Full wwPDB EM Validation Report

Feb 26, 2024 – 12:59 PM JST

PDB ID	:	8X15
EMDB ID	:	EMD-37984
Title	:	Structure of nucleosome-bound SRCAP-C in the apo 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:

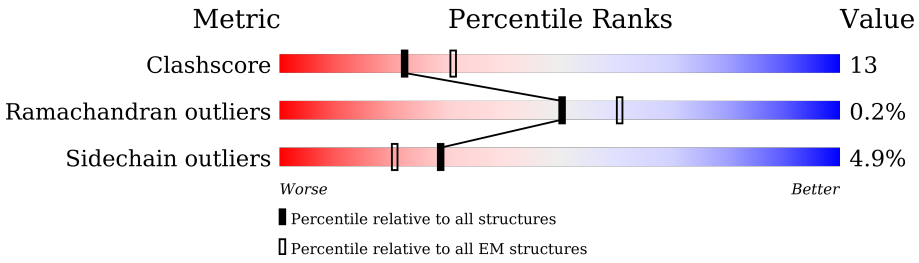
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	26% 62% 20% • 17%
1	E	130	16% 66% 12% • 19%
2	B	126	11% 56% 21% 24%
2	F	126	10% 66% 6% •• 25%
3	C	136	17% 51% 18% • 30%
3	G	136	21% 59% 12% 29%
4	D	103	13% 63% 16% 21%
4	H	103	10% 61% 16% • 22%

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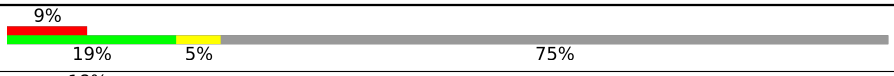
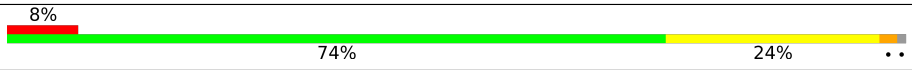
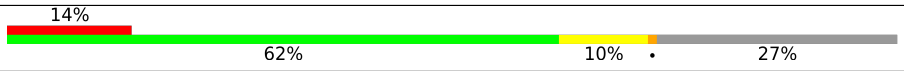
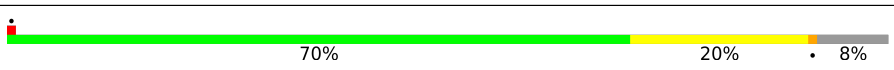
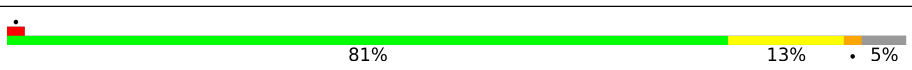
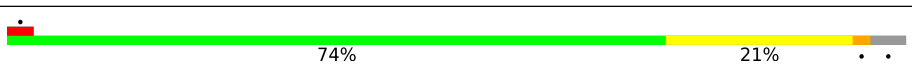
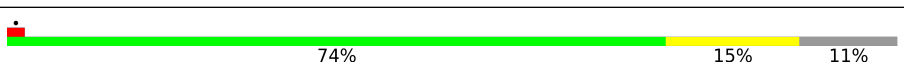
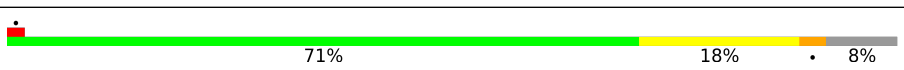
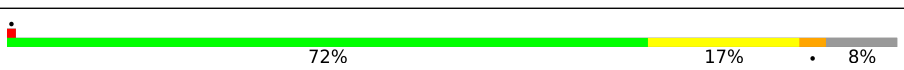
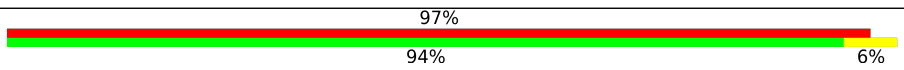
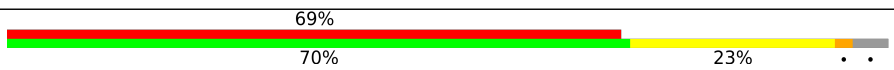
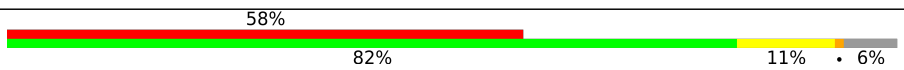
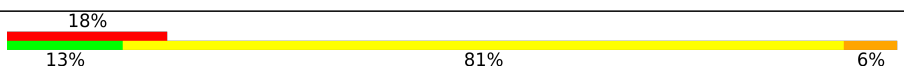
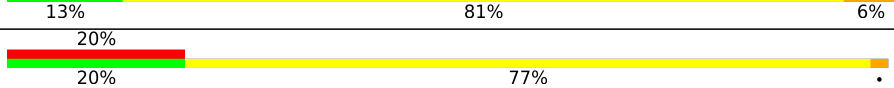
Mol	Chain	Length	Quality of chain
5	I	3230	
6	J	364	
7	K	396	
8	L	154	
9	M	456	
9	O	456	
9	Q	456	
10	N	463	
10	P	463	
10	R	463	
11	S	375	
11	U	375	
12	T	429	
13	V	467	
14	W	227	
15	X	137	
16	Y	137	

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
17	ADP	M	501	-	-	X	-
17	ADP	N	501	-	-	X	-
17	ADP	O	501	-	-	X	-
17	ADP	P	501	-	-	X	-
17	ADP	Q	501	-	-	X	-
17	ADP	R	501	-	-	X	-
18	ATP	U	401	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 55488 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	792	Total	C	N	O	S	0	0
			6519	4147	1202	1134	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	158	Total	C	N	O	S	0	0
			1316	826	252	234	4		

- 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, N-terminally processed.

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	187	Total	C	N	O	S	0	0
			1617	1032	299	282	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		

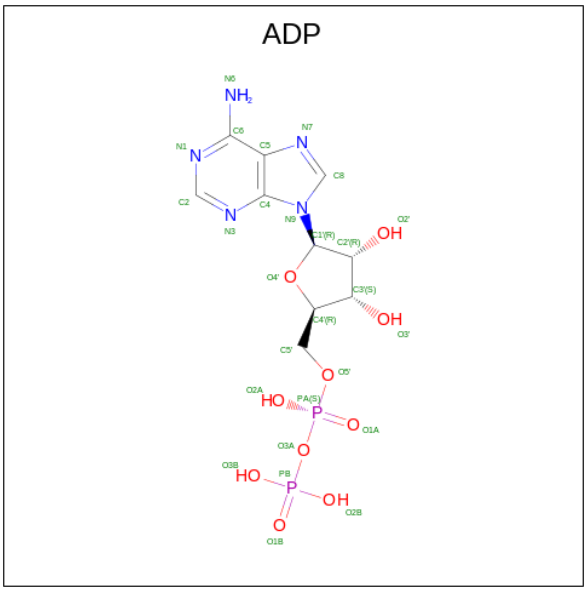
- Molecule 15 is a DNA chain called DNA (137-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	137	Total	C	N	O	P	0	0
			2829	1338	537	818	136		

- Molecule 16 is a DNA chain called DNA (137-MER).

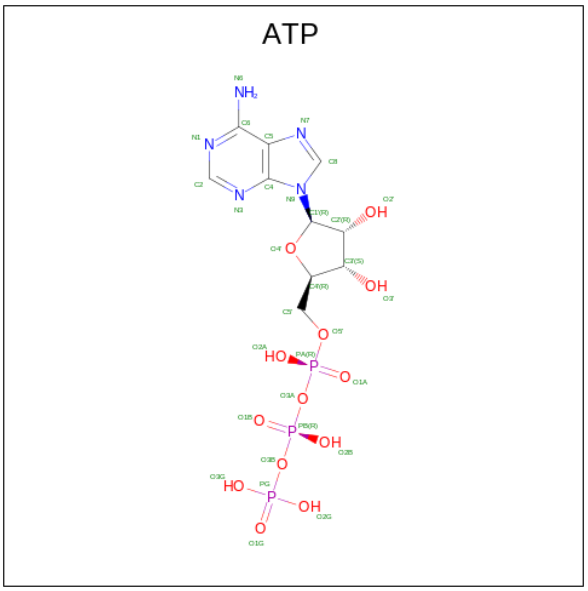
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	137	Total	C	N	O	P	0	0
			2785	1323	501	824	137		

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

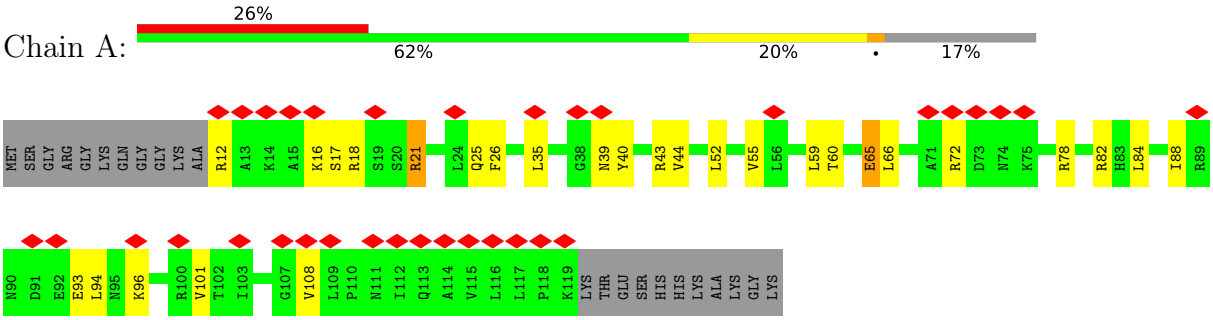


Mol	Chain	Residues	Atoms					AltConf
18	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	U	1	Total	C	N	O	P	0
			31	10	5	13	3	

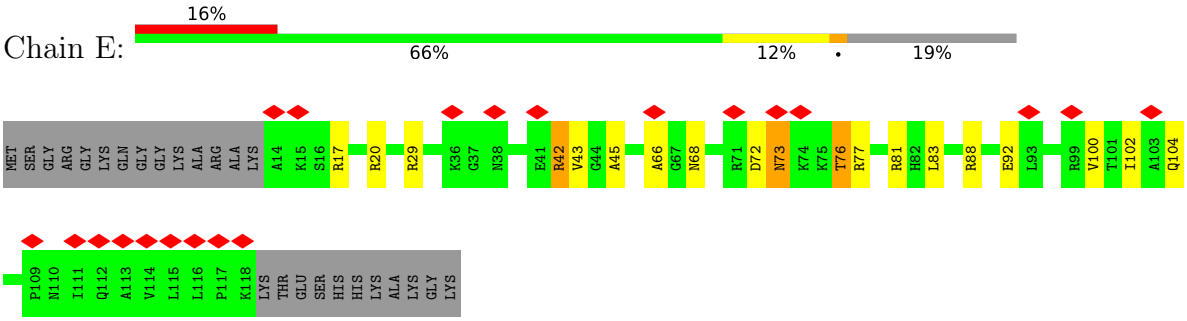
3 Residue-property plots (i)

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.

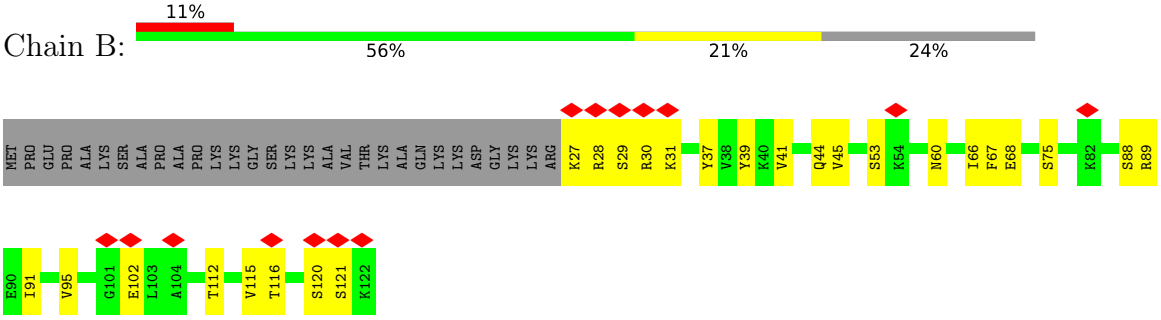
• Molecule 1: Histone H2A type 1-C



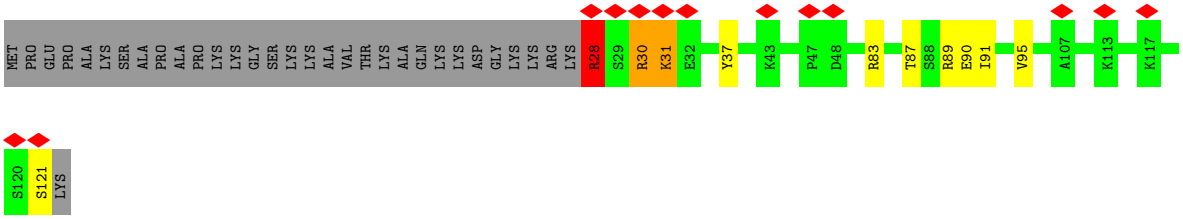
• Molecule 1: Histone H2A type 1-C



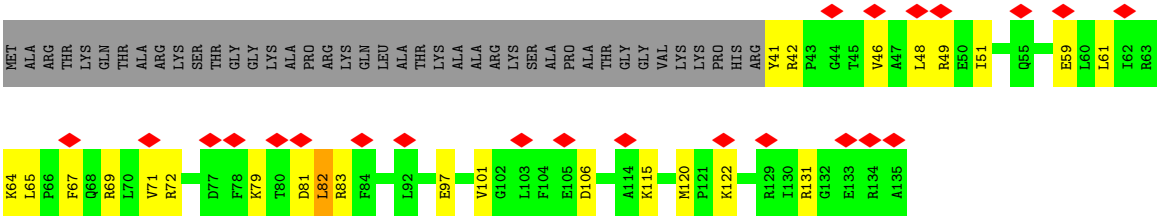
• Molecule 2: Histone H2B type 1-C/E/F/G/I



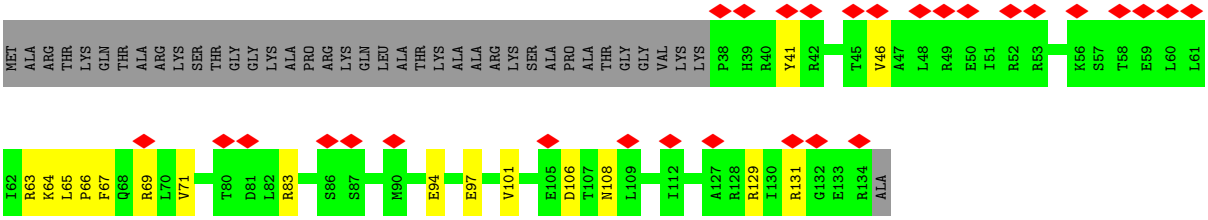
• Molecule 2: Histone H2B type 1-C/E/F/G/I



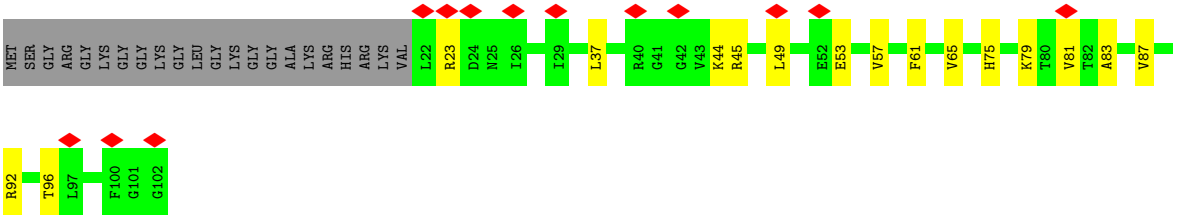
• Molecule 3: Histone H3.1



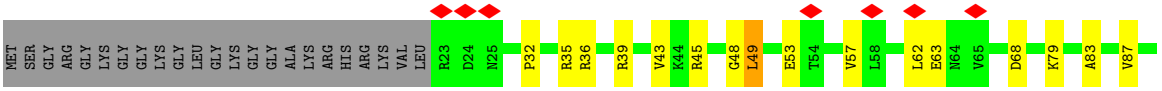
• Molecule 3: Histone H3.1

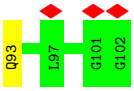


• Molecule 4: Histone H4

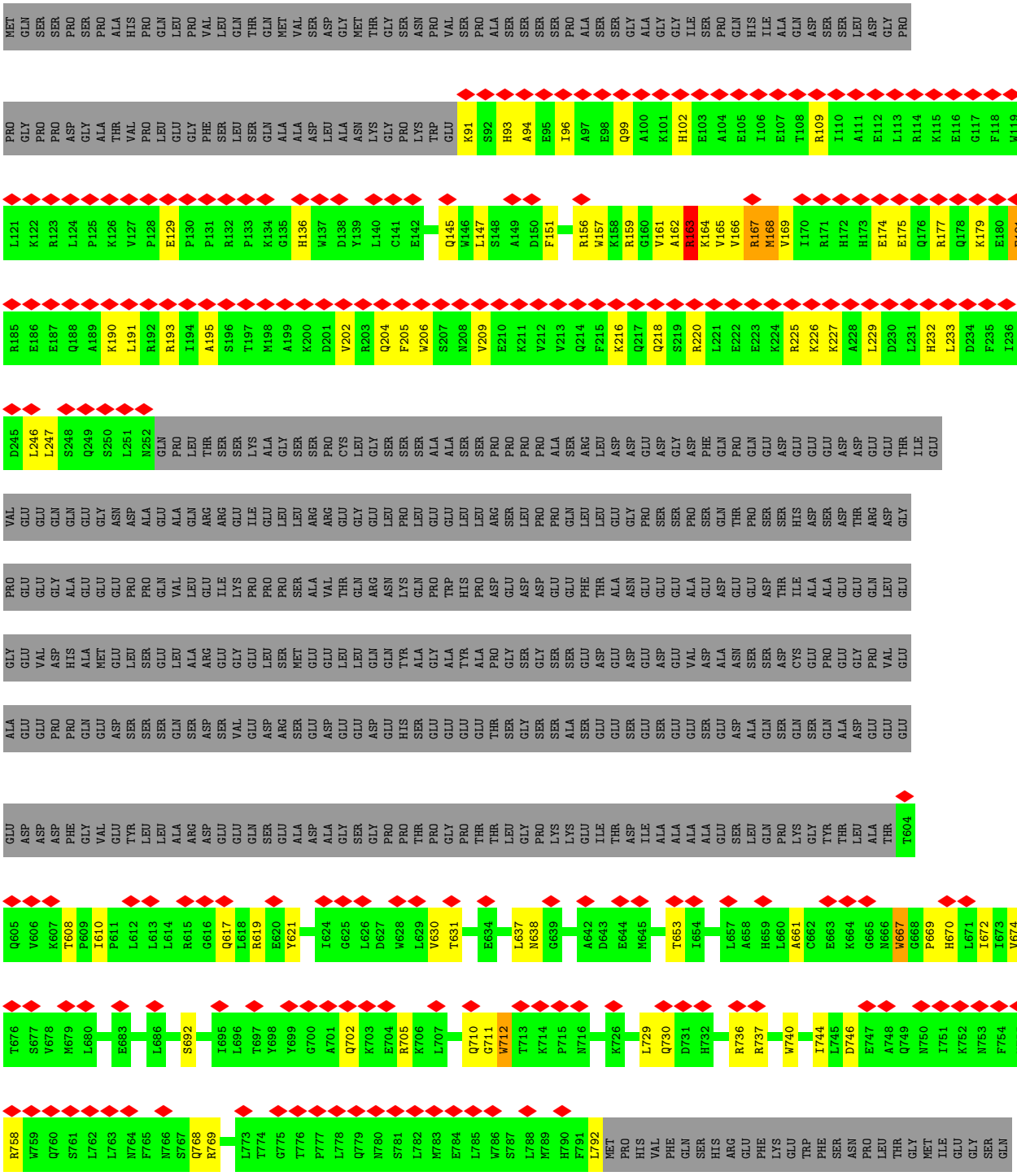


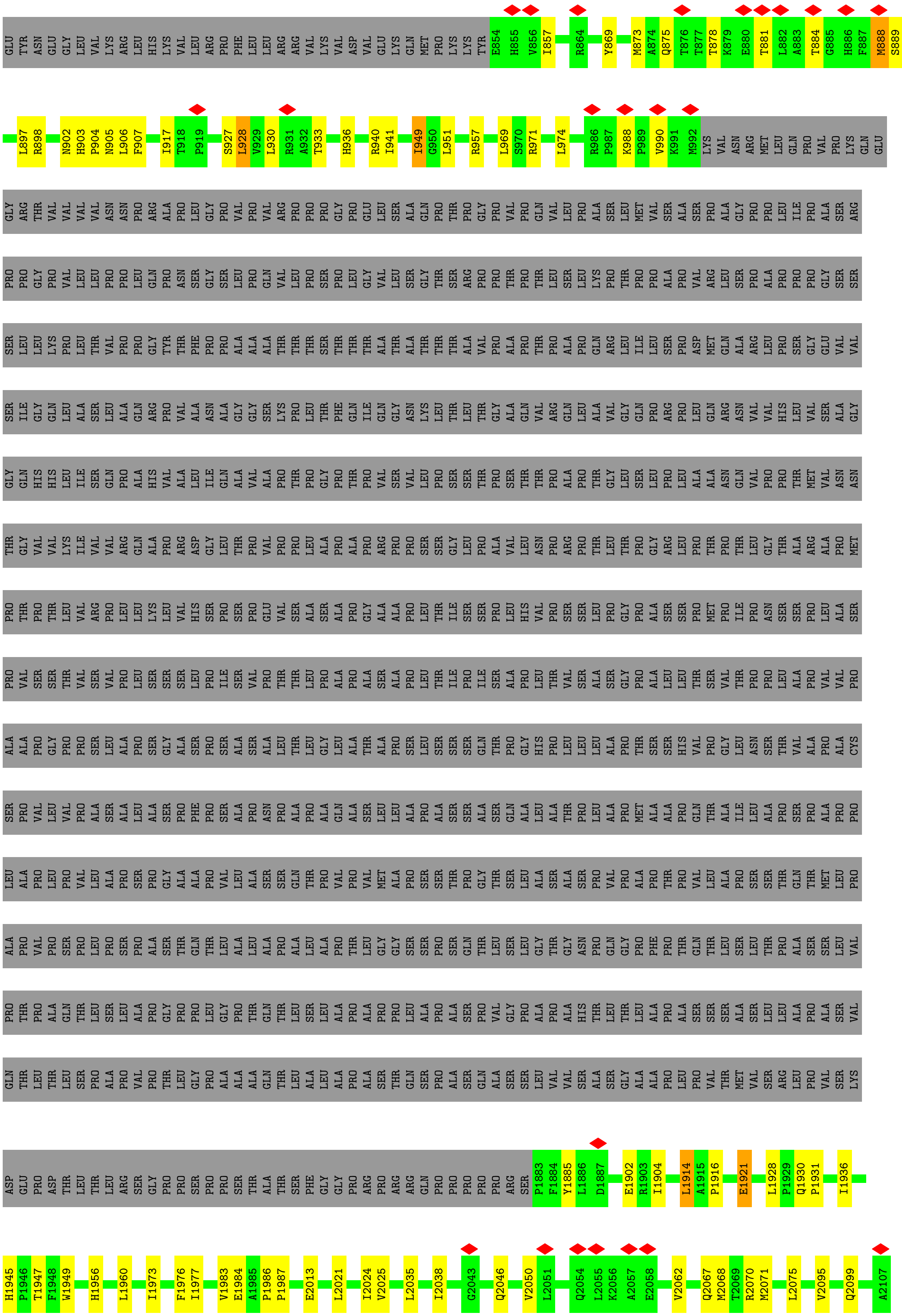
• Molecule 4: Histone H4

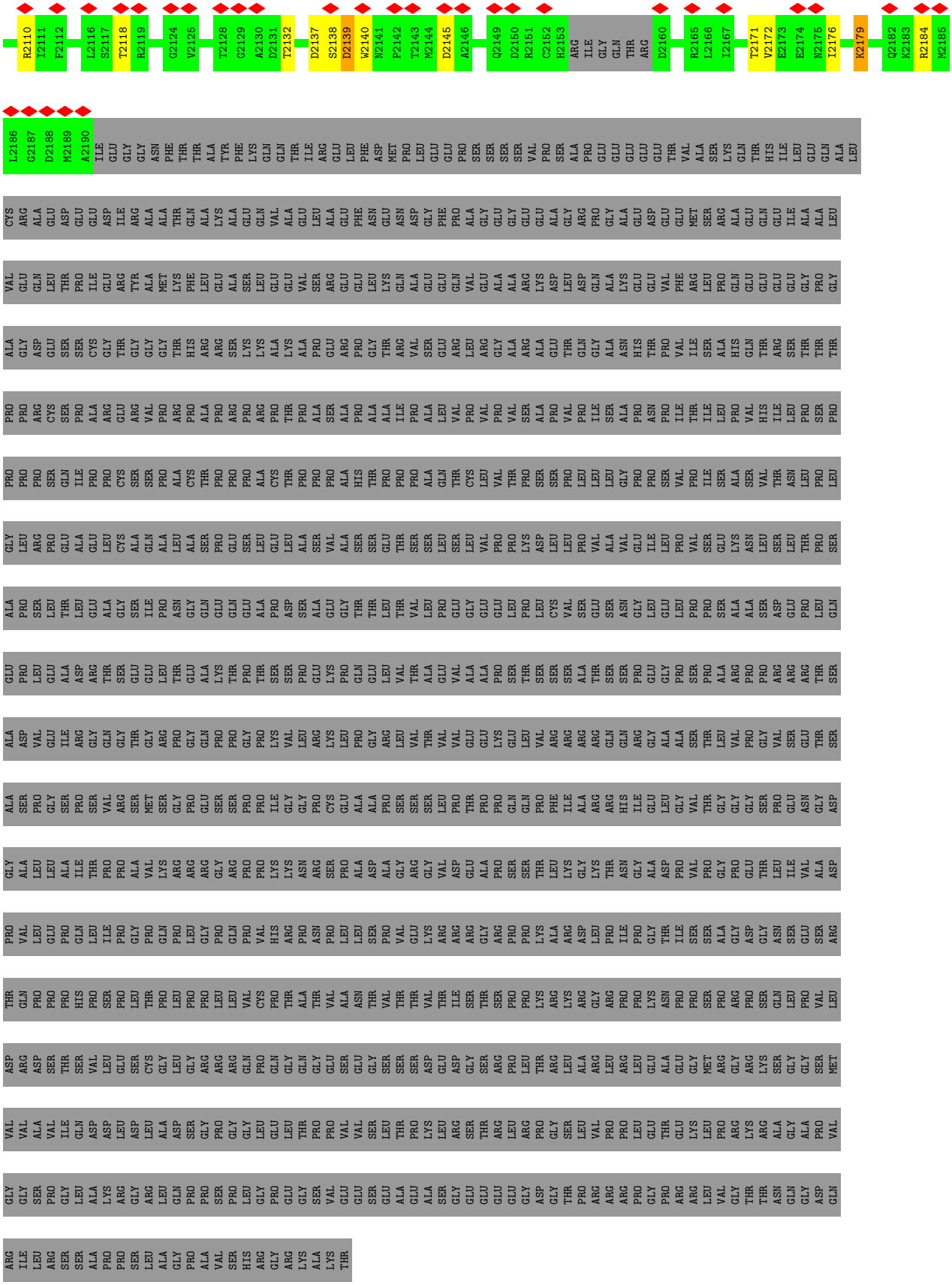




• Molecule 5: Helicase SRCAP

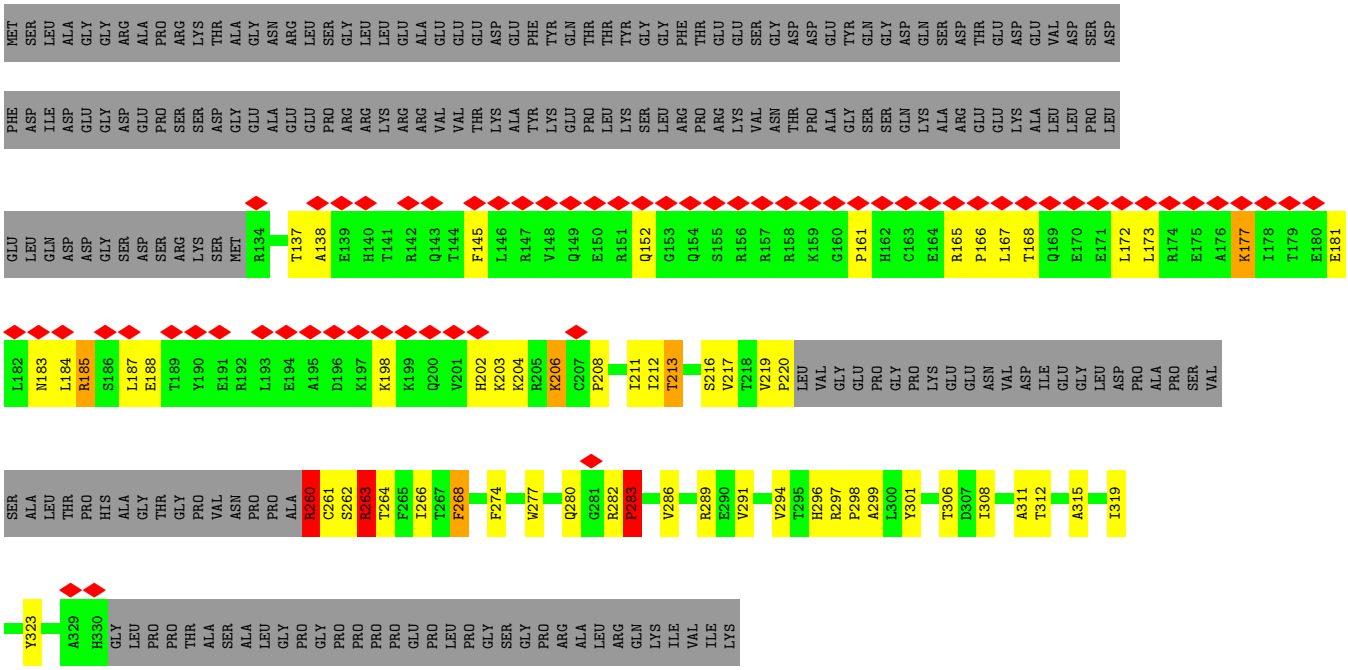



E854 H855 V856 I857 R864 Y869 M873 A874 Q875 T876 T877 T878 K879 E880 T881 L882 A883 T884 G885 H886 F887 M888 S889
L897 R898 N902 H903 P904 N905 L906 F907 I917 T918 P919 S927 L928 V929 L930 R931 A932 T933 H936 R940 I941 I949 G950 L951 R957 L969 S970 R971 L974 R986 P987 K988 P989 V990 K991 M992
P1883 F1884 Y1885 L1886 D1887 E1902 R1903 I1904 L1914 A1915 P1916 E1921 L1928 P1929 Q1930 P1931 I1936
H1945 P1946 T1947 F1948 W1949 H1956 L1960 I1973 F1976 I1977 V1983 E1984 A1985 P1986 P1987 E2013 L2021 I2024 V2025 L2035 I2038 G2043 Q2046 V2050 L2051 Q2054 L2055 K2056 A2057 E2058 V2062 Q2067 M2068 T2069 R2070 M2071 L2075 V2095 Q2099 A2107



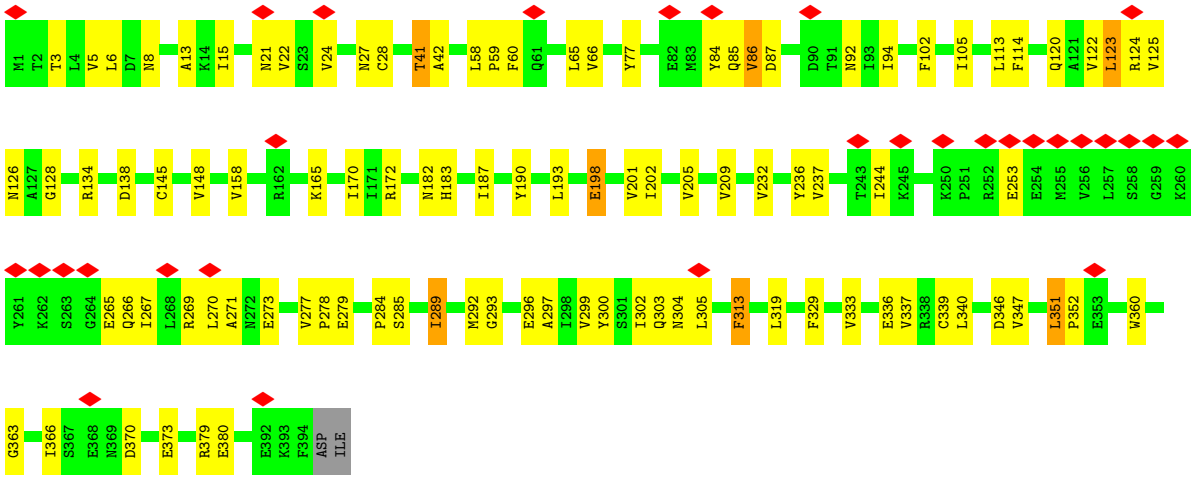
• Molecule 6: Vacuolar protein sorting-associated protein 72 homolog

Chain J:



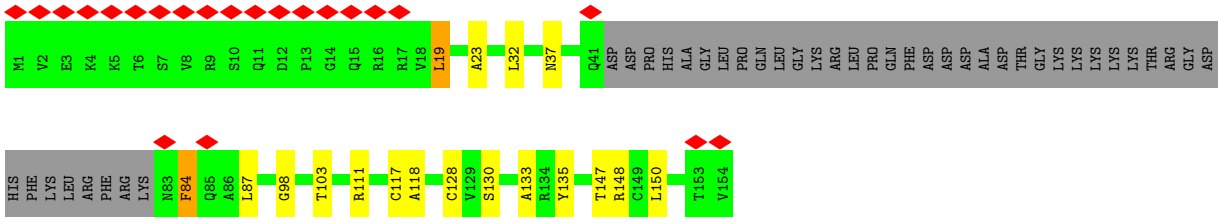
• Molecule 7: Actin-related protein 6

Chain K:



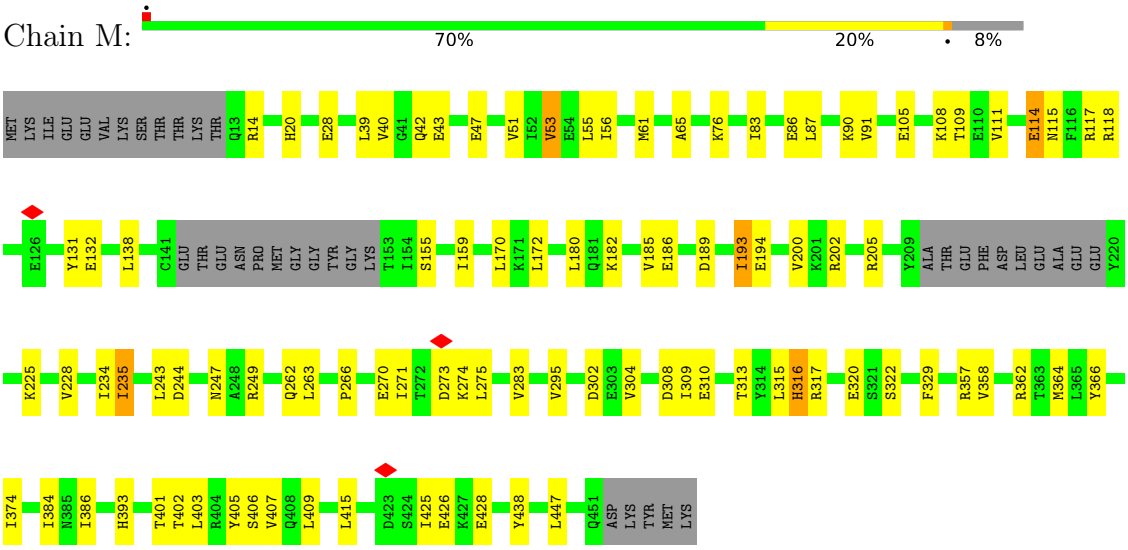
• Molecule 8: Zinc finger HIT domain-containing protein 1

Chain L:



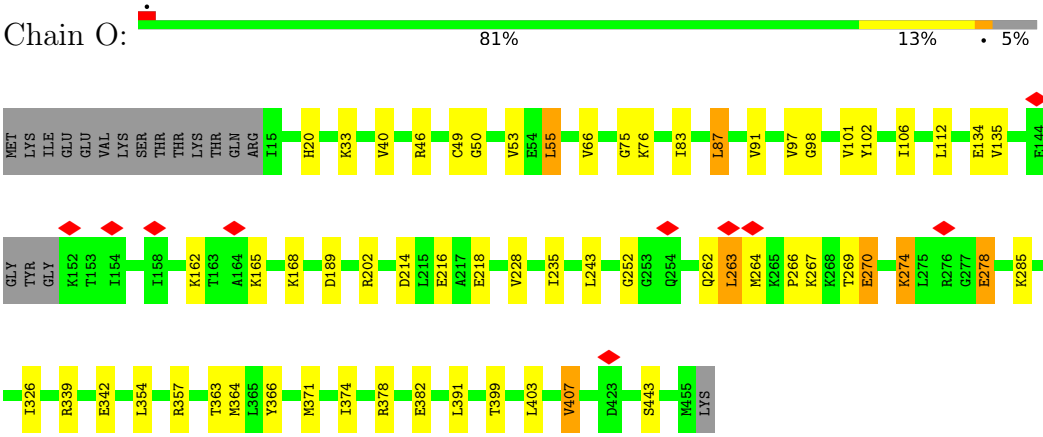
• Molecule 9: RuvB-like 1

Chain M:



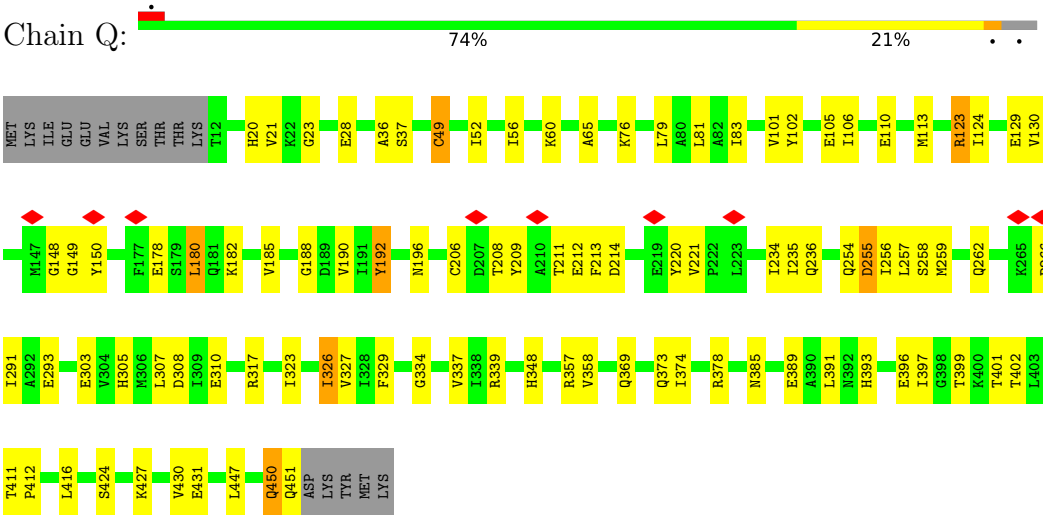
• Molecule 9: RuvB-like 1

Chain O:



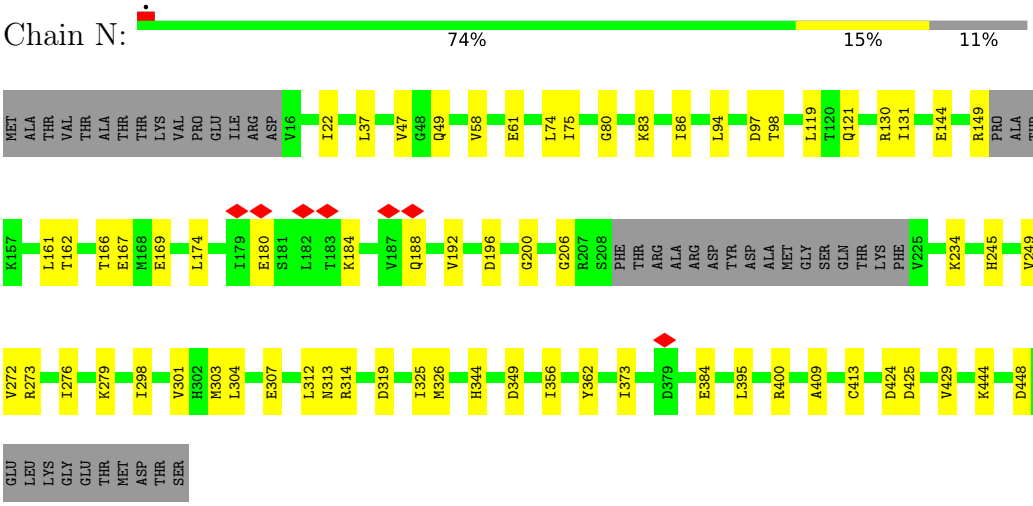
• Molecule 9: RuvB-like 1

Chain Q:



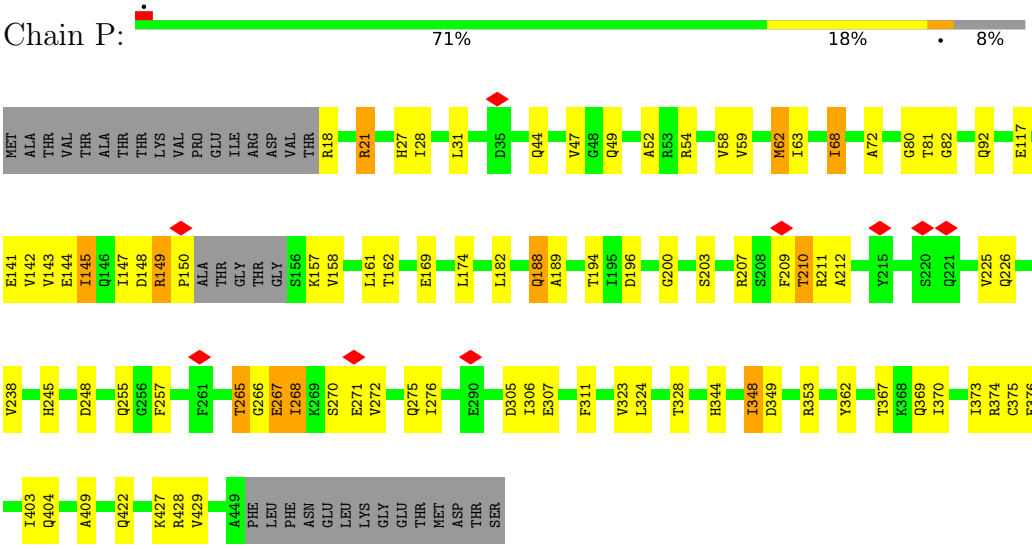
• Molecule 10: RuvB-like 2

Chain N:



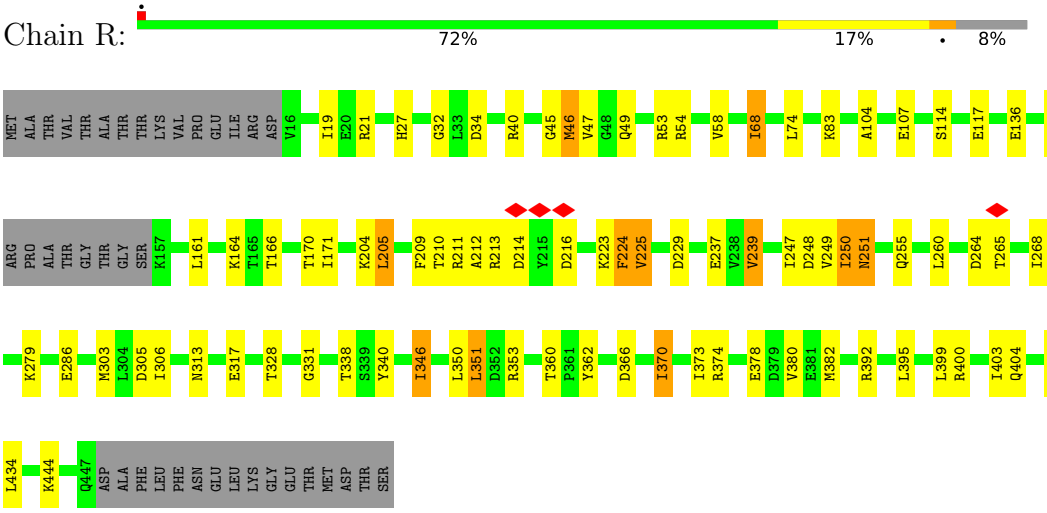
• Molecule 10: RuvB-like 2

Chain P:



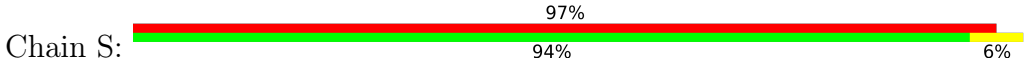
• Molecule 10: RuvB-like 2

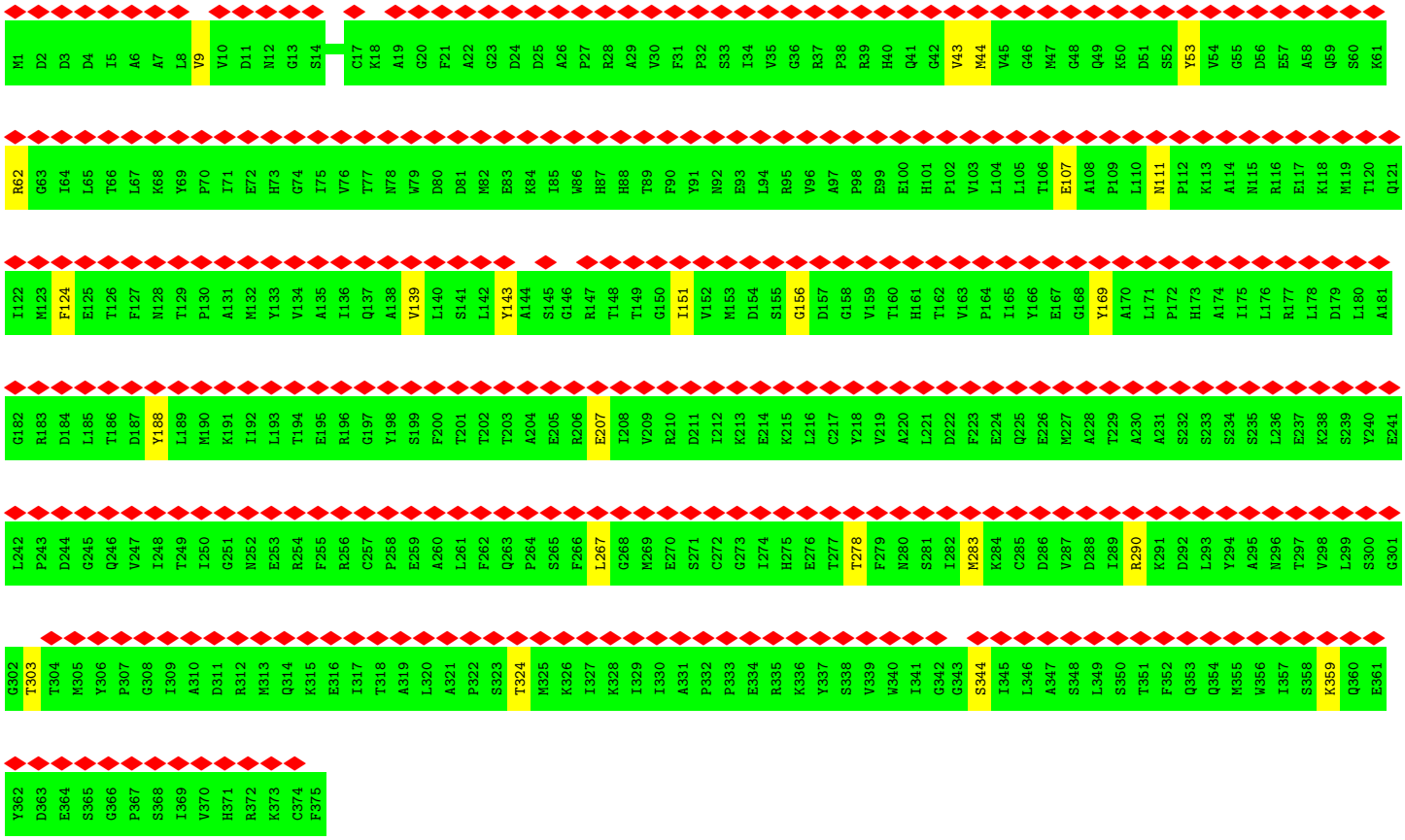
Chain R:



• Molecule 11: Actin, cytoplasmic 1, N-terminally processed

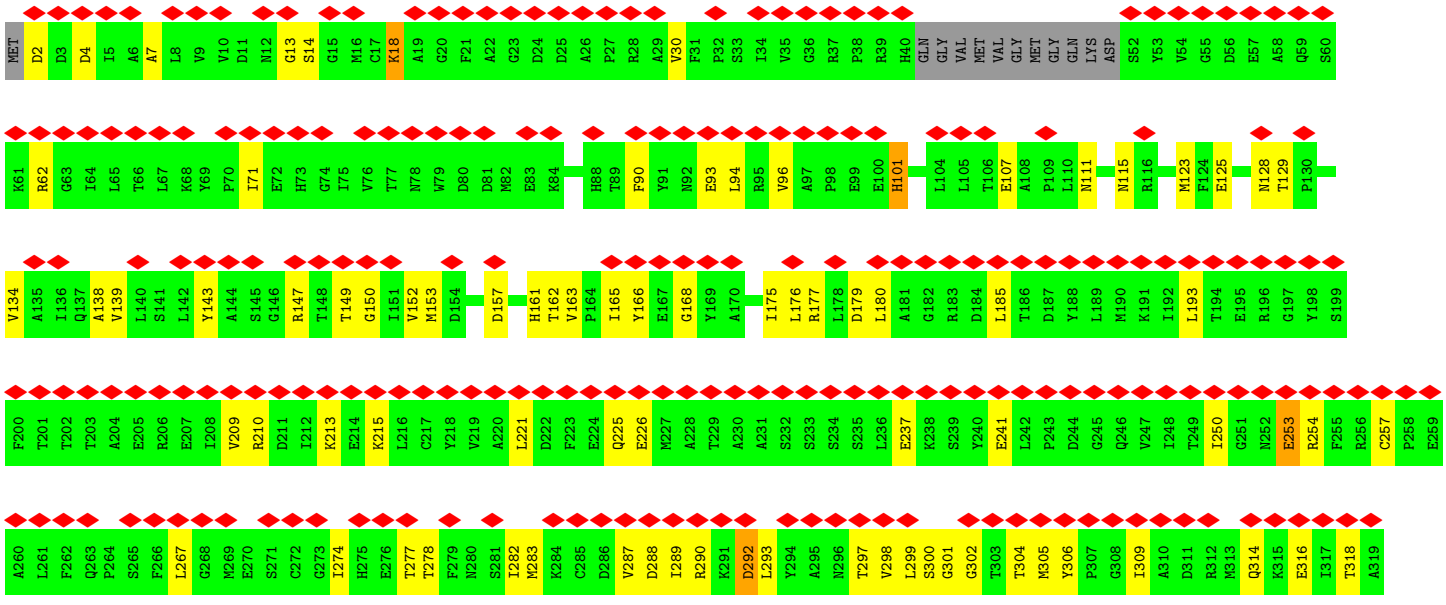
Chain S:

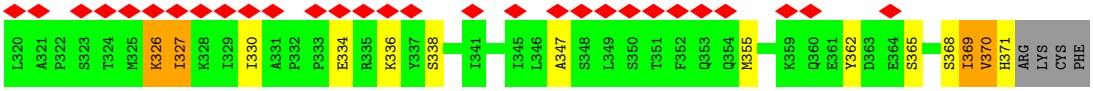




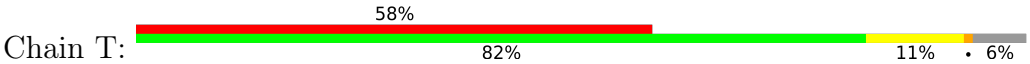
• Molecule 11: Actin, cytoplasmic 1, N-terminally processed

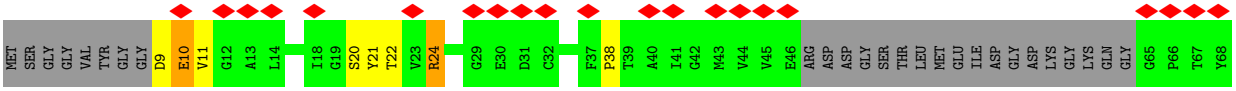
Chain U:

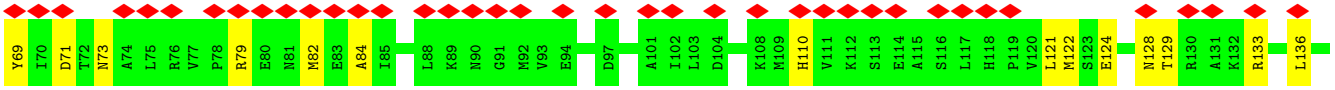


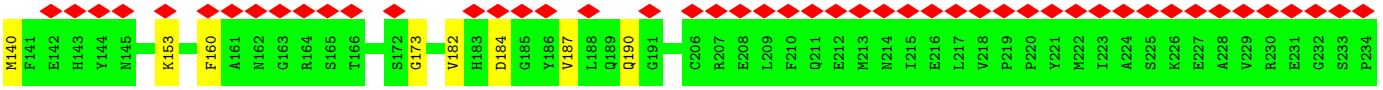


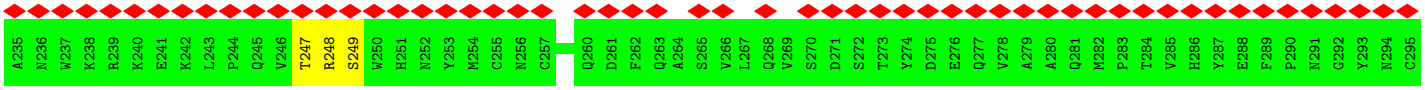
• Molecule 12: Actin-like protein 6A

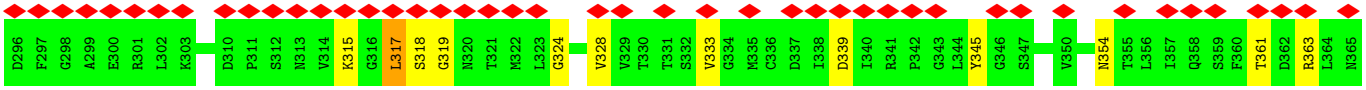


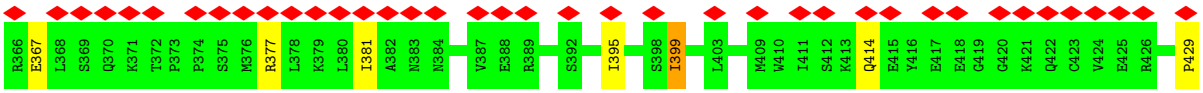




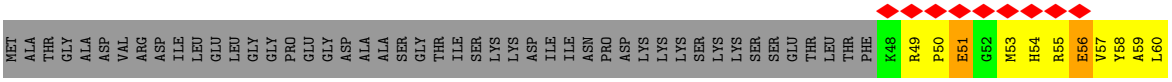


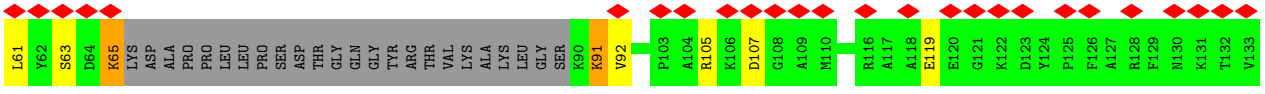


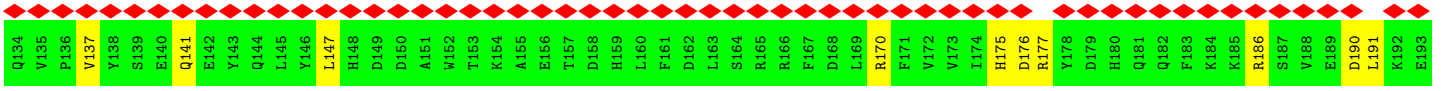


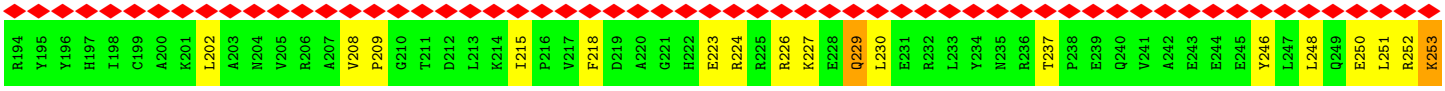


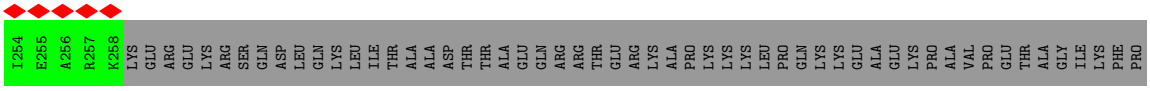
• Molecule 13: DNA methyltransferase 1-associated protein 1

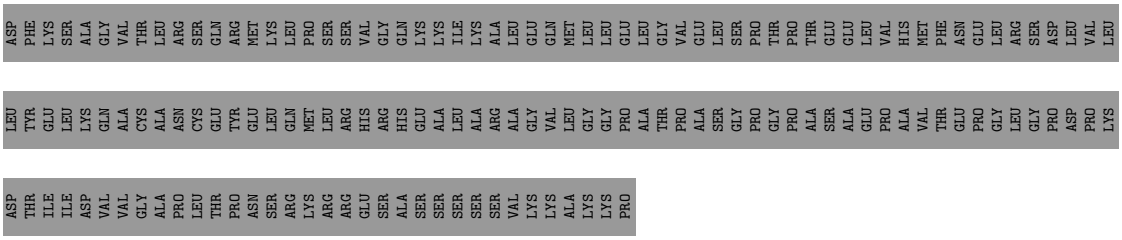






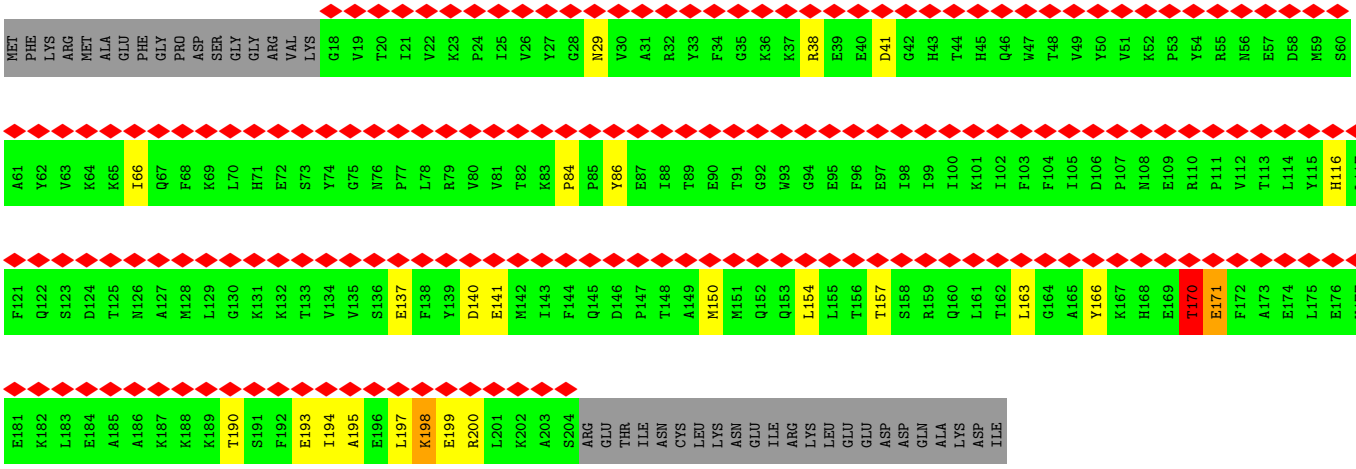






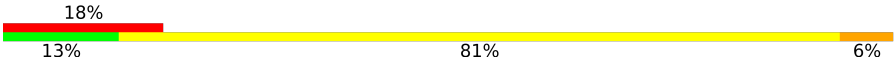
• Molecule 14: YEATS domain-containing protein 4

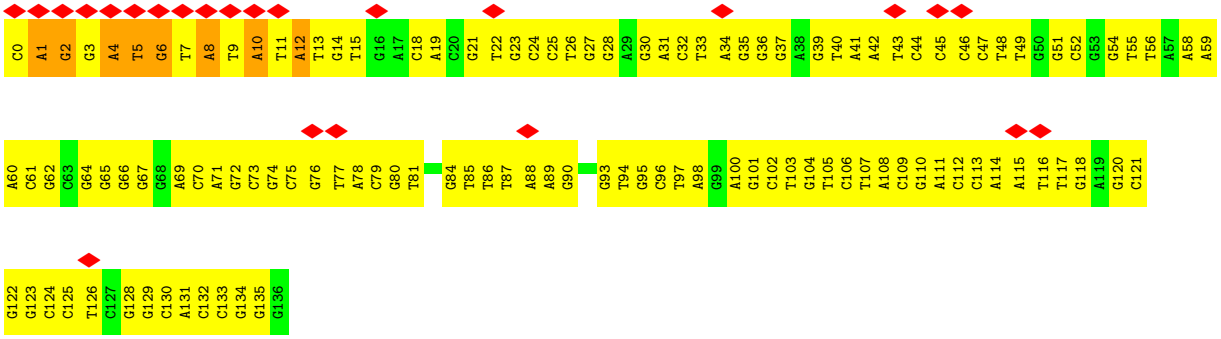
Chain W:



• Molecule 15: DNA (137-MER)

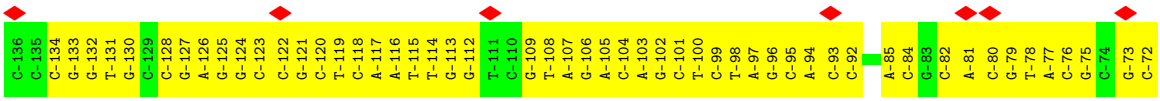
Chain X:

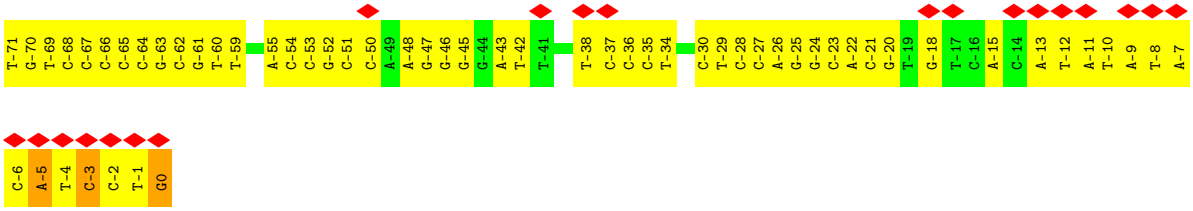




• Molecule 16: DNA (137-MER)

Chain Y:




T-71
G-70
T-69
C-68
C-67
C-66
C-65
C-64
G-63
C-62
G-61
T-60
T-59
A-55
C-54
C-53
G-52
C-51
C-50
A-49
A-48
G-47
G-46
G-45
G-44
A-43
T-42
T-41
T-38
C-37
C-36
C-35
T-34
C-30
T-29
C-28
C-27
A-26
G-25
G-24
C-23
A-22
C-21
G-20
T-19
G-18
T-17
C-16
A-15
C-14
A-13
T-12
A-11
T-10
A-9
T-8
A-7
C-6
A-5
T-4
C-3
C-2
T-1
G0

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1092654	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	0.195	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	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: ADP, ATP

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	0.24	0/843	0.39	0/1136
1	E	0.24	0/818	0.39	0/1104
2	B	0.24	0/766	0.38	0/1026
2	F	0.27	0/747	0.40	0/1004
3	C	0.24	0/789	0.38	0/1057
3	G	0.23	0/813	0.37	0/1090
4	D	0.24	0/653	0.42	0/873
4	H	0.24	0/645	0.42	0/862
5	I	0.25	0/6675	0.41	1/9019 (0.0%)
6	J	0.31	0/1347	0.51	1/1818 (0.1%)
7	K	0.24	0/3283	0.42	0/4445
8	L	0.25	0/909	0.42	0/1227
9	M	0.24	0/3253	0.43	1/4382 (0.0%)
9	O	0.24	0/3382	0.42	0/4559
9	Q	0.24	0/3413	0.42	0/4603
10	N	0.23	0/3217	0.42	0/4328
10	P	0.25	0/3324	0.43	0/4477
10	R	0.24	0/3329	0.42	0/4479
11	S	0.24	0/2988	0.40	0/4045
11	U	0.24	0/2863	0.42	0/3882
12	T	0.24	0/3217	0.40	0/4362
13	V	0.24	0/1661	0.41	0/2234
14	W	0.37	1/1578 (0.1%)	0.53	0/2128
15	X	0.62	7/3179 (0.2%)	0.85	3/4911 (0.1%)
16	Y	0.59	2/3118 (0.1%)	0.84	1/4804 (0.0%)
All	All	0.31	10/56810 (0.0%)	0.49	7/77855 (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
2	F	0	1
5	I	0	2
6	J	0	2
9	Q	0	1
11	U	0	1
14	W	0	1
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	X	12	DA	C1'-N9	-7.16	1.37	1.47
16	Y	0	DG	C1'-N9	-6.97	1.37	1.47
15	X	6	DG	C1'-N9	-6.81	1.37	1.47
15	X	8	DA	C1'-N9	-6.60	1.38	1.47
15	X	2	DG	C1'-N9	-6.59	1.38	1.47
15	X	10	DA	C1'-N9	-6.49	1.38	1.47
14	W	198	LYS	CD-CE	6.45	1.67	1.51
16	Y	-5	DA	C1'-N9	-6.33	1.38	1.47
15	X	1	DA	C1'-N9	-5.25	1.39	1.47
15	X	0	DC	C1'-N1	5.07	1.55	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	-3	DC	P-O3'-C3'	-10.46	107.14	119.70
15	X	5	DT	P-O3'-C3'	-9.41	108.41	119.70
6	J	283	PRO	CA-N-CD	-8.45	99.68	111.50
15	X	8	DA	P-O3'-C3'	-8.20	109.86	119.70
5	I	667	TRP	N-CA-C	-7.08	91.89	111.00
15	X	4	DA	P-O3'-C3'	-6.51	111.88	119.70
9	M	234	ILE	CG1-CB-CG2	6.49	125.68	111.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	28	ARG	Sidechain
5	I	163	ARG	Sidechain
5	I	167	ARG	Sidechain
6	J	260	ARG	Sidechain
6	J	263	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	Q	255	ASP	Peptide
11	U	257	CYS	Peptide
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	890	40	0
1	E	808	0	864	24	0
2	B	755	0	780	55	0
2	F	736	0	755	24	0
3	C	779	0	816	27	0
3	G	801	0	839	22	0
4	D	646	0	687	14	0
4	H	638	0	676	23	0
5	I	6519	0	6602	168	0
6	J	1316	0	1330	54	0
7	K	3209	0	3132	63	0
8	L	893	0	880	15	0
9	M	3213	0	3331	80	0
9	O	3339	0	3425	48	0
9	Q	3368	0	3452	75	0
10	N	3185	0	3271	55	0
10	P	3287	0	3335	89	0
10	R	3293	0	3373	76	0
11	S	2925	0	2891	15	0
11	U	2802	0	2760	85	0
12	T	3146	0	3086	37	0
13	V	1617	0	1584	57	0
14	W	1542	0	1556	27	0
15	X	2829	0	1537	290	0
16	Y	2785	0	1538	289	0
17	M	27	0	12	13	0
17	N	27	0	12	11	0
17	O	27	0	12	12	0
17	P	27	0	12	27	0
17	Q	27	0	12	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	27	0	11	17	0
18	T	31	0	12	6	0
18	U	31	0	12	25	0
All	All	55488	0	53485	1381	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 13.

All (1381) 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:I:711:GLY:H	15:X:135:DG:P	1.29	1.54
1:A:43:ARG:NE	16:Y:-34:DT:H5"	1.20	1.51
2:B:30:ARG:HH11	16:Y:-24:DG:C4'	1.31	1.44
2:B:89:ARG:HE	13:V:63:SER:CB	1.33	1.39
15:X:27:DG:N2	16:Y:-26:DA:H2	0.91	1.38
1:A:43:ARG:CZ	16:Y:-34:DT:H5"	1.52	1.37
16:Y:-35:DC:C2'	16:Y:-34:DT:H73	1.55	1.36
16:Y:-35:DC:N1	16:Y:-34:DT:H72	1.40	1.34
5:I:711:GLY:CA	15:X:135:DG:OP1	1.76	1.33
1:A:43:ARG:NH1	16:Y:-34:DT:C5'	1.89	1.31
15:X:74:DG:C2	16:Y:-73:DG:N2	1.97	1.31
16:Y:-35:DC:C2'	16:Y:-34:DT:C7	2.10	1.30
6:J:277:TRP:O	6:J:280:GLN:HG3	1.32	1.29
5:I:711:GLY:N	15:X:135:DG:P	2.06	1.28
10:P:47:VAL:O	17:P:501:ADP:N6	1.62	1.28
16:Y:-35:DC:C6	16:Y:-34:DT:H72	1.68	1.28
6:J:282:ARG:NH2	9:Q:139:THR:HG22	1.43	1.28
1:A:43:ARG:NE	16:Y:-34:DT:C5'	1.94	1.28
1:A:43:ARG:HH22	16:Y:-35:DC:C4'	1.43	1.28
5:I:736:ARG:NE	16:Y:-130:DG:P	2.07	1.27
15:X:21:DG:C2	16:Y:-20:DG:N2	2.00	1.27
1:A:43:ARG:NH1	16:Y:-34:DT:H5'	1.49	1.26
11:U:302:GLY:N	18:U:401:ATP:O2A	1.66	1.25
12:T:377:ARG:NH1	15:X:24:DC:OP1	1.68	1.24
1:A:43:ARG:CZ	16:Y:-34:DT:C5'	2.12	1.24
2:B:30:ARG:NH1	16:Y:-24:DG:O4'	1.71	1.24
10:P:27:HIS:CE1	17:P:501:ADP:O2'	1.89	1.24
1:A:43:ARG:HE	16:Y:-34:DT:C5'	1.48	1.23
2:B:28:ARG:NH2	16:Y:-22:DA:H5"	1.54	1.23
11:U:13:GLY:HA2	18:U:401:ATP:O1G	1.33	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:39:DG:C2'	15:X:40:DT:H71	1.70	1.22
1:A:18:ARG:N	15:X:30:DG:OP1	1.71	1.22
1:A:16:LYS:O	15:X:30:DG:H5"	1.36	1.21
15:X:110:DG:C2	16:Y:-109:DG:N2	2.08	1.20
12:T:20:SER:HB2	18:T:501:ATP:O3G	1.45	1.16
6:J:161:PRO:HG3	16:Y:-133:DG:OP1	1.46	1.16
13:V:49:ARG:NH2	15:X:41:DA:OP1	1.79	1.16
5:I:711:GLY:N	15:X:135:DG:OP1	1.77	1.14
1:A:43:ARG:NH2	16:Y:-35:DC:H4'	1.39	1.14
15:X:27:DG:N2	16:Y:-26:DA:C2	1.82	1.14
15:X:74:DG:C2	16:Y:-73:DG:C2	2.34	1.13
2:B:29:SER:OG	15:X:102:DC:OP1	1.66	1.12
15:X:74:DG:N2	16:Y:-73:DG:C2	2.17	1.12
5:I:156:ARG:NH2	16:Y:-27:DC:OP1	1.82	1.12
11:U:13:GLY:CA	18:U:401:ATP:O1G	1.97	1.12
2:B:89:ARG:HE	13:V:63:SER:HB3	1.03	1.10
3:C:81:ASP:OD2	14:W:163:LEU:HD11	1.50	1.10
2:B:89:ARG:NE	13:V:63:SER:HB3	1.65	1.10
2:B:28:ARG:NH2	16:Y:-22:DA:C5'	2.16	1.08
10:N:400:ARG:NH2	17:N:501:ADP:O3A	1.86	1.08
11:U:157:ASP:OD1	18:U:401:ATP:O3'	1.70	1.07
16:Y:-35:DC:H2"	16:Y:-34:DT:H73	1.15	1.07
15:X:39:DG:H2"	15:X:40:DT:C7	1.84	1.07
2:F:83:ARG:NH2	16:Y:-106:DG:O5'	1.87	1.06
16:Y:-35:DC:H2'	16:Y:-34:DT:C7	1.86	1.06
2:B:89:ARG:NE	13:V:63:SER:CB	2.17	1.06
4:D:23:ARG:HD2	14:W:84:PRO:O	1.55	1.06
5:I:736:ARG:NH2	16:Y:-130:DG:H3'	1.69	1.06
15:X:8:DA:H2'	15:X:9:DT:H71	1.34	1.05
13:V:49:ARG:CZ	15:X:41:DA:OP1	2.06	1.04
15:X:21:DG:C2	16:Y:-20:DG:C2	2.46	1.03
10:R:47:VAL:O	17:R:501:ADP:N6	1.91	1.03
6:J:161:PRO:CG	16:Y:-133:DG:OP1	2.06	1.03
2:B:30:ARG:NH1	16:Y:-24:DG:C4'	2.16	1.03
5:I:96:ILE:HD11	14:W:197:LEU:HD21	1.38	1.02
11:U:306:TYR:HE1	18:U:401:ATP:C2	1.76	1.02
15:X:76:DG:N2	16:Y:-75:DG:C2	2.28	1.02
16:Y:-35:DC:C1'	16:Y:-34:DT:H72	1.90	1.01
3:C:49:ARG:HD3	15:X:7:DT:P	2.00	1.01
3:G:63:ARG:NH2	16:Y:-55:DA:O3'	1.93	1.01
6:J:277:TRP:HE3	6:J:280:GLN:HE21	1.04	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:711:GLY:HA2	15:X:135:DG:OP1	1.59	1.00
4:D:79:LYS:HB2	15:X:100:DA:OP1	1.61	1.00
1:A:43:ARG:HB2	16:Y:-34:DT:OP1	1.60	0.99
9:O:374:ILE:HG23	17:O:501:ADP:N3	1.78	0.99
9:Q:374:ILE:HG23	17:Q:501:ADP:N3	1.77	0.99
2:F:83:ARG:CD	16:Y:-106:DG:OP1	2.12	0.98
11:U:306:TYR:CE1	18:U:401:ATP:H2	1.82	0.98
2:F:83:ARG:NH2	16:Y:-106:DG:H3'	1.79	0.97
5:I:736:ARG:NE	16:Y:-130:DG:OP2	1.97	0.97
5:I:737:ARG:NH1	15:X:132:DC:O2	1.98	0.97
3:C:69:ARG:NH1	15:X:89:DA:OP2	1.98	0.96
10:P:80:GLY:HA2	17:P:501:ADP:O3B	1.64	0.96
15:X:74:DG:N3	16:Y:-73:DG:N2	2.13	0.95
2:B:30:ARG:HH11	16:Y:-24:DG:H4'	1.32	0.95
6:J:282:ARG:NH2	9:Q:139:THR:CG2	2.30	0.94
5:I:711:GLY:N	15:X:135:DG:OP2	1.92	0.94
4:H:45:ARG:HG3	16:Y:-64:DC:OP1	1.66	0.94
9:M:20:HIS:HE1	17:M:501:ADP:O2'	1.49	0.94
6:J:260:ARG:HA	10:P:210:THR:HA	1.47	0.94
5:I:736:ARG:HD3	16:Y:-130:DG:O5'	1.63	0.94
15:X:6:DG:C2	15:X:7:DT:C2	2.56	0.94
11:U:306:TYR:CE1	18:U:401:ATP:C2	2.56	0.93
2:B:27:LYS:HG3	15:X:103:DT:OP1	1.67	0.93
6:J:282:ARG:HH22	9:Q:139:THR:HG22	1.29	0.93
9:M:76:LYS:NZ	17:M:501:ADP:O2B	2.00	0.93
9:O:374:ILE:HG12	17:O:501:ADP:C2	2.02	0.93
16:Y:-35:DC:H2'	16:Y:-34:DT:H73	1.39	0.92
16:Y:-35:DC:C6	16:Y:-34:DT:C7	2.52	0.92
10:P:27:HIS:CE1	17:P:501:ADP:HO2'	1.81	0.91
5:I:96:ILE:CD1	14:W:197:LEU:HD21	2.01	0.91
16:Y:-115:DT:H2'	16:Y:-114:DT:H72	1.51	0.91
2:F:83:ARG:HD2	16:Y:-106:DG:OP1	1.70	0.90
16:Y:-115:DT:C2'	16:Y:-114:DT:H72	2.01	0.90
16:Y:-5:DA:H2"	16:Y:-4:DT:H5'	1.54	0.90
15:X:110:DG:N2	16:Y:-109:DG:N2	2.18	0.90
1:E:42:ARG:HG3	15:X:111:DA:H5'	1.52	0.90
2:B:116:THR:HG22	13:V:57:VAL:CG1	2.02	0.90
5:I:737:ARG:CZ	16:Y:-132:DG:H21	1.85	0.90
15:X:39:DG:H2"	15:X:40:DT:H71	0.91	0.89
16:Y:-35:DC:N1	16:Y:-34:DT:C7	2.33	0.89
16:Y:-35:DC:H2"	16:Y:-34:DT:C7	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:501:ADP:O3B	9:O:357:ARG:NH1	2.05	0.89
3:C:49:ARG:HD3	15:X:6:DG:O3'	1.72	0.89
16:Y:-10:DT:H2"	16:Y:-9:DA:H5"	1.53	0.89
3:G:63:ARG:HG2	16:Y:-55:DA:H5"	1.52	0.88
10:R:362:TYR:OH	17:R:501:ADP:N7	2.06	0.88
9:Q:404:ARG:NH1	17:Q:501:ADP:O3B	2.07	0.87
1:A:12:ARG:NH1	16:Y:-29:DT:H1'	1.90	0.87
2:F:83:ARG:HH21	16:Y:-106:DG:P	1.98	0.87
5:I:167:ARG:HB3	15:X:33:DT:OP1	1.75	0.87
11:U:215:LYS:O	11:U:254:ARG:NH2	2.07	0.87
15:X:76:DG:C2	16:Y:-75:DG:C2	2.63	0.87
9:O:270:GLU:OE2	9:O:274:LYS:NZ	2.09	0.86
2:F:83:ARG:HH22	16:Y:-106:DG:C3'	1.88	0.86
15:X:98:DA:C2	16:Y:-97:DA:H2	1.93	0.86
5:I:730:GLN:NE2	15:X:56:DT:OP1	2.10	0.85
5:I:737:ARG:CZ	16:Y:-132:DG:N2	2.40	0.85
2:B:37:TYR:OH	16:Y:-25:DG:H5"	1.76	0.85
15:X:125:DC:H2"	15:X:126:DT:H71	1.59	0.84
16:Y:-35:DC:C2'	16:Y:-34:DT:H72	1.92	0.84
2:F:83:ARG:HD3	16:Y:-106:DG:OP1	1.76	0.84
12:T:20:SER:CB	18:T:501:ATP:O3G	2.25	0.84
4:D:23:ARG:CD	14:W:84:PRO:O	2.26	0.83
6:J:161:PRO:CB	16:Y:-133:DG:OP1	2.25	0.83
9:M:20:HIS:CE1	17:M:501:ADP:O2'	2.32	0.83
5:I:711:GLY:CA	15:X:135:DG:P	2.61	0.83
15:X:95:DG:C6	15:X:96:DC:N4	2.47	0.82
10:P:47:VAL:C	17:P:501:ADP:HN62	1.81	0.82
11:U:283:MET:SD	11:U:290:ARG:NH2	2.53	0.82
3:G:63:ARG:CZ	16:Y:-55:DA:H4'	2.09	0.82
16:Y:-48:DA:C2	16:Y:-47:DG:C2	2.68	0.82
6:J:185:ARG:NH2	6:J:188:GLU:OE1	2.13	0.81
2:B:89:ARG:CZ	13:V:63:SER:HB3	2.09	0.81
15:X:98:DA:C2	16:Y:-97:DA:C2	2.69	0.81
15:X:21:DG:N1	16:Y:-20:DG:C2	2.49	0.81
10:N:400:ARG:NH2	17:N:501:ADP:PA	2.53	0.81
10:P:27:HIS:NE2	17:P:501:ADP:O2'	2.01	0.81
2:B:29:SER:HG	15:X:102:DC:P	2.04	0.80
15:X:6:DG:N2	15:X:7:DT:C2	2.50	0.80
9:M:76:LYS:NZ	17:M:501:ADP:PB	2.55	0.80
7:K:15:ILE:O	7:K:21:ASN:ND2	2.14	0.80
5:I:96:ILE:HD11	14:W:197:LEU:CD2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:277:TRP:HE3	6:J:280:GLN:NE2	1.79	0.80
10:R:47:VAL:H	17:R:501:ADP:HN62	1.29	0.80
3:C:81:ASP:OD2	14:W:163:LEU:CD1	2.28	0.79
7:K:134:ARG:NH2	7:K:138:ASP:OD1	2.16	0.79
8:L:98:GLY:O	8:L:103:THR:OG1	2.00	0.79
15:X:21:DG:N3	16:Y:-20:DG:N2	2.29	0.79
16:Y:-10:DT:H2"	16:Y:-9:DA:C5'	2.11	0.79
10:R:313:ASN:O	10:R:353:ARG:NH2	2.15	0.79
5:I:166:VAL:HG21	11:U:168:GLY:HA3	1.63	0.79
15:X:98:DA:N1	16:Y:-97:DA:C2	2.50	0.79
10:N:400:ARG:HH22	17:N:501:ADP:PA	2.05	0.79
5:I:96:ILE:CG1	14:W:197:LEU:HD21	2.12	0.79
15:X:34:DA:C6	15:X:35:DG:C6	2.72	0.78
10:R:45:GLY:O	17:R:501:ADP:H2	1.66	0.78
15:X:48:DT:C6	15:X:49:DT:H72	2.19	0.78
9:M:322:SER:OG	10:R:21:ARG:O	2.00	0.78
15:X:97:DT:O2	16:Y:-96:DG:N2	2.17	0.78
2:B:28:ARG:CZ	16:Y:-22:DA:H5"	2.14	0.77
15:X:78:DA:H2"	15:X:79:DC:C5	2.20	0.77
2:B:116:THR:HG22	13:V:57:VAL:HG11	1.65	0.77
3:C:49:ARG:NH2	15:X:6:DG:O3'	2.18	0.77
5:I:711:GLY:C	15:X:135:DG:OP1	2.23	0.77
12:T:339:ASP:OD2	13:V:227:LYS:NZ	2.17	0.77
6:J:277:TRP:O	6:J:280:GLN:CG	2.23	0.77
2:B:112:THR:CG2	13:V:61:LEU:HD21	2.15	0.76
6:J:282:ARG:HH21	9:Q:139:THR:HG22	1.44	0.76
5:I:96:ILE:HG12	14:W:197:LEU:CD2	2.15	0.76
10:P:27:HIS:HE1	17:P:501:ADP:O2'	1.62	0.76
5:I:736:ARG:CD	16:Y:-130:DG:O5'	2.28	0.76
15:X:21:DG:N2	16:Y:-20:DG:C2	2.52	0.76
15:X:125:DC:H2"	15:X:126:DT:C7	2.14	0.76
15:X:108:DA:H2"	15:X:109:DC:C5	2.21	0.76
16:Y:-10:DT:C2'	16:Y:-9:DA:H5"	2.16	0.76
5:I:1945:HIS:NE2	5:I:1947:THR:OG1	2.19	0.76
6:J:260:ARG:CA	10:P:210:THR:HA	2.17	0.75
3:C:49:ARG:HD3	15:X:7:DT:OP1	1.84	0.75
6:J:217:VAL:HA	10:P:144:GLU:HG3	1.67	0.75
2:F:83:ARG:HH22	16:Y:-106:DG:C2'	1.99	0.75
10:N:400:ARG:NH2	17:N:501:ADP:O5'	2.19	0.75
9:O:366:TYR:OH	17:O:501:ADP:N7	2.18	0.75
15:X:27:DG:H2"	15:X:28:DG:H5"	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:6:DG:N2	15:X:7:DT:O2	2.20	0.75
15:X:44:DC:H2"	15:X:45:DC:C5	2.21	0.75
9:M:357:ARG:O	10:R:404:GLN:NE2	2.20	0.75
10:R:114:SER:OG	10:R:117:GLU:OE1	2.05	0.75
5:I:736:ARG:HH22	16:Y:-130:DG:H3'	1.51	0.74
10:P:149:ARG:NH2	10:P:150:PRO:O	2.19	0.74
5:I:159:ARG:O	5:I:163:ARG:HB2	1.86	0.74
10:P:82:GLY:HA2	17:P:501:ADP:O1A	1.87	0.74
10:P:194:THR:OG1	10:P:203:SER:OG	2.05	0.74
16:Y:-35:DC:C1'	16:Y:-34:DT:C7	2.59	0.74
15:X:21:DG:N1	16:Y:-20:DG:N1	2.36	0.73
10:P:63:ILE:HG12	10:P:323:VAL:HG21	1.69	0.73
1:A:16:LYS:O	15:X:30:DG:C5'	2.27	0.73
3:C:49:ARG:NH2	15:X:6:DG:H4'	2.04	0.73
5:I:711:GLY:HA2	15:X:135:DG:P	2.26	0.73
16:Y:-115:DT:C6	16:Y:-114:DT:H72	2.23	0.73
5:I:736:ARG:CZ	16:Y:-130:DG:O5'	2.36	0.73
9:O:278:GLU:OE1	9:O:278:GLU:N	2.22	0.73
9:M:76:LYS:HG2	17:M:501:ADP:O3B	1.88	0.73
2:B:31:LYS:O	16:Y:-23:DC:OP1	2.06	0.73
2:F:83:ARG:NH2	16:Y:-106:DG:C3'	2.46	0.73
15:X:39:DG:C2'	15:X:40:DT:C7	2.54	0.73
9:Q:20:HIS:CE1	17:Q:501:ADP:O2'	2.42	0.72
2:B:39:TYR:HH	15:X:19:DA:P	2.13	0.71
2:B:89:ARG:NH1	13:V:63:SER:HB3	2.04	0.71
9:M:76:LYS:HZ2	17:M:501:ADP:PB	2.14	0.71
11:U:302:GLY:CA	18:U:401:ATP:O2A	2.38	0.71
9:Q:211:THR:HG21	9:Q:214:ASP:HB2	1.70	0.71
4:D:79:LYS:CB	15:X:100:DA:OP1	2.38	0.71
9:M:304:VAL:HG21	9:M:329:PHE:HB3	1.72	0.71
1:A:43:ARG:HH22	16:Y:-35:DC:H4'	0.60	0.71
10:N:80:GLY:HA2	17:N:501:ADP:O3A	1.89	0.71
5:I:96:ILE:CD1	14:W:197:LEU:CD2	2.69	0.70
5:I:881:THR:O	5:I:884:THR:OG1	2.08	0.70
15:X:125:DC:H2"	15:X:126:DT:C5	2.26	0.70
10:P:142:VAL:HG22	10:P:161:LEU:HD11	1.72	0.70
9:Q:255:ASP:O	9:Q:257:LEU:N	2.24	0.70
3:G:63:ARG:CG	16:Y:-55:DA:H5"	2.20	0.70
2:F:30:ARG:HD3	15:X:122:DG:H5'	1.72	0.70
3:G:64:LYS:HB3	16:Y:-54:DC:OP2	1.92	0.70
15:X:133:DC:H2"	15:X:134:DG:N7	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:166:VAL:CG2	11:U:168:GLY:HA3	2.21	0.70
11:S:324:THR:HG21	15:X:117:DT:H73	1.72	0.70
16:Y:-115:DT:C2'	16:Y:-114:DT:C7	2.70	0.70
5:I:736:ARG:CZ	16:Y:-130:DG:P	2.79	0.70
1:A:43:ARG:NH1	16:Y:-35:DC:C1'	2.50	0.69
3:C:49:ARG:CZ	15:X:6:DG:H4'	2.22	0.69
5:I:247:LEU:HD11	5:I:631:THR:HG22	1.74	0.69
7:K:265:GLU:OE1	7:K:265:GLU:N	2.25	0.69
15:X:74:DG:N2	16:Y:-73:DG:N3	2.40	0.69
15:X:74:DG:N1	16:Y:-73:DG:N1	2.41	0.69
5:I:96:ILE:CG1	14:W:197:LEU:CD2	2.70	0.69
16:Y:-30:DC:H2'	16:Y:-29:DT:H72	1.75	0.69
15:X:106:DC:C6	15:X:107:DT:H72	2.27	0.69
1:E:77:ARG:HH11	15:X:129:DG:H4'	1.58	0.68
10:R:370:ILE:HD11	10:R:399:LEU:HD11	1.76	0.68
15:X:76:DG:C2	16:Y:-75:DG:N1	2.61	0.68
11:S:156:GLY:O	11:S:303:THR:OG1	2.11	0.68
9:M:117:ARG:NH2	9:M:244:ASP:OD2	2.26	0.68
9:O:374:ILE:CG2	17:O:501:ADP:N3	2.56	0.68
9:Q:374:ILE:HG23	17:Q:501:ADP:C2	2.28	0.68
12:T:173:GLY:O	12:T:354:ASN:ND2	2.27	0.68
15:X:116:DT:H2'	15:X:117:DT:H72	1.74	0.68
10:R:366:ASP:O	10:R:370:ILE:HG23	1.92	0.68
12:T:21:TYR:CD2	18:T:501:ATP:H5'2	2.28	0.68
13:V:250:GLU:OE1	13:V:253:LYS:NZ	2.22	0.68
15:X:118:DG:N2	16:Y:-117:DA:C2	2.60	0.68
11:U:250:ILE:HG23	11:U:253:GLU:OE2	1.93	0.68
9:M:28:GLU:N	9:M:28:GLU:OE1	2.27	0.67
2:B:89:ARG:HH11	13:V:63:SER:HB3	1.60	0.67
9:M:186:GLU:OE2	9:M:205:ARG:NH2	2.27	0.67
9:O:49:CYS:O	9:O:53:VAL:HG13	1.95	0.67
12:T:395:ILE:O	12:T:399:ILE:HG23	1.94	0.67
15:X:74:DG:N2	16:Y:-73:DG:N2	2.28	0.67
15:X:76:DG:C2	16:Y:-75:DG:N2	2.63	0.67
1:A:21:ARG:NH1	15:X:31:DA:OP1	2.28	0.67
10:N:362:TYR:OH	17:N:501:ADP:N6	2.18	0.67
12:T:184:ASP:OD2	13:V:170:ARG:NH2	2.28	0.67
10:R:47:VAL:H	17:R:501:ADP:N6	1.93	0.67
2:F:83:ARG:HH22	16:Y:-106:DG:H2'	1.58	0.67
5:I:674:VAL:HG12	5:I:746:ASP:CB	2.25	0.67
5:I:736:ARG:NE	16:Y:-130:DG:O5'	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:20:HIS:HE1	17:Q:501:ADP:O2'	1.79	0.66
15:X:21:DG:N1	16:Y:-20:DG:N2	2.43	0.66
14:W:29:ASN:OD1	14:W:116:HIS:NE2	2.29	0.66
5:I:669:PRO:HB2	5:I:740:TRP:CZ3	2.30	0.66
10:R:209:PHE:O	10:R:210:THR:OG1	2.09	0.66
5:I:2145:ASP:OD2	5:I:2184:ARG:NH1	2.29	0.66
10:P:80:GLY:CA	17:P:501:ADP:O3B	2.41	0.66
11:S:188:TYR:HB2	11:S:267:LEU:HD21	1.78	0.66
5:I:2118:THR:HG21	5:I:2139:ASP:OD2	1.96	0.66
3:G:46:VAL:HG21	16:Y:-63:DG:H3'	1.77	0.66
10:N:384:GLU:OE1	10:N:384:GLU:N	2.28	0.66
15:X:116:DT:C2'	15:X:117:DT:H72	2.26	0.66
5:I:710:GLN:HA	15:X:135:DG:OP2	1.95	0.66
12:T:10:GLU:OE1	12:T:11:VAL:N	2.28	0.66
11:U:305:MET:HB2	18:U:401:ATP:C6	2.30	0.66
3:C:83:ARG:NH2	16:Y:-96:DG:H4'	2.11	0.66
15:X:21:DG:H2'	15:X:22:DT:H71	1.78	0.66
15:X:98:DA:N1	16:Y:-97:DA:H2	1.92	0.66
2:B:31:LYS:N	16:Y:-23:DC:OP1	2.29	0.65
4:D:45:ARG:CZ	15:X:79:DC:H4'	2.26	0.65
3:G:63:ARG:NE	16:Y:-55:DA:H4'	2.11	0.65
5:I:161:VAL:O	5:I:165:VAL:HG23	1.96	0.65
2:B:112:THR:HG21	13:V:61:LEU:CD2	2.27	0.65
10:P:271:GLU:O	10:P:275:GLN:N	2.24	0.65
16:Y:-5:DA:C2'	16:Y:-4:DT:H5'	2.25	0.65
10:P:47:VAL:H	17:P:501:ADP:N6	1.93	0.65
15:X:48:DT:C2'	15:X:49:DT:H72	2.27	0.65
10:P:47:VAL:H	17:P:501:ADP:HN62	1.44	0.65
16:Y:-121:DG:H2"	16:Y:-120:DC:C5	2.31	0.65
1:E:43:VAL:N	15:X:111:DA:OP1	2.28	0.65
5:I:736:ARG:CZ	16:Y:-130:DG:OP2	2.44	0.65
10:N:121:GLN:OE1	10:N:273:ARG:NH1	2.30	0.65
15:X:107:DT:H2"	15:X:108:DA:N7	2.12	0.65
4:H:45:ARG:CG	16:Y:-64:DC:OP1	2.42	0.65
6:J:283:PRO:HD2	6:J:283:PRO:O	1.96	0.65
2:B:112:THR:CG2	13:V:61:LEU:CD2	2.76	0.64
2:B:115:VAL:HG11	13:V:60:LEU:CD1	2.27	0.64
3:C:51:ILE:HD11	4:D:44:LYS:HA	1.78	0.64
7:K:284:PRO:O	7:K:285:SER:OG	2.11	0.64
10:R:247:ILE:HG12	10:R:272:VAL:HG22	1.79	0.64
15:X:110:DG:N2	16:Y:-109:DG:C2	2.64	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:128:DG:N2	16:Y:-127:DG:N2	2.45	0.64
5:I:162:ALA:O	5:I:166:VAL:HG23	1.97	0.64
9:O:135:VAL:HG12	9:O:189:ASP:O	1.97	0.64
1:E:92:GLU:OE1	1:E:92:GLU:N	2.31	0.64
5:I:881:THR:HG22	5:I:889:SER:HB3	1.79	0.64
15:X:112:DC:C4	15:X:113:DC:N4	2.65	0.64
2:F:28:ARG:HD3	15:X:122:DG:H4'	1.79	0.64
4:H:79:LYS:N	16:Y:-45:DG:OP1	2.31	0.64
10:P:80:GLY:HA2	17:P:501:ADP:PB	2.37	0.64
4:H:36:ARG:NH1	15:X:59:DA:OP1	2.30	0.64
11:U:162:THR:HG21	11:U:277:THR:HG22	1.80	0.64
5:I:927:SER:HB3	5:I:930:LEU:HD23	1.80	0.64
16:Y:-115:DT:H2'	16:Y:-114:DT:C7	2.26	0.64
15:X:42:DA:H2"	15:X:43:DT:H5"	1.79	0.64
5:I:730:GLN:OE1	15:X:56:DT:OP1	2.15	0.64
12:T:190:GLN:OE1	12:T:190:GLN:N	2.31	0.64
16:Y:-13:DA:H2"	16:Y:-12:DT:H5'	1.78	0.64
3:C:49:ARG:CG	15:X:7:DT:OP1	2.46	0.64
7:K:85:GLN:O	7:K:87:ASP:N	2.31	0.63
9:M:415:LEU:HD21	10:N:61:GLU:HB2	1.79	0.63
10:N:180:GLU:OE2	10:N:184:LYS:NZ	2.27	0.63
9:M:108:LYS:NZ	9:M:310:GLU:OE2	2.17	0.63
10:R:117:GLU:OE1	10:R:117:GLU:N	2.31	0.63
11:U:157:ASP:HB2	18:U:401:ATP:H4'	1.81	0.63
5:I:737:ARG:HG2	16:Y:-131:DT:H4'	1.81	0.63
10:R:305:ASP:OD1	10:R:306:ILE:N	2.30	0.63
10:R:382:MET:HE2	10:R:426:ILE:HD11	1.79	0.63
11:U:125:GLU:O	13:V:91:LYS:NZ	2.32	0.63
5:I:1984:GLU:OE2	9:O:252:GLY:N	2.30	0.63
7:K:5:VAL:HG21	7:K:363:GLY:HA3	1.80	0.63
9:Q:374:ILE:HG12	17:Q:501:ADP:N1	2.13	0.63
10:R:268:ILE:O	10:R:272:VAL:HG23	1.97	0.63
3:G:83:ARG:HH21	16:Y:-46:DG:H4'	1.64	0.63
9:M:39:LEU:HA	17:M:501:ADP:N1	2.14	0.63
11:U:152:VAL:HG22	11:U:298:VAL:HB	1.79	0.63
10:R:370:ILE:HD11	10:R:399:LEU:HD21	1.78	0.63
16:Y:-132:DG:H2"	16:Y:-131:DT:C6	2.34	0.63
16:Y:-65:DC:H2"	16:Y:-64:DC:C6	2.33	0.63
3:C:65:LEU:HB2	15:X:90:DG:OP2	1.99	0.63
5:I:2068:MET:HB3	5:I:2071:MET:HB2	1.79	0.63
15:X:84:DG:H2'	15:X:85:DT:H72	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:299:ALA:HA	6:J:311:ALA:HB2	1.81	0.63
5:I:91:LYS:N	14:W:197:LEU:HD11	2.14	0.62
9:M:438:TYR:N	10:N:356:ILE:O	2.32	0.62
9:Q:65:ALA:HB3	9:Q:358:VAL:HG12	1.81	0.62
5:I:730:GLN:CD	15:X:56:DT:OP1	2.37	0.62
10:P:267:GLU:OE1	10:P:267:GLU:N	2.31	0.62
12:T:21:TYR:CG	18:T:501:ATP:H5'2	2.34	0.62
12:T:24:ARG:NH1	18:T:501:ATP:O1A	2.32	0.62
14:W:190:THR:HG22	14:W:194:ILE:HD12	1.81	0.62
2:B:116:THR:HG22	13:V:57:VAL:HG13	1.81	0.62
9:M:428:GLU:N	9:M:428:GLU:OE1	2.32	0.62
5:I:91:LYS:HG2	5:I:96:ILE:HD11	1.81	0.62
9:Q:212:GLU:N	9:Q:212:GLU:OE1	2.31	0.62
16:Y:-96:DG:C8	16:Y:-95:DC:C5	2.87	0.62
9:Q:206:CYS:SG	9:Q:208:THR:HG22	2.39	0.62
2:B:116:THR:CG2	13:V:57:VAL:HG13	2.30	0.62
10:R:370:ILE:CD1	10:R:399:LEU:HD21	2.30	0.62
10:P:400:ARG:NH1	17:P:501:ADP:O2A	2.33	0.62
3:G:66:PRO:HD3	16:Y:-55:DA:O5'	1.99	0.62
10:N:196:ASP:O	10:N:200:GLY:N	2.33	0.62
1:E:76:THR:O	1:E:76:THR:OG1	2.18	0.62
10:R:45:GLY:O	17:R:501:ADP:C2	2.51	0.61
10:R:223:LYS:O	10:R:225:VAL:N	2.33	0.61
3:G:97:GLU:O	3:G:101:VAL:HG23	2.01	0.61
6:J:219:VAL:HB	6:J:261:CYS:HB3	1.82	0.61
9:Q:404:ARG:NH1	17:Q:501:ADP:O2A	2.33	0.61
10:P:47:VAL:N	17:P:501:ADP:N1	2.48	0.61
5:I:175:GLU:O	5:I:179:LYS:N	2.33	0.61
6:J:277:TRP:CE3	6:J:280:GLN:NE2	2.60	0.61
9:M:189:ASP:OD2	9:M:202:ARG:NH1	2.33	0.61
9:M:313:THR:HG21	10:R:303:MET:HG3	1.83	0.61
10:R:136:GLU:N	10:R:136:GLU:OE1	2.34	0.61
11:U:157:ASP:HB2	18:U:401:ATP:C5'	2.30	0.61
15:X:114:DA:C2	16:Y:-113:DG:N2	2.69	0.61
16:Y:-72:DC:C6	16:Y:-71:DT:H72	2.35	0.61
2:B:29:SER:CB	15:X:102:DC:OP1	2.48	0.61
9:M:270:GLU:N	9:M:270:GLU:OE1	2.33	0.61
10:R:362:TYR:CZ	17:R:501:ADP:N7	2.67	0.61
15:X:122:DG:C2	16:Y:-121:DG:N2	2.69	0.61
16:Y:-100:DT:H2"	16:Y:-99:DC:C5	2.36	0.61
3:C:49:ARG:CD	15:X:7:DT:OP1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ARG:CG	2:F:121:SER:OG	2.48	0.61
2:F:87:THR:OG1	2:F:90:GLU:OE1	2.19	0.61
16:Y:-79:DG:H2"	16:Y:-78:DT:C5	2.36	0.61
5:I:1973:ILE:HG23	5:I:1977:ILE:HD12	1.82	0.61
9:O:97:VAL:HG11	10:P:311:PHE:HA	1.82	0.61
9:Q:374:ILE:HG12	17:Q:501:ADP:C2	2.36	0.61
15:X:4:DA:N6	16:Y:-5:DA:N6	2.48	0.61
1:A:43:ARG:NH1	16:Y:-35:DC:H1'	2.16	0.60
12:T:182:VAL:HG22	12:T:187:VAL:HG22	1.81	0.60
16:Y:-13:DA:H2"	16:Y:-12:DT:C5'	2.31	0.60
5:I:156:ARG:HG3	16:Y:-28:DC:OP1	2.00	0.60
9:O:339:ARG:NH1	10:P:307:GLU:OE2	2.33	0.60
15:X:76:DG:H2"	15:X:77:DT:C6	2.36	0.60
15:X:80:DG:C2	16:Y:-79:DG:N2	2.69	0.60
16:Y:-132:DG:H2"	16:Y:-131:DT:C5	2.35	0.60
9:Q:374:ILE:CG2	17:Q:501:ADP:N3	2.59	0.60
15:X:110:DG:C2	16:Y:-109:DG:C2	2.88	0.60
5:I:164:LYS:O	5:I:168:MET:HG2	2.01	0.60
5:I:957:ARG:N	5:I:1921:GLU:OE2	2.32	0.60
8:L:135:TYR:OH	10:N:169:GLU:O	2.18	0.60
10:P:47:VAL:N	17:P:501:ADP:HN62	1.99	0.60
4:H:45:ARG:HA	16:Y:-64:DC:OP1	2.00	0.60
5:I:166:VAL:O	5:I:169:VAL:HB	2.01	0.60
5:I:736:ARG:NH2	16:Y:-130:DG:O5'	2.35	0.60
12:T:69:TYR:OH	12:T:79:ARG:NH2	2.34	0.60
4:H:48:GLY:HA3	16:Y:-65:DC:OP2	2.01	0.60
15:X:64:DG:C2	15:X:65:DG:N2	2.69	0.60
4:D:75:HIS:O	2:F:89:ARG:NH2	2.33	0.60
7:K:148:VAL:HB	7:K:319:LEU:HD23	1.82	0.60
9:Q:404:ARG:CZ	17:Q:501:ADP:O3B	2.50	0.60
15:X:10:DA:C8	15:X:11:DT:C7	2.85	0.60
16:Y:-96:DG:C8	16:Y:-95:DC:H5	2.19	0.60
16:Y:-124:DG:C4	16:Y:-123:DC:C5	2.90	0.60
10:N:74:LEU:HD23	10:N:75:ILE:N	2.17	0.60
13:V:141:GLN:N	13:V:141:GLN:OE1	2.34	0.60
10:P:31:LEU:O	10:P:44:GLN:NE2	2.35	0.59
10:P:362:TYR:OH	17:P:501:ADP:N7	2.31	0.59
9:Q:190:VAL:HG11	9:Q:221:VAL:HG11	1.84	0.59
11:U:138:ALA:CB	11:U:163:VAL:HG21	2.32	0.59
14:W:38:ARG:NH2	14:W:41:ASP:OD2	2.36	0.59
2:B:39:TYR:CE2	15:X:19:DA:OP2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:201:VAL:O	7:K:205:VAL:HG23	2.03	0.59
12:T:73:ASN:ND2	11:U:277:THR:HG23	2.17	0.59
15:X:44:DC:H2"	15:X:45:DC:H5	1.63	0.59
2:B:30:ARG:NH1	16:Y:-24:DG:H4'	2.03	0.59
4:H:68:ASP:OD2	4:H:93:GLN:NE2	2.34	0.59
5:I:151:PHE:CD2	12:T:399:ILE:HG22	2.38	0.59
5:I:674:VAL:HG12	5:I:746:ASP:HB3	1.83	0.59
15:X:8:DA:H61	16:Y:-8:DT:H3	1.50	0.59
16:Y:-2:DC:H2"	16:Y:-1:DT:C5	2.38	0.59
10:P:381:GLU:N	10:P:381:GLU:OE1	2.34	0.59
10:R:370:ILE:HD12	17:R:501:ADP:N9	2.17	0.59
5:I:181:GLU:N	5:I:181:GLU:OE1	2.36	0.59
7:K:299:VAL:O	7:K:303:GLN:NE2	2.36	0.59
15:X:25:DC:H2"	15:X:26:DT:C5	2.37	0.59
7:K:60:PHE:CZ	7:K:65:LEU:HD13	2.38	0.59
12:T:333:VAL:HG11	12:T:345:TYR:CZ	2.38	0.59
5:I:157:TRP:CZ2	5:I:161:VAL:HG21	2.38	0.59
5:I:174:GLU:OE1	15:X:34:DA:OP2	2.20	0.59
5:I:906:LEU:HD13	5:I:2068:MET:HE1	1.83	0.59
10:P:349:ASP:OD1	10:P:353:ARG:NH2	2.32	0.59
12:T:124:GLU:OE2	12:T:133:ARG:NH2	2.35	0.59
16:Y:-34:DT:H5'	16:Y:-34:DT:H6	1.67	0.59
9:M:386:ILE:HG22	9:M:425:ILE:HB	1.85	0.59
16:Y:-67:DC:H2"	16:Y:-66:DC:C5	2.38	0.59
2:F:83:ARG:CZ	16:Y:-106:DG:H3'	2.32	0.58
7:K:289:ILE:HG22	8:L:32:LEU:HD13	1.84	0.58
9:Q:123:ARG:HE	9:Q:235:ILE:HD11	1.68	0.58
13:V:176:ASP:OD2	13:V:177:ARG:NH2	2.36	0.58
1:A:59:LEU:HD12	2:B:66:ILE:HG21	1.84	0.58
7:K:380:GLU:OE1	7:K:380:GLU:N	2.36	0.58
10:P:68:ILE:HD13	10:P:68:ILE:H	1.69	0.58
1:A:66:LEU:HD12	1:A:94:LEU:HD12	1.86	0.58
9:Q:451:GLN:N	9:Q:451:GLN:OE1	2.35	0.58
11:U:157:ASP:HB2	18:U:401:ATP:C4'	2.34	0.58
3:C:46:VAL:HB	15:X:81:DT:OP1	2.03	0.58
10:P:21:ARG:NH1	9:Q:323:ILE:O	2.36	0.58
10:P:145:ILE:HG23	10:P:161:LEU:HD13	1.86	0.58
13:V:190:ASP:OD1	13:V:191:LEU:N	2.36	0.58
16:Y:-54:DC:C2	16:Y:-53:DC:C5	2.92	0.58
16:Y:-9:DA:H2"	16:Y:-8:DT:C6	2.39	0.58
5:I:669:PRO:HB2	5:I:740:TRP:CE3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:362:TYR:CZ	17:P:501:ADP:N7	2.71	0.58
11:U:111:ASN:ND2	11:U:115:ASN:OD1	2.37	0.58
15:X:54:DG:H2'	15:X:55:DT:H71	1.86	0.58
16:Y:-38:DT:H2"	16:Y:-37:DC:C5	2.39	0.58
2:B:39:TYR:OH	15:X:19:DA:OP2	2.22	0.58
11:U:306:TYR:HB2	11:U:309:ILE:HG23	1.85	0.58
10:R:237:GLU:OE2	10:R:239:VAL:HG13	2.04	0.57
13:V:51:GLU:HB3	13:V:58:TYR:CZ	2.39	0.57
1:A:55:VAL:HG21	2:B:95:VAL:HG21	1.86	0.57
2:B:89:ARG:HE	13:V:63:SER:HB2	1.53	0.57
2:B:116:THR:CG2	13:V:57:VAL:CG1	2.78	0.57
3:C:97:GLU:O	3:C:101:VAL:HG23	2.04	0.57
3:G:65:LEU:HD23	16:Y:-55:DA:OP2	2.05	0.57
5:I:906:LEU:HD13	5:I:2068:MET:CE	2.33	0.57
15:X:74:DG:N1	16:Y:-73:DG:C2	2.71	0.57
4:H:36:ARG:HH22	15:X:59:DA:P	2.27	0.57
10:P:47:VAL:HG23	17:P:501:ADP:N1	2.19	0.57
13:V:105:ARG:NH1	13:V:107:ASP:OD2	2.38	0.57
15:X:125:DC:H2"	15:X:126:DT:C6	2.39	0.57
3:C:82:LEU:HD22	4:D:81:VAL:HG23	1.87	0.57
2:F:90:GLU:OE1	2:F:90:GLU:N	2.37	0.57
10:R:204:LYS:HB3	10:R:205:LEU:HD22	1.87	0.57
1:E:42:ARG:HG3	15:X:111:DA:C5'	2.30	0.57
5:I:2176:ILE:HA	5:I:2179:LYS:HD2	1.85	0.57
10:N:97:ASP:OD1	10:N:130:ARG:NH1	2.37	0.57
10:P:142:VAL:HG12	10:P:189:ALA:HA	1.86	0.57
9:Q:293:GLU:OE1	9:Q:293:GLU:N	2.37	0.57
11:U:149:THR:HG21	11:U:293:LEU:HD22	1.86	0.57
11:U:292:ASP:N	11:U:292:ASP:OD1	2.37	0.57
10:P:196:ASP:O	10:P:200:GLY:N	2.33	0.57
2:B:89:ARG:NE	13:V:63:SER:OG	2.36	0.57
5:I:705:ARG:NH2	5:I:730:GLN:OE1	2.36	0.57
7:K:158:VAL:HG13	7:K:170:ILE:HD13	1.87	0.57
5:I:2110:ARG:NH2	9:O:214:ASP:O	2.38	0.57
9:M:47:GLU:O	9:M:51:VAL:HG23	2.04	0.57
12:T:414:GLN:N	12:T:414:GLN:OE1	2.38	0.57
10:R:49:GLN:NE2	10:R:360:THR:O	2.35	0.56
5:I:737:ARG:HH22	15:X:133:DC:C1'	2.18	0.56
9:M:55:LEU:HD21	9:M:61:MET:HB3	1.86	0.56
11:U:93:GLU:OE1	11:U:93:GLU:N	2.36	0.56
11:U:149:THR:HG21	11:U:293:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-35:DC:C2	16:Y:-34:DT:H72	2.33	0.56
5:I:674:VAL:HG12	5:I:746:ASP:HB2	1.88	0.56
9:O:235:ILE:HG23	9:O:235:ILE:O	2.05	0.56
1:E:20:ARG:HG2	2:F:121:SER:OG	2.05	0.56
7:K:182:ASN:ND2	8:L:37:ASN:O	2.39	0.56
8:L:19:LEU:CD2	8:L:150:LEU:HD22	2.35	0.56
9:O:53:VAL:HG12	9:O:83:ILE:HG23	1.88	0.56
13:V:50:PRO:O	13:V:51:GLU:HG3	2.06	0.56
16:Y:-7:DA:H1'	16:Y:-6:DC:H5"	1.86	0.56
7:K:114:PHE:O	7:K:379:ARG:NH2	2.38	0.56
9:M:76:LYS:HZ3	17:M:501:ADP:PB	2.18	0.56
9:Q:378:ARG:HG3	9:Q:407:VAL:HG21	1.87	0.56
5:I:928:LEU:HD13	5:I:928:LEU:N	2.21	0.56
1:E:88:ARG:NH1	1:E:100:VAL:O	2.36	0.56
9:M:53:VAL:HA	9:M:56:ILE:HD12	1.87	0.56
3:C:41:TYR:OH	15:X:6:DG:H5'	2.05	0.56
3:G:69:ARG:NH1	16:Y:-55:DA:OP2	2.39	0.56
5:I:129:GLU:N	5:I:129:GLU:OE1	2.37	0.56
9:Q:129:GLU:OE2	9:Q:196:ASN:N	2.36	0.56
10:R:83:LYS:N	17:R:501:ADP:O3B	2.39	0.56
10:R:317:GLU:OE2	10:R:353:ARG:NH2	2.38	0.56
5:I:246:LEU:O	5:I:246:LEU:HD23	2.06	0.55
10:P:47:VAL:CG2	10:P:373:ILE:HD12	2.36	0.55
14:W:137:GLU:HG2	14:W:170:THR:HB	1.88	0.55
15:X:128:DG:C2	16:Y:-127:DG:N2	2.74	0.55
16:Y:-11:DA:H2"	16:Y:-10:DT:H5'	1.86	0.55
5:I:229:LEU:O	5:I:233:LEU:HD23	2.05	0.55
5:I:737:ARG:NH1	16:Y:-132:DG:N2	2.53	0.55
5:I:902:ASN:ND2	5:I:2137:ASP:OD2	2.39	0.55
9:O:378:ARG:NH2	9:O:382:GLU:OE2	2.38	0.55
2:F:83:ARG:NH2	16:Y:-106:DG:C5'	2.67	0.55
3:G:106:ASP:OD2	3:G:131:ARG:NE	2.40	0.55
8:L:128:CYS:N	8:L:133:ALA:O	2.38	0.55
10:N:362:TYR:CE2	17:N:501:ADP:N7	2.75	0.55
9:O:55:LEU:HD12	9:O:55:LEU:O	2.07	0.55
16:Y:-100:DT:H2"	16:Y:-99:DC:C6	2.42	0.55
5:I:2068:MET:CB	5:I:2071:MET:HB2	2.36	0.55
9:Q:235:ILE:HG23	9:Q:235:ILE:O	2.06	0.55
2:B:39:TYR:OH	15:X:19:DA:P	2.65	0.55
7:K:41:THR:HG22	7:K:42:ALA:H	1.72	0.55
9:O:112:LEU:HD21	9:O:315:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:108:ASN:HB2	4:H:43:VAL:HG22	1.88	0.55
5:I:169:VAL:HG21	11:U:143:TYR:CD1	2.41	0.55
15:X:10:DA:C8	15:X:11:DT:H73	2.41	0.55
15:X:125:DC:C2'	15:X:126:DT:H71	2.33	0.55
12:T:82:MET:O	12:T:247:THR:OG1	2.15	0.55
9:Q:180:LEU:HD13	9:Q:185:VAL:CG2	2.36	0.55
9:Q:374:ILE:HD13	17:Q:501:ADP:C5	2.42	0.55
11:U:365:SER:O	11:U:368:SER:OG	2.18	0.55
15:X:114:DA:C2	16:Y:-113:DG:C2	2.94	0.55
7:K:253:GLU:N	7:K:253:GLU:OE1	2.38	0.55
3:G:83:ARG:NH2	16:Y:-46:DG:H4'	2.21	0.55
5:I:2095:VAL:HG12	5:I:2099:GLN:HE21	1.72	0.55
10:N:192:VAL:HG12	10:N:206:GLY:O	2.07	0.55
1:E:42:ARG:HG2	15:X:110:DG:H4'	1.90	0.54
10:R:54:ARG:O	10:R:58:VAL:HG23	2.08	0.54
10:R:370:ILE:HD12	17:R:501:ADP:C1'	2.37	0.54
15:X:54:DG:C2'	15:X:55:DT:H71	2.37	0.54
1:E:77:ARG:HH11	15:X:129:DG:C4'	2.20	0.54
5:I:930:LEU:HD21	10:N:131:ILE:CD1	2.37	0.54
5:I:2062:VAL:HG13	5:I:2132:THR:OG1	2.07	0.54
7:K:289:ILE:H	7:K:289:ILE:HD13	1.73	0.54
9:M:426:GLU:N	9:M:426:GLU:OE1	2.39	0.54
12:T:153:LYS:NZ	12:T:429:PRO:OXT	2.39	0.54
13:V:54:HIS:O	13:V:58:TYR:HB3	2.07	0.54
16:Y:-23:DC:H2"	16:Y:-22:DA:C8	2.42	0.54
16:Y:-12:DT:H2"	16:Y:-11:DA:H5'	1.89	0.54
2:B:27:LYS:N	15:X:103:DT:OP1	2.39	0.54
10:P:409:ALA:HA	10:P:429:VAL:HG21	1.88	0.54
10:R:286:GLU:OE1	10:R:286:GLU:N	2.40	0.54
15:X:10:DA:H1'	15:X:11:DT:H5'	1.90	0.54
5:I:164:LYS:O	5:I:167:ARG:HB2	2.07	0.54
12:T:317:LEU:O	12:T:319:GLY:N	2.41	0.54
11:U:128:ASN:O	11:U:128:ASN:ND2	2.41	0.54
15:X:8:DA:H2"	15:X:9:DT:H6	1.71	0.54
16:Y:-43:DA:H2'	16:Y:-42:DT:H71	1.90	0.54
16:Y:-11:DA:H1'	16:Y:-10:DT:H5"	1.88	0.54
7:K:232:VAL:HG23	7:K:271:ALA:HB1	1.89	0.54
10:N:301:VAL:HG21	10:N:326:MET:CB	2.37	0.54
10:N:301:VAL:HG21	10:N:326:MET:HB2	1.88	0.54
9:Q:148:GLY:O	9:Q:150:TYR:N	2.38	0.54
11:S:44:MET:SD	11:S:53:TYR:OH	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:366:TYR:OH	17:M:501:ADP:N7	2.33	0.54
10:P:47:VAL:CA	17:P:501:ADP:HN62	2.20	0.54
11:S:324:THR:HG21	15:X:117:DT:C7	2.36	0.54
11:U:316:GLU:N	11:U:316:GLU:OE1	2.40	0.54
15:X:23:DG:C6	15:X:24:DC:N4	2.75	0.54
15:X:87:DT:H2"	15:X:88:DA:C8	2.42	0.54
15:X:95:DG:C6	15:X:96:DC:C4	2.96	0.54
16:Y:-124:DG:C5	16:Y:-123:DC:N4	2.76	0.54
7:K:205:VAL:HG22	7:K:236:TYR:CE2	2.43	0.54
9:Q:396:GLU:O	9:Q:399:THR:OG1	2.24	0.54
15:X:34:DA:N1	15:X:35:DG:C6	2.76	0.54
5:I:768:GLN:O	5:I:769:ARG:NH2	2.39	0.54
6:J:173:LEU:O	6:J:177:LYS:NZ	2.30	0.54
6:J:206:LYS:C	6:J:208:PRO:HD3	2.28	0.54
7:K:266:GLN:N	7:K:266:GLN:OE1	2.41	0.54
8:L:128:CYS:SG	8:L:130:SER:OG	2.65	0.54
11:S:9:VAL:HG21	11:S:344:SER:HA	1.90	0.54
13:V:49:ARG:NH1	15:X:41:DA:OP1	2.41	0.54
2:B:112:THR:HG21	13:V:61:LEU:HD21	1.89	0.53
4:H:32:PRO:HG3	15:X:59:DA:H3'	1.90	0.53
10:P:147:ILE:HD11	10:P:157:LYS:HB2	1.89	0.53
11:U:138:ALA:CB	11:U:163:VAL:HG11	2.39	0.53
15:X:13:DT:H2"	15:X:14:DG:C8	2.44	0.53
16:Y:-35:DC:C2	16:Y:-34:DT:C5	2.97	0.53
10:P:370:ILE:HG12	17:P:501:ADP:C2	2.44	0.53
9:Q:450:GLN:OE1	9:Q:450:GLN:N	2.41	0.53
11:U:306:TYR:CD1	18:U:401:ATP:H2	2.26	0.53
3:C:72:ARG:NH2	16:Y:-95:DC:OP1	2.41	0.53
9:O:366:TYR:CZ	17:O:501:ADP:N7	2.75	0.53
7:K:333:VAL:O	7:K:337:VAL:HG22	2.09	0.53
8:L:147:THR:OG1	8:L:148:ARG:NH2	2.42	0.53
11:U:7:ALA:HB1	11:U:347:ALA:HB1	1.91	0.53
1:A:17:SER:HA	15:X:30:DG:OP1	2.08	0.53
9:O:374:ILE:HG12	17:O:501:ADP:N1	2.22	0.53
5:I:96:ILE:HG12	14:W:197:LEU:HD22	1.87	0.53
10:P:207:ARG:O	10:P:225:VAL:HG12	2.09	0.53
13:V:248:LEU:HD13	13:V:252:ARG:HD3	1.90	0.53
15:X:47:DC:H2"	15:X:48:DT:C6	2.44	0.53
15:X:76:DG:H2"	15:X:77:DT:C5	2.43	0.53
7:K:187:ILE:HG21	7:K:273:GLU:HG3	1.90	0.53
10:R:74:LEU:HD11	10:R:328:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-60:DT:C6	16:Y:-59:DT:H72	2.44	0.53
5:I:247:LEU:HD22	5:I:637:LEU:HD12	1.89	0.53
16:Y:-30:DC:H2'	16:Y:-29:DT:C7	2.38	0.53
6:J:212:ILE:HG23	6:J:268:PHE:CD2	2.44	0.53
6:J:306:THR:HG22	6:J:323:TYR:CB	2.38	0.53
10:P:255:GLN:OE1	10:P:255:GLN:N	2.42	0.53
2:B:115:VAL:HG11	13:V:60:LEU:HD11	1.90	0.53
4:H:48:GLY:H	16:Y:-65:DC:P	2.31	0.53
10:P:47:VAL:HG11	10:P:369:GLN:HB3	1.90	0.53
11:U:210:ARG:CZ	18:U:401:ATP:H2'	2.38	0.53
13:V:50:PRO:C	13:V:51:GLU:HG3	2.28	0.53
15:X:1:DA:N1	15:X:2:DG:N1	2.57	0.53
5:I:166:VAL:HG13	11:U:143:TYR:HE1	1.73	0.52
10:N:47:VAL:O	17:N:501:ADP:N6	2.39	0.52
15:X:7:DT:H2"	15:X:8:DA:H5"	1.91	0.52
15:X:71:DA:C2	16:Y:-70:DG:C2	2.98	0.52
9:O:40:VAL:H	17:O:501:ADP:HN62	1.54	0.52
10:P:370:ILE:HG23	17:P:501:ADP:N3	2.25	0.52
11:S:62:ARG:NH1	11:S:207:GLU:OE2	2.42	0.52
16:Y:-12:DT:H1'	16:Y:-11:DA:H5"	1.90	0.52
5:I:930:LEU:N	5:I:930:LEU:HD22	2.24	0.52
9:M:320:GLU:OE2	9:M:357:ARG:NH2	2.42	0.52
10:N:307:GLU:OE1	10:N:307:GLU:N	2.42	0.52
10:N:424:ASP:OD1	10:N:425:ASP:N	2.42	0.52
9:Q:404:ARG:NE	17:Q:501:ADP:H5'2	2.24	0.52
15:X:74:DG:H2"	15:X:75:DC:C5	2.44	0.52
16:Y:-26:DA:H2"	16:Y:-25:DG:C8	2.44	0.52
15:X:34:DA:C2	15:X:35:DG:C4	2.96	0.52
15:X:84:DG:C2'	15:X:85:DT:H72	2.39	0.52
2:F:37:TYR:OH	15:X:120:DG:H5"	2.08	0.52
10:P:80:GLY:CA	17:P:501:ADP:PB	2.98	0.52
7:K:41:THR:HG21	7:K:77:TYR:HB2	1.90	0.52
11:U:14:SER:N	18:U:401:ATP:O1G	2.43	0.52
15:X:66:DG:H2"	15:X:67:DG:C8	2.45	0.52
16:Y:-69:DT:H2"	16:Y:-68:DC:C6	2.45	0.52
1:A:43:ARG:NE	16:Y:-34:DT:O5'	2.19	0.52
5:I:156:ARG:NH2	16:Y:-27:DC:P	2.83	0.52
6:J:137:THR:HG22	6:J:138:ALA:H	1.75	0.52
7:K:205:VAL:O	7:K:209:VAL:HG22	2.09	0.52
16:Y:-94:DA:C4	16:Y:-93:DC:C5	2.98	0.52
2:F:91:ILE:O	2:F:95:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:79:LYS:HB2	16:Y:-45:DG:P	2.49	0.52
9:O:371:MET:HG3	9:O:403:LEU:HD13	1.91	0.52
10:R:249:VAL:C	10:R:250:ILE:HD13	2.30	0.52
15:X:76:DG:N3	16:Y:-75:DG:N2	2.58	0.52
1:A:26:PHE:HZ	1:A:60:THR:HG21	1.74	0.52
8:L:19:LEU:HD23	8:L:150:LEU:HD22	1.92	0.52
16:Y:-115:DT:H2"	16:Y:-114:DT:C7	2.39	0.52
3:C:67:PHE:O	3:C:71:VAL:HG23	2.10	0.52
6:J:286:VAL:HG22	6:J:286:VAL:O	2.10	0.52
7:K:28:CYS:HB3	7:K:58:LEU:HD23	1.92	0.52
9:Q:337:VAL:HG22	10:R:340:TYR:OH	2.10	0.52
15:X:106:DC:H2'	15:X:107:DT:H72	1.92	0.52
5:I:940:ARG:NH1	9:M:194:GLU:OE1	2.41	0.51
15:X:76:DG:N2	16:Y:-75:DG:N1	2.58	0.51
9:M:65:ALA:HB3	9:M:358:VAL:HG22	1.92	0.51
11:U:193:LEU:HD22	11:U:209:VAL:HG22	1.93	0.51
15:X:36:DG:N2	16:Y:-35:DC:O2	2.42	0.51
15:X:64:DG:C2	15:X:65:DG:C2	2.98	0.51
16:Y:-77:DA:H2"	16:Y:-76:DC:C5	2.45	0.51
9:M:42:GLN:NE2	9:M:364:MET:O	2.39	0.51
9:M:415:LEU:HD23	10:N:58:VAL:HG13	1.93	0.51
15:X:1:DA:N1	15:X:2:DG:C6	2.78	0.51
5:I:164:LYS:HA	5:I:167:ARG:HB2	1.93	0.51
5:I:653:THR:HG21	5:I:744:ILE:HD13	1.91	0.51
10:N:409:ALA:HA	10:N:429:VAL:HG21	1.93	0.51
9:O:76:LYS:HG2	17:O:501:ADP:O2B	2.10	0.51
9:O:267:LYS:HE2	10:P:268:ILE:HG22	1.93	0.51
3:G:63:ARG:NH2	16:Y:-54:DC:P	2.83	0.51
4:H:36:ARG:NH2	15:X:59:DA:OP1	2.44	0.51
5:I:917:ILE:HG23	5:I:917:ILE:O	2.11	0.51
10:R:166:THR:HG22	10:R:229:ASP:HA	1.91	0.51
11:U:18:LYS:HA	11:U:30:VAL:HG12	1.92	0.51
15:X:3:DG:H1'	15:X:4:DA:H5'	1.91	0.51
15:X:8:DA:C2	16:Y:-7:DA:C2	2.99	0.51
2:B:88:SER:HB2	13:V:60:LEU:HD21	1.92	0.51
5:I:712:TRP:N	15:X:135:DG:OP1	2.44	0.51
5:I:736:ARG:HE	16:Y:-130:DG:P	2.19	0.51
10:R:370:ILE:HD12	17:R:501:ADP:C8	2.46	0.51
15:X:8:DA:H2"	15:X:9:DT:C6	2.46	0.51
3:C:106:ASP:OD2	3:C:131:ARG:NH1	2.41	0.51
9:M:283:VAL:HG11	10:R:19:ILE:HD11	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:327:VAL:HG11	9:Q:329:PHE:CZ	2.45	0.51
15:X:47:DC:H2"	15:X:48:DT:C5	2.45	0.51
16:Y:-65:DC:H2"	16:Y:-64:DC:C5	2.46	0.51
1:A:93:GLU:OE2	2:B:102:GLU:N	2.44	0.51
5:I:710:GLN:CA	15:X:135:DG:OP2	2.59	0.51
5:I:736:ARG:HD3	16:Y:-130:DG:C5'	2.41	0.51
16:Y:-67:DC:H2"	16:Y:-66:DC:C6	2.45	0.51
4:D:53:GLU:O	4:D:57:VAL:HG23	2.10	0.51
9:Q:36:ALA:O	9:Q:37:SER:OG	2.27	0.51
10:R:214:ASP:OD1	10:R:214:ASP:N	2.44	0.51
5:I:2038:ILE:HD12	5:I:2038:ILE:H	1.76	0.51
15:X:11:DT:H2"	15:X:12:DA:H5'	1.93	0.51
13:V:92:VAL:O	13:V:92:VAL:HG13	2.11	0.50
15:X:1:DA:C2	15:X:2:DG:C2	2.99	0.50
16:Y:-124:DG:H2"	16:Y:-123:DC:C6	2.46	0.50
16:Y:-96:DG:C5	16:Y:-95:DC:C5	2.98	0.50
9:Q:76:LYS:NZ	17:Q:501:ADP:O2B	2.44	0.50
1:A:59:LEU:CD1	2:B:66:ILE:HG21	2.41	0.50
1:E:42:ARG:CG	15:X:111:DA:H5'	2.34	0.50
5:I:202:VAL:HG21	11:S:143:TYR:CD1	2.46	0.50
6:J:137:THR:HG22	6:J:138:ALA:N	2.26	0.50
9:O:106:ILE:HG23	9:O:267:LYS:HB2	1.93	0.50
11:S:124:PHE:O	11:S:359:LYS:NZ	2.41	0.50
18:U:401:ATP:O2B	18:U:401:ATP:H5'1	2.11	0.50
6:J:263:ARG:CZ	6:J:264:THR:H	2.25	0.50
7:K:41:THR:HG21	7:K:77:TYR:CB	2.41	0.50
9:Q:208:THR:HG23	9:Q:209:TYR:CD1	2.46	0.50
16:Y:-106:DG:H2"	16:Y:-105:DA:C8	2.46	0.50
16:Y:-27:DC:H1'	16:Y:-26:DA:H5'	1.94	0.50
5:I:930:LEU:HD21	10:N:131:ILE:HD12	1.93	0.50
9:M:14:ARG:NH2	10:N:319:ASP:O	2.40	0.50
10:N:144:GLU:N	10:N:162:THR:OG1	2.44	0.50
15:X:6:DG:C2	15:X:7:DT:N3	2.78	0.50
15:X:60:DA:C4	15:X:61:DC:C5	2.99	0.50
6:J:306:THR:HG21	6:J:319:ILE:HG22	1.93	0.50
10:P:82:GLY:N	17:P:501:ADP:O3A	2.36	0.50
10:R:400:ARG:NH2	17:R:501:ADP:O1A	2.44	0.50
11:U:305:MET:HB2	18:U:401:ATP:N1	2.27	0.50
11:U:369:ILE:O	11:U:371:HIS:N	2.44	0.50
13:V:49:ARG:CZ	15:X:41:DA:P	3.00	0.50
16:Y:-8:DT:H2"	16:Y:-7:DA:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-3:DC:H2'	16:Y:-2:DC:C5	2.46	0.50
5:I:933:THR:O	10:N:279:LYS:NZ	2.45	0.50
9:O:75:GLY:HA2	17:O:501:ADP:O1A	2.12	0.50
10:P:210:THR:C	10:P:212:ALA:H	2.14	0.50
10:R:47:VAL:N	17:R:501:ADP:N1	2.60	0.50
11:U:326:LYS:C	11:U:327:ILE:HD13	2.31	0.50
15:X:96:DC:C2'	15:X:97:DT:H72	2.42	0.50
15:X:128:DG:N2	16:Y:-127:DG:H21	2.10	0.50
5:I:156:ARG:CD	16:Y:-28:DC:OP1	2.60	0.50
6:J:219:VAL:O	6:J:261:CYS:HB2	2.11	0.50
15:X:3:DG:H2"	15:X:4:DA:H5'	1.94	0.50
15:X:105:DT:H2"	15:X:106:DC:C6	2.47	0.50
5:I:2021:LEU:O	5:I:2025:VAL:HG23	2.11	0.50
9:O:303:GLU:OE1	9:O:305:HIS:NE2	2.44	0.50
12:T:363:ARG:NE	12:T:367:GLU:OE2	2.45	0.50
16:Y:-43:DA:C4	16:Y:-42:DT:C5	3.00	0.50
1:E:76:THR:HG23	15:X:130:DC:OP2	2.12	0.49
3:G:63:ARG:HG2	16:Y:-55:DA:C5'	2.33	0.49
5:I:1983:VAL:HG11	9:O:243:LEU:HD23	1.93	0.49
11:U:162:THR:CG2	11:U:277:THR:HG22	2.41	0.49
15:X:2:DG:H2"	15:X:3:DG:N7	2.27	0.49
15:X:48:DT:H2"	15:X:49:DT:C7	2.42	0.49
2:B:27:LYS:N	15:X:103:DT:P	2.86	0.49
9:M:273:ASP:OD1	9:M:274:LYS:N	2.45	0.49
10:R:142:VAL:HG13	10:R:161:LEU:HD11	1.94	0.49
10:R:211:ARG:O	10:R:212:ALA:HB3	2.12	0.49
12:T:324:GLY:O	12:T:328:VAL:HG23	2.11	0.49
9:M:249:ARG:NH1	9:M:266:PRO:O	2.45	0.49
10:P:47:VAL:HG23	17:P:501:ADP:C2	2.47	0.49
10:P:374:ARG:HG2	10:P:403:ILE:HG23	1.94	0.49
10:R:32:GLY:O	10:R:53:ARG:NH2	2.44	0.49
12:T:9:ASP:OD1	12:T:10:GLU:N	2.45	0.49
11:U:175:ILE:O	11:U:176:LEU:HD23	2.12	0.49
15:X:8:DA:C8	15:X:9:DT:C7	2.95	0.49
5:I:163:ARG:O	5:I:167:ARG:HG3	2.13	0.49
9:O:202:ARG:NH1	9:O:218:GLU:OE1	2.40	0.49
9:Q:28:GLU:OE1	9:Q:28:GLU:N	2.44	0.49
15:X:1:DA:C6	15:X:2:DG:C6	3.00	0.49
1:A:52:LEU:HD21	2:B:67:PHE:CD2	2.48	0.49
10:R:249:VAL:HG12	10:R:249:VAL:O	2.12	0.49
12:T:173:GLY:HA3	18:T:501:ATP:O2G	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:10:DA:H2"	15:X:11:DT:OP2	2.12	0.49
15:X:48:DT:C2	15:X:49:DT:C4	3.01	0.49
15:X:76:DG:N1	16:Y:-75:DG:N1	2.61	0.49
16:Y:-109:DG:H2"	16:Y:-108:DT:C5	2.48	0.49
16:Y:-5:DA:C2	16:Y:-4:DT:C2	3.01	0.49
9:M:109:THR:HG21	10:R:107:GLU:HG2	1.95	0.49
1:A:35:LEU:HB3	1:A:44:VAL:HG21	1.94	0.49
9:O:306:MET:SD	9:O:306:MET:N	2.85	0.49
11:U:306:TYR:HE1	18:U:401:ATP:N3	2.07	0.49
10:R:346:ILE:HD11	10:R:351:LEU:HD13	1.94	0.49
10:R:378:GLU:HG2	10:R:380:VAL:HG23	1.95	0.49
11:S:283:MET:O	11:S:290:ARG:NH1	2.46	0.49
2:B:53:SER:HB3	15:X:18:DC:OP2	2.13	0.49
3:C:69:ARG:HH12	15:X:89:DA:P	2.35	0.49
5:I:903:HIS:O	5:I:905:ASN:N	2.45	0.49
6:J:308:ILE:HD12	6:J:319:ILE:HG23	1.94	0.49
10:P:268:ILE:H	10:P:268:ILE:HD13	1.78	0.49
11:U:163:VAL:O	11:U:163:VAL:HG13	2.13	0.49
15:X:60:DA:C4	15:X:61:DC:C4	3.00	0.49
3:C:83:ARG:HH21	16:Y:-96:DG:H4'	1.75	0.49
10:P:404:GLN:NE2	9:Q:357:ARG:O	2.40	0.49
11:U:157:ASP:HB2	18:U:401:ATP:H5'1	1.95	0.49
2:F:83:ARG:NH1	16:Y:-105:DA:OP2	2.46	0.48
6:J:260:ARG:HH21	10:P:209:PHE:HB2	1.77	0.48
6:J:283:PRO:O	6:J:283:PRO:CD	2.61	0.48
7:K:292:MET:HE1	7:K:297:ALA:H	1.79	0.48
10:P:59:VAL:HG23	10:P:62:MET:HE3	1.94	0.48
9:Q:49:CYS:HB2	9:Q:83:ILE:HD11	1.94	0.48
9:Q:385:ASN:O	9:Q:424:SER:OG	2.14	0.48
15:X:123:DG:C5	15:X:124:DC:C4	3.01	0.48
2:B:39:TYR:CZ	15:X:19:DA:OP2	2.66	0.48
9:M:131:TYR:HB2	9:M:193:ILE:HG23	1.94	0.48
9:M:235:ILE:HG23	9:M:235:ILE:O	2.12	0.48
9:M:317:ARG:HG2	10:R:104:ALA:HB2	1.95	0.48
9:O:134:GLU:N	9:O:162:LYS:O	2.46	0.48
10:P:81:THR:N	17:P:501:ADP:O2B	2.36	0.48
9:Q:56:ILE:CG1	9:Q:326:ILE:HD13	2.43	0.48
11:U:139:VAL:HG12	11:U:143:TYR:CE2	2.48	0.48
15:X:8:DA:C2'	15:X:9:DT:H71	2.25	0.48
1:A:17:SER:CA	15:X:30:DG:OP1	2.62	0.48
1:E:42:ARG:HA	15:X:111:DA:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:339:ARG:HE	10:R:306:ILE:HD11	1.78	0.48
15:X:80:DG:N1	16:Y:-79:DG:N2	2.61	0.48
9:Q:259:MET:O	9:Q:262:GLN:NE2	2.47	0.48
10:R:47:VAL:HG21	10:R:373:ILE:HD12	1.96	0.48
10:R:141:GLU:N	10:R:164:LYS:O	2.46	0.48
3:G:67:PHE:O	3:G:71:VAL:HG23	2.12	0.48
9:M:308:ASP:OD1	9:M:309:ILE:N	2.43	0.48
11:U:157:ASP:CB	18:U:401:ATP:H4'	2.44	0.48
16:Y:-64:DC:H2"	16:Y:-63:DG:C8	2.48	0.48
5:I:91:LYS:HG3	14:W:193:GLU:HG3	1.96	0.48
5:I:729:LEU:HD11	5:I:758:ARG:HG2	1.95	0.48
6:J:208:PRO:HD2	6:J:211:ILE:CG2	2.43	0.48
9:M:76:LYS:HG2	17:M:501:ADP:PB	2.53	0.48
9:Q:101:VAL:HG21	9:Q:307:LEU:CD2	2.43	0.48
10:R:47:VAL:N	17:R:501:ADP:HN62	2.06	0.48
12:T:160:PHE:O	12:T:399:ILE:HD11	2.13	0.48
11:U:71:ILE:N	11:U:71:ILE:HD12	2.28	0.48
11:U:297:THR:HG23	11:U:297:THR:O	2.14	0.48
15:X:121:DC:H2"	15:X:122:DG:C8	2.49	0.48
1:A:82:ARG:NH1	1:A:108:VAL:O	2.44	0.48
5:I:2046:GLN:O	5:I:2050:VAL:HG23	2.13	0.48
12:T:128:ASN:OD1	12:T:129:THR:N	2.47	0.48
15:X:21:DG:C4	16:Y:-20:DG:N2	2.80	0.48
9:M:111:VAL:O	9:M:115:ASN:ND2	2.43	0.48
10:P:210:THR:C	10:P:212:ALA:N	2.67	0.48
1:E:68:ASN:O	1:E:68:ASN:ND2	2.46	0.48
7:K:113:LEU:HD12	7:K:122:VAL:HG11	1.96	0.48
16:Y:-134:DC:H2"	16:Y:-133:DG:C8	2.48	0.48
1:A:101:VAL:HG22	4:D:96:THR:HB	1.95	0.48
6:J:308:ILE:HD12	6:J:319:ILE:CG2	2.44	0.48
9:M:316:HIS:O	9:M:357:ARG:NH2	2.47	0.48
5:I:1945:HIS:CD2	5:I:1947:THR:HG1	2.29	0.47
9:M:315:LEU:HD21	9:M:329:PHE:CZ	2.48	0.47
9:M:415:LEU:HD21	10:N:61:GLU:CB	2.42	0.47
11:U:138:ALA:HB2	11:U:163:VAL:HG11	1.96	0.47
15:X:4:DA:H2"	15:X:5:DT:H5"	1.95	0.47
4:H:32:PRO:CG	15:X:59:DA:H3'	2.44	0.47
4:H:53:GLU:O	4:H:57:VAL:HG23	2.14	0.47
6:J:212:ILE:HG23	6:J:268:PHE:CE2	2.49	0.47
15:X:66:DG:H2"	15:X:67:DG:N7	2.29	0.47
2:F:31:LYS:H	2:F:31:LYS:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:617:GLN:OE1	5:I:617:GLN:N	2.43	0.47
9:M:53:VAL:HG11	9:M:86:GLU:OE1	2.15	0.47
10:P:265:THR:HG22	10:P:266:GLY:H	1.78	0.47
13:V:175:HIS:NE2	13:V:186:ARG:O	2.46	0.47
16:Y:-48:DA:C2	16:Y:-47:DG:N2	2.82	0.47
7:K:126:ASN:OD1	7:K:128:GLY:N	2.47	0.47
9:M:172:LEU:HD11	10:R:216:ASP:OD2	2.15	0.47
10:N:188:GLN:N	10:N:188:GLN:OE1	2.46	0.47
11:U:301:GLY:O	11:U:304:THR:OG1	2.32	0.47
16:Y:-10:DT:H2"	16:Y:-9:DA:H5'	1.95	0.47
16:Y:-9:DA:H2'	16:Y:-8:DT:C7	2.44	0.47
1:A:25:GLN:OE1	1:A:25:GLN:N	2.47	0.47
3:C:42:ARG:NH1	16:Y:-77:DA:H5"	2.29	0.47
3:C:49:ARG:CD	15:X:6:DG:O3'	2.56	0.47
6:J:294:VAL:HG21	6:J:315:ALA:HB1	1.96	0.47
10:N:362:TYR:HE2	17:N:501:ADP:N7	2.13	0.47
16:Y:-7:DA:H2"	16:Y:-6:DC:H5'	1.95	0.47
5:I:164:LYS:HG2	15:X:32:DC:OP1	2.15	0.47
6:J:219:VAL:HG13	6:J:220:PRO:HD2	1.97	0.47
7:K:292:MET:CE	7:K:293:GLY:O	2.62	0.47
10:N:298:ILE:HG22	10:N:301:VAL:HG22	1.95	0.47
9:Q:374:ILE:HG12	17:Q:501:ADP:C6	2.50	0.47
10:R:46:MET:HA	17:R:501:ADP:N1	2.30	0.47
5:I:2013:GLU:N	5:I:2013:GLU:OE1	2.48	0.47
7:K:346:ASP:OD1	7:K:347:VAL:N	2.48	0.47
9:M:43:GLU:OE1	9:M:43:GLU:N	2.44	0.47
9:M:180:LEU:HD23	9:M:200:VAL:HG11	1.96	0.47
11:U:153:MET:CG	11:U:274:ILE:HD11	2.45	0.47
11:U:177:ARG:NH1	11:U:179:ASP:OD1	2.48	0.47
15:X:73:DC:H2"	15:X:74:DG:C8	2.50	0.47
15:X:85:DT:C6	15:X:86:DT:H72	2.50	0.47
16:Y:-1:DT:H2"	16:Y:0:DG:H5"	1.97	0.47
6:J:172:LEU:HD12	6:J:172:LEU:O	2.15	0.47
15:X:2:DG:H2"	15:X:3:DG:C8	2.49	0.47
15:X:3:DG:C2'	15:X:4:DA:H5'	2.45	0.47
15:X:65:DG:H2"	15:X:66:DG:C8	2.50	0.47
5:I:974:LEU:HD21	5:I:1904:ILE:HG23	1.97	0.47
7:K:351:LEU:HD23	7:K:352:PRO:O	2.15	0.47
9:M:362:ARG:HD2	10:R:434:LEU:HD11	1.97	0.47
10:R:248:ASP:OD1	10:R:251:ASN:ND2	2.48	0.47
16:Y:-115:DT:N1	16:Y:-114:DT:H72	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ALA:HB2	15:X:110:DG:OP2	2.15	0.47
16:Y:-102:DG:H1'	16:Y:-101:DC:H5'	1.96	0.47
2:B:89:ARG:HH11	13:V:63:SER:CB	2.27	0.46
9:M:53:VAL:HG22	9:M:87:LEU:HD21	1.96	0.46
9:O:106:ILE:HG22	9:O:269:THR:HG22	1.97	0.46
10:P:72:ALA:HB1	10:P:324:LEU:HD11	1.97	0.46
15:X:75:DC:H2"	15:X:76:DG:C8	2.49	0.46
15:X:95:DG:C5	15:X:96:DC:C4	3.03	0.46
15:X:95:DG:C5	15:X:96:DC:N4	2.83	0.46
15:X:126:DT:H6	15:X:126:DT:OP2	1.98	0.46
16:Y:-99:DC:H2"	16:Y:-98:DT:C7	2.44	0.46
9:Q:56:ILE:HG13	9:Q:326:ILE:HD13	1.97	0.46
10:R:68:ILE:HD13	10:R:68:ILE:H	1.80	0.46
11:U:336:LYS:HE3	18:U:401:ATP:N7	2.30	0.46
15:X:19:DA:N3	16:Y:-18:DG:N2	2.63	0.46
15:X:72:DG:C6	15:X:73:DC:N4	2.83	0.46
5:I:1930:GLN:HB3	5:I:1931:PRO:HD3	1.97	0.46
5:I:2172:VAL:HG12	5:I:2172:VAL:O	2.15	0.46
9:Q:334:GLY:O	9:Q:348:HIS:N	2.47	0.46
13:V:59:ALA:O	13:V:63:SER:HB2	2.15	0.46
13:V:202:LEU:HD23	13:V:202:LEU:O	2.14	0.46
15:X:133:DC:H2"	15:X:134:DG:C8	2.51	0.46
16:Y:-96:DG:C4	16:Y:-95:DC:C5	3.04	0.46
5:I:608:THR:HG21	5:I:630:VAL:HG11	1.97	0.46
8:L:19:LEU:HD23	8:L:150:LEU:HD13	1.96	0.46
15:X:77:DT:H2"	15:X:78:DA:C8	2.49	0.46
16:Y:-128:DC:H2"	16:Y:-127:DG:N7	2.30	0.46
5:I:737:ARG:NH2	15:X:133:DC:O4'	2.45	0.46
9:M:114:GLU:N	9:M:114:GLU:OE1	2.49	0.46
9:M:132:GLU:O	9:M:228:VAL:HG23	2.15	0.46
10:N:47:VAL:CG2	10:N:373:ILE:HD12	2.46	0.46
9:O:264:MET:C	9:O:266:PRO:HD3	2.36	0.46
10:P:49:GLN:HG3	10:P:52:ALA:HB3	1.97	0.46
12:T:21:TYR:CD2	12:T:22:THR:HG23	2.50	0.46
15:X:14:DG:H2"	15:X:15:DT:C5	2.51	0.46
7:K:86:VAL:O	7:K:86:VAL:HG12	2.16	0.46
9:M:170:LEU:HB3	10:R:216:ASP:HB2	1.98	0.46
10:N:272:VAL:O	10:N:276:ILE:HD13	2.16	0.46
9:O:40:VAL:O	17:O:501:ADP:N6	2.49	0.46
10:P:54:ARG:O	10:P:58:VAL:HG23	2.16	0.46
9:Q:255:ASP:OD1	9:Q:258:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:381:ILE:N	12:T:381:ILE:HD12	2.30	0.46
15:X:131:DA:C6	16:Y:-130:DG:N2	2.83	0.46
1:A:17:SER:HA	15:X:30:DG:C5'	2.46	0.46
8:L:87:LEU:C	8:L:87:LEU:HD13	2.35	0.46
5:I:1936:ILE:HG22	5:I:1956:HIS:HA	1.97	0.46
11:U:185:LEU:HD13	11:U:185:LEU:O	2.15	0.46
15:X:116:DT:H2"	15:X:117:DT:C7	2.46	0.46
16:Y:-124:DG:C4	16:Y:-123:DC:C4	3.04	0.46
4:H:43:VAL:HG12	4:H:45:ARG:H	1.81	0.46
5:I:156:ARG:CG	16:Y:-28:DC:OP1	2.64	0.46
7:K:102:PHE:CG	7:K:105:ILE:HD12	2.51	0.46
9:M:115:ASN:OD1	9:M:118:ARG:NH1	2.49	0.46
9:M:159:ILE:HG22	9:M:172:LEU:HD13	1.98	0.46
10:N:166:THR:HG23	10:N:167:GLU:HG3	1.97	0.46
16:Y:-126:DA:H2"	16:Y:-125:DG:C8	2.51	0.46
16:Y:-93:DC:C2	16:Y:-92:DC:C5	3.04	0.46
4:H:79:LYS:HB2	16:Y:-45:DG:OP1	2.15	0.46
5:I:120:SER:OG	13:V:229:GLN:NE2	2.49	0.46
9:M:403:LEU:O	9:M:407:VAL:HG23	2.16	0.46
10:P:144:GLU:O	10:P:161:LEU:HD12	2.16	0.46
12:T:84:ALA:HB2	12:T:249:SER:CB	2.46	0.46
11:U:241:GLU:N	11:U:241:GLU:OE1	2.48	0.46
15:X:96:DC:H2"	15:X:97:DT:C7	2.46	0.46
16:Y:-80:DC:H2"	16:Y:-79:DG:C8	2.50	0.46
9:M:53:VAL:HG23	9:M:83:ILE:HG23	1.98	0.45
10:N:119:LEU:HD21	10:N:312:LEU:HD21	1.98	0.45
9:Q:374:ILE:CG2	17:Q:501:ADP:C4	2.99	0.45
9:Q:397:ILE:O	9:Q:401:THR:HG22	2.16	0.45
15:X:76:DG:N2	16:Y:-75:DG:N3	2.63	0.45
16:Y:-104:DC:H2"	16:Y:-103:DA:C8	2.51	0.45
9:O:315:LEU:HD23	9:O:354:LEU:HD21	1.98	0.45
10:R:141:GLU:O	10:R:164:LYS:N	2.49	0.45
16:Y:-124:DG:N9	16:Y:-123:DC:C5	2.84	0.45
7:K:24:VAL:HG22	7:K:24:VAL:O	2.16	0.45
13:V:55:ARG:HB2	16:Y:-36:DC:OP1	2.17	0.45
15:X:64:DG:C5	15:X:65:DG:N1	2.85	0.45
1:A:108:VAL:HG11	3:C:101:VAL:HG11	1.98	0.45
6:J:277:TRP:C	6:J:280:GLN:HG3	2.24	0.45
7:K:123:LEU:HG	7:K:125:VAL:HG13	1.98	0.45
10:N:313:ASN:ND2	10:N:349:ASP:OD2	2.45	0.45
9:O:326:ILE:N	9:O:326:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:382:MET:CE	10:R:426:ILE:HD11	2.45	0.45
13:V:56:GLU:N	13:V:56:GLU:OE1	2.49	0.45
15:X:21:DG:N2	16:Y:-20:DG:N3	2.65	0.45
7:K:269:ARG:NE	7:K:270:LEU:O	2.47	0.45
7:K:289:ILE:HG23	8:L:32:LEU:HD22	1.97	0.45
9:Q:303:GLU:OE1	9:Q:305:HIS:NE2	2.45	0.45
9:Q:369:GLN:OE1	9:Q:373:GLN:NE2	2.48	0.45
11:U:210:ARG:NE	18:U:401:ATP:H2'	2.32	0.45
13:V:56:GLU:CD	13:V:56:GLU:H	2.19	0.45
15:X:64:DG:H2"	15:X:65:DG:C8	2.52	0.45
15:X:89:DA:H2"	15:X:90:DG:H8	1.80	0.45
16:Y:-23:DC:H2"	16:Y:-22:DA:H8	1.81	0.45
2:B:116:THR:HG22	13:V:57:VAL:CG2	2.47	0.45
5:I:151:PHE:HD2	12:T:399:ILE:HG22	1.79	0.45
6:J:291:VAL:HG13	6:J:296:HIS:HA	1.98	0.45
9:O:102:TYR:OH	9:O:306:MET:O	2.23	0.45
11:U:101:HIS:CG	11:U:129:THR:HG22	2.52	0.45
15:X:72:DG:C5	15:X:73:DC:C4	3.04	0.45
5:I:928:LEU:HD13	5:I:928:LEU:H	1.81	0.45
9:O:98:GLY:O	9:O:101:VAL:HG22	2.16	0.45
10:P:403:ILE:CD1	17:P:501:ADP:H4'	2.47	0.45
10:R:170:THR:OG1	10:R:171:ILE:N	2.49	0.45
15:X:10:DA:C5	15:X:11:DT:C4	3.05	0.45
1:E:17:ARG:NH1	16:Y:-115:DT:OP2	2.49	0.45
3:G:41:TYR:HD2	16:Y:-62:DC:OP1	2.00	0.45
5:I:737:ARG:HG2	16:Y:-131:DT:C4'	2.46	0.45
5:I:737:ARG:NH2	16:Y:-132:DG:N2	2.64	0.45
7:K:13:ALA:HB2	7:K:27:ASN:HB2	1.99	0.45
10:P:210:THR:O	10:P:212:ALA:N	2.50	0.45
10:P:268:ILE:HD13	10:P:268:ILE:N	2.31	0.45
9:Q:106:ILE:HD11	9:Q:110:GLU:CG	2.47	0.45
11:S:107:GLU:OE1	11:S:111:ASN:ND2	2.48	0.45
11:U:162:THR:HG22	11:U:278:THR:HG22	1.99	0.45
11:U:163:VAL:HG22	11:U:165:ILE:HG23	1.99	0.45
15:X:6:DG:N1	15:X:7:DT:N3	2.65	0.45
15:X:49:DT:H5"	15:X:49:DT:H6	1.81	0.45
4:H:83:ALA:O	4:H:87:VAL:HG23	2.17	0.45
5:I:2062:VAL:HG22	5:I:2132:THR:OG1	2.17	0.45
5:I:2171:THR:OG1	5:I:2172:VAL:N	2.50	0.45
9:Q:404:ARG:NH2	17:Q:501:ADP:O3B	2.50	0.45
11:U:149:THR:HG22	11:U:150:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:46:DC:H2"	15:X:47:DC:C5	2.51	0.45
15:X:86:DT:C2'	15:X:87:DT:H72	2.46	0.45
16:Y:-9:DA:H2"	16:Y:-8:DT:C5	2.52	0.45
5:I:949:ILE:HD13	5:I:949:ILE:O	2.17	0.45
7:K:237:VAL:HG22	7:K:267:ILE:HD12	1.99	0.45
16:Y:-35:DC:H2"	16:Y:-34:DT:C6	2.52	0.45
16:Y:-1:DT:C2'	16:Y:0:DG:H5"	2.47	0.45
1:A:17:SER:C	15:X:30:DG:OP1	2.50	0.44
7:K:302:ILE:HD12	7:K:313:PHE:HB3	1.99	0.44
15:X:54:DG:C6	16:Y:-55:DA:N6	2.85	0.44
5:I:941:ILE:HD12	5:I:941:ILE:N	2.32	0.44
7:K:296:GLU:OE1	7:K:296:GLU:N	2.47	0.44
10:P:236:LYS:HE3	10:P:238:VAL:HG13	1.99	0.44
16:Y:-43:DA:C6	16:Y:-42:DT:C4	3.05	0.44
16:Y:-35:DC:H2"	16:Y:-34:DT:C5	2.50	0.44
9:O:20:HIS:CE1	17:O:501:ADP:O2'	2.70	0.44
11:S:43:VAL:HG12	11:S:43:VAL:O	2.18	0.44
13:V:223:GLU:OE2	13:V:226:ARG:NH1	2.43	0.44
15:X:51:DG:C5	15:X:52:DC:N4	2.85	0.44
6:J:308:ILE:CG2	6:J:319:ILE:HD13	2.47	0.44
9:M:401:THR:HG22	9:M:402:THR:HG22	1.98	0.44
10:P:348:ILE:HD13	10:P:348:ILE:N	2.32	0.44
9:Q:21:VAL:HG21	9:Q:81:LEU:HD11	1.99	0.44
14:W:140:ASP:OD1	14:W:141:GLU:N	2.47	0.44
1:E:29:ARG:HA	16:Y:-116:DA:OP1	2.17	0.44
4:H:48:GLY:N	16:Y:-65:DC:O5'	2.50	0.44
5:I:904:PRO:O	5:I:907:PHE:N	2.51	0.44
5:I:971:ARG:NH2	5:I:1902:GLU:OE1	2.50	0.44
9:Q:401:THR:OG1	9:Q:402:THR:N	2.50	0.44
12:T:22:THR:HG22	12:T:38:PRO:HA	1.98	0.44
15:X:96:DC:H2"	15:X:97:DT:C6	2.53	0.44
1:E:73:ASN:O	1:E:73:ASN:ND2	2.45	0.44
5:I:869:TYR:CE2	5:I:897:LEU:HD22	2.53	0.44
13:V:65:LYS:O	13:V:65:LYS:HG2	2.17	0.44
15:X:36:DG:H2"	15:X:37:DG:C8	2.53	0.44
15:X:108:DA:H2"	15:X:109:DC:C6	2.52	0.44
16:Y:-34:DT:H5'	16:Y:-34:DT:C6	2.50	0.44
5:I:737:ARG:NH1	16:Y:-132:DG:H22	2.15	0.44
9:O:168:LYS:CG	9:O:228:VAL:HG11	2.47	0.44
10:R:264:ASP:OD1	10:R:265:THR:N	2.51	0.44
15:X:69:DA:H2"	15:X:70:DC:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:-96:DG:H2”	16:Y:-95:DC:H6	1.82	0.44
16:Y:-12:DT:H1’	16:Y:-11:DA:C5’	2.48	0.44
4:D:49:LEU:H	4:D:49:LEU:HD12	1.81	0.44
5:I:109:ARG:HB2	13:V:246:TYR:CZ	2.52	0.44
5:I:692:SER:OG	6:J:181:GLU:OE1	2.35	0.44
6:J:260:ARG:HA	6:J:260:ARG:HD3	1.38	0.44
7:K:86:VAL:O	7:K:87:ASP:C	2.55	0.44
8:L:84:PHE:CE2	8:L:87:LEU:HD12	2.52	0.44
9:M:20:HIS:CE1	17:M:501:ADP:HO2’	2.32	0.44
10:N:119:LEU:HD21	10:N:312:LEU:CD2	2.48	0.44
15:X:51:DG:C6	15:X:52:DC:N4	2.86	0.44
5:I:619:ARG:NH2	5:I:621:TYR:OH	2.43	0.44
9:O:33:LYS:O	9:O:46:ARG:NH1	2.48	0.44
9:O:87:LEU:HD12	9:O:91:VAL:HG21	1.99	0.44
11:U:149:THR:HG23	11:U:166:TYR:HA	1.99	0.44
15:X:15:DT:H3	16:Y:-15:DA:H61	1.66	0.44
16:Y:-51:DC:H2”	16:Y:-50:DC:C6	2.53	0.44
7:K:198:GLU:OE2	7:K:202:ILE:N	2.50	0.43
7:K:277:VAL:HG22	7:K:278:PRO:HD3	2.00	0.43
9:M:40:VAL:O	17:M:501:ADP:N6	2.51	0.43
9:M:405:TYR:CE2	9:M:409:LEU:HD11	2.53	0.43
12:T:122:MET:SD	12:T:136:LEU:HD21	2.57	0.43
15:X:112:DC:H2”	15:X:113:DC:H6	1.83	0.43
16:Y:-3:DC:H2’	16:Y:-2:DC:C6	2.53	0.43
6:J:262:SER:N	10:P:212:ALA:O	2.50	0.43
9:M:275:LEU:HD22	10:R:260:LEU:O	2.18	0.43
16:Y:-15:DA:O5’	16:Y:-15:DA:H8	2.01	0.43
2:F:83:ARG:HH22	16:Y:-106:DG:H3’	1.46	0.43
5:I:147:LEU:HD11	5:I:151:PHE:CE1	2.53	0.43
5:I:157:TRP:CE2	5:I:161:VAL:HG21	2.53	0.43
5:I:1976:PHE:CZ	10:P:131:ILE:HD12	2.53	0.43
9:Q:49:CYS:O	9:Q:52:ILE:HG13	2.18	0.43
15:X:95:DG:C4	15:X:96:DC:C5	3.07	0.43
16:Y:-113:DG:C6	16:Y:-112:DG:O6	2.71	0.43
16:Y:-47:DG:H2”	16:Y:-46:DG:C8	2.53	0.43
1:E:29:ARG:HH12	15:X:121:DC:P	2.41	0.43
7:K:329:PHE:O	7:K:333:VAL:HG23	2.17	0.43
11:U:327:ILE:HD13	11:U:327:ILE:N	2.34	0.43
5:I:990:VAL:HG12	5:I:990:VAL:O	2.18	0.43
7:K:124:ARG:HG3	7:K:124:ARG:O	2.18	0.43
11:U:107:GLU:OE2	11:U:134:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:21:ASN:ND2	7:K:21:ASN:O	2.50	0.43
9:Q:105:GLU:OE1	9:Q:105:GLU:N	2.51	0.43
9:Q:393:HIS:HD2	9:Q:430:VAL:HG13	1.83	0.43
13:V:147:LEU:N	13:V:147:LEU:HD22	2.34	0.43
15:X:8:DA:C8	15:X:9:DT:H73	2.53	0.43
15:X:125:DC:C2'	15:X:126:DT:C7	2.89	0.43
1:E:104:GLN:NE2	3:G:94:GLU:OE2	2.52	0.43
5:I:875:GLN:OE1	5:I:878:THR:HG23	2.19	0.43
5:I:906:LEU:HD22	5:I:2070:ARG:HB3	2.00	0.43
7:K:3:THR:HG22	7:K:92:ASN:OD1	2.18	0.43
7:K:277:VAL:N	7:K:278:PRO:CD	2.81	0.43
8:L:19:LEU:CD1	8:L:23:ALA:HB3	2.49	0.43
9:Q:447:LEU:HD22	10:R:331:GLY:HA2	2.00	0.43
11:U:149:THR:CG2	11:U:293:LEU:HD22	2.49	0.43
11:U:306:TYR:CD1	18:U:401:ATP:C2	3.03	0.43
5:I:638:ASN:ND2	5:I:792:LEU:O	2.48	0.43
5:I:888:MET:SD	5:I:888:MET:N	2.91	0.43
9:M:302:ASP:OD2	10:N:314:ARG:NE	2.48	0.43
9:M:447:LEU:HD11	10:N:344:HIS:CE1	2.53	0.43
10:N:298:ILE:CG2	10:N:301:VAL:HG22	2.49	0.43
10:N:409:ALA:CA	10:N:429:VAL:HG21	2.49	0.43
12:T:333:VAL:HG11	12:T:345:TYR:CE2	2.54	0.43
13:V:137:VAL:O	13:V:137:VAL:HG13	2.19	0.43
15:X:1:DA:C2	15:X:2:DG:C6	3.07	0.43
15:X:44:DC:C2'	15:X:45:DC:C5	2.97	0.43
15:X:131:DA:C5	16:Y:-130:DG:N2	2.87	0.43
5:I:610:ILE:HD12	5:I:610:ILE:N	2.34	0.43
5:I:1986:PRO:O	5:I:1987:PRO:C	2.57	0.43
6:J:216:SER:HB3	10:P:145:ILE:HG13	2.00	0.43
7:K:347:VAL:HG13	7:K:347:VAL:O	2.19	0.43
9:M:295:VAL:HG23	9:M:295:VAL:O	2.19	0.43
11:U:221:LEU:O	11:U:225:GLN:N	2.50	0.43
15:X:112:DC:H2"	15:X:113:DC:C6	2.54	0.43
16:Y:-124:DG:H2"	16:Y:-123:DC:H6	1.84	0.43
5:I:957:ARG:NH2	5:I:1916:PRO:O	2.52	0.43
10:N:245:HIS:O	10:N:249:VAL:HG23	2.18	0.43
14:W:195:ALA:O	14:W:199:GLU:HG2	2.19	0.43
15:X:110:DG:N1	16:Y:-109:DG:N2	2.60	0.43
15:X:115:DA:C8	15:X:116:DT:H72	2.54	0.43
1:A:84:LEU:O	1:A:88:ILE:HD12	2.19	0.42
9:M:243:LEU:O	9:M:247:ASN:ND2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:161:LEU:HD12	10:N:162:THR:H	1.84	0.42
15:X:8:DA:C5	15:X:9:DT:C4	3.07	0.42
16:Y:-85:DA:C4	16:Y:-84:DC:C5	3.07	0.42
7:K:22:VAL:HG22	7:K:360:TRP:CE2	2.53	0.42
10:N:161:LEU:HB2	10:N:174:LEU:HD11	2.00	0.42
13:V:215:ILE:N	13:V:215:ILE:HD12	2.34	0.42
7:K:59:PRO:O	7:K:66:VAL:N	2.51	0.42
10:P:188:GLN:HE21	10:P:188:GLN:HB3	1.57	0.42
9:Q:404:ARG:NE	17:Q:501:ADP:C5'	2.82	0.42
11:U:289:ILE:HG22	11:U:293:LEU:HD21	2.01	0.42
14:W:150:MET:O	14:W:154:LEU:HG	2.19	0.42
14:W:194:ILE:CG2	14:W:198:LYS:HE2	2.49	0.42
15:X:8:DA:C2'	15:X:9:DT:C6	3.01	0.42
15:X:48:DT:N1	15:X:49:DT:H72	2.34	0.42
15:X:84:DG:C8	15:X:85:DT:H72	2.54	0.42
16:Y:-132:DG:H2"	16:Y:-131:DT:C7	2.48	0.42
1:E:66:ALA:HB2	1:E:83:LEU:HD23	2.01	0.42
5:I:165:VAL:HG22	11:U:355:MET:SD	2.59	0.42
5:I:166:VAL:HG21	11:U:168:GLY:CA	2.43	0.42
6:J:308:ILE:HG21	6:J:319:ILE:HD13	2.01	0.42
9:O:304:VAL:HG22	9:O:304:VAL:O	2.19	0.42
9:O:443:SER:OG	10:P:344:HIS:NE2	2.40	0.42
10:P:169:GLU:N	10:P:169:GLU:OE1	2.52	0.42
10:P:270:SER:O	10:P:272:VAL:N	2.52	0.42
13:V:250:GLU:HA	13:V:253:LYS:HD2	2.02	0.42
15:X:106:DC:C2'	15:X:107:DT:H72	2.49	0.42
16:Y:-1:DT:H2"	16:Y:0:DG:C5'	2.50	0.42
2:B:120:SER:O	2:B:121:SER:OG	2.35	0.42
10:N:22:ILE:HD12	10:N:22:ILE:N	2.34	0.42
10:P:367:THR:HG23	10:P:399:LEU:HD13	2.01	0.42
10:R:306:ILE:HD13	10:R:338:THR:CG2	2.50	0.42
14:W:190:THR:HG22	14:W:194:ILE:CD1	2.47	0.42
15:X:77:DT:H2"	15:X:78:DA:N7	2.35	0.42
15:X:100:DA:C6	15:X:101:DG:C6	3.07	0.42
16:Y:-119:DT:H2"	16:Y:-118:DC:C5	2.54	0.42
16:Y:-66:DC:H2"	16:Y:-65:DC:C6	2.55	0.42
16:Y:-30:DC:H2"	16:Y:-29:DT:C6	2.55	0.42
5:I:1949:TRP:O	9:Q:234:ILE:HG23	2.19	0.42
5:I:2140:TRP:CH2	5:I:2176:ILE:HG23	2.55	0.42
9:M:384:ILE:HG21	9:M:425:ILE:HD12	2.01	0.42
10:P:245:HIS:HA	10:P:248:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:57:VAL:O	13:V:61:LEU:HG	2.19	0.42
13:V:208:VAL:N	13:V:209:PRO:CD	2.83	0.42
14:W:66:ILE:HD12	14:W:86:TYR:CG	2.55	0.42
15:X:34:DA:N6	15:X:35:DG:O6	2.51	0.42
15:X:54:DG:H2"	15:X:55:DT:H5'	2.01	0.42
15:X:129:DG:H2"	15:X:130:DC:C6	2.55	0.42
5:I:951:LEU:HD11	5:I:1914:LEU:HD13	2.01	0.42
9:M:105:GLU:OE1	9:M:105:GLU:N	2.51	0.42
9:Q:106:ILE:HD11	9:Q:110:GLU:HG2	2.02	0.42
4:H:62:LEU:O	4:H:63:GLU:C	2.57	0.42
5:I:216:LYS:O	5:I:220:ARG:HG2	2.19	0.42
5:I:927:SER:OG	5:I:928:LEU:N	2.53	0.42
6:J:297:ARG:HB3	6:J:298:PRO:HD2	2.02	0.42
9:M:270:GLU:HB3	9:M:275:LEU:HD23	2.02	0.42
10:P:348:ILE:HD13	10:P:348:ILE:H	1.84	0.42
12:T:247:THR:HG22	12:T:248:ARG:N	2.34	0.42
11:U:302:GLY:HA3	18:U:401:ATP:O2A	2.18	0.42
15:X:114:DA:C6	15:X:115:DA:C6	3.08	0.42
16:Y:-8:DT:H2"	16:Y:-7:DA:C8	2.53	0.42
1:A:43:ARG:NH2	16:Y:-35:DC:C4'	2.20	0.42
2:B:41:VAL:O	2:B:45:VAL:HG22	2.19	0.42
2:B:91:ILE:O	2:B:95:VAL:HG23	2.20	0.42
6:J:165:ARG:N	6:J:166:PRO:HD3	2.35	0.42
10:N:256:GLY:O	10:N:258:LEU:N	2.45	0.42
9:Q:135:VAL:HG13	9:Q:188:GLY:H	1.85	0.42
9:Q:308:ASP:OD1	9:Q:310:GLU:N	2.53	0.42
11:S:151:ILE:HD13	11:S:278:THR:HG23	2.02	0.42
14:W:157:THR:HG22	14:W:157:THR:O	2.20	0.42
15:X:72:DG:C4	15:X:73:DC:C5	3.08	0.42
15:X:103:DT:H2"	15:X:104:DG:C8	2.55	0.42
16:Y:-107:DA:C6	16:Y:-106:DG:C6	3.08	0.42
16:Y:-102:DG:C5	16:Y:-101:DC:N4	2.88	0.42
16:Y:-65:DC:C2'	16:Y:-64:DC:C5	3.03	0.42
5:I:161:VAL:HG12	5:I:162:ALA:N	2.34	0.42
5:I:672:ILE:HG22	5:I:674:VAL:HG13	2.02	0.42
10:R:27:HIS:NE2	17:R:501:ADP:N3	2.68	0.42
14:W:194:ILE:CG2	14:W:198:LYS:HD2	2.50	0.42
15:X:88:DA:H1'	15:X:89:DA:C8	2.55	0.42
16:Y:-1:DT:H1'	16:Y:0:DG:H5"	2.01	0.42
1:A:55:VAL:O	1:A:59:LEU:HG	2.20	0.41
1:A:65:GLU:N	1:A:65:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1928:LEU:HD22	10:R:279:LYS:CD	2.50	0.41
7:K:123:LEU:CD1	7:K:125:VAL:HG13	2.50	0.41
9:M:316:HIS:CD2	9:M:316:HIS:C	2.93	0.41
9:O:378:ARG:HG2	9:O:407:VAL:HG22	2.01	0.41
10:P:174:LEU:HD13	10:P:182:LEU:CD1	2.50	0.41
11:U:96:VAL:O	11:U:96:VAL:HG13	2.18	0.41
14:W:194:ILE:HG23	14:W:198:LYS:CE	2.50	0.41
15:X:10:DA:C4	15:X:11:DT:C5	3.08	0.41
16:Y:-132:DG:H2"	16:Y:-131:DT:H71	2.02	0.41
9:M:90:LYS:HG3	9:M:91:VAL:HG13	2.03	0.41
10:N:37:LEU:HD21	10:N:61:GLU:HG3	2.02	0.41
9:O:50:GLY:O	9:O:53:VAL:HG22	2.20	0.41
15:X:13:DT:H2"	15:X:14:DG:N7	2.35	0.41
15:X:72:DG:C6	15:X:73:DC:C4	3.08	0.41
16:Y:-125:DG:C2	16:Y:-124:DG:C6	3.08	0.41
16:Y:-82:DC:H2"	16:Y:-81:DA:C8	2.56	0.41
1:A:40:TYR:O	2:B:75:SER:OG	2.28	0.41
4:D:83:ALA:O	4:D:87:VAL:HG23	2.20	0.41
5:I:163:ARG:HB3	5:I:167:ARG:NH1	2.36	0.41
5:I:653:THR:CG2	5:I:744:ILE:HD13	2.51	0.41
9:Q:56:ILE:HG12	9:Q:326:ILE:HG21	2.01	0.41
9:Q:130:VAL:HG13	9:Q:192:TYR:CD2	2.56	0.41
11:S:139:VAL:HG12	11:S:143:TYR:CE2	2.56	0.41
11:U:369:ILE:HG23	11:U:370:VAL:N	2.35	0.41
16:Y:-122:DC:C4	16:Y:-121:DG:C6	3.09	0.41
4:H:49:LEU:HD12	4:H:49:LEU:N	2.36	0.41
6:J:167:LEU:O	6:J:168:THR:HG23	2.19	0.41
9:M:374:ILE:HG12	17:M:501:ADP:C2	2.55	0.41
11:U:289:ILE:CG2	11:U:293:LEU:HD21	2.51	0.41
11:U:289:ILE:N	11:U:289:ILE:HD12	2.35	0.41
15:X:10:DA:C2'	15:X:11:DT:H71	2.50	0.41
15:X:21:DG:N2	16:Y:-20:DG:N2	2.53	0.41
16:Y:-52:DG:H2"	16:Y:-51:DC:C6	2.56	0.41
16:Y:-7:DA:H2"	16:Y:-6:DC:C5'	2.51	0.41
10:P:143:VAL:HG23	10:P:162:THR:O	2.20	0.41
9:Q:124:ILE:HG13	9:Q:291:ILE:HG22	2.02	0.41
9:Q:255:ASP:OD1	9:Q:258:SER:HB3	2.21	0.41
9:Q:411:THR:N	9:Q:412:PRO:HD2	2.36	0.41
15:X:89:DA:H2"	15:X:90:DG:C8	2.55	0.41
15:X:131:DA:C6	16:Y:-130:DG:C2	3.09	0.41
5:I:195:ALA:HB3	11:S:169:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1960:LEU:N	5:I:1960:LEU:HD22	2.36	0.41
6:J:216:SER:O	10:P:144:GLU:HA	2.20	0.41
7:K:6:LEU:C	7:K:6:LEU:HD23	2.41	0.41
7:K:84:TYR:O	7:K:84:TYR:CG	2.74	0.41
7:K:183:HIS:CD2	7:K:187:ILE:HD11	2.55	0.41
9:M:263:LEU:HD12	9:O:263:LEU:O	2.20	0.41
10:N:301:VAL:HG13	10:N:304:LEU:CD1	2.49	0.41
15:X:5:DT:H2"	15:X:6:DG:O5'	2.20	0.41
16:Y:-9:DA:C2'	16:Y:-8:DT:H71	2.51	0.41
5:I:661:ALA:HB1	5:I:667:TRP:CE2	2.56	0.41
9:M:172:LEU:HD12	9:M:172:LEU:N	2.36	0.41
9:M:180:LEU:HD22	9:M:185:VAL:HG21	2.03	0.41
10:N:94:LEU:HD21	10:N:98:THR:CG2	2.50	0.41
10:P:328:THR:HG21	10:P:344:HIS:HD1	1.86	0.41
10:R:346:ILE:HD12	10:R:350:LEU:HD23	2.01	0.41
15:X:60:DA:C5	15:X:61:DC:N4	2.88	0.41
16:Y:-100:DT:H6	16:Y:-100:DT:H2'	1.74	0.41
6:J:183:ASN:O	6:J:187:LEU:HD23	2.20	0.41
8:L:117:CYS:SG	8:L:118:ALA:N	2.94	0.41
9:M:47:GLU:OE2	10:R:428:ARG:NH2	2.49	0.41
9:M:155:SER:O	10:R:213:ARG:NH1	2.54	0.41
9:O:76:LYS:HG3	17:O:501:ADP:O1B	2.20	0.41
9:Q:102:TYR:OH	9:Q:339:ARG:NH2	2.54	0.41
11:U:210:ARG:CZ	18:U:401:ATP:C2'	2.98	0.41
11:U:299:LEU:HD13	11:U:309:ILE:HD12	2.02	0.41
3:C:61:LEU:HD12	4:D:37:LEU:HD23	2.02	0.41
4:D:61:PHE:O	4:D:65:VAL:HG23	2.20	0.41
1:E:68:ASN:HB2	6:J:145:PHE:CZ	2.56	0.41
3:G:41:TYR:O	16:Y:-63:DG:H4'	2.21	0.41
4:H:36:ARG:CZ	15:X:59:DA:OP1	2.69	0.41
5:I:1977:ILE:HD13	5:I:2024:ILE:HG23	2.03	0.41
6:J:268:PHE:CD1	6:J:268:PHE:N	2.89	0.41
7:K:292:MET:SD	7:K:296:GLU:HB2	2.61	0.41
7:K:302:ILE:HB	7:K:303:GLN:OE1	2.20	0.41
9:M:262:GLN:O	9:M:263:LEU:HB3	2.21	0.41
10:N:47:VAL:HG23	10:N:373:ILE:HD12	2.02	0.41
10:P:147:ILE:HD12	10:P:158:VAL:O	2.21	0.41
9:Q:374:ILE:CD1	17:Q:501:ADP:C5	3.04	0.41
10:R:34:ASP:OD1	10:R:40:ARG:NE	2.48	0.41
10:R:224:PHE:O	10:R:225:VAL:C	2.60	0.41
11:U:153:MET:SD	11:U:274:ILE:HD11	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:287:VAL:HG13	11:U:288:ASP:N	2.35	0.41
11:U:293:LEU:N	11:U:293:LEU:HD23	2.35	0.41
11:U:300:SER:OG	11:U:338:SER:OG	2.33	0.41
15:X:12:DA:H2"	15:X:13:DT:C6	2.56	0.41
15:X:24:DC:H6	15:X:24:DC:H2'	1.74	0.41
15:X:93:DG:C6	15:X:94:DT:C4	3.08	0.41
15:X:116:DT:C2'	15:X:117:DT:C7	2.96	0.41
16:Y:-25:DG:H2"	16:Y:-24:DG:C8	2.56	0.41
12:T:121:LEU:C	12:T:121:LEU:HD23	2.42	0.41
11:U:267:LEU:C	11:U:267:LEU:HD23	2.41	0.41
16:Y:-102:DG:C5	16:Y:-101:DC:C4	3.09	0.41
1:E:102:ILE:HD12	1:E:102:ILE:N	2.35	0.40
7:K:13:ALA:HB2	7:K:27:ASN:CB	2.52	0.40
7:K:292:MET:HE1	7:K:297:ALA:N	2.35	0.40
15:X:58:DA:H2"	15:X:59:DA:C8	2.56	0.40
15:X:110:DG:N2	16:Y:-109:DG:H21	2.08	0.40
16:Y:-22:DA:H1'	16:Y:-21:DC:H5'	2.04	0.40
4:H:35:ARG:O	4:H:39:ARG:HG2	2.21	0.40
10:P:117:GLU:OE1	10:P:121:GLN:NE2	2.54	0.40
10:P:225:VAL:HG22	10:P:226:GLN:N	2.36	0.40
15:X:25:DC:H2"	15:X:26:DT:C4	2.56	0.40
5:I:873:MET:SD	5:I:897:LEU:HD21	2.60	0.40
6:J:213:THR:O	6:J:266:ILE:HG23	2.22	0.40
10:N:80:GLY:HA2	17:N:501:ADP:PA	2.62	0.40
15:X:22:DT:C4	15:X:23:DG:C6	3.10	0.40
3:G:66:PRO:HG3	16:Y:-55:DA:OP1	2.22	0.40
7:K:285:SER:H	7:K:289:ILE:HD11	1.86	0.40
10:N:49:GLN:HG2	10:N:86:ILE:HD11	2.02	0.40
10:N:119:LEU:HD21	10:N:312:LEU:HG	2.03	0.40
10:P:47:VAL:CB	17:P:501:ADP:N1	2.85	0.40
10:P:305:ASP:OD1	10:P:306:ILE:N	2.48	0.40
10:P:349:ASP:O	10:P:353:ARG:NH2	2.48	0.40
9:Q:23:GLY:O	9:Q:37:SER:OG	2.38	0.40
10:R:204:LYS:O	10:R:223:LYS:HE2	2.21	0.40
15:X:62:DG:C2	16:Y:-61:DG:C2	3.10	0.40
15:X:86:DT:H2"	15:X:87:DT:H72	2.03	0.40
5:I:205:PHE:O	5:I:209:VAL:HG23	2.21	0.40
10:P:272:VAL:O	10:P:276:ILE:HD13	2.22	0.40
10:R:403:ILE:CD1	17:R:501:ADP:H4'	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	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
1	E	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
2	B	94/126 (75%)	93 (99%)	1 (1%)	0	100	100
2	F	92/126 (73%)	87 (95%)	5 (5%)	0	100	100
3	C	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
3	G	95/136 (70%)	95 (100%)	0	0	100	100
4	D	79/103 (77%)	79 (100%)	0	0	100	100
4	H	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
5	I	782/3230 (24%)	742 (95%)	38 (5%)	2 (0%)	41	74
6	J	154/364 (42%)	129 (84%)	24 (16%)	1 (1%)	25	64
7	K	392/396 (99%)	359 (92%)	32 (8%)	1 (0%)	41	74
8	L	109/154 (71%)	105 (96%)	4 (4%)	0	100	100
9	M	412/456 (90%)	399 (97%)	13 (3%)	0	100	100
9	O	431/456 (94%)	412 (96%)	19 (4%)	0	100	100
9	Q	438/456 (96%)	416 (95%)	19 (4%)	3 (1%)	22	61
10	N	405/463 (88%)	396 (98%)	9 (2%)	0	100	100
10	P	423/463 (91%)	402 (95%)	20 (5%)	1 (0%)	47	79
10	R	420/463 (91%)	393 (94%)	25 (6%)	2 (0%)	29	67
11	S	373/375 (100%)	369 (99%)	4 (1%)	0	100	100
11	U	355/375 (95%)	311 (88%)	43 (12%)	1 (0%)	41	74
12	T	399/429 (93%)	389 (98%)	9 (2%)	1 (0%)	41	74
13	V	183/467 (39%)	174 (95%)	9 (5%)	0	100	100
14	W	185/227 (82%)	182 (98%)	2 (1%)	1 (0%)	29	67
All	All	6201/9764 (64%)	5904 (95%)	284 (5%)	13 (0%)	50	79

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	R	224	PHE
5	I	670	HIS
7	K	86	VAL
9	Q	256	ILE
6	J	283	PRO
14	W	171	GLU
10	P	211	ARG
9	Q	149	GLY
12	T	318	SER
5	I	94	ALA
9	Q	266	PRO
10	R	225	VAL
11	U	370	VAL

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%)	78 (93%)	6 (7%)	14 47
1	E	82/99 (83%)	77 (94%)	5 (6%)	18 54
2	B	83/106 (78%)	80 (96%)	3 (4%)	35 69
2	F	81/106 (76%)	78 (96%)	3 (4%)	34 68
3	C	82/111 (74%)	74 (90%)	8 (10%)	8 31
3	G	85/111 (77%)	84 (99%)	1 (1%)	71 88
4	D	66/79 (84%)	65 (98%)	1 (2%)	65 85
4	H	65/79 (82%)	64 (98%)	1 (2%)	65 85
5	I	710/2721 (26%)	670 (94%)	40 (6%)	21 57
6	J	144/312 (46%)	127 (88%)	17 (12%)	5 23
7	K	359/361 (99%)	334 (93%)	25 (7%)	15 48
8	L	98/133 (74%)	95 (97%)	3 (3%)	40 72
9	M	353/387 (91%)	342 (97%)	11 (3%)	40 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	O	364/387 (94%)	346 (95%)	18 (5%)	25 61
9	Q	366/387 (95%)	342 (93%)	24 (7%)	16 51
10	N	347/390 (89%)	338 (97%)	9 (3%)	46 76
10	P	352/390 (90%)	328 (93%)	24 (7%)	16 49
10	R	358/390 (92%)	342 (96%)	16 (4%)	27 63
11	S	318/318 (100%)	318 (100%)	0	100 100
11	U	305/318 (96%)	280 (92%)	25 (8%)	11 41
12	T	346/364 (95%)	337 (97%)	9 (3%)	46 76
13	V	168/400 (42%)	155 (92%)	13 (8%)	13 44
14	W	168/203 (83%)	164 (98%)	4 (2%)	49 77
All	All	5384/8251 (65%)	5118 (95%)	266 (5%)	29 61

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	39	ASN
1	A	65	GLU
1	A	72	ARG
1	A	78	ARG
1	A	96	LYS
2	B	44	GLN
2	B	60	ASN
2	B	68	GLU
3	C	48	LEU
3	C	59	GLU
3	C	64	LYS
3	C	79	LYS
3	C	82	LEU
3	C	115	LYS
3	C	120	MET
3	C	122	LYS
4	D	92	ARG
1	E	42	ARG
1	E	72	ASP
1	E	73	ASN
1	E	76	THR
1	E	81	ARG

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Mol	Chain	Res	Type
2	F	28	ARG
2	F	30	ARG
2	F	31	LYS
3	G	129	ARG
4	H	49	LEU
5	I	93	HIS
5	I	99	GLN
5	I	102	HIS
5	I	136	HIS
5	I	145	GLN
5	I	163	ARG
5	I	168	MET
5	I	177	ARG
5	I	181	GLU
5	I	190	LYS
5	I	191	LEU
5	I	193	ARG
5	I	204	GLN
5	I	206	TRP
5	I	218	GLN
5	I	225	ARG
5	I	226	LYS
5	I	227	LYS
5	I	232	HIS
5	I	239	GLN
5	I	243	TYR
5	I	702	GLN
5	I	712	TRP
5	I	857	ILE
5	I	888	MET
5	I	898	ARG
5	I	928	LEU
5	I	936	HIS
5	I	949	ILE
5	I	969	LEU
5	I	988	LYS
5	I	1885	TYR
5	I	1914	LEU
5	I	1921	GLU
5	I	2035	LEU
5	I	2067	GLN
5	I	2075	LEU

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Mol	Chain	Res	Type
5	I	2138	SER
5	I	2139	ASP
5	I	2179	LYS
6	J	152	GLN
6	J	177	LYS
6	J	184	LEU
6	J	185	ARG
6	J	198	LYS
6	J	202	HIS
6	J	203	LYS
6	J	204	LYS
6	J	206	LYS
6	J	213	THR
6	J	260	ARG
6	J	263	ARG
6	J	268	PHE
6	J	274	PHE
6	J	289	ARG
6	J	301	TYR
6	J	312	THR
7	K	8	ASN
7	K	41	THR
7	K	94	ILE
7	K	120	GLN
7	K	123	LEU
7	K	145	CYS
7	K	165	LYS
7	K	172	ARG
7	K	190	TYR
7	K	193	LEU
7	K	198	GLU
7	K	244	ILE
7	K	279	GLU
7	K	289	ILE
7	K	300	TYR
7	K	304	ASN
7	K	305	LEU
7	K	313	PHE
7	K	336	GLU
7	K	339	CYS
7	K	340	LEU
7	K	351	LEU

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Mol	Chain	Res	Type
7	K	366	ILE
7	K	370	ASP
7	K	373	GLU
8	L	19	LEU
8	L	84	PHE
8	L	111	ARG
9	M	53	VAL
9	M	114	GLU
9	M	138	LEU
9	M	182	LYS
9	M	193	ILE
9	M	225	LYS
9	M	235	ILE
9	M	271	ILE
9	M	316	HIS
9	M	393	HIS
9	M	406	SER
10	N	83	LYS
10	N	149	ARG
10	N	234	LYS
10	N	303	MET
10	N	325	ILE
10	N	395	LEU
10	N	413	CYS
10	N	444	LYS
10	N	448	ASP
9	O	55	LEU
9	O	66	VAL
9	O	87	LEU
9	O	165	LYS
9	O	216	GLU
9	O	262	GLN
9	O	263	LEU
9	O	270	GLU
9	O	274	LYS
9	O	278	GLU
9	O	285	LYS
9	O	306	MET
9	O	342	GLU
9	O	363	THR
9	O	364	MET
9	O	391	LEU

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Mol	Chain	Res	Type
9	O	399	THR
9	O	407	VAL
10	P	18	ARG
10	P	21	ARG
10	P	28	ILE
10	P	62	MET
10	P	68	ILE
10	P	92	GLN
10	P	141	GLU
10	P	145	ILE
10	P	148	ASP
10	P	149	ARG
10	P	188	GLN
10	P	210	THR
10	P	232	LEU
10	P	236	LYS
10	P	257	PHE
10	P	265	THR
10	P	267	GLU
10	P	268	ILE
10	P	348	ILE
10	P	375	CYS
10	P	376	GLU
10	P	422	GLN
10	P	427	LYS
10	P	428	ARG
9	Q	49	CYS
9	Q	60	LYS
9	Q	79	LEU
9	Q	113	MET
9	Q	123	ARG
9	Q	178	GLU
9	Q	180	LEU
9	Q	182	LYS
9	Q	192	TYR
9	Q	213	PHE
9	Q	220	TYR
9	Q	236	GLN
9	Q	254	GLN
9	Q	275	LEU
9	Q	276	ARG
9	Q	317	ARG

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Mol	Chain	Res	Type
9	Q	326	ILE
9	Q	389	GLU
9	Q	391	LEU
9	Q	404	ARG
9	Q	416	LEU
9	Q	427	LYS
9	Q	431	GLU
9	Q	450	GLN
10	R	46	MET
10	R	68	ILE
10	R	205	LEU
10	R	239	VAL
10	R	250	ILE
10	R	251	ASN
10	R	255	GLN
10	R	269	LYS
10	R	346	ILE
10	R	351	LEU
10	R	370	ILE
10	R	374	ARG
10	R	392	ARG
10	R	395	LEU
10	R	428	ARG
10	R	444	LYS
12	T	10	GLU
12	T	24	ARG
12	T	71	ASP
12	T	110	HIS
12	T	140	MET
12	T	315	LYS
12	T	317	LEU
12	T	361	THR
12	T	399	ILE
11	U	2	ASP
11	U	4	ASP
11	U	18	LYS
11	U	62	ARG
11	U	90	PHE
11	U	94	LEU
11	U	101	HIS
11	U	123	MET
11	U	147	ARG

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Mol	Chain	Res	Type
11	U	161	HIS
11	U	180	LEU
11	U	213	LYS
11	U	226	GLU
11	U	237	GLU
11	U	253	GLU
11	U	282	ILE
11	U	292	ASP
11	U	314	GLN
11	U	318	THR
11	U	326	LYS
11	U	327	ILE
11	U	330	ILE
11	U	334	GLU
11	U	362	TYR
11	U	369	ILE
13	V	51	GLU
13	V	53	MET
13	V	56	GLU
13	V	65	LYS
13	V	91	LYS
13	V	119	GLU
13	V	218	PHE
13	V	224	ARG
13	V	229	GLN
13	V	230	LEU
13	V	237	THR
13	V	251	LEU
13	V	253	LYS
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 (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	44	GLN
4	D	25	ASN
4	D	75	HIS
1	E	104	GLN
2	F	81	ASN

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Mol	Chain	Res	Type
2	F	92	GLN
3	G	76	GLN
5	I	99	GLN
5	I	145	GLN
5	I	178	GLN
5	I	204	GLN
5	I	218	GLN
5	I	716	ASN
5	I	936	HIS
5	I	2099	GLN
6	J	280	GLN
7	K	174	ASN
7	K	304	ASN
9	M	18	HIS
9	M	20	HIS
9	M	316	HIS
10	N	275	GLN
9	O	20	HIS
9	O	34	GLN
9	O	156	HIS
9	O	251	GLN
9	O	289	GLN
10	P	27	HIS
10	P	44	GLN
10	P	121	GLN
9	Q	20	HIS
9	Q	115	ASN
9	Q	196	ASN
9	Q	236	GLN
9	Q	262	GLN
9	Q	393	HIS
10	R	302	HIS
12	T	73	ASN
11	U	78	ASN
11	U	111	ASN
11	U	353	GLN
11	U	371	HIS

5.3.3 RNA

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)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
18	ATP	U	401	-	26,33,33	0.88	1 (3%)	31,52,52	1.97	5 (16%)
17	ADP	R	501	10	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
17	ADP	O	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.54	4 (13%)
17	ADP	N	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
18	ATP	T	501	-	26,33,33	0.99	1 (3%)	31,52,52	1.85	5 (16%)
17	ADP	M	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.39	4 (13%)
17	ADP	Q	501	9	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
17	ADP	P	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)

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
18	ATP	U	401	-	-	6/18/38/38	0/3/3/3
17	ADP	R	501	10	-	3/12/32/32	0/3/3/3
17	ADP	O	501	-	-	3/12/32/32	0/3/3/3
17	ADP	N	501	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ATP	T	501	-	-	5/18/38/38	0/3/3/3
17	ADP	M	501	-	-	4/12/32/32	0/3/3/3
17	ADP	Q	501	9	-	4/12/32/32	0/3/3/3
17	ADP	P	501	-	-	7/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	501	ATP	C2'-C1'	-2.72	1.49	1.53
17	M	501	ADP	C5-C4	2.45	1.47	1.40
17	N	501	ADP	C5-C4	2.37	1.47	1.40
17	R	501	ADP	C5-C4	2.36	1.47	1.40
17	P	501	ADP	C5-C4	2.35	1.47	1.40
17	O	501	ADP	C5-C4	2.30	1.47	1.40
17	Q	501	ADP	C5-C4	2.20	1.46	1.40
18	U	401	ATP	C5-C4	2.02	1.46	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	U	401	ATP	PA-O3A-PB	-5.73	113.16	132.83
18	U	401	ATP	PB-O3B-PG	-5.54	113.82	132.83
18	T	501	ATP	PA-O3A-PB	-5.39	114.34	132.83
18	T	501	ATP	PB-O3B-PG	-4.80	116.37	132.83
17	O	501	ADP	PA-O3A-PB	-3.92	119.37	132.83
17	Q	501	ADP	PA-O3A-PB	-3.81	119.75	132.83
17	N	501	ADP	PA-O3A-PB	-3.78	119.84	132.83
17	R	501	ADP	PA-O3A-PB	-3.76	119.94	132.83
17	P	501	ADP	PA-O3A-PB	-3.63	120.37	132.83
18	U	401	ATP	C3'-C2'-C1'	3.53	106.29	100.98
17	R	501	ADP	C3'-C2'-C1'	3.48	106.22	100.98
18	T	501	ATP	N3-C2-N1	-3.39	123.37	128.68
17	O	501	ADP	C3'-C2'-C1'	3.37	106.06	100.98
17	M	501	ADP	N3-C2-N1	-3.36	123.43	128.68
17	M	501	ADP	PA-O3A-PB	-3.29	121.55	132.83
17	O	501	ADP	N3-C2-N1	-3.28	123.55	128.68
17	Q	501	ADP	N3-C2-N1	-3.14	123.76	128.68
17	N	501	ADP	N3-C2-N1	-3.11	123.81	128.68
17	P	501	ADP	N3-C2-N1	-3.11	123.81	128.68
17	R	501	ADP	N3-C2-N1	-3.03	123.95	128.68
17	Q	501	ADP	C3'-C2'-C1'	3.02	105.52	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	U	401	ATP	N3-C2-N1	-2.92	124.12	128.68
17	N	501	ADP	C3'-C2'-C1'	2.86	105.28	100.98
17	P	501	ADP	C4-C5-N7	-2.85	106.43	109.40
18	U	401	ATP	C4-C5-N7	-2.85	106.43	109.40
17	M	501	ADP	C3'-C2'-C1'	2.75	105.12	100.98
17	O	501	ADP	C4-C5-N7	-2.70	106.58	109.40
17	Q	501	ADP	C4-C5-N7	-2.66	106.63	109.40
17	P	501	ADP	C3'-C2'-C1'	2.63	104.94	100.98
17	R	501	ADP	C4-C5-N7	-2.61	106.68	109.40
17	N	501	ADP	C4-C5-N7	-2.54	106.75	109.40
18	T	501	ATP	C3'-C2'-C1'	2.35	104.51	100.98
17	M	501	ADP	C4-C5-N7	-2.26	107.04	109.40
18	T	501	ATP	C4-C5-N7	-2.16	107.14	109.40

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	M	501	ADP	PA-O3A-PB-O2B
17	N	501	ADP	PA-O3A-PB-O2B
17	N	501	ADP	C5'-O5'-PA-O1A
17	N	501	ADP	C5'-O5'-PA-O2A
17	O	501	ADP	C5'-O5'-PA-O1A
17	O	501	ADP	C5'-O5'-PA-O2A
17	P	501	ADP	C5'-O5'-PA-O3A
17	Q	501	ADP	C5'-O5'-PA-O1A
17	Q	501	ADP	C5'-O5'-PA-O2A
17	R	501	ADP	C5'-O5'-PA-O1A
17	R	501	ADP	C5'-O5'-PA-O2A
18	T	501	ATP	C5'-O5'-PA-O3A
18	U	401	ATP	C5'-O5'-PA-O1A
18	U	401	ATP	C5'-O5'-PA-O2A
17	M	501	ADP	O4'-C4'-C5'-O5'
17	P	501	ADP	O4'-C4'-C5'-O5'
18	T	501	ATP	O4'-C4'-C5'-O5'
17	P	501	ADP	C3'-C4'-C5'-O5'
18	T	501	ATP	C3'-C4'-C5'-O5'
17	Q	501	ADP	C5'-O5'-PA-O3A
18	U	401	ATP	PG-O3B-PB-O1B
17	P	501	ADP	C5'-O5'-PA-O1A
18	T	501	ATP	C5'-O5'-PA-O1A
18	T	501	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
17	M	501	ADP	C3'-C4'-C5'-O5'
17	P	501	ADP	PB-O3A-PA-O2A
17	P	501	ADP	C4'-C5'-O5'-PA
17	Q	501	ADP	PB-O3A-PA-O2A
17	M	501	ADP	C5'-O5'-PA-O3A
17	N	501	ADP	C5'-O5'-PA-O3A
17	O	501	ADP	C5'-O5'-PA-O3A
17	R	501	ADP	C5'-O5'-PA-O3A
18	U	401	ATP	C5'-O5'-PA-O3A
17	N	501	ADP	O4'-C4'-C5'-O5'
17	P	501	ADP	PB-O3A-PA-O1A
18	U	401	ATP	PG-O3B-PB-O2B
18	U	401	ATP	PA-O3A-PB-O2B

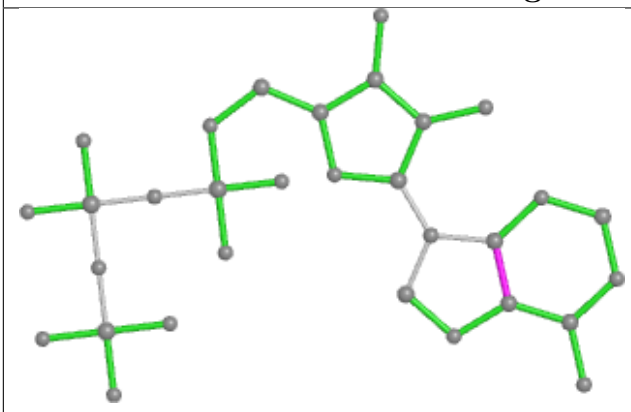
There are no ring outliers.

8 monomers are involved in 129 short contacts:

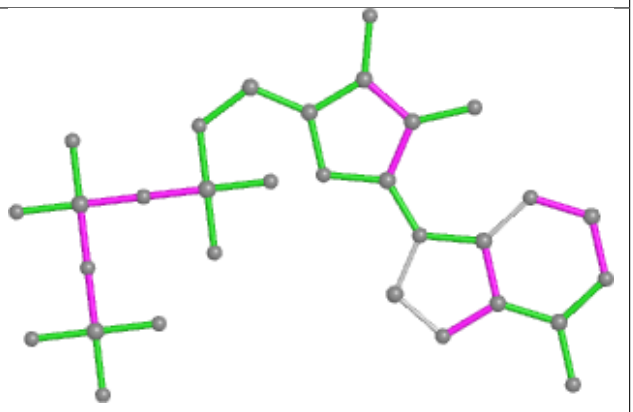
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	401	ATP	25	0
17	R	501	ADP	17	0
17	O	501	ADP	12	0
17	N	501	ADP	11	0
18	T	501	ATP	6	0
17	M	501	ADP	13	0
17	Q	501	ADP	18	0
17	P	501	ADP	27	0

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.

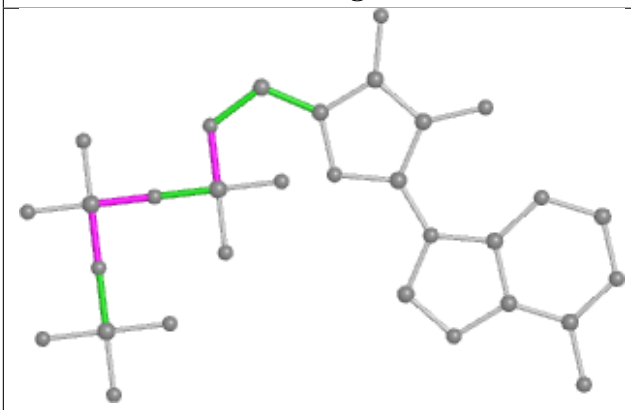
Ligand ATP U 401



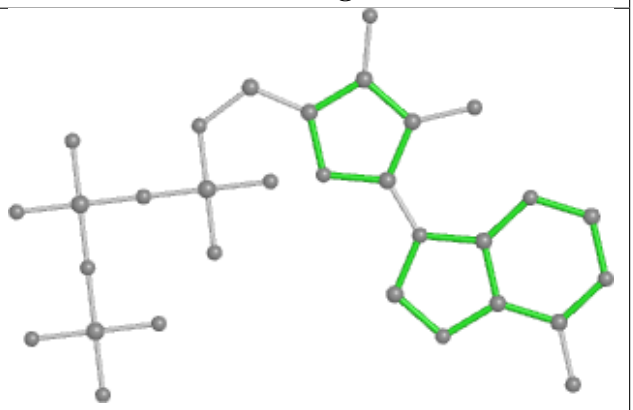
Bond lengths



Bond angles

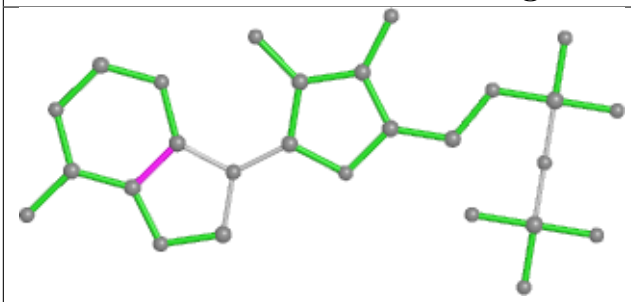


Torsions

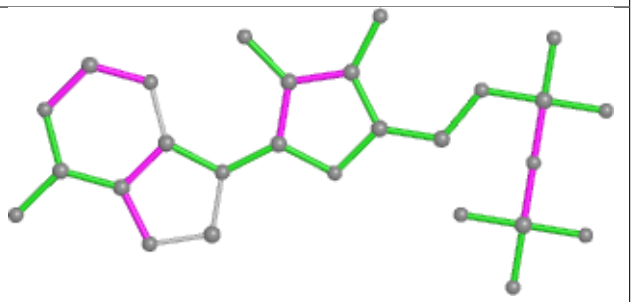


Rings

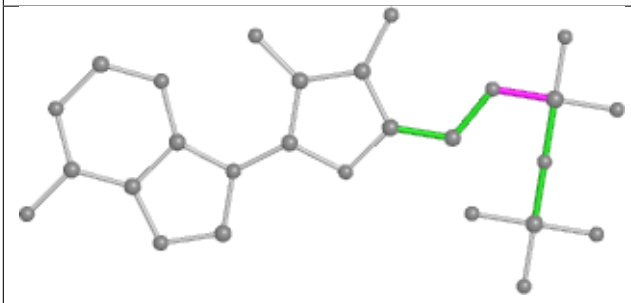
Ligand ADP R 501



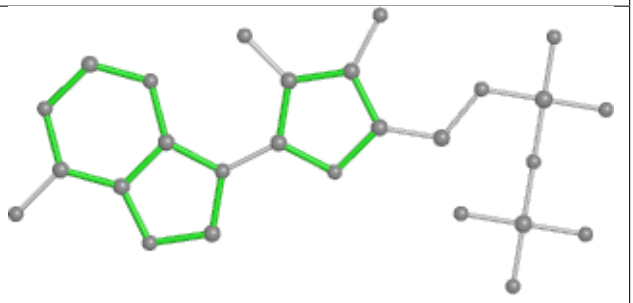
Bond lengths



Bond angles

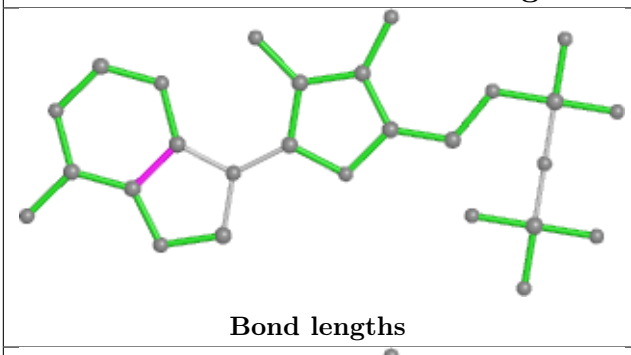


Torsions

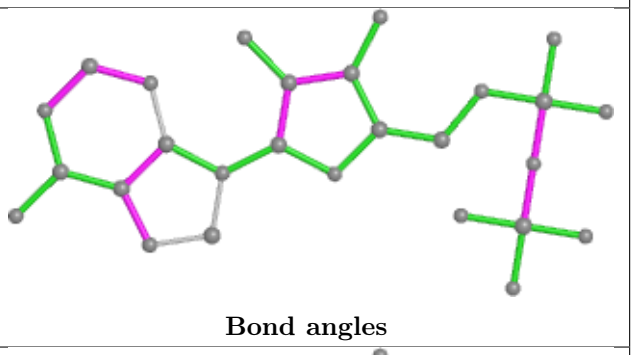


Rings

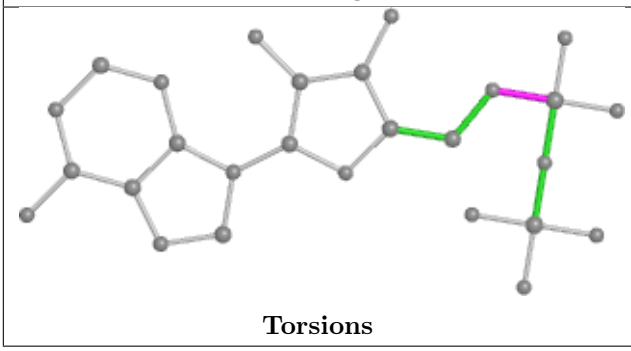
Ligand ADP O 501



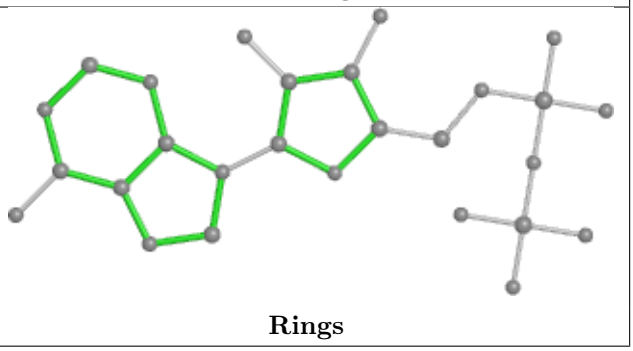
Bond lengths



Bond angles

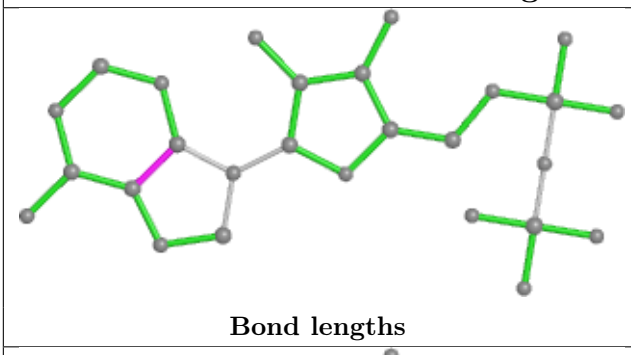


Torsions

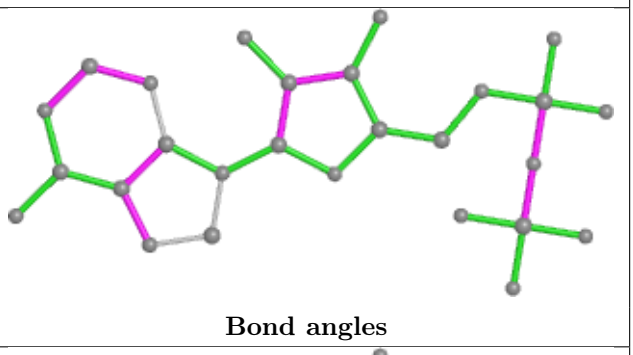


Rings

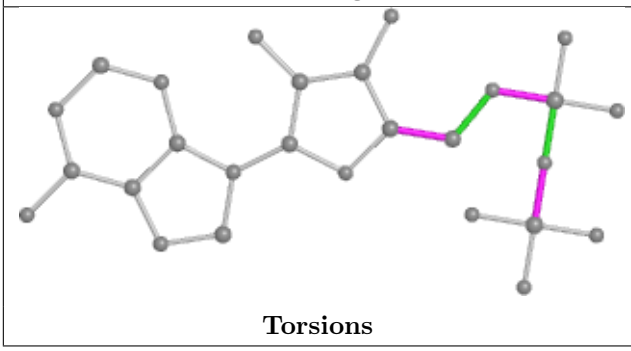
Ligand ADP N 501



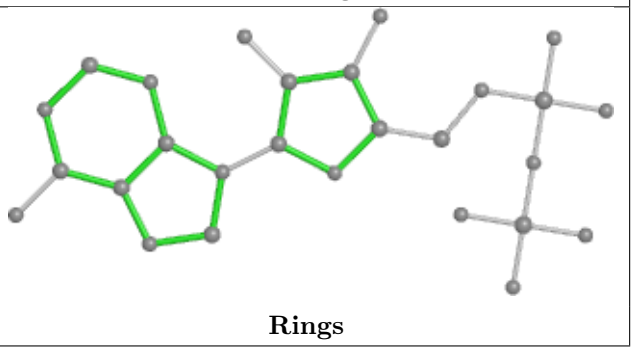
Bond lengths



Bond angles

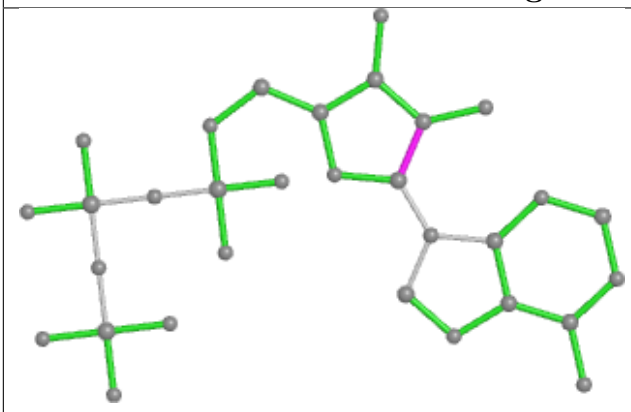


Torsions

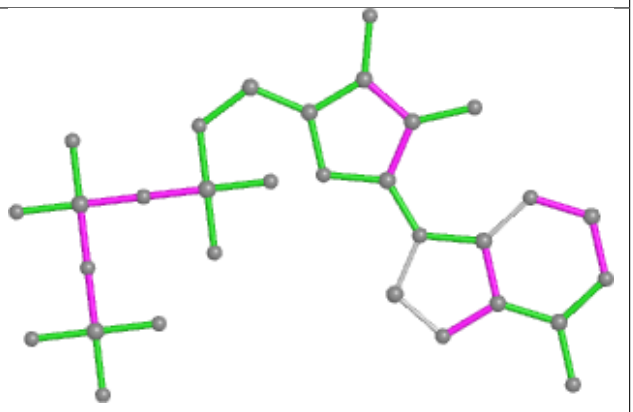


Rings

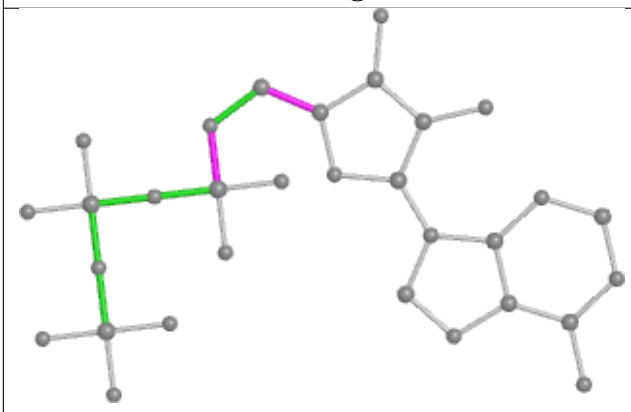
Ligand ATP T 501



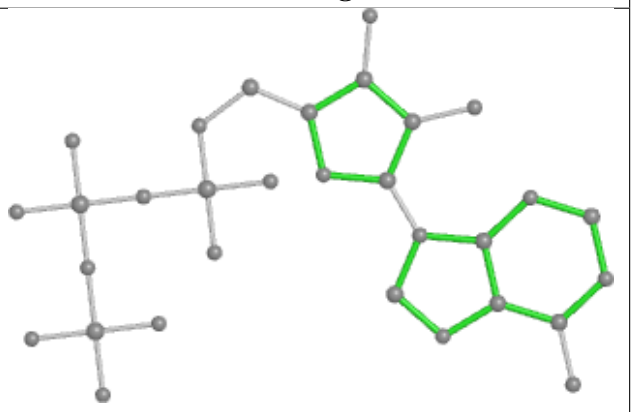
Bond lengths



Bond angles

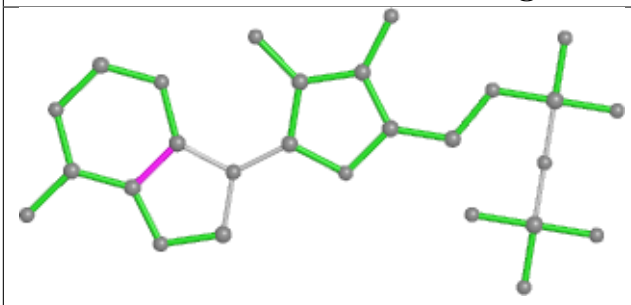


Torsions

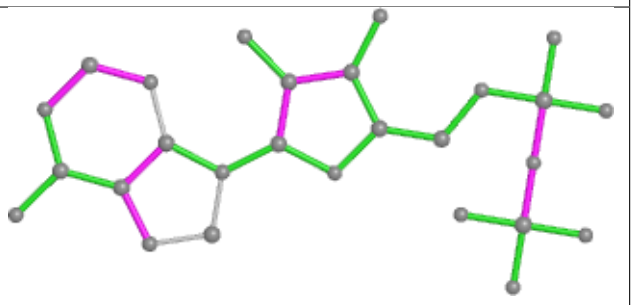


Rings

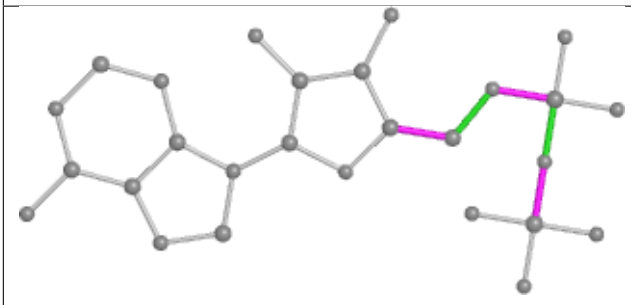
Ligand ADP M 501



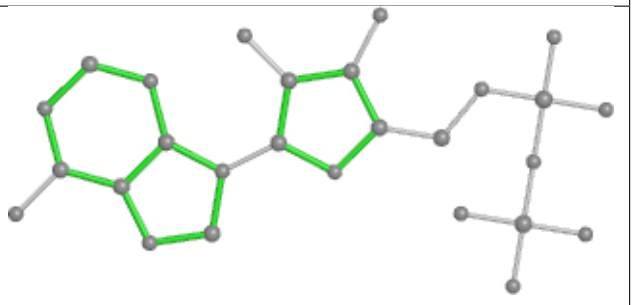
Bond lengths



Bond angles

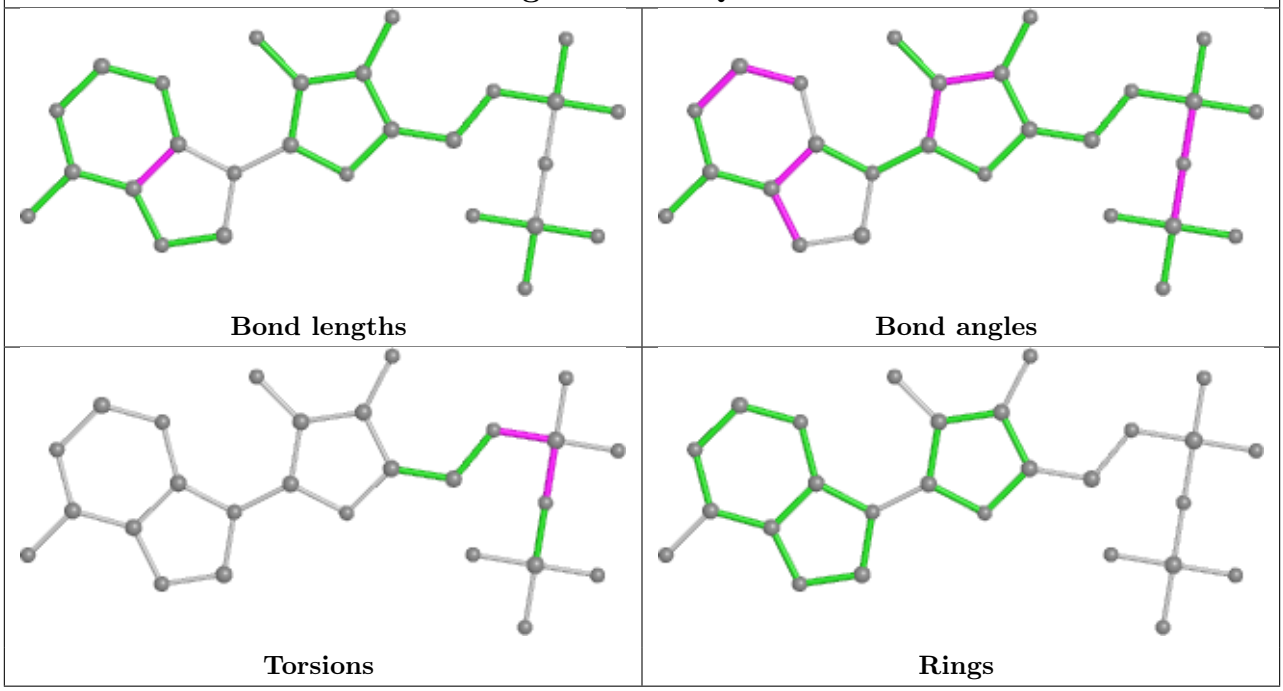


Torsions

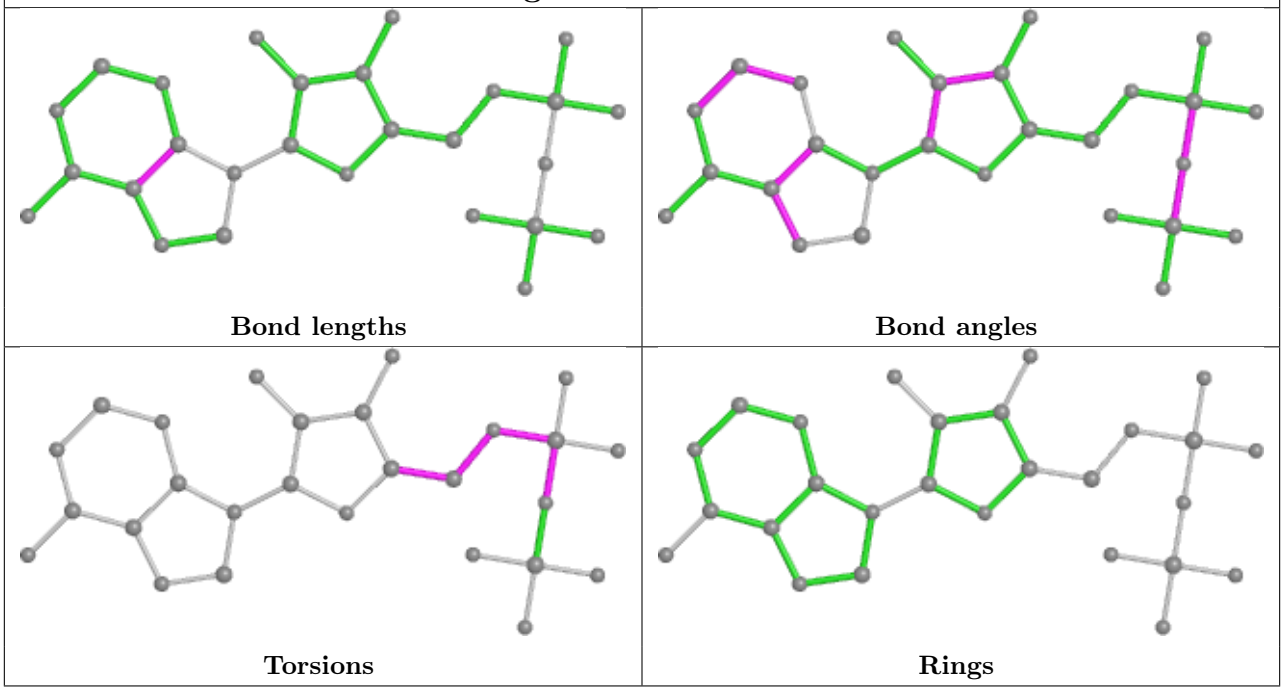


Rings

Ligand ADP Q 501



Ligand ADP P 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.

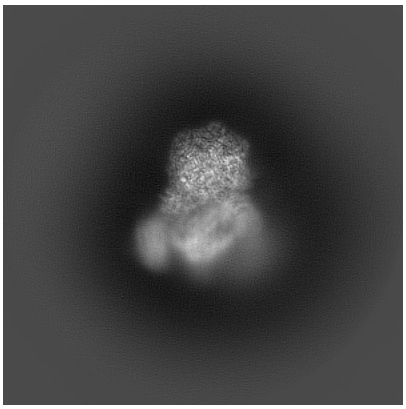
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37984. These allow visual inspection of the internal detail of the map and identification of artifacts.

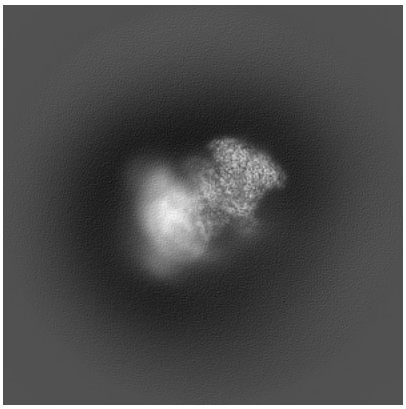
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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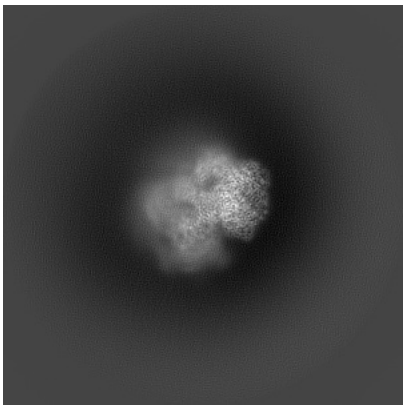
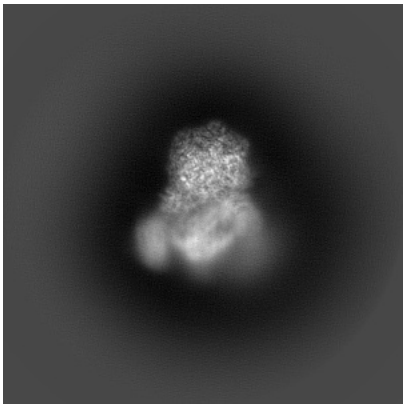


Z

6.1.2 Raw map



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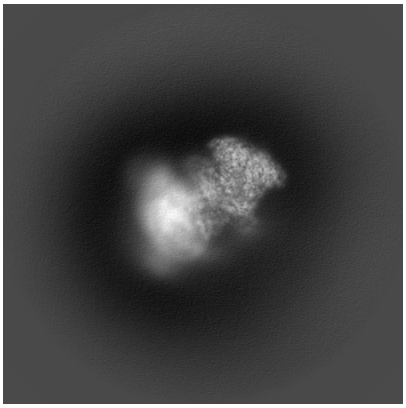
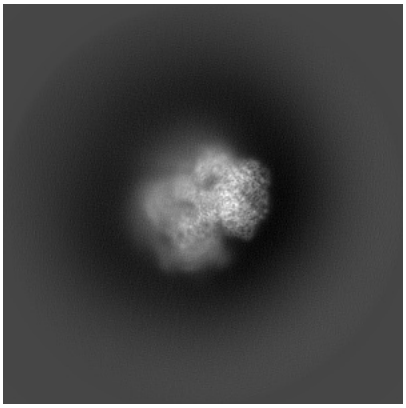


Y

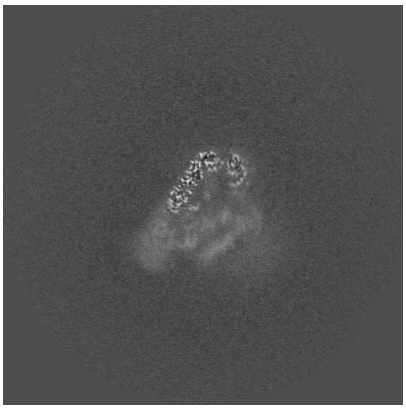


Z

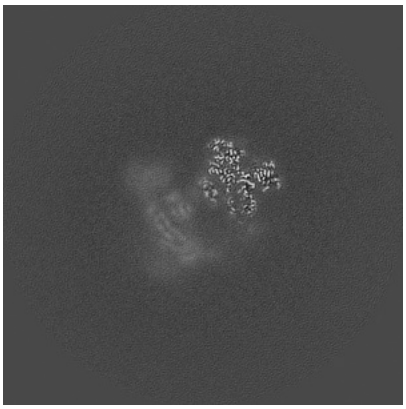
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

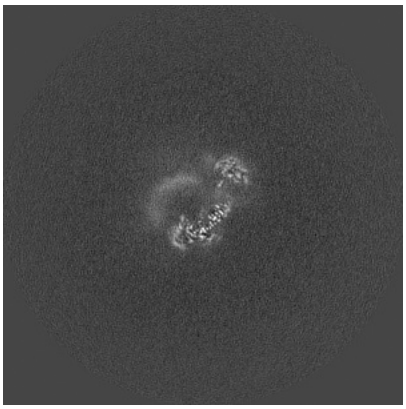
6.2.1 Primary map



X Index: 200

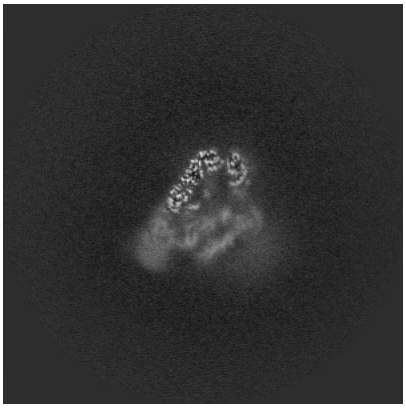


Y Index: 200

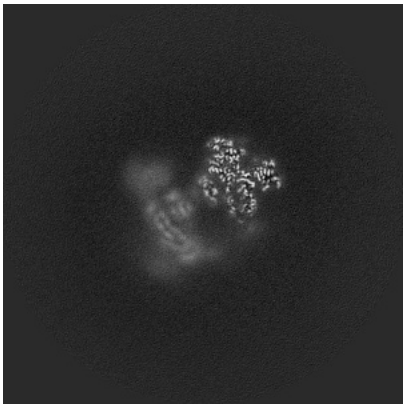


Z Index: 200

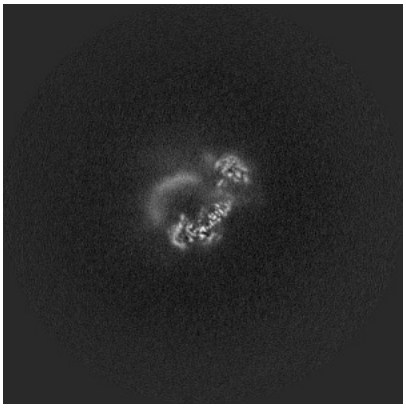
6.2.2 Raw map



X Index: 200



Y Index: 200

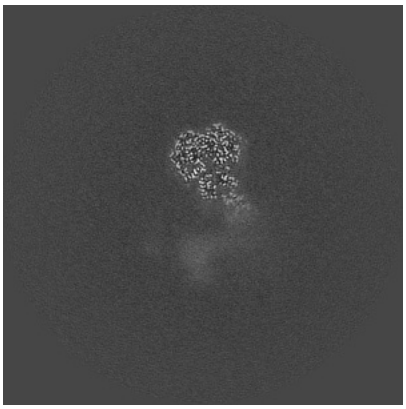


Z Index: 200

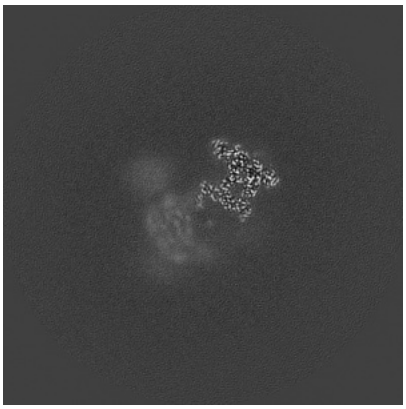
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

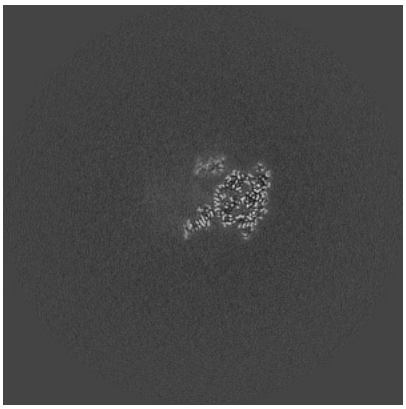
6.3.1 Primary map



X Index: 232

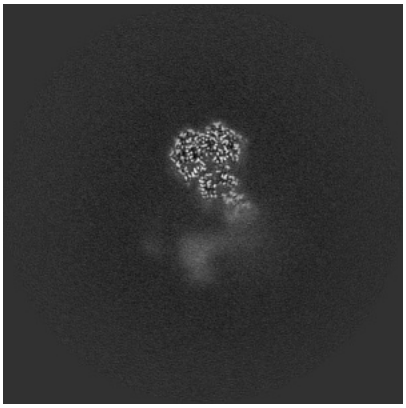


Y Index: 191

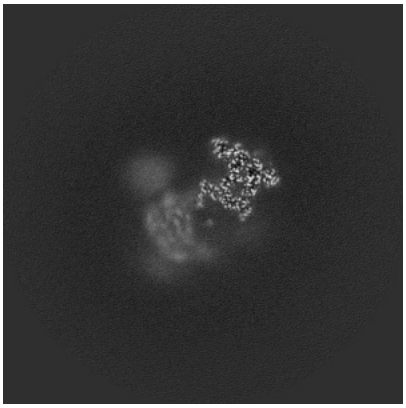


Z Index: 224

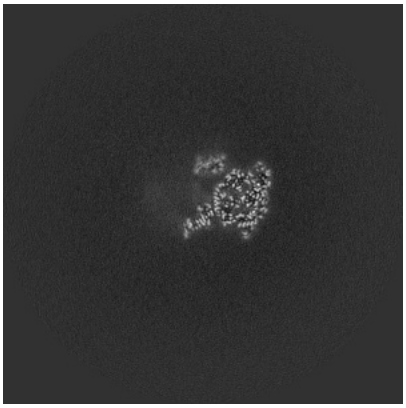
6.3.2 Raw map



X Index: 232



Y Index: 191

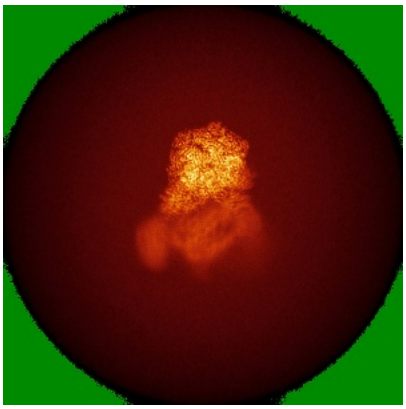


Z Index: 224

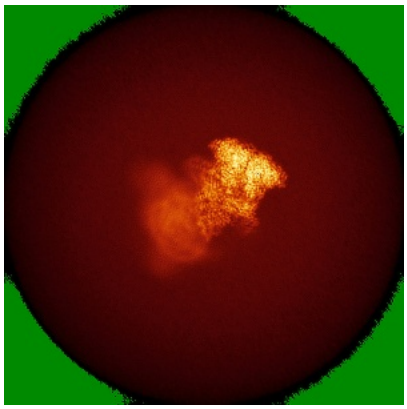
The images above show the largest variance slices of the map in three orthogonal directions.

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

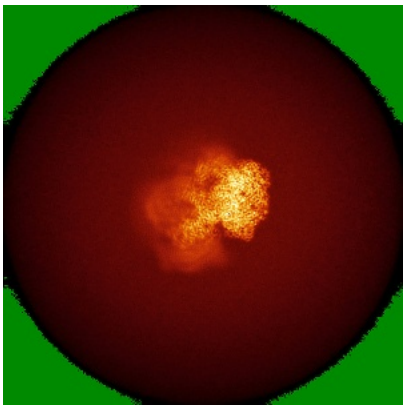
6.4.1 Primary map



X

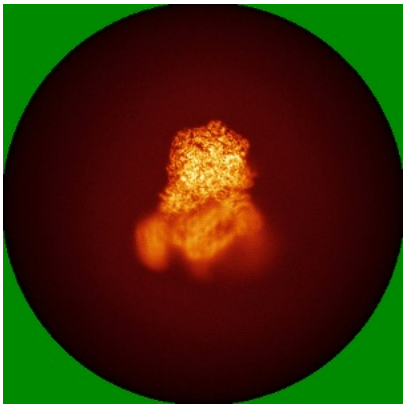


Y

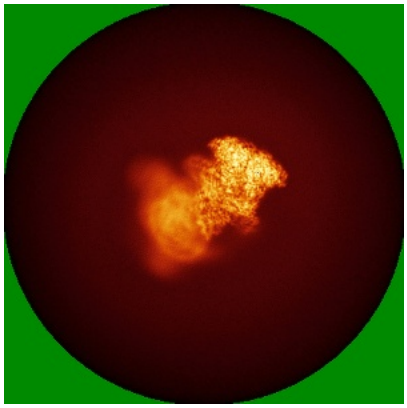


Z

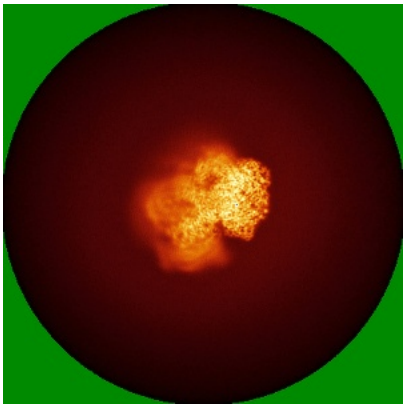
6.4.2 Raw map



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.

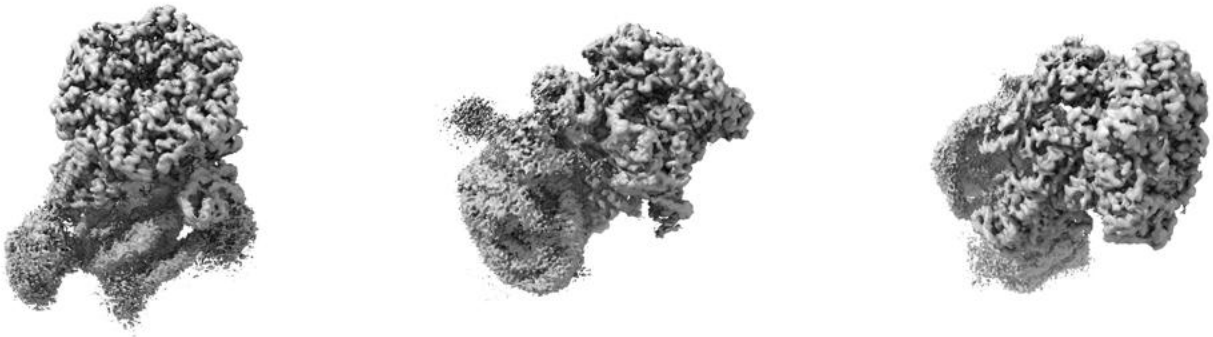
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. 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.

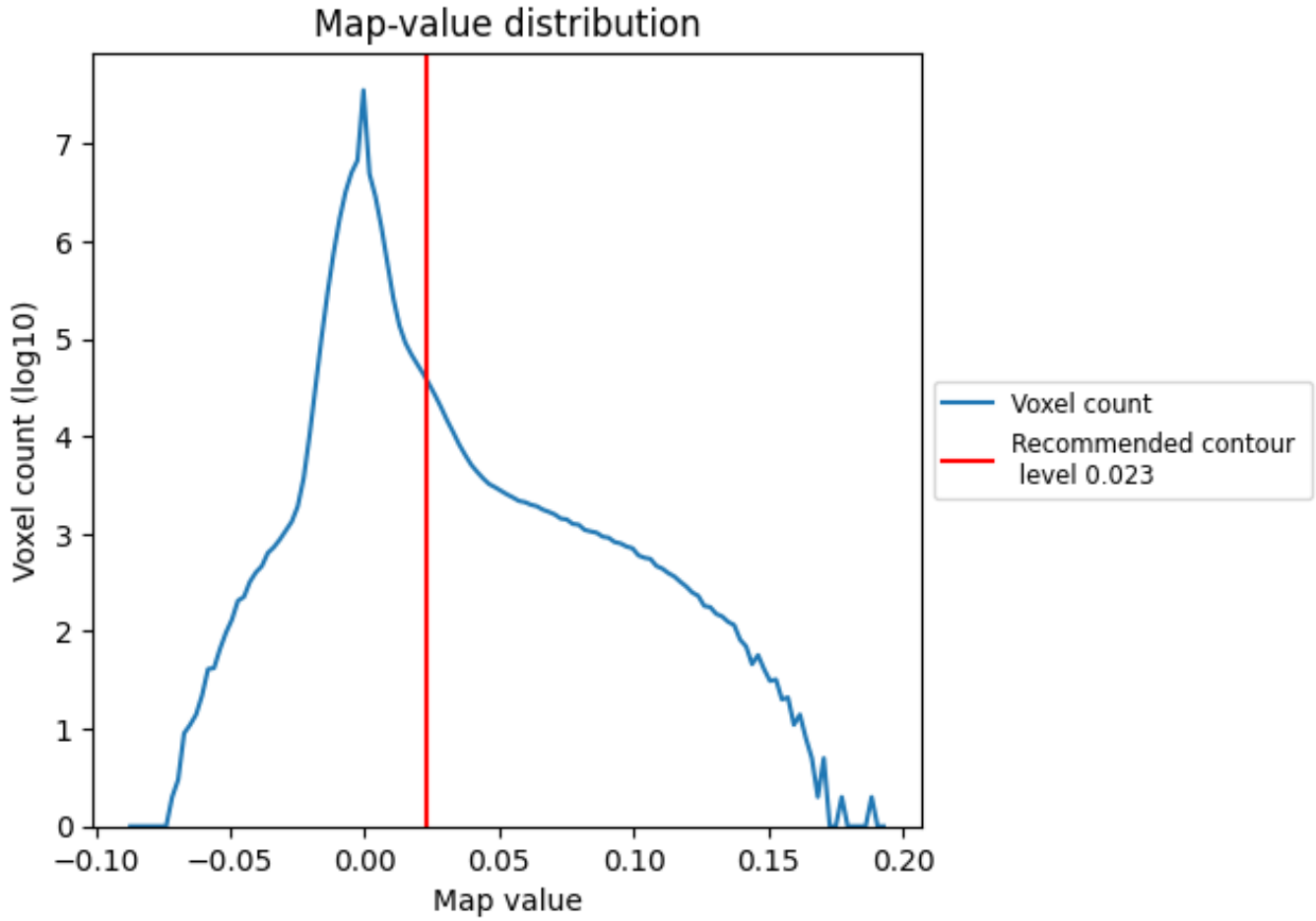
6.6 Mask visualisation (i)

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

7 Map analysis

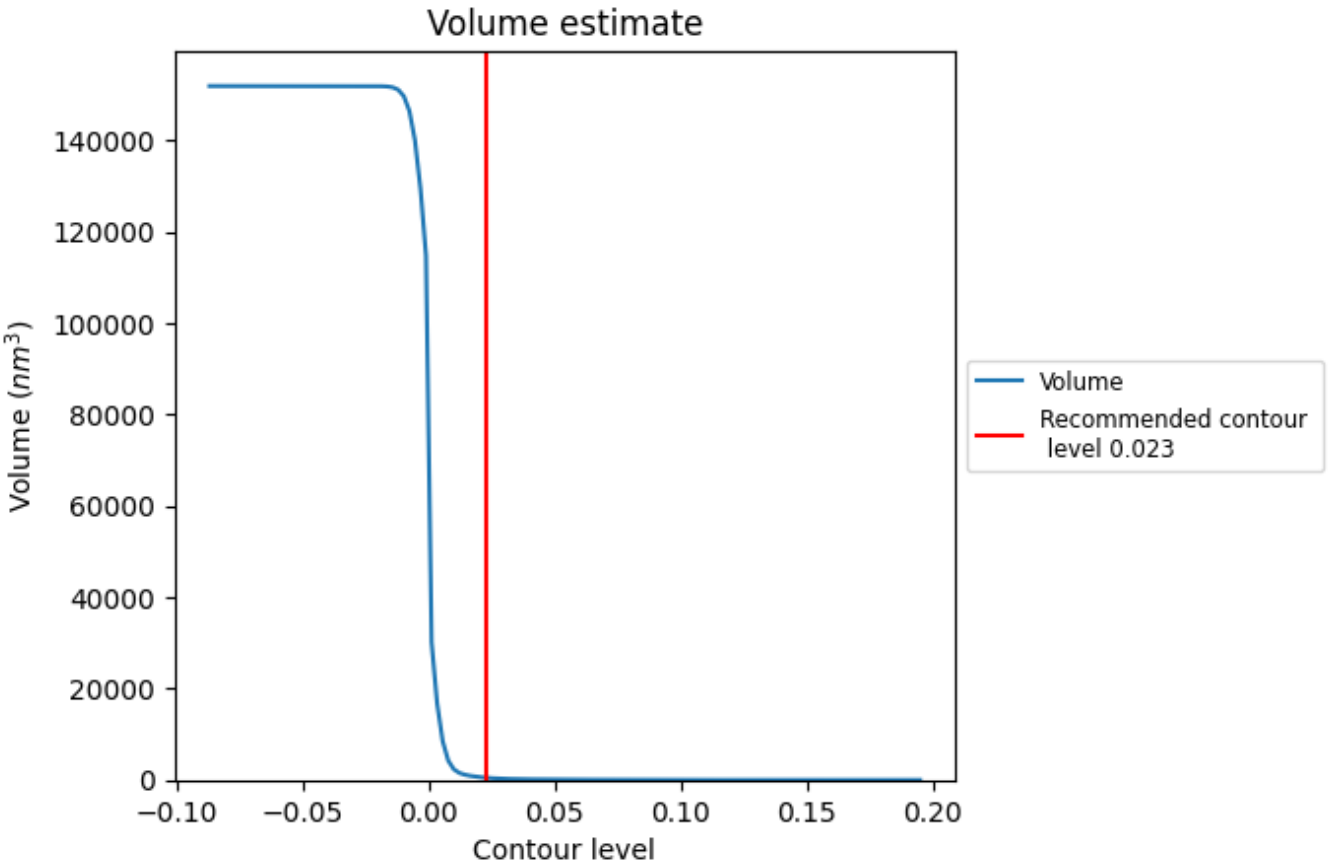
This section contains the results of statistical analysis of the map.

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.

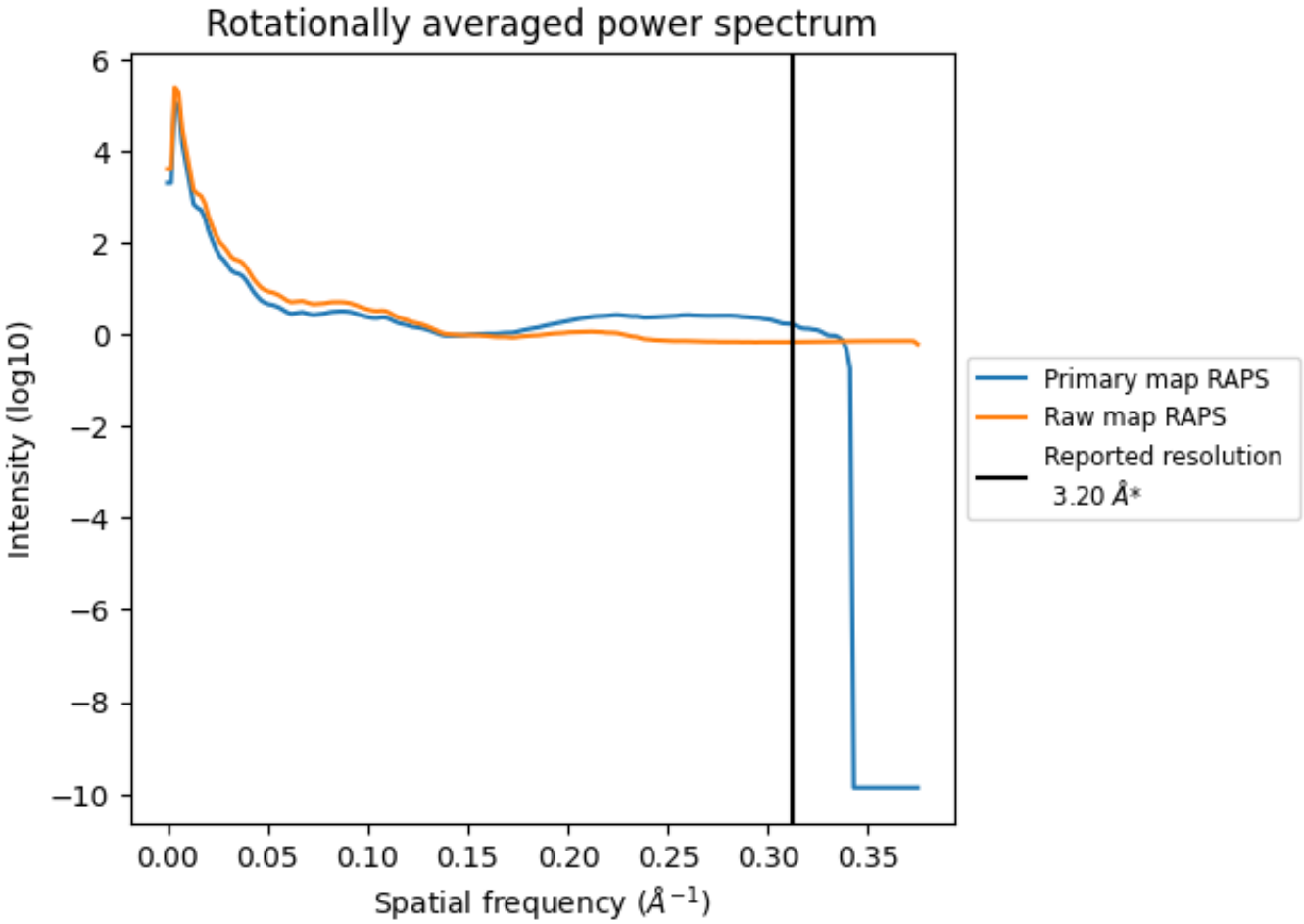
7.2 Volume estimate



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 424 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)

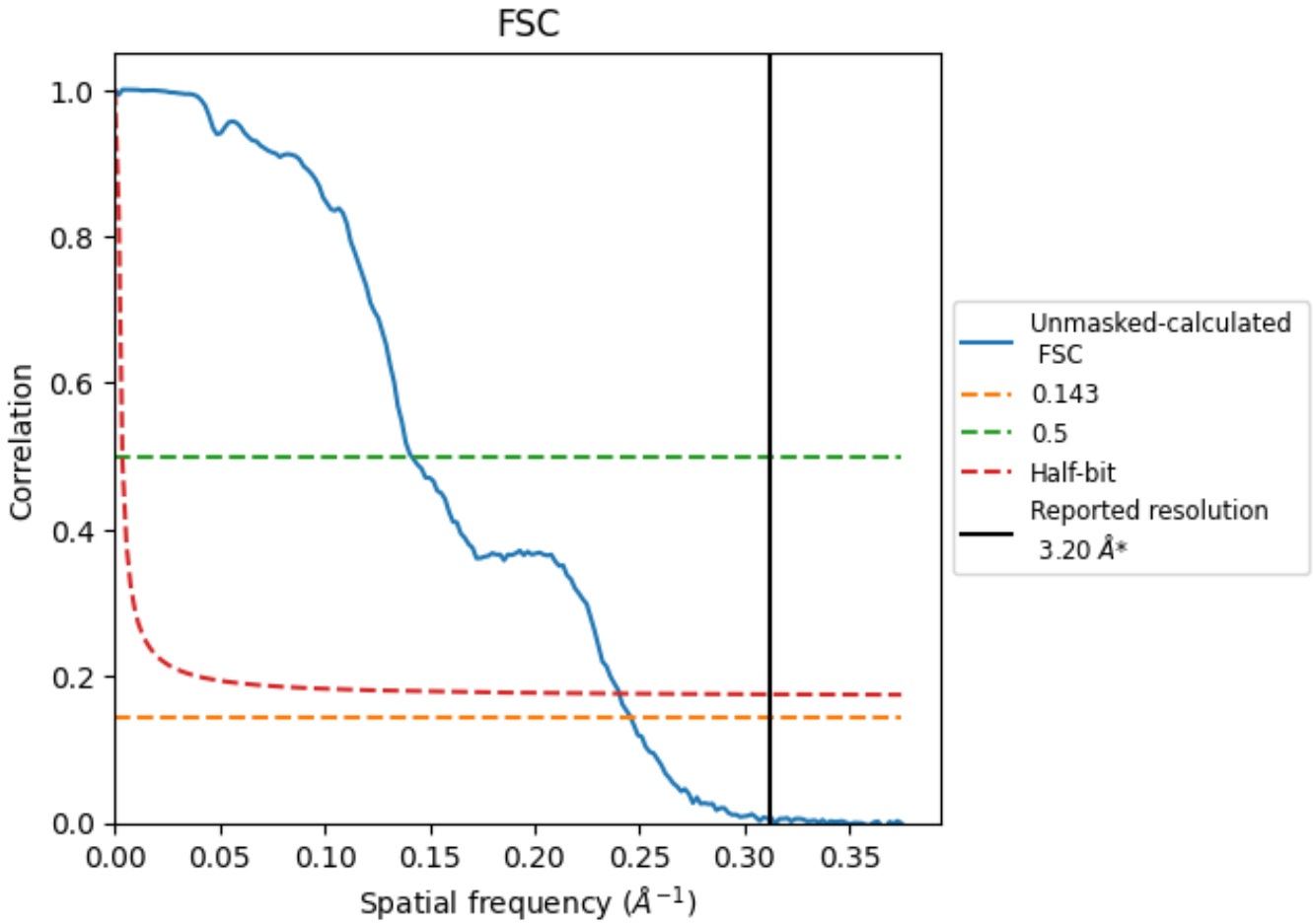


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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)

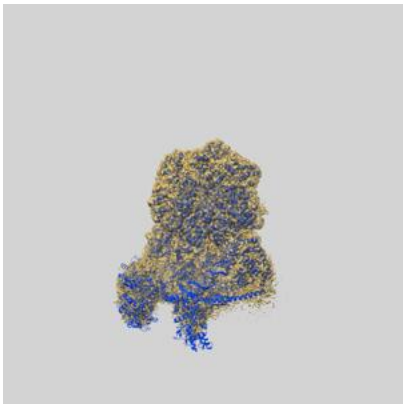
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	7.08	4.16

*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 4.07 differs from the reported value 3.2 by more than 10 %

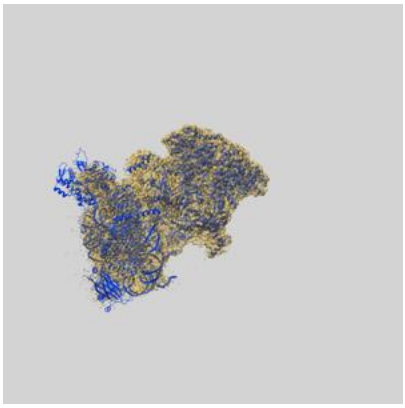
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37984 and PDB model 8X15. Per-residue inclusion information can be found in section 3 on page 9.

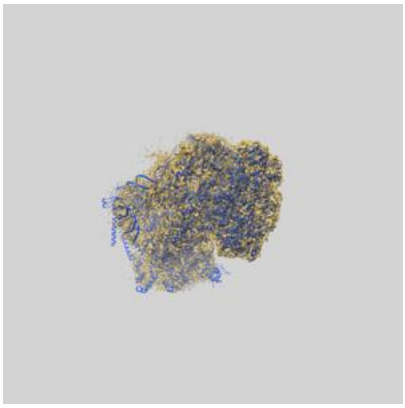
9.1 Map-model overlay



X



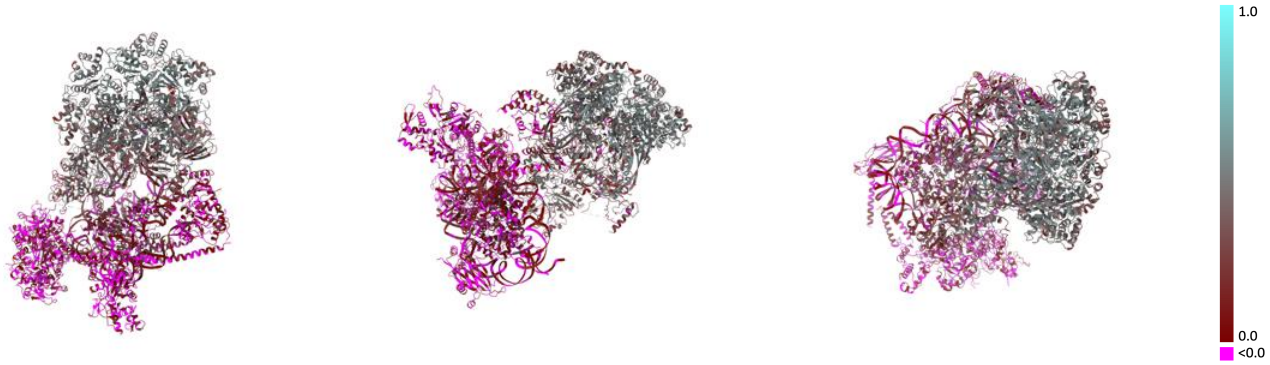
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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.

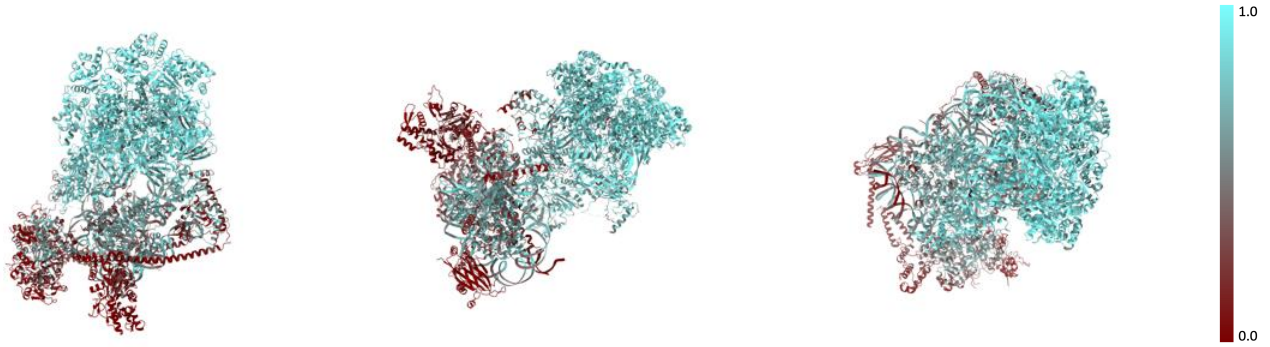
9.2 Q-score mapped to coordinate model (i)



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.

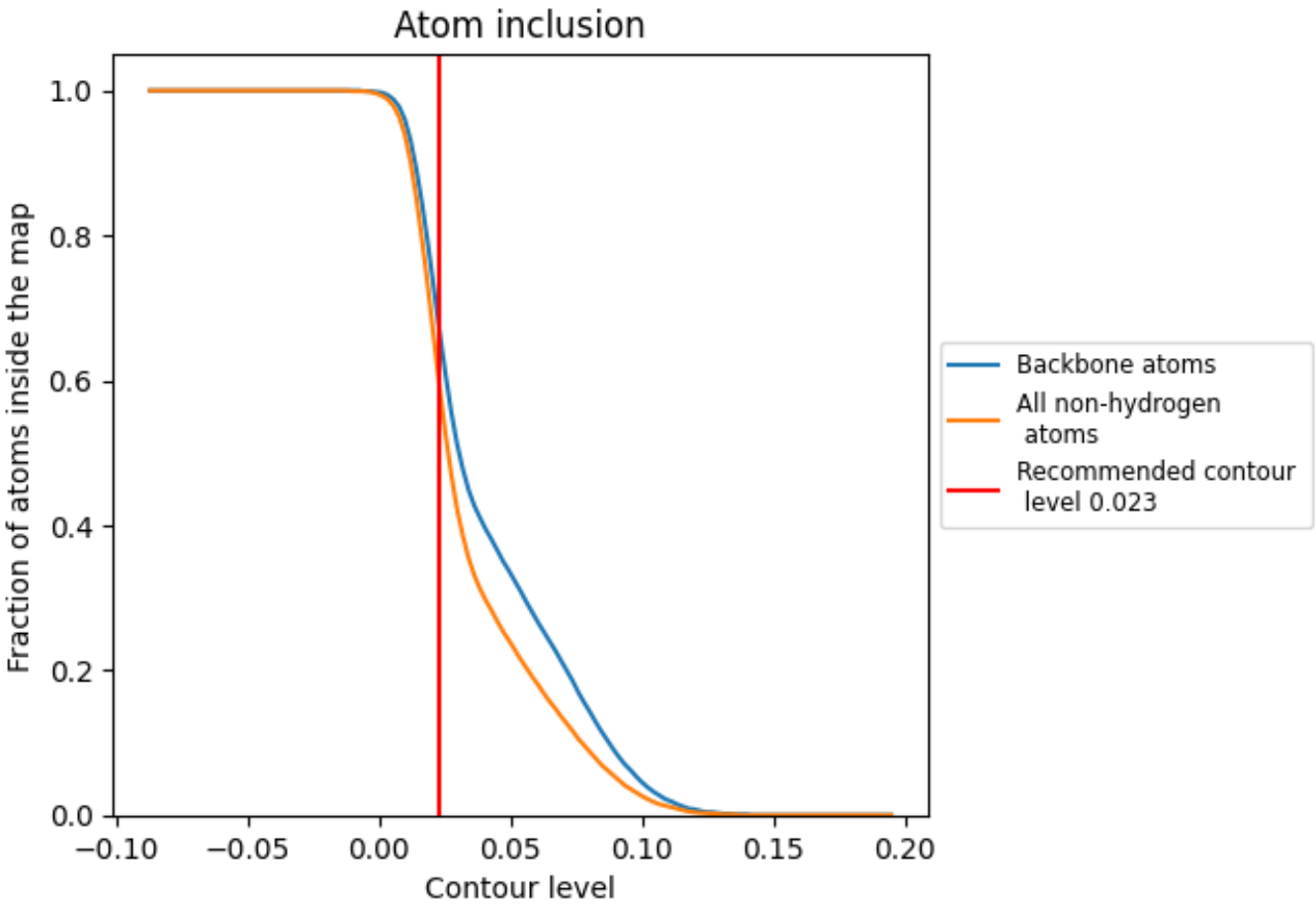
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 59% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5930	0.2180
A	0.5380	0.1040
B	0.6600	0.1240
C	0.5960	0.0760
D	0.6390	0.0780
E	0.6000	0.0860
F	0.6600	0.1180
G	0.5700	0.0790
H	0.6960	0.1250
I	0.5440	0.1840
J	0.4560	0.1500
K	0.7550	0.3060
L	0.6730	0.2840
M	0.8550	0.4390
N	0.8200	0.3990
O	0.8140	0.3810
P	0.8380	0.4260
Q	0.8350	0.4240
R	0.8540	0.4480
S	0.0530	0.0050
T	0.3200	0.0250
U	0.2550	0.0090
V	0.1740	0.0130
W	0.0150	0.0040
X	0.5980	0.0610
Y	0.5650	0.0730