Full wwPDB EM Validation Report

May 18, 2024 – 10:25 AM EDT

PDB ID	:	6W5M
EMDB ID	:	EMD-21543
Title	:	Cryo-EM structure of MLL1 in complex with RbBP5, WDR5, SET1, and ASH2L bound to the nucleosome (Class02)
Authors	:	Park, S.H.; Lee, Y.T.; Ayoub, A.; Dou, Y.; Cho, U.
Deposited on	:	2020-03-13
Resolution	:	4.60 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:

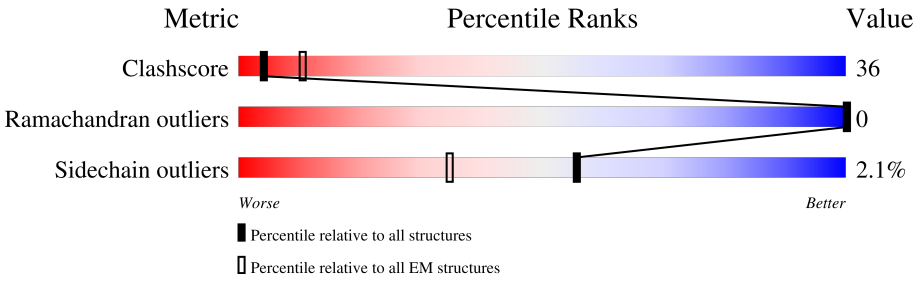
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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	538	31% 26% 30% 43%
2	B	313	55% 48% 47% 5%
3	C	209	36% 44% 27% 29%
4	D	534	11% 19% 21% 59%
5	G	136	18% 51% 28%
5	K	136	19% 49% 28%
6	H	103	25% 50% 5% 20%
6	L	103	27% 48% 5% 20%

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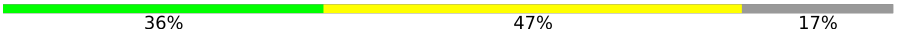
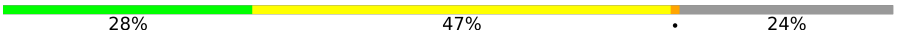
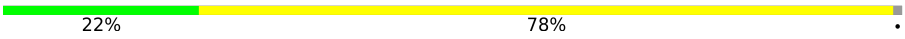
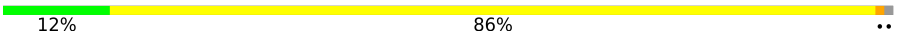
Mol	Chain	Length	Quality of chain
7	I	129	
7	M	129	
8	J	123	
8	N	123	
9	O	147	
10	P	147	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19574 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 Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2381	1505	422	439	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q15291

- Molecule 2 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	3	0
			2302	1470	382	439	11		

- Molecule 3 is a protein called Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	S	0	0
			1185	751	213	208	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3761	SER	-	expression tag	UNP Q03164
C	3861	ILE	ASN	conflict	UNP Q03164
C	3867	LEU	GLN	conflict	UNP Q03164

- Molecule 4 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	217	Total	C	N	O	S	0	0
			1742	1124	295	316	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP Q9UBL3

- Molecule 5 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
5	K	98	Total	C	N	O	S	0	0
			801	506	153	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	102	ALA	GLY	engineered mutation	UNP P84233
K	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
6	L	82	Total	C	N	O	S	0	0
			653	413	127	112	1		

- Molecule 7 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	107	Total	C	N	O	0	0
			811	510	158	143		
7	M	107	Total	C	N	O	0	0
			815	513	159	143		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	99	ARG	GLY	engineered mutation	UNP P06897
I	123	SER	ALA	engineered mutation	UNP P06897
M	99	ARG	GLY	engineered mutation	UNP P06897
M	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
8	N	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	MET	-	initiating methionine	UNP P02281
J	29	THR	SER	engineered mutation	UNP P02281
N	0	MET	-	initiating methionine	UNP P02281
N	29	THR	SER	engineered mutation	UNP P02281

- Molecule 9 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 10 is a DNA chain called DNA (147-MER).

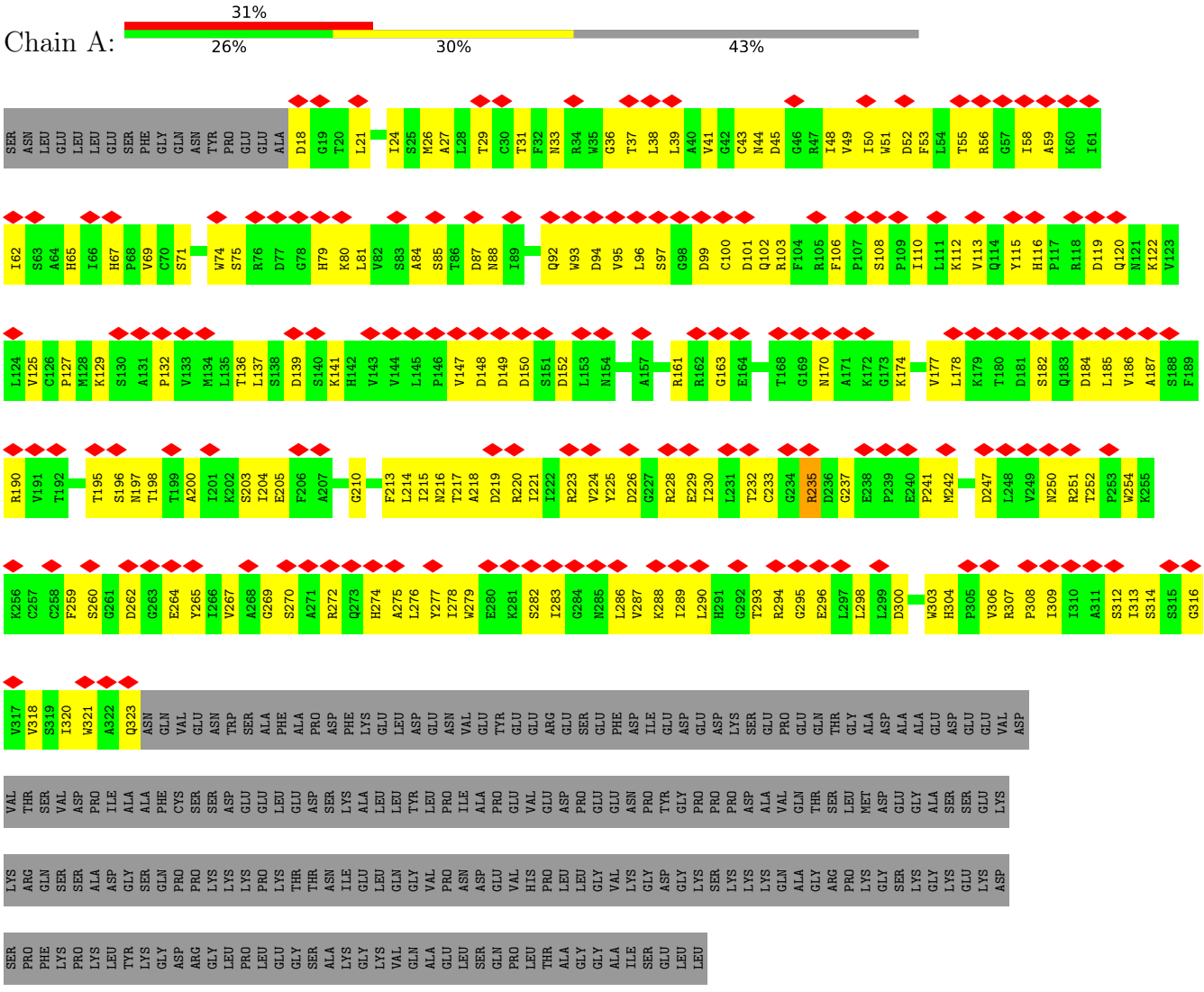
Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

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.

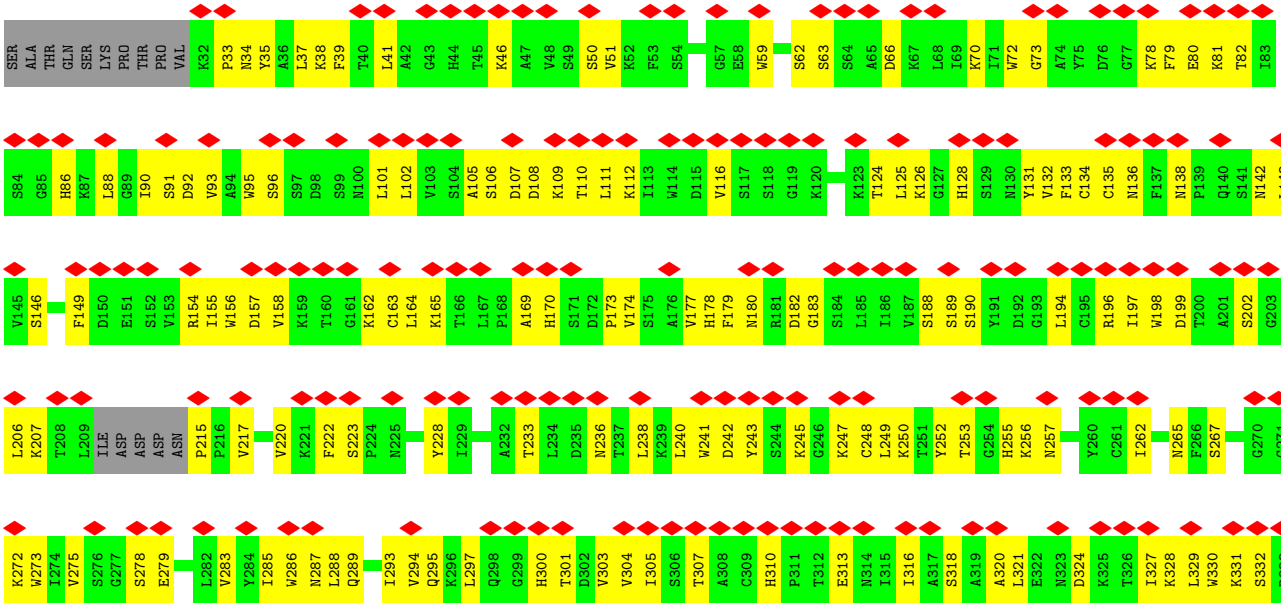
• Molecule 1: Retinoblastoma-binding protein 5

Chain A:



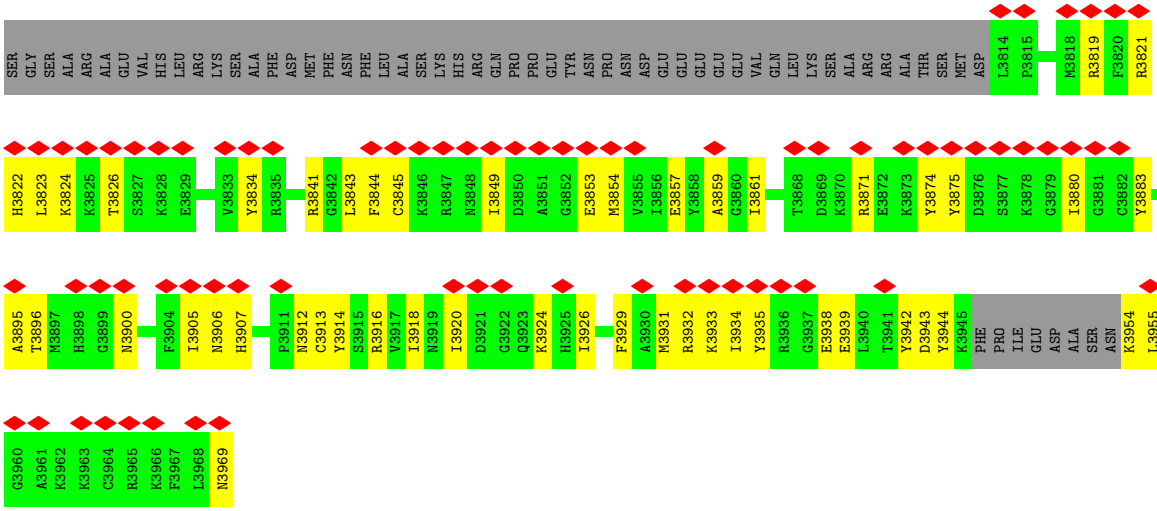
• Molecule 2: WD repeat-containing protein 5

Chain B:



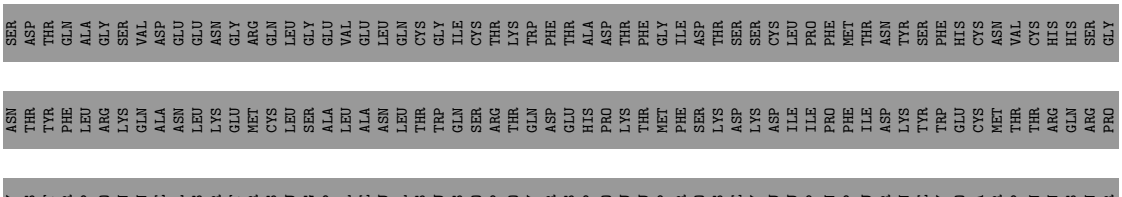
• Molecule 3: Histone-lysine N-methyltransferase 2A

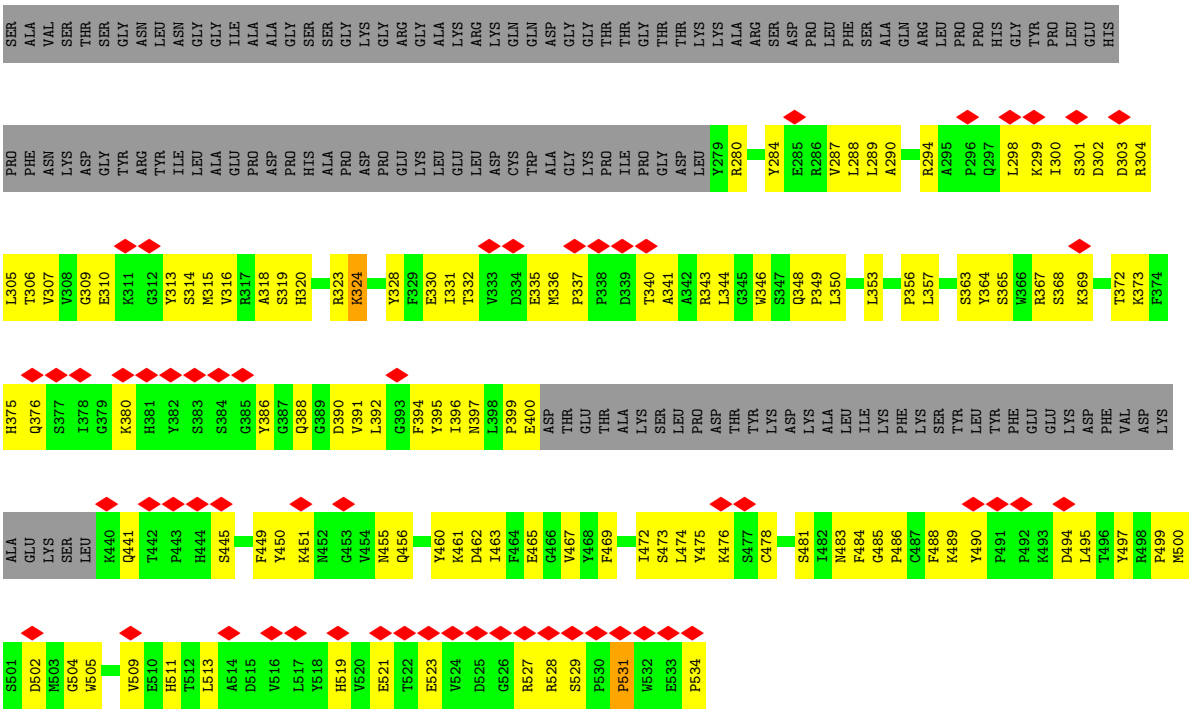
Chain C:



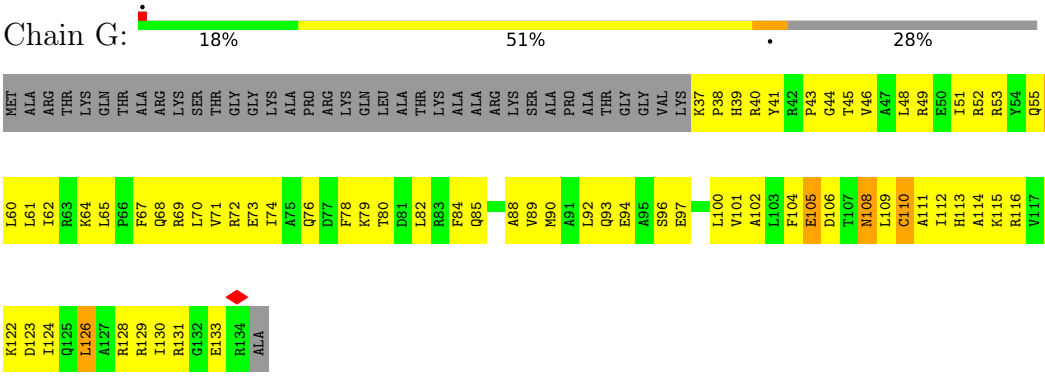
• Molecule 4: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain D:

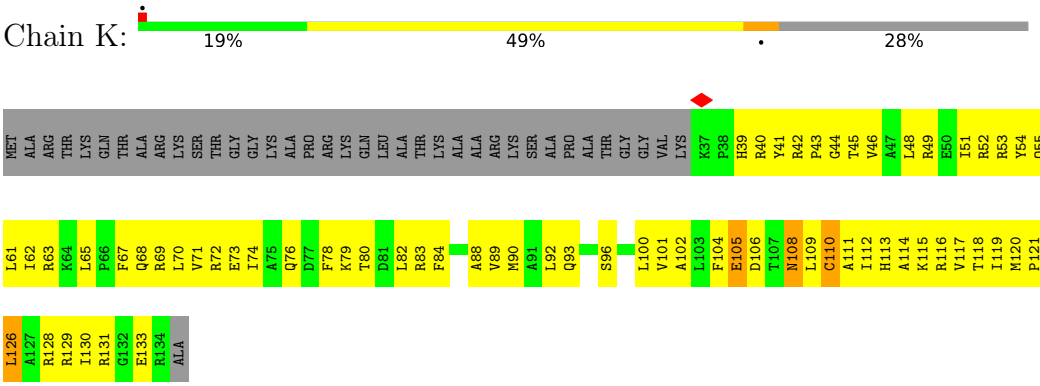




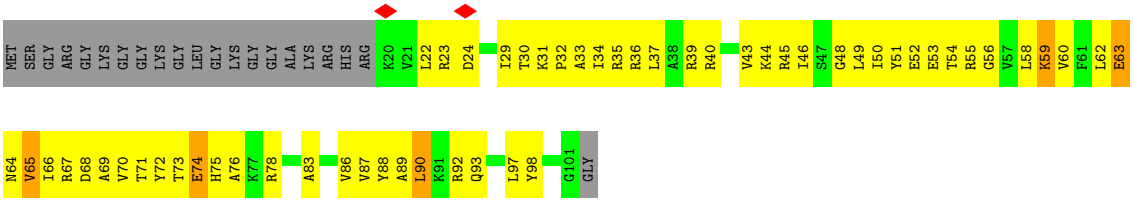
• Molecule 5: Histone H3.2

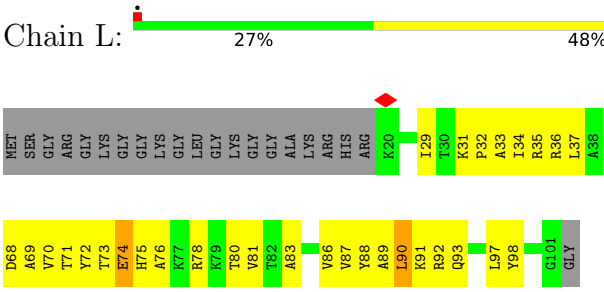


• Molecule 5: Histone H3.2



• Molecule 6: Histone H4



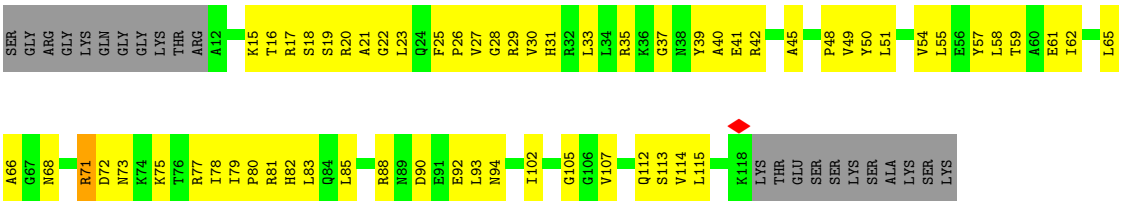


• Molecule 6: Histone H4

Chain L:

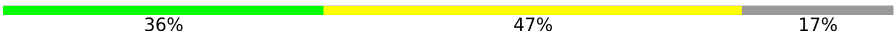
• Molecule 7: Histone H2A type 1

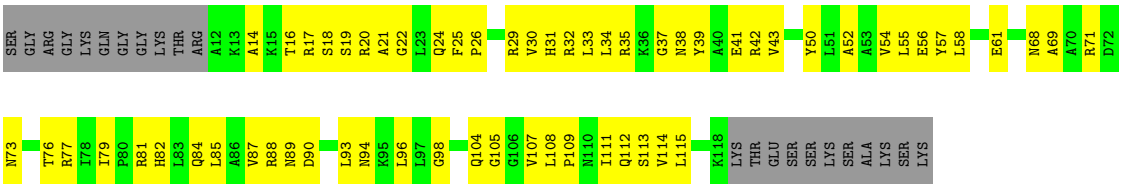
Chain I:



• Molecule 7: Histone H2A type 1

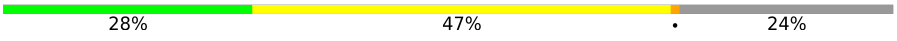
Chain M:

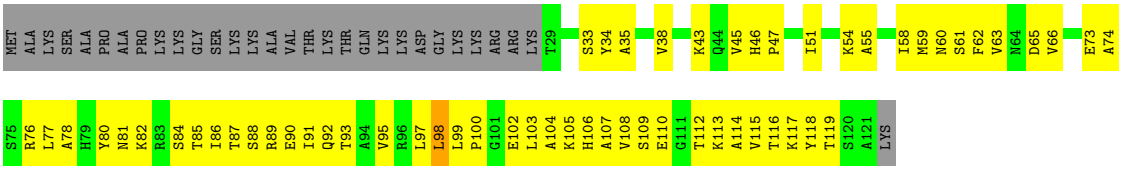




• Molecule 8: Histone H2B 1.1

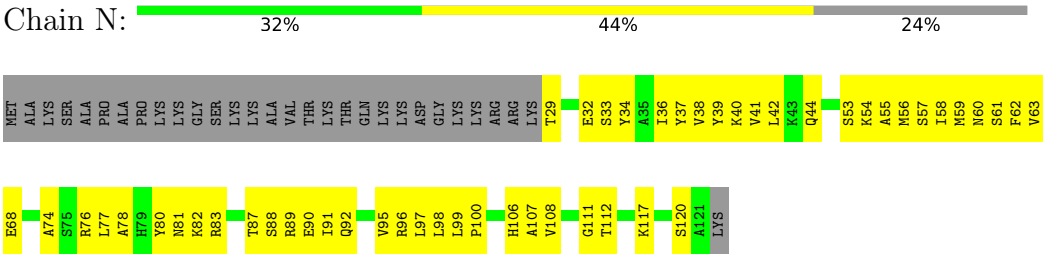
Chain J:





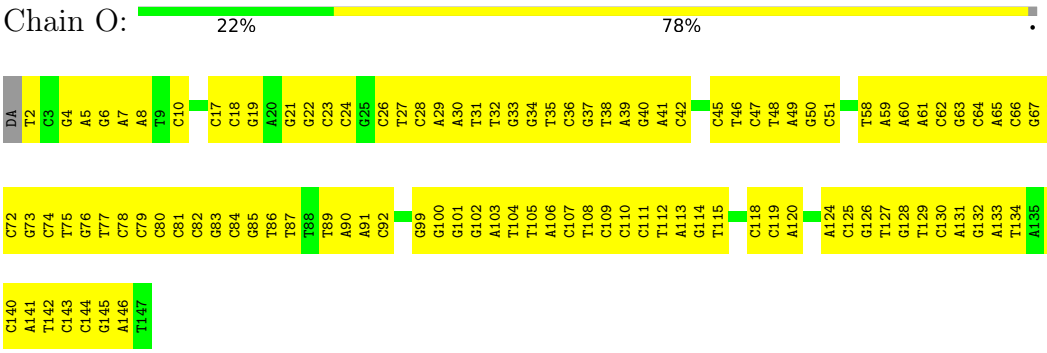
• Molecule 8: Histone H2B 1.1

Chain N:



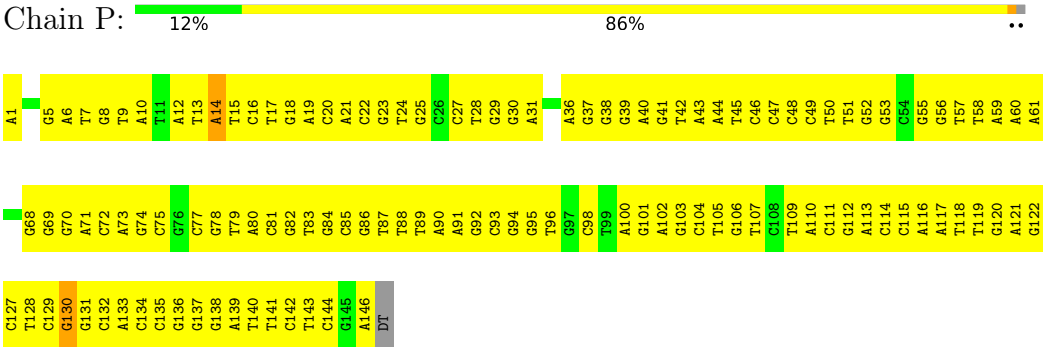
• Molecule 9: DNA (147-MER)

Chain O:



• Molecule 10: DNA (147-MER)

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27730	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0073	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/2431	0.48	0/3301
2	B	0.28	0/2372	0.47	0/3216
3	C	0.28	0/1208	0.42	0/1616
4	D	0.30	0/1797	0.49	0/2438
5	G	0.31	0/813	0.43	0/1093
5	K	0.31	0/813	0.43	0/1093
6	H	0.33	0/660	0.50	0/885
6	L	0.33	0/660	0.50	0/885
7	I	0.30	0/821	0.46	0/1112
7	M	0.29	0/825	0.45	0/1116
8	J	0.32	0/729	0.47	1/985 (0.1%)
8	N	0.31	0/737	0.45	0/993
9	O	0.75	0/3333	0.95	0/5137
10	P	0.77	0/3381	0.93	2/5221 (0.0%)
All	All	0.50	0/20580	0.67	3/29091 (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
4	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	98	LEU	C-N-CA	-5.41	108.18	121.70
10	P	14	DA	O4'-C4'-C3'	-5.23	102.41	104.50
10	P	130	DG	O4'-C4'-C3'	-5.15	102.44	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	531	PRO	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	2381	0	2394	126	0
2	B	2302	0	2269	118	0
3	C	1185	0	1190	53	0
4	D	1742	0	1685	93	0
5	G	801	0	831	140	0
5	K	801	0	831	134	0
6	H	653	0	695	92	0
6	L	653	0	695	111	0
7	I	811	0	849	79	0
7	M	815	0	860	90	0
8	J	718	0	725	94	0
8	N	726	0	747	94	0
9	O	2975	0	1639	205	0
10	P	3011	0	1639	228	0
All	All	19574	0	17049	1282	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 36.

All (1282) 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)
5:G:115:LYS:NZ	5:K:122:LYS:HE2	1.32	1.41
5:G:122:LYS:HE2	5:K:115:LYS:NZ	1.33	1.38
5:G:113:HIS:CE1	5:K:122:LYS:HG3	1.62	1.34
2:B:247:LYS:HB3	3:C:3834:TYR:CE1	1.64	1.31
5:G:122:LYS:HG3	5:K:113:HIS:CE1	1.70	1.26
5:G:122:LYS:CE	5:K:115:LYS:HZ3	1.50	1.24
5:G:115:LYS:NZ	5:K:122:LYS:CE	2.08	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:122:LYS:CE	5:K:115:LYS:NZ	2.06	1.16
7:I:77:ARG:NH2	9:O:132:DG:H5'	1.61	1.16
7:I:112:GLN:HG3	5:K:112:ILE:HD11	1.31	1.13
9:O:79:DC:N4	10:P:68:DG:O6	1.84	1.11
6:L:91:LYS:HE2	8:N:76:ARG:HH12	1.05	1.07
2:B:247:LYS:CB	3:C:3834:TYR:HE1	1.68	1.07
5:G:122:LYS:HG3	5:K:113:HIS:HE1	1.04	1.07
5:G:43:PRO:HG2	10:P:69:DG:H5"	1.37	1.04
5:G:113:HIS:CE1	5:K:122:LYS:CG	2.41	1.03
5:G:115:LYS:HZ1	5:K:122:LYS:CE	1.69	1.00
6:L:91:LYS:CE	8:N:76:ARG:HH12	1.73	0.99
5:G:122:LYS:CG	5:K:113:HIS:CE1	2.46	0.99
8:J:65:ASP:OD2	6:L:98:TYR:HE1	1.43	0.98
5:G:115:LYS:HZ3	5:K:122:LYS:HE2	1.29	0.98
7:I:77:ARG:HH22	9:O:132:DG:H5'	1.25	0.98
6:L:74:GLU:O	8:N:89:ARG:NH2	1.96	0.97
9:O:28:DC:N4	10:P:119:DT:C4	2.34	0.96
2:B:247:LYS:CB	3:C:3834:TYR:CE1	2.45	0.95
5:G:113:HIS:HE1	5:K:122:LYS:HG3	0.94	0.95
8:J:65:ASP:OD2	6:L:98:TYR:CE1	2.18	0.95
8:N:29:THR:OG1	9:O:104:DT:OP1	1.83	0.95
7:M:29:ARG:NH1	8:N:33:SER:O	2.00	0.95
6:L:91:LYS:HD3	8:N:76:ARG:HH22	1.34	0.93
9:O:76:DG:O6	10:P:71:DA:N6	2.01	0.93
6:H:44:LYS:HD2	7:M:115:LEU:HG	1.50	0.92
6:L:91:LYS:HE2	8:N:76:ARG:NH1	1.85	0.91
9:O:2:DT:H71	10:P:146:DA:C4	2.06	0.90
7:I:112:GLN:HG3	5:K:112:ILE:CD1	2.01	0.90
5:G:106:ASP:HB2	5:K:130:ILE:CD1	2.02	0.90
5:G:115:LYS:HZ3	5:K:122:LYS:CE	1.78	0.90
5:G:123:ASP:N	5:K:113:HIS:CE1	2.39	0.90
5:G:112:ILE:HD11	7:M:112:GLN:HG3	1.54	0.90
8:J:62:PHE:HA	6:L:98:TYR:CZ	2.07	0.89
4:D:313:TYR:HA	4:D:474:LEU:O	1.71	0.89
9:O:67:DG:N1	10:P:80:DA:N1	2.21	0.89
2:B:247:LYS:HB3	3:C:3834:TYR:CD1	2.07	0.89
9:O:78:DC:N4	10:P:69:DG:O6	2.06	0.88
5:G:122:LYS:NZ	5:K:115:LYS:HZ3	1.70	0.88
7:I:77:ARG:NH2	9:O:131:DA:O4'	2.07	0.87
5:G:122:LYS:HE2	5:K:115:LYS:HZ1	1.38	0.87
6:H:71:THR:O	6:H:74:GLU:HB3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:71:THR:O	6:L:74:GLU:HB3	1.75	0.85
5:K:61:LEU:HD12	6:L:36:ARG:HD2	1.58	0.85
7:M:24:GLN:CD	8:N:44:GLN:HE22	1.79	0.85
5:G:130:ILE:HD12	5:K:106:ASP:HB2	1.59	0.84
5:G:122:LYS:HE2	5:K:115:LYS:CE	2.06	0.84
7:M:54:VAL:HG13	8:N:107:ALA:HB1	1.59	0.84
9:O:2:DT:C6	10:P:146:DA:C2	2.66	0.84
9:O:83:DG:N1	10:P:65:DC:N3	2.26	0.83
9:O:101:DG:O6	10:P:46:DC:N4	2.11	0.83
7:M:77:ARG:HG3	10:P:132:DC:H5"	1.60	0.82
5:G:130:ILE:CD1	5:K:106:ASP:HB2	2.09	0.82
5:G:122:LYS:HE2	5:K:115:LYS:HZ3	0.99	0.82
5:G:115:LYS:HZ1	5:K:122:LYS:HE2	1.01	0.82
2:B:111:LEU:HB2	2:B:125:LEU:HB2	1.60	0.81
9:O:67:DG:O6	10:P:80:DA:N6	2.12	0.81
7:I:50:TYR:CZ	8:J:92:GLN:HG2	2.15	0.81
6:H:74:GLU:O	8:J:89:ARG:NH2	2.15	0.80
7:M:77:ARG:N	10:P:132:DC:OP1	2.14	0.80
5:G:46:VAL:HB	9:O:83:DG:P	2.22	0.80
2:B:178:HIS:HD2	2:B:222:PHE:H	1.27	0.80
6:L:70:VAL:O	6:L:74:GLU:N	2.15	0.79
9:O:83:DG:N2	10:P:65:DC:O2	2.16	0.79
8:J:61:SER:OG	6:L:98:TYR:HB3	1.83	0.79
5:G:106:ASP:HB2	5:K:130:ILE:HD12	1.63	0.79
6:H:70:VAL:O	6:H:74:GLU:N	2.15	0.78
9:O:90:DA:H1'	9:O:91:DA:N7	1.98	0.78
4:D:451:LYS:HB2	4:D:456:GLN:HE21	1.47	0.78
5:G:61:LEU:HD12	6:H:36:ARG:HD2	1.66	0.78
2:B:38:LYS:HE3	2:B:331:LYS:HB3	1.65	0.78
5:G:115:LYS:CE	5:K:122:LYS:HE2	2.14	0.78
9:O:76:DG:N1	10:P:71:DA:N1	2.31	0.78
1:A:300:ASP:HB3	1:A:313:ILE:HB	1.66	0.77
5:G:115:LYS:HZ3	5:K:122:LYS:NZ	1.82	0.77
2:B:283:VAL:HB	2:B:297:LEU:HB2	1.66	0.77
1:A:224:VAL:O	1:A:242:MET:N	2.18	0.77
6:H:88:TYR:CE1	8:J:80:TYR:CE1	2.72	0.76
1:A:100:CYS:SG	1:A:103:ARG:NH2	2.58	0.76
7:I:21:ALA:HA	8:J:117:LYS:HG2	1.68	0.76
9:O:77:DT:O4	10:P:70:DG:C6	2.39	0.76
5:G:55:GLN:HG2	7:M:107:VAL:HG13	1.65	0.76
5:G:90:MET:SD	5:G:93:GLN:NE2	2.59	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3906:ASN:ND2	3:C:3939:GLU:OE2	2.17	0.76
6:L:78:ARG:HD2	10:P:102:DA:H5"	1.67	0.76
6:L:91:LYS:CD	8:N:76:ARG:HH22	1.97	0.76
5:G:79:LYS:HB3	5:G:82:LEU:HD11	1.67	0.76
6:L:31:LYS:HA	6:L:34:ILE:HD12	1.68	0.76
5:G:113:HIS:CE1	5:K:123:ASP:N	2.53	0.76
5:K:79:LYS:HB3	5:K:82:LEU:HD11	1.67	0.75
4:D:484:PHE:HD2	4:D:486:PRO:HD2	1.52	0.75
6:H:88:TYR:CD1	8:J:80:TYR:CZ	2.73	0.75
7:I:73:ASN:O	7:I:75:LYS:NZ	2.17	0.75
5:K:90:MET:SD	5:K:93:GLN:NE2	2.59	0.75
10:P:86:DG:H3'	10:P:87:DT:H71	1.69	0.75
2:B:50[B]:SER:HG	2:B:63:SER:HG	1.32	0.75
5:G:65:LEU:HG	9:O:92:DC:OP2	1.86	0.75
5:G:55:GLN:CD	7:M:109:PRO:HA	2.07	0.74
8:N:55:ALA:HA	8:N:58:ILE:HD12	1.69	0.74
5:G:56:LYS:NZ	9:O:10:DC:OP1	2.20	0.74
6:H:23:ARG:O	6:H:24:ASP:CG	2.25	0.74
7:M:20:ARG:O	8:N:117:LYS:NZ	2.19	0.74
7:M:69:ALA:O	7:M:73:ASN:ND2	2.21	0.74
9:O:2:DT:C6	10:P:146:DA:N1	2.56	0.74
5:G:123:ASP:N	5:K:113:HIS:HE1	1.86	0.73
1:A:252:THR:HG21	1:A:270:SER:HB2	1.70	0.73
2:B:41:LEU:N	2:B:327:ILE:O	2.18	0.73
2:B:247:LYS:HB3	3:C:3834:TYR:HE1	1.02	0.73
3:C:3955:LEU:H	3:C:3969:ASN:HD21	1.35	0.73
9:O:76:DG:C6	10:P:71:DA:N6	2.55	0.73
6:H:31:LYS:HA	6:H:34:ILE:HD12	1.68	0.73
8:J:62:PHE:HB2	6:L:98:TYR:CE2	2.24	0.73
5:G:113:HIS:ND1	5:K:122:LYS:HD2	2.04	0.73
8:J:65:ASP:CG	6:L:98:TYR:HE1	1.90	0.73
1:A:278:ILE:O	1:A:287:VAL:N	2.22	0.72
10:P:112:DG:H2"	10:P:113:DA:C8	2.25	0.72
7:M:42:ARG:NH2	10:P:112:DG:O4'	2.21	0.72
4:D:441:GLN:HG3	4:D:463:ILE:H	1.54	0.72
5:G:115:LYS:NZ	5:K:122:LYS:NZ	2.37	0.72
7:I:57:TYR:CZ	8:J:106:HIS:HB3	2.23	0.72
9:O:69:DA:C2	10:P:78:DG:C2	2.77	0.72
2:B:136:ASN:ND2	2:B:177:VAL:O	2.23	0.72
2:B:285:ILE:HD12	2:B:295:GLN:HB3	1.70	0.72
7:I:30:VAL:HA	7:I:33:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:122:LYS:CE	5:K:115:LYS:HZ1	1.94	0.72
6:H:98:TYR:HB3	8:N:61:SER:OG	1.88	0.72
10:P:89:DT:H2"	10:P:90:DA:C8	2.24	0.72
7:I:88:ARG:NH1	7:I:94:ASN:OD1	2.23	0.71
6:H:75:HIS:CE1	8:J:89:ARG:HG2	2.25	0.71
1:A:278:ILE:HD13	1:A:288:LYS:HG3	1.71	0.71
9:O:67:DG:C6	10:P:80:DA:N1	2.58	0.71
5:G:118:THR:HG23	10:P:71:DA:OP1	1.90	0.71
9:O:17:DC:C4	10:P:130:DG:C6	2.78	0.71
1:A:161:ARG:NE	1:A:210:GLY:O	2.23	0.71
7:M:31:HIS:CD2	7:M:35:ARG:HH11	2.08	0.71
5:G:43:PRO:CG	10:P:69:DG:H5"	2.17	0.70
5:K:44:GLY:O	5:K:48:LEU:N	2.22	0.70
3:C:3887:ILE:HD12	3:C:3891:GLU:HB3	1.73	0.70
9:O:2:DT:H6	10:P:146:DA:C2	2.08	0.70
5:G:128:ARG:HB3	5:G:133:GLU:HB2	1.74	0.70
6:H:75:HIS:O	8:J:89:ARG:NH1	2.18	0.70
5:G:57:SER:OG	6:H:40:ARG:NH2	2.24	0.70
6:H:88:TYR:CZ	8:J:80:TYR:CD1	2.78	0.70
7:I:92:GLU:O	8:J:100:PRO:HG2	1.91	0.70
9:O:118:DC:N4	10:P:29:DG:O6	2.24	0.70
4:D:309:GLY:HA3	4:D:474:LEU:HD13	1.74	0.70
5:G:44:GLY:O	5:G:48:LEU:N	2.21	0.70
9:O:67:DG:O6	10:P:80:DA:C6	2.44	0.70
5:K:128:ARG:HB3	5:K:133:GLU:HB2	1.74	0.69
6:H:52:GLU:OE1	6:H:52:GLU:N	2.25	0.69
9:O:79:DC:C4	10:P:68:DG:O6	2.45	0.69
1:A:288:LYS:NZ	1:A:323:GLN:OE1	2.22	0.69
5:K:116:ARG:NH1	5:K:118:THR:O	2.26	0.69
2:B:272:LYS:HB3	2:B:288:LEU:HD13	1.74	0.69
6:L:52:GLU:N	6:L:52:GLU:OE1	2.25	0.69
4:D:289:LEU:HA	4:D:318:ALA:HA	1.75	0.69
5:G:116:ARG:NH1	5:G:118:THR:O	2.26	0.69
2:B:305:ILE:HB	2:B:321:LEU:HG	1.74	0.69
1:A:217:THR:OG1	1:A:219:ASP:OD1	2.11	0.69
4:D:287:VAL:HG21	4:D:504:GLY:HA3	1.75	0.69
4:D:284:TYR:OH	4:D:289:LEU:O	2.10	0.69
6:L:80:THR:HG22	10:P:102:DA:H5'	1.73	0.68
7:M:25:PHE:N	7:M:56:GLU:OE2	2.25	0.68
2:B:180:ASN:ND2	2:B:182:ASP:OD1	2.25	0.68
10:P:111:DC:H2"	10:P:112:DG:C8	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3954:LYS:N	4:D:523:GLU:OE2	2.26	0.68
6:L:75:HIS:HA	8:N:89:ARG:NH1	2.09	0.68
9:O:18:DC:N4	10:P:129:DC:C4	2.62	0.68
10:P:87:DT:H3'	10:P:88:DT:H71	1.75	0.68
4:D:331:ILE:HD12	4:D:472:ILE:HD11	1.77	0.67
10:P:52:DG:H2'	10:P:53:DG:H8	1.59	0.67
5:G:94:GLU:OE1	7:M:104:GLN:NE2	2.28	0.67
7:I:107:VAL:HG13	5:K:55:GLN:HG2	1.76	0.67
7:M:88:ARG:NH1	7:M:94:ASN:OD1	2.28	0.67
1:A:122:LYS:HG2	1:A:136:THR:HG22	1.77	0.67
6:H:88:TYR:CG	8:J:80:TYR:CE2	2.82	0.67
8:J:78:ALA:HA	8:J:81:ASN:HD22	1.59	0.67
2:B:199:ASP:HB2	2:B:206:LEU:HD21	1.77	0.67
7:I:92:GLU:HG2	8:J:100:PRO:HB2	1.76	0.66
3:C:3932:ARG:NH2	3:C:3938:GLU:OE2	2.24	0.66
4:D:357:LEU:HG	4:D:365:SER:HB3	1.77	0.66
5:G:122:LYS:NZ	5:K:115:LYS:NZ	2.38	0.66
6:L:88:TYR:CE2	8:N:80:TYR:CG	2.83	0.66
7:M:17:ARG:HG3	9:O:31:DT:OP1	1.94	0.66
3:C:3849:ILE:N	3:C:3934:ILE:O	2.28	0.66
7:M:20:ARG:C	8:N:117:LYS:HZ2	1.97	0.66
7:M:94:ASN:O	7:M:98:GLY:N	2.29	0.66
6:L:75:HIS:HA	8:N:89:ARG:CZ	2.26	0.66
1:A:170:ASN:OD1	1:A:174:LYS:N	2.28	0.66
3:C:3886:ARG:HA	3:C:3892:VAL:HG22	1.78	0.66
7:I:68:ASN:O	7:I:71:ARG:NH1	2.29	0.66
6:L:88:TYR:CD2	8:N:80:TYR:CD2	2.84	0.65
10:P:112:DG:H2"	10:P:113:DA:H8	1.61	0.65
2:B:247:LYS:CD	3:C:3834:TYR:CE1	2.79	0.65
7:I:77:ARG:HE	9:O:131:DA:H4'	1.61	0.65
2:B:273:TRP:HE3	2:B:287:ASN:HA	1.61	0.65
5:G:94:GLU:OE2	7:M:104:GLN:N	2.22	0.65
9:O:30:DA:H2'	9:O:31:DT:H71	1.79	0.65
5:G:65:LEU:HD12	9:O:91:DA:H2'	1.77	0.65
6:H:92:ARG:NH2	8:J:98:LEU:HA	2.10	0.65
7:I:51:LEU:O	7:I:55:LEU:HG	1.95	0.65
1:A:87:ASP:OD2	6:H:23:ARG:NH2	2.30	0.65
5:K:104:PHE:HE2	6:L:37:LEU:HB2	1.61	0.65
1:A:195:THR:OG1	1:A:196:SER:N	2.28	0.65
5:G:126:LEU:HD12	5:K:113:HIS:HB2	1.78	0.65
9:O:28:DC:C4	10:P:119:DT:C4	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:20:ARG:O	8:N:117:LYS:HG2	1.96	0.64
8:J:100:PRO:HD2	8:J:103:LEU:HD12	1.79	0.64
4:D:301:SER:OG	4:D:306:THR:OG1	2.13	0.64
6:L:92:ARG:NH2	8:N:98:LEU:HA	2.11	0.64
7:M:79:ILE:HG12	7:M:82:HIS:CE1	2.33	0.64
9:O:17:DC:N3	10:P:130:DG:N1	2.46	0.64
9:O:45:DC:H2'	9:O:46:DT:C6	2.32	0.64
5:G:41:TYR:HD1	10:P:144:DC:OP1	1.80	0.64
5:K:109:LEU:HA	5:K:112:ILE:HD12	1.79	0.64
5:G:109:LEU:HA	5:G:112:ILE:HD12	1.79	0.64
6:L:29:ILE:O	6:L:55:ARG:NH2	2.20	0.63
6:H:89:ALA:O	6:H:93:GLN:N	2.29	0.63
7:I:93:LEU:HD23	8:J:103:LEU:HD11	1.78	0.63
9:O:132:DG:N2	10:P:17:DT:O2	2.31	0.63
10:P:48:DC:H1'	10:P:49:DC:C4	2.32	0.63
6:H:75:HIS:ND1	8:J:89:ARG:HG2	2.12	0.63
6:H:68:ASP:O	6:H:71:THR:HB	1.99	0.63
7:I:57:TYR:OH	8:J:106:HIS:HB3	1.99	0.63
7:I:77:ARG:CZ	9:O:132:DG:H5'	2.29	0.63
1:A:304:HIS:CG	1:A:307:ARG:HB2	2.33	0.63
5:G:113:HIS:CE1	5:K:122:LYS:NZ	2.67	0.63
6:L:68:ASP:O	6:L:71:THR:HB	1.99	0.63
1:A:33:ASN:ND2	1:A:37:THR:OG1	2.31	0.62
1:A:229:GLU:N	1:A:229:GLU:OE1	2.32	0.62
9:O:45:DC:H3'	9:O:46:DT:H71	1.81	0.62
9:O:138:DT:H2"	9:O:139:DA:C8	2.34	0.62
6:H:88:TYR:CE2	8:J:80:TYR:CG	2.86	0.62
7:M:50:TYR:OH	8:N:108:VAL:O	2.18	0.62
6:L:39:ARG:NH1	6:L:43:VAL:O	2.33	0.62
1:A:220:ARG:NH1	1:A:251:ARG:O	2.33	0.62
2:B:41:LEU:HB2	2:B:327:ILE:HB	1.82	0.62
5:G:43:PRO:HG2	10:P:69:DG:C5'	2.23	0.62
5:G:118:THR:HG21	10:P:71:DA:H5"	1.82	0.62
2:B:80:GLU:HG3	2:B:81:LYS:HG2	1.80	0.62
6:H:39:ARG:NH1	6:H:43:VAL:O	2.32	0.62
5:K:118:THR:N	9:O:71:DG:OP1	2.24	0.62
5:K:43:PRO:HG2	9:O:69:DA:H5"	1.82	0.62
6:L:89:ALA:O	6:L:93:GLN:N	2.28	0.62
4:D:399:PRO:HD3	4:D:445:SER:HB2	1.82	0.62
8:J:102:GLU:HG3	8:J:106:HIS:CD2	2.34	0.62
8:N:81:ASN:O	8:N:83:ARG:NE	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:HIS:CG	1:A:85:SER:HB3	2.35	0.62
3:C:3821:ARG:HA	3:C:3824:LYS:HE3	1.81	0.62
4:D:451:LYS:HB2	4:D:456:GLN:NE2	2.15	0.62
6:H:75:HIS:HB2	8:J:93:THR:HG21	1.81	0.62
9:O:103:DA:N6	10:P:44:DA:N6	2.48	0.62
8:J:109:SER:O	8:J:112:THR:OG1	2.12	0.61
5:K:40:ARG:HH12	10:P:83:DT:H1'	1.65	0.61
4:D:336:MET:HB3	4:D:388:GLN:HG3	1.81	0.61
6:H:29:ILE:O	6:H:55:ARG:NH2	2.20	0.61
2:B:34:ASN:OD1	2:B:332:SER:OG	2.18	0.61
3:C:3849:ILE:O	3:C:3934:ILE:N	2.31	0.61
5:G:113:HIS:CE1	5:K:122:LYS:CD	2.82	0.61
9:O:28:DC:C4	10:P:119:DT:N3	2.69	0.61
2:B:88:LEU:HD12	2:B:108:ASP:HA	1.81	0.61
4:D:392:LEU:HD22	4:D:449:PHE:HE1	1.66	0.61
8:J:35:ALA:HA	8:J:38:VAL:HG22	1.83	0.61
8:N:90:GLU:OE1	8:N:90:GLU:N	2.25	0.61
1:A:147:VAL:HG12	1:A:150:ASP:H	1.66	0.61
9:O:2:DT:C6	10:P:146:DA:C6	2.88	0.61
1:A:38:LEU:HD12	1:A:50:ILE:HG22	1.81	0.61
5:K:57:SER:OG	6:L:40:ARG:NH2	2.33	0.61
9:O:77:DT:N3	10:P:70:DG:N1	2.49	0.61
8:J:115:VAL:O	8:J:119:THR:N	2.28	0.60
10:P:17:DT:H2"	10:P:18:DG:C5	2.35	0.60
2:B:70:LYS:HB3	2:B:72:TRP:HE1	1.67	0.60
5:G:112:ILE:CD1	7:M:112:GLN:HG3	2.30	0.60
6:H:48:GLY:HA2	6:H:51:TYR:CE2	2.36	0.60
6:H:88:TYR:CD2	8:J:80:TYR:CD2	2.88	0.60
7:I:77:ARG:HH21	9:O:131:DA:C4'	2.14	0.60
1:A:113:VAL:HG12	1:A:125:VAL:HG22	1.82	0.60
4:D:521:GLU:HG2	4:D:527:ARG:HE	1.67	0.60
6:L:48:GLY:HA2	6:L:51:TYR:CE2	2.36	0.60
5:G:113:HIS:CE1	5:K:122:LYS:HZ3	2.19	0.60
7:I:80:PRO:HA	7:I:83:LEU:HD13	1.84	0.60
10:P:52:DG:H2'	10:P:53:DG:C8	2.37	0.60
4:D:343:ARG:HG2	4:D:367:ARG:HA	1.84	0.60
10:P:85:DC:H2"	10:P:86:DG:H8	1.67	0.60
5:G:46:VAL:HB	9:O:83:DG:OP1	2.02	0.60
6:H:75:HIS:HA	8:J:89:ARG:CZ	2.32	0.60
10:P:58:DT:H2"	10:P:59:DA:N7	2.16	0.60
5:G:67:PHE:O	5:G:71:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:33:ALA:O	6:L:37:LEU:HG	2.02	0.60
9:O:67:DG:N1	10:P:80:DA:C2	2.70	0.60
9:O:103:DA:H61	10:P:44:DA:N6	2.00	0.60
2:B:188:SER:HG	2:B:198:TRP:HE1	1.50	0.60
7:I:81:ARG:O	7:I:85:LEU:HG	2.02	0.60
5:K:67:PHE:O	5:K:71:VAL:HG23	2.02	0.60
7:M:29:ARG:O	7:M:33:LEU:HG	2.00	0.60
9:O:106:DA:H2"	9:O:107:DC:H5"	1.83	0.60
5:G:96:SER:O	5:G:100:LEU:HG	2.02	0.59
5:K:101:VAL:HG21	6:L:40:ARG:HG2	1.83	0.59
10:P:38:DG:H4'	10:P:39:DG:H5'	1.83	0.59
1:A:26:MET:HB3	1:A:44:ASN:H	1.67	0.59
4:D:502:ASP:HA	4:D:505:TRP:CE2	2.37	0.59
5:G:55:GLN:NE2	7:M:109:PRO:HA	2.16	0.59
8:N:33:SER:OG	8:N:60:ASN:ND2	2.35	0.59
9:O:30:DA:N6	10:P:117:DA:N6	2.50	0.59
1:A:51:TRP:HA	1:A:58:ILE:HA	1.84	0.59
8:J:33:SER:OG	8:J:60:ASN:ND2	2.36	0.59
5:K:46:VAL:HB	10:P:83:DT:OP2	2.02	0.59
9:O:85:DG:H2'	9:O:86:DT:H71	1.83	0.59
10:P:130:DG:H1'	10:P:131:DG:C5	2.37	0.59
2:B:301:THR:N	2:B:324:ASP:OD2	2.31	0.59
7:I:16:THR:HG23	7:I:19:SER:H	1.67	0.59
6:L:75:HIS:C	8:N:89:ARG:HH12	2.06	0.59
9:O:77:DT:C4	10:P:70:DG:C6	2.91	0.59
10:P:28:DT:H1'	10:P:29:DG:C5	2.37	0.59
9:O:114:DG:H1'	9:O:115:DT:H5'	1.85	0.59
7:I:77:ARG:HH22	9:O:132:DG:C5'	2.08	0.59
7:M:31:HIS:HA	7:M:34:LEU:HD12	1.83	0.59
9:O:19:DG:O6	10:P:128:DT:C4	2.55	0.59
2:B:70:LYS:NZ	2:B:82:THR:OG1	2.34	0.58
5:K:108:ASN:O	5:K:112:ILE:HG13	2.03	0.58
7:M:41:GLU:OE1	7:M:41:GLU:N	2.36	0.58
3:C:3907:HIS:HB2	3:C:3944:TYR:CD1	2.38	0.58
7:I:22:GLY:N	8:J:117:LYS:HE3	2.19	0.58
8:N:33:SER:OG	8:N:34:TYR:N	2.35	0.58
2:B:111:LEU:HD21	2:B:146:SER:HB3	1.85	0.58
2:B:149:PHE:HA	2:B:173:PRO:HB3	1.84	0.58
4:D:367:ARG:HH21	4:D:372:THR:HG21	1.68	0.58
4:D:392:LEU:HD13	4:D:449:PHE:HZ	1.68	0.58
5:G:108:ASN:O	5:G:112:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:33:ALA:O	6:H:37:LEU:HG	2.02	0.58
8:J:99:LEU:HB2	8:J:104:ALA:HB2	1.86	0.58
5:K:96:SER:O	5:K:100:LEU:HG	2.02	0.58
6:L:75:HIS:NE2	8:N:90:GLU:HG3	2.18	0.58
4:D:299:LYS:NZ	4:D:310:GLU:OE1	2.34	0.58
1:A:110:ILE:HA	1:A:127:PRO:HA	1.84	0.58
8:J:62:PHE:HB2	6:L:98:TYR:CD2	2.38	0.58
1:A:197:ASN:OD1	1:A:198:THR:N	2.36	0.58
2:B:215:PRO:HG3	3:C:3841:ARG:NH1	2.19	0.58
7:I:42:ARG:NH2	10:P:39:DG:O4'	2.37	0.58
6:L:91:LYS:HD3	8:N:76:ARG:NH2	2.13	0.58
10:P:7:DT:H2"	10:P:8:DG:C8	2.39	0.58
7:I:31:HIS:CD2	7:I:35:ARG:HE	2.22	0.58
8:N:87:THR:H	8:N:90:GLU:CD	2.06	0.58
9:O:66:DC:N4	10:P:81:DC:N4	2.51	0.58
5:K:46:VAL:HB	10:P:83:DT:P	2.44	0.57
9:O:103:DA:N6	10:P:44:DA:H61	2.00	0.57
10:P:106:DG:H2"	10:P:107:DT:H5"	1.85	0.57
3:C:3916:ARG:HB2	3:C:3929:PHE:CE1	2.39	0.57
6:L:75:HIS:CE1	8:N:89:ARG:HG2	2.39	0.57
6:L:97:LEU:HD12	6:L:98:TYR:H	1.69	0.57
9:O:60:DA:H2"	9:O:61:DA:H8	1.69	0.57
9:O:128:DG:H2'	9:O:129:DT:H71	1.85	0.57
6:H:36:ARG:NH2	10:P:61:DA:OP1	2.37	0.57
7:I:77:ARG:HH21	9:O:131:DA:C1'	2.16	0.57
9:O:4:DG:H2"	9:O:5:DA:C8	2.39	0.57
2:B:96:SER:HB3	2:B:101:LEU:HB2	1.87	0.57
5:G:122:LYS:C	5:K:113:HIS:CE1	2.77	0.57
1:A:139:ASP:OD1	1:A:139:ASP:N	2.38	0.57
2:B:169:ALA:O	2:B:196:ARG:NH1	2.36	0.57
5:G:78:PHE:CE1	6:H:67:ARG:HD3	2.40	0.57
3:C:3887:ILE:HG12	3:C:3926:ILE:HD11	1.84	0.57
4:D:314:SER:O	4:D:473:SER:HA	2.04	0.57
6:L:73:THR:HA	6:L:76:ALA:HB3	1.85	0.57
9:O:28:DC:N4	10:P:119:DT:N3	2.51	0.57
1:A:182:SER:OG	1:A:184:ASP:OD1	2.20	0.57
2:B:310:HIS:CD2	2:B:313:GLU:H	2.23	0.57
4:D:335:GLU:HG2	4:D:337:PRO:HD3	1.87	0.57
7:I:49:VAL:HG12	8:J:114:ALA:HB1	1.87	0.57
9:O:36:DC:H2"	9:O:37:DG:C8	2.40	0.57
1:A:102:GLN:NE2	1:A:137:LEU:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LYS:NZ	2:B:124:THR:OG1	2.30	0.57
1:A:108:SER:HB2	1:A:129:LYS:H	1.70	0.57
4:D:294:ARG:HH12	4:D:300:ILE:HG12	1.69	0.57
4:D:450:TYR:CD1	4:D:455:ASN:HA	2.38	0.57
1:A:67:HIS:CG	1:A:87:ASP:HB2	2.40	0.56
6:H:88:TYR:CZ	8:J:80:TYR:CE1	2.93	0.56
5:K:119:ILE:HG22	6:L:46:ILE:HA	1.86	0.56
6:L:36:ARG:NH2	9:O:61:DA:OP1	2.37	0.56
8:N:91:ILE:O	8:N:95:VAL:HG23	2.04	0.56
2:B:138:ASN:ND2	2:B:142:ASN:OD1	2.32	0.56
4:D:475:TYR:CZ	4:D:476:LYS:HE2	2.39	0.56
7:I:77:ARG:HG2	8:J:51:ILE:H	1.70	0.56
1:A:92:GLN:O	1:A:101:ASP:N	2.37	0.56
5:G:68:GLN:HE21	5:G:72:ARG:HE	1.53	0.56
6:H:73:THR:HA	6:H:76:ALA:HB3	1.85	0.56
7:M:37:GLY:HA3	7:M:39:TYR:CE2	2.40	0.56
7:M:87:VAL:HA	7:M:93:LEU:HD22	1.86	0.56
9:O:78:DC:N3	10:P:69:DG:N1	2.49	0.56
6:H:97:LEU:HD12	6:H:98:TYR:H	1.69	0.56
8:J:62:PHE:HA	6:L:98:TYR:CE2	2.39	0.56
1:A:286:LEU:HD21	1:A:289:ILE:HG13	1.85	0.56
4:D:494:ASP:OD2	4:D:497:TYR:N	2.33	0.56
1:A:39:LEU:HB2	1:A:53:PHE:CE1	2.41	0.56
1:A:177:VAL:HB	1:A:187:ALA:HB3	1.88	0.56
6:L:88:TYR:CZ	8:N:80:TYR:CD1	2.94	0.56
10:P:79:DT:H2"	10:P:80:DA:C8	2.41	0.56
6:H:69:ALA:HA	6:H:72:TYR:HD2	1.71	0.56
7:I:20:ARG:O	8:J:117:LYS:HG2	2.05	0.56
7:M:26:PRO:O	7:M:30:VAL:HG23	2.06	0.56
10:P:15:DT:H4'	10:P:16:DC:OP1	2.06	0.56
2:B:138:ASN:OD1	2:B:143:LEU:N	2.35	0.56
2:B:310:HIS:HD2	2:B:313:GLU:H	1.54	0.56
3:C:3843:LEU:HD22	3:C:3905:ILE:HG12	1.88	0.56
3:C:3857:GLU:O	3:C:3900:ASN:ND2	2.33	0.56
4:D:330:GLU:HB3	4:D:488:PHE:CE1	2.40	0.56
6:H:51:TYR:O	6:H:54:THR:HB	2.06	0.56
5:K:41:TYR:HA	9:O:144:DC:H5"	1.86	0.56
9:O:18:DC:C4	10:P:129:DC:N4	2.73	0.56
9:O:31:DT:C6	9:O:32:DT:H72	2.41	0.56
9:O:90:DA:H1'	9:O:91:DA:C5	2.40	0.56
2:B:91:SER:OG	2:B:107:ASP:OD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:57:TYR:OH	8:J:106:HIS:CB	2.54	0.56
5:G:55:GLN:OE1	7:M:109:PRO:HA	2.06	0.55
6:H:78:ARG:HB3	9:O:102:DG:OP1	2.06	0.55
7:M:16:THR:HG23	7:M:19:SER:H	1.71	0.55
7:M:18:SER:O	7:M:22:GLY:N	2.39	0.55
7:I:17:ARG:HA	7:I:20:ARG:HD2	1.89	0.55
9:O:77:DT:C4	10:P:70:DG:N1	2.74	0.55
10:P:100:DA:H1'	10:P:101:DG:O4'	2.05	0.55
6:H:54:THR:O	6:H:58:LEU:HG	2.06	0.55
5:K:68:GLN:HE21	5:K:72:ARG:HE	1.53	0.55
5:K:78:PHE:CE1	6:L:67:ARG:HD3	2.41	0.55
7:M:20:ARG:C	8:N:117:LYS:NZ	2.58	0.55
7:M:32:ARG:HD2	7:M:33:LEU:HD23	1.88	0.55
10:P:127:DC:C6	10:P:128:DT:H72	2.41	0.55
2:B:242:ASP:HB3	2:B:245:LYS:HB2	1.88	0.55
5:K:48:LEU:HA	5:K:51:ILE:HD12	1.89	0.55
6:L:69:ALA:HA	6:L:72:TYR:HD2	1.71	0.55
3:C:3871:ARG:O	3:C:3874:TYR:HB3	2.06	0.55
4:D:301:SER:O	4:D:305:LEU:N	2.39	0.55
5:K:63:ARG:NH1	9:O:61:DA:OP1	2.40	0.55
7:M:111:ILE:HG23	7:M:115:LEU:HD22	1.87	0.55
9:O:67:DG:C6	10:P:80:DA:C6	2.95	0.55
10:P:141:DT:H2"	10:P:142:DC:C5	2.41	0.55
6:H:92:ARG:HH21	8:J:98:LEU:HD23	1.72	0.55
5:K:65:LEU:O	5:K:69:ARG:HG3	2.06	0.55
6:L:51:TYR:O	6:L:54:THR:HB	2.06	0.55
2:B:267:SER:HG	2:B:273:TRP:HD1	1.54	0.55
5:G:122:LYS:HD2	5:K:113:HIS:ND1	2.22	0.55
3:C:3888:ASP:OD2	3:C:3924:LYS:NZ	2.32	0.55
5:G:46:VAL:CB	9:O:83:DG:OP1	2.54	0.55
10:P:48:DC:H4'	10:P:49:DC:H5'	1.89	0.55
5:G:113:HIS:HE1	5:K:123:ASP:N	2.05	0.55
1:A:205:GLU:HB2	1:A:214:LEU:HG	1.89	0.55
10:P:104:DC:H2'	10:P:105:DT:C6	2.42	0.55
3:C:3883:TYR:O	3:C:3895:ALA:N	2.35	0.54
2:B:157:ASP:OD1	2:B:158:VAL:N	2.40	0.54
3:C:3854:MET:SD	3:C:3854:MET:N	2.80	0.54
4:D:509:VAL:O	4:D:513:LEU:HG	2.07	0.54
8:J:90:GLU:OE1	8:J:90:GLU:N	2.29	0.54
5:K:88:ALA:O	5:K:92:LEU:HG	2.08	0.54
9:O:27:DT:N3	10:P:120:DG:C6	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:37:DG:N2	10:P:38:DG:C2	2.75	0.54
4:D:300:ILE:HG22	4:D:307:VAL:HG12	1.88	0.54
5:G:48:LEU:HA	5:G:51:ILE:HD12	1.89	0.54
6:H:60:VAL:O	6:H:63:GLU:HB2	2.07	0.54
5:K:89:VAL:HA	5:K:92:LEU:HG	1.90	0.54
1:A:53:PHE:O	1:A:56:ARG:HG2	2.08	0.54
1:A:65:HIS:HD2	1:A:69:VAL:HG22	1.73	0.54
1:A:116:HIS:HB3	1:A:119:ASP:O	2.08	0.54
4:D:441:GLN:NE2	4:D:461:LYS:O	2.41	0.54
5:G:122:LYS:CG	5:K:113:HIS:HE1	1.91	0.54
6:L:34:ILE:HD13	6:L:51:TYR:HB3	1.90	0.54
6:L:54:THR:O	6:L:58:LEU:HG	2.06	0.54
9:O:74:DC:H1'	9:O:75:DT:H5'	1.88	0.54
9:O:76:DG:H1'	9:O:77:DT:H5'	1.89	0.54
1:A:88:ASN:ND2	1:A:106:PHE:O	2.41	0.54
2:B:253:THR:O	2:B:286:TRP:NE1	2.40	0.54
3:C:3887:ILE:HD11	3:C:3893:VAL:HG23	1.90	0.54
5:G:88:ALA:O	5:G:92:LEU:HG	2.08	0.54
7:I:112:GLN:HG2	7:I:115:LEU:HD11	1.89	0.54
6:L:60:VAL:O	6:L:63:GLU:HB2	2.07	0.54
10:P:44:DA:H1'	10:P:45:DT:H5'	1.90	0.54
6:L:88:TYR:CG	8:N:80:TYR:CE2	2.95	0.54
3:C:3916:ARG:HB2	3:C:3929:PHE:HE1	1.72	0.54
5:G:104:PHE:HE2	6:H:37:LEU:HB2	1.72	0.54
7:I:92:GLU:OE2	8:J:100:PRO:O	2.26	0.54
9:O:80:DC:H2"	9:O:81:DC:C5	2.43	0.54
10:P:105:DT:H2"	10:P:106:DG:C8	2.43	0.54
1:A:308:PRO:HB2	1:A:323:GLN:HB3	1.89	0.53
2:B:33:PRO:HD2	2:B:294:VAL:HB	1.89	0.53
2:B:236:ASN:OD1	2:B:257:ASN:N	2.36	0.53
5:G:115:LYS:HZ3	5:K:122:LYS:HZ1	1.55	0.53
10:P:38:DG:H1'	10:P:39:DG:C5	2.42	0.53
10:P:91:DA:H2"	10:P:92:DG:H8	1.73	0.53
5:K:83:ARG:HG2	9:O:51:DC:H5"	1.89	0.53
5:K:117:VAL:HG13	6:L:45:ARG:HB2	1.89	0.53
8:N:59:MET:O	8:N:63:VAL:HG23	2.07	0.53
1:A:93:TRP:HA	1:A:99:ASP:O	2.08	0.53
5:G:65:LEU:O	5:G:69:ARG:HG3	2.07	0.53
8:J:61:SER:OG	6:L:98:TYR:CB	2.54	0.53
9:O:41:DA:C8	9:O:41:DA:H5'	2.44	0.53
10:P:36:DA:H2"	10:P:37:DG:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ASP:OD1	2:B:202:SER:N	2.38	0.53
5:G:122:LYS:CD	5:K:113:HIS:CE1	2.91	0.53
5:G:89:VAL:HA	5:G:92:LEU:HG	1.90	0.53
10:P:50:DT:H2"	10:P:51:DT:C6	2.44	0.53
1:A:75:SER:HB3	1:A:80:LYS:HB2	1.91	0.53
2:B:128:HIS:CE1	2:B:154:ARG:HB2	2.43	0.53
1:A:252:THR:HG23	1:A:272:ARG:HB3	1.91	0.53
6:L:75:HIS:CE1	8:N:90:GLU:HG3	2.44	0.53
7:M:81:ARG:NH1	7:M:105:GLY:O	2.37	0.53
8:N:77:LEU:HA	8:N:80:TYR:CD2	2.44	0.53
10:P:141:DT:H2"	10:P:142:DC:H5	1.73	0.53
7:I:42:ARG:HB2	8:J:85:THR:HG22	1.90	0.53
1:A:260:SER:HB3	1:A:265:TYR:HB2	1.91	0.53
2:B:35:TYR:H	2:B:295:GLN:HE22	1.56	0.53
5:K:62:ILE:HG21	5:K:67:PHE:HD2	1.74	0.53
5:K:126:LEU:O	5:K:130:ILE:HG12	2.09	0.53
9:O:111:DC:N4	10:P:36:DA:N6	2.57	0.53
7:M:31:HIS:HE1	7:M:43:VAL:HB	1.74	0.53
7:M:85:LEU:O	7:M:89:ASN:ND2	2.42	0.53
10:P:5:DG:H1'	10:P:6:DA:H5'	1.90	0.53
10:P:83:DT:H2"	10:P:84:DG:C8	2.44	0.53
1:A:178:LEU:HD23	1:A:185:LEU:HA	1.91	0.52
2:B:242:ASP:HB2	2:B:249:LEU:HD11	1.90	0.52
7:M:84:GLN:HE22	7:M:108:LEU:N	2.06	0.52
9:O:136:DT:H2"	9:O:137:DA:C8	2.44	0.52
1:A:52:ASP:HB3	1:A:55:THR:HG22	1.90	0.52
5:G:111:ALA:HA	5:G:114:ALA:HB3	1.91	0.52
6:H:23:ARG:O	6:H:24:ASP:OD1	2.28	0.52
6:H:34:ILE:HD13	6:H:51:TYR:HB3	1.90	0.52
5:K:108:ASN:HB2	6:L:43:VAL:HG22	1.90	0.52
9:O:66:DC:H2"	9:O:67:DG:C8	2.44	0.52
9:O:86:DT:H2'	9:O:87:DT:H72	1.90	0.52
10:P:7:DT:H2"	10:P:8:DG:H8	1.74	0.52
5:G:46:VAL:HG23	9:O:83:DG:OP1	2.08	0.52
5:G:62:ILE:HG21	5:G:67:PHE:HD2	1.74	0.52
7:I:50:TYR:O	7:I:54:VAL:HG23	2.08	0.52
2:B:178:HIS:CD2	2:B:222:PHE:H	2.17	0.52
2:B:179:PHE:HD2	2:B:183:GLY:HA2	1.73	0.52
5:G:126:LEU:O	5:G:130:ILE:HG12	2.09	0.52
7:I:17:ARG:NH2	7:I:28:GLY:HA2	2.25	0.52
8:J:87:THR:OG1	8:J:90:GLU:OE1	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:32:ARG:NH2	8:N:32:GLU:OE2	2.42	0.52
8:N:64:ASN:O	8:N:68:GLU:HG2	2.10	0.52
9:O:23:DC:H1'	9:O:24:DC:H5'	1.91	0.52
10:P:19:DA:H1'	10:P:20:DC:H5'	1.91	0.52
3:C:3907:HIS:CE1	3:C:3943:ASP:HA	2.44	0.52
5:G:124:ILE:O	5:G:128:ARG:HG3	2.10	0.52
6:H:50:ILE:HA	6:H:53:GLU:OE1	2.10	0.52
8:J:113:LYS:O	8:J:116:THR:OG1	2.19	0.52
6:L:50:ILE:HA	6:L:53:GLU:OE1	2.10	0.52
5:G:74:ILE:HG13	6:H:62:LEU:CD1	2.40	0.52
9:O:30:DA:H61	10:P:117:DA:N6	2.07	0.52
7:I:79:ILE:HG12	7:I:82:HIS:CE1	2.45	0.52
9:O:17:DC:N4	10:P:130:DG:C6	2.78	0.52
4:D:280:ARG:HD3	4:D:511:HIS:HB3	1.90	0.52
7:I:112:GLN:HB2	7:I:115:LEU:HG	1.92	0.52
5:K:111:ALA:HA	5:K:114:ALA:HB3	1.91	0.52
2:B:238:LEU:HB2	2:B:252:TYR:HB2	1.91	0.52
5:G:126:LEU:HD11	5:K:109:LEU:O	2.09	0.52
6:H:62:LEU:HA	6:H:65:VAL:HG13	1.92	0.52
8:J:88:SER:HA	8:J:91:ILE:HG12	1.91	0.52
7:M:25:PHE:CD2	7:M:56:GLU:HG2	2.45	0.52
2:B:73:GLY:N	2:B:78:LYS:O	2.28	0.51
2:B:90:ILE:HA	2:B:106:SER:HA	1.92	0.51
6:H:88:TYR:CE1	8:J:80:TYR:CZ	2.97	0.51
7:M:37:GLY:HA3	7:M:39:TYR:CZ	2.44	0.51
8:N:98:LEU:HG	8:N:99:LEU:HD23	1.91	0.51
9:O:48:DT:H1'	9:O:49:DA:C4	2.45	0.51
10:P:129:DC:H1'	10:P:130:DG:C5	2.44	0.51
3:C:3912:ASN:O	3:C:3931:MET:N	2.42	0.51
4:D:298:LEU:HD11	4:D:316:VAL:HB	1.91	0.51
4:D:331:ILE:HG21	4:D:344:LEU:HD22	1.91	0.51
5:G:113:HIS:ND1	5:K:122:LYS:CG	2.73	0.51
6:H:90:LEU:HA	6:H:93:GLN:HB2	1.92	0.51
6:L:90:LEU:HA	6:L:93:GLN:HB2	1.92	0.51
9:O:48:DT:H1'	9:O:49:DA:C5	2.45	0.51
10:P:113:DA:C8	10:P:113:DA:H5'	2.46	0.51
4:D:288:LEU:HD22	4:D:305:LEU:HD22	1.92	0.51
8:J:78:ALA:O	8:J:82:LYS:N	2.43	0.51
5:K:124:ILE:O	5:K:128:ARG:HG3	2.10	0.51
8:N:87:THR:OG1	8:N:90:GLU:OE1	2.26	0.51
6:L:62:LEU:HA	6:L:65:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:76:THR:HG1	10:P:132:DC:P	2.33	0.51
1:A:71:SER:HB3	1:A:113:VAL:HG22	1.93	0.51
1:A:190:ARG:HD3	1:A:198:THR:HG22	1.92	0.51
2:B:279:GLU:HA	2:B:303:VAL:HG13	1.91	0.51
7:M:33:LEU:HD11	8:N:34:TYR:OH	2.11	0.51
5:G:113:HIS:ND1	5:K:122:LYS:CD	2.71	0.51
5:G:123:ASP:CA	5:K:113:HIS:CE1	2.93	0.51
6:H:92:ARG:NE	8:J:97:LEU:HD21	2.26	0.51
9:O:7:DA:H2"	9:O:8:DA:C8	2.45	0.51
9:O:79:DC:N4	10:P:68:DG:C6	2.70	0.51
7:I:37:GLY:HA3	7:I:39:TYR:CE2	2.46	0.51
1:A:260:SER:N	1:A:265:TYR:O	2.43	0.51
1:A:269:GLY:HA2	1:A:276:LEU:HD13	1.93	0.51
7:I:17:ARG:HG2	8:J:118:TYR:CE1	2.46	0.51
8:J:77:LEU:HG	8:J:81:ASN:HD21	1.75	0.51
7:M:57:TYR:O	7:M:61:GLU:HG2	2.10	0.51
4:D:328:TYR:HB2	4:D:395:TYR:HD1	1.76	0.50
5:G:120:MET:HG2	5:G:122:LYS:HE3	1.93	0.50
8:J:62:PHE:HA	6:L:98:TYR:CE1	2.46	0.50
9:O:18:DC:N4	10:P:129:DC:N4	2.60	0.50
2:B:285:ILE:O	2:B:294:VAL:N	2.42	0.50
4:D:341:ALA:HB2	4:D:369:LYS:HE2	1.92	0.50
5:K:120:MET:HG2	5:K:122:LYS:HE3	1.93	0.50
8:N:34:TYR:H	8:N:60:ASN:ND2	2.10	0.50
9:O:68:DT:O4	10:P:79:DT:O4	2.29	0.50
4:D:315:MET:HB3	4:D:353:LEU:HA	1.92	0.50
10:P:41:DG:H1'	10:P:42:DT:H5'	1.94	0.50
8:J:110:GLU:O	8:J:113:LYS:HB2	2.10	0.50
6:L:75:HIS:ND1	8:N:89:ARG:HG2	2.27	0.50
10:P:139:DA:H1'	10:P:140:DT:H5'	1.94	0.50
1:A:303:TRP:HD1	1:A:304:HIS:N	2.10	0.50
2:B:255:HIS:HB2	2:B:278:SER:HB2	1.94	0.50
6:H:75:HIS:HA	8:J:89:ARG:NH2	2.27	0.50
8:J:85:THR:HG23	10:P:40:DA:OP1	2.11	0.50
8:N:67:PHE:HD2	8:N:68:GLU:OE2	1.95	0.50
9:O:30:DA:N6	10:P:117:DA:H61	2.09	0.50
3:C:3823:LEU:HD22	3:C:3854:MET:HB3	1.94	0.50
4:D:531:PRO:O	4:D:534:PRO:HD2	2.12	0.50
6:L:45:ARG:HH11	9:O:70:DC:H4'	1.75	0.50
10:P:51:DT:H2"	10:P:52:DG:H8	1.76	0.50
1:A:31:THR:HG23	1:A:74:TRP:NE1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:HB3	1:A:314:SER:OG	2.12	0.50
6:L:55:ARG:HA	6:L:58:LEU:HD12	1.94	0.50
9:O:26:DC:H2"	9:O:27:DT:H71	1.94	0.50
10:P:68:DG:H2"	10:P:69:DG:C8	2.46	0.50
1:A:50:ILE:O	1:A:59:ALA:N	2.37	0.50
1:A:95:VAL:HG23	1:A:96:LEU:HD22	1.94	0.50
1:A:108:SER:HA	1:A:129:LYS:NZ	2.27	0.49
1:A:270:SER:O	1:A:270:SER:OG	2.30	0.49
4:D:346:TRP:CZ2	4:D:394:PHE:HB3	2.47	0.49
6:H:40:ARG:O	7:M:107:VAL:HG11	2.12	0.49
4:D:324:LYS:HB2	4:D:400:GLU:HA	1.93	0.49
6:H:55:ARG:HA	6:H:58:LEU:HD12	1.93	0.49
6:L:91:LYS:NZ	8:N:76:ARG:HH12	2.10	0.49
1:A:312:SER:O	1:A:318:VAL:HA	2.12	0.49
2:B:303:VAL:HB	2:B:321:LEU:HD12	1.94	0.49
4:D:346:TRP:CH2	4:D:394:PHE:HB3	2.47	0.49
7:I:21:ALA:O	8:J:117:LYS:HD3	2.12	0.49
8:J:33:SER:OG	8:J:34:TYR:N	2.44	0.49
8:J:63:VAL:HA	8:J:66:VAL:HG22	1.93	0.49
9:O:2:DT:H71	10:P:146:DA:N9	2.24	0.49
10:P:126:DC:H2"	10:P:127:DC:O5'	2.12	0.49
2:B:105:ALA:HB1	2:B:132:VAL:HG12	1.94	0.49
6:H:30:THR:HG21	10:P:61:DA:H5"	1.94	0.49
7:I:26:PRO:HB2	7:I:29:ARG:HB3	1.95	0.49
8:J:105:LYS:O	8:J:108:VAL:HG22	2.12	0.49
3:C:3886:ARG:NH1	3:C:3888:ASP:O	2.44	0.49
7:M:31:HIS:CE1	7:M:43:VAL:HB	2.48	0.49
9:O:2:DT:H71	10:P:146:DA:C5	2.48	0.49
9:O:112:DT:H2"	9:O:113:DA:C8	2.47	0.49
8:J:88:SER:O	8:J:92:GLN:HG3	2.13	0.49
10:P:80:DA:H8	10:P:80:DA:OP2	1.95	0.49
10:P:136:DG:H2"	10:P:137:DG:OP2	2.11	0.49
3:C:3854:MET:HG3	3:C:3929:PHE:CE2	2.47	0.49
5:G:85:GLN:HA	10:P:50:DT:OP1	2.12	0.49
8:N:108:VAL:O	8:N:112:THR:OG1	2.27	0.49
9:O:6:DG:H2"	9:O:7:DA:C8	2.47	0.49
4:D:330:GLU:HG2	4:D:483:ASN:HB3	1.94	0.49
5:G:68:GLN:HE21	5:G:72:ARG:NE	2.11	0.49
9:O:101:DG:H2"	9:O:102:DG:C8	2.47	0.49
2:B:37:LEU:HD13	2:B:328:LYS:HB3	1.95	0.49
4:D:502:ASP:HA	4:D:505:TRP:NE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:31:LYS:HD3	6:H:35:ARG:HH11	1.77	0.49
6:H:35:ARG:NH2	9:O:82:DC:OP2	2.28	0.49
8:J:45:VAL:HG12	8:J:46:HIS:CE1	2.48	0.49
6:L:69:ALA:O	6:L:72:TYR:HB2	2.13	0.49
7:M:50:TYR:CD1	8:N:111:GLY:HA3	2.48	0.49
8:N:78:ALA:O	8:N:82:LYS:N	2.46	0.49
10:P:30:DG:H2"	10:P:31:DA:H8	1.78	0.49
2:B:79:PHE:HZ	2:B:82:THR:HG1	1.60	0.49
2:B:107:ASP:HB3	2:B:131:TYR:HD1	1.77	0.49
4:D:288:LEU:O	4:D:319:SER:N	2.46	0.49
5:K:40:ARG:NH2	10:P:82:DG:H21	2.11	0.49
6:L:75:HIS:HA	8:N:89:ARG:NH2	2.27	0.49
7:M:50:TYR:O	7:M:54:VAL:HG23	2.13	0.49
8:N:74:ALA:O	8:N:77:LEU:HG	2.13	0.49
1:A:187:ALA:HA	1:A:235:ARG:HD3	1.94	0.48
4:D:307:VAL:HG11	4:D:316:VAL:HG11	1.95	0.48
5:G:126:LEU:HD13	5:K:110:CYS:HA	1.95	0.48
8:J:73:GLU:HA	8:J:76:ARG:NH1	2.28	0.48
9:O:129:DT:H2"	9:O:130:DC:C5	2.47	0.48
7:I:102:ILE:HG23	7:I:105:GLY:HA3	1.94	0.48
8:J:106:HIS:O	8:J:109:SER:OG	2.16	0.48
5:K:90:MET:HA	5:K:93:GLN:NE2	2.28	0.48
10:P:69:DG:N2	10:P:70:DG:C2	2.81	0.48
5:G:90:MET:HA	5:G:93:GLN:NE2	2.28	0.48
6:H:45:ARG:HH11	10:P:70:DG:H5'	1.79	0.48
7:M:16:THR:O	7:M:19:SER:OG	2.18	0.48
4:D:304:ARG:HH22	4:D:332:THR:HB	1.79	0.48
8:J:76:ARG:HG2	8:J:80:TYR:CZ	2.48	0.48
5:G:48:LEU:O	5:G:52:ARG:HG3	2.13	0.48
7:I:107:VAL:CG1	5:K:55:GLN:HG2	2.42	0.48
9:O:33:DG:H2"	9:O:34:DG:H8	1.78	0.48
5:G:110:CYS:HA	5:K:126:LEU:HD13	1.95	0.48
7:I:66:ALA:HB1	7:I:78:ILE:HG21	1.95	0.48
5:K:70:LEU:O	5:K:74:ILE:HG12	2.14	0.48
6:L:45:ARG:HH11	9:O:70:DC:C4'	2.26	0.48
9:O:72:DC:H2"	9:O:73:DG:H8	1.79	0.48
10:P:90:DA:H2"	10:P:91:DA:C8	2.47	0.48
1:A:229:GLU:HA	1:A:232:THR:HG22	1.96	0.48
2:B:131:TYR:O	2:B:149:PHE:N	2.38	0.48
4:D:330:GLU:CG	4:D:483:ASN:HB3	2.44	0.48
8:J:43:LYS:NZ	8:J:47:PRO:O	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:48:LEU:O	5:K:52:ARG:HG3	2.13	0.48
6:L:31:LYS:HD3	6:L:35:ARG:HH11	1.78	0.48
5:G:70:LEU:O	5:G:74:ILE:HG12	2.14	0.48
5:G:120:MET:HG3	5:G:121:PRO:HD2	1.96	0.48
6:H:35:ARG:O	6:H:39:ARG:HG2	2.13	0.48
5:K:68:GLN:HE21	5:K:72:ARG:NE	2.11	0.48
7:M:55:LEU:HD12	7:M:58:LEU:HD11	1.96	0.48
8:N:117:LYS:O	8:N:120:SER:OG	2.20	0.48
10:P:37:DG:C2	10:P:38:DG:C2	3.02	0.48
2:B:72:TRP:HA	2:B:80:GLU:H	1.78	0.48
2:B:170:HIS:CD2	2:B:194:LEU:HB2	2.48	0.48
5:K:83:ARG:O	6:L:81:VAL:N	2.41	0.48
6:L:35:ARG:O	6:L:39:ARG:HG2	2.13	0.48
8:N:34:TYR:H	8:N:60:ASN:HD21	1.62	0.48
2:B:247:LYS:CG	3:C:3834:TYR:CE1	2.97	0.48
4:D:489:LYS:HG2	4:D:490:TYR:CE2	2.49	0.48
6:H:69:ALA:O	6:H:72:TYR:HB2	2.13	0.48
9:O:110:DC:H1’	9:O:111:DC:O4’	2.14	0.48
6:H:22:LEU:O	6:H:23:ARG:HB2	2.14	0.47
7:M:55:LEU:HD11	8:N:63:VAL:HG13	1.96	0.47
9:O:47:DC:N3	10:P:100:DA:N6	2.62	0.47
10:P:13:DT:H2”	10:P:14:DA:C8	2.49	0.47
1:A:79:HIS:HA	1:A:95:VAL:HG22	1.95	0.47
8:N:61:SER:HA	8:N:64:ASN:HD22	1.79	0.47
9:O:63:DG:H1’	9:O:64:DC:H5’	1.96	0.47
9:O:76:DG:N1	10:P:71:DA:C6	2.82	0.47
10:P:133:DA:H1’	10:P:134:DC:H5’	1.96	0.47
2:B:41:LEU:O	2:B:327:ILE:N	2.25	0.47
7:I:92:GLU:OE1	8:J:103:LEU:HG	2.14	0.47
2:B:189:SER:HB3	2:B:220:VAL:HB	1.96	0.47
7:M:32:ARG:HA	7:M:35:ARG:CZ	2.44	0.47
7:M:81:ARG:NH2	7:M:107:VAL:O	2.29	0.47
7:M:87:VAL:HG22	7:M:93:LEU:HD21	1.95	0.47
9:O:38:DT:H2”	9:O:39:DA:N7	2.29	0.47
5:G:64:LYS:HG2	9:O:92:DC:OP1	2.14	0.47
5:G:119:ILE:HG22	6:H:46:ILE:HA	1.97	0.47
6:H:88:TYR:CD2	8:J:80:TYR:CE2	3.02	0.47
7:I:40:ALA:HB1	8:J:84:SER:O	2.14	0.47
9:O:29:DA:N6	10:P:118:DT:C4	2.82	0.47
4:D:300:ILE:HD12	4:D:302:ASP:OD1	2.15	0.47
4:D:391:VAL:HG21	4:D:489:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:42:ARG:O	5:K:45:THR:OG1	2.27	0.47
7:M:76:THR:OG1	10:P:132:DC:P	2.73	0.47
7:M:81:ARG:HH12	7:M:107:VAL:N	2.12	0.47
8:N:78:ALA:O	8:N:83:ARG:N	2.41	0.47
9:O:18:DC:H2"	9:O:19:DG:N7	2.30	0.47
10:P:37:DG:H1'	10:P:38:DG:H5'	1.96	0.47
1:A:26:MET:O	1:A:43:CYS:HA	2.15	0.47
1:A:71:SER:HB2	1:A:84:ALA:HB3	1.96	0.47
1:A:80:LYS:NZ	1:A:94:ASP:HB2	2.30	0.47
2:B:164:LEU:HD12	2:B:165:LYS:HG3	1.97	0.47
2:B:273:TRP:CE3	2:B:287:ASN:HA	2.46	0.47
2:B:283:VAL:HG22	2:B:304:VAL:HG11	1.97	0.47
4:D:349:PRO:O	4:D:350:LEU:HB2	2.15	0.47
5:G:102:ALA:C	5:G:131:ARG:HH22	2.18	0.47
5:G:124:ILE:HD12	5:G:124:ILE:H	1.79	0.47
6:H:63:GLU:O	6:H:67:ARG:NH1	2.47	0.47
6:H:98:TYR:CZ	8:N:62:PHE:HA	2.50	0.47
5:K:124:ILE:H	5:K:124:ILE:HD12	1.79	0.47
6:L:78:ARG:HB3	10:P:102:DA:OP1	2.15	0.47
6:L:91:LYS:CE	8:N:76:ARG:NH1	2.58	0.47
10:P:24:DT:H2"	10:P:25:DG:C8	2.49	0.47
1:A:247:ASP:OD2	1:A:250:ASN:HB3	2.14	0.47
5:G:40:ARG:HH12	9:O:83:DG:H1'	1.79	0.47
5:G:69:ARG:NH1	9:O:91:DA:OP2	2.48	0.47
6:H:83:ALA:O	6:H:86:VAL:HG12	2.15	0.47
5:K:105:GLU:O	5:K:109:LEU:HG	2.15	0.47
6:L:63:GLU:O	6:L:67:ARG:NH1	2.47	0.47
6:L:92:ARG:HH21	8:N:98:LEU:HD13	1.80	0.47
9:O:2:DT:H2"	10:P:146:DA:N1	2.29	0.47
10:P:37:DG:H2'	10:P:37:DG:OP2	2.15	0.47
10:P:72:DC:H2"	10:P:73:DA:C8	2.50	0.47
1:A:260:SER:OG	1:A:262:ASP:OD1	2.23	0.47
3:C:3888:ASP:OD1	3:C:3888:ASP:N	2.47	0.47
4:D:519:HIS:O	4:D:523:GLU:HB2	2.15	0.47
8:J:62:PHE:CB	6:L:98:TYR:CE2	2.95	0.47
8:J:116:THR:HA	8:J:119:THR:HG1	1.79	0.47
10:P:9:DT:H2"	10:P:10:DA:C8	2.50	0.47
2:B:275:VAL:HG21	2:B:316:ILE:HD13	1.97	0.47
3:C:3859:ALA:H	3:C:3900:ASN:ND2	2.13	0.47
4:D:288:LEU:HD13	4:D:305:LEU:HD13	1.97	0.47
9:O:125:DC:H2"	9:O:126:DG:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:HB3	2:B:72:TRP:NE1	2.28	0.46
2:B:155:ILE:O	2:B:164:LEU:HG	2.14	0.46
2:B:267:SER:HB3	2:B:273:TRP:HB2	1.96	0.46
3:C:3845:CYS:N	3:C:3938:GLU:O	2.40	0.46
5:G:101:VAL:HG21	6:H:40:ARG:HG2	1.97	0.46
7:I:65:LEU:HA	7:I:68:ASN:ND2	2.31	0.46
8:J:91:ILE:O	8:J:95:VAL:HG22	2.15	0.46
5:K:63:ARG:HH21	9:O:60:DA:H5"	1.80	0.46
7:M:29:ARG:HD2	8:N:34:TYR:CE1	2.49	0.46
7:M:32:ARG:NH2	8:N:32:GLU:OE1	2.48	0.46
9:O:78:DC:H2"	9:O:79:DC:C6	2.50	0.46
9:O:131:DA:H1'	9:O:132:DG:O4'	2.15	0.46
10:P:85:DC:H2"	10:P:86:DG:C8	2.47	0.46
1:A:36:GLY:O	1:A:304:HIS:NE2	2.48	0.46
1:A:149:ASP:HB2	1:A:152:ASP:OD1	2.15	0.46
5:G:46:VAL:CG2	9:O:83:DG:OP1	2.64	0.46
7:I:15:LYS:O	7:I:20:ARG:NE	2.39	0.46
6:L:83:ALA:O	6:L:86:VAL:HG12	2.15	0.46
9:O:101:DG:H2"	9:O:102:DG:H8	1.80	0.46
2:B:157:ASP:HB3	2:B:162:LYS:H	1.78	0.46
4:D:392:LEU:HD22	4:D:449:PHE:CE1	2.48	0.46
10:P:61:DA:H1'	10:P:62:DA:H5'	1.96	0.46
10:P:63:DC:C2	10:P:64:DG:N7	2.83	0.46
1:A:203:SER:OG	1:A:216:ASN:HB3	2.16	0.46
4:D:346:TRP:NE1	4:D:396:ILE:HG21	2.30	0.46
5:K:102:ALA:C	5:K:131:ARG:HH22	2.19	0.46
9:O:28:DC:N3	10:P:119:DT:N3	2.63	0.46
10:P:115:DC:H2"	10:P:116:DA:H8	1.81	0.46
1:A:125:VAL:O	1:A:132:PRO:HA	2.16	0.46
1:A:127:PRO:HD3	1:A:132:PRO:HA	1.98	0.46
4:D:349:PRO:HD2	4:D:467:VAL:O	2.15	0.46
5:G:109:LEU:O	5:K:126:LEU:HD11	2.15	0.46
5:K:120:MET:HG3	5:K:121:PRO:HD2	1.96	0.46
9:O:111:DC:H2'	9:O:112:DT:H72	1.97	0.46
6:H:44:LYS:CD	7:M:115:LEU:HG	2.35	0.46
7:I:21:ALA:C	8:J:117:LYS:HE3	2.36	0.46
10:P:105:DT:H2"	10:P:106:DG:H8	1.80	0.46
1:A:115:TYR:HB3	1:A:120:GLN:HE22	1.81	0.46
1:A:270:SER:O	1:A:274:HIS:N	2.49	0.46
3:C:3859:ALA:H	3:C:3900:ASN:HD21	1.62	0.46
4:D:356:PRO:HA	4:D:473:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:73:GLU:O	5:G:76:GLN:HG2	2.15	0.46
5:K:63:ARG:CZ	9:O:61:DA:OP1	2.64	0.46
6:L:88:TYR:CE2	8:N:80:TYR:CD1	3.03	0.46
9:O:67:DG:C6	10:P:80:DA:N6	2.84	0.46
9:O:72:DC:H2"	9:O:73:DG:C8	2.51	0.46
9:O:89:DT:H1'	9:O:90:DA:C4	2.50	0.46
1:A:94:ASP:OD2	1:A:97:SER:N	2.42	0.46
1:A:108:SER:O	1:A:108:SER:OG	2.33	0.46
2:B:297:LEU:HD13	2:B:330:TRP:CD2	2.51	0.46
4:D:336:MET:SD	4:D:369:LYS:NZ	2.70	0.46
4:D:364:TYR:HB3	4:D:460:TYR:CE1	2.50	0.46
6:H:35:ARG:HH22	9:O:82:DC:P	2.36	0.46
7:I:41:GLU:CD	7:M:38:ASN:HD21	2.19	0.46
6:L:75:HIS:CA	8:N:89:ARG:NH1	2.79	0.46
10:P:52:DG:C2	10:P:53:DG:C5	3.04	0.46
1:A:186:VAL:O	1:A:235:ARG:NH1	2.43	0.46
1:A:267:VAL:HA	1:A:277:TYR:O	2.16	0.46
5:G:105:GLU:O	5:G:109:LEU:HG	2.15	0.46
5:G:109:LEU:C	5:K:126:LEU:HD11	2.36	0.46
5:K:78:PHE:CE1	6:L:67:ARG:HB2	2.51	0.46
9:O:58:DT:H2"	9:O:59:DA:N7	2.30	0.46
9:O:84:DC:H2"	9:O:85:DG:H8	1.81	0.46
10:P:135:DC:H2"	10:P:136:DG:C8	2.51	0.46
4:D:328:TYR:HA	4:D:394:PHE:O	2.16	0.46
4:D:368:SER:HB3	4:D:386:TYR:CZ	2.51	0.46
5:G:45:THR:HA	5:G:48:LEU:HD12	1.98	0.46
6:H:56:GLY:O	6:H:60:VAL:HG23	2.16	0.46
6:L:60:VAL:O	6:L:63:GLU:CB	2.64	0.46
10:P:109:DT:H2"	10:P:110:DA:C8	2.51	0.46
1:A:26:MET:SD	1:A:44:ASN:HB3	2.56	0.45
1:A:226:ASP:HB2	1:A:242:MET:SD	2.56	0.45
2:B:59:TRP:HB2	2:B:95:TRP:CH2	2.51	0.45
3:C:3918:ILE:HD12	3:C:3920:ILE:HD11	1.98	0.45
4:D:323:ARG:HG3	4:D:467:VAL:HG12	1.98	0.45
7:I:15:LYS:HB3	7:I:20:ARG:NH2	2.31	0.45
5:K:118:THR:HG23	9:O:71:DG:OP1	2.16	0.45
6:L:92:ARG:CD	8:N:97:LEU:HD21	2.47	0.45
7:M:90:ASP:HB3	7:M:93:LEU:HB3	1.97	0.45
7:M:113:SER:OG	7:M:114:VAL:N	2.49	0.45
10:P:43:DA:H2"	10:P:44:DA:C8	2.52	0.45
10:P:120:DG:H1'	10:P:121:DA:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:138:DG:H2"	10:P:139:DA:C8	2.52	0.45
1:A:116:HIS:NE2	1:A:163:GLY:O	2.43	0.45
1:A:274:HIS:CE1	1:A:298:LEU:HD13	2.52	0.45
2:B:286:TRP:HA	2:B:293:ILE:HA	1.96	0.45
7:I:27:VAL:HG11	7:I:49:VAL:HG22	1.96	0.45
7:M:77:ARG:HG3	10:P:132:DC:C5'	2.38	0.45
1:A:71:SER:OG	1:A:112:LYS:HA	2.16	0.45
1:A:304:HIS:HB2	1:A:309:ILE:HB	1.98	0.45
2:B:33:PRO:HG2	2:B:295:GLN:HB2	1.98	0.45
2:B:46:LYS:HD2	2:B:66:ASP:HA	1.98	0.45
7:I:77:ARG:HG2	8:J:51:ILE:N	2.32	0.45
7:I:79:ILE:CD1	7:I:81:ARG:HB3	2.46	0.45
9:O:129:DT:N3	10:P:18:DG:C6	2.85	0.45
10:P:109:DT:H2"	10:P:110:DA:N7	2.32	0.45
5:K:45:THR:HA	5:K:48:LEU:HD12	1.98	0.45
5:K:73:GLU:O	5:K:76:GLN:HG2	2.15	0.45
6:L:56:GLY:O	6:L:60:VAL:HG23	2.16	0.45
2:B:102:LEU:HD12	2:B:116:VAL:HG12	1.99	0.45
2:B:126:LYS:O	2:B:156:TRP:HH2	1.99	0.45
2:B:256:LYS:N	2:B:278:SER:OG	2.45	0.45
7:I:41:GLU:OE2	7:M:38:ASN:ND2	2.48	0.45
7:M:76:THR:OG1	7:M:77:ARG:N	2.50	0.45
8:N:58:ILE:O	8:N:61:SER:OG	2.30	0.45
9:O:40:DG:H1'	9:O:41:DA:C8	2.51	0.45
9:O:100:DG:H1'	9:O:101:DG:C8	2.51	0.45
10:P:77:DC:H2"	10:P:78:DG:C8	2.51	0.45
10:P:113:DA:H1'	10:P:114:DC:H5'	1.99	0.45
1:A:29:THR:O	1:A:41:VAL:HA	2.17	0.45
6:H:88:TYR:CG	8:J:80:TYR:CZ	3.04	0.45
6:H:98:TYR:OH	8:N:65:ASP:CB	2.65	0.45
8:J:59:MET:O	8:J:63:VAL:HG13	2.16	0.45
9:O:100:DG:N2	9:O:101:DG:C2	2.85	0.45
10:P:55:DG:C2	10:P:56:DG:C6	3.04	0.45
1:A:279:TRP:HA	1:A:286:LEU:HA	1.99	0.45
1:A:282:SER:OG	1:A:283:ILE:N	2.49	0.45
2:B:247:LYS:CB	3:C:3834:TYR:CD1	2.91	0.45
4:D:357:LEU:HB3	4:D:473:SER:HB2	1.99	0.45
5:K:83:ARG:HG2	9:O:51:DC:C5'	2.47	0.45
7:M:26:PRO:HD3	8:N:37:TYR:CZ	2.52	0.45
7:M:50:TYR:CE1	8:N:111:GLY:HA3	2.52	0.45
8:N:34:TYR:O	8:N:38:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:2:DT:C7	10:P:146:DA:C5	2.99	0.45
10:P:17:DT:H2"	10:P:18:DG:C4	2.52	0.45
1:A:18:ASP:HB3	1:A:320:ILE:O	2.16	0.45
2:B:223:SER:N	2:B:228:TYR:O	2.50	0.45
5:G:78:PHE:HZ	6:H:63:GLU:OE2	1.99	0.45
6:H:60:VAL:O	6:H:63:GLU:CB	2.65	0.45
6:L:36:ARG:NH1	9:O:61:DA:OP2	2.49	0.45
7:M:25:PHE:HE2	7:M:55:LEU:HG	1.82	0.45
8:N:34:TYR:N	8:N:60:ASN:HD21	2.15	0.45
10:P:59:DA:C6	10:P:60:DA:C6	3.05	0.45
2:B:154:ARG:NH1	2:B:163:CYS:SG	2.88	0.45
3:C:3913:CYS:HA	3:C:3931:MET:H	1.82	0.45
4:D:294:ARG:NH2	4:D:298:LEU:O	2.35	0.45
5:G:122:LYS:CD	5:K:115:LYS:HZ1	2.29	0.45
7:I:15:LYS:HG2	7:I:20:ARG:HG3	1.98	0.45
2:B:51:VAL:HG12	2:B:62:SER:HB3	1.97	0.45
2:B:134:CYS:SG	2:B:135:CYS:N	2.90	0.45
3:C:3819:ARG:NH2	3:C:3853:GLU:OE2	2.50	0.45
6:L:88:TYR:CE1	8:N:80:TYR:CE1	3.05	0.45
7:M:76:THR:OG1	10:P:132:DC:OP1	2.34	0.45
2:B:217:VAL:HG22	2:B:233:THR:HG22	1.99	0.44
3:C:3822:HIS:O	3:C:3826:THR:HG22	2.17	0.44
5:G:58:THR:HG21	7:M:104:GLN:O	2.17	0.44
5:G:78:PHE:CE1	6:H:67:ARG:HB2	2.52	0.44
7:I:42:ARG:HG2	9:O:113:DA:H5'	1.98	0.44
8:N:61:SER:HA	8:N:64:ASN:ND2	2.31	0.44
2:B:91:SER:HB2	2:B:133:PHE:HA	2.00	0.44
3:C:3861:ILE:HG21	3:C:3871:ARG:HH22	1.83	0.44
4:D:303:ASP:OD1	4:D:304:ARG:N	2.51	0.44
4:D:390:ASP:OD1	4:D:451:LYS:HE3	2.17	0.44
5:G:74:ILE:HG13	6:H:62:LEU:HD13	1.98	0.44
5:G:114:ALA:HB1	5:G:116:ARG:HE	1.82	0.44
7:I:40:ALA:HB3	8:J:86:ILE:HG22	1.99	0.44
8:J:43:LYS:CD	8:J:47:PRO:HA	2.47	0.44
9:O:35:DT:H2"	9:O:36:DC:OP2	2.17	0.44
9:O:109:DC:C2	10:P:38:DG:N1	2.85	0.44
10:P:12:DA:C5	10:P:13:DT:C4	3.05	0.44
10:P:120:DG:H1'	10:P:121:DA:C8	2.52	0.44
1:A:24:ILE:HG12	1:A:49:VAL:HG11	2.00	0.44
1:A:48:ILE:HB	1:A:62:ILE:HB	1.99	0.44
1:A:205:GLU:O	1:A:213:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ALA:HB3	2:B:324:ASP:HB3	1.97	0.44
3:C:3907:HIS:ND1	3:C:3942:TYR:O	2.51	0.44
9:O:18:DC:C4	10:P:129:DC:C4	3.05	0.44
9:O:28:DC:H2"	9:O:29:DA:C8	2.52	0.44
3:C:3844:PHE:HA	3:C:3939:GLU:HA	1.98	0.44
3:C:3912:ASN:C	3:C:3931:MET:HB2	2.38	0.44
4:D:348:GLN:NE2	4:D:465:GLU:O	2.34	0.44
5:K:104:PHE:CE2	6:L:37:LEU:HB2	2.46	0.44
7:M:77:ARG:HG2	10:P:132:DC:OP1	2.18	0.44
9:O:132:DG:H1'	9:O:133:DA:C8	2.51	0.44
5:G:46:VAL:HG21	9:O:83:DG:H3'	2.00	0.44
5:G:131:ARG:HG3	5:K:130:ILE:CG2	2.47	0.44
9:O:67:DG:H2'	9:O:68:DT:H71	1.99	0.44
9:O:89:DT:H1'	9:O:90:DA:C5	2.53	0.44
10:P:15:DT:H1'	10:P:16:DC:O5'	2.18	0.44
10:P:58:DT:H1'	10:P:59:DA:C4	2.52	0.44
10:P:63:DC:C2	10:P:64:DG:C8	3.06	0.44
10:P:120:DG:H1'	10:P:121:DA:C5	2.52	0.44
1:A:293:THR:HG22	1:A:295:GLY:H	1.83	0.44
6:H:75:HIS:NE2	8:J:90:GLU:HG3	2.32	0.44
7:I:41:GLU:OE1	7:I:41:GLU:N	2.49	0.44
6:L:88:TYR:CD2	8:N:80:TYR:CG	3.05	0.44
9:O:33:DG:H2"	9:O:34:DG:C8	2.51	0.44
9:O:127:DT:H1'	9:O:128:DG:C8	2.52	0.44
10:P:30:DG:H8	10:P:30:DG:OP2	2.00	0.44
10:P:104:DC:H2'	10:P:105:DT:C5	2.52	0.44
1:A:81:LEU:HD12	1:A:95:VAL:HG12	2.00	0.44
1:A:200:ALA:HB3	1:A:218:ALA:HB2	2.00	0.44
1:A:233:CYS:SG	1:A:237:GLY:HA3	2.57	0.44
2:B:38:LYS:HG3	2:B:331:LYS:HB3	1.99	0.44
2:B:257:ASN:HB2	2:B:262:ILE:HD12	2.00	0.44
5:G:55:GLN:O	7:M:81:ARG:NH2	2.51	0.44
5:K:51:ILE:HG13	6:L:39:ARG:HD2	2.00	0.44
10:P:133:DA:H8	10:P:133:DA:OP2	2.00	0.44
1:A:220:ARG:O	1:A:254:TRP:NE1	2.37	0.44
1:A:290:LEU:HD13	1:A:321:TRP:CE3	2.53	0.44
5:K:72:ARG:HG2	5:K:84:PHE:CE2	2.53	0.44
5:K:114:ALA:HB1	5:K:116:ARG:HE	1.82	0.44
10:P:42:DT:H1'	10:P:43:DA:H5'	2.00	0.44
7:I:18:SER:O	7:I:22:GLY:N	2.51	0.44
8:J:54:LYS:O	8:J:58:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:92:GLN:O	8:N:96:ARG:HG3	2.17	0.44
10:P:55:DG:OP2	10:P:55:DG:H2'	2.18	0.44
10:P:104:DC:H2'	10:P:105:DT:H71	2.00	0.44
10:P:132:DC:H2"	10:P:133:DA:C8	2.53	0.44
1:A:204:ILE:HG12	1:A:215:ILE:HD12	2.00	0.43
1:A:307:ARG:HD3	1:A:307:ARG:HA	1.85	0.43
5:G:72:ARG:HG2	5:G:84:PHE:CE2	2.53	0.43
6:L:88:TYR:CD1	8:N:80:TYR:CZ	3.06	0.43
7:M:52:ALA:O	7:M:56:GLU:HG3	2.18	0.43
7:M:68:ASN:HA	7:M:71:ARG:NH2	2.32	0.43
10:P:37:DG:OP2	10:P:37:DG:H8	2.01	0.43
10:P:87:DT:H2'	10:P:88:DT:C6	2.52	0.43
10:P:88:DT:H1'	10:P:89:DT:H5'	1.99	0.43
1:A:219:ASP:O	1:A:221:ILE:HG13	2.18	0.43
4:D:289:LEU:H	4:D:305:LEU:HD21	1.84	0.43
6:L:75:HIS:CA	8:N:89:ARG:HH12	2.31	0.43
7:M:81:ARG:NH1	7:M:84:GLN:OE1	2.51	0.43
8:N:95:VAL:O	8:N:99:LEU:N	2.33	0.43
9:O:37:DG:C8	9:O:38:DT:H72	2.53	0.43
1:A:67:HIS:CD2	1:A:87:ASP:HB2	2.52	0.43
1:A:92:GLN:HG2	1:A:101:ASP:OD2	2.19	0.43
5:K:74:ILE:HG13	6:L:62:LEU:CD1	2.48	0.43
7:M:31:HIS:HD2	7:M:35:ARG:HH11	1.58	0.43
8:N:88:SER:HA	8:N:91:ILE:HG12	2.00	0.43
10:P:121:DA:C6	10:P:122:DG:C6	3.07	0.43
1:A:31:THR:O	1:A:74:TRP:NE1	2.45	0.43
1:A:33:ASN:OD1	1:A:37:THR:N	2.49	0.43
2:B:35:TYR:N	2:B:295:GLN:OE1	2.51	0.43
6:H:59:LYS:O	6:H:63:GLU:N	2.37	0.43
8:J:55:ALA:HA	8:J:58:ILE:HD12	1.99	0.43
7:M:26:PRO:HG3	8:N:37:TYR:CZ	2.54	0.43
9:O:119:DC:H2"	9:O:120:DA:N7	2.34	0.43
9:O:131:DA:C6	9:O:132:DG:C6	3.07	0.43
10:P:37:DG:H2"	10:P:38:DG:C8	2.54	0.43
1:A:136:THR:OG1	1:A:139:ASP:OD1	2.35	0.43
1:A:262:ASP:OD2	1:A:264:GLU:HB2	2.19	0.43
2:B:250:LYS:HE3	2:B:289:GLN:HA	2.00	0.43
3:C:3875:TYR:HB3	3:C:3880:ILE:O	2.19	0.43
5:G:46:VAL:N	9:O:83:DG:OP1	2.52	0.43
6:H:52:GLU:HG2	6:H:53:GLU:N	2.34	0.43
7:I:18:SER:OG	7:I:23:LEU:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:52:GLU:HG2	6:L:53:GLU:N	2.33	0.43
6:L:88:TYR:CG	8:N:80:TYR:CZ	3.07	0.43
9:O:19:DG:O6	10:P:128:DT:O4	2.36	0.43
9:O:107:DC:C6	9:O:108:DT:H72	2.54	0.43
9:O:143:DC:H2"	9:O:144:DC:C6	2.54	0.43
10:P:16:DC:H1'	10:P:17:DT:O4'	2.19	0.43
10:P:103:DG:C4	10:P:104:DC:C4	3.06	0.43
5:G:109:LEU:CB	5:K:126:LEU:HD21	2.49	0.43
5:G:109:LEU:HB2	5:K:126:LEU:HD21	2.01	0.43
8:J:104:ALA:O	8:J:108:VAL:HG13	2.18	0.43
10:P:129:DC:H1'	10:P:130:DG:N7	2.33	0.43
1:A:31:THR:HG23	1:A:74:TRP:HE1	1.83	0.43
7:M:79:ILE:H	7:M:82:HIS:CE1	2.37	0.43
9:O:29:DA:N1	10:P:119:DT:C4	2.86	0.43
10:P:22:DC:H2"	10:P:23:DG:H8	1.83	0.43
2:B:197:ILE:O	2:B:206:LEU:N	2.51	0.43
2:B:240:LEU:O	2:B:249:LEU:N	2.44	0.43
8:J:95:VAL:O	8:J:99:LEU:N	2.50	0.43
10:P:58:DT:H2"	10:P:59:DA:C8	2.53	0.43
10:P:98:DC:H5'	10:P:98:DC:C6	2.54	0.43
1:A:306:VAL:O	1:A:307:ARG:NH1	2.46	0.43
3:C:3914:TYR:CZ	3:C:3929:PHE:HB2	2.53	0.43
4:D:495:LEU:H	4:D:495:LEU:HD23	1.84	0.43
5:G:128:ARG:HA	5:G:131:ARG:HB2	2.01	0.43
8:J:85:THR:HG23	10:P:39:DG:O3'	2.19	0.43
9:O:2:DT:C7	10:P:146:DA:C4	2.92	0.43
1:A:110:ILE:HG23	1:A:125:VAL:HG13	2.01	0.43
4:D:340:THR:HG23	4:D:478:CYS:SG	2.59	0.43
5:G:122:LYS:CB	5:K:113:HIS:CE1	3.01	0.43
8:J:60:ASN:O	8:J:63:VAL:HG22	2.19	0.43
5:K:54:TYR:O	6:L:40:ARG:NH2	2.50	0.43
6:L:75:HIS:O	8:N:89:ARG:NH1	2.30	0.43
7:M:21:ALA:O	8:N:117:LYS:HD3	2.19	0.43
7:M:24:GLN:HG3	8:N:41:VAL:HG12	2.00	0.43
7:M:42:ARG:HB2	10:P:112:DG:O3'	2.19	0.43
7:M:96:LEU:HD11	8:N:100:PRO:HD3	2.01	0.43
9:O:21:DG:H2"	9:O:22:DG:H8	1.83	0.43
1:A:26:MET:CB	1:A:44:ASN:H	2.32	0.42
1:A:38:LEU:HD13	1:A:52:ASP:HA	2.00	0.42
2:B:92:ASP:HB2	2:B:133:PHE:O	2.19	0.42
2:B:108:ASP:O	2:B:110:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:320:HIS:CD2	4:D:500:MET:HG3	2.53	0.42
4:D:485:GLY:O	4:D:488:PHE:HB2	2.19	0.42
4:D:528:ARG:HE	4:D:529:SER:H	1.67	0.42
6:L:50:ILE:O	6:L:53:GLU:HB3	2.19	0.42
9:O:62:DC:H5'	9:O:62:DC:C6	2.54	0.42
10:P:8:DG:C8	10:P:9:DT:H72	2.54	0.42
10:P:46:DC:H2"	10:P:47:DC:OP2	2.18	0.42
4:D:528:ARG:HE	4:D:529:SER:N	2.15	0.42
6:L:92:ARG:HG3	8:N:97:LEU:HD21	2.01	0.42
1:A:43:CYS:HB2	1:A:45:ASP:OD1	2.19	0.42
1:A:177:VAL:O	1:A:186:VAL:HG22	2.19	0.42
2:B:39:PHE:HB2	2:B:329:LEU:HD12	2.01	0.42
6:H:50:ILE:O	6:H:53:GLU:HB3	2.19	0.42
5:K:110:CYS:HB3	5:K:123:ASP:OD2	2.20	0.42
9:O:109:DC:OP2	9:O:109:DC:H2'	2.19	0.42
1:A:27:ALA:O	1:A:316:GLY:HA2	2.19	0.42
1:A:251:ARG:HA	1:A:251:ARG:HH11	1.85	0.42
6:H:35:ARG:NH1	6:H:46:ILE:HD11	2.35	0.42
7:I:45:ALA:O	7:I:48:PRO:HD2	2.20	0.42
8:N:53:SER:HA	8:N:56:MET:SD	2.60	0.42
10:P:14:DA:C4	10:P:15:DT:C4	3.07	0.42
10:P:72:DC:H2"	10:P:73:DA:H8	1.84	0.42
10:P:102:DA:C6	10:P:103:DG:C6	3.07	0.42
5:G:60:LEU:HD12	5:G:60:LEU:H	1.84	0.42
5:G:110:CYS:HB3	5:G:123:ASP:OD2	2.20	0.42
6:H:60:VAL:HA	6:H:63:GLU:HB2	2.01	0.42
6:L:35:ARG:NH1	6:L:46:ILE:HD11	2.35	0.42
6:L:64:ASN:HA	6:L:67:ARG:NH2	2.35	0.42
9:O:146:DA:N6	10:P:1:DA:N6	2.66	0.42
10:P:21:DA:H1'	10:P:22:DC:H5'	2.00	0.42
10:P:124:DG:C2	10:P:125:DG:C4	3.07	0.42
1:A:226:ASP:OD2	1:A:228:ARG:NH2	2.53	0.42
4:D:357:LEU:CB	4:D:473:SER:HB2	2.49	0.42
5:K:128:ARG:HA	5:K:131:ARG:HB2	2.01	0.42
7:M:14:ALA:HB1	9:O:31:DT:H4'	2.01	0.42
8:N:54:LYS:O	8:N:57:SER:OG	2.32	0.42
9:O:144:DC:H2"	9:O:145:DG:C8	2.55	0.42
6:L:55:ARG:O	6:L:58:LEU:HB2	2.19	0.42
9:O:62:DC:H5'	9:O:62:DC:H6	1.83	0.42
9:O:142:DT:H2"	9:O:143:DC:C5	2.55	0.42
1:A:26:MET:HE3	1:A:43:CYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:LEU:HD23	2:B:144:ILE:N	2.35	0.42
4:D:294:ARG:NH2	4:D:300:ILE:HG23	2.34	0.42
5:G:106:ASP:HA	5:G:109:LEU:HG	2.01	0.42
5:K:90:MET:HA	5:K:93:GLN:HE21	1.84	0.42
7:M:31:HIS:O	7:M:35:ARG:HG3	2.20	0.42
9:O:124:DA:N6	10:P:23:DG:N1	2.67	0.42
10:P:94:DG:C6	10:P:95:DG:C6	3.07	0.42
10:P:95:DG:H2"	10:P:96:DT:OP2	2.20	0.42
10:P:143:DT:H2"	10:P:144:DC:C5	2.55	0.42
2:B:35:TYR:H	2:B:295:GLN:NE2	2.18	0.42
2:B:133:PHE:CZ	2:B:149:PHE:HD2	2.38	0.42
2:B:155:ILE:HB	2:B:165:LYS:HB2	2.02	0.42
2:B:241:TRP:HA	2:B:248:CYS:HA	2.01	0.42
5:G:90:MET:HA	5:G:93:GLN:HE21	1.84	0.42
5:G:126:LEU:O	5:G:129:ARG:HB3	2.20	0.42
7:I:58:LEU:HD12	7:I:59:THR:N	2.35	0.42
5:K:106:ASP:HA	5:K:109:LEU:HG	2.02	0.42
7:M:42:ARG:HA	10:P:113:DA:OP1	2.20	0.42
9:O:125:DC:H2"	9:O:126:DG:C8	2.55	0.42
10:P:74:DG:C4	10:P:75:DC:C5	3.08	0.42
10:P:103:DG:C5	10:P:104:DC:C4	3.08	0.42
10:P:116:DA:H2"	10:P:117:DA:H8	1.85	0.42
10:P:131:DG:C5	10:P:132:DC:C4	3.08	0.42
1:A:21:LEU:HD13	1:A:51:TRP:CE2	2.54	0.42
1:A:252:THR:HG23	1:A:272:ARG:HD2	2.01	0.42
2:B:300:HIS:NE2	2:B:318:SER:O	2.52	0.42
3:C:3849:ILE:HB	3:C:3934:ILE:HB	2.00	0.42
6:H:48:GLY:HA2	6:H:51:TYR:CZ	2.55	0.42
7:I:77:ARG:NH2	9:O:131:DA:C1'	2.80	0.42
6:L:60:VAL:HA	6:L:63:GLU:HB2	2.01	0.42
9:O:21:DG:H2"	9:O:22:DG:C8	2.55	0.42
9:O:99:DG:H2"	9:O:100:DG:N7	2.35	0.42
9:O:128:DG:P	9:O:128:DG:H8	2.42	0.42
10:P:92:DG:C4	10:P:93:DC:C4	3.08	0.42
2:B:109:LYS:HA	2:B:132:VAL:HG23	2.02	0.41
4:D:369:LYS:HD3	4:D:369:LYS:HA	1.84	0.41
5:G:106:ASP:CB	5:K:130:ILE:HD12	2.43	0.41
7:M:25:PHE:CE2	7:M:56:GLU:HG2	2.55	0.41
9:O:38:DT:OP2	9:O:38:DT:H2'	2.19	0.41
9:O:131:DA:C4	9:O:132:DG:C5	3.08	0.41
1:A:148:ASP:OD2	1:A:174:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:115:LYS:HZ1	5:K:122:LYS:CD	2.29	0.41
6:H:32:PRO:HA	6:H:35:ARG:HG2	2.01	0.41
6:H:64:ASN:HA	6:H:67:ARG:NH2	2.35	0.41
7:I:71:ARG:NH1	7:I:72:ASP:HB2	2.35	0.41
5:K:84:PHE:O	9:O:50:DG:H3'	2.20	0.41
5:K:126:LEU:O	5:K:129:ARG:HB3	2.20	0.41
5:K:126:LEU:HD23	5:K:129:ARG:HB3	2.02	0.41
6:L:66:ILE:HD12	6:L:66:ILE:H	1.85	0.41
9:O:47:DC:H2"	9:O:48:DT:H71	2.03	0.41
10:P:59:DA:C5	10:P:60:DA:C5	3.09	0.41
10:P:123:DC:H2'	10:P:123:DC:OP2	2.19	0.41
1:A:214:LEU:HD23	1:A:259:PHE:CZ	2.55	0.41
4:D:373:LYS:HE3	4:D:373:LYS:HB2	1.85	0.41
5:G:49:ARG:O	5:G:53:ARG:HG2	2.21	0.41
6:H:55:ARG:O	6:H:58:LEU:HB2	2.19	0.41
6:H:88:TYR:CE2	8:J:80:TYR:CD1	3.08	0.41
7:I:68:ASN:O	7:I:71:ARG:HD3	2.20	0.41
8:J:55:ALA:O	8:J:59:MET:HG2	2.20	0.41
5:K:60:LEU:HD12	5:K:60:LEU:H	1.85	0.41
6:L:46:ILE:HD12	6:L:51:TYR:CE1	2.56	0.41
10:P:57:DT:H6	10:P:57:DT:H2'	1.65	0.41
10:P:94:DG:C4	10:P:95:DG:C5	3.08	0.41
10:P:113:DA:H8	10:P:113:DA:H5'	1.83	0.41
10:P:125:DG:C4	10:P:126:DC:C5	3.09	0.41
1:A:214:LEU:HD23	1:A:259:PHE:CE2	2.55	0.41
1:A:223:ARG:HH21	1:A:241:PRO:HG2	1.86	0.41
2:B:143:LEU:HD21	2:B:155:ILE:CG2	2.50	0.41
2:B:174:VAL:HA	2:B:190:SER:HB2	2.02	0.41
2:B:242:ASP:HB2	2:B:249:LEU:HD21	2.03	0.41
2:B:297:LEU:HB3	2:B:330:TRP:CZ3	2.55	0.41
6:H:46:ILE:HD12	6:H:51:TYR:CE1	2.56	0.41
7:I:58:LEU:HA	7:I:61:GLU:OE1	2.21	0.41
8:J:43:LYS:HD3	8:J:47:PRO:HA	2.03	0.41
8:N:40:LYS:O	8:N:44:GLN:HG3	2.20	0.41
9:O:36:DC:OP2	9:O:36:DC:H2'	2.20	0.41
9:O:68:DT:C4	10:P:79:DT:O4	2.73	0.41
9:O:112:DT:H2"	9:O:113:DA:H8	1.85	0.41
4:D:290:ALA:HB2	4:D:319:SER:HA	2.02	0.41
5:G:39:HIS:HE1	5:G:41:TYR:CE2	2.39	0.41
5:G:126:LEU:HD23	5:G:129:ARG:HB3	2.02	0.41
8:J:104:ALA:O	8:J:107:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:49:ARG:O	5:K:53:ARG:HG2	2.21	0.41
6:L:32:PRO:HA	6:L:35:ARG:HG2	2.01	0.41
7:M:57:TYR:CZ	8:N:106:HIS:HB2	2.55	0.41
10:P:58:DT:H6	10:P:58:DT:H2'	1.63	0.41
2:B:143:LEU:HD22	2:B:179:PHE:HZ	1.86	0.41
4:D:357:LEU:HD12	4:D:363:SER:OG	2.21	0.41
4:D:375:HIS:CE1	4:D:376:GLN:HG3	2.56	0.41
4:D:485:GLY:HA3	4:D:499:PRO:HB3	2.01	0.41
6:H:54:THR:H	6:H:54:THR:HG1	1.55	0.41
9:O:29:DA:C2	10:P:119:DT:N3	2.88	0.41
9:O:65:DA:H1'	9:O:66:DC:H5'	2.03	0.41
9:O:91:DA:C8	9:O:92:DC:C5	3.08	0.41
10:P:128:DT:H2"	10:P:129:DC:C5	2.56	0.41
3:C:3933:LYS:HE3	3:C:3935:TYR:CZ	2.55	0.41
7:I:81:ARG:CZ	7:I:85:LEU:HD21	2.51	0.41
7:I:112:GLN:H	7:I:115:LEU:HD12	1.85	0.41
5:K:53:ARG:HA	5:K:56:LYS:HB2	2.02	0.41
9:O:41:DA:H1'	9:O:42:DC:O4'	2.20	0.41
9:O:105:DT:H2"	9:O:106:DA:H8	1.85	0.41
1:A:307:ARG:HB3	1:A:309:ILE:HG13	2.02	0.41
3:C:3883:TYR:HB2	3:C:3896:THR:HA	2.03	0.41
6:H:83:ALA:O	6:H:87:VAL:HG23	2.20	0.41
7:I:25:PHE:CE2	7:I:55:LEU:HB2	2.56	0.41
10:P:73:DA:H8	10:P:73:DA:OP2	2.04	0.41
10:P:119:DT:H2"	10:P:120:DG:N7	2.35	0.41
1:A:225:TYR:HB3	1:A:230:ILE:HD11	2.02	0.41
2:B:93:VAL:HG22	2:B:102:LEU:HD22	2.02	0.41
4:D:288:LEU:HB3	4:D:305:LEU:HD21	2.03	0.41
4:D:304:ARG:NH2	4:D:481:SER:OG	2.54	0.41
5:G:37:LYS:HA	5:G:38:PRO:HD3	1.94	0.41
6:H:36:ARG:NH1	10:P:61:DA:OP2	2.46	0.41
6:H:46:ILE:HD12	6:H:51:TYR:HE1	1.86	0.41
6:H:66:ILE:HD12	6:H:66:ILE:H	1.85	0.41
7:I:113:SER:OG	7:I:114:VAL:N	2.54	0.41
8:J:112:THR:O	8:J:116:THR:HG23	2.21	0.41
5:K:40:ARG:HH12	10:P:83:DT:C1'	2.34	0.41
6:L:46:ILE:HD12	6:L:51:TYR:HE1	1.86	0.41
6:L:48:GLY:HA2	6:L:51:TYR:CZ	2.55	0.41
6:L:59:LYS:O	6:L:63:GLU:N	2.37	0.41
6:L:88:TYR:HB3	8:N:80:TYR:CE2	2.56	0.41
8:N:87:THR:O	8:N:91:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:50:DG:C5	9:O:51:DC:C4	3.09	0.41
9:O:79:DC:H2'	9:O:79:DC:OP2	2.20	0.41
10:P:37:DG:H4'	10:P:38:DG:OP1	2.20	0.41
2:B:267:SER:OG	2:B:273:TRP:HD1	2.04	0.41
5:G:43:PRO:CD	10:P:69:DG:H5"	2.52	0.41
7:I:42:ARG:HA	9:O:113:DA:OP1	2.21	0.41
7:I:62:ILE:HG22	7:I:93:LEU:HD13	2.02	0.41
7:I:90:ASP:OD1	7:I:93:LEU:N	2.34	0.41
9:O:58:DT:H2"	9:O:59:DA:C8	2.55	0.41
9:O:120:DA:N6	10:P:27:DC:C4	2.89	0.41
9:O:133:DA:H2'	9:O:134:DT:H71	2.03	0.41
1:A:195:THR:H	1:A:195:THR:HG23	1.67	0.40
4:D:313:TYR:CZ	4:D:475:TYR:HB2	2.56	0.40
4:D:386:TYR:CE1	4:D:392:LEU:HD11	2.56	0.40
4:D:397:ASN:O	4:D:445:SER:HA	2.21	0.40
6:L:50:ILE:HG22	6:L:54:THR:OG1	2.21	0.40
10:P:83:DT:C2	10:P:84:DG:C5	3.09	0.40
2:B:59:TRP:CZ3	2:B:80:GLU:HB2	2.57	0.40
3:C:3834:TYR:HD2	3:C:3844:PHE:CD1	2.38	0.40
6:L:83:ALA:O	6:L:87:VAL:HG23	2.20	0.40
8:N:36:ILE:HG13	8:N:37:TYR:N	2.36	0.40
9:O:28:DC:C4	10:P:119:DT:O4	2.74	0.40
9:O:137:DA:H8	9:O:137:DA:OP2	2.05	0.40
9:O:140:DC:H1'	9:O:141:DA:H5'	2.02	0.40
2:B:86:HIS:NE2	2:B:112:LYS:HB2	2.36	0.40
4:D:441:GLN:HB2	4:D:462:ASP:OD1	2.21	0.40
5:G:60:LEU:HD23	5:G:97:GLU:OE2	2.21	0.40
5:K:39:HIS:HE1	5:K:41:TYR:CE2	2.39	0.40
5:K:42:ARG:N	9:O:144:DC:OP1	2.46	0.40
6:L:54:THR:H	6:L:54:THR:HG1	1.60	0.40
6:L:76:ALA:O	6:L:78:ARG:HG3	2.21	0.40
9:O:35:DT:H1'	9:O:36:DC:O5'	2.21	0.40
9:O:113:DA:C4	9:O:114:DG:C8	3.10	0.40
1:A:275:ALA:C	1:A:276:LEU:HD22	2.41	0.40
2:B:207:LYS:NZ	2:B:243:TYR:O	2.51	0.40
2:B:265:ASN:HD21	2:B:307:THR:C	2.25	0.40
3:C:3821:ARG:O	3:C:3824:LYS:HG2	2.21	0.40
4:D:349:PRO:HD3	4:D:469:PHE:CE2	2.56	0.40
4:D:375:HIS:O	4:D:380:LYS:NZ	2.54	0.40
6:H:98:TYR:CB	8:N:61:SER:OG	2.64	0.40
7:I:81:ARG:HH12	7:I:107:VAL:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:74:ALA:HB1	8:J:86:ILE:HD11	2.04	0.40
5:K:84:PHE:HD1	6:L:81:VAL:HB	1.87	0.40
8:N:39:TYR:HE1	9:O:21:DG:OP1	2.04	0.40
9:O:60:DA:H2"	9:O:61:DA:C8	2.51	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	304/538 (56%)	286 (94%)	18 (6%)	0	100	100
2	B	297/313 (95%)	281 (95%)	16 (5%)	0	100	100
3	C	144/209 (69%)	139 (96%)	5 (4%)	0	100	100
4	D	213/534 (40%)	194 (91%)	19 (9%)	0	100	100
5	G	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
5	K	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
6	H	80/103 (78%)	69 (86%)	11 (14%)	0	100	100
6	L	80/103 (78%)	70 (88%)	10 (12%)	0	100	100
7	I	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
7	M	105/129 (81%)	101 (96%)	4 (4%)	0	100	100
8	J	91/123 (74%)	86 (94%)	5 (6%)	0	100	100
8	N	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
All	All	1702/2576 (66%)	1601 (94%)	101 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	266/462 (58%)	263 (99%)	3 (1%)	73 85
2	B	258/274 (94%)	258 (100%)	0	100 100
3	C	127/182 (70%)	127 (100%)	0	100 100
4	D	185/460 (40%)	184 (100%)	1 (0%)	88 93
5	G	84/111 (76%)	78 (93%)	6 (7%)	14 41
5	K	84/111 (76%)	78 (93%)	6 (7%)	14 41
6	H	67/79 (85%)	61 (91%)	6 (9%)	9 32
6	L	67/79 (85%)	61 (91%)	6 (9%)	9 32
7	I	81/101 (80%)	80 (99%)	1 (1%)	71 84
7	M	82/101 (81%)	82 (100%)	0	100 100
8	J	77/103 (75%)	77 (100%)	0	100 100
8	N	79/103 (77%)	78 (99%)	1 (1%)	69 82
All	All	1457/2166 (67%)	1427 (98%)	30 (2%)	56 72

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	235	ARG
1	A	294	ARG
4	D	324	LYS
5	G	56	LYS
5	G	80	THR
5	G	105	GLU
5	G	108	ASN
5	G	110	CYS
5	G	126	LEU
6	H	49	LEU
6	H	59	LYS
6	H	63	GLU
6	H	65	VAL

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Mol	Chain	Res	Type
6	H	74	GLU
6	H	90	LEU
7	I	71	ARG
5	K	56	LYS
5	K	80	THR
5	K	105	GLU
5	K	108	ASN
5	K	110	CYS
5	K	126	LEU
6	L	49	LEU
6	L	59	LYS
6	L	63	GLU
6	L	65	VAL
6	L	74	GLU
6	L	90	LEU
8	N	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	120	GLN
1	A	285	ASN
2	B	178	HIS
2	B	255	HIS
2	B	265	ASN
2	B	289	GLN
2	B	323	ASN
4	D	441	GLN
4	D	483	ASN
5	G	39	HIS
5	G	68	GLN
5	G	113	HIS
6	H	25	ASN
7	I	31	HIS
7	I	68	ASN
7	I	89	ASN
8	J	60	ASN
8	J	64	ASN
8	J	81	ASN
8	J	106	HIS
5	K	39	HIS

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Mol	Chain	Res	Type
5	K	68	GLN
6	L	25	ASN
7	M	31	HIS
7	M	89	ASN
7	M	104	GLN
7	M	112	GLN
8	N	44	GLN
8	N	46	HIS
8	N	60	ASN
8	N	64	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

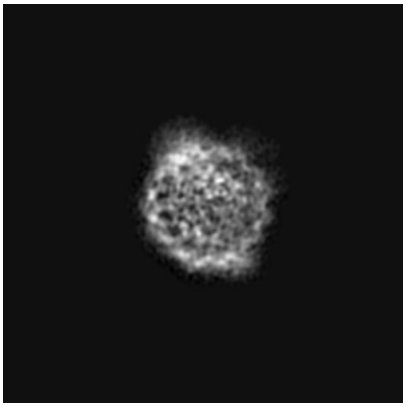
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21543. These allow visual inspection of the internal detail of the map and identification of artifacts.

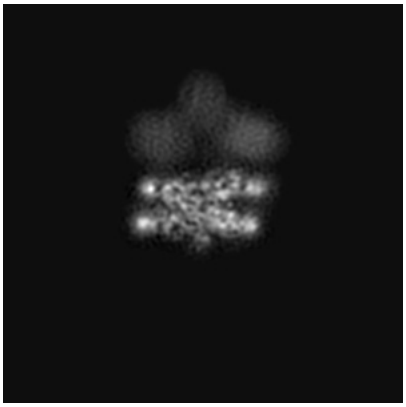
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

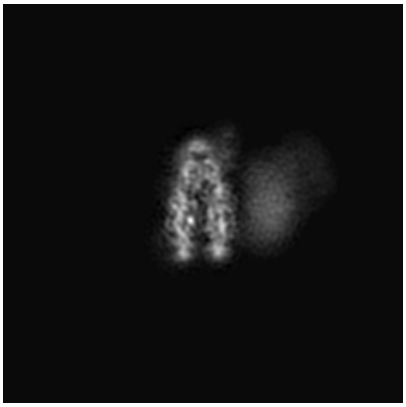
6.1.1 Primary map



X



Y

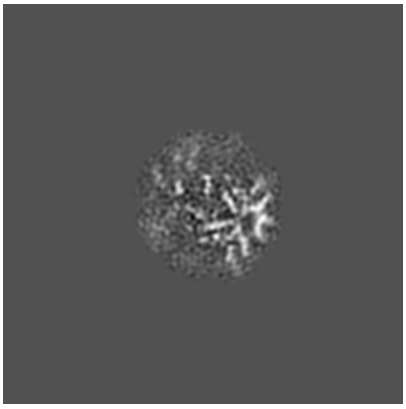


Z

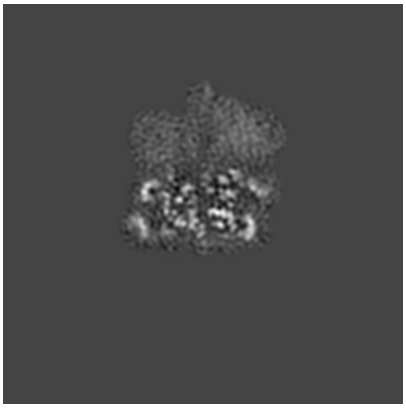
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 150



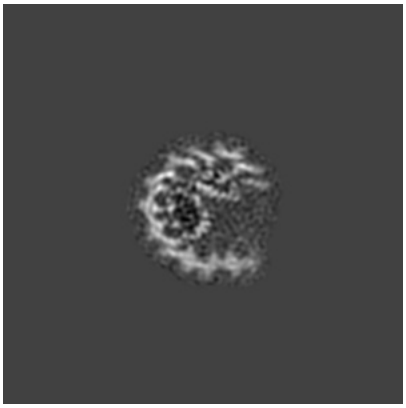
Y Index: 150

Z Index: 150

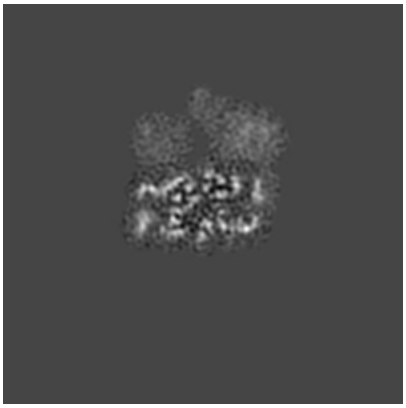
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

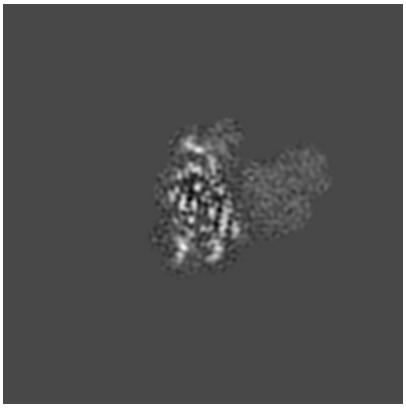
6.3.1 Primary map



X Index: 135



Y Index: 145

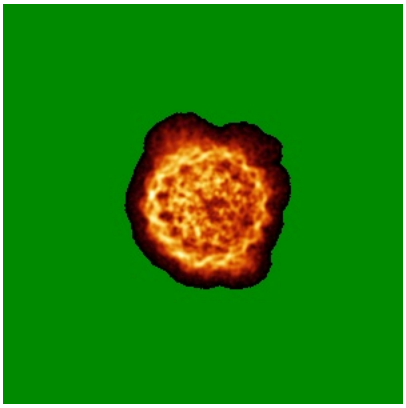


Z Index: 162

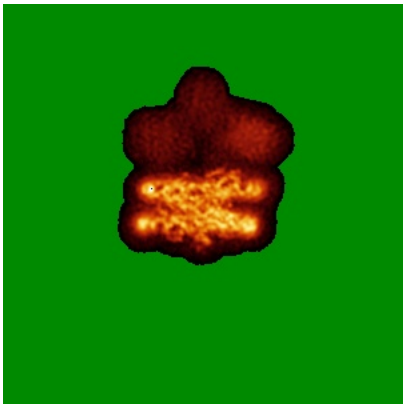
The images above show the largest variance slices of the map in three orthogonal directions.

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

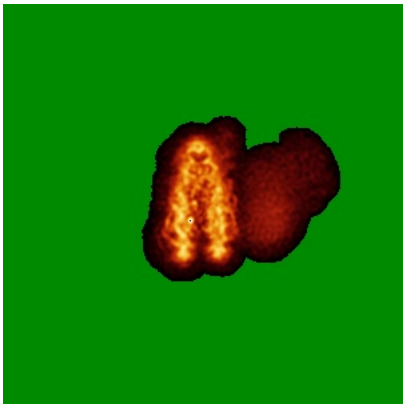
6.4.1 Primary map



X



Y

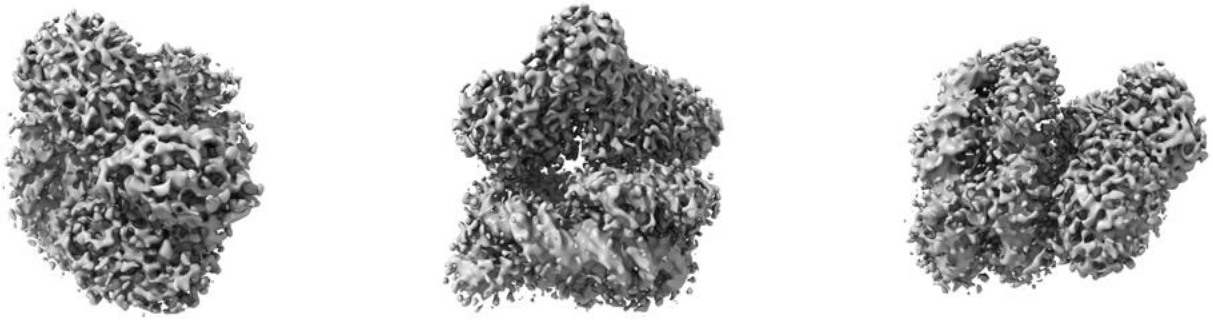


Z

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 0.0073. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

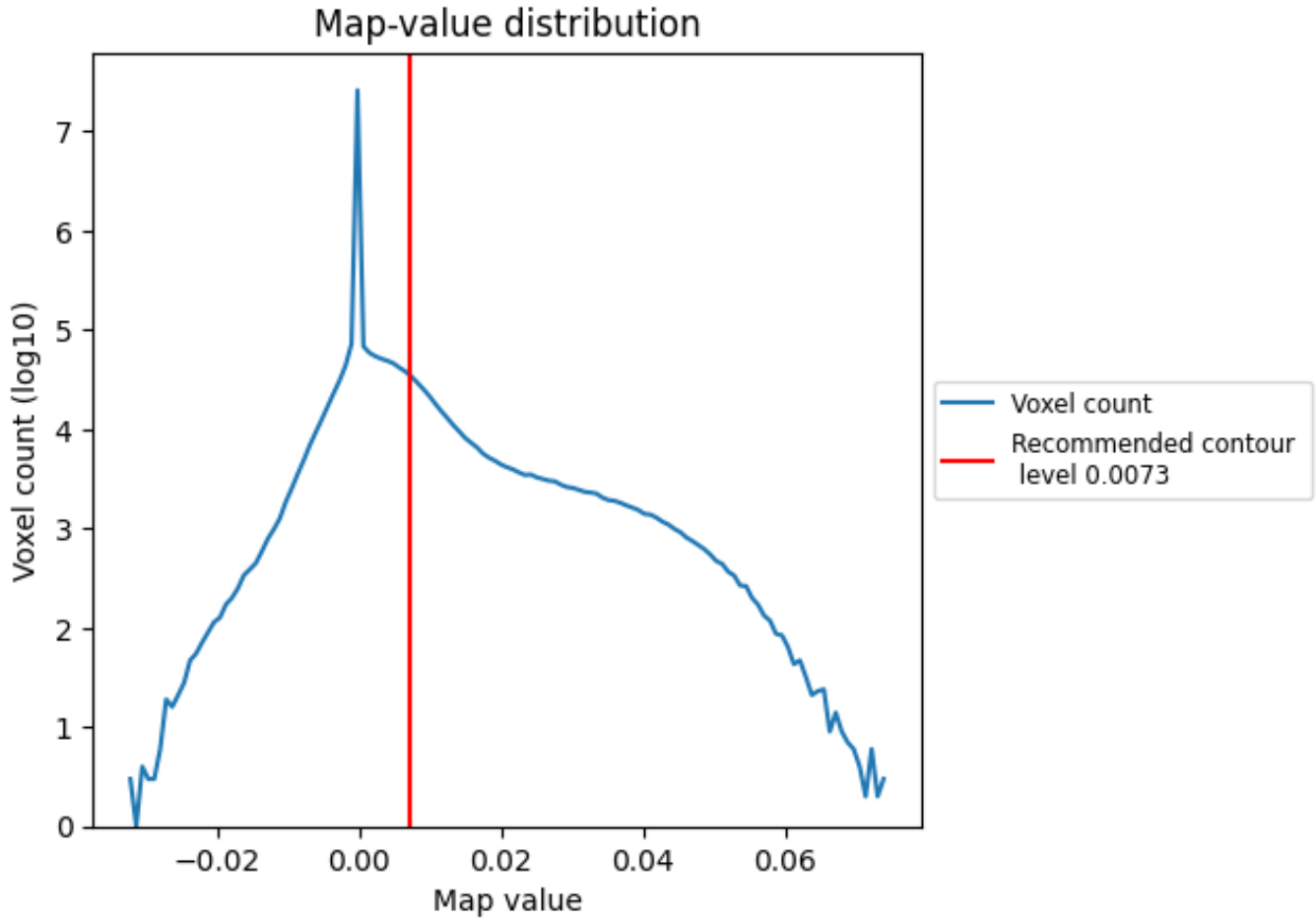
6.6 Mask visualisation (i)

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

7 Map analysis

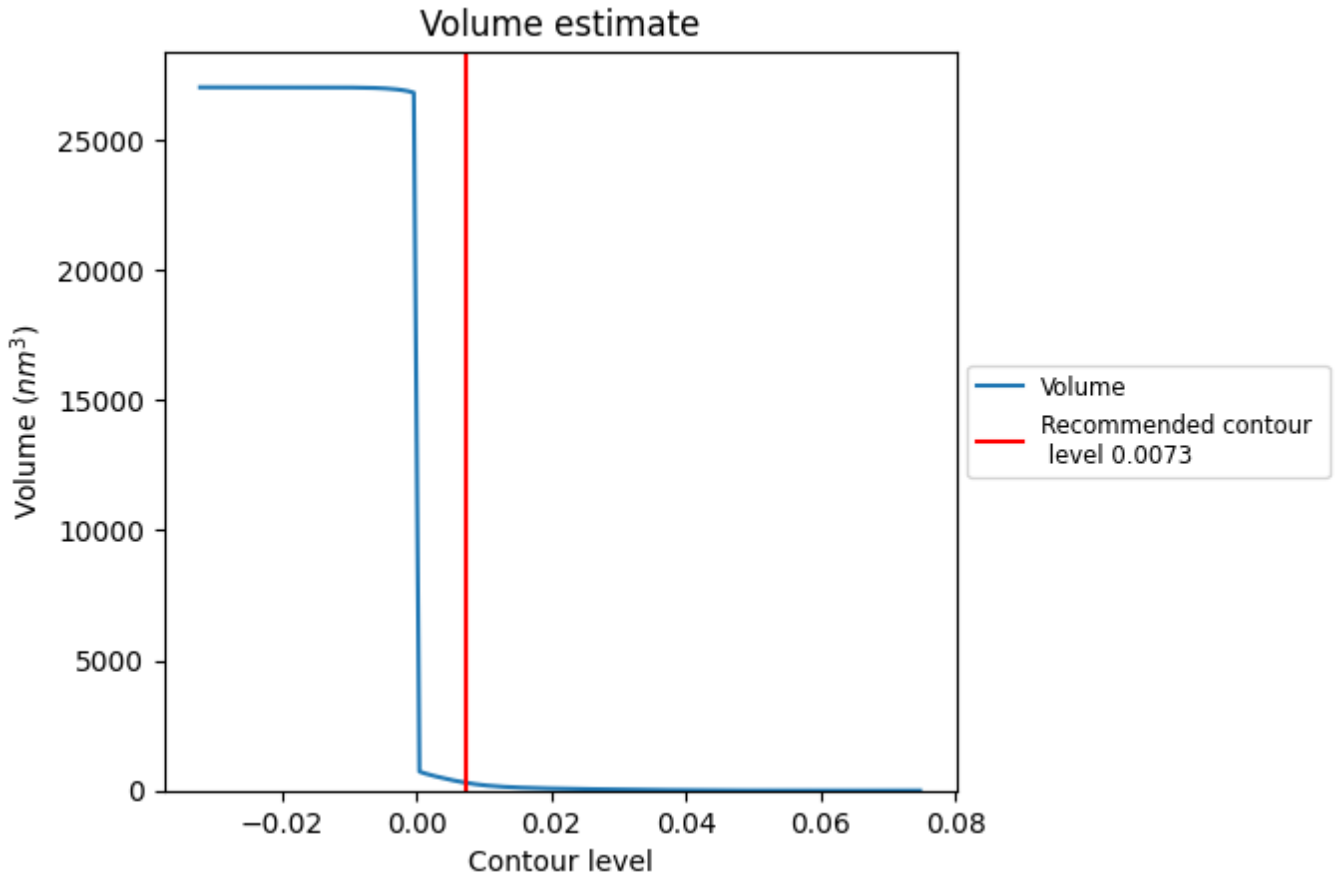
This section contains the results of statistical analysis of the map.

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.

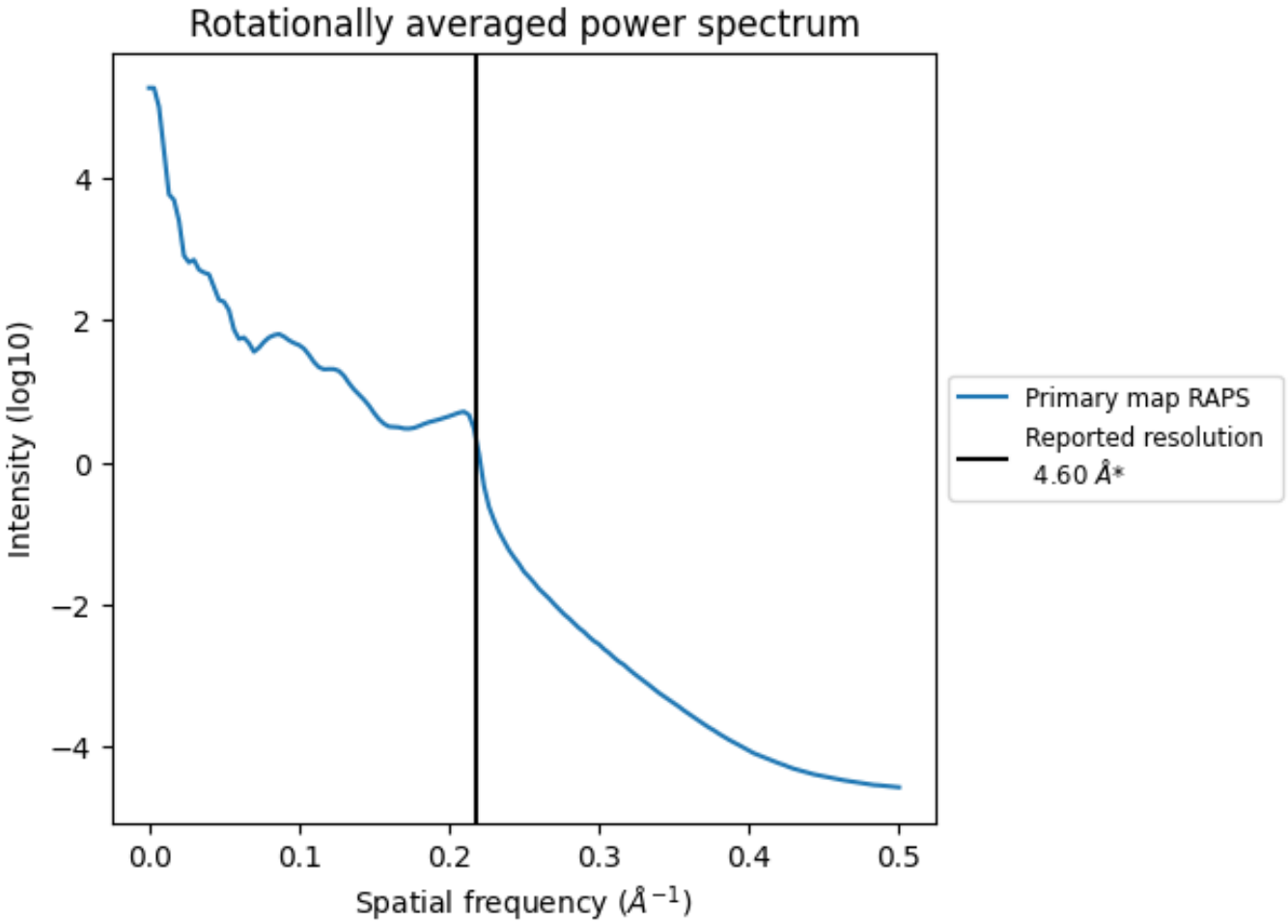
7.2 Volume estimate



The volume at the recommended contour level is 299 nm^3; this corresponds to an approximate mass of 270 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)

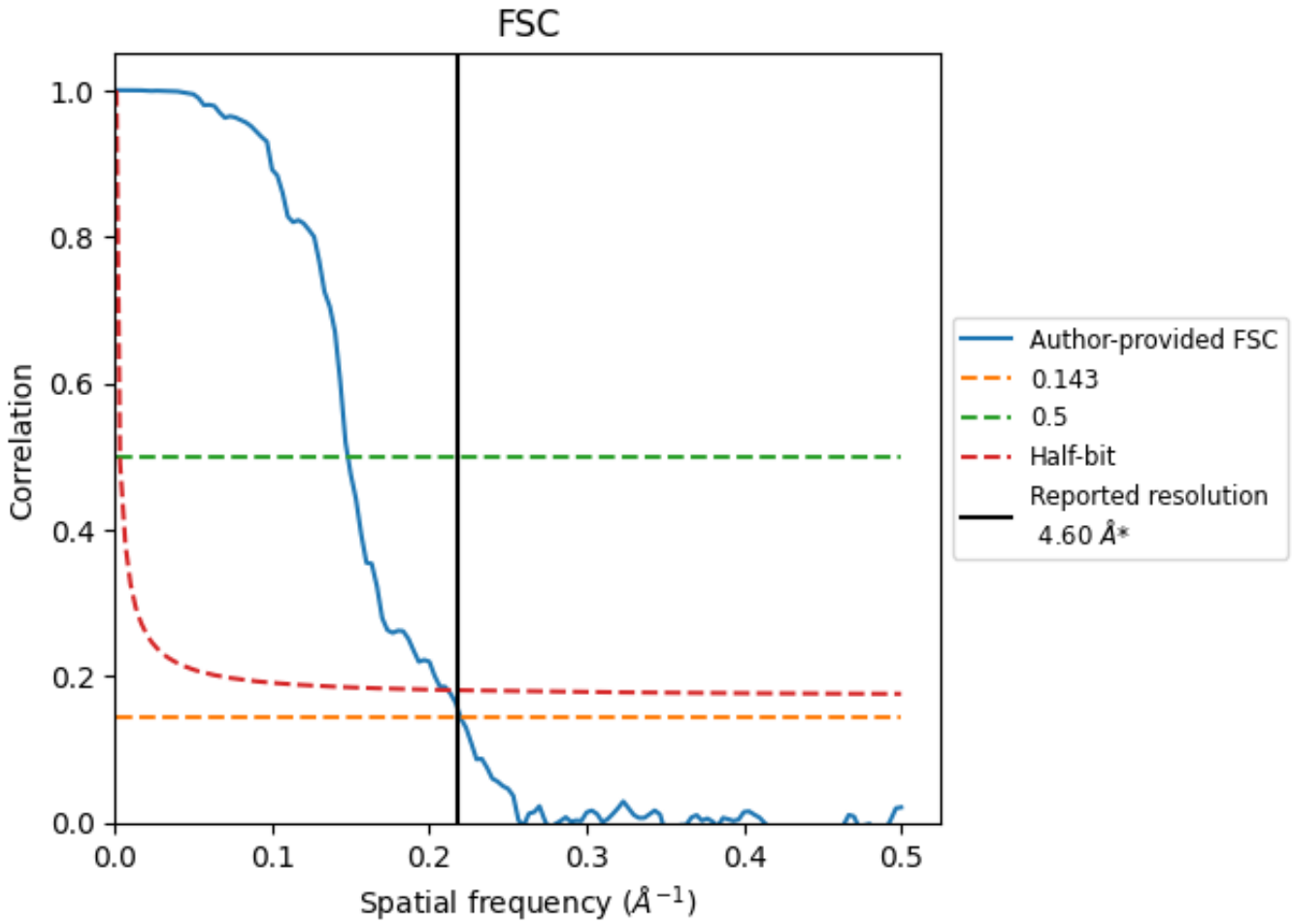


*Reported resolution corresponds to spatial frequency of 0.217 $Å^{-1}$

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

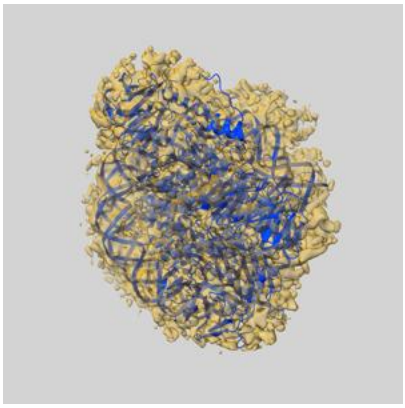
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.55	6.75	4.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

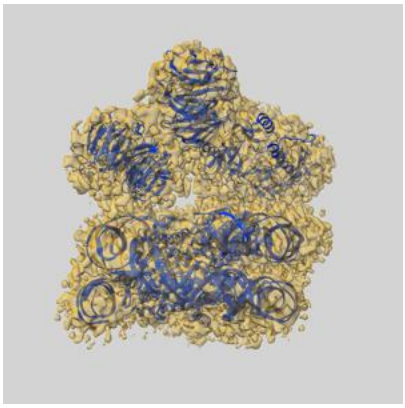
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21543 and PDB model 6W5M. Per-residue inclusion information can be found in section 3 on page 7.

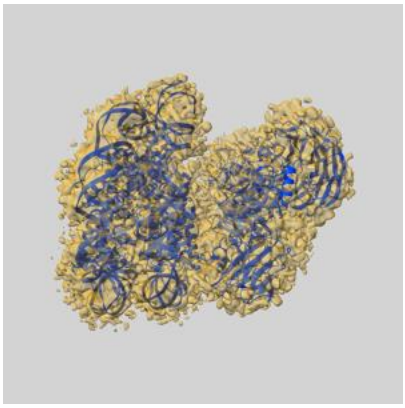
9.1 Map-model overlay



X



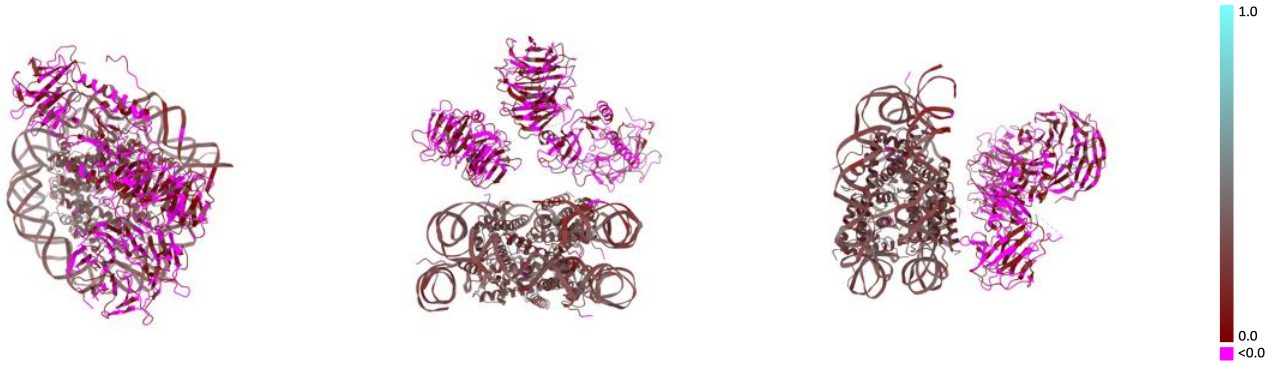
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0073 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.

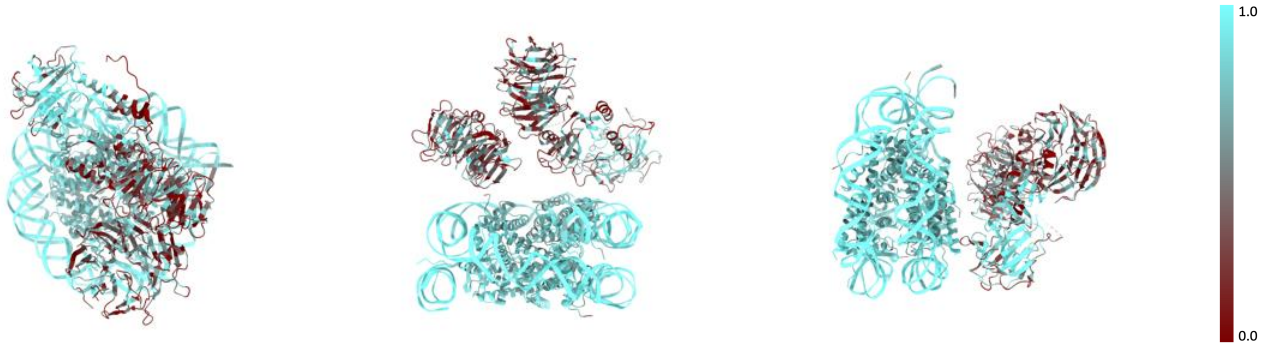
9.2 Q-score mapped to coordinate model (i)



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.

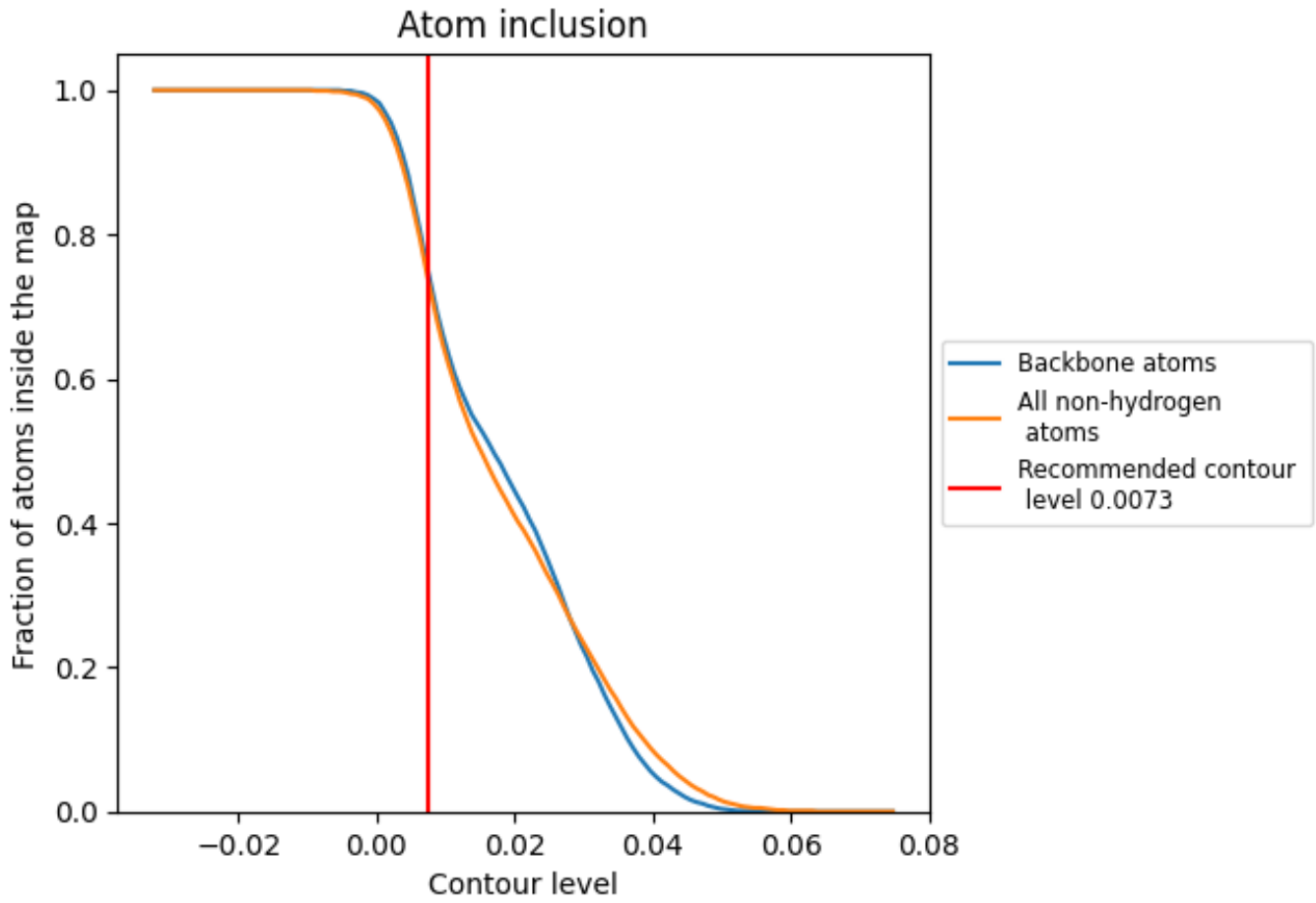
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0073).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.1770
A	0.3940	-0.0000
B	0.3860	0.0510
C	0.4390	0.0070
D	0.6570	0.0150
G	0.8380	0.2660
H	0.8710	0.2960
I	0.8560	0.2810
J	0.8760	0.2660
K	0.8510	0.2630
L	0.8840	0.2790
M	0.8800	0.2670
N	0.8750	0.2590
O	0.9790	0.2820
P	0.9790	0.2810