16:Y:-100:DC:H5'	1.72	0.71
13:V:239:GLU:CD	13:V:240:GLN:HG2	2.10	0.71
16:Y:-10:DA:H2"	16:Y:-9:DT:H5"	1.71	0.71
2:B:117:LYS:HE2	2:B:122:LYS:HD2	1.72	0.71
1:A:27:PRO:HD2	2:B:34:TYR:CE1	2.26	0.71
7:K:82:GLU:HG2	7:K:83:MET:HG2	1.71	0.71
7:K:133:HIS:CE1	7:K:137:ARG:HD2	2.26	0.71
15:X:36:DG:H2"	15:X:37:DG:OP2	1.90	0.71
3:G:107:THR:HG21	3:G:124:ILE:HG12	1.73	0.70
13:V:261:ARG:HB3	13:V:262:GLU:OE2	1.91	0.70
7:K:93:ILE:O	7:K:122:VAL:HA	1.91	0.70
13:V:124:TYR:CD1	13:V:125:PRO:HD2	2.25	0.70
5:I:969:LEU:HB2	10:R:225:VAL:HA	1.72	0.70
7:K:314:PHE:HZ	7:K:345:TYR:HD2	1.39	0.70
5:I:2014:LEU:HD11	9:Q:259:MET:SD	2.31	0.70
13:V:96:LYS:HB3	13:V:98:MET:HE3	1.73	0.70
5:I:916:PHE:HB3	5:I:1983:VAL:HG22	1.71	0.70
13:V:147:LEU:CD1	13:V:198:ILE:HG23	2.21	0.70
16:Y:-98:DA:H2"	16:Y:-97:DG:H8	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HB2	2:B:86:ILE:CG1	2.21	0.70
1:A:63:ILE:CG2	2:B:59:MET:HE1	2.22	0.70
16:Y:-142:DA:H1'	16:Y:-141:DG:H5'	1.72	0.70
7:K:377:VAL:HG23	7:K:393:LYS:HG3	1.74	0.70
7:K:309:MET:HG2	7:K:313:PHE:CE2	2.26	0.70
13:V:96:LYS:O	13:V:98:MET:HG3	1.91	0.70
16:Y:-44:DA:H2'	16:Y:-43:DT:H72	1.72	0.70
3:G:74:ILE:HD13	4:H:62:LEU:HB3	1.74	0.70
7:K:218:ARG:O	7:K:222:ILE:HG12	1.91	0.70
9:M:110:GLU:CG	9:M:269:THR:HG22	2.19	0.70
16:Y:-54:DC:H2"	16:Y:-53:DG:C8	2.27	0.70
7:K:114:PHE:HE1	7:K:122:VAL:HB	1.56	0.69
7:K:152:TYR:CZ	7:K:178:LYS:HG2	2.27	0.69
13:V:258:LYS:HB3	13:V:259:LYS:HZ2	1.55	0.69
15:X:59:DA:H2"	15:X:60:DA:C5'	2.22	0.69
3:G:74:ILE:HG23	4:H:63:GLU:HG2	1.74	0.69
7:K:150:SER:HB2	7:K:323:ASN:HB2	1.74	0.69
3:C:61:LEU:HD12	4:D:37:LEU:HD23	1.74	0.69
5:I:1992:ALA:HB2	10:N:201:LYS:NZ	2.06	0.69
7:K:120:GLN:N	7:K:120:GLN:HE21	1.90	0.69
1:A:26:PHE:CZ	1:A:60:THR:HG21	2.27	0.69
5:I:694:LYS:HB2	5:I:719:HIS:HD2	1.56	0.69
1:A:41:ALA:HB2	2:B:86:ILE:CD1	2.22	0.69
5:I:1983:VAL:CG2	9:O:238:VAL:CG1	2.61	0.69
13:V:239:GLU:O	13:V:243:GLU:N	2.25	0.69
3:G:118:THR:OG1	4:H:45:ARG:HD3	1.90	0.69
5:I:141:CYS:O	5:I:145:GLN:HG3	1.92	0.69
16:Y:-98:DA:H2"	16:Y:-97:DG:C8	2.27	0.69
1:E:92:GLU:HG2	2:F:103:LEU:HB2	1.75	0.69
3:G:116:ARG:NH2	3:G:123:ASP:OD1	2.25	0.69
5:I:2154:ARG:NH1	17:I:3301:ADP:O2A	2.26	0.69
7:K:156:HIS:CD2	7:K:170:ILE:HD11	2.28	0.69
13:V:261:ARG:HD2	14:W:198:LYS:HG2	1.73	0.69
16:Y:-146:DC:H5'	16:Y:-146:DC:C6	2.27	0.69
16:Y:-10:DA:H2"	16:Y:-9:DT:C5'	2.23	0.69
7:K:335:SER:HA	7:K:338:ARG:HE	1.58	0.69
5:I:2060:HIS:CD2	5:I:2131:ASP:OD2	2.46	0.69
5:I:2088:ARG:HD3	5:I:2115:ILE:CG2	2.23	0.69
7:K:108:SER:O	7:K:112:ILE:HD12	1.93	0.69
5:I:633:TYR:CD1	5:I:742:TYR:CE1	2.78	0.68
5:I:923:PHE:CD1	10:N:201:LYS:NZ	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2063:LEU:HD21	5:I:2127:LEU:HD22	1.66	0.68
7:K:239:PRO:HD3	7:K:247:GLY:CA	2.22	0.68
5:I:116:GLU:CD	13:V:240:GLN:HG3	2.13	0.68
16:Y:-99:DT:H2"	16:Y:-98:DA:H5"	1.75	0.68
1:A:88:ILE:HG12	1:A:98:LEU:HD12	1.74	0.68
13:V:105:ARG:NH2	13:V:107:ASP:OD2	2.25	0.68
1:A:80:ILE:HG13	1:A:82:ARG:HB3	1.75	0.68
9:M:413:ALA:CB	9:M:433:ILE:HD12	2.23	0.68
5:I:930:LEU:HD21	10:N:250:ILE:CD1	2.24	0.68
13:V:239:GLU:HA	13:V:243:GLU:H	1.58	0.68
15:X:141:DC:H2'	15:X:142:DT:H71	1.73	0.68
5:I:621:TYR:HE2	5:I:846:GLU:CD	1.97	0.68
7:K:295:PRO:O	7:K:299:VAL:HG23	1.93	0.68
5:I:2088:ARG:HD3	5:I:2115:ILE:HG21	1.76	0.68
7:K:220:MET:O	7:K:224:LYS:HG2	1.94	0.68
2:F:53:SER:N	16:Y:-127:DA:OP1	2.20	0.68
7:K:282:PHE:O	7:K:284:PRO:HD3	1.93	0.68
9:M:313:THR:CA	9:M:316:HIS:HE1	1.80	0.68
13:V:92:VAL:O	13:V:94:PRO:HD3	1.94	0.68
5:I:621:TYR:CZ	5:I:846:GLU:OE1	2.47	0.68
5:I:917:ILE:HD12	9:O:128:LYS:NZ	2.09	0.68
7:K:56:TYR:HB2	8:L:39:ASN:CG	2.14	0.68
13:V:55:ARG:NH2	15:X:39:DA:H5"	2.10	0.68
5:I:118:PHE:CE2	13:V:247:LEU:HD13	2.30	0.67
10:R:117:GLU:OE1	10:R:117:GLU:N	2.27	0.67
15:X:73:DG:H1'	15:X:74:DC:H5'	1.74	0.67
1:A:66:LEU:HD12	1:A:94:LEU:HD12	1.76	0.67
5:I:949:ILE:CD1	9:M:249:ARG:O	2.41	0.67
7:K:146:ILE:HB	7:K:148:VAL:HG23	1.75	0.67
7:K:312:HIS:HA	7:K:315:LYS:HE3	1.76	0.67
13:V:95:TRP:CE2	13:V:116:ARG:HG2	2.30	0.67
13:V:179:ASP:O	13:V:183:PHE:HB2	1.93	0.67
7:K:233:MET:HG2	7:K:252:ARG:CD	2.24	0.67
1:A:30:ARG:HH22	2:B:34:TYR:HA	1.59	0.67
4:H:97:LEU:HD11	4:H:100:PHE:CD1	2.30	0.67
7:K:319:LEU:HD21	7:K:333:VAL:HG11	1.75	0.67
9:M:26:LEU:CD2	9:M:30:GLY:O	2.31	0.67
13:V:257:ARG:O	13:V:261:ARG:HG2	1.94	0.67
15:X:131:DC:H2"	15:X:132:DA:C8	2.30	0.67
7:K:157:ILE:HG21	7:K:298:ILE:HA	1.76	0.67
7:K:302:ILE:HD12	7:K:313:PHE:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2088:ARG:NH1	5:I:2090:ASP:OD1	2.28	0.67
7:K:232:VAL:HG22	7:K:233:MET:H	1.58	0.67
10:N:38:GLU:CD	10:N:54:ARG:NH1	2.48	0.67
15:X:68:DG:H2'	15:X:68:DG:OP2	1.94	0.67
16:Y:-3:DC:H2'	16:Y:-2:DT:C5	2.30	0.67
1:E:35:ARG:HB3	1:E:43:VAL:CG2	2.24	0.67
1:E:49:VAL:HG21	2:F:118:TYR:CD2	2.30	0.67
3:G:107:THR:OG1	3:G:124:ILE:HG12	1.94	0.67
6:J:260:ARG:HB2	10:P:210:THR:HB	1.75	0.67
7:K:120:GLN:CA	7:K:378:THR:HG21	2.25	0.67
15:X:123:DG:H2"	15:X:124:DG:H8	1.60	0.67
1:E:117:PRO:HD3	3:G:48:LEU:CD1	2.25	0.67
7:K:16:GLY:HA2	7:K:84:TYR:OH	1.94	0.67
15:X:136:DG:H2'	15:X:137:DG:C8	2.30	0.66
1:A:52:LEU:HD21	2:B:67:PHE:CE2	2.30	0.66
7:K:361:GLU:O	7:K:365:LEU:HD22	1.95	0.66
10:P:68:ILE:HD13	10:P:68:ILE:H	1.60	0.66
15:X:81:DG:H2'	15:X:82:DT:H71	1.78	0.66
3:G:82:LEU:HD11	4:H:70:VAL:HG13	1.77	0.66
7:K:198:GLU:HB2	7:K:201:VAL:HG23	1.76	0.66
7:K:265:GLU:HB2	7:K:267:ILE:HG23	1.77	0.66
15:X:79:DA:H2"	15:X:80:DC:C5	2.29	0.66
5:I:694:LYS:H	5:I:719:HIS:CD2	2.13	0.66
7:K:68:TRP:HE1	7:K:112:ILE:HD13	1.61	0.66
15:X:44:DT:H2"	15:X:45:DC:H5"	1.78	0.66
16:Y:-87:DA:H2"	16:Y:-86:DA:C8	2.31	0.66
5:I:936:HIS:CE1	10:N:279:LYS:HZ1	1.81	0.66
5:I:1886:LEU:HD11	7:K:311:PRO:HB2	1.78	0.66
5:I:2063:LEU:CD2	5:I:2127:LEU:HD23	2.16	0.66
7:K:230:ASN:ND2	7:K:232:VAL:HB	2.08	0.66
13:V:265:SER:OG	14:W:195:ALA:HA	1.95	0.66
2:F:33:SER:HB2	2:F:60:ASN:OD1	1.95	0.66
1:A:30:ARG:HG3	1:A:33:ARG:HH21	1.60	0.66
3:C:120:MET:HB3	3:C:122:LYS:HD2	1.77	0.66
13:V:163:LEU:HD22	13:V:167:PHE:HE2	1.60	0.66
13:V:244:GLU:HA	13:V:247:LEU:CD2	2.26	0.66
5:I:819:GLN:O	5:I:821:TYR:N	2.29	0.66
5:I:1914:LEU:HD13	9:M:282:VAL:HG11	1.77	0.66
7:K:74:VAL:O	7:K:78:LEU:HG	1.96	0.66
7:K:187:ILE:HA	7:K:190:TYR:CD2	2.30	0.66
13:V:265:SER:CB	14:W:198:LYS:HD3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-5:DT:C2'	16:Y:-4:DC:H5'	2.23	0.66
3:G:110:CYS:HB2	3:G:123:ASP:HB3	1.78	0.65
10:N:324:LEU:HD13	10:N:326:MET:HE2	1.78	0.65
13:V:239:GLU:O	13:V:244:GLU:N	2.26	0.65
5:I:810:PRO:O	5:I:814:MET:CG	2.37	0.65
7:K:133:HIS:CG	7:K:366:ILE:HG12	2.31	0.65
13:V:268:LEU:HD22	14:W:191:SER:CB	2.26	0.65
15:X:100:DG:H1'	15:X:101:DA:C8	2.31	0.65
16:Y:-146:DC:H2'	16:Y:-145:DT:H72	1.79	0.65
16:Y:-134:DG:H1'	16:Y:-133:DG:H5'	1.78	0.65
1:E:20:ARG:HD3	2:F:121:SER:OG	1.95	0.65
1:E:85:LEU:O	1:E:89:ASN:ND2	2.21	0.65
5:I:921:ILE:HG23	5:I:1986:PRO:HD2	1.74	0.65
7:K:287:ILE:HG23	8:L:35:LEU:HD13	1.79	0.65
7:K:336:GLU:O	7:K:340:LEU:HD22	1.95	0.65
16:Y:-145:DT:H2"	16:Y:-144:DG:C5'	2.22	0.65
16:Y:-142:DA:H5'	16:Y:-142:DA:H8	1.61	0.65
5:I:1914:LEU:HD13	9:M:282:VAL:CG1	2.26	0.65
7:K:38:LYS:HB3	7:K:40:PHE:CE1	2.32	0.65
7:K:81:LYS:HA	7:K:85:GLN:CA	2.20	0.65
16:Y:-23:DA:H2"	16:Y:-22:DC:H5'	1.79	0.65
16:Y:-21:DG:H2'	16:Y:-20:DT:C6	2.32	0.65
2:B:89:ARG:CZ	13:V:63:SER:HB3	2.27	0.65
3:G:63:ARG:HH21	15:X:59:DA:H4'	1.62	0.65
5:I:949:ILE:CG2	10:R:260:LEU:HD22	2.21	0.65
2:B:90:GLU:HA	2:B:93:THR:HG22	1.79	0.65
4:D:45:ARG:CZ	15:X:80:DC:H4'	2.26	0.65
5:I:2014:LEU:CG	5:I:2017:ARG:HD2	2.27	0.65
7:K:106:GLN:HA	7:K:109:MET:HB3	1.77	0.65
7:K:233:MET:HA	7:K:255:MET:CE	2.25	0.65
15:X:71:DC:H2"	15:X:72:DA:C8	2.31	0.65
15:X:108:DT:H2"	15:X:109:DA:C8	2.31	0.65
3:C:128:ARG:NH1	3:C:133:GLU:OE1	2.23	0.65
7:K:156:HIS:HD2	7:K:170:ILE:HD11	1.62	0.65
7:K:185:LYS:HG2	7:K:202:ILE:HG21	1.77	0.65
7:K:220:MET:SD	7:K:275:PHE:HE1	2.19	0.65
13:V:247:LEU:HD12	13:V:248:LEU:N	2.12	0.65
1:E:114:VAL:HG12	3:G:117:VAL:CG2	2.27	0.65
14:W:29:ASN:OD1	14:W:116:HIS:NE2	2.29	0.65
7:K:211:TYR:O	7:K:275:PHE:HA	1.97	0.65
1:A:21:ARG:HH11	1:A:21:ARG:CB	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG13	2:B:67:PHE:HE2	1.58	0.64
7:K:107:GLU:HA	7:K:110:ASN:ND2	2.13	0.64
7:K:299:VAL:O	7:K:303:GLN:HG2	1.97	0.64
7:K:187:ILE:HA	7:K:190:TYR:CE2	2.32	0.64
13:V:115:ARG:HB3	13:V:119:GLU:OE2	1.97	0.64
16:Y:-112:DT:H1'	16:Y:-111:DC:H5'	1.79	0.64
16:Y:-39:DT:H2"	16:Y:-38:DC:H5"	1.78	0.64
1:A:33:ARG:HA	1:A:36:ARG:HG3	1.78	0.64
1:E:42:ARG:HG2	15:X:111:DG:H4'	1.79	0.64
1:E:101:THR:HG23	4:H:96:THR:O	1.97	0.64
7:K:88:PHE:HB3	7:K:119:PHE:CD2	2.31	0.64
5:I:118:PHE:CZ	13:V:247:LEU:HB2	2.33	0.64
5:I:657:LEU:HD23	5:I:670:HIS:ND1	2.11	0.64
7:K:211:TYR:CE1	7:K:274:ARG:HD3	2.25	0.64
15:X:25:DC:OP2	15:X:25:DC:H2'	1.97	0.64
15:X:113:DC:H2"	15:X:114:DC:O5'	1.96	0.64
9:M:413:ALA:N	9:M:433:ILE:HD13	2.13	0.64
15:X:131:DC:H2"	15:X:132:DA:H8	1.63	0.64
5:I:2088:ARG:CD	5:I:2115:ILE:CG2	2.76	0.64
7:K:68:TRP:NE1	7:K:112:ILE:HD13	2.12	0.64
9:M:96:MET:SD	9:M:115:ASN:ND2	2.71	0.64
1:E:81:ARG:O	1:E:81:ARG:HD3	1.98	0.64
7:K:220:MET:HE3	8:L:122:PHE:CD2	2.33	0.64
2:B:88:SER:OG	13:V:60:LEU:HD21	1.98	0.64
2:F:77:LEU:HD11	2:F:93:THR:CG2	2.28	0.64
7:K:121:ALA:CB	7:K:376:VAL:HG22	2.28	0.64
7:K:331:ASP:O	7:K:335:SER:OG	2.16	0.64
13:V:244:GLU:O	13:V:248:LEU:HG	1.98	0.64
13:V:258:LYS:HE3	13:V:259:LYS:HG3	1.79	0.64
16:Y:-120:DT:H1'	16:Y:-119:DC:H5'	1.78	0.64
7:K:314:PHE:CE2	7:K:345:TYR:HB3	2.33	0.64
9:M:56:ILE:HG12	9:M:326:ILE:HG21	1.80	0.64
16:Y:-10:DA:C2'	16:Y:-9:DT:H5"	2.28	0.64
1:A:33:ARG:HA	1:A:36:ARG:NE	2.13	0.63
1:A:91:ASP:OD1	8:L:17:ARG:NH2	2.31	0.63
2:B:75:SER:HB2	2:B:86:ILE:HD11	1.80	0.63
3:C:61:LEU:HD11	4:D:40:ARG:CZ	2.29	0.63
3:G:102:GLY:O	3:G:131:ARG:NH2	2.31	0.63
9:M:235:ILE:O	9:M:235:ILE:CG2	2.46	0.63
9:O:447:LEU:HD12	10:P:343:PRO:HB3	1.79	0.63
15:X:92:DC:H2"	15:X:93:DG:O5'	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-84:DG:H1'	16:Y:-83:DC:H5'	1.79	0.63
1:E:21:ALA:C	2:F:117:LYS:HD3	2.18	0.63
1:E:56:GLU:HG2	6:J:130:ARG:NH2	2.13	0.63
7:K:93:ILE:HD13	7:K:113:LEU:HD21	1.80	0.63
7:K:158:VAL:HG22	7:K:170:ILE:HD13	1.80	0.63
7:K:376:VAL:HG13	7:K:377:VAL:H	1.61	0.63
10:R:247:ILE:HG12	10:R:272:VAL:HG22	1.80	0.63
13:V:100:PHE:CD1	13:V:113:HIS:HB2	2.33	0.63
13:V:239:GLU:CA	13:V:243:GLU:H	2.10	0.63
16:Y:-142:DA:H5'	16:Y:-142:DA:C8	2.33	0.63
5:I:2091:GLY:HA3	15:X:55:DG:H5'	1.80	0.63
7:K:81:LYS:HB2	7:K:85:GLN:NE2	2.14	0.63
9:M:270:GLU:HB2	9:M:276:ARG:HE	1.62	0.63
1:A:42:GLU:CG	2:B:84:SER:HB2	2.28	0.63
1:A:58:TYR:CE2	2:B:106:HIS:HB2	2.33	0.63
3:C:63:ARG:CZ	3:C:66:PRO:HG2	2.29	0.63
4:H:39:ARG:HH12	4:H:46:ILE:HD11	1.62	0.63
5:I:694:LYS:CB	5:I:719:HIS:HD2	2.12	0.63
7:K:222:ILE:O	7:K:225:LEU:HB3	1.98	0.63
5:I:732:HIS:HD2	5:I:736:ARG:HH12	0.65	0.63
10:R:268:ILE:O	10:R:272:VAL:HG23	1.99	0.63
13:V:221:GLY:O	13:V:225:ARG:HG3	1.98	0.63
2:F:28:ARG:HG3	15:X:123:DG:H5'	1.79	0.63
7:K:334:TYR:HA	7:K:349:VAL:HG21	1.80	0.63
1:E:67:GLY:HA2	1:E:78:ILE:CG1	2.20	0.63
12:T:338:ILE:CD1	13:V:230:LEU:HD22	2.29	0.63
5:I:112:GLU:OE1	13:V:247:LEU:HD23	1.99	0.63
5:I:613:LEU:CD1	6:J:178:ILE:HD13	2.29	0.63
7:K:67:ASN:O	7:K:69:ASP:N	2.31	0.63
10:P:305:ASP:OD1	10:P:306:ILE:N	2.31	0.63
7:K:4:LEU:HB2	7:K:93:ILE:HG13	1.81	0.63
13:V:100:PHE:CE1	13:V:113:HIS:HB2	2.33	0.63
1:A:51:TYR:HE1	2:B:95:VAL:HG21	1.64	0.62
1:A:56:LEU:HD11	2:B:67:PHE:CD2	2.34	0.62
1:A:116:LEU:HD11	3:C:108:ASN:ND2	2.11	0.62
5:I:660:LEU:HD21	5:I:742:TYR:OH	1.96	0.62
5:I:2037:LEU:HD11	5:I:2039:GLN:CG	2.29	0.62
5:I:2063:LEU:CD2	5:I:2127:LEU:HD21	2.18	0.62
16:Y:-68:DC:H2"	16:Y:-67:DC:C5	2.34	0.62
1:A:89:ARG:HB3	1:A:109:LEU:HD11	1.80	0.62
5:I:842:LYS:O	5:I:842:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:269:SER:HB3	9:Q:150:TYR:CG	2.30	0.62
1:E:73:ASN:O	1:E:73:ASN:ND2	2.32	0.62
7:K:335:SER:HA	7:K:338:ARG:HH21	1.63	0.62
2:B:90:GLU:HG3	4:H:75:HIS:CE1	2.34	0.62
1:E:42:ARG:HB3	2:F:85:THR:OG1	1.98	0.62
10:R:305:ASP:OD1	10:R:306:ILE:N	2.32	0.62
13:V:167:PHE:O	13:V:170:ARG:HG2	1.99	0.62
15:X:11:DA:H2"	15:X:12:DT:H5'	1.80	0.62
15:X:94:DG:H2"	15:X:95:DT:H5'	1.81	0.62
1:A:33:ARG:CD	1:A:37:LYS:HE2	2.29	0.62
5:I:935:VAL:O	5:I:936:HIS:ND1	2.33	0.62
7:K:144:CYS:O	7:K:316:ASN:HB2	1.99	0.62
10:R:286:GLU:N	10:R:286:GLU:OE1	2.32	0.62
13:V:270:LYS:HE2	13:V:270:LYS:N	2.13	0.62
2:B:34:TYR:H	2:B:60:ASN:ND2	1.98	0.62
5:I:124:LEU:H	13:V:226:ARG:HD2	1.65	0.62
5:I:129:GLU:HG3	13:V:196:TYR:CE2	2.34	0.62
2:B:75:SER:HA	2:B:86:ILE:HD11	1.82	0.62
14:W:190:THR:HG22	14:W:194:ILE:HD12	1.81	0.62
1:E:117:PRO:HD3	3:G:48:LEU:HD11	1.82	0.62
8:L:4:LYS:O	8:L:4:LYS:HG2	1.99	0.62
13:V:268:LEU:HD13	14:W:191:SER:HA	1.80	0.62
1:A:56:LEU:HD21	2:B:67:PHE:CA	2.30	0.62
3:G:118:THR:HG23	4:H:45:ARG:HG2	1.82	0.62
5:I:1914:LEU:HD11	9:M:282:VAL:HB	1.80	0.62
7:K:56:TYR:HB3	8:L:39:ASN:HD21	1.61	0.62
16:Y:-22:DC:H2"	16:Y:-21:DG:C8	2.34	0.62
1:A:26:PHE:CG	1:A:57:GLU:HB2	2.35	0.62
1:E:100:VAL:HG11	4:H:98:TYR:CE2	2.34	0.62
7:K:228:GLU:O	7:K:229:GLU:HG2	2.00	0.62
7:K:364:LYS:O	7:K:368:GLU:HG2	2.00	0.62
13:V:90:LYS:O	13:V:90:LYS:HG2	1.99	0.62
13:V:220:ALA:HB1	13:V:224:ARG:NH2	2.15	0.62
1:A:32:HIS:CG	1:A:49:PRO:HG3	2.35	0.61
5:I:106:ILE:HD11	13:V:254:ILE:HG22	1.80	0.61
7:K:133:HIS:HE2	7:K:365:LEU:HB2	1.65	0.61
9:M:135:VAL:HG22	9:M:161:LEU:CD2	2.30	0.61
16:Y:-133:DG:H2'	16:Y:-132:DT:H72	1.81	0.61
1:E:18:SER:HB2	1:E:25:PHE:O	2.00	0.61
2:F:59:MET:O	2:F:63:VAL:HG23	2.00	0.61
13:V:95:TRP:CZ2	13:V:116:ARG:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:95:TRP:HB3	13:V:114:TRP:CZ3	2.34	0.61
1:A:41:ALA:HB2	2:B:86:ILE:HD12	1.81	0.61
7:K:165:LYS:HG2	7:K:167:LYS:CD	2.28	0.61
7:K:181:THR:O	7:K:185:LYS:HG3	2.01	0.61
7:K:185:LYS:HA	7:K:202:ILE:HD13	1.81	0.61
13:V:96:LYS:HB3	13:V:98:MET:CE	2.29	0.61
13:V:258:LYS:HB3	13:V:259:LYS:NZ	2.14	0.61
13:V:259:LYS:HZ2	13:V:259:LYS:H	1.48	0.61
15:X:123:DG:H2"	15:X:124:DG:C8	2.35	0.61
1:A:58:TYR:CZ	2:B:106:HIS:HB2	2.36	0.61
2:B:39:TYR:HE1	2:B:43:LYS:HE3	1.66	0.61
12:T:190:GLN:OE1	12:T:190:GLN:N	2.32	0.61
3:C:42:ARG:HB3	3:C:42:ARG:HH11	1.65	0.61
1:E:114:VAL:HG12	3:G:117:VAL:HG23	1.82	0.61
15:X:94:DG:H2'	15:X:95:DT:C6	2.35	0.61
1:A:29:GLY:O	1:A:36:ARG:NH2	2.33	0.61
15:X:43:DA:H2'	15:X:44:DT:H72	1.82	0.61
1:A:52:LEU:HD21	2:B:67:PHE:CZ	2.36	0.61
5:I:622:GLN:CD	17:I:3301:ADP:HN61	2.04	0.61
7:K:89:LEU:HD13	7:K:89:LEU:H	1.65	0.61
7:K:306:PRO:HB2	7:K:309:MET:HB2	1.83	0.61
16:Y:-109:DT:H2"	16:Y:-108:DA:N7	2.15	0.61
2:B:34:TYR:HB2	2:B:60:ASN:ND2	2.16	0.61
2:F:53:SER:H	16:Y:-127:DA:P	2.22	0.61
9:Q:254:GLN:OE1	9:Q:254:GLN:N	2.33	0.61
13:V:206:ARG:O	13:V:208:VAL:N	2.33	0.61
13:V:244:GLU:HB2	13:V:247:LEU:HD21	1.82	0.61
13:V:264:ARG:HB3	14:W:198:LYS:HE3	1.83	0.61
15:X:8:DT:H2"	15:X:9:DA:H5'	1.81	0.61
7:K:26:PRO:HG2	7:K:42:ALA:CA	2.29	0.60
7:K:190:TYR:HB2	8:L:148:ARG:HH22	1.66	0.60
16:Y:-146:DC:H2"	16:Y:-145:DT:C6	2.36	0.60
7:K:225:LEU:HD23	7:K:230:ASN:HA	1.83	0.60
9:M:270:GLU:HB2	9:M:276:ARG:NE	2.15	0.60
13:V:192:LYS:HB3	13:V:218:PHE:CE1	2.36	0.60
16:Y:-102:DC:C2'	16:Y:-101:DT:H72	2.29	0.60
6:J:269:SER:HB2	9:Q:150:TYR:HB3	1.59	0.60
7:K:149:ASP:O	7:K:155:THR:HA	2.02	0.60
7:K:161:CYS:H	7:K:166:LYS:HE2	1.65	0.60
10:N:231:GLU:HB2	10:N:234:LYS:HE2	1.81	0.60
13:V:235:ASN:O	13:V:235:ASN:ND2	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:46:DC:H2”	15:X:47:DC:C6	2.36	0.60
16:Y:-52:DC:H4’	16:Y:-51:DC:OP1	2.00	0.60
5:I:921:ILE:HD13	5:I:1986:PRO:CB	2.32	0.60
13:V:147:LEU:HD12	13:V:198:ILE:HG23	1.82	0.60
13:V:237:THR:HG23	13:V:238:PRO:CD	2.25	0.60
5:I:949:ILE:HG22	10:R:260:LEU:CD2	2.24	0.60
16:Y:-44:DA:H2’	16:Y:-43:DT:C7	2.32	0.60
16:Y:-3:DC:H2’	16:Y:-2:DT:C6	2.36	0.60
2:B:111:GLY:O	2:B:115:VAL:HG23	2.02	0.60
1:E:68:ASN:ND2	1:E:68:ASN:O	2.33	0.60
1:E:115:LEU:HD22	4:H:44:LYS:HG2	1.84	0.60
7:K:123:LEU:HD22	7:K:372:PHE:HE1	1.65	0.60
7:K:230:ASN:HD21	7:K:232:VAL:HB	1.65	0.60
2:B:41:VAL:O	2:B:44:GLN:HG2	2.01	0.60
15:X:13:DA:H2”	15:X:14:DT:C5	2.36	0.60
2:B:89:ARG:NE	13:V:63:SER:HB3	2.17	0.60
5:I:921:ILE:HG21	5:I:1986:PRO:N	2.17	0.60
5:I:694:LYS:H	5:I:719:HIS:HD2	1.50	0.60
5:I:754:PHE:HD1	5:I:755:LYS:HG3	1.65	0.60
7:K:29:GLN:HG3	7:K:70:VAL:HG12	1.83	0.60
7:K:232:VAL:HG13	7:K:233:MET:N	2.16	0.60
7:K:302:ILE:CD1	7:K:313:PHE:HB3	2.31	0.60
1:E:56:GLU:HG3	2:F:41:VAL:HG21	1.83	0.60
5:I:613:LEU:HD13	6:J:178:ILE:HD13	1.84	0.60
5:I:1954:ALA:HB3	9:Q:124:ILE:HD11	1.83	0.60
1:E:20:ARG:HG2	1:E:20:ARG:O	2.02	0.59
1:E:102:ILE:HG23	2:F:58:ILE:CD1	2.31	0.59
5:I:949:ILE:HG21	9:M:247:ASN:C	2.12	0.59
7:K:133:HIS:CD2	7:K:366:ILE:HG12	2.35	0.59
7:K:279:GLU:OE2	7:K:283:ASN:HB2	2.02	0.59
7:K:319:LEU:HD12	7:K:330:ARG:HG2	1.82	0.59
11:U:363:ASP:O	13:V:95:TRP:HH2	1.85	0.59
15:X:56:DT:H2”	15:X:57:DT:H5”	1.84	0.59
15:X:99:DA:H1’	15:X:100:DG:C5’	2.31	0.59
2:B:99:LEU:HB3	2:B:103:LEU:HB3	1.83	0.59
5:I:888:MET:SD	15:X:51:DG:C6	2.95	0.59
7:K:159:PRO:HA	7:K:313:PHE:HE1	1.67	0.59
13:V:257:ARG:HA	13:V:260:GLU:HB2	1.83	0.59
7:K:292:MET:H	7:K:292:MET:HE2	1.67	0.59
7:K:364:LYS:HG2	7:K:368:GLU:OE2	2.02	0.59
15:X:51:DG:C1’	15:X:52:DG:H5’	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HG2	1:A:37:LYS:NZ	2.17	0.59
3:G:107:THR:OG1	3:G:124:ILE:HA	2.02	0.59
5:I:667:TRP:CD1	5:I:719:HIS:ND1	2.60	0.59
7:K:139:ASN:HB3	7:K:142:GLU:CG	2.32	0.59
7:K:356:ILE:HD13	7:K:356:ILE:H	1.68	0.59
1:A:52:LEU:HD12	1:A:56:LEU:HG	1.83	0.59
3:C:121:PRO:HB3	4:D:53:GLU:HG3	1.83	0.59
1:E:35:ARG:HB3	1:E:43:VAL:HG21	1.85	0.59
5:I:1972:ILE:HD13	10:P:242:VAL:CG1	2.32	0.59
7:K:183:HIS:HD2	7:K:277:VAL:HG13	1.67	0.59
7:K:305:LEU:CB	7:K:306:PRO:HD3	2.32	0.59
13:V:141:GLN:OE1	13:V:141:GLN:N	2.35	0.59
15:X:72:DA:H1'	15:X:73:DG:H5'	1.84	0.59
7:K:11:TYR:HB2	7:K:152:TYR:CE2	2.38	0.59
7:K:25:ILE:HG22	7:K:26:PRO:HD2	1.84	0.59
7:K:314:PHE:HZ	7:K:345:TYR:CD2	2.21	0.59
15:X:40:DG:H2"	15:X:41:DT:O5'	2.03	0.59
15:X:69:DG:H2"	15:X:70:DA:C8	2.37	0.59
7:K:11:TYR:HB2	7:K:152:TYR:CD2	2.37	0.59
7:K:101:ASN:ND2	7:K:106:GLN:HB2	2.17	0.59
11:U:364:GLU:O	13:V:116:ARG:NH2	2.36	0.59
13:V:246:TYR:HA	13:V:249:GLN:NE2	2.18	0.59
3:C:42:ARG:HB3	3:C:42:ARG:NH1	2.17	0.59
3:C:115:LYS:HD3	3:C:115:LYS:N	2.17	0.59
2:F:28:ARG:HD2	2:F:29:SER:H	1.68	0.59
5:I:713:THR:HG1	15:X:136:DG:P	2.26	0.59
7:K:15:ILE:HD13	7:K:78:LEU:HD13	1.85	0.59
13:V:237:THR:CB	13:V:238:PRO:HD3	2.33	0.59
1:A:43:ARG:HG3	2:B:85:THR:HB	1.85	0.59
5:I:2088:ARG:CD	5:I:2115:ILE:HG22	2.33	0.59
14:W:38:ARG:NH2	14:W:41:ASP:OD2	2.36	0.59
15:X:129:DG:H2"	15:X:130:DG:C8	2.37	0.59
1:A:84:LEU:HD13	2:B:58:ILE:CG2	2.32	0.59
2:B:77:LEU:HD23	2:B:93:THR:HG23	1.83	0.59
5:I:1914:LEU:HD22	9:M:282:VAL:HG12	1.84	0.59
7:K:159:PRO:CG	7:K:169:ALA:HB3	2.32	0.59
7:K:378:THR:HG22	7:K:379:ARG:N	2.17	0.59
13:V:264:ARG:CZ	14:W:198:LYS:HZ3	2.16	0.59
15:X:141:DC:H6	15:X:141:DC:C5'	2.16	0.59
16:Y:-118:DA:H2"	16:Y:-117:DA:C8	2.36	0.59
1:A:35:LEU:HD11	1:A:52:LEU:CD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:OE1	2:F:45:VAL:HG12	2.03	0.58
7:K:212:VAL:CG1	7:K:332:ARG:HG3	2.32	0.58
9:M:35:ALA:HB1	9:M:40:VAL:HG22	1.85	0.58
15:X:128:DC:H2"	15:X:129:DG:C8	2.37	0.58
3:C:49:ARG:HD3	15:X:7:DG:P	2.44	0.58
5:I:633:TYR:HD1	5:I:742:TYR:CE1	2.20	0.58
5:I:657:LEU:HD22	5:I:670:HIS:ND1	2.17	0.58
5:I:935:VAL:O	5:I:936:HIS:CG	2.56	0.58
7:K:232:VAL:HG13	7:K:233:MET:SD	2.43	0.58
7:K:306:PRO:HB2	7:K:309:MET:CB	2.33	0.58
5:I:751:ILE:O	5:I:751:ILE:HG22	2.03	0.58
5:I:921:ILE:CD1	5:I:1986:PRO:HB2	2.33	0.58
3:G:83:ARG:HE	4:H:80:THR:HG22	1.69	0.58
7:K:193:LEU:O	7:K:195:VAL:N	2.37	0.58
10:N:165:THR:HG22	10:N:228:PRO:HG2	1.85	0.58
10:N:301:VAL:CG2	10:N:326:MET:HB2	2.33	0.58
15:X:57:DT:H5'	15:X:57:DT:C6	2.35	0.58
16:Y:-104:DA:H2"	16:Y:-103:DG:O5'	2.02	0.58
7:K:239:PRO:HD3	7:K:247:GLY:HA3	1.85	0.58
13:V:113:HIS:HD2	13:V:115:ARG:HE	1.51	0.58
3:C:100:LEU:HD11	4:D:58:LEU:HD22	1.85	0.58
1:E:111:ILE:HD13	3:G:51:ILE:HG21	1.85	0.58
2:F:85:THR:HG22	16:Y:-107:DG:OP1	2.03	0.58
13:V:264:ARG:HH22	14:W:194:ILE:HG12	1.68	0.58
15:X:87:DT:H1'	15:X:88:DT:C5	2.38	0.58
15:X:121:DG:H2"	15:X:122:DC:C5	2.38	0.58
15:X:138:DA:H2"	15:X:139:DT:H71	1.86	0.58
1:A:51:TYR:CE2	2:B:92:GLN:HB2	2.39	0.58
16:Y:-115:DT:H2"	16:Y:-114:DG:H8	1.67	0.58
1:A:43:ARG:CG	2:B:85:THR:HB	2.34	0.58
5:I:2105:PHE:HE2	5:I:2127:LEU:HD21	1.68	0.58
7:K:198:GLU:O	7:K:200:HIS:N	2.37	0.58
13:V:147:LEU:HD11	13:V:198:ILE:HG23	1.85	0.58
15:X:37:DG:H2"	15:X:38:DG:C8	2.38	0.58
16:Y:-146:DC:H2'	16:Y:-145:DT:C7	2.33	0.58
16:Y:-86:DA:H2"	16:Y:-85:DC:O5'	2.02	0.58
16:Y:-7:DC:H2"	16:Y:-6:DA:H5'	1.86	0.58
2:B:89:ARG:NH2	13:V:63:SER:HB3	2.19	0.58
5:I:649:LYS:NZ	19:I:3303:BEF:F1	2.23	0.58
7:K:205:VAL:HG22	7:K:236:TYR:CE1	2.39	0.58
13:V:236:ARG:NH2	13:V:240:GLN:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLN:HG2	2:B:40:LYS:HB3	1.86	0.58
2:B:38:VAL:HG11	2:B:59:MET:CG	2.34	0.58
3:C:109:LEU:CD1	3:G:129:ARG:HG2	2.32	0.58
5:I:163:ARG:O	5:I:166:VAL:HG23	2.00	0.58
5:I:726:LYS:HD2	15:X:56:DT:H4'	1.84	0.58
7:K:193:LEU:HG	7:K:268:LEU:HD13	1.86	0.58
7:K:351:LEU:HD23	7:K:352:PRO:O	2.03	0.58
15:X:28:DG:H2"	15:X:29:DG:H8	1.67	0.58
15:X:71:DC:H2"	15:X:72:DA:H8	1.68	0.58
1:A:25:GLN:OE1	2:B:41:VAL:HG22	2.03	0.57
2:B:90:GLU:HA	2:B:93:THR:CG2	2.34	0.57
2:F:77:LEU:CD1	2:F:93:THR:HB	2.34	0.57
3:G:103:LEU:HD11	3:G:128:ARG:CG	2.33	0.57
4:H:49:LEU:H	4:H:49:LEU:HD12	1.69	0.57
5:I:2079:LEU:HD12	5:I:2115:ILE:HD11	1.86	0.57
7:K:66:VAL:O	7:K:67:ASN:ND2	2.37	0.57
7:K:159:PRO:HB3	7:K:313:PHE:CZ	2.38	0.57
13:V:262:GLU:CG	14:W:202:LYS:NZ	2.65	0.57
2:B:46:HIS:HB3	2:B:49:THR:HB	1.86	0.57
3:C:128:ARG:O	3:C:131:ARG:HB2	2.04	0.57
4:H:35:ARG:NH1	4:H:35:ARG:HB2	2.19	0.57
9:M:312:PHE:O	9:M:316:HIS:ND1	2.26	0.57
15:X:121:DG:H2"	15:X:122:DC:C6	2.39	0.57
1:A:35:LEU:HD21	2:B:67:PHE:HE1	1.63	0.57
3:G:118:THR:HG23	4:H:45:ARG:HB3	1.87	0.57
12:T:12:GLY:H	13:V:97:TRP:HH2	1.51	0.57
16:Y:-106:DA:H2"	16:Y:-105:DC:C6	2.39	0.57
7:K:32:SER:HB2	7:K:54:LEU:CD2	2.34	0.57
7:K:282:PHE:CE2	7:K:332:ARG:HB3	2.38	0.57
7:K:376:VAL:O	7:K:377:VAL:HB	2.04	0.57
13:V:51:GLU:HB3	13:V:58:TYR:CZ	2.39	0.57
13:V:182:GLN:HB2	13:V:183:PHE:CE1	2.38	0.57
15:X:118:DT:H2"	15:X:119:DG:C8	2.39	0.57
2:B:75:SER:CA	2:B:86:ILE:HD11	2.34	0.57
3:G:73:GLU:CA	4:H:23:ARG:HH12	2.17	0.57
7:K:159:PRO:HG2	7:K:169:ALA:HB3	1.85	0.57
10:P:248:ASP:OD2	10:P:273:ARG:NH1	2.38	0.57
10:R:43:SER:O	10:R:45:GLY:N	2.37	0.57
7:K:96:THR:HA	7:K:125:VAL:O	2.05	0.57
7:K:131:SER:OG	7:K:147:ILE:HD12	2.04	0.57
7:K:315:LYS:HA	7:K:348:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:313:THR:CB	9:M:316:HIS:CE1	2.88	0.57
10:N:123:PHE:HE1	10:N:324:LEU:HD23	1.69	0.57
13:V:147:LEU:CD1	13:V:198:ILE:HA	2.35	0.57
16:Y:-13:DT:H71	16:Y:-13:DT:OP2	2.04	0.57
3:G:118:THR:HG23	4:H:45:ARG:CG	2.35	0.57
3:G:120:MET:HB2	3:G:121:PRO:CD	2.35	0.57
7:K:101:ASN:HD21	7:K:106:GLN:H	1.51	0.57
7:K:102:PHE:O	7:K:104:SER:N	2.37	0.57
7:K:305:LEU:HB2	7:K:306:PRO:HD3	1.87	0.57
13:V:219:ASP:O	13:V:223:GLU:HB2	2.04	0.57
13:V:239:GLU:OE2	13:V:240:GLN:HG2	2.05	0.57
15:X:48:DC:H1'	15:X:49:DT:C6	2.40	0.57
1:A:29:GLY:O	1:A:33:ARG:HB2	2.05	0.57
1:E:25:PHE:CD2	1:E:26:PRO:HD2	2.40	0.57
7:K:44:GLN:HG3	7:K:77:TYR:CE2	2.40	0.57
7:K:68:TRP:O	7:K:72:ARG:HG2	2.05	0.57
15:X:33:DC:H2'	15:X:34:DT:H71	1.84	0.57
1:E:76:THR:O	1:E:76:THR:OG1	2.16	0.57
2:F:77:LEU:HD11	2:F:93:THR:HG22	1.86	0.57
7:K:93:ILE:HG21	7:K:113:LEU:HD11	1.87	0.57
16:Y:-80:DG:H2"	16:Y:-79:DT:C6	2.39	0.57
2:B:75:SER:CB	2:B:86:ILE:HD11	2.35	0.57
7:K:105:ILE:HG12	8:L:90:GLU:OE1	2.04	0.57
13:V:189:GLU:CG	13:V:224:ARG:HD3	2.35	0.57
3:C:130:ILE:HD12	3:G:130:ILE:HD12	1.86	0.56
7:K:273:GLU:O	7:K:277:VAL:HG23	2.05	0.56
16:Y:-42:DT:H2"	16:Y:-41:DA:H5'	1.87	0.56
2:B:73:GLU:OE2	4:H:72:TYR:OH	2.13	0.56
7:K:195:VAL:HG22	7:K:198:GLU:HG3	1.87	0.56
9:M:416:LEU:HB2	9:M:433:ILE:HD11	1.86	0.56
13:V:143:TYR:HA	13:V:147:LEU:HB2	1.87	0.56
13:V:268:LEU:HD22	14:W:191:SER:OG	2.04	0.56
15:X:8:DT:H2"	15:X:9:DA:H8	1.69	0.56
5:I:125:PRO:HD2	13:V:222:HIS:CE1	2.40	0.56
5:I:210:GLU:O	5:I:214:GLN:HG3	2.04	0.56
5:I:921:ILE:HG22	5:I:1985:ALA:CB	2.19	0.56
5:I:1992:ALA:HB2	10:N:201:LYS:HZ2	1.68	0.56
7:K:205:VAL:HG11	7:K:269:ARG:CZ	2.35	0.56
7:K:311:PRO:HA	7:K:314:PHE:CE2	2.40	0.56
13:V:233:LEU:N	13:V:233:LEU:HD23	2.20	0.56
13:V:262:GLU:HG3	14:W:202:LYS:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-56:DA:H2"	16:Y:-55:DC:C5	2.40	0.56
1:A:35:LEU:HD11	1:A:52:LEU:HD23	1.88	0.56
1:E:20:ARG:HG3	2:F:121:SER:CB	2.35	0.56
7:K:36:ARG:NH2	7:K:37:LEU:HG	2.20	0.56
7:K:232:VAL:HG22	7:K:233:MET:N	2.20	0.56
13:V:264:ARG:NH1	14:W:194:ILE:HG21	2.21	0.56
13:V:265:SER:OG	14:W:198:LYS:HD3	2.06	0.56
1:A:56:LEU:HD11	2:B:67:PHE:HD2	1.70	0.56
1:E:85:LEU:HD22	1:E:108:LEU:HD23	1.87	0.56
4:H:79:LYS:HB3	4:H:79:LYS:NZ	2.21	0.56
5:I:2131:ASP:O	5:I:2132:THR:OG1	2.23	0.56
7:K:13:ALA:HB3	7:K:25:ILE:HG12	1.87	0.56
7:K:176:GLY:H	7:K:179:LEU:HD13	1.71	0.56
14:W:137:GLU:HG2	14:W:170:THR:HB	1.88	0.56
15:X:137:DG:H2"	15:X:138:DA:C8	2.41	0.56
1:A:18:ARG:HH22	1:A:36:ARG:HH12	1.54	0.56
1:E:81:ARG:HD3	1:E:81:ARG:C	2.25	0.56
2:F:111:GLY:O	2:F:115:VAL:HG23	2.06	0.56
7:K:81:LYS:HD2	7:K:82:GLU:N	2.21	0.56
7:K:113:LEU:HA	7:K:117:TYR:HD2	1.70	0.56
7:K:306:PRO:HB3	7:K:308:GLU:OE2	2.05	0.56
13:V:156:GLU:OE1	13:V:183:PHE:CD2	2.59	0.56
13:V:255:GLU:HA	13:V:259:LYS:HE2	1.86	0.56
16:Y:-56:DA:H2"	16:Y:-55:DC:C6	2.40	0.56
1:A:57:GLU:OE2	8:L:9:ARG:NH2	2.39	0.56
1:E:85:LEU:HD22	1:E:108:LEU:CD2	2.36	0.56
13:V:50:PRO:O	13:V:51:GLU:HG3	2.06	0.56
13:V:182:GLN:C	13:V:183:PHE:CD1	2.79	0.56
9:M:180:LEU:HD21	9:M:193:ILE:HD11	1.88	0.56
9:M:317:ARG:CD	10:R:104:ALA:HB2	2.36	0.56
15:X:125:DC:H2"	15:X:126:DC:H5'	1.88	0.56
1:A:56:LEU:HD11	2:B:67:PHE:HB2	1.88	0.56
2:B:28:ARG:HH12	16:Y:-21:DG:P	2.29	0.56
1:E:95:LYS:HZ2	1:E:95:LYS:HB3	1.71	0.56
4:H:97:LEU:HD11	4:H:100:PHE:HD1	1.71	0.56
5:I:118:PHE:CG	13:V:247:LEU:HD13	2.40	0.56
7:K:13:ALA:O	7:K:15:ILE:N	2.39	0.56
7:K:183:HIS:O	7:K:187:ILE:HG12	2.05	0.56
7:K:237:VAL:CG1	7:K:250:LYS:HE2	2.35	0.56
7:K:337:VAL:O	7:K:341:THR:HG23	2.06	0.56
9:M:416:LEU:HD22	9:M:433:ILE:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:338:ILE:HD11	13:V:230:LEU:HD22	1.87	0.56
5:I:167:ARG:HG2	15:X:31:DG:H5"	1.88	0.55
7:K:133:HIS:O	7:K:137:ARG:HG3	2.06	0.55
7:K:324:SER:HB2	7:K:351:LEU:HD11	1.88	0.55
13:V:128:ARG:HG3	13:V:129:PHE:CD1	2.41	0.55
13:V:143:TYR:CE1	13:V:154:LYS:HG3	2.40	0.55
1:A:55:VAL:HG13	2:B:107:ALA:CB	2.34	0.55
2:F:39:TYR:CZ	2:F:43:LYS:HE3	2.41	0.55
7:K:62:LYS:HD2	7:K:172:ARG:HH12	1.71	0.55
7:K:233:MET:HA	7:K:255:MET:HE3	1.87	0.55
7:K:377:VAL:HG22	7:K:389:VAL:HG22	1.88	0.55
10:N:39:PRO:HD3	10:N:54:ARG:HB2	1.88	0.55
13:V:250:GLU:OE2	13:V:253:LYS:HD3	2.05	0.55
13:V:261:ARG:HA	14:W:198:LYS:CE	2.37	0.55
16:Y:-21:DG:H2'	16:Y:-20:DT:C7	2.33	0.55
3:C:96:CYS:SG	4:D:62:LEU:HD21	2.46	0.55
4:H:92:ARG:HB3	4:H:92:ARG:CZ	2.37	0.55
15:X:8:DT:H2"	15:X:9:DA:C8	2.42	0.55
15:X:119:DG:H1'	15:X:120:DA:C8	2.42	0.55
16:Y:-77:DC:H2"	16:Y:-76:DG:C8	2.41	0.55
2:F:99:LEU:HB2	2:F:104:ALA:CB	2.36	0.55
7:K:159:PRO:HB3	7:K:313:PHE:HZ	1.72	0.55
15:X:110:DC:H2"	15:X:111:DG:C8	2.42	0.55
1:A:110:PRO:HA	3:C:55:GLN:OE1	2.06	0.55
7:K:72:ARG:NH1	7:K:117:TYR:OH	2.39	0.55
13:V:229:GLN:OE1	13:V:229:GLN:N	2.38	0.55
16:Y:-110:DG:H4'	16:Y:-110:DG:OP1	2.06	0.55
1:A:85:GLN:O	1:A:89:ARG:HG2	2.07	0.55
2:B:73:GLU:OE1	2:B:73:GLU:HA	2.07	0.55
5:I:1914:LEU:CD1	9:M:282:VAL:HB	2.36	0.55
13:V:96:LYS:N	13:V:114:TRP:HZ3	2.05	0.55
15:X:51:DG:H1'	15:X:52:DG:C5'	2.31	0.55
15:X:141:DC:H6	15:X:141:DC:H5'	1.71	0.55
1:A:55:VAL:CG1	2:B:107:ALA:HB1	2.37	0.55
4:D:23:ARG:NH2	14:W:81:VAL:CG1	2.63	0.55
7:K:29:GLN:HB3	7:K:39:THR:HG22	1.88	0.55
7:K:128:GLY:O	7:K:147:ILE:HG13	2.06	0.55
7:K:223:ALA:HA	7:K:230:ASN:O	2.06	0.55
11:U:257:CYS:HB3	11:U:258:PRO:CD	2.37	0.55
16:Y:-24:DC:H2"	16:Y:-23:DA:C8	2.41	0.55
4:D:75:HIS:CD2	2:F:89:ARG:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:237:VAL:HG12	7:K:267:ILE:HG22	1.89	0.55
16:Y:-78:DA:H2"	16:Y:-77:DC:C6	2.41	0.55
5:I:128:PRO:CB	13:V:216:PRO:HG2	2.37	0.55
5:I:670:HIS:CD2	5:I:742:TYR:HD2	2.21	0.55
7:K:75:TRP:HB3	7:K:79:PHE:CZ	2.42	0.55
7:K:78:LEU:O	7:K:84:TYR:HB2	2.07	0.55
15:X:12:DT:H2"	15:X:13:DA:C8	2.42	0.55
4:H:73:THR:OG1	4:H:85:ASP:OD2	2.18	0.54
7:K:180:LEU:HB3	7:K:277:VAL:HG12	1.89	0.54
5:I:921:ILE:CG2	5:I:1985:ALA:HB1	2.20	0.54
7:K:376:VAL:CG1	7:K:377:VAL:N	2.67	0.54
15:X:4:DG:H2"	15:X:5:DA:H5"	1.89	0.54
15:X:35:DA:H4'	15:X:35:DA:OP1	2.07	0.54
7:K:17:TYR:H	7:K:21:ASN:CG	2.11	0.54
7:K:172:ARG:NH2	7:K:174:ASN:HD21	2.05	0.54
11:U:117:GLU:OE1	13:V:114:TRP:NE1	2.39	0.54
15:X:100:DG:H1'	15:X:101:DA:N7	2.22	0.54
16:Y:-39:DT:H4'	16:Y:-39:DT:OP1	2.06	0.54
1:A:25:GLN:N	8:L:9:ARG:HH22	2.04	0.54
2:B:93:THR:HG21	4:H:75:HIS:CD2	2.42	0.54
2:B:116:THR:HG22	13:V:57:VAL:HG13	1.90	0.54
13:V:104:ALA:HB2	13:V:127:ALA:HB1	1.89	0.54
15:X:120:DA:H2"	15:X:121:DG:C8	2.42	0.54
1:A:66:LEU:CD1	1:A:94:LEU:HD12	2.38	0.54
3:C:130:ILE:HG21	3:G:130:ILE:HB	1.89	0.54
1:E:25:PHE:HB2	1:E:56:GLU:OE1	2.07	0.54
7:K:110:ASN:HB2	7:K:387:HIS:CD2	2.42	0.54
7:K:377:VAL:HG21	7:K:393:LYS:HG3	1.90	0.54
9:M:26:LEU:CD1	9:M:50:GLY:HA3	2.35	0.54
11:U:362:TYR:HE2	13:V:91:LYS:HD3	1.73	0.54
13:V:54:HIS:O	13:V:58:TYR:HB3	2.07	0.54
15:X:120:DA:C2'	15:X:121:DG:C8	2.91	0.54
16:Y:-12:DA:H2"	16:Y:-11:DT:H5'	1.89	0.54
3:G:83:ARG:O	4:H:80:THR:HA	2.08	0.54
5:I:128:PRO:CG	13:V:218:PHE:HA	2.38	0.54
5:I:633:TYR:HD1	5:I:742:TYR:HE1	1.56	0.54
5:I:2072:LEU:HB3	5:I:2088:ARG:CD	2.29	0.54
13:V:258:LYS:O	13:V:262:GLU:N	2.36	0.54
1:A:51:TYR:CD1	2:B:91:ILE:HG22	2.42	0.54
3:G:55:GLN:HG2	3:G:55:GLN:O	2.07	0.54
5:I:236:ILE:HA	5:I:239:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2092:SER:HA	15:X:56:DT:H73	1.90	0.54
7:K:99:TYR:CE2	7:K:158:VAL:HG21	2.43	0.54
7:K:120:GLN:C	7:K:378:THR:HG21	2.28	0.54
7:K:121:ALA:HA	7:K:378:THR:OG1	2.07	0.54
7:K:176:GLY:O	7:K:180:LEU:HG	2.07	0.54
13:V:236:ARG:NH2	13:V:241:VAL:HA	2.23	0.54
13:V:272:ILE:HD13	14:W:191:SER:HB2	1.88	0.54
15:X:36:DG:N2	16:Y:-35:DT:O2	2.41	0.54
1:A:51:TYR:CE1	2:B:95:VAL:HG21	2.43	0.54
13:V:206:ARG:O	13:V:209:PRO:HD2	2.08	0.54
15:X:39:DA:H2"	15:X:40:DG:H8	1.73	0.54
15:X:109:DA:H61	16:Y:-109:DT:H3	1.55	0.54
1:A:30:ARG:NH1	2:B:33:SER:O	2.34	0.54
1:A:71:ALA:HA	1:A:83:HIS:CD2	2.42	0.54
4:H:38:ALA:HB1	4:H:43:VAL:HB	1.90	0.54
5:I:2087:LEU:HD11	5:I:2104:ARG:CZ	2.37	0.54
7:K:222:ILE:HG22	7:K:230:ASN:HA	1.90	0.54
15:X:7:DG:C1'	15:X:8:DT:H5"	2.38	0.54
15:X:135:DG:H2"	15:X:136:DG:O5'	2.07	0.54
5:I:800:HIS:CG	5:I:801:ARG:H	2.26	0.54
7:K:6:LEU:HD13	7:K:95:ILE:HG12	1.90	0.54
7:K:225:LEU:HG	7:K:230:ASN:HB3	1.89	0.54
7:K:294:ILE:N	7:K:295:PRO:HD2	2.23	0.54
7:K:375:MET:O	7:K:376:VAL:CG1	2.54	0.54
9:O:15:ILE:CG2	10:P:69:ALA:HB2	2.38	0.54
15:X:57:DT:C6	15:X:57:DT:C5'	2.91	0.54
13:V:225:ARG:O	13:V:229:GLN:OE1	2.25	0.53
15:X:35:DA:H2"	15:X:36:DG:C8	2.43	0.53
15:X:81:DG:C2'	15:X:82:DT:H71	2.38	0.53
16:Y:-109:DT:H2"	16:Y:-108:DA:C5	2.43	0.53
3:C:126:LEU:HD22	3:G:113:HIS:CG	2.43	0.53
1:E:78:ILE:HG13	2:F:49:THR:CG2	2.38	0.53
4:H:97:LEU:HD11	4:H:100:PHE:CE1	2.43	0.53
7:K:62:LYS:HD2	7:K:172:ARG:HH22	1.72	0.53
13:V:247:LEU:HD12	13:V:248:LEU:HD23	1.89	0.53
13:V:258:LYS:CE	13:V:259:LYS:HG3	2.37	0.53
15:X:75:DG:H2"	15:X:76:DC:C6	2.43	0.53
16:Y:-60:DT:H71	16:Y:-60:DT:OP2	2.08	0.53
3:C:47:ALA:O	3:C:51:ILE:HG13	2.08	0.53
5:I:846:GLU:CG	5:I:848:GLN:HG2	2.36	0.53
7:K:279:GLU:O	7:K:283:ASN:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:251:LEU:O	13:V:255:GLU:HB2	2.09	0.53
13:V:266:GLN:HA	13:V:266:GLN:NE2	2.23	0.53
16:Y:-91:DC:H1'	16:Y:-90:DT:H5'	1.90	0.53
16:Y:-13:DT:H2"	16:Y:-12:DA:H5'	1.89	0.53
1:A:13:ALA:N	5:I:164:LYS:HB2	2.23	0.53
1:A:116:LEU:HD22	3:C:117:VAL:HG13	1.90	0.53
2:B:87:THR:O	2:B:91:ILE:HG12	2.07	0.53
4:D:23:ARG:HH21	14:W:81:VAL:HG13	1.71	0.53
1:E:42:ARG:NH1	15:X:112:DA:H5'	2.23	0.53
5:I:128:PRO:HG3	13:V:216:PRO:O	2.08	0.53
13:V:233:LEU:CA	13:V:236:ARG:HD3	2.27	0.53
13:V:265:SER:OG	14:W:198:LYS:CD	2.56	0.53
15:X:141:DC:C5'	15:X:141:DC:C6	2.92	0.53
3:C:49:ARG:HD3	15:X:7:DG:OP1	2.09	0.53
1:E:99:ARG:O	4:H:96:THR:HB	2.08	0.53
7:K:50:ASP:OD1	7:K:52:SER:HB2	2.08	0.53
7:K:72:ARG:HA	7:K:72:ARG:HH11	1.72	0.53
7:K:241:PHE:HA	7:K:244:ILE:O	2.09	0.53
1:A:26:PHE:HE2	2:B:63:VAL:CG1	2.21	0.53
2:B:39:TYR:CE1	2:B:43:LYS:HE3	2.43	0.53
5:I:667:TRP:CZ2	5:I:719:HIS:CE1	2.97	0.53
5:I:969:LEU:CB	10:R:225:VAL:HA	2.38	0.53
7:K:377:VAL:HG23	7:K:393:LYS:HZ3	1.73	0.53
9:M:113:MET:CG	9:M:276:ARG:HH12	2.18	0.53
13:V:50:PRO:C	13:V:51:GLU:HG3	2.28	0.53
13:V:202:LEU:HD13	13:V:206:ARG:HH22	1.72	0.53
1:A:32:HIS:CA	1:A:49:PRO:HB3	2.39	0.53
2:B:65:ASP:OD2	4:D:98:TYR:OH	2.26	0.53
5:I:649:LYS:NZ	19:I:3303:BEF:F3	2.31	0.53
5:I:1972:ILE:HG21	10:P:242:VAL:HG11	1.91	0.53
7:K:133:HIS:NE2	7:K:362:GLY:O	2.42	0.53
15:X:117:DT:H2"	15:X:118:DT:C6	2.44	0.53
1:A:71:ALA:HA	1:A:83:HIS:NE2	2.24	0.53
7:K:164:LYS:HZ1	7:K:166:LYS:HA	1.73	0.53
10:N:59:VAL:HG21	10:N:325:ILE:HD11	1.91	0.53
13:V:244:GLU:HA	13:V:247:LEU:HD21	1.90	0.53
13:V:261:ARG:CB	14:W:198:LYS:HG2	2.39	0.53
13:V:262:GLU:HG3	14:W:202:LYS:HG3	1.90	0.53
1:A:33:ARG:O	1:A:36:ARG:HG3	2.08	0.53
1:A:39:ASN:ND2	1:E:40:ALA:HA	2.24	0.53
5:I:2088:ARG:HA	5:I:2115:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:333:VAL:O	7:K:337:VAL:HG13	2.09	0.53
16:Y:-116:DT:H5'	16:Y:-116:DT:H6	1.73	0.53
16:Y:-85:DC:H1'	16:Y:-84:DG:C8	2.44	0.53
16:Y:-41:DA:H2"	16:Y:-40:DC:C6	2.44	0.53
1:A:51:TYR:CZ	2:B:92:GLN:HA	2.44	0.53
3:C:113:HIS:NE2	3:G:110:CYS:O	2.42	0.53
1:E:35:ARG:HB3	1:E:43:VAL:HG23	1.90	0.53
16:Y:-25:DG:H1'	16:Y:-24:DC:C5	2.44	0.53
4:D:45:ARG:NH2	15:X:80:DC:O4'	2.42	0.52
5:I:726:LYS:NZ	15:X:55:DG:H1'	2.25	0.52
15:X:59:DA:H2"	15:X:60:DA:OP2	2.08	0.52
1:A:52:LEU:HD11	2:B:67:PHE:HA	1.90	0.52
2:B:116:THR:HG22	13:V:57:VAL:CG1	2.40	0.52
4:H:46:ILE:CG2	4:H:50:ILE:HG21	2.35	0.52
7:K:88:PHE:CB	7:K:119:PHE:HD2	2.22	0.52
7:K:191:ARG:NH1	7:K:273:GLU:OE1	2.42	0.52
7:K:233:MET:HG2	7:K:252:ARG:HG3	1.91	0.52
7:K:357:THR:O	7:K:361:GLU:HG3	2.09	0.52
13:V:96:LYS:HD2	13:V:98:MET:HE2	1.91	0.52
5:I:2063:LEU:CD1	5:I:2127:LEU:HD23	2.38	0.52
5:I:2098:ARG:NH1	15:X:56:DT:OP2	2.40	0.52
16:Y:-108:DA:H2"	16:Y:-107:DG:O5'	2.09	0.52
1:E:17:ARG:N	16:Y:-116:DT:OP1	2.39	0.52
13:V:96:LYS:HD3	13:V:97:TRP:O	2.09	0.52
13:V:182:GLN:HB2	13:V:183:PHE:CD1	2.45	0.52
13:V:189:GLU:HG3	13:V:224:ARG:HD3	1.91	0.52
16:Y:-115:DT:H2"	16:Y:-114:DG:C8	2.44	0.52
1:E:25:PHE:N	1:E:56:GLU:OE1	2.43	0.52
7:K:107:GLU:HG3	7:K:108:SER:N	2.25	0.52
7:K:338:ARG:HB2	7:K:347:VAL:HG11	1.90	0.52
13:V:206:ARG:C	13:V:209:PRO:HD2	2.30	0.52
1:A:66:LEU:HB2	1:A:87:ALA:HB1	1.91	0.52
5:I:1992:ALA:HB2	10:N:201:LYS:HZ3	1.75	0.52
15:X:49:DT:H2'	15:X:50:DT:H71	1.92	0.52
16:Y:-25:DG:H4'	16:Y:-24:DC:OP1	2.10	0.52
7:K:287:ILE:HG23	8:L:35:LEU:CD1	2.38	0.52
3:C:42:ARG:NH2	16:Y:-78:DA:O5'	2.41	0.52
5:I:888:MET:SD	15:X:51:DG:N1	2.82	0.52
7:K:377:VAL:HG23	7:K:393:LYS:NZ	2.25	0.52
9:M:36:ALA:O	9:M:38:GLY:N	2.42	0.52
13:V:261:ARG:O	14:W:198:LYS:CE	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TYR:N	2:B:60:ASN:HD21	2.04	0.52
3:C:103:LEU:HD11	3:C:128:ARG:HG2	1.92	0.52
7:K:93:ILE:CG2	7:K:113:LEU:HD11	2.40	0.52
7:K:157:ILE:O	7:K:170:ILE:HA	2.09	0.52
7:K:376:VAL:O	7:K:377:VAL:CB	2.58	0.52
15:X:66:DG:H2"	15:X:67:DG:N7	2.25	0.52
1:E:101:THR:N	4:H:96:THR:O	2.32	0.52
9:M:271:ILE:HD12	9:M:271:ILE:N	2.25	0.52
9:O:447:LEU:HD11	10:P:344:HIS:CE1	2.44	0.52
13:V:98:MET:HB3	13:V:120:GLU:OE2	2.09	0.52
13:V:187:SER:N	13:V:190:ASP:OD2	2.43	0.52
15:X:105:DG:H1'	15:X:106:DT:H5'	1.91	0.52
3:G:103:LEU:HD11	3:G:128:ARG:HG2	1.92	0.51
13:V:147:LEU:HD12	13:V:198:ILE:HG12	1.92	0.51
13:V:219:ASP:OD1	13:V:223:GLU:N	2.43	0.51
16:Y:-13:DT:H2"	16:Y:-12:DA:C5'	2.41	0.51
7:K:76:ASP:O	7:K:80:GLY:N	2.43	0.51
7:K:119:PHE:O	7:K:120:GLN:O	2.28	0.51
7:K:233:MET:HG2	7:K:252:ARG:HD2	1.91	0.51
13:V:201:LYS:O	13:V:205:VAL:HG13	2.10	0.51
15:X:59:DA:C2'	15:X:60:DA:H5"	2.39	0.51
15:X:76:DC:H2'	15:X:76:DC:OP2	2.11	0.51
16:Y:-12:DA:H1'	16:Y:-11:DT:H5"	1.92	0.51
1:A:33:ARG:HB2	1:A:36:ARG:NH2	2.24	0.51
1:A:60:THR:CG2	2:B:63:VAL:HG22	2.40	0.51
7:K:174:ASN:HB2	7:K:291:GLU:OE1	2.10	0.51
7:K:282:PHE:CZ	7:K:333:VAL:HG23	2.46	0.51
7:K:385:ASN:OD1	7:K:385:ASN:N	2.43	0.51
9:M:274:LYS:O	9:M:278:GLU:HG2	2.10	0.51
15:X:68:DG:H1'	15:X:69:DG:C8	2.45	0.51
1:A:33:ARG:HG3	15:X:28:DG:OP2	2.09	0.51
1:A:84:LEU:O	1:A:88:ILE:HD12	2.10	0.51
7:K:380:GLU:OE1	7:K:381:ASP:N	2.40	0.51
11:U:117:GLU:CD	13:V:114:TRP:HE1	2.14	0.51
13:V:98:MET:CE	13:V:120:GLU:HB2	2.41	0.51
13:V:138:TYR:HB3	13:V:202:LEU:HD21	1.93	0.51
13:V:271:LEU:HB3	14:W:187:LYS:HZ1	1.76	0.51
3:C:74:ILE:HG23	4:D:63:GLU:HG2	1.93	0.51
1:E:87:ILE:HD13	1:E:97:LEU:HD12	1.92	0.51
5:I:895:MET:HE1	15:X:52:DG:H5"	1.91	0.51
7:K:112:ILE:O	7:K:116:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:280:ILE:HG12	7:K:287:ILE:HG12	1.92	0.51
7:K:285:SER:HA	7:K:289:ILE:O	2.11	0.51
15:X:111:DG:C2	16:Y:-110:DG:N2	2.78	0.51
16:Y:-9:DT:H2"	16:Y:-8:DA:C8	2.45	0.51
1:A:58:TYR:OH	1:A:62:GLU:OE2	2.25	0.51
2:B:77:LEU:CD2	2:B:93:THR:HG23	2.41	0.51
2:B:122:LYS:HB3	8:L:2:VAL:HG12	1.90	0.51
1:E:81:ARG:HG2	3:G:58:THR:HG23	1.93	0.51
4:H:92:ARG:HB3	4:H:92:ARG:NH1	2.26	0.51
7:K:13:ALA:HB3	7:K:25:ILE:CG1	2.41	0.51
7:K:67:ASN:C	7:K:69:ASP:H	2.14	0.51
7:K:106:GLN:CB	7:K:124:ARG:HH22	2.18	0.51
13:V:92:VAL:O	13:V:92:VAL:HG22	2.10	0.51
15:X:138:DA:H2"	15:X:139:DT:C7	2.40	0.51
1:A:33:ARG:HH22	2:B:32:GLU:CD	2.13	0.51
1:E:65:LEU:CB	1:E:86:ALA:HB1	2.39	0.51
3:G:41:TYR:CD1	3:G:45:THR:HG21	2.45	0.51
5:I:895:MET:CE	15:X:52:DG:H4'	2.40	0.51
5:I:1886:LEU:HB2	5:I:1889:LEU:HB2	1.93	0.51
12:T:340:ILE:HD13	13:V:172:VAL:HG11	1.92	0.51
13:V:225:ARG:O	13:V:228:GLU:N	2.43	0.51
3:C:121:PRO:HA	4:D:50:ILE:CD1	2.41	0.51
5:I:918:THR:O	5:I:921:ILE:HG23	2.10	0.51
7:K:234:ILE:CD1	7:K:271:ALA:HA	2.32	0.51
9:O:235:ILE:HG23	9:O:235:ILE:O	2.11	0.51
11:U:101:HIS:CD2	11:U:101:HIS:N	2.78	0.51
1:A:33:ARG:HG2	1:A:37:LYS:HZ1	1.75	0.51
1:A:89:ARG:NH1	1:A:95:ASN:OD1	2.39	0.51
5:I:619:ARG:NH1	17:I:3301:ADP:C6	2.79	0.51
5:I:1954:ALA:CB	9:Q:124:ILE:HD11	2.41	0.51
7:K:13:ALA:O	7:K:15:ILE:HG23	2.11	0.51
7:K:171:ILE:HG22	7:K:173:ILE:HG12	1.92	0.51
10:N:324:LEU:HD13	10:N:326:MET:CE	2.40	0.51
10:P:205:LEU:H	10:P:205:LEU:HD22	1.76	0.51
15:X:10:DT:H2"	15:X:11:DA:OP2	2.10	0.51
15:X:21:DC:H1'	15:X:22:DG:H5"	1.91	0.51
15:X:47:DC:H2"	15:X:48:DC:C6	2.45	0.51
15:X:57:DT:H6	15:X:57:DT:C5'	2.21	0.51
3:C:96:CYS:HB3	4:D:58:LEU:HD11	1.92	0.51
3:G:120:MET:HB2	3:G:121:PRO:HD2	1.91	0.51
5:I:126:LYS:HE2	13:V:216:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:313:THR:HG21	10:R:303:MET:CG	2.40	0.51
1:A:67:ALA:HA	1:A:83:HIS:O	2.11	0.50
7:K:38:LYS:HD2	7:K:40:PHE:CG	2.46	0.50
7:K:232:VAL:HG13	7:K:233:MET:H	1.75	0.50
15:X:22:DG:H2"	15:X:23:DT:C5'	2.17	0.50
15:X:103:DC:C6	15:X:104:DT:H72	2.46	0.50
16:Y:-11:DT:H2"	16:Y:-10:DA:H5'	1.92	0.50
16:Y:-11:DT:H1'	16:Y:-10:DA:H5"	1.91	0.50
1:E:57:TYR:CD1	2:F:110:GLU:HG3	2.46	0.50
1:E:71:ARG:HA	1:E:75:LYS:O	2.11	0.50
3:G:116:ARG:HH21	3:G:122:LYS:HE3	1.76	0.50
5:I:180:GLU:N	5:I:180:GLU:OE1	2.43	0.50
5:I:621:TYR:OH	5:I:846:GLU:OE1	2.28	0.50
5:I:917:ILE:HD12	9:O:128:LYS:HZ1	1.75	0.50
5:I:921:ILE:HD13	5:I:1986:PRO:HB2	1.92	0.50
5:I:1941:PRO:HG2	5:I:1945:HIS:HD2	1.76	0.50
9:O:401:THR:O	9:O:402:THR:HG23	2.11	0.50
15:X:133:DC:H1'	15:X:134:DC:H5'	1.93	0.50
1:E:100:VAL:HA	4:H:96:THR:O	2.12	0.50
5:I:1992:ALA:CB	10:N:201:LYS:HZ3	2.25	0.50
7:K:237:VAL:CG1	7:K:267:ILE:HG22	2.40	0.50
7:K:337:VAL:HG23	7:K:347:VAL:HG21	1.92	0.50
9:M:310:GLU:HA	9:M:313:THR:HG22	1.93	0.50
9:Q:255:ASP:O	9:Q:257:LEU:N	2.45	0.50
16:Y:-138:DT:H2"	16:Y:-137:DC:C6	2.46	0.50
5:I:904:PRO:O	5:I:908:ASP:N	2.43	0.50
7:K:88:PHE:O	7:K:119:PHE:HB2	2.11	0.50
7:K:284:PRO:HG3	7:K:293:GLY:N	2.27	0.50
13:V:226:ARG:HA	13:V:229:GLN:OE1	2.11	0.50
15:X:70:DA:H8	15:X:70:DA:OP2	1.94	0.50
1:E:74:LYS:HD3	6:J:151:ARG:CD	2.40	0.50
1:E:81:ARG:NH2	1:E:107:VAL:O	2.43	0.50
3:G:48:LEU:HD23	3:G:51:ILE:HD12	1.94	0.50
7:K:89:LEU:HD13	7:K:89:LEU:N	2.26	0.50
7:K:122:VAL:C	7:K:123:LEU:HD23	2.32	0.50
13:V:255:GLU:C	13:V:259:LYS:HE2	2.32	0.50
16:Y:-56:DA:H1'	16:Y:-55:DC:C6	2.46	0.50
16:Y:-24:DC:H1'	16:Y:-23:DA:C8	2.46	0.50
16:Y:-23:DA:H2'	16:Y:-22:DC:C5	2.46	0.50
7:K:56:TYR:C	8:L:39:ASN:ND2	2.65	0.50
7:K:310:GLN:O	7:K:313:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:117:GLU:HB2	13:V:114:TRP:HE1	1.77	0.50
13:V:98:MET:HE1	13:V:120:GLU:HB2	1.94	0.50
16:Y:-84:DG:OP2	16:Y:-84:DG:H8	1.94	0.50
3:C:46:VAL:HG22	3:C:49:ARG:HH21	1.77	0.50
7:K:157:ILE:CG2	7:K:298:ILE:HA	2.42	0.50
7:K:79:PHE:HB3	7:K:88:PHE:CE1	2.47	0.50
15:X:75:DG:H1	16:Y:-75:DC:N4	2.06	0.50
1:E:64:GLU:HA	2:F:46:HIS:CE1	2.46	0.50
5:I:726:LYS:HD2	15:X:56:DT:C4'	2.42	0.50
5:I:2060:HIS:CD2	5:I:2132:THR:HG21	2.39	0.50
7:K:133:HIS:HE1	7:K:137:ARG:HD2	1.76	0.50
7:K:160:TYR:CE1	7:K:165:LYS:HB2	2.47	0.50
11:U:237:GLU:OE1	11:U:237:GLU:N	2.44	0.50
13:V:169:LEU:HD21	13:V:195:TYR:CE2	2.47	0.50
3:C:73:GLU:O	3:C:76:GLN:HB2	2.11	0.49
1:E:70:ALA:O	1:E:75:LYS:HB2	2.12	0.49
5:I:1914:LEU:CD2	9:M:285:LYS:HD2	2.42	0.49
5:I:2072:LEU:HD13	5:I:2088:ARG:HH11	1.77	0.49
7:K:233:MET:HG2	7:K:252:ARG:CG	2.42	0.49
13:V:91:LYS:O	13:V:91:LYS:NZ	2.29	0.49
13:V:249:GLN:HG2	13:V:250:GLU:N	2.24	0.49
15:X:128:DC:H2"	15:X:129:DG:H5"	1.92	0.49
16:Y:-125:DG:C2'	16:Y:-124:DC:H5"	2.36	0.49
16:Y:-103:DG:OP1	16:Y:-103:DG:H4'	2.12	0.49
1:A:33:ARG:HD2	1:A:37:LYS:HE2	1.94	0.49
2:B:119:THR:HB	13:V:54:HIS:CD2	2.47	0.49
7:K:175:VAL:HG21	7:K:289:ILE:HG21	1.94	0.49
7:K:378:THR:HB	7:K:380:GLU:HG3	1.93	0.49
9:M:113:MET:CG	9:M:276:ARG:NH1	2.56	0.49
12:T:408:GLN:HA	13:V:105:ARG:HH11	1.76	0.49
13:V:104:ALA:HB1	13:V:130:ASN:HD22	1.77	0.49
15:X:11:DA:H2'	15:X:12:DT:H71	1.94	0.49
16:Y:-133:DG:C2'	16:Y:-132:DT:H72	2.42	0.49
16:Y:-75:DC:H1'	16:Y:-74:DG:H5'	1.94	0.49
1:A:66:LEU:HD13	1:A:91:ASP:HB2	1.94	0.49
5:I:112:GLU:OE1	13:V:247:LEU:CD2	2.60	0.49
5:I:622:GLN:NE2	17:I:3301:ADP:HN61	2.11	0.49
5:I:913:THR:HG23	5:I:2031:GLN:HB2	1.93	0.49
5:I:2167:ILE:HD11	5:I:2177:LEU:HD22	1.93	0.49
7:K:64:TYR:O	7:K:66:VAL:HG22	2.13	0.49
7:K:121:ALA:CA	7:K:378:THR:OG1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:78:DT:H2”	15:X:79:DA:C8	2.46	0.49
16:Y:-83:DC:H1’	16:Y:-82:DA:H5’	1.93	0.49
2:B:38:VAL:HG11	2:B:59:MET:HG2	1.95	0.49
3:C:127:ALA:O	3:G:130:ILE:HG21	2.13	0.49
3:G:124:ILE:O	3:G:128:ARG:HG3	2.12	0.49
5:I:888:MET:CE	15:X:51:DG:N1	2.76	0.49
7:K:119:PHE:O	7:K:119:PHE:CD1	2.65	0.49
7:K:156:HIS:NE2	7:K:172:ARG:HB2	2.28	0.49
7:K:234:ILE:HG13	7:K:271:ALA:HB2	1.94	0.49
13:V:265:SER:HG	14:W:195:ALA:HA	1.76	0.49
16:Y:-12:DA:H1’	16:Y:-11:DT:C5’	2.42	0.49
3:C:76:GLN:OE1	3:C:76:GLN:HA	2.13	0.49
3:C:127:ALA:HA	3:G:130:ILE:HG21	1.95	0.49
5:I:2014:LEU:CD1	9:Q:256:ILE:HG13	2.33	0.49
7:K:87:ASP:HB2	7:K:91:THR:HG21	1.93	0.49
7:K:187:ILE:O	7:K:191:ARG:HG3	2.12	0.49
8:L:27:ARG:HE	8:L:153:THR:HG21	1.65	0.49
10:N:38:GLU:OE2	10:N:54:ARG:NH1	2.45	0.49
13:V:119:GLU:OE1	13:V:119:GLU:CA	2.59	0.49
13:V:152:TRP:CZ3	13:V:194:ARG:HG2	2.47	0.49
13:V:256:ALA:HB1	13:V:260:GLU:OE2	2.12	0.49
16:Y:-119:DC:H1’	16:Y:-118:DA:O4’	2.13	0.49
16:Y:-61:DT:H2”	16:Y:-60:DT:C5	2.48	0.49
16:Y:-7:DC:H1’	16:Y:-6:DA:H5”	1.94	0.49
16:Y:-1:DG:H2”	16:Y:0:DT:H5”	1.94	0.49
1:A:63:ILE:HG23	2:B:59:MET:HE1	1.93	0.49
3:C:128:ARG:HD2	3:C:133:GLU:OE1	2.12	0.49
5:I:2014:LEU:HG	5:I:2017:ARG:CD	2.37	0.49
7:K:64:TYR:HH	8:L:101:TYR:HE2	1.51	0.49
7:K:120:GLN:C	7:K:378:THR:CG2	2.81	0.49
7:K:239:PRO:HG3	7:K:247:GLY:N	2.28	0.49
10:N:38:GLU:OE1	10:N:54:ARG:CZ	2.57	0.49
2:F:99:LEU:HB2	2:F:104:ALA:CA	2.42	0.49
3:G:94:GLU:HG3	4:H:100:PHE:HZ	1.78	0.49
5:I:811:LEU:HA	5:I:814:MET:HG2	1.95	0.49
10:N:52:ALA:CB	10:N:359:THR:HG22	2.41	0.49
10:P:272:VAL:O	10:P:276:ILE:HG12	2.12	0.49
13:V:261:ARG:HB3	14:W:198:LYS:HG2	1.94	0.49
16:Y:-146:DC:H2”	16:Y:-145:DT:H6	1.76	0.49
2:B:77:LEU:HD13	4:H:72:TYR:CE1	2.47	0.49
1:E:42:ARG:HB3	2:F:85:THR:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:118:THR:HG23	4:H:45:ARG:CB	2.42	0.49
7:K:99:TYR:CZ	7:K:158:VAL:HG21	2.47	0.49
15:X:39:DA:H2"	15:X:40:DG:C8	2.48	0.49
16:Y:-142:DA:C1'	16:Y:-141:DG:H5'	2.42	0.49
16:Y:-27:DA:H2"	16:Y:-26:DG:C8	2.47	0.49
3:C:82:LEU:HD13	4:D:81:VAL:CG2	2.43	0.49
2:F:110:GLU:HA	2:F:110:GLU:OE1	2.11	0.49
3:G:61:LEU:HD22	4:H:36:ARG:HD2	1.95	0.49
3:G:94:GLU:HG3	4:H:100:PHE:CZ	2.47	0.49
7:K:112:ILE:HG23	7:K:116:GLU:CD	2.33	0.49
7:K:165:LYS:HZ3	7:K:167:LYS:HE2	1.78	0.49
7:K:237:VAL:HG22	7:K:250:LYS:HG3	1.95	0.49
15:X:145:DA:H2"	15:X:146:DG:H5"	1.95	0.49
16:Y:-101:DT:C2'	16:Y:-100:DC:H5'	2.42	0.49
16:Y:-49:DA:H2"	16:Y:-48:DG:C8	2.48	0.49
16:Y:-22:DC:C2'	16:Y:-21:DG:C8	2.96	0.49
1:A:48:ALA:HA	2:B:91:ILE:HG13	1.95	0.49
3:G:107:THR:HG21	3:G:124:ILE:CG1	2.43	0.49
5:I:163:ARG:HA	5:I:166:VAL:HG22	1.95	0.49
7:K:173:ILE:HG22	7:K:174:ASN:H	1.77	0.49
7:K:179:LEU:H	7:K:179:LEU:HD12	1.77	0.49
15:X:40:DG:H2'	15:X:41:DT:H71	1.94	0.49
1:A:35:LEU:HD22	1:A:40:TYR:HD2	1.78	0.48
2:B:75:SER:HA	2:B:86:ILE:CD1	2.43	0.48
5:I:2014:LEU:HG	5:I:2017:ARG:HB2	1.94	0.48
7:K:62:LYS:O	7:K:62:LYS:HD3	2.12	0.48
7:K:78:LEU:HD23	7:K:83:MET:CE	2.43	0.48
7:K:306:PRO:O	7:K:309:MET:N	2.43	0.48
7:K:314:PHE:CZ	7:K:345:TYR:HB3	2.47	0.48
11:U:118:LYS:HZ2	13:V:97:TRP:HB2	1.77	0.48
15:X:2:DA:H2"	15:X:3:DG:C8	2.46	0.48
16:Y:-19:DG:H2"	16:Y:-18:DT:H5"	1.95	0.48
1:A:101:VAL:HG22	4:D:96:THR:HB	1.94	0.48
2:B:89:ARG:NH2	4:H:75:HIS:HA	2.29	0.48
3:C:128:ARG:HA	3:C:131:ARG:HD2	1.94	0.48
5:I:102:HIS:CE1	13:V:253:LYS:HE2	2.48	0.48
15:X:23:DT:H2"	15:X:24:DG:C8	2.48	0.48
16:Y:-98:DA:C2'	16:Y:-97:DG:C8	2.95	0.48
3:C:119:ILE:O	3:C:119:ILE:HG13	2.13	0.48
7:K:51:PRO:O	7:K:54:LEU:HG	2.14	0.48
7:K:145:CYS:O	7:K:160:TYR:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:152:TYR:CE2	7:K:178:LYS:HG2	2.48	0.48
12:T:338:ILE:CD1	13:V:234:TYR:HB2	2.44	0.48
13:V:184:LYS:HE2	13:V:186:ARG:NH2	2.28	0.48
1:A:31:VAL:HG12	1:A:32:HIS:N	2.29	0.48
2:B:99:LEU:HD23	2:B:99:LEU:N	2.28	0.48
3:G:73:GLU:N	4:H:23:ARG:HH12	2.12	0.48
5:I:106:ILE:CD1	13:V:254:ILE:HG22	2.43	0.48
7:K:196:MET:HG3	8:L:41:GLN:HE22	1.79	0.48
13:V:91:LYS:NZ	13:V:91:LYS:HB3	2.22	0.48
13:V:245:GLU:O	13:V:248:LEU:HB2	2.14	0.48
13:V:264:ARG:HH12	14:W:194:ILE:CD1	2.12	0.48
7:K:146:ILE:HG13	7:K:317:ILE:HA	1.94	0.48
7:K:183:HIS:CD2	7:K:277:VAL:HG13	2.48	0.48
7:K:294:ILE:O	7:K:298:ILE:HG13	2.13	0.48
7:K:330:ARG:CG	7:K:351:LEU:HB2	2.43	0.48
8:L:15:GLN:O	8:L:15:GLN:HG2	2.13	0.48
13:V:196:TYR:HB3	13:V:217:VAL:HG13	1.95	0.48
13:V:238:PRO:O	13:V:240:GLN:N	2.47	0.48
13:V:245:GLU:OE2	13:V:246:TYR:HB2	2.13	0.48
16:Y:-20:DT:H2"	16:Y:-19:DG:H8	1.79	0.48
2:F:86:ILE:O	2:F:86:ILE:HG22	2.13	0.48
3:G:82:LEU:CD1	4:H:70:VAL:HG13	2.42	0.48
17:I:3301:ADP:O2B	19:I:3303:BEF:F3	2.22	0.48
7:K:15:ILE:CD1	7:K:78:LEU:HB3	2.44	0.48
7:K:134:ARG:HD2	7:K:361:GLU:HB2	1.94	0.48
8:L:27:ARG:HH21	8:L:153:THR:HG23	1.78	0.48
11:U:117:GLU:HB2	13:V:114:TRP:NE1	2.28	0.48
11:U:117:GLU:CB	13:V:114:TRP:HE1	2.27	0.48
13:V:261:ARG:CA	14:W:198:LYS:HG2	2.43	0.48
15:X:116:DA:H2'	15:X:117:DT:C6	2.48	0.48
2:B:90:GLU:HG3	4:H:75:HIS:NE2	2.29	0.48
2:B:112:THR:O	2:B:116:THR:HG23	2.14	0.48
1:E:64:GLU:CB	2:F:45:VAL:HG11	2.37	0.48
7:K:81:LYS:HB2	7:K:85:GLN:HE22	1.78	0.48
7:K:314:PHE:HA	7:K:317:ILE:HG13	1.95	0.48
10:N:324:LEU:CD1	10:N:326:MET:CE	2.92	0.48
15:X:128:DC:H6	15:X:128:DC:H5"	1.78	0.48
5:I:1972:ILE:CG2	5:I:1976:PHE:CD2	2.74	0.48
7:K:316:ASN:O	7:K:318:VAL:HG23	2.14	0.48
16:Y:-130:DC:OP2	16:Y:-130:DC:H6	1.97	0.48
16:Y:-42:DT:H2"	16:Y:-41:DA:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:TYR:HB2	15:X:83:DG:P	2.54	0.48
1:E:47:ALA:HB3	1:E:48:PRO:HD3	1.96	0.48
5:I:125:PRO:HD2	13:V:222:HIS:NE2	2.29	0.48
7:K:16:GLY:HA3	7:K:360:TRP:HE1	1.79	0.48
7:K:88:PHE:O	7:K:119:PHE:CB	2.61	0.48
7:K:89:LEU:HD23	7:K:90:ASP:H	1.79	0.48
7:K:97:GLU:HG3	7:K:126:ASN:HD22	1.77	0.48
7:K:167:LYS:HZ2	7:K:170:ILE:HG21	1.78	0.48
13:V:206:ARG:O	13:V:208:VAL:HG13	2.14	0.48
16:Y:-54:DC:C2'	16:Y:-53:DG:C8	2.95	0.48
5:I:2000:ALA:HB3	5:I:2001:PRO:HD3	1.95	0.48
7:K:56:TYR:CA	8:L:39:ASN:ND2	2.77	0.48
7:K:229:GLU:HG2	7:K:230:ASN:N	2.29	0.48
7:K:277:VAL:HB	7:K:278:PRO:CD	2.41	0.48
7:K:292:MET:HB2	7:K:296:GLU:HB2	1.96	0.48
7:K:379:ARG:O	7:K:383:GLU:N	2.41	0.48
15:X:7:DG:C2'	15:X:8:DT:H5"	2.44	0.48
15:X:48:DC:H2"	15:X:49:DT:C5	2.48	0.48
1:A:32:HIS:HB2	1:A:49:PRO:CG	2.43	0.47
5:I:754:PHE:CE1	5:I:755:LYS:HG3	2.48	0.47
7:K:89:LEU:CD2	7:K:90:ASP:H	2.25	0.47
7:K:131:SER:OG	7:K:147:ILE:HG23	2.14	0.47
11:U:363:ASP:O	13:V:95:TRP:CH2	2.66	0.47
13:V:264:ARG:HH11	13:V:264:ARG:CG	2.17	0.47
4:D:38:ALA:HB3	4:D:46:ILE:HD11	1.96	0.47
3:G:73:GLU:HB2	4:H:25:ASN:OD1	2.14	0.47
5:I:814:MET:SD	5:I:819:GLN:HA	2.54	0.47
7:K:94:ILE:HA	7:K:122:VAL:O	2.13	0.47
7:K:98:PRO:HD2	7:K:106:GLN:OE1	2.14	0.47
7:K:235:ASP:CG	7:K:255:MET:HG2	2.34	0.47
9:M:196:ASN:OD1	9:M:197:SER:N	2.47	0.47
9:M:425:ILE:CG2	9:M:430:VAL:HG23	2.43	0.47
9:O:135:VAL:HG12	9:O:189:ASP:O	2.14	0.47
12:T:340:ILE:HD13	13:V:172:VAL:CG1	2.44	0.47
11:U:367:PRO:HD3	13:V:95:TRP:CG	2.49	0.47
13:V:265:SER:OG	14:W:198:LYS:HB2	2.14	0.47
1:A:52:LEU:O	1:A:56:LEU:HG	2.14	0.47
1:E:49:VAL:HG21	2:F:118:TYR:CE2	2.49	0.47
5:I:129:GLU:CG	13:V:196:TYR:CE2	2.98	0.47
5:I:2088:ARG:HG3	5:I:2115:ILE:HG22	1.97	0.47
7:K:220:MET:CE	8:L:122:PHE:CD2	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:323:ILE:O	9:Q:323:ILE:HG22	2.14	0.47
10:R:412:VAL:HG11	10:R:428:ARG:HG2	1.96	0.47
15:X:125:DC:H2"	15:X:126:DC:C6	2.49	0.47
1:A:63:ILE:HG23	1:A:64:LEU:N	2.29	0.47
5:I:2055:LEU:HD22	5:I:2060:HIS:CE1	2.49	0.47
7:K:381:ASP:HA	7:K:384:GLU:OE1	2.14	0.47
8:L:6:THR:O	8:L:9:ARG:NH1	2.47	0.47
9:M:91:VAL:CG1	9:M:297:GLY:HA2	2.44	0.47
13:V:265:SER:HB2	14:W:198:LYS:HD3	1.95	0.47
15:X:28:DG:C2'	15:X:29:DG:H8	2.28	0.47
15:X:141:DC:C2'	15:X:142:DT:H5'	2.41	0.47
2:F:75:SER:N	2:F:86:ILE:HD11	2.29	0.47
3:G:68:GLN:O	3:G:72:ARG:HG3	2.15	0.47
7:K:221:ASP:HA	7:K:224:LYS:NZ	2.24	0.47
9:M:313:THR:CB	9:M:316:HIS:HE1	2.25	0.47
15:X:6:DT:H2"	15:X:7:DG:OP2	2.13	0.47
1:A:66:LEU:N	1:A:66:LEU:HD23	2.30	0.47
7:K:334:TYR:HB2	7:K:349:VAL:HB	1.96	0.47
7:K:375:MET:O	7:K:376:VAL:CB	2.62	0.47
10:R:389:VAL:HG21	10:R:423:VAL:HG23	1.97	0.47
13:V:261:ARG:HD3	14:W:198:LYS:HZ2	1.78	0.47
16:Y:-112:DT:H1'	16:Y:-111:DC:C5'	2.44	0.47
16:Y:-102:DC:H2"	16:Y:-101:DT:C7	2.36	0.47
1:A:32:HIS:O	1:A:32:HIS:HD2	1.97	0.47
1:A:72:ARG:CZ	8:L:154:VAL:HG11	2.43	0.47
3:C:42:ARG:NE	16:Y:-78:DA:OP1	2.37	0.47
1:E:100:VAL:HG11	4:H:98:TYR:CD2	2.49	0.47
3:G:107:THR:HG23	3:G:124:ILE:N	2.30	0.47
5:I:921:ILE:HD12	5:I:1986:PRO:HB2	1.96	0.47
5:I:1886:LEU:HD21	7:K:315:LYS:CE	2.41	0.47
7:K:66:VAL:C	7:K:68:TRP:H	2.18	0.47
7:K:172:ARG:NH1	8:L:101:TYR:CE2	2.83	0.47
7:K:189:SER:OG	7:K:195:VAL:N	2.47	0.47
8:L:38:ASP:OD1	8:L:39:ASN:N	2.44	0.47
10:P:348:ILE:H	10:P:348:ILE:HD13	1.78	0.47
10:R:408:ALA:HB3	10:R:429:VAL:HG11	1.96	0.47
12:T:186:TYR:HB2	13:V:173:VAL:HG21	1.97	0.47
13:V:244:GLU:HG2	13:V:248:LEU:HG	1.96	0.47
13:V:254:ILE:HG13	13:V:255:GLU:OE1	2.15	0.47
13:V:261:ARG:CD	14:W:198:LYS:HZ2	2.28	0.47
15:X:8:DT:C2'	15:X:9:DA:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:11:DA:C2'	15:X:12:DT:H71	2.45	0.47
16:Y:-8:DA:H2"	16:Y:-7:DC:C6	2.49	0.47
3:C:121:PRO:HA	4:D:50:ILE:HD11	1.96	0.47
1:E:64:GLU:O	2:F:46:HIS:HE1	1.98	0.47
5:I:116:GLU:OE2	13:V:240:GLN:HG3	2.15	0.47
5:I:163:ARG:CA	5:I:166:VAL:HG22	2.44	0.47
5:I:694:LYS:CB	5:I:719:HIS:CD2	2.92	0.47
7:K:11:TYR:HB2	7:K:152:TYR:CZ	2.49	0.47
7:K:79:PHE:HB3	7:K:88:PHE:HE1	1.79	0.47
7:K:200:HIS:O	7:K:204:GLN:HG3	2.14	0.47
7:K:224:LYS:CB	8:L:122:PHE:CE2	2.94	0.47
9:Q:395:GLY:O	9:Q:399:THR:HG23	2.14	0.47
12:T:184:ASP:HB3	13:V:170:ARG:HH11	1.80	0.47
15:X:87:DT:H2"	15:X:88:DT:H72	1.96	0.47
1:A:63:ILE:HG12	1:A:88:ILE:HD11	1.97	0.47
3:C:128:ARG:HD2	3:C:133:GLU:CD	2.35	0.47
3:G:106:ASP:O	3:G:127:ALA:HB2	2.15	0.47
5:I:742:TYR:CD1	5:I:769:ARG:HB2	2.50	0.47
5:I:895:MET:HE2	15:X:52:DG:H4'	1.97	0.47
5:I:975:LEU:HD23	5:I:1901:LEU:HD13	1.96	0.47
9:M:394:LEU:HD13	9:M:430:VAL:HG11	1.97	0.47
10:N:110:SER:OG	10:N:113:MET:O	2.32	0.47
9:O:401:THR:O	9:O:402:THR:CG2	2.63	0.47
13:V:179:ASP:HB3	13:V:183:PHE:CD2	2.50	0.47
15:X:141:DC:C6	15:X:141:DC:H5"	2.50	0.47
3:G:90:MET:CE	3:G:90:MET:HA	2.45	0.47
5:I:2030:THR:HG21	9:O:199:ALA:CB	2.45	0.47
13:V:270:LYS:HD3	13:V:270:LYS:HA	1.59	0.47
1:A:66:LEU:CD1	1:A:91:ASP:HB2	2.45	0.46
7:K:371:ASP:O	7:K:375:MET:HG2	2.15	0.46
7:K:377:VAL:CG2	7:K:389:VAL:HG22	2.44	0.46
9:M:135:VAL:HG22	9:M:161:LEU:HD21	1.96	0.46
11:U:262:PHE:HA	11:U:273:GLY:HA3	1.96	0.46
13:V:264:ARG:HH12	14:W:194:ILE:HG21	1.80	0.46
15:X:68:DG:H1'	15:X:69:DG:N7	2.30	0.46
1:A:95:ASN:O	1:A:99:GLY:N	2.49	0.46
1:E:80:PRO:HA	1:E:83:LEU:HB2	1.96	0.46
7:K:160:TYR:OH	7:K:165:LYS:HD3	2.15	0.46
7:K:228:GLU:O	7:K:229:GLU:CG	2.63	0.46
7:K:299:VAL:HG11	7:K:340:LEU:HB3	1.96	0.46
7:K:311:PRO:O	7:K:315:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:112:DA:H2"	15:X:113:DC:H6	1.81	0.46
1:A:80:ILE:HG13	1:A:82:ARG:H	1.81	0.46
1:E:42:ARG:HA	15:X:112:DA:OP1	2.15	0.46
3:G:95:ALA:CB	4:H:90:LEU:HD11	2.45	0.46
5:I:167:ARG:HD2	15:X:31:DG:O3'	2.14	0.46
5:I:843:VAL:HG13	5:I:844:ASP:N	2.31	0.46
7:K:198:GLU:HB2	7:K:201:VAL:CG2	2.46	0.46
7:K:332:ARG:O	7:K:336:GLU:CG	2.61	0.46
13:V:268:LEU:HD12	14:W:194:ILE:HG21	1.97	0.46
15:X:38:DG:H2"	15:X:39:DA:C8	2.51	0.46
15:X:54:DG:H2'	15:X:54:DG:P	2.55	0.46
16:Y:-79:DT:H2"	16:Y:-78:DA:OP2	2.15	0.46
1:A:32:HIS:HB2	1:A:49:PRO:HB3	1.94	0.46
3:C:49:ARG:HD3	15:X:6:DT:O3'	2.15	0.46
5:I:654:ILE:HA	5:I:657:LEU:HD12	1.97	0.46
5:I:1904:ILE:HD13	10:R:211:ARG:HG2	1.98	0.46
10:N:324:LEU:HD11	10:N:326:MET:HE3	1.97	0.46
10:P:394:GLY:HA3	10:P:402:ALA:HB2	1.96	0.46
10:R:205:LEU:CG	10:R:225:VAL:HG22	2.43	0.46
13:V:237:THR:OG1	13:V:238:PRO:HD3	2.15	0.46
13:V:245:GLU:HA	13:V:248:LEU:HD12	1.97	0.46
15:X:6:DT:H1'	15:X:7:DG:H5'	1.97	0.46
16:Y:-81:DC:H2"	16:Y:-80:DG:O5'	2.15	0.46
2:B:73:GLU:HB3	2:B:94:ALA:HB1	1.96	0.46
3:G:107:THR:CB	3:G:124:ILE:HG12	2.46	0.46
5:I:201:ASP:OD1	5:I:202:VAL:N	2.47	0.46
5:I:918:THR:O	5:I:918:THR:HG23	2.16	0.46
5:I:1930:GLN:HB3	5:I:1931:PRO:HD3	1.98	0.46
7:K:78:LEU:O	7:K:83:MET:HB2	2.16	0.46
7:K:128:GLY:CA	7:K:147:ILE:HG13	2.45	0.46
7:K:164:LYS:NZ	7:K:166:LYS:HD3	2.31	0.46
15:X:41:DT:H2"	15:X:42:DA:H5'	1.97	0.46
15:X:120:DA:H8	15:X:120:DA:H5"	1.80	0.46
3:C:110:CYS:O	3:C:113:HIS:HB3	2.16	0.46
3:C:120:MET:C	4:D:50:ILE:HD11	2.35	0.46
5:I:916:PHE:O	5:I:1983:VAL:HG13	2.16	0.46
7:K:286:ASP:OD1	7:K:286:ASP:N	2.48	0.46
7:K:319:LEU:CD1	7:K:330:ARG:HA	2.46	0.46
10:P:349:ASP:OD1	10:P:353:ARG:NH1	2.49	0.46
13:V:145:LEU:HB3	13:V:146:TYR:CE1	2.51	0.46
13:V:224:ARG:O	13:V:228:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HG3	1:A:30:ARG:HE	1.80	0.46
4:D:23:ARG:NH2	14:W:81:VAL:HG13	2.31	0.46
4:D:79:LYS:N	15:X:101:DA:OP2	2.36	0.46
7:K:36:ARG:NE	7:K:36:ARG:CA	2.78	0.46
7:K:51:PRO:HG2	7:K:241:PHE:CE1	2.51	0.46
9:M:333:ARG:O	9:M:348:HIS:HA	2.15	0.46
11:U:162:THR:HG21	11:U:277:THR:HG22	1.96	0.46
13:V:222:HIS:CE1	13:V:226:ARG:HB2	2.49	0.46
13:V:239:GLU:HB2	13:V:240:GLN:NE2	2.29	0.46
15:X:45:DC:H2"	15:X:46:DC:C5'	2.39	0.46
2:B:96:ARG:HE	13:V:64:ASP:HB3	1.81	0.46
5:I:705:ARG:HH22	15:X:58:DA:P	2.38	0.46
7:K:62:LYS:CD	7:K:172:ARG:HH12	2.28	0.46
9:M:317:ARG:HD2	10:R:104:ALA:HB2	1.98	0.46
11:S:103:VAL:O	11:S:132:MET:HA	2.16	0.46
13:V:134:GLN:OE1	13:V:134:GLN:HA	2.14	0.46
13:V:212:ASP:C	13:V:214:LYS:H	2.19	0.46
13:V:261:ARG:HD3	14:W:198:LYS:NZ	2.31	0.46
13:V:272:ILE:HD13	14:W:191:SER:CB	2.46	0.46
1:E:20:ARG:HD2	2:F:118:TYR:CD1	2.50	0.46
5:I:977:VAL:O	5:I:977:VAL:HG12	2.16	0.46
7:K:114:PHE:O	7:K:118:GLN:N	2.49	0.46
7:K:135:TYR:CE2	7:K:145:CYS:HB3	2.50	0.46
12:T:338:ILE:HD13	13:V:230:LEU:HD22	1.96	0.46
13:V:247:LEU:HA	13:V:250:GLU:HB2	1.98	0.46
13:V:261:ARG:HA	14:W:198:LYS:HE3	1.97	0.46
16:Y:-139:DA:H2'	16:Y:-138:DT:H72	1.97	0.46
10:R:211:ARG:HG2	10:R:212:ALA:H	1.81	0.46
11:U:165:ILE:HG22	11:U:170:ALA:HA	1.97	0.46
11:U:188:TYR:CZ	11:U:192:ILE:HD11	2.51	0.46
16:Y:-111:DC:H2'	16:Y:-111:DC:O5'	2.16	0.46
1:A:114:ALA:HA	1:A:117:LEU:HD12	1.97	0.45
7:K:160:TYR:CZ	7:K:165:LYS:HB2	2.51	0.45
7:K:200:HIS:CE1	7:K:201:VAL:HG22	2.51	0.45
7:K:310:GLN:HA	7:K:313:PHE:HB2	1.98	0.45
13:V:59:ALA:O	13:V:63:SER:HB2	2.15	0.45
13:V:259:LYS:H	13:V:259:LYS:NZ	2.14	0.45
1:A:32:HIS:HB2	1:A:49:PRO:HG3	1.98	0.45
7:K:6:LEU:HB2	7:K:94:ILE:O	2.16	0.45
7:K:93:ILE:HG23	7:K:122:VAL:HG23	1.98	0.45
7:K:315:LYS:HE3	7:K:315:LYS:HB2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:117:GLU:HA	10:N:120:THR:HG22	1.98	0.45
13:V:261:ARG:HA	14:W:198:LYS:NZ	2.31	0.45
15:X:109:DA:H2"	15:X:110:DC:OP2	2.17	0.45
3:C:103:LEU:HD22	4:D:57:VAL:HG11	1.97	0.45
2:F:75:SER:CA	2:F:86:ILE:HD11	2.46	0.45
3:G:61:LEU:H	3:G:97:GLU:CD	2.20	0.45
7:K:181:THR:OG1	7:K:206:LYS:NZ	2.48	0.45
9:M:40:VAL:CG2	9:M:377:ILE:CD1	2.94	0.45
10:P:180:GLU:O	10:P:184:LYS:HG2	2.17	0.45
13:V:257:ARG:H	13:V:257:ARG:HG2	1.47	0.45
2:B:100:PRO:HG2	2:B:103:LEU:HB2	1.98	0.45
1:E:66:ALA:CB	1:E:83:LEU:HD23	2.47	0.45
2:F:65:ASP:OD2	4:H:98:TYR:OH	2.31	0.45
7:K:11:TYR:HB2	7:K:152:TYR:CG	2.51	0.45
7:K:156:HIS:HB3	7:K:170:ILE:HD11	1.99	0.45
10:N:324:LEU:CD1	10:N:326:MET:HE3	2.46	0.45
13:V:98:MET:HB3	13:V:120:GLU:OE1	2.16	0.45
13:V:98:MET:HE1	13:V:116:ARG:O	2.17	0.45
15:X:5:DA:H2'	15:X:6:DT:C7	2.47	0.45
15:X:23:DT:C2'	15:X:24:DG:C8	3.00	0.45
1:A:48:ALA:N	1:A:49:PRO:HD2	2.32	0.45
1:A:81:PRO:HB2	1:A:105:GLN:C	2.37	0.45
2:B:28:ARG:HA	2:B:28:ARG:HE	1.79	0.45
1:E:28:GLY:HA3	16:Y:-117:DA:H3'	1.96	0.45
1:E:51:LEU:O	1:E:55:LEU:HG	2.16	0.45
3:G:59:GLU:H	4:H:40:ARG:HH22	1.65	0.45
3:G:116:ARG:HH22	3:G:123:ASP:CG	2.19	0.45
7:K:171:ILE:HG21	7:K:292:MET:HE1	1.99	0.45
7:K:230:ASN:O	7:K:232:VAL:N	2.50	0.45
9:O:366:TYR:OH	17:O:501:ADP:N7	2.41	0.45
13:V:258:LYS:C	13:V:261:ARG:H	2.20	0.45
7:K:75:TRP:CZ3	7:K:113:LEU:HD23	2.52	0.45
13:V:183:PHE:CD1	13:V:183:PHE:N	2.83	0.45
15:X:59:DA:H1'	15:X:60:DA:H5"	1.97	0.45
16:Y:-13:DT:C4	16:Y:-12:DA:N6	2.85	0.45
1:E:62:ILE:HG12	1:E:93:LEU:HD13	1.97	0.45
1:E:111:ILE:CG2	1:E:116:LEU:HG	2.47	0.45
3:G:129:ARG:HA	3:G:134:ARG:HB2	1.98	0.45
5:I:733:GLN:OE1	5:I:736:ARG:NH2	2.50	0.45
5:I:2072:LEU:HD22	5:I:2115:ILE:HG22	1.99	0.45
9:Q:268:LYS:O	9:Q:268:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:220:ALA:CB	13:V:224:ARG:NH2	2.79	0.45
15:X:99:DA:C1'	15:X:100:DG:H5'	2.41	0.45
16:Y:-1:DG:C2'	16:Y:0:DT:H5"	2.47	0.45
1:A:18:ARG:HH22	1:A:36:ARG:NH1	2.15	0.45
1:E:18:SER:HB3	1:E:27:VAL:H	1.82	0.45
1:E:84:GLN:O	1:E:88:ARG:HG2	2.17	0.45
1:E:88:ARG:NH2	1:E:100:VAL:O	2.49	0.45
5:I:2087:LEU:HD11	5:I:2104:ARG:HH11	1.71	0.45
7:K:7:ASP:O	7:K:9:GLY:N	2.47	0.45
7:K:379:ARG:CZ	7:K:379:ARG:HB3	2.47	0.45
9:O:276:ARG:HH11	9:O:276:ARG:CG	2.30	0.45
9:Q:233:GLU:HG3	9:Q:233:GLU:O	2.17	0.45
15:X:49:DT:C6	15:X:50:DT:H71	2.52	0.45
16:Y:-10:DA:H2"	16:Y:-9:DT:H5'	1.99	0.45
1:A:82:ARG:HA	1:A:106:GLY:O	2.16	0.45
1:A:94:LEU:HD23	2:B:103:LEU:HD21	1.99	0.45
2:B:88:SER:HA	2:B:91:ILE:HB	1.98	0.45
3:C:82:LEU:HD23	3:C:82:LEU:HA	1.80	0.45
3:G:103:LEU:CD1	3:G:128:ARG:HG2	2.47	0.45
5:I:754:PHE:CZ	5:I:801:ARG:HD3	2.52	0.45
7:K:214:GLN:NE2	7:K:332:ARG:HG2	2.32	0.45
7:K:344:ASP:OD1	7:K:344:ASP:N	2.50	0.45
9:M:192:TYR:O	9:M:192:TYR:CG	2.70	0.45
9:O:308:ASP:OD1	9:O:309:ILE:N	2.50	0.45
10:R:416:ARG:O	10:R:416:ARG:HG2	2.17	0.45
13:V:147:LEU:CD2	13:V:201:LYS:HB3	2.47	0.45
1:A:32:HIS:HB3	1:A:36:ARG:HH12	1.82	0.45
1:A:117:LEU:HB3	1:A:118:PRO:CD	2.47	0.45
2:F:34:TYR:CE2	2:F:63:VAL:HB	2.52	0.45
7:K:82:GLU:N	7:K:82:GLU:OE1	2.49	0.45
7:K:308:GLU:O	7:K:311:PRO:HD2	2.17	0.45
9:O:428:GLU:OE1	9:O:429:HIS:ND1	2.50	0.45
13:V:94:PRO:HD2	13:V:117:ALA:CB	2.47	0.45
13:V:255:GLU:CA	13:V:259:LYS:HE2	2.47	0.45
16:Y:-53:DG:C5	16:Y:-52:DC:C4	3.05	0.45
2:B:102:GLU:OE1	2:B:102:GLU:HA	2.18	0.44
9:M:40:VAL:HG21	9:M:377:ILE:CD1	2.46	0.44
13:V:161:PHE:CE1	13:V:198:ILE:HG21	2.52	0.44
15:X:44:DT:H2"	15:X:45:DC:C6	2.51	0.44
1:A:26:PHE:HE2	2:B:63:VAL:CG2	2.30	0.44
1:A:81:PRO:HB3	1:A:104:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:112:ILE:HG23	7:K:116:GLU:OE1	2.16	0.44
7:K:307:GLU:O	7:K:310:GLN:HG3	2.17	0.44
9:M:135:VAL:HG22	9:M:161:LEU:HD23	1.97	0.44
9:M:357:ARG:HB3	10:R:400:ARG:HD2	1.99	0.44
10:P:33:LEU:HD23	10:P:39:PRO:HA	1.97	0.44
13:V:56:GLU:H	13:V:56:GLU:CD	2.19	0.44
15:X:93:DG:C4	15:X:94:DG:C8	3.06	0.44
1:A:33:ARG:NH2	2:B:32:GLU:OE1	2.41	0.44
1:A:39:ASN:HD22	1:E:40:ALA:HA	1.82	0.44
1:A:59:LEU:HG	1:A:59:LEU:H	1.54	0.44
1:A:59:LEU:HD13	2:B:66:ILE:HG13	1.99	0.44
1:E:32:ARG:O	1:E:36:LYS:HB2	2.17	0.44
3:G:129:ARG:HD3	3:G:134:ARG:HH21	1.82	0.44
7:K:295:PRO:HG2	7:K:296:GLU:OE1	2.17	0.44
7:K:334:TYR:O	7:K:337:VAL:HG22	2.17	0.44
7:K:335:SER:HA	7:K:338:ARG:NH2	2.32	0.44
9:O:50:GLY:O	9:O:53:VAL:HG22	2.17	0.44
9:Q:49:CYS:HB2	9:Q:83:ILE:HD11	1.98	0.44
11:U:124:PHE:HB3	13:V:91:LYS:HE2	1.98	0.44
13:V:98:MET:HB3	13:V:120:GLU:CD	2.38	0.44
15:X:52:DG:C4	15:X:53:DC:C5	3.04	0.44
1:A:32:HIS:CB	1:A:49:PRO:HB3	2.48	0.44
3:C:82:LEU:HD11	4:D:70:VAL:HG22	1.99	0.44
3:C:103:LEU:HA	3:C:131:ARG:NH2	2.33	0.44
1:E:29:ARG:NH1	2:F:33:SER:O	2.44	0.44
5:I:612:LEU:O	5:I:614:LEU:N	2.50	0.44
7:K:186:GLU:HA	7:K:196:MET:HE3	1.98	0.44
7:K:189:SER:CB	7:K:194:HIS:HA	2.47	0.44
7:K:213:SER:HB3	7:K:275:PHE:HB2	1.98	0.44
7:K:279:GLU:HG2	7:K:283:ASN:OD1	2.18	0.44
10:N:298:ILE:O	10:N:301:VAL:HG23	2.17	0.44
10:N:298:ILE:CG2	10:N:301:VAL:HG22	2.48	0.44
13:V:56:GLU:OE1	13:V:56:GLU:N	2.50	0.44
13:V:152:TRP:CE2	13:V:194:ARG:HD3	2.52	0.44
13:V:214:LYS:N	13:V:214:LYS:HD2	2.33	0.44
13:V:264:ARG:CB	14:W:198:LYS:HE3	2.47	0.44
1:A:59:LEU:CD1	2:B:66:ILE:HG13	2.48	0.44
1:E:106:GLY:CA	3:G:58:THR:HG22	2.38	0.44
2:F:29:SER:O	2:F:31:LYS:N	2.50	0.44
3:G:57:SER:O	4:H:40:ARG:NH2	2.51	0.44
3:G:63:ARG:HE	15:X:59:DA:H4'	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:752:LYS:HE2	16:Y:-52:DC:OP2	2.18	0.44
5:I:2067:GLN:O	5:I:2068:MET:HB2	2.18	0.44
7:K:99:TYR:HE2	7:K:158:VAL:CG2	2.31	0.44
7:K:159:PRO:HB2	7:K:166:LYS:HE3	2.00	0.44
7:K:287:ILE:HD13	7:K:287:ILE:HA	1.80	0.44
10:N:301:VAL:HG21	10:N:326:MET:HB3	1.97	0.44
13:V:264:ARG:HG2	13:V:264:ARG:NH1	2.17	0.44
15:X:127:DT:H6	15:X:127:DT:H2'	1.65	0.44
1:A:79:ILE:HA	1:A:83:HIS:ND1	2.32	0.44
3:C:130:ILE:CG2	3:G:130:ILE:HB	2.48	0.44
1:E:73:ASN:HD22	1:E:73:ASN:C	2.20	0.44
5:I:664:LYS:HA	5:I:664:LYS:HE2	1.99	0.44
5:I:888:MET:HE1	16:Y:-51:DC:N3	2.33	0.44
5:I:921:ILE:O	5:I:921:ILE:HG13	2.17	0.44
5:I:2050:VAL:O	5:I:2054:GLN:HG2	2.18	0.44
7:K:229:GLU:CG	7:K:230:ASN:H	2.30	0.44
7:K:282:PHE:HB3	7:K:332:ARG:NH2	2.32	0.44
7:K:352:PRO:O	7:K:355:PRO:HD3	2.17	0.44
12:T:374:PRO:HD2	13:V:241:VAL:HG21	1.99	0.44
13:V:262:GLU:O	13:V:266:GLN:HG2	2.17	0.44
15:X:92:DC:H2"	15:X:93:DG:C5'	2.48	0.44
2:B:41:VAL:O	2:B:45:VAL:HG13	2.18	0.44
5:I:128:PRO:HG3	13:V:218:PHE:HA	1.99	0.44
5:I:612:LEU:HD22	5:I:612:LEU:N	2.33	0.44
5:I:948:LEU:N	9:M:247:ASN:OD1	2.50	0.44
7:K:150:SER:O	7:K:323:ASN:N	2.47	0.44
7:K:302:ILE:HG23	7:K:313:PHE:CB	2.48	0.44
7:K:336:GLU:HG2	7:K:336:GLU:H	1.48	0.44
9:O:264:MET:HG2	9:O:266:PRO:HD3	2.00	0.44
9:O:276:ARG:HH11	9:O:276:ARG:HG3	1.82	0.44
10:R:49:GLN:NE2	10:R:360:THR:O	2.44	0.44
15:X:55:DG:C2'	15:X:56:DT:H5"	2.45	0.44
16:Y:-21:DG:H2'	16:Y:-20:DT:H6	1.82	0.44
5:I:206:TRP:O	5:I:210:GLU:HG2	2.18	0.44
7:K:44:GLN:HG3	7:K:77:TYR:HE2	1.81	0.44
7:K:165:LYS:HZ2	7:K:167:LYS:HD3	1.82	0.44
9:O:341:THR:O	9:O:342:GLU:CG	2.66	0.44
13:V:264:ARG:NH2	14:W:198:LYS:HZ3	2.15	0.44
16:Y:-75:DC:H2"	16:Y:-74:DG:O5'	2.18	0.44
1:A:60:THR:HG21	2:B:63:VAL:HG22	1.98	0.44
5:I:949:ILE:HD12	9:M:249:ARG:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:147:ILE:HG12	7:K:160:TYR:CE2	2.52	0.44
7:K:265:GLU:HB2	7:K:267:ILE:CG2	2.47	0.44
10:R:74:LEU:HB2	10:R:354:LEU:HD13	2.00	0.44
10:R:430:TYR:O	10:R:438:ARG:NH2	2.51	0.44
13:V:147:LEU:HD22	13:V:201:LYS:HB3	1.99	0.44
13:V:238:PRO:HG2	13:V:239:GLU:HG3	1.99	0.44
14:W:190:THR:HG22	14:W:194:ILE:CD1	2.47	0.44
15:X:70:DA:H2"	15:X:71:DC:H5"	2.00	0.44
16:Y:-21:DG:C2'	16:Y:-20:DT:C6	2.99	0.44
1:A:25:GLN:O	2:B:37:TYR:CD1	2.71	0.43
1:A:93:GLU:OE1	2:B:102:GLU:HB2	2.18	0.43
2:B:73:GLU:OE2	2:B:97:LEU:HD13	2.17	0.43
2:B:77:LEU:HD13	4:H:72:TYR:HE1	1.81	0.43
2:F:99:LEU:HD12	2:F:107:ALA:HB3	2.00	0.43
4:H:35:ARG:O	4:H:39:ARG:HG2	2.18	0.43
7:K:236:TYR:H	7:K:269:ARG:HB2	1.82	0.43
8:L:33:GLU:O	8:L:37:ASN:N	2.51	0.43
10:P:324:LEU:HD12	10:P:324:LEU:O	2.18	0.43
11:U:96:VAL:HG22	11:U:96:VAL:O	2.18	0.43
11:U:121:GLN:OE1	13:V:114:TRP:HH2	2.01	0.43
13:V:90:LYS:HB3	13:V:90:LYS:HE3	1.38	0.43
13:V:187:SER:O	13:V:191:LEU:HG	2.18	0.43
13:V:272:ILE:HD12	14:W:187:LYS:HZ2	1.83	0.43
15:X:29:DG:H2"	15:X:30:DA:H8	1.83	0.43
1:A:60:THR:HA	2:B:59:MET:CE	2.48	0.43
2:B:92:GLN:HG3	2:B:108:VAL:HG13	1.99	0.43
5:I:1886:LEU:HD11	7:K:312:HIS:CD2	2.53	0.43
7:K:43:ASN:OD1	7:K:43:ASN:N	2.51	0.43
7:K:81:LYS:HE3	7:K:81:LYS:HB3	1.58	0.43
7:K:100:PHE:HE1	7:K:167:LYS:HZ1	1.66	0.43
7:K:148:VAL:HB	7:K:319:LEU:HA	1.99	0.43
7:K:269:ARG:HA	7:K:269:ARG:HD2	1.76	0.43
9:M:275:LEU:HD13	10:R:260:LEU:HD23	1.99	0.43
3:G:111:ALA:HA	3:G:123:ASP:CG	2.37	0.43
7:K:164:LYS:HD2	7:K:164:LYS:HA	1.57	0.43
7:K:205:VAL:HG11	7:K:269:ARG:NH2	2.33	0.43
7:K:205:VAL:HA	7:K:208:ASP:HB2	2.00	0.43
7:K:216:PHE:HE2	8:L:116:PHE:CZ	2.37	0.43
7:K:375:MET:N	7:K:375:MET:SD	2.91	0.43
7:K:376:VAL:HG22	7:K:377:VAL:H	1.84	0.43
10:P:329:ASN:ND2	9:Q:353:ASP:OD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:408:GLN:HA	13:V:105:ARG:HD2	2.01	0.43
15:X:99:DA:C2'	15:X:100:DG:H5'	2.49	0.43
1:E:54:VAL:HG21	2:F:95:VAL:HG21	1.99	0.43
1:E:62:ILE:HD12	2:F:62:PHE:CE2	2.53	0.43
3:G:118:THR:HA	4:H:45:ARG:HB3	2.00	0.43
7:K:133:HIS:CE1	7:K:366:ILE:HG12	2.53	0.43
7:K:157:ILE:HG12	7:K:173:ILE:HD11	2.01	0.43
7:K:162:ARG:O	7:K:163:SER:OG	2.31	0.43
7:K:220:MET:HE3	7:K:220:MET:HB3	1.91	0.43
15:X:7:DG:C2	16:Y:-6:DA:C2	3.06	0.43
5:I:124:LEU:H	13:V:226:ARG:HH11	1.67	0.43
7:K:3:THR:HB	7:K:94:ILE:HG22	2.01	0.43
7:K:120:GLN:N	7:K:378:THR:HG21	2.34	0.43
7:K:233:MET:CG	7:K:252:ARG:HG3	2.47	0.43
9:M:384:ILE:HG22	9:M:386:ILE:HG23	2.01	0.43
9:M:394:LEU:HD13	9:M:430:VAL:CG1	2.48	0.43
13:V:203:ALA:HA	13:V:206:ARG:HD2	2.00	0.43
15:X:5:DA:H2'	15:X:6:DT:H72	2.00	0.43
15:X:126:DC:H5'	15:X:126:DC:C6	2.53	0.43
16:Y:-144:DG:H2"	16:Y:-143:DG:H5'	2.00	0.43
3:C:126:LEU:HD22	3:G:113:HIS:CD2	2.54	0.43
1:E:74:LYS:HD3	6:J:151:ARG:HD2	2.00	0.43
2:F:65:ASP:OD2	2:F:69:ARG:NH2	2.38	0.43
3:G:72:ARG:HH12	3:G:84:PHE:HB2	1.84	0.43
7:K:75:TRP:HA	7:K:78:LEU:HD12	2.00	0.43
7:K:148:VAL:HG22	7:K:157:ILE:HD12	2.00	0.43
7:K:177:GLY:O	7:K:181:THR:OG1	2.32	0.43
7:K:190:TYR:HB2	8:L:148:ARG:NH2	2.31	0.43
13:V:96:LYS:HE2	13:V:120:GLU:OE1	2.19	0.43
16:Y:-30:DT:H2'	16:Y:-29:DC:C6	2.54	0.43
1:A:85:GLN:NE2	1:A:89:ARG:HE	2.17	0.43
1:A:89:ARG:CB	1:A:109:LEU:HD11	2.46	0.43
1:E:118:LYS:HD2	1:E:118:LYS:C	2.39	0.43
3:G:63:ARG:HH21	15:X:59:DA:H5"	1.84	0.43
5:I:128:PRO:CD	13:V:218:PHE:HA	2.48	0.43
5:I:898:ARG:HA	5:I:898:ARG:NE	2.33	0.43
7:K:14:LYS:HA	7:K:23:SER:O	2.18	0.43
7:K:156:HIS:HB3	7:K:170:ILE:CD1	2.49	0.43
7:K:270:LEU:O	7:K:271:ALA:HB3	2.19	0.43
7:K:317:ILE:HD12	7:K:349:VAL:HG22	2.00	0.43
12:T:340:ILE:HG21	13:V:172:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:247:LEU:CD1	13:V:248:LEU:HD23	2.48	0.43
15:X:138:DA:H2"	15:X:139:DT:C5	2.53	0.43
1:A:26:PHE:CE2	2:B:63:VAL:HG11	2.53	0.43
1:A:78:ARG:CZ	15:X:18:DA:H4'	2.49	0.43
3:C:41:TYR:HB2	15:X:83:DG:OP1	2.18	0.43
1:E:58:LEU:HD12	2:F:66:ILE:HG21	2.00	0.43
3:G:116:ARG:NH2	3:G:122:LYS:HE3	2.34	0.43
5:I:129:GLU:CG	13:V:196:TYR:HE2	2.32	0.43
5:I:921:ILE:CG2	5:I:1986:PRO:CD	2.51	0.43
7:K:103:THR:O	7:K:107:GLU:HB3	2.18	0.43
7:K:184:LEU:HD12	7:K:184:LEU:HA	1.87	0.43
7:K:302:ILE:HG23	7:K:313:PHE:HB3	2.01	0.43
7:K:319:LEU:CD2	7:K:333:VAL:HG11	2.45	0.43
7:K:366:ILE:HD13	7:K:366:ILE:HA	1.82	0.43
9:M:40:VAL:HG21	9:M:377:ILE:HD11	2.00	0.43
11:U:151:ILE:O	11:U:152:VAL:C	2.56	0.43
13:V:65:LYS:O	13:V:65:LYS:HG2	2.17	0.43
13:V:136:PRO:HG3	13:V:199:CYS:SG	2.59	0.43
13:V:147:LEU:HD11	13:V:198:ILE:HA	2.00	0.43
13:V:262:GLU:CG	14:W:202:LYS:CE	2.96	0.43
1:A:26:PHE:CE2	2:B:63:VAL:HG21	2.54	0.43
1:A:30:ARG:NH2	2:B:34:TYR:HA	2.31	0.43
1:A:56:LEU:CD2	2:B:67:PHE:N	2.77	0.43
5:I:2034:ASP:O	5:I:2035:LEU:HB2	2.19	0.43
7:K:15:ILE:O	7:K:15:ILE:HG13	2.18	0.43
7:K:109:MET:SD	7:K:124:ARG:NH2	2.91	0.43
7:K:146:ILE:CG2	7:K:158:VAL:H	2.21	0.43
7:K:270:LEU:O	7:K:270:LEU:HD22	2.19	0.43
13:V:139:SER:HB3	13:V:142:GLU:CG	2.45	0.43
13:V:143:TYR:CE1	13:V:154:LYS:CG	3.02	0.43
15:X:28:DG:H2"	15:X:29:DG:C8	2.52	0.43
15:X:114:DC:H2'	15:X:114:DC:OP2	2.19	0.43
16:Y:-78:DA:H2"	16:Y:-77:DC:C5	2.54	0.43
1:A:33:ARG:HD3	1:A:37:LYS:HE2	1.99	0.43
1:A:65:GLU:N	1:A:65:GLU:OE1	2.52	0.43
4:H:31:LYS:N	4:H:32:PRO:HD2	2.33	0.43
5:I:1993:CYS:SG	5:I:1994:HIS:N	2.92	0.43
7:K:106:GLN:O	7:K:109:MET:HB3	2.18	0.43
7:K:220:MET:CE	8:L:123:PRO:HD3	2.43	0.43
7:K:261:TYR:CD1	7:K:267:ILE:HB	2.53	0.43
7:K:371:ASP:HA	7:K:374:ASP:CG	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:76:LYS:HZ2	17:Q:501:ADP:PB	2.41	0.43
13:V:143:TYR:CD1	13:V:143:TYR:C	2.92	0.43
16:Y:-107:DG:C1'	16:Y:-106:DA:C8	2.97	0.43
1:A:70:ALA:O	1:A:73:ASP:HB2	2.19	0.42
3:C:96:CYS:SG	4:D:62:LEU:CD2	3.07	0.42
3:C:128:ARG:NH1	3:C:133:GLU:HB3	2.34	0.42
7:K:60:PHE:HB3	7:K:63:GLY:HA2	2.00	0.42
7:K:224:LYS:CG	8:L:122:PHE:CE2	3.02	0.42
7:K:358:TYR:HA	7:K:361:GLU:OE1	2.19	0.42
12:T:338:ILE:HD11	13:V:234:TYR:HB2	2.01	0.42
12:T:376:MET:HE1	13:V:234:TYR:CE2	2.54	0.42
11:U:140:LEU:O	11:U:342:GLY:HA3	2.19	0.42
13:V:271:LEU:HB3	14:W:187:LYS:NZ	2.34	0.42
16:Y:-21:DG:H2'	16:Y:-20:DT:C5	2.54	0.42
16:Y:-14:DA:O3'	16:Y:-13:DT:C6	2.72	0.42
7:K:159:PRO:HG3	7:K:169:ALA:HB3	2.01	0.42
12:T:184:ASP:HB3	13:V:170:ARG:NH1	2.34	0.42
13:V:57:VAL:O	13:V:61:LEU:HG	2.19	0.42
13:V:261:ARG:O	14:W:198:LYS:CD	2.66	0.42
15:X:2:DA:C2'	15:X:3:DG:N7	2.74	0.42
1:A:55:VAL:HG21	2:B:95:VAL:HG21	2.01	0.42
3:C:99:TYR:HA	4:D:95:ARG:NH2	2.35	0.42
1:E:26:PRO:HB3	2:F:37:TYR:CZ	2.53	0.42
4:H:35:ARG:HB2	4:H:35:ARG:HH11	1.80	0.42
6:J:155:SER:HA	16:Y:-135:DC:OP1	2.19	0.42
7:K:36:ARG:HG3	7:K:36:ARG:HH21	1.84	0.42
7:K:88:PHE:CA	7:K:119:PHE:HD2	2.32	0.42
7:K:121:ALA:N	7:K:378:THR:OG1	2.52	0.42
7:K:220:MET:O	7:K:224:LYS:CG	2.64	0.42
7:K:282:PHE:CE2	7:K:333:VAL:HG23	2.54	0.42
7:K:306:PRO:HB2	7:K:309:MET:HB3	2.02	0.42
7:K:315:LYS:HG3	7:K:346:ASP:O	2.19	0.42
9:M:401:THR:CG2	9:M:402:THR:N	2.83	0.42
10:N:249:VAL:HG12	10:N:256:GLY:O	2.19	0.42
11:U:332:PRO:O	11:U:335:ARG:HD2	2.19	0.42
16:Y:-20:DT:H2"	16:Y:-19:DG:OP2	2.19	0.42
3:C:61:LEU:N	3:C:97:GLU:OE2	2.51	0.42
1:E:34:LEU:HD13	1:E:43:VAL:HG13	2.01	0.42
3:G:63:ARG:HH21	15:X:59:DA:C4'	2.31	0.42
3:G:73:GLU:HA	4:H:23:ARG:CZ	2.50	0.42
7:K:65:LEU:HB3	7:K:68:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:206:LYS:HA	7:K:210:CYS:SG	2.60	0.42
7:K:330:ARG:HG2	7:K:351:LEU:HB2	2.02	0.42
7:K:338:ARG:HA	7:K:347:VAL:HG11	2.00	0.42
9:M:35:ALA:HB2	9:M:40:VAL:HG22	1.99	0.42
11:U:150:GLY:HA2	11:U:296:ASN:O	2.19	0.42
14:W:150:MET:O	14:W:154:LEU:HG	2.19	0.42
15:X:7:DG:H2"	15:X:8:DT:H5"	2.00	0.42
15:X:98:DT:H1'	15:X:99:DA:C8	2.55	0.42
15:X:110:DC:H2"	15:X:111:DG:H8	1.82	0.42
16:Y:-67:DC:H1'	16:Y:-66:DC:C6	2.55	0.42
1:A:57:GLU:HG3	2:B:41:VAL:HG21	2.01	0.42
1:A:58:TYR:HH	2:B:106:HIS:HD1	1.56	0.42
1:E:67:GLY:CA	1:E:78:ILE:HG12	2.23	0.42
1:E:95:LYS:HB3	1:E:95:LYS:NZ	2.35	0.42
5:I:1883:PRO:HG2	7:K:308:GLU:HG2	2.00	0.42
7:K:32:SER:HB2	7:K:54:LEU:HD21	2.00	0.42
7:K:216:PHE:HE2	8:L:116:PHE:HZ	1.67	0.42
10:P:227:CYS:HB2	10:P:228:PRO:HD2	2.02	0.42
11:U:111:ASN:O	11:U:115:ASN:HB2	2.19	0.42
13:V:202:LEU:HD23	13:V:202:LEU:HA	1.74	0.42
15:X:99:DA:H2"	15:X:100:DG:H5'	2.01	0.42
2:B:102:GLU:O	2:B:103:LEU:C	2.58	0.42
1:E:66:ALA:HB2	1:E:83:LEU:HD23	2.02	0.42
1:E:118:LYS:HE2	1:E:118:LYS:HB3	1.81	0.42
3:G:107:THR:O	3:G:123:ASP:HB3	2.20	0.42
5:I:102:HIS:CE1	13:V:253:LYS:HB3	2.55	0.42
5:I:834:ARG:N	5:I:835:PRO:CD	2.82	0.42
5:I:2123:VAL:HG13	5:I:2124:GLY:N	2.34	0.42
7:K:36:ARG:NH2	7:K:36:ARG:HG3	2.34	0.42
7:K:100:PHE:HZ	7:K:170:ILE:HG12	1.83	0.42
7:K:135:TYR:HA	7:K:138:ASP:OD1	2.20	0.42
7:K:220:MET:HE3	8:L:122:PHE:HD2	1.83	0.42
9:M:401:THR:HG21	9:M:405:TYR:CD2	2.55	0.42
13:V:196:TYR:HB3	13:V:217:VAL:CG1	2.49	0.42
14:W:194:ILE:CG2	14:W:198:LYS:HD2	2.50	0.42
15:X:112:DA:C2'	15:X:113:DC:C6	3.03	0.42
16:Y:-133:DG:C2'	16:Y:-132:DT:C7	2.97	0.42
16:Y:-130:DC:OP2	16:Y:-130:DC:C6	2.72	0.42
1:A:56:LEU:CD1	2:B:67:PHE:HB2	2.50	0.42
2:F:77:LEU:HD23	2:F:80:TYR:HD2	1.85	0.42
3:G:74:ILE:HD12	4:H:62:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:122:LYS:HE2	5:I:122:LYS:HA	2.02	0.42
5:I:2088:ARG:HB2	5:I:2115:ILE:HB	2.02	0.42
7:K:92:ASN:HA	7:K:119:PHE:O	2.19	0.42
7:K:97:GLU:OE2	7:K:124:ARG:HD3	2.19	0.42
7:K:102:PHE:HD2	8:L:90:GLU:HG3	1.85	0.42
10:R:249:VAL:O	10:R:249:VAL:HG12	2.19	0.42
13:V:113:HIS:CD2	13:V:115:ARG:HE	2.32	0.42
16:Y:-126:DG:H2"	16:Y:-125:DG:H8	1.84	0.42
3:C:120:MET:O	3:C:123:ASP:N	2.49	0.42
3:G:63:ARG:HB3	3:G:66:PRO:HG2	2.00	0.42
5:I:892:ASN:CG	15:X:51:DG:H4'	2.40	0.42
5:I:2037:LEU:HD11	5:I:2039:GLN:CD	2.39	0.42
7:K:71:GLN:OE1	7:K:72:ARG:HG2	2.20	0.42
7:K:106:GLN:CA	7:K:109:MET:HB3	2.46	0.42
7:K:244:ILE:HD13	7:K:248:PHE:HE1	1.85	0.42
7:K:319:LEU:O	7:K:352:PRO:HD2	2.20	0.42
8:L:114:ARG:NE	8:L:114:ARG:HA	2.35	0.42
11:U:326:LYS:HE2	11:U:328:LYS:HB2	2.01	0.42
13:V:248:LEU:O	13:V:252:ARG:CZ	2.67	0.42
14:W:195:ALA:O	14:W:199:GLU:HG2	2.19	0.42
16:Y:-124:DC:H1'	16:Y:-123:DC:H5'	2.02	0.42
16:Y:-6:DA:H2"	16:Y:-5:DT:O5'	2.20	0.42
1:E:88:ARG:CB	1:E:108:LEU:HD11	2.49	0.42
5:I:930:LEU:CD2	10:N:250:ILE:CD1	2.96	0.42
6:J:162:HIS:CE1	15:X:137:DG:C4'	2.92	0.42
7:K:93:ILE:O	7:K:122:VAL:CA	2.65	0.42
7:K:158:VAL:HG13	7:K:170:ILE:HB	2.02	0.42
7:K:230:ASN:C	7:K:231:THR:HG1	2.20	0.42
7:K:284:PRO:HG3	7:K:293:GLY:H	1.83	0.42
7:K:387:HIS:O	7:K:391:GLU:HG3	2.19	0.42
8:L:8:VAL:O	8:L:9:ARG:C	2.58	0.42
11:U:275:HIS:CG	11:U:276:GLU:N	2.88	0.42
15:X:87:DT:P	15:X:87:DT:H2'	2.60	0.42
15:X:114:DC:C2	15:X:115:DA:C5	3.08	0.42
16:Y:-24:DC:C6	16:Y:-24:DC:H5'	2.54	0.42
1:A:43:ARG:HG2	2:B:85:THR:HB	2.01	0.42
1:A:93:GLU:HG2	2:B:100:PRO:HB2	2.02	0.42
5:I:1928:LEU:HD22	10:R:279:LYS:HD2	2.02	0.42
7:K:235:ASP:OD2	7:K:250:LYS:HD2	2.20	0.42
9:M:354:LEU:O	9:M:358:VAL:CG2	2.68	0.42
11:U:256:ARG:O	11:U:257:CYS:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:257:ARG:O	13:V:261:ARG:CG	2.65	0.42
14:W:157:THR:O	14:W:157:THR:HG22	2.20	0.42
15:X:60:DA:H5"	15:X:60:DA:H8	1.84	0.42
15:X:128:DC:H6	15:X:128:DC:C5'	2.33	0.42
1:E:42:ARG:O	2:F:85:THR:OG1	2.20	0.41
5:I:1914:LEU:HD23	9:M:285:LYS:HD2	2.01	0.41
5:I:2060:HIS:HD2	5:I:2132:THR:HG23	1.78	0.41
5:I:2091:GLY:O	15:X:56:DT:H73	2.20	0.41
7:K:146:ILE:O	7:K:318:VAL:HB	2.20	0.41
7:K:175:VAL:CG2	7:K:289:ILE:HG21	2.50	0.41
7:K:234:ILE:O	7:K:235:ASP:OD1	2.37	0.41
15:X:5:DA:H2"	15:X:6:DT:O5'	2.20	0.41
15:X:16:DT:C7	15:X:16:DT:OP2	2.68	0.41
15:X:37:DG:OP2	15:X:37:DG:H8	2.02	0.41
16:Y:-23:DA:H2"	16:Y:-22:DC:C5'	2.50	0.41
1:A:51:TYR:OH	2:B:108:VAL:HA	2.20	0.41
1:A:113:GLN:HB2	1:A:116:LEU:HG	2.02	0.41
1:E:36:LYS:HA	1:E:36:LYS:HD3	1.86	0.41
1:E:57:TYR:CA	6:J:130:ARG:HH12	2.22	0.41
1:E:83:LEU:HD13	2:F:58:ILE:HG21	2.02	0.41
1:E:88:ARG:HB3	1:E:108:LEU:HD11	2.02	0.41
5:I:694:LYS:N	5:I:719:HIS:HD2	2.15	0.41
7:K:120:GLN:HE21	7:K:120:GLN:H	1.65	0.41
7:K:125:VAL:CG1	7:K:129:ALA:HB3	2.50	0.41
7:K:185:LYS:HE2	7:K:185:LYS:HB3	1.87	0.41
7:K:261:TYR:HB2	7:K:267:ILE:HG12	2.02	0.41
7:K:284:PRO:HG3	7:K:292:MET:HA	2.02	0.41
7:K:292:MET:HE3	7:K:292:MET:O	2.21	0.41
9:Q:237:ASP:OD1	9:Q:237:ASP:N	2.51	0.41
12:T:198:ALA:H	12:T:201:PHE:HB3	1.86	0.41
11:U:170:ALA:HB1	11:U:175:ILE:HD11	2.02	0.41
1:A:26:PHE:CE2	2:B:63:VAL:CG2	3.03	0.41
7:K:10:ALA:HB3	7:K:152:TYR:HD2	1.85	0.41
7:K:119:PHE:CD1	7:K:119:PHE:N	2.86	0.41
7:K:276:ALA:O	7:K:279:GLU:HB3	2.21	0.41
7:K:364:LYS:HE2	7:K:365:LEU:HD13	2.02	0.41
9:M:317:ARG:CG	10:R:104:ALA:HB2	2.50	0.41
11:U:188:TYR:CE1	11:U:192:ILE:HD11	2.55	0.41
13:V:182:GLN:C	13:V:183:PHE:HD1	2.22	0.41
15:X:122:DC:C2	15:X:123:DG:C5	3.08	0.41
16:Y:-146:DC:C2'	16:Y:-145:DT:C6	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-133:DG:H2'	16:Y:-132:DT:C7	2.48	0.41
16:Y:-118:DA:H2"	16:Y:-117:DA:N7	2.35	0.41
16:Y:-55:DC:H2'	16:Y:-54:DC:C6	2.55	0.41
1:A:40:TYR:O	2:B:86:ILE:HD11	2.19	0.41
1:A:117:LEU:HA	3:C:48:LEU:HD11	2.03	0.41
2:F:77:LEU:HD23	2:F:77:LEU:HA	1.81	0.41
7:K:75:TRP:HB3	7:K:79:PHE:CE2	2.56	0.41
10:R:112:GLU:HB2	10:R:265:THR:CG2	2.51	0.41
10:R:264:ASP:OD1	10:R:265:THR:N	2.53	0.41
10:R:328:THR:HG21	10:R:344:HIS:HB3	2.02	0.41
15:X:87:DT:C1'	15:X:88:DT:H72	2.51	0.41
16:Y:-120:DT:H1'	16:Y:-119:DC:C5'	2.47	0.41
1:A:84:LEU:HD12	2:B:58:ILE:HD13	2.02	0.41
1:A:101:VAL:HG11	4:D:98:TYR:CE2	2.55	0.41
2:B:75:SER:HA	2:B:86:ILE:CG1	2.50	0.41
2:B:106:HIS:CD2	2:B:106:HIS:N	2.88	0.41
1:E:68:ASN:CG	6:J:144:THR:HG21	2.40	0.41
1:E:74:LYS:HD3	6:J:151:ARG:HD3	2.02	0.41
5:I:128:PRO:HG3	13:V:218:PHE:N	2.36	0.41
5:I:979:THR:HG23	5:I:980:ALA:N	2.36	0.41
7:K:146:ILE:HG21	7:K:157:ILE:HG23	2.02	0.41
7:K:162:ARG:HA	7:K:162:ARG:HE	1.85	0.41
13:V:171:PHE:HZ	13:V:195:TYR:CD2	2.37	0.41
15:X:114:DC:O5'	15:X:114:DC:H2'	2.21	0.41
1:A:33:ARG:HA	1:A:36:ARG:CZ	2.50	0.41
3:C:41:TYR:HD2	15:X:83:DG:OP1	2.04	0.41
4:H:84:MET:HE2	4:H:101:GLY:O	2.19	0.41
7:K:99:TYR:CE2	7:K:158:VAL:HG11	2.56	0.41
9:M:270:GLU:HB3	9:M:276:ARG:HG3	2.01	0.41
13:V:175:HIS:O	13:V:178:TYR:HB2	2.21	0.41
14:W:190:THR:O	14:W:194:ILE:HD12	2.21	0.41
15:X:8:DT:C2'	15:X:9:DA:C8	3.02	0.41
16:Y:-140:DA:C2'	16:Y:-139:DA:H5"	2.27	0.41
1:A:55:VAL:O	1:A:59:LEU:CG	2.64	0.41
3:C:61:LEU:HD11	4:D:40:ARG:NE	2.35	0.41
1:E:18:SER:CB	1:E:27:VAL:H	2.33	0.41
7:K:135:TYR:O	7:K:139:ASN:N	2.53	0.41
13:V:239:GLU:OE1	13:V:240:GLN:HG2	2.21	0.41
13:V:259:LYS:C	13:V:261:ARG:N	2.73	0.41
14:W:194:ILE:CG2	14:W:198:LYS:HE2	2.50	0.41
15:X:25:DC:H1'	15:X:26:DC:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:HB2	2:B:110:GLU:CD	2.41	0.41
1:A:63:ILE:HG23	1:A:64:LEU:H	1.86	0.41
3:C:124:ILE:HG13	4:D:50:ILE:HD12	2.02	0.41
1:E:26:PRO:HG3	2:F:37:TYR:CE2	2.56	0.41
1:E:31:HIS:CE1	1:E:35:ARG:HH11	2.38	0.41
1:E:47:ALA:N	1:E:48:PRO:CD	2.84	0.41
3:G:107:THR:HG21	3:G:119:ILE:HD12	2.03	0.41
4:H:89:ALA:O	4:H:93:GLN:HG2	2.20	0.41
5:I:120:SER:CB	13:V:233:LEU:HD12	2.44	0.41
6:J:177:LYS:HA	6:J:180:GLU:HG2	2.02	0.41
9:M:416:LEU:HD22	9:M:433:ILE:HG12	2.02	0.41
9:O:171:LYS:C	9:O:172:LEU:HD22	2.41	0.41
13:V:236:ARG:HH21	13:V:241:VAL:HA	1.83	0.41
13:V:272:ILE:HD12	14:W:187:LYS:NZ	2.36	0.41
15:X:36:DG:H1'	15:X:37:DG:C8	2.56	0.41
15:X:112:DA:C2'	15:X:113:DC:H6	2.34	0.41
16:Y:-49:DA:H2"	16:Y:-48:DG:N7	2.36	0.41
2:B:90:GLU:CA	2:B:93:THR:HG22	2.47	0.41
3:C:48:LEU:HA	3:C:51:ILE:HD12	2.02	0.41
2:F:34:TYR:CE1	2:F:63:VAL:HG11	2.56	0.41
5:I:124:LEU:N	5:I:125:PRO:HD3	2.35	0.41
5:I:895:MET:O	5:I:898:ARG:HB2	2.21	0.41
5:I:1886:LEU:CD1	7:K:311:PRO:HB2	2.49	0.41
5:I:1941:PRO:HG2	5:I:1945:HIS:CD2	2.56	0.41
5:I:2088:ARG:HG3	5:I:2115:ILE:C	2.41	0.41
7:K:110:ASN:HB2	7:K:387:HIS:HD2	1.86	0.41
7:K:226:LYS:HB3	7:K:226:LYS:HE3	1.62	0.41
10:N:22:ILE:N	10:N:22:ILE:HD12	2.36	0.41
10:P:19:ILE:HG13	9:Q:287:ILE:HG21	2.02	0.41
14:W:66:ILE:HD12	14:W:86:TYR:CG	2.55	0.41
14:W:140:ASP:OD1	14:W:141:GLU:N	2.47	0.41
16:Y:-17:DC:H6	16:Y:-17:DC:H2'	1.78	0.41
1:A:59:LEU:HD13	2:B:66:ILE:HG21	1.98	0.41
5:I:815:ILE:HG23	5:I:816:GLU:N	2.36	0.41
5:I:2131:ASP:OD2	5:I:2132:THR:HG23	2.21	0.41
7:K:106:GLN:HA	7:K:109:MET:CB	2.50	0.41
7:K:120:GLN:H	7:K:379:ARG:HH22	1.68	0.41
7:K:183:HIS:CE1	7:K:187:ILE:HG13	2.56	0.41
7:K:380:GLU:HG3	7:K:380:GLU:H	1.52	0.41
11:S:252:ASN:HA	11:S:255:PHE:CE1	2.55	0.41
13:V:228:GLU:O	13:V:231:GLU:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:194:ILE:HG23	14:W:198:LYS:CE	2.50	0.41
15:X:60:DA:H5"	15:X:60:DA:C8	2.56	0.41
16:Y:-116:DT:C6	16:Y:-116:DT:H5'	2.54	0.41
16:Y:-91:DC:H2"	16:Y:-90:DT:OP2	2.21	0.41
16:Y:-33:DG:H2'	16:Y:-32:DT:H71	2.03	0.41
16:Y:-1:DG:H1'	16:Y:0:DT:H5"	2.03	0.41
2:B:98:LEU:HD13	2:B:98:LEU:HA	1.94	0.40
2:B:112:THR:CG2	13:V:61:LEU:HD21	2.51	0.40
7:K:72:ARG:NH1	7:K:72:ARG:HA	2.36	0.40
7:K:123:LEU:HD13	7:K:372:PHE:CD1	2.56	0.40
7:K:335:SER:HA	7:K:338:ARG:NE	2.31	0.40
7:K:378:THR:HB	7:K:380:GLU:CD	2.41	0.40
9:Q:129:GLU:HG2	9:Q:195:ALA:HB3	2.03	0.40
9:Q:137:GLU:O	9:Q:159:ILE:HA	2.22	0.40
12:T:157:LEU:O	12:T:396:GLY:HA3	2.21	0.40
13:V:224:ARG:HE	13:V:224:ARG:HB2	1.50	0.40
15:X:87:DT:H2'	15:X:87:DT:OP2	2.21	0.40
16:Y:-15:DC:H6	16:Y:-15:DC:H5"	1.86	0.40
16:Y:-11:DT:H2"	16:Y:-10:DA:OP2	2.21	0.40
3:C:73:GLU:HB3	4:D:25:ASN:HD22	1.86	0.40
3:G:110:CYS:HB2	3:G:123:ASP:CB	2.48	0.40
4:H:70:VAL:O	4:H:74:GLU:HG3	2.20	0.40
5:I:903:HIS:CG	5:I:904:PRO:HD2	2.56	0.40
7:K:59:PRO:HA	7:K:67:ASN:HD22	1.85	0.40
7:K:171:ILE:HD11	7:K:300:TYR:HD1	1.87	0.40
9:M:389:GLU:HG2	9:M:427:LYS:HB2	2.02	0.40
9:M:416:LEU:HD22	9:M:433:ILE:HG13	2.02	0.40
10:P:68:ILE:HD13	10:P:68:ILE:N	2.33	0.40
10:R:207:ARG:HD3	10:R:207:ARG:H	1.87	0.40
10:R:211:ARG:HB3	10:R:211:ARG:CZ	2.51	0.40
11:U:193:LEU:C	11:U:195:GLU:H	2.22	0.40
11:U:256:ARG:O	11:U:257:CYS:HB3	2.21	0.40
13:V:128:ARG:HG3	13:V:129:PHE:HD1	1.84	0.40
15:X:10:DT:C2	15:X:11:DA:N7	2.89	0.40
15:X:47:DC:H2"	15:X:48:DC:C5	2.56	0.40
1:A:52:LEU:HD11	1:A:56:LEU:HD11	2.03	0.40
5:I:887:PHE:O	5:I:890:VAL:HG22	2.20	0.40
7:K:4:LEU:HB2	7:K:93:ILE:CG1	2.50	0.40
7:K:36:ARG:HA	7:K:36:ARG:HE	1.82	0.40
7:K:98:PRO:HG2	7:K:101:ASN:HB2	2.02	0.40
7:K:156:HIS:HA	7:K:171:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:144:GLU:N	10:R:162:THR:OG1	2.55	0.40
15:X:115:DA:H2"	15:X:116:DA:H8	1.85	0.40
1:E:62:ILE:HD12	2:F:62:PHE:CZ	2.56	0.40
5:I:154:GLU:OE2	5:I:158:LYS:NZ	2.41	0.40
7:K:120:GLN:HA	7:K:378:THR:HG21	2.01	0.40
7:K:214:GLN:NE2	7:K:331:ASP:OD2	2.54	0.40
7:K:224:LYS:HG2	8:L:122:PHE:CE2	2.56	0.40
10:P:147:ILE:HD12	10:P:148:ASP:N	2.36	0.40
15:X:28:DG:C2'	15:X:29:DG:C8	3.04	0.40
15:X:101:DA:C2'	15:X:102:DG:C8	3.04	0.40
16:Y:-61:DT:H2"	16:Y:-60:DT:C6	2.57	0.40
1:E:70:ALA:HA	1:E:82:HIS:ND1	2.37	0.40
3:G:68:GLN:OE1	3:G:72:ARG:NH2	2.49	0.40
3:G:74:ILE:CD1	4:H:62:LEU:HB3	2.48	0.40
3:G:83:ARG:HB2	4:H:80:THR:HG22	2.02	0.40
4:H:26:ILE:HG13	4:H:26:ILE:O	2.20	0.40
5:I:105:GLU:OE2	13:V:246:TYR:OH	2.35	0.40
7:K:113:LEU:HD12	7:K:114:PHE:CD1	2.56	0.40
7:K:377:VAL:HG22	7:K:389:VAL:CG2	2.52	0.40
8:L:92:ASN:C	8:L:92:ASN:OD1	2.60	0.40
9:O:334:GLY:O	9:O:348:HIS:N	2.53	0.40
10:R:116:THR:HG23	10:R:311:PHE:CE1	2.56	0.40
12:T:353:GLY:N	20:T:501:ATP:O2A	2.49	0.40
13:V:211:THR:O	13:V:212:ASP:C	2.60	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	106/130 (82%)	97 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	103/130 (79%)	93 (90%)	10 (10%)	0	100 100
2	B	94/126 (75%)	87 (93%)	7 (7%)	0	100 100
2	F	92/126 (73%)	88 (96%)	2 (2%)	2 (2%)	6 35
3	C	93/136 (68%)	91 (98%)	2 (2%)	0	100 100
3	G	95/136 (70%)	91 (96%)	4 (4%)	0	100 100
4	D	79/103 (77%)	78 (99%)	1 (1%)	0	100 100
4	H	78/103 (76%)	72 (92%)	6 (8%)	0	100 100
5	I	858/3230 (27%)	792 (92%)	63 (7%)	3 (0%)	41 74
6	J	158/364 (43%)	145 (92%)	13 (8%)	0	100 100
7	K	392/396 (99%)	295 (75%)	84 (21%)	13 (3%)	4 25
8	L	109/154 (71%)	96 (88%)	13 (12%)	0	100 100
9	M	412/456 (90%)	395 (96%)	16 (4%)	1 (0%)	47 79
9	O	431/456 (94%)	409 (95%)	19 (4%)	3 (1%)	22 61
9	Q	438/456 (96%)	417 (95%)	20 (5%)	1 (0%)	47 79
10	N	405/463 (88%)	386 (95%)	19 (5%)	0	100 100
10	P	423/463 (91%)	396 (94%)	26 (6%)	1 (0%)	47 79
10	R	420/463 (91%)	393 (94%)	26 (6%)	1 (0%)	47 79
11	S	373/375 (100%)	366 (98%)	7 (2%)	0	100 100
11	U	355/375 (95%)	325 (92%)	29 (8%)	1 (0%)	41 74
12	T	399/429 (93%)	381 (96%)	18 (4%)	0	100 100
13	V	200/467 (43%)	178 (89%)	19 (10%)	3 (2%)	10 44
14	W	185/227 (82%)	182 (98%)	2 (1%)	1 (0%)	29 67
All	All	6298/9764 (64%)	5853 (93%)	415 (7%)	30 (0%)	32 67

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	820	GLU
7	K	89	LEU
7	K	103	THR
7	K	120	GLN
7	K	376	VAL
7	K	377	VAL
9	O	264	MET

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Mol	Chain	Res	Type
11	U	257	CYS
13	V	207	ALA
13	V	238	PRO
13	V	239	GLU
2	F	30	ARG
7	K	68	TRP
7	K	173	ILE
7	K	199	THR
7	K	231	THR
9	O	17	SER
9	O	266	PRO
10	P	21	ARG
2	F	29	SER
7	K	232	VAL
14	W	171	GLU
5	I	1993	CYS
9	M	37	SER
7	K	269	ARG
9	Q	256	ILE
7	K	175	VAL
7	K	305	LEU
10	R	44	GLN
5	I	133	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 PDB entries followed by that with respect to all EM entries.

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	84/99 (85%)	64 (76%)	20 (24%)	0 3
1	E	82/99 (83%)	64 (78%)	18 (22%)	1 5
2	B	83/106 (78%)	71 (86%)	12 (14%)	3 15
2	F	81/106 (76%)	73 (90%)	8 (10%)	8 30
3	C	82/111 (74%)	68 (83%)	14 (17%)	2 10
3	G	85/111 (77%)	80 (94%)	5 (6%)	19 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	66/79 (84%)	66 (100%)	0	100 100
4	H	65/79 (82%)	54 (83%)	11 (17%)	2 10
5	I	775/2721 (28%)	759 (98%)	16 (2%)	53 79
6	J	148/312 (47%)	147 (99%)	1 (1%)	84 94
7	K	359/361 (99%)	238 (66%)	121 (34%)	0 0
8	L	98/133 (74%)	96 (98%)	2 (2%)	55 80
9	M	353/387 (91%)	346 (98%)	7 (2%)	55 80
9	O	364/387 (94%)	344 (94%)	20 (6%)	21 57
9	Q	366/387 (95%)	344 (94%)	22 (6%)	19 54
10	N	347/390 (89%)	340 (98%)	7 (2%)	55 80
10	P	352/390 (90%)	331 (94%)	21 (6%)	19 54
10	R	358/390 (92%)	329 (92%)	29 (8%)	11 42
11	S	318/318 (100%)	318 (100%)	0	100 100
11	U	305/318 (96%)	291 (95%)	14 (5%)	27 63
12	T	346/364 (95%)	338 (98%)	8 (2%)	50 78
13	V	183/400 (46%)	129 (70%)	54 (30%)	0 1
14	W	168/203 (83%)	164 (98%)	4 (2%)	49 77
All	All	5468/8251 (66%)	5054 (92%)	414 (8%)	17 45

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	21	ARG
1	A	36	ARG
1	A	37	LYS
1	A	42	GLU
1	A	44	VAL
1	A	59	LEU
1	A	65	GLU
1	A	66	LEU
1	A	72	ARG
1	A	78	ARG
1	A	80	ILE
1	A	82	ARG
1	A	92	GLU

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Mol	Chain	Res	Type
1	A	96	LYS
1	A	100	ARG
1	A	102	THR
1	A	109	LEU
1	A	115	VAL
1	A	119	LYS
2	B	28	ARG
2	B	46	HIS
2	B	60	ASN
2	B	68	GLU
2	B	77	LEU
2	B	85	THR
2	B	88	SER
2	B	89	ARG
2	B	98	LEU
2	B	103	LEU
2	B	106	HIS
2	B	113	LYS
3	C	41	TYR
3	C	42	ARG
3	C	48	LEU
3	C	56	LYS
3	C	59	GLU
3	C	64	LYS
3	C	76	GLN
3	C	77	ASP
3	C	79	LYS
3	C	82	LEU
3	C	115	LYS
3	C	120	MET
3	C	122	LYS
3	C	129	ARG
1	E	15	LYS
1	E	25	PHE
1	E	35	ARG
1	E	42	ARG
1	E	64	GLU
1	E	68	ASN
1	E	71	ARG
1	E	72	ASP
1	E	73	ASN
1	E	74	LYS

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Mol	Chain	Res	Type
1	E	75	LYS
1	E	76	THR
1	E	81	ARG
1	E	90	ASP
1	E	92	GLU
1	E	95	LYS
1	E	101	THR
1	E	111	ILE
2	F	28	ARG
2	F	30	ARG
2	F	31	LYS
2	F	45	VAL
2	F	60	ASN
2	F	79	HIS
2	F	84	SER
2	F	102	GLU
3	G	59	GLU
3	G	76	GLN
3	G	77	ASP
3	G	129	ARG
3	G	134	ARG
4	H	25	ASN
4	H	44	LYS
4	H	46	ILE
4	H	49	LEU
4	H	50	ILE
4	H	59	LYS
4	H	62	LEU
4	H	79	LYS
4	H	84	MET
4	H	91	LYS
4	H	97	LEU
5	I	132	ARG
5	I	144	MET
5	I	225	ARG
5	I	226	LYS
5	I	239	GLN
5	I	241	GLU
5	I	712	TRP
5	I	737	ARG
5	I	803	PHE
5	I	866	ARG

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Mol	Chain	Res	Type
5	I	972	ARG
5	I	992	MET
5	I	2015	TRP
5	I	2034	ASP
5	I	2040	TYR
5	I	2109	LYS
6	J	289	ARG
7	K	1	MET
7	K	5	VAL
7	K	6	LEU
7	K	7	ASP
7	K	8	ASN
7	K	14	LYS
7	K	17	TYR
7	K	23	SER
7	K	24	VAL
7	K	25	ILE
7	K	33	LYS
7	K	34	THR
7	K	36	ARG
7	K	38	LYS
7	K	52	SER
7	K	62	LYS
7	K	65	LEU
7	K	66	VAL
7	K	67	ASN
7	K	68	TRP
7	K	69	ASP
7	K	70	VAL
7	K	71	GLN
7	K	72	ARG
7	K	79	PHE
7	K	81	LYS
7	K	82	GLU
7	K	83	MET
7	K	87	ASP
7	K	89	LEU
7	K	94	ILE
7	K	95	ILE
7	K	97	GLU
7	K	107	GLU
7	K	115	GLU

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Mol	Chain	Res	Type
7	K	119	PHE
7	K	120	GLN
7	K	124	ARG
7	K	133	HIS
7	K	137	ARG
7	K	138	ASP
7	K	146	ILE
7	K	153	SER
7	K	154	PHE
7	K	155	THR
7	K	158	VAL
7	K	164	LYS
7	K	166	LYS
7	K	167	LYS
7	K	168	GLU
7	K	170	ILE
7	K	174	ASN
7	K	178	LYS
7	K	181	THR
7	K	183	HIS
7	K	185	LYS
7	K	186	GLU
7	K	190	TYR
7	K	192	GLN
7	K	193	LEU
7	K	197	ASP
7	K	198	GLU
7	K	201	VAL
7	K	206	LYS
7	K	207	GLU
7	K	209	VAL
7	K	213	SER
7	K	214	GLN
7	K	217	TYR
7	K	218	ARG
7	K	222	ILE
7	K	224	LYS
7	K	225	LEU
7	K	226	LYS
7	K	228	GLU
7	K	229	GLU
7	K	233	MET

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Mol	Chain	Res	Type
7	K	237	VAL
7	K	238	LEU
7	K	242	SER
7	K	244	ILE
7	K	266	GLN
7	K	269	ARG
7	K	270	LEU
7	K	273	GLU
7	K	274	ARG
7	K	287	ILE
7	K	289	ILE
7	K	291	GLU
7	K	292	MET
7	K	294	ILE
7	K	304	ASN
7	K	305	LEU
7	K	309	MET
7	K	310	GLN
7	K	312	HIS
7	K	313	PHE
7	K	314	PHE
7	K	325	LEU
7	K	326	PHE
7	K	330	ARG
7	K	331	ASP
7	K	335	SER
7	K	336	GLU
7	K	338	ARG
7	K	339	CYS
7	K	340	LEU
7	K	347	VAL
7	K	350	VAL
7	K	356	ILE
7	K	365	LEU
7	K	366	ILE
7	K	368	GLU
7	K	371	ASP
7	K	372	PHE
7	K	374	ASP
7	K	379	ARG
7	K	380	GLU
7	K	383	GLU

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Mol	Chain	Res	Type
7	K	385	ASN
7	K	391	GLU
8	L	40	PHE
8	L	111	ARG
9	M	129	GLU
9	M	184	ARG
9	M	186	GLU
9	M	192	TYR
9	M	317	ARG
9	M	362	ARG
9	M	378	ARG
10	N	149	ARG
10	N	194	THR
10	N	258	LEU
10	N	283	TRP
10	N	380	VAL
10	N	407	THR
10	N	413	CYS
9	O	18	HIS
9	O	37	SER
9	O	109	THR
9	O	137	GLU
9	O	194	GLU
9	O	216	GLU
9	O	228	VAL
9	O	264	MET
9	O	265	LYS
9	O	266	PRO
9	O	278	GLU
9	O	315	LEU
9	O	319	LEU
9	O	333	ARG
9	O	342	GLU
9	O	378	ARG
9	O	391	LEU
9	O	407	VAL
9	O	428	GLU
9	O	451	GLN
10	P	18	ARG
10	P	21	ARG
10	P	28	ILE
10	P	62	MET

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Mol	Chain	Res	Type
10	P	68	ILE
10	P	116	THR
10	P	147	ILE
10	P	236	LYS
10	P	257	PHE
10	P	261	PHE
10	P	267	GLU
10	P	268	ILE
10	P	286	GLU
10	P	323	VAL
10	P	324	LEU
10	P	328	THR
10	P	348	ILE
10	P	407	THR
10	P	424	ASP
10	P	428	ARG
10	P	429	VAL
9	Q	40	VAL
9	Q	52	ILE
9	Q	91	VAL
9	Q	113	MET
9	Q	138	LEU
9	Q	165	LYS
9	Q	185	VAL
9	Q	211	THR
9	Q	212	GLU
9	Q	215	LEU
9	Q	237	ASP
9	Q	262	GLN
9	Q	264	MET
9	Q	265	LYS
9	Q	268	LYS
9	Q	270	GLU
9	Q	276	ARG
9	Q	308	ASP
9	Q	316	HIS
9	Q	326	ILE
9	Q	430	VAL
9	Q	450	GLN
10	R	21	ARG
10	R	166	THR
10	R	168	MET

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Mol	Chain	Res	Type
10	R	185	ASP
10	R	207	ARG
10	R	215	TYR
10	R	225	VAL
10	R	246	GLU
10	R	250	ILE
10	R	255	GLN
10	R	267	GLU
10	R	269	LYS
10	R	279	LYS
10	R	285	GLU
10	R	286	GLU
10	R	308	SER
10	R	316	LEU
10	R	323	VAL
10	R	324	LEU
10	R	346	ILE
10	R	351	LEU
10	R	353	ARG
10	R	374	ARG
10	R	392	ARG
10	R	395	LEU
10	R	407	THR
10	R	422	GLN
10	R	423	VAL
10	R	444	LYS
12	T	10	GLU
12	T	24	ARG
12	T	70	ILE
12	T	82	MET
12	T	132	LYS
12	T	140	MET
12	T	317	LEU
12	T	389	ARG
11	U	101	HIS
11	U	107	GLU
11	U	147	ARG
11	U	151	ILE
11	U	161	HIS
11	U	163	VAL
11	U	198	TYR
11	U	210	ARG

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Mol	Chain	Res	Type
11	U	226	GLU
11	U	297	THR
11	U	326	LYS
11	U	330	ILE
11	U	335	ARG
11	U	353	GLN
13	V	51	GLU
13	V	53	MET
13	V	56	GLU
13	V	65	LYS
13	V	90	LYS
13	V	91	LYS
13	V	93	ARG
13	V	96	LYS
13	V	114	TRP
13	V	119	GLU
13	V	124	TYR
13	V	131	LYS
13	V	134	GLN
13	V	135	VAL
13	V	145	LEU
13	V	147	LEU
13	V	153	THR
13	V	156	GLU
13	V	169	LEU
13	V	190	ASP
13	V	196	TYR
13	V	202	LEU
13	V	205	VAL
13	V	206	ARG
13	V	208	VAL
13	V	214	LYS
13	V	218	PHE
13	V	219	ASP
13	V	222	HIS
13	V	223	GLU
13	V	224	ARG
13	V	225	ARG
13	V	229	GLN
13	V	230	LEU
13	V	232	ARG
13	V	235	ASN

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Mol	Chain	Res	Type
13	V	237	THR
13	V	239	GLU
13	V	241	VAL
13	V	244	GLU
13	V	245	GLU
13	V	249	GLN
13	V	250	GLU
13	V	252	ARG
13	V	255	GLU
13	V	257	ARG
13	V	258	LYS
13	V	259	LYS
13	V	263	LYS
13	V	265	SER
13	V	267	ASP
13	V	270	LYS
13	V	271	LEU
13	V	272	ILE
14	W	166	TYR
14	W	170	THR
14	W	171	GLU
14	W	200	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
2	B	44	GLN
2	B	60	ASN
2	B	92	GLN
3	C	108	ASN
4	D	25	ASN
4	D	75	HIS
1	E	24	GLN
1	E	31	HIS
1	E	68	ASN
1	E	104	GLN
2	F	46	HIS
2	F	92	GLN
3	G	76	GLN
4	H	75	HIS
5	I	239	GLN

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Mol	Chain	Res	Type
5	I	719	HIS
5	I	732	HIS
5	I	936	HIS
5	I	967	HIS
5	I	1945	HIS
5	I	1963	GLN
5	I	1964	GLN
5	I	2060	HIS
6	J	162	HIS
7	K	19	HIS
7	K	29	GLN
7	K	67	ASN
7	K	73	GLN
7	K	85	GLN
7	K	101	ASN
7	K	120	GLN
7	K	156	HIS
7	K	174	ASN
7	K	183	HIS
7	K	192	GLN
7	K	200	HIS
7	K	214	GLN
7	K	304	ASN
7	K	310	GLN
7	K	312	HIS
7	K	316	ASN
7	K	387	HIS
8	L	39	ASN
9	M	156	HIS
9	M	280	ASN
10	N	277	ASN
10	N	329	ASN
9	O	18	HIS
9	O	34	GLN
9	O	229	HIS
9	O	348	HIS
9	O	451	GLN
10	P	44	GLN
10	P	313	ASN
10	P	447	GLN
9	Q	196	ASN
9	Q	284	ASN

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Mol	Chain	Res	Type
10	R	233	GLN
12	T	143	HIS
11	U	101	HIS
11	U	353	GLN
13	V	204	ASN
13	V	249	GLN
13	V	266	GLN
13	V	269	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	ADP	N	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.33	4 (13%)
20	ATP	T	501	-	26,33,33	0.62	1 (3%)	31,52,52	1.12	4 (12%)
20	ATP	U	401	-	26,33,33	0.63	1 (3%)	31,52,52	1.06	2 (6%)
17	ADP	R	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	5 (17%)
17	ADP	I	3301	-	24,29,29	0.90	1 (4%)	29,45,45	1.64	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BEF	I	3303	-	0,3,3	-	-	-		
17	ADP	O	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	5 (17%)
17	ADP	P	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.57	6 (20%)
17	ADP	Q	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	5 (17%)
17	ADP	M	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	N	501	-	-	4/12/32/32	0/3/3/3
20	ATP	T	501	-	-	1/18/38/38	0/3/3/3
20	ATP	U	401	-	-	2/18/38/38	0/3/3/3
17	ADP	R	501	-	-	1/12/32/32	0/3/3/3
17	ADP	I	3301	-	-	5/12/32/32	0/3/3/3
17	ADP	O	501	-	-	6/12/32/32	0/3/3/3
17	ADP	P	501	-	-	2/12/32/32	0/3/3/3
17	ADP	Q	501	-	-	3/12/32/32	0/3/3/3
17	ADP	M	501	-	-	2/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	501	ADP	C5-C4	2.67	1.48	1.40
17	R	501	ADP	C5-C4	2.60	1.47	1.40
17	P	501	ADP	C5-C4	2.60	1.47	1.40
17	Q	501	ADP	C5-C4	2.59	1.47	1.40
17	M	501	ADP	C5-C4	2.58	1.47	1.40
17	N	501	ADP	C5-C4	2.50	1.47	1.40
17	I	3301	ADP	C5-C4	2.49	1.47	1.40
20	U	401	ATP	C8-N7	-2.05	1.31	1.34
20	T	501	ATP	C8-N7	-2.02	1.31	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	3301	ADP	PA-O3A-PB	-4.37	117.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	501	ADP	C3'-C2'-C1'	3.73	106.60	100.98
17	Q	501	ADP	PA-O3A-PB	-3.64	120.34	132.83
17	I	3301	ADP	N3-C2-N1	-3.53	123.16	128.68
17	M	501	ADP	PA-O3A-PB	-3.51	120.79	132.83
17	R	501	ADP	PA-O3A-PB	-3.40	121.17	132.83
17	I	3301	ADP	C3'-C2'-C1'	3.40	106.09	100.98
17	O	501	ADP	PA-O3A-PB	-3.39	121.19	132.83
17	O	501	ADP	N3-C2-N1	-3.38	123.40	128.68
17	N	501	ADP	N3-C2-N1	-3.36	123.43	128.68
17	Q	501	ADP	N3-C2-N1	-3.35	123.44	128.68
17	R	501	ADP	N3-C2-N1	-3.31	123.50	128.68
17	M	501	ADP	N3-C2-N1	-3.30	123.52	128.68
17	P	501	ADP	N3-C2-N1	-3.24	123.62	128.68
17	N	501	ADP	PA-O3A-PB	-3.21	121.83	132.83
17	P	501	ADP	PA-O3A-PB	-3.18	121.93	132.83
17	N	501	ADP	C4-C5-N7	-2.91	106.37	109.40
17	P	501	ADP	C4-C5-N7	-2.90	106.38	109.40
17	O	501	ADP	C4-C5-N7	-2.80	106.48	109.40
17	R	501	ADP	C4-C5-N7	-2.75	106.53	109.40
17	Q	501	ADP	C4-C5-N7	-2.71	106.57	109.40
17	M	501	ADP	C4-C5-N7	-2.51	106.78	109.40
20	U	401	ATP	C5-C6-N6	2.36	123.94	120.35
17	Q	501	ADP	C2-N1-C6	2.33	122.73	118.75
20	T	501	ATP	C5-C6-N6	2.30	123.84	120.35
17	O	501	ADP	C2-N1-C6	2.26	122.62	118.75
17	Q	501	ADP	C3'-C2'-C1'	2.22	104.33	100.98
20	T	501	ATP	O3'-C3'-C2'	-2.19	104.72	111.82
20	U	401	ATP	O3'-C3'-C2'	-2.18	104.77	111.82
20	T	501	ATP	O3'-C3'-C4'	-2.17	104.77	111.05
17	I	3301	ADP	C2-N1-C6	2.16	122.45	118.75
17	O	501	ADP	C3'-C2'-C1'	2.16	104.23	100.98
17	I	3301	ADP	C4-C5-N7	-2.16	107.15	109.40
17	R	501	ADP	C2-N1-C6	2.08	122.32	118.75
17	R	501	ADP	C3'-C2'-C1'	2.07	104.10	100.98
20	T	501	ATP	PB-O3B-PG	2.07	139.92	132.83
17	P	501	ADP	C2-N1-C6	2.04	122.25	118.75
17	P	501	ADP	O3B-PB-O2B	2.03	115.41	107.64
17	N	501	ADP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	I	3301	ADP	C5'-O5'-PA-O2A
17	N	501	ADP	C5'-O5'-PA-O1A
17	N	501	ADP	O4'-C4'-C5'-O5'
17	O	501	ADP	C5'-O5'-PA-O2A
17	P	501	ADP	PA-O3A-PB-O2B
17	N	501	ADP	C3'-C4'-C5'-O5'
20	U	401	ATP	C3'-C4'-C5'-O5'
17	I	3301	ADP	O4'-C4'-C5'-O5'
17	I	3301	ADP	C3'-C4'-C5'-O5'
17	O	501	ADP	O4'-C4'-C5'-O5'
17	M	501	ADP	O4'-C4'-C5'-O5'
17	I	3301	ADP	C5'-O5'-PA-O3A
17	O	501	ADP	C5'-O5'-PA-O3A
17	O	501	ADP	C3'-C4'-C5'-O5'
17	Q	501	ADP	O4'-C4'-C5'-O5'
17	I	3301	ADP	C5'-O5'-PA-O1A
17	O	501	ADP	C4'-C5'-O5'-PA
20	U	401	ATP	O4'-C4'-C5'-O5'
17	Q	501	ADP	C4'-C5'-O5'-PA
17	Q	501	ADP	C3'-C4'-C5'-O5'
17	P	501	ADP	PA-O3A-PB-O3B
17	M	501	ADP	C5'-O5'-PA-O3A
17	N	501	ADP	C5'-O5'-PA-O3A
20	T	501	ATP	C3'-C4'-C5'-O5'
17	R	501	ADP	C4'-C5'-O5'-PA
17	O	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

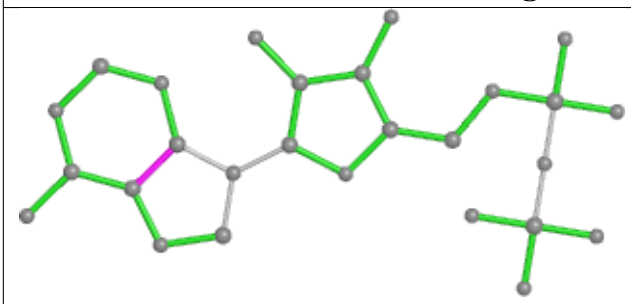
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	T	501	ATP	1	0
17	I	3301	ADP	6	0
19	I	3303	BEF	3	0
17	O	501	ADP	1	0
17	Q	501	ADP	1	0

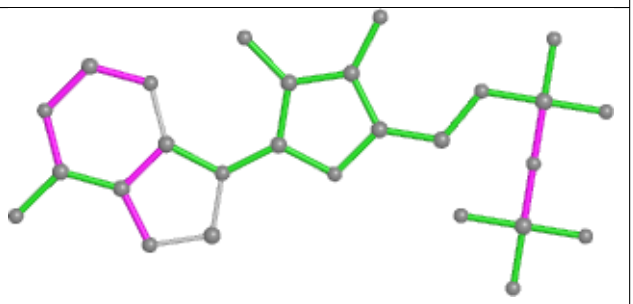
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

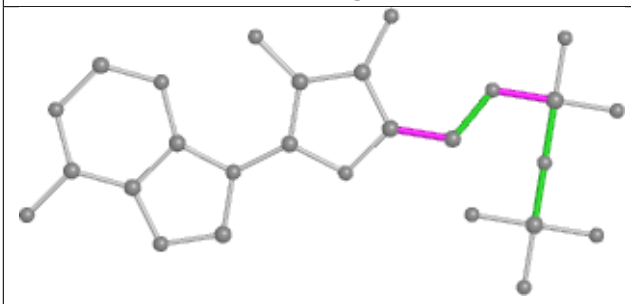
Ligand ADP N 501



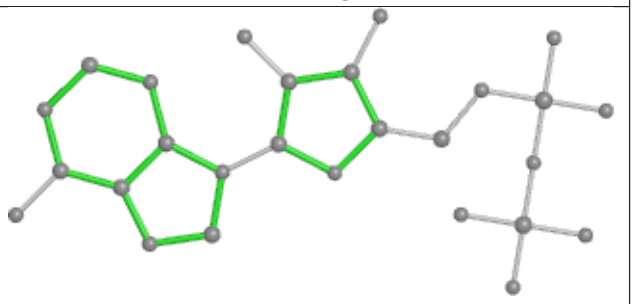
Bond lengths



Bond angles

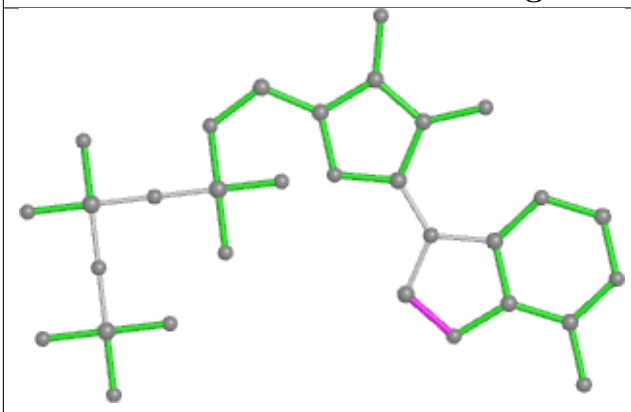


Torsions



Rings

Ligand ATP T 501



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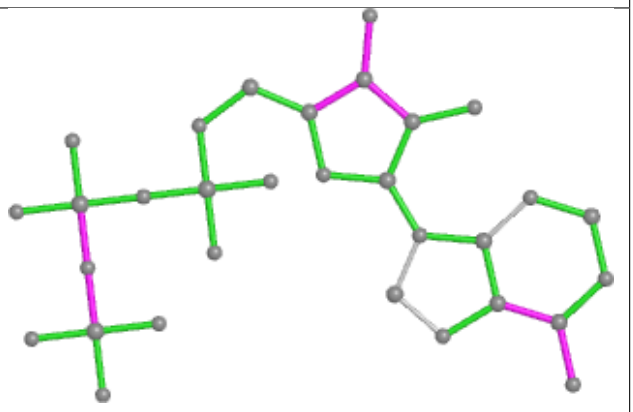

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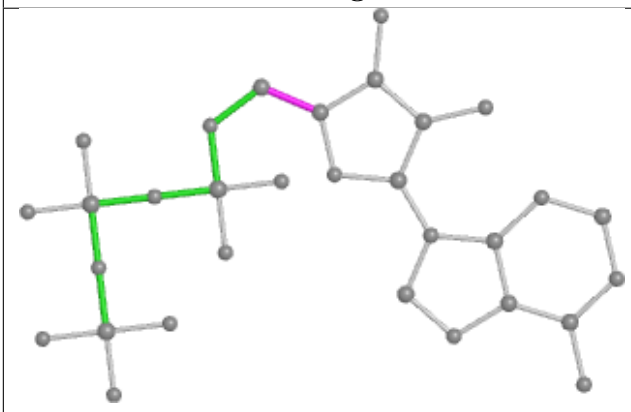

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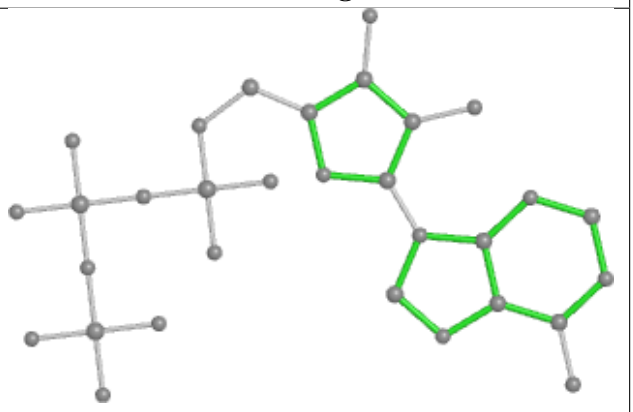
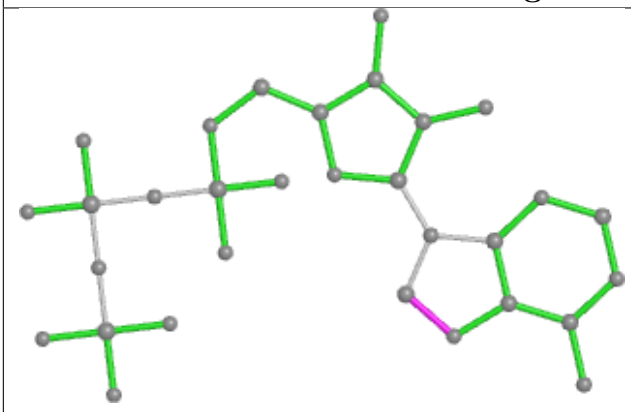


Rings

Ligand ATP U 401



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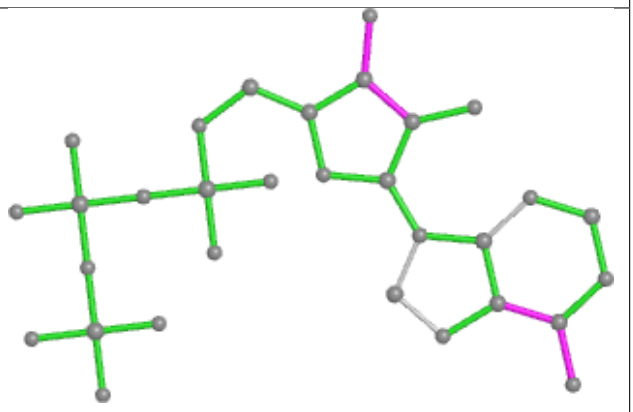

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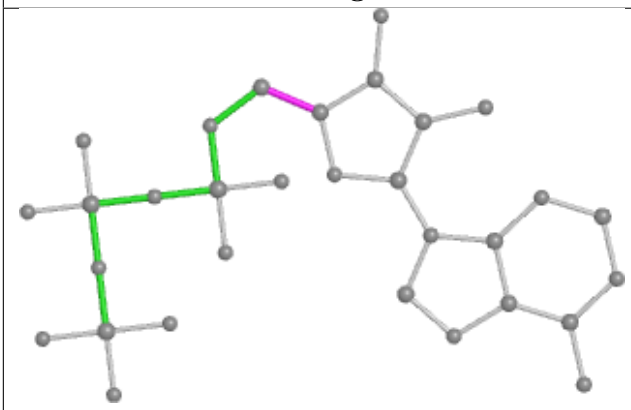

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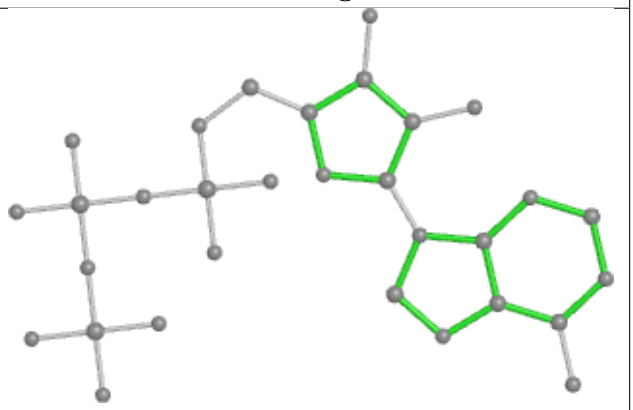
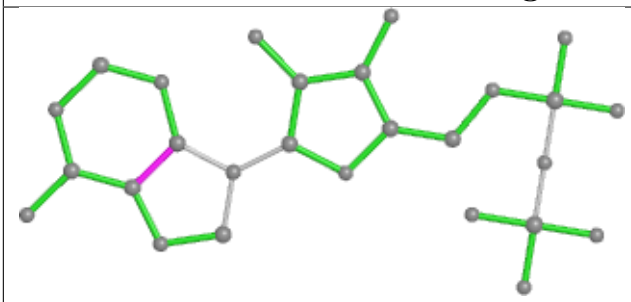


Rings

Ligand ADP R 501



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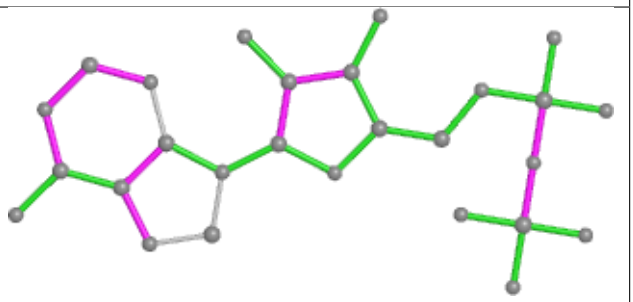
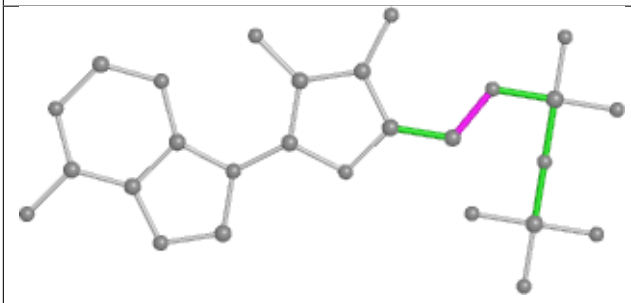


Bond angles



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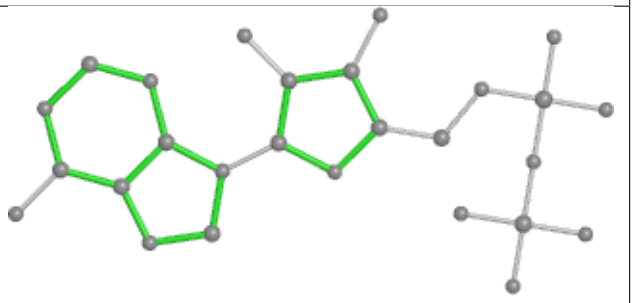
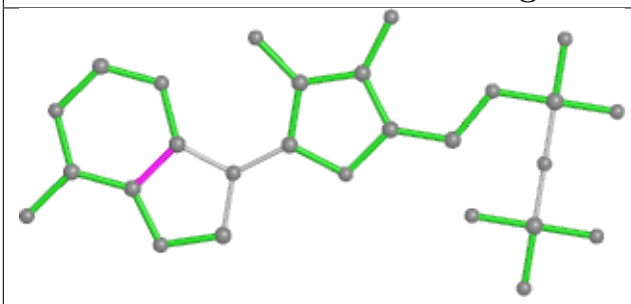
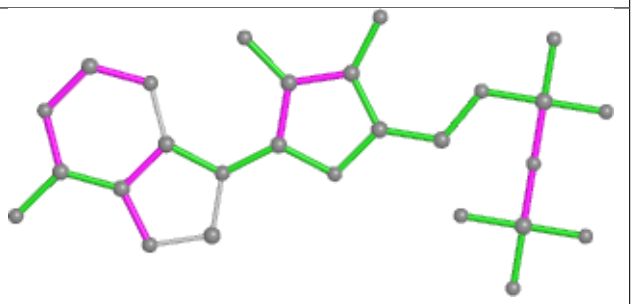


Rings

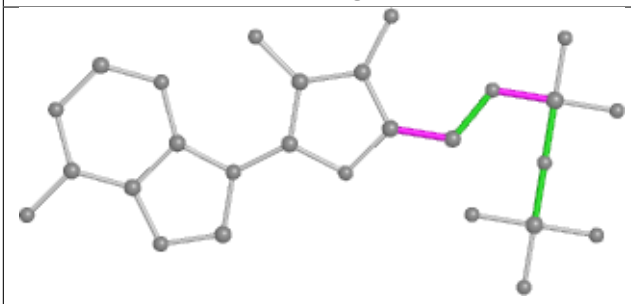
Ligand ADP I 3301



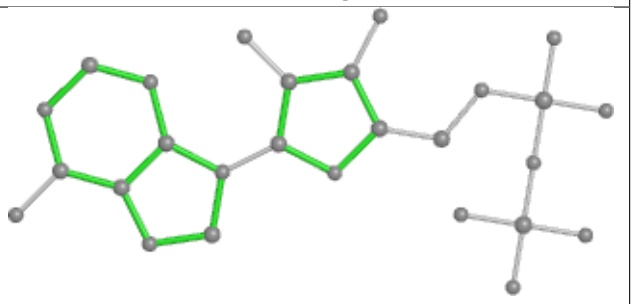
Bond lengths



Bond angles

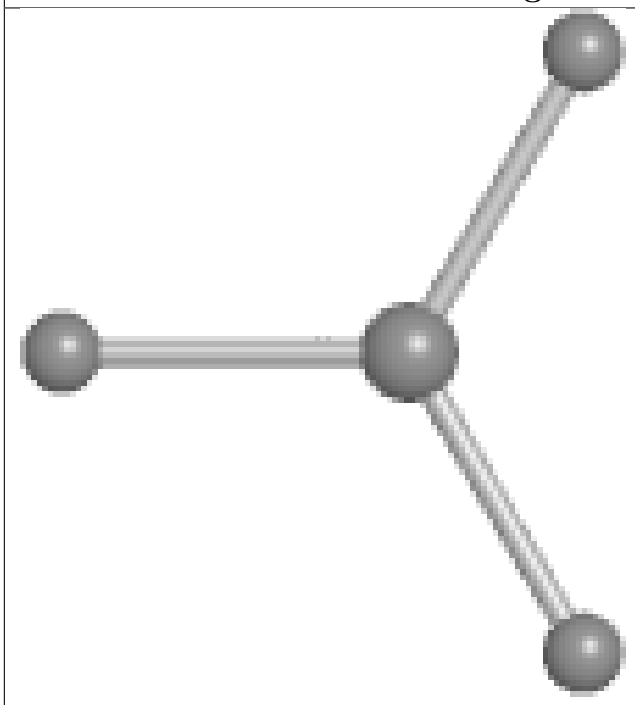


Torsions

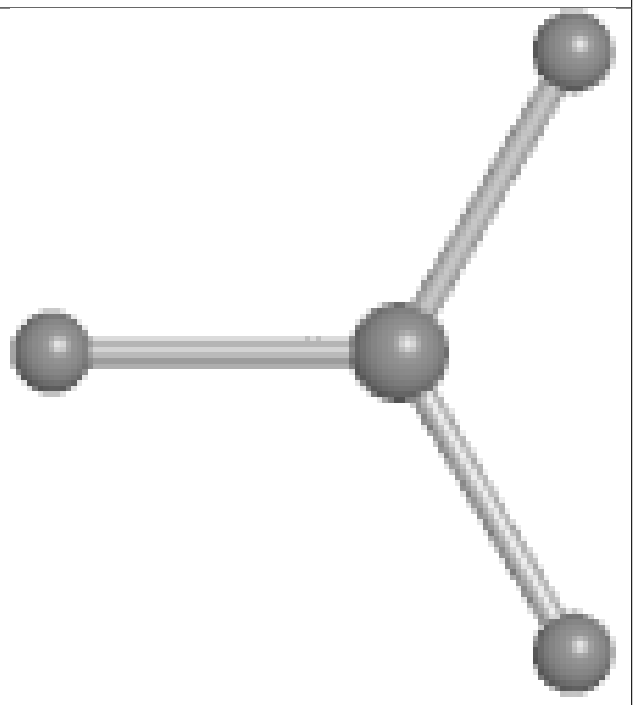


Rings

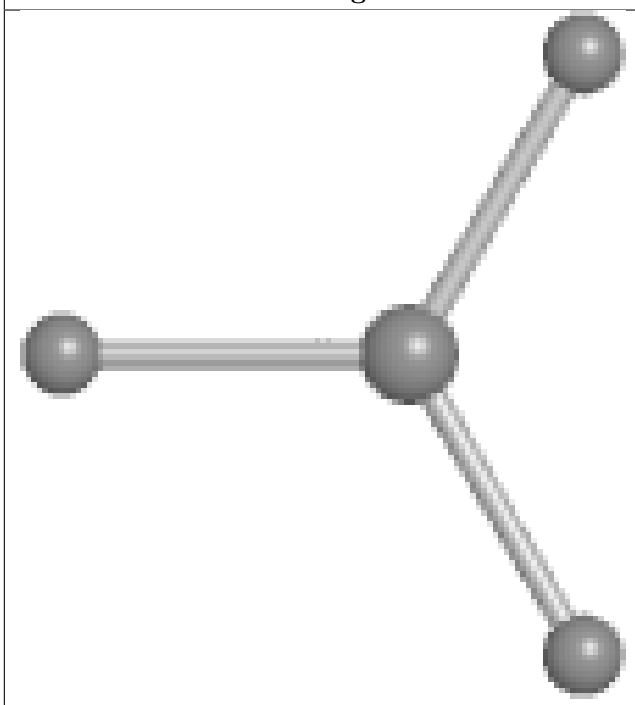
Ligand BEF I 3303



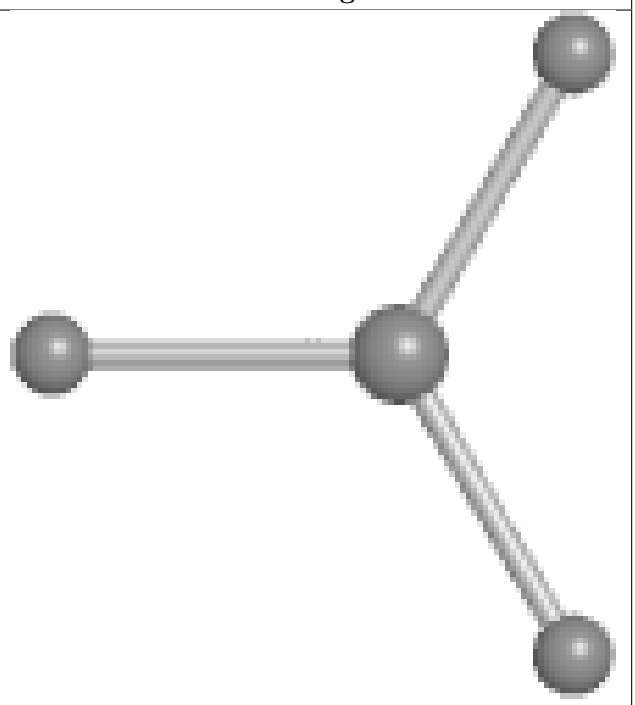
Bond lengths



Bond angles

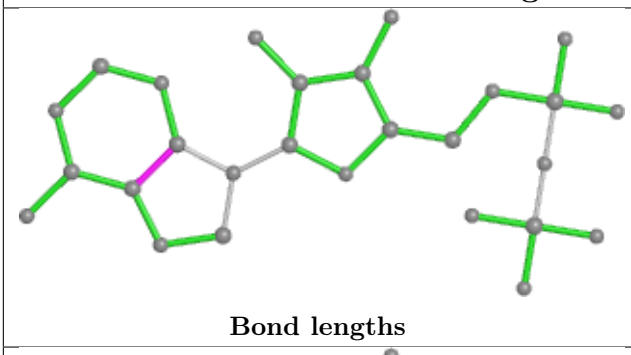


Torsions

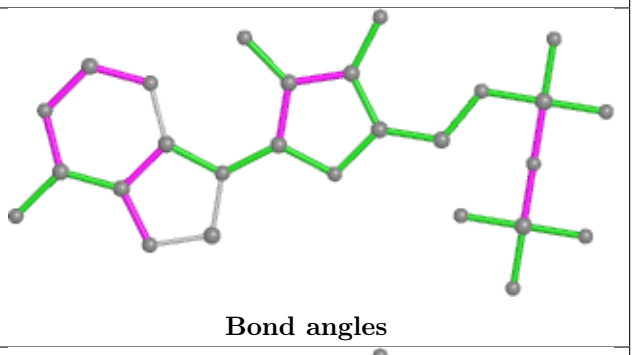


Rings

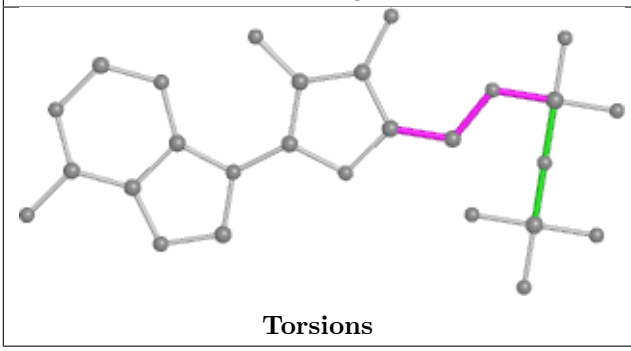
Ligand ADP O 501



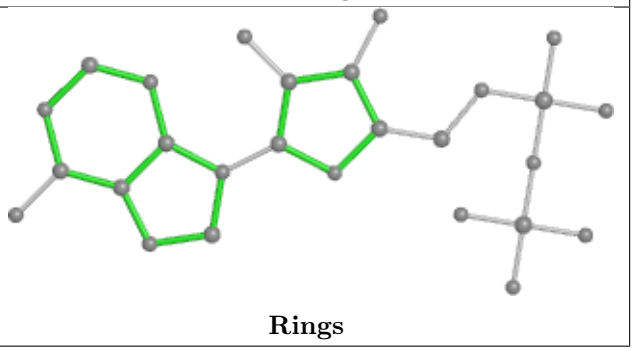
Bond lengths



Bond angles

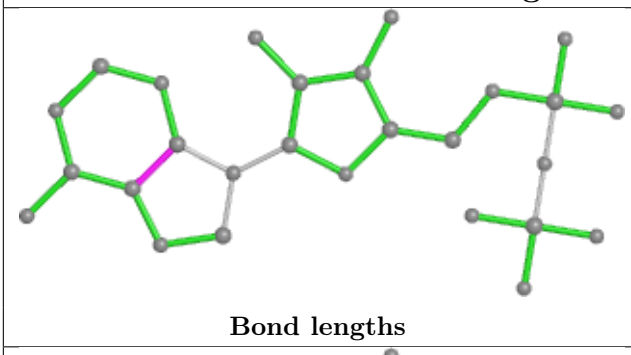


Torsions

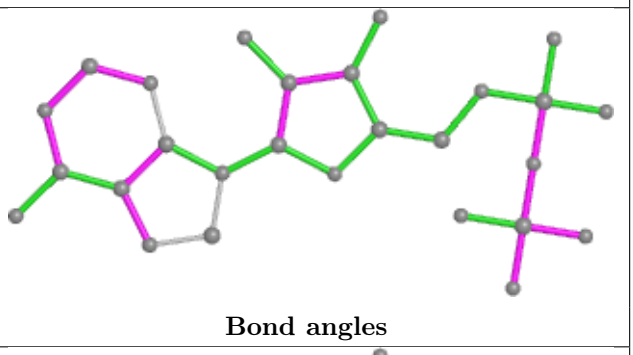


Rings

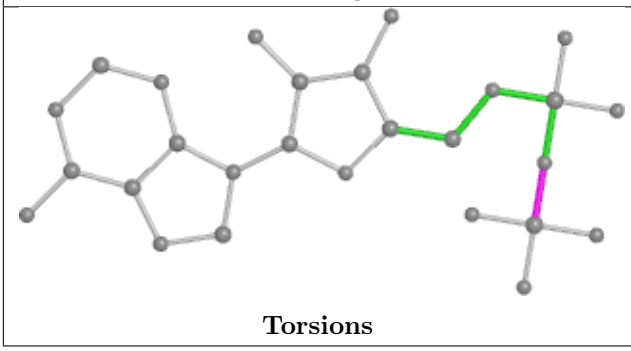
Ligand ADP P 501



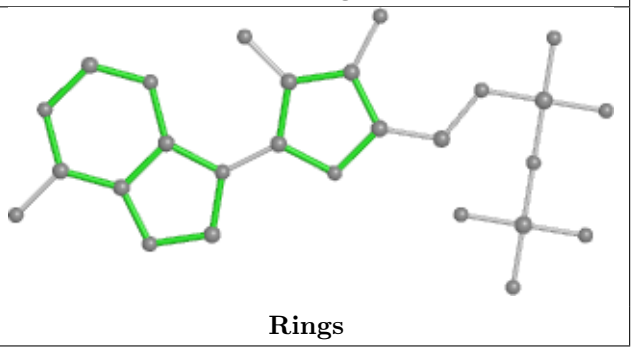
Bond lengths



Bond angles

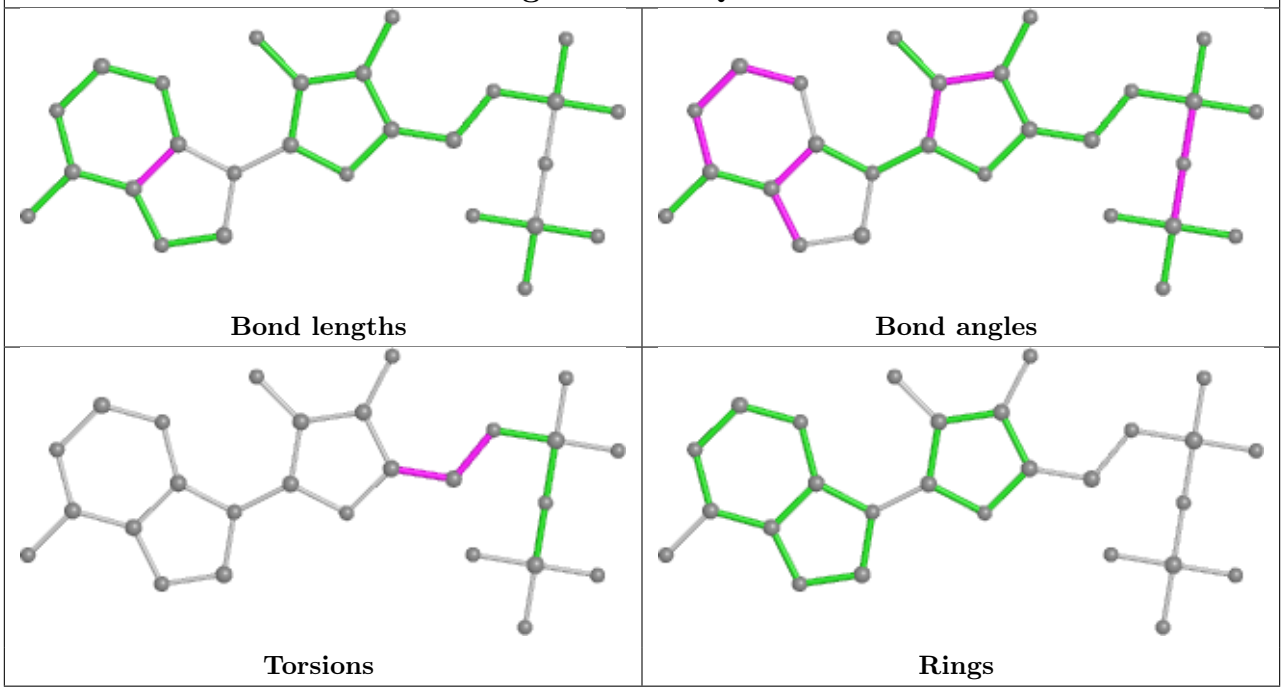


Torsions

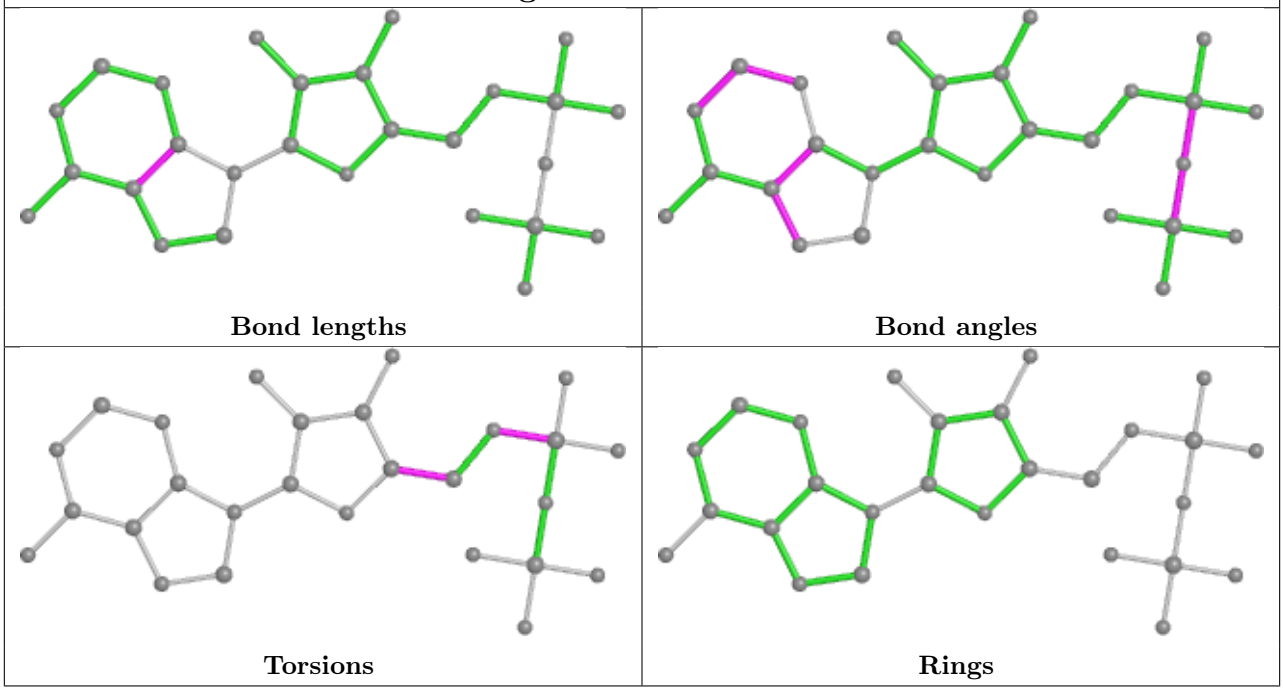


Rings

Ligand ADP Q 501



Ligand ADP M 501



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.

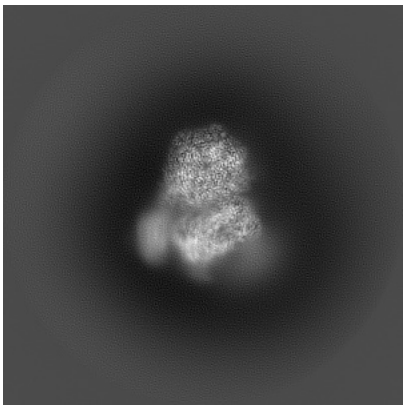
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37988. These allow visual inspection of the internal detail of the map and identification of artifacts.

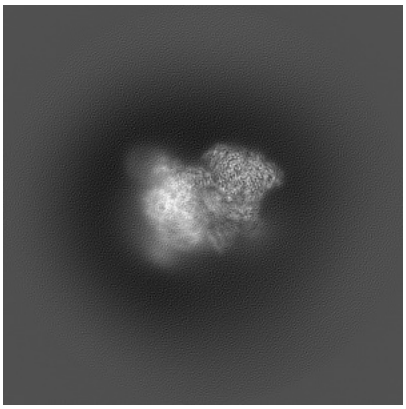
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

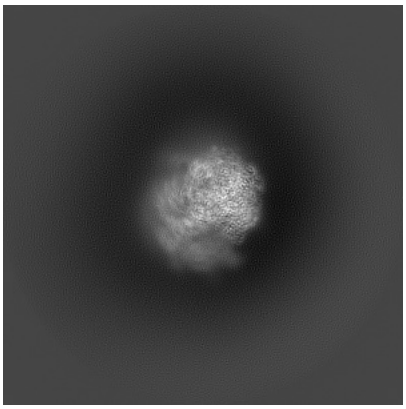
6.1.1 Primary map



X

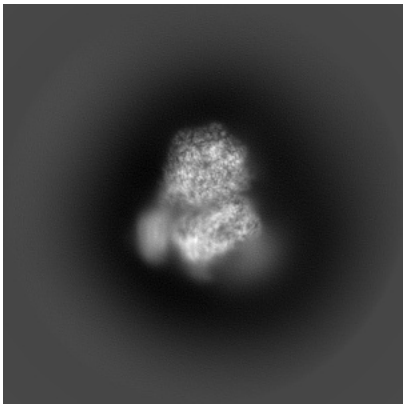


Y

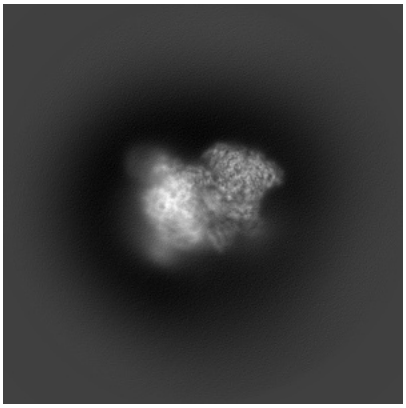


Z

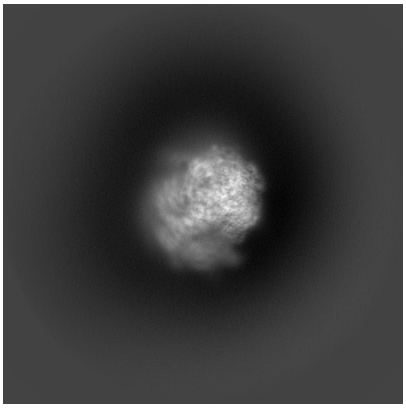
6.1.2 Raw map



X



Y

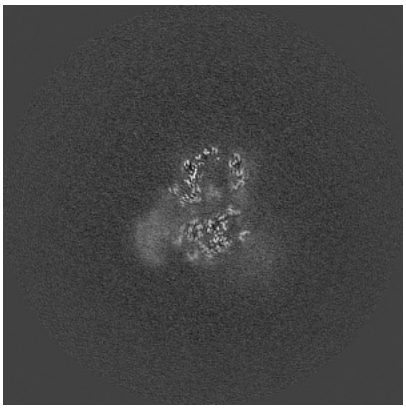


Z

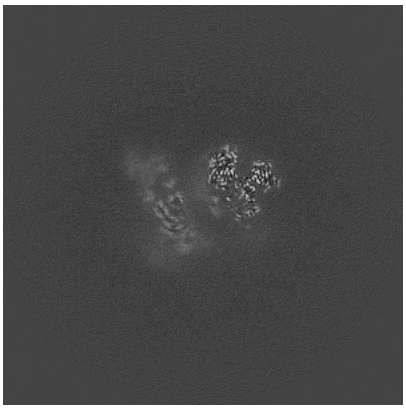
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

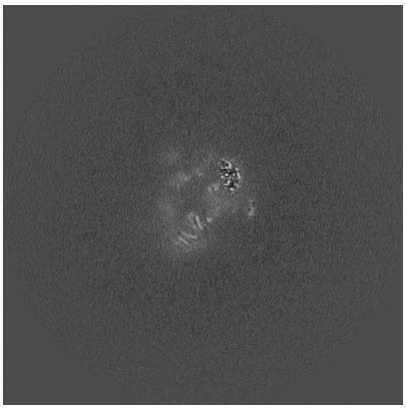
6.2.1 Primary map



X Index: 200

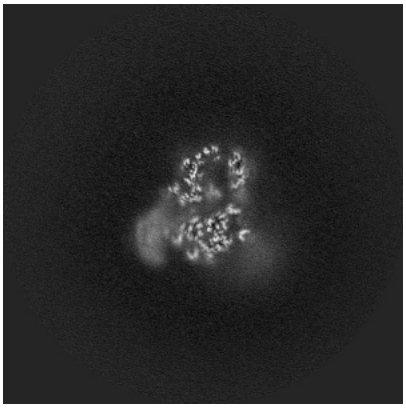


Y Index: 200

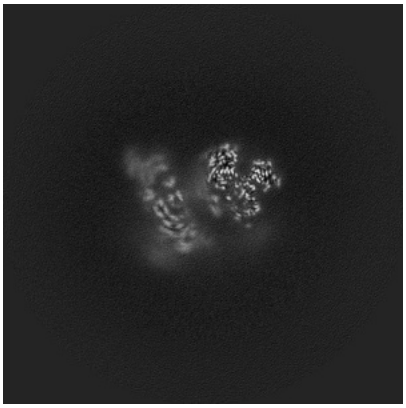


Z Index: 200

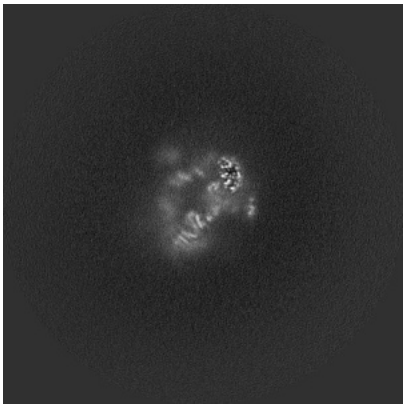
6.2.2 Raw map



X Index: 200



Y Index: 200

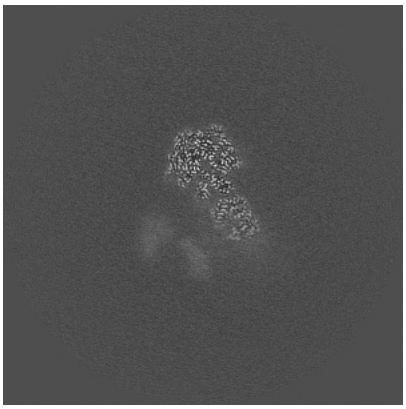


Z Index: 200

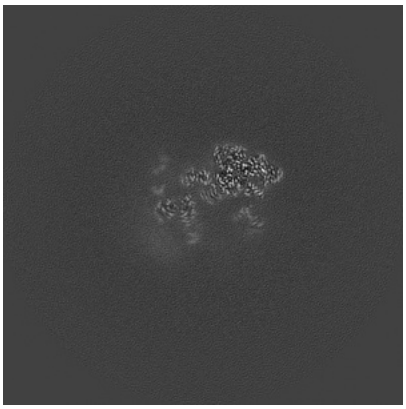
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

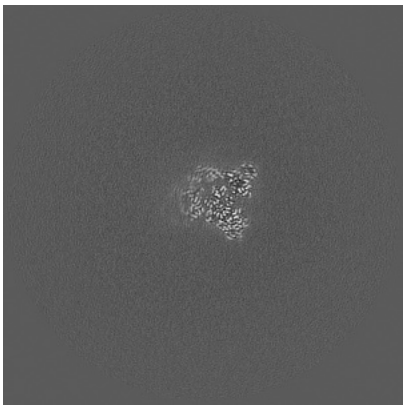
6.3.1 Primary map



X Index: 228

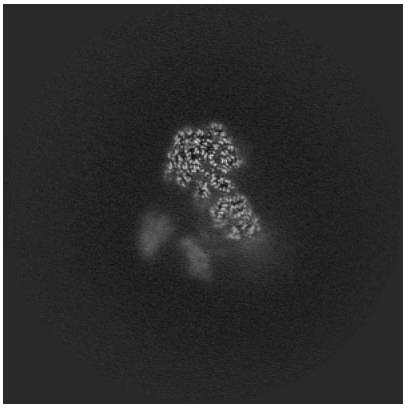


Y Index: 217

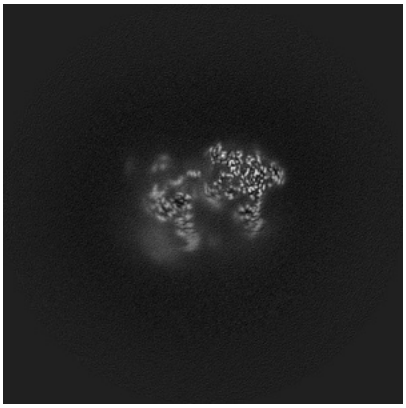


Z Index: 246

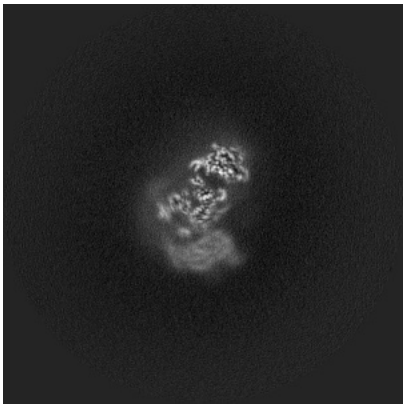
6.3.2 Raw map



X Index: 228



Y Index: 210

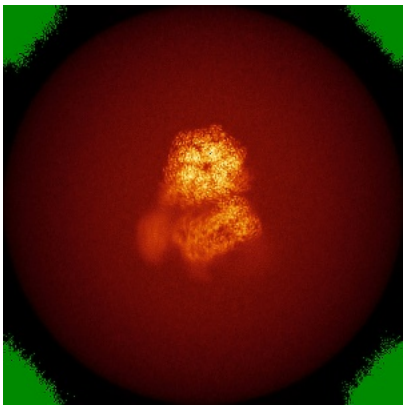


Z Index: 173

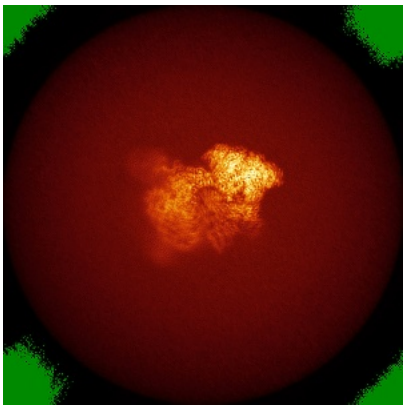
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

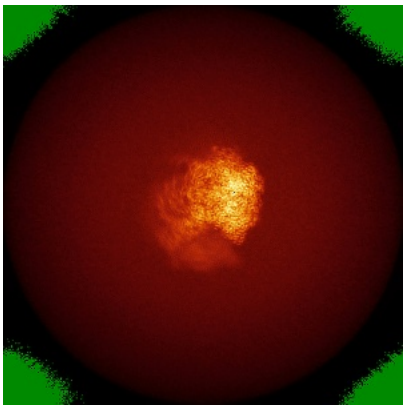
6.4.1 Primary map



X

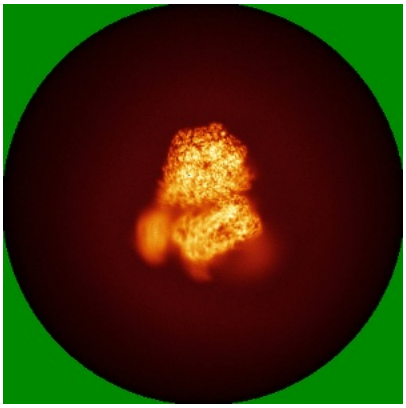


Y

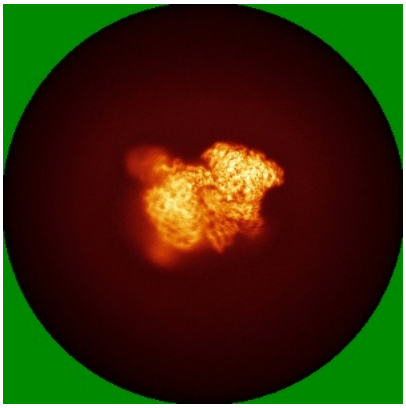


Z

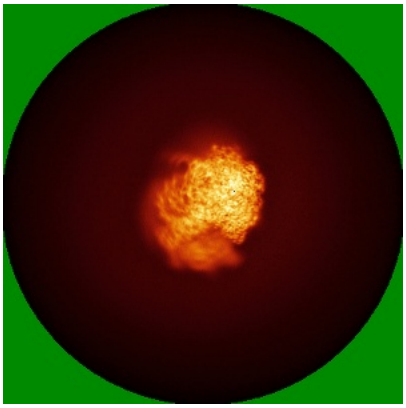
6.4.2 Raw map



X



Y

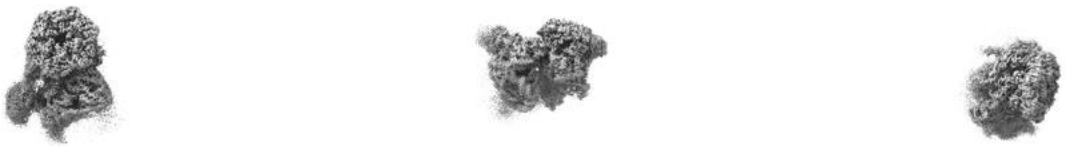


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

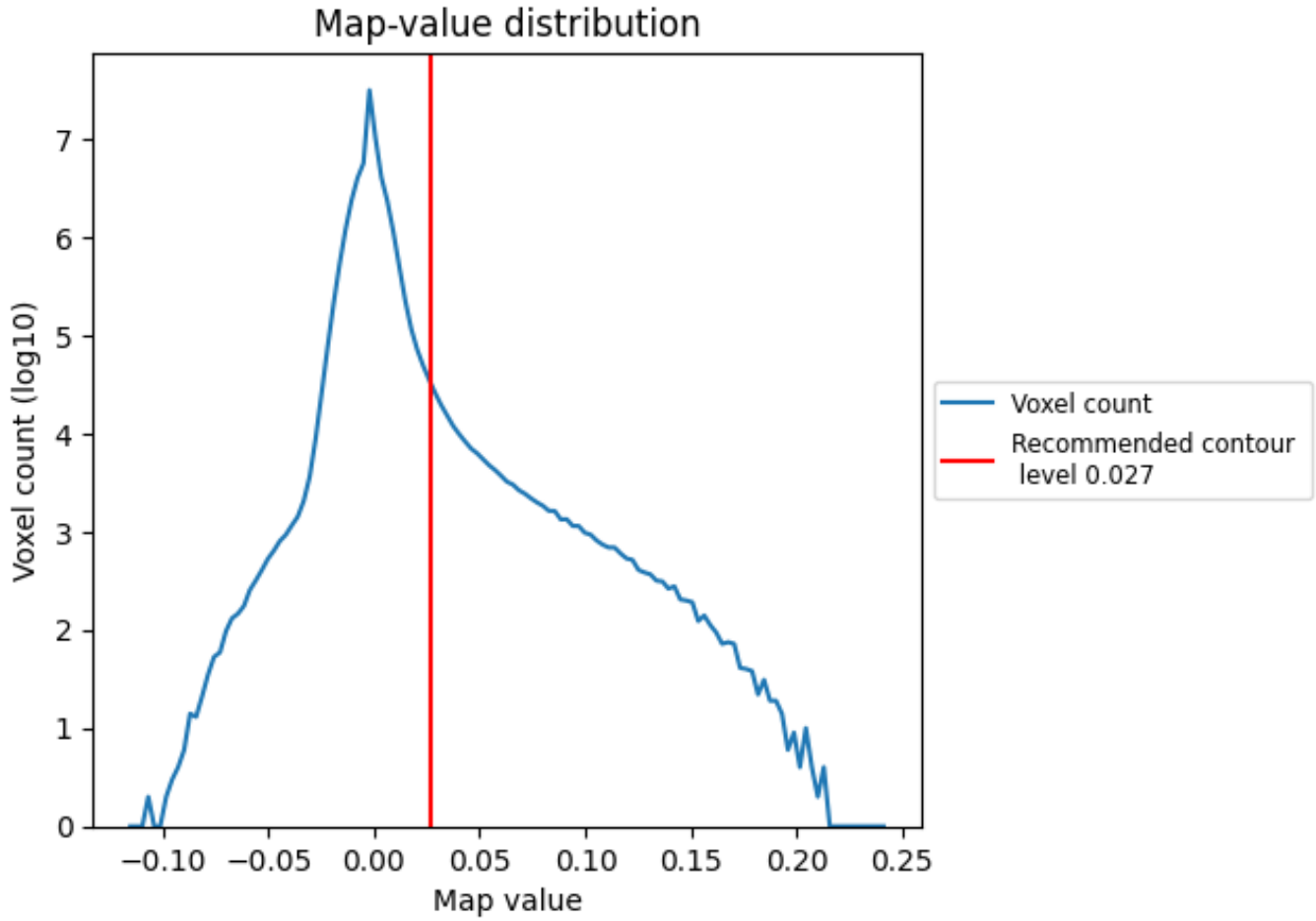
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

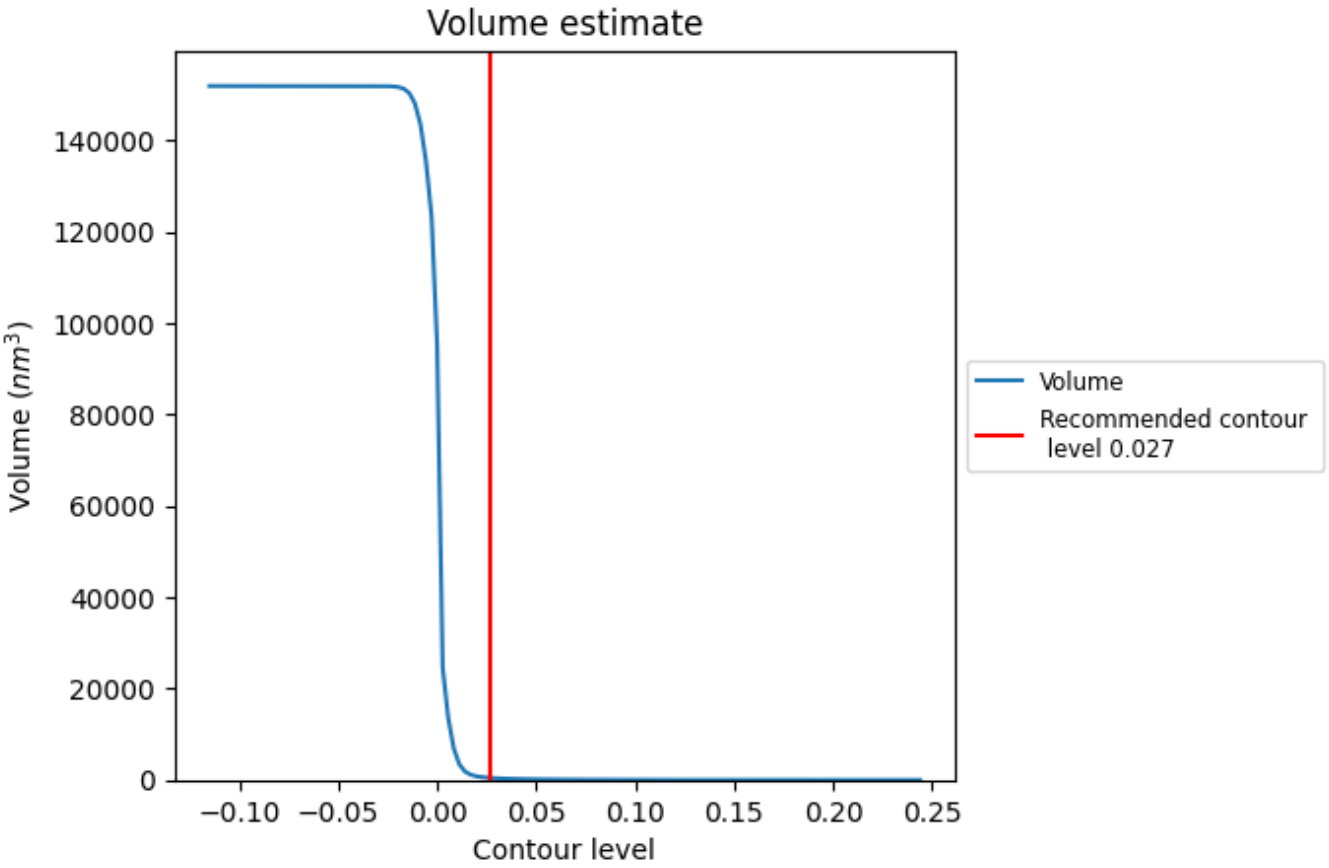
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

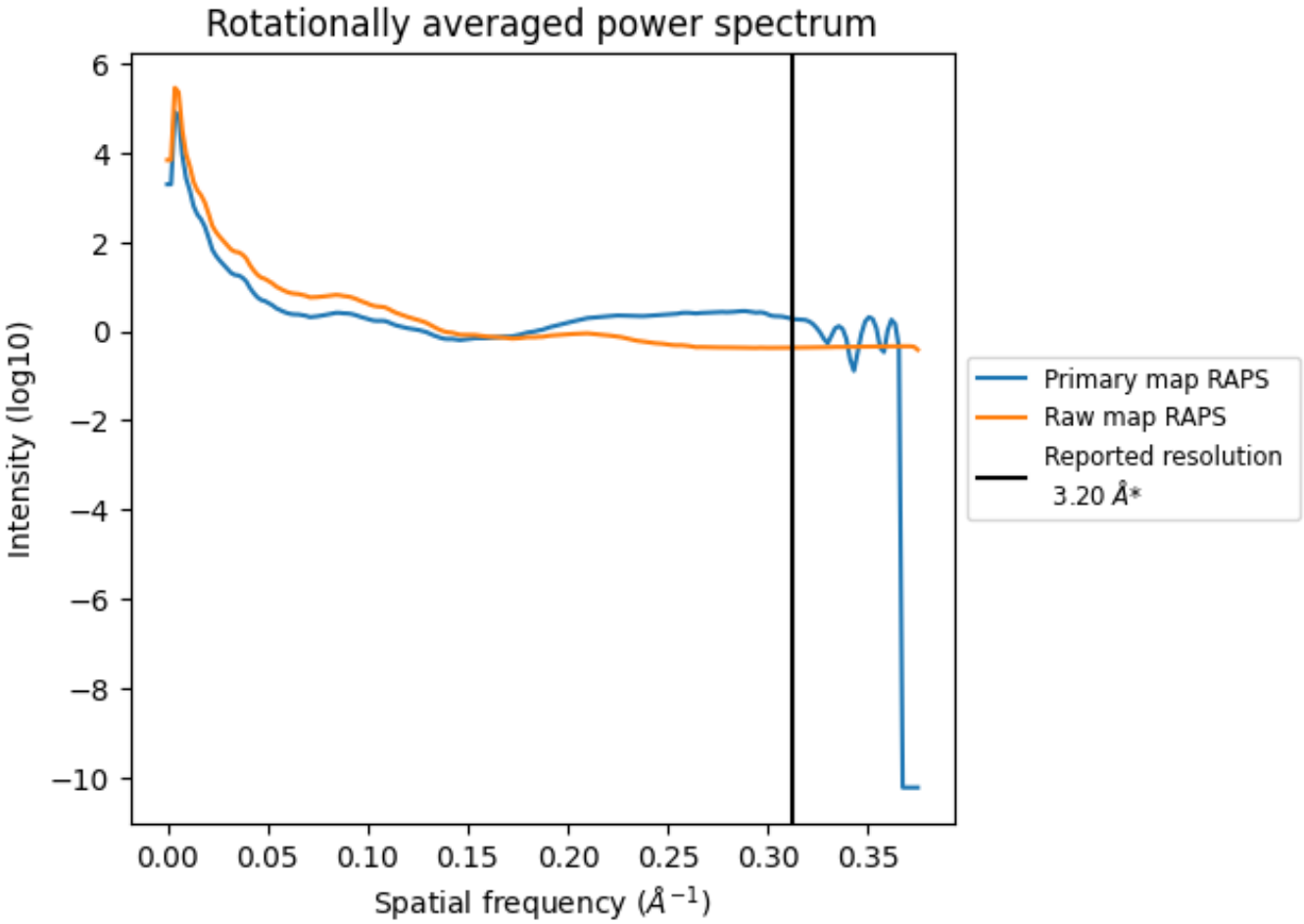
7.2 Volume estimate



The volume at the recommended contour level is 435 nm^3; this corresponds to an approximate mass of 393 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

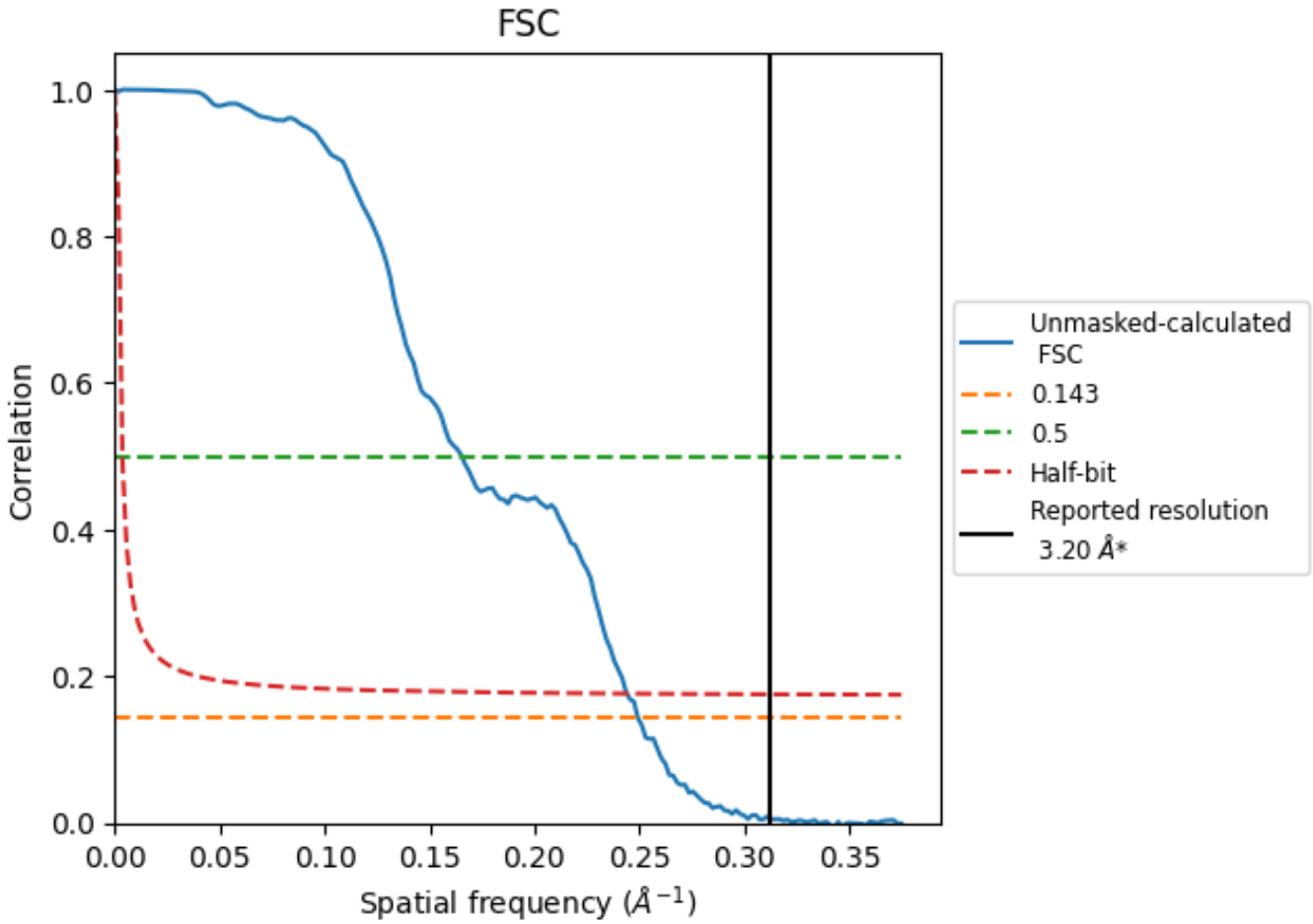


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

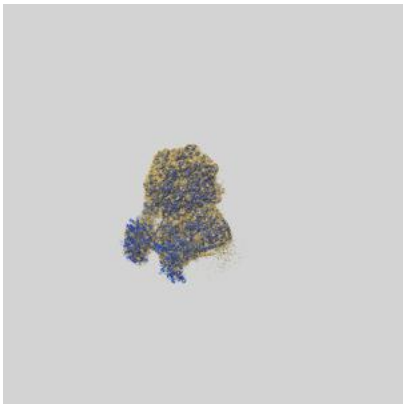
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.05	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.2 by more than 10 %

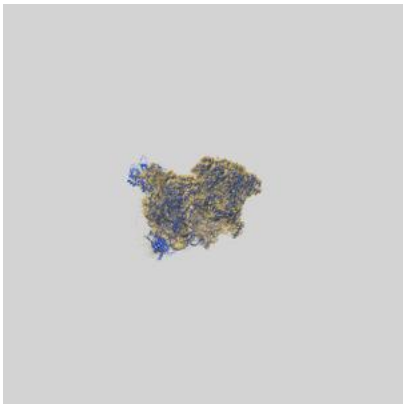
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37988 and PDB model 8X19. Per-residue inclusion information can be found in section 3 on page 9.

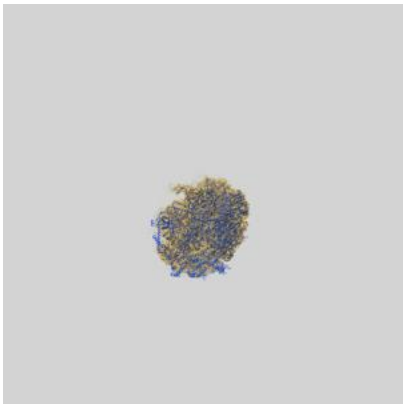
9.1 Map-model overlay



X



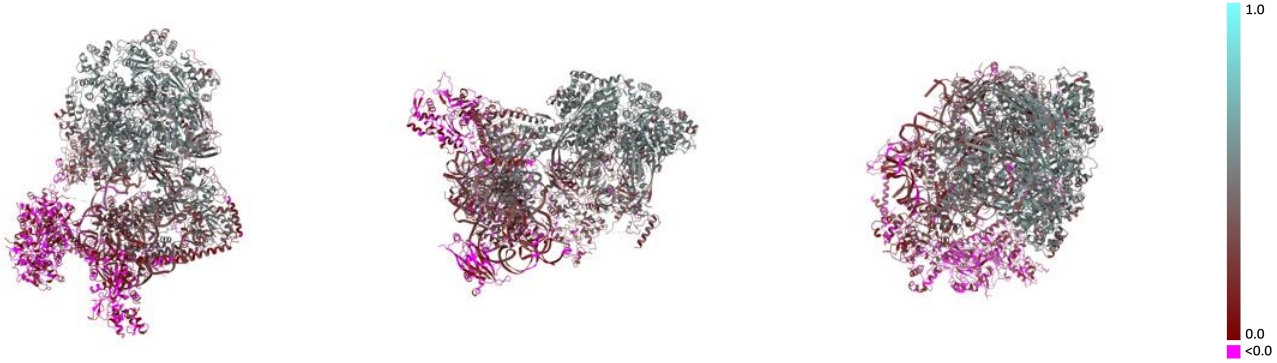
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

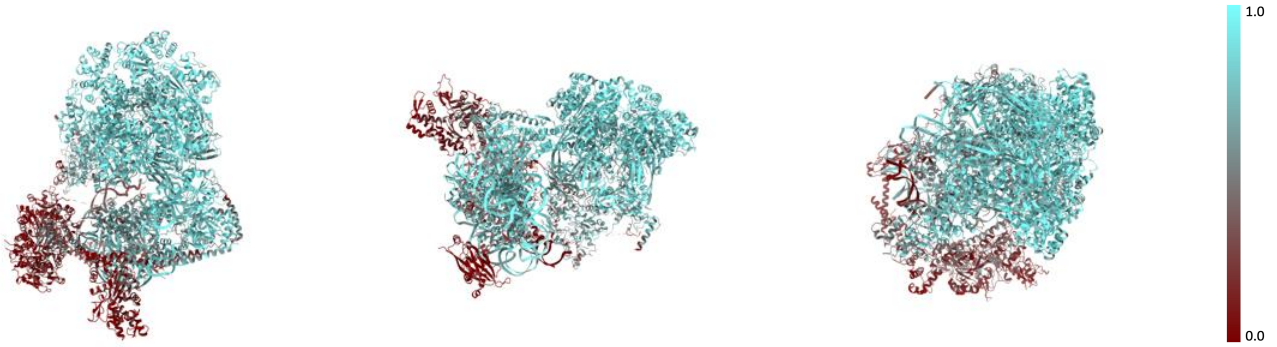
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

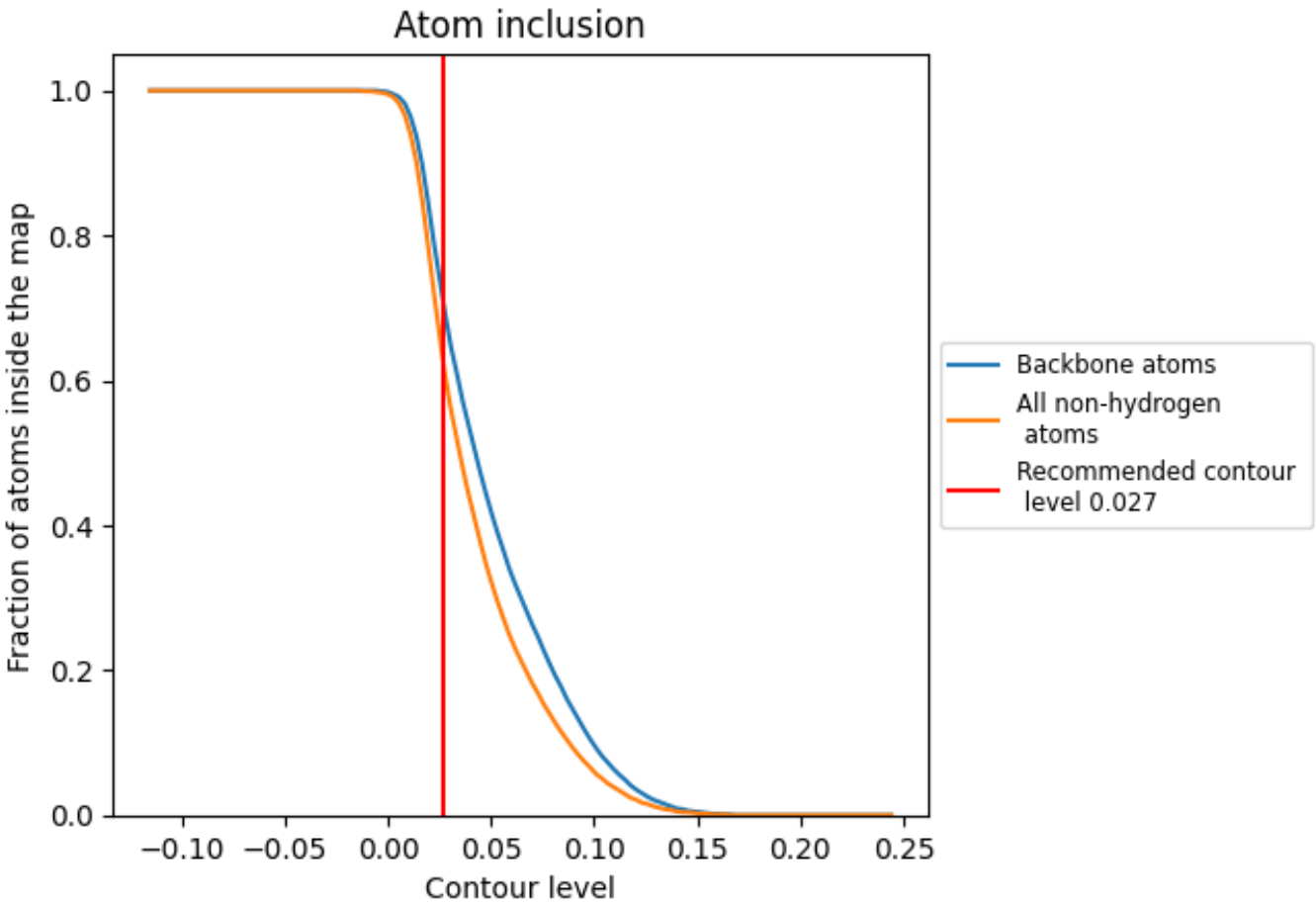
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.2920
A	0.6500	0.2420
B	0.6660	0.2500
C	0.6640	0.2180
D	0.7370	0.2590
E	0.7430	0.3420
F	0.7460	0.3170
G	0.8160	0.3950
H	0.8380	0.4060
I	0.7210	0.3600
J	0.4800	0.2110
K	0.6010	0.2190
L	0.5320	0.1960
M	0.8670	0.4860
N	0.8400	0.4560
O	0.8280	0.4490
P	0.8460	0.4690
Q	0.8370	0.4600
R	0.8400	0.4790
S	0.1210	0.0340
T	0.1710	0.0240
U	0.1460	0.0250
V	0.1000	0.0420
W	0.0160	0.0120
X	0.7320	0.2290
Y	0.7400	0.2360