Full wwPDB EM Validation Report

Sep 28, 2024 – 10:07 PM EDT

PDB ID	:	8T9G
EMDB ID	:	EMD-41110
Title	:	Automethylated PRC2 dimer bound to nucleosome
Authors	:	Sauer, P.V.; Pavlenko, E.; Nogales, E.; Poepsel, S.
Deposited on	:	2023-06-23
Resolution	:	6.20 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:

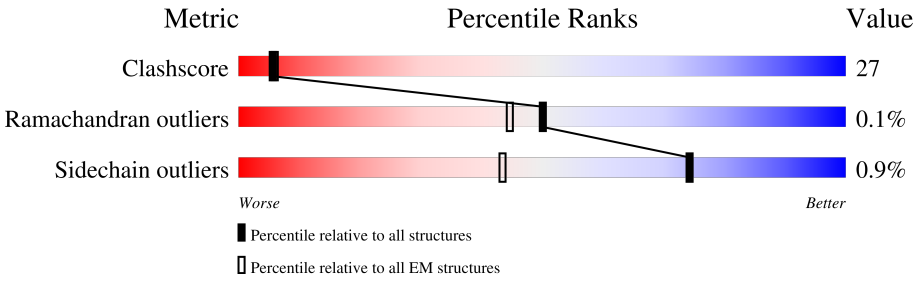
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	619	12% 35% 36% • 28%
1	G	619	• 28% 43% 28%
2	C	753	• 36% 35% • 29%
2	I	753	• 38% 42% • 20%
3	F	441	• 40% 42% 18%
3	K	441	23% 59% 18%
4	L	425	• 40% 53% • 7%
4	O	425	35% 58% 7%

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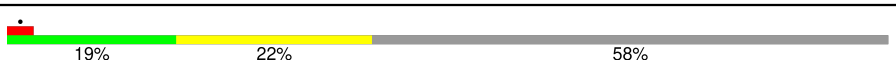
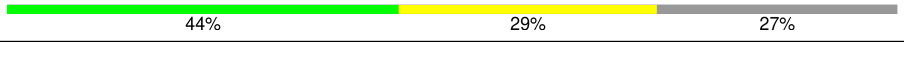
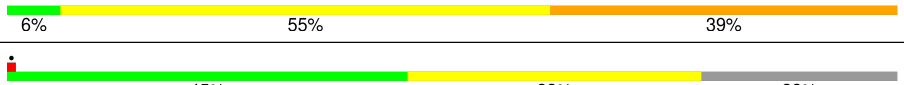
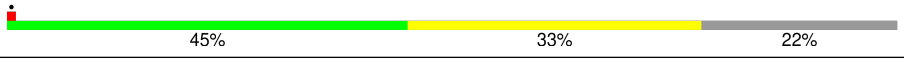
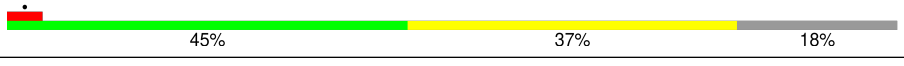
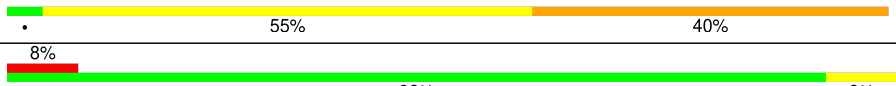
Mol	Chain	Length	Quality of chain
5	M	303	
5	Y	303	
6	A	136	
6	W	136	
7	H	215	
8	J	106	
8	X	106	
9	R	133	
9	U	133	
10	S	123	
10	V	123	
11	T	215	
12	E	12	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 45911 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	443	Total	C	N	O	S	0	0
			3665	2326	656	656	27		
1	G	443	Total	C	N	O	S	0	0
			3665	2326	656	656	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP Q15022
G	67	MET	-	initiating methionine	UNP Q15022

- Molecule 2 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	536	Total	C	N	O	S	0	0
			4304	2696	765	801	42		
2	I	605	Total	C	N	O	S	0	0
			4863	3049	863	908	43		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q15910
C	0	ASN	-	expression tag	UNP Q15910
C	1	ALA	-	expression tag	UNP Q15910
C	14	ALA	CYS	conflict	UNP Q15910
C	15	CYS	TRP	conflict	UNP Q15910
I	-1	SER	-	expression tag	UNP Q15910
I	0	ASN	-	expression tag	UNP Q15910
I	1	ALA	-	expression tag	UNP Q15910
I	14	ALA	CYS	conflict	UNP Q15910
I	15	CYS	TRP	conflict	UNP Q15910

- Molecule 3 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	362	Total	C	N	O	S	0	0
			2930	1855	513	541	21		
3	K	362	Total	C	N	O	S	0	0
			2930	1855	513	541	21		

- Molecule 4 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		
4	O	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		

- Molecule 5 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	126	Total	C	N	O	S	0	0
			1047	664	206	174	3		
5	Y	126	Total	C	N	O	S	0	0
			1047	664	206	174	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	7	SER	-	expression tag	UNP Q6ZN18
M	8	ASN	-	expression tag	UNP Q6ZN18
M	9	ALA	MET	conflict	UNP Q6ZN18
Y	7	SER	-	expression tag	UNP Q6ZN18
Y	8	ASN	-	expression tag	UNP Q6ZN18
Y	9	ALA	MET	conflict	UNP Q6ZN18

- Molecule 6 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	117	Total	C	N	O	S	0	0
			939	590	183	163	3		
6	W	99	Total	C	N	O	S	0	0
			817	515	158	141	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
W	102	ALA	GLY	conflict	UNP P84233

- Molecule 7 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	215	Total	C	N	O	P	0	0
			4421	2085	846	1275	215		

- Molecule 8 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
8	X	87	Total	C	N	O	S	0	0
			702	442	142	117	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	103	SER	-	expression tag	UNP P62799
J	104	SER	-	expression tag	UNP P62799
J	105	GLY	-	expression tag	UNP P62799
X	103	SER	-	expression tag	UNP P62799
X	104	SER	-	expression tag	UNP P62799
X	105	GLY	-	expression tag	UNP P62799

- Molecule 9 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	108	Total	C	N	O	S	0	0
			829	522	162	144	1		
9	U	108	Total	C	N	O	S	0	0
			829	522	162	144	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	SER	-	expression tag	UNP P06897
R	-2	ASN	-	expression tag	UNP P06897
R	-1	ALA	-	expression tag	UNP P06897
R	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
R	119	CYS	LYS	conflict	UNP P06897
R	123	SER	ALA	conflict	UNP P06897
U	-3	SER	-	expression tag	UNP P06897
U	-2	ASN	-	expression tag	UNP P06897
U	-1	ALA	-	expression tag	UNP P06897
U	99	ARG	GLY	conflict	UNP P06897
U	119	CYS	LYS	conflict	UNP P06897
U	123	SER	ALA	conflict	UNP P06897

- Molecule 10 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	96	Total	C	N	O	S	0	0
			752	472	137	141	2		
10	V	95	Total	C	N	O	S	0	0
			741	466	133	140	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	MET	-	initiating methionine	UNP P02281
S	29	THR	SER	conflict	UNP P02281
V	0	MET	-	initiating methionine	UNP P02281
V	29	THR	SER	conflict	UNP P02281

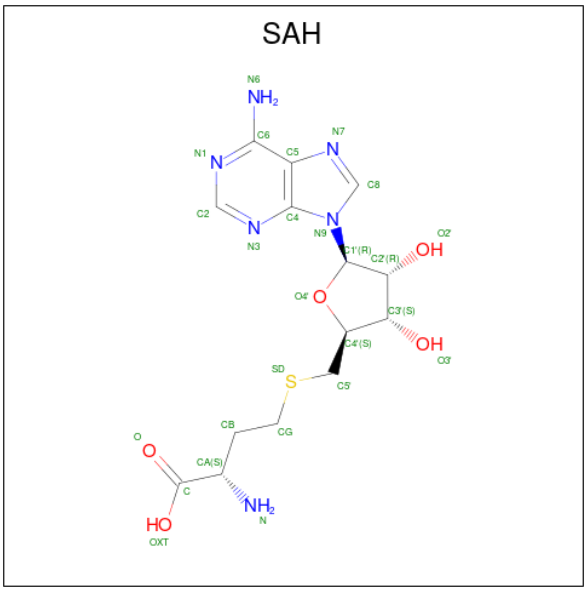
- Molecule 11 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	215	Total	C	N	O	P	0	0
			4372	2067	807	1283	215		

- Molecule 12 is a protein called activating methylated peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	E	12	Total	C	N	O	0	0
			67	42	13	12		

- Molecule 13 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



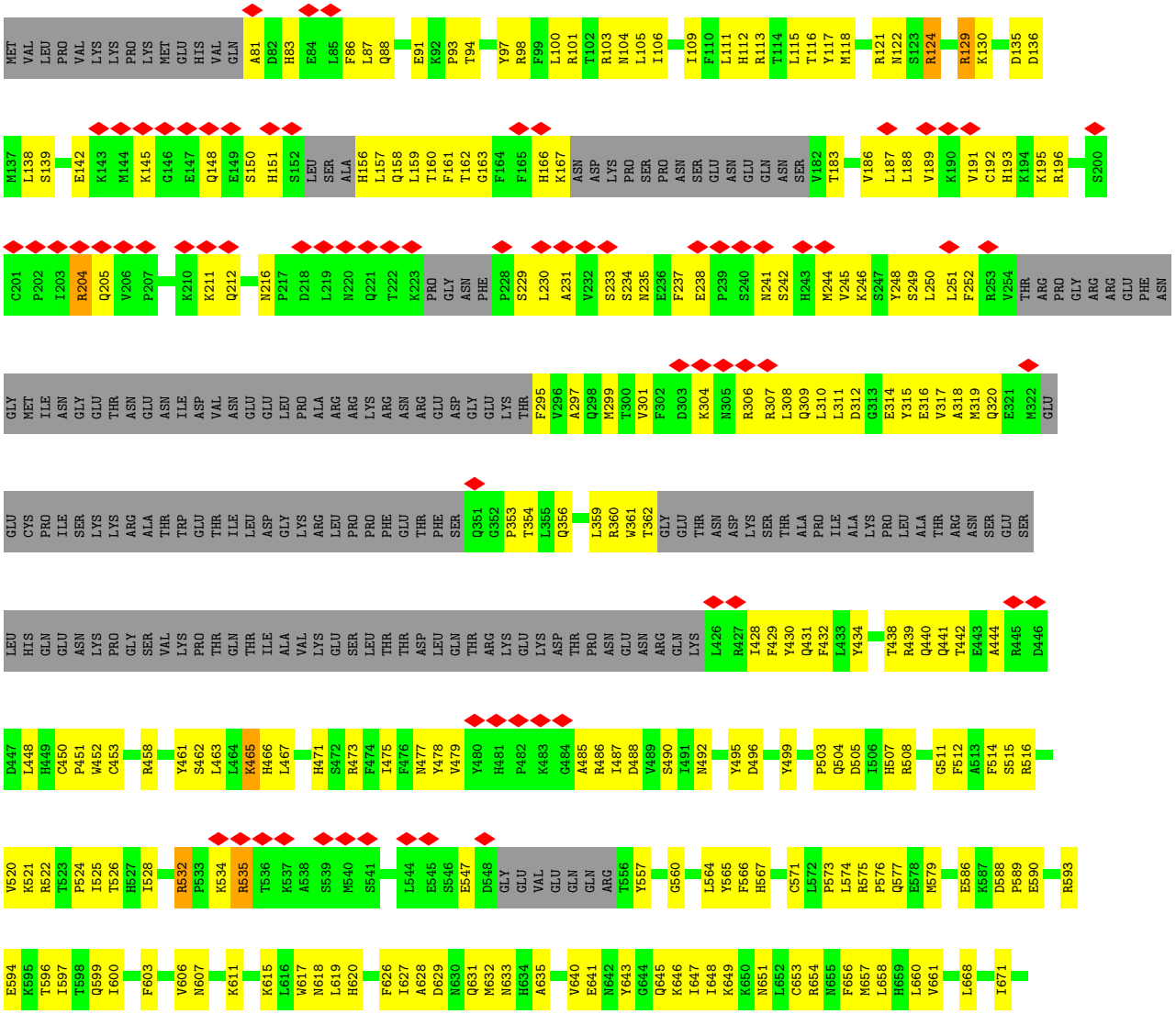
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	S	0
			26	14	6	5	1	
13	I	1	Total	C	N	O	S	0
			26	14	6	5	1	

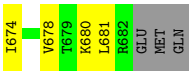
3 Residue-property plots (i)

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: Polycomb protein SUZ12

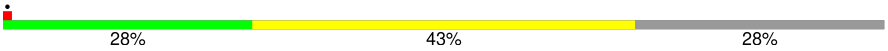
Chain B:

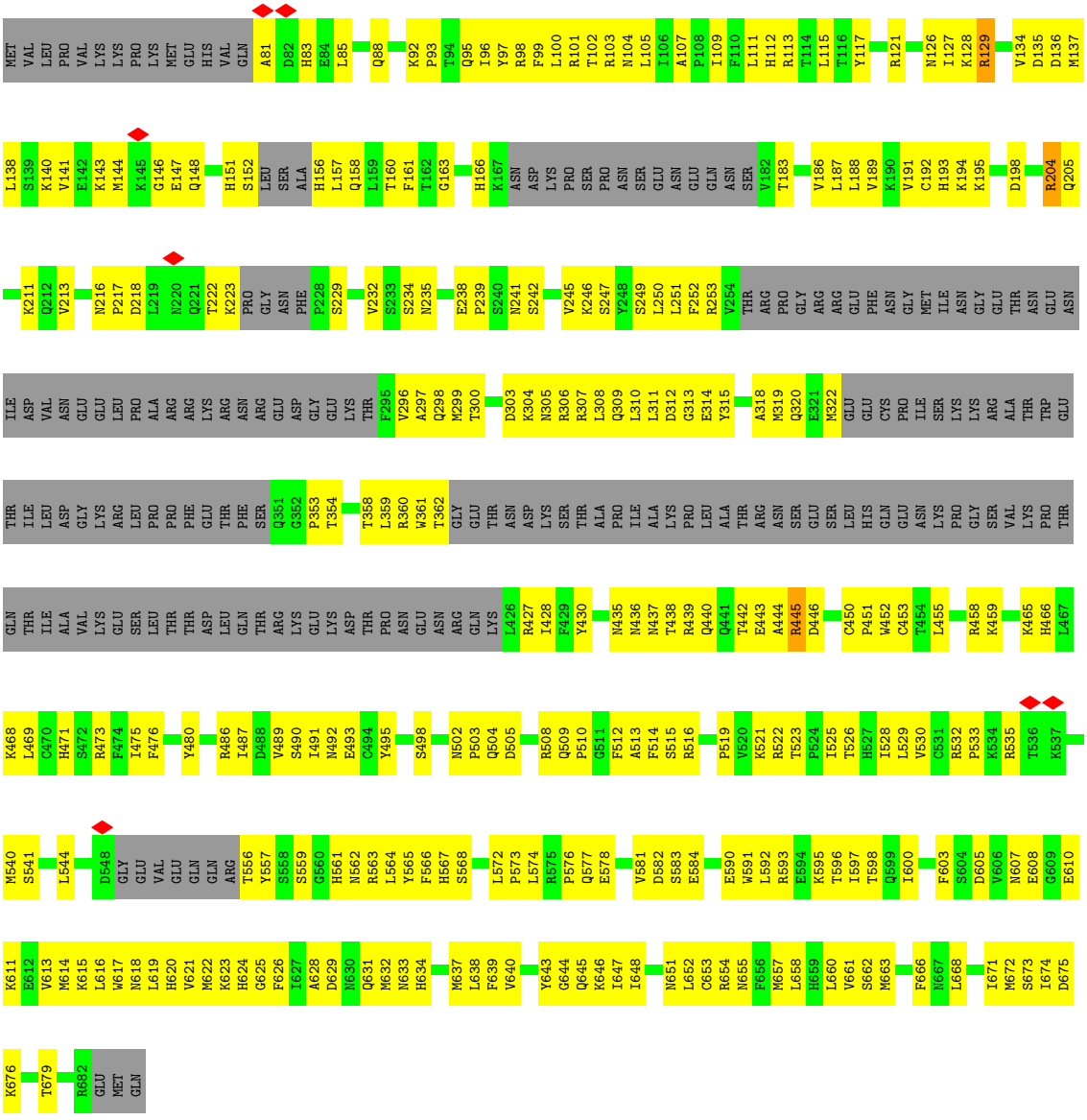




• Molecule 1: Polycomb protein SUZ12

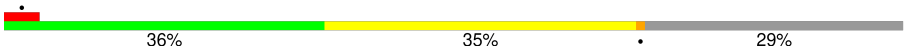
Chain G:

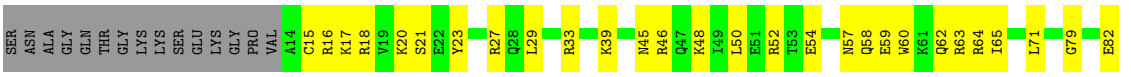


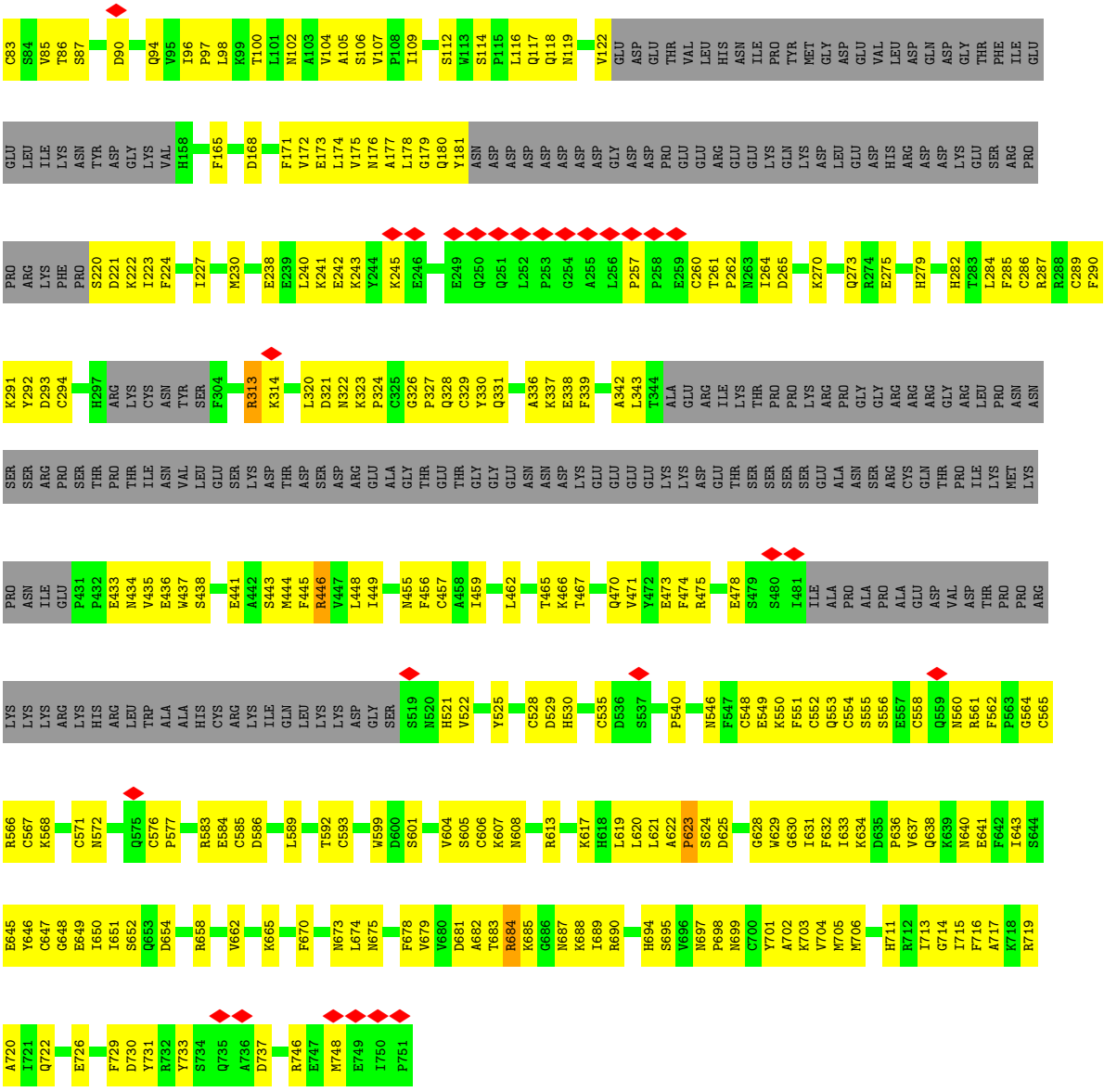


• Molecule 2: Histone-lysine N-methyltransferase EZH2

Chain C:

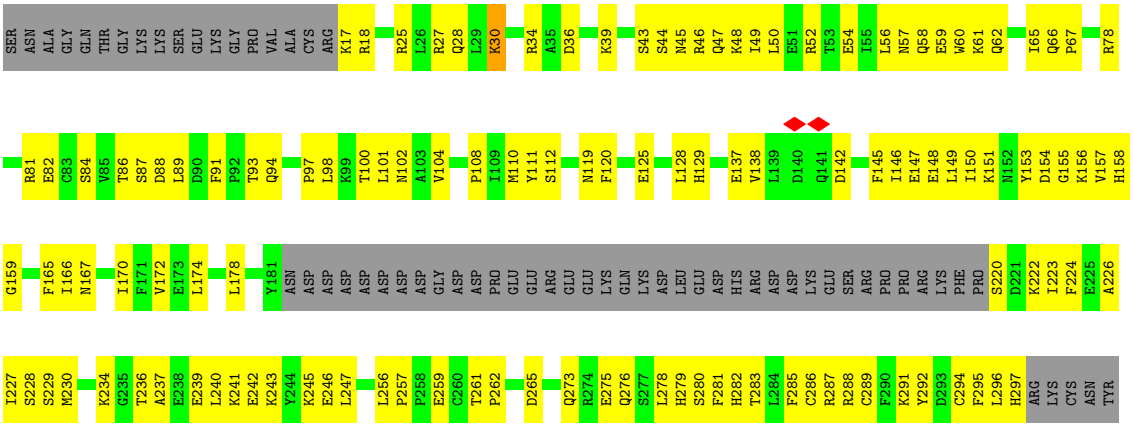


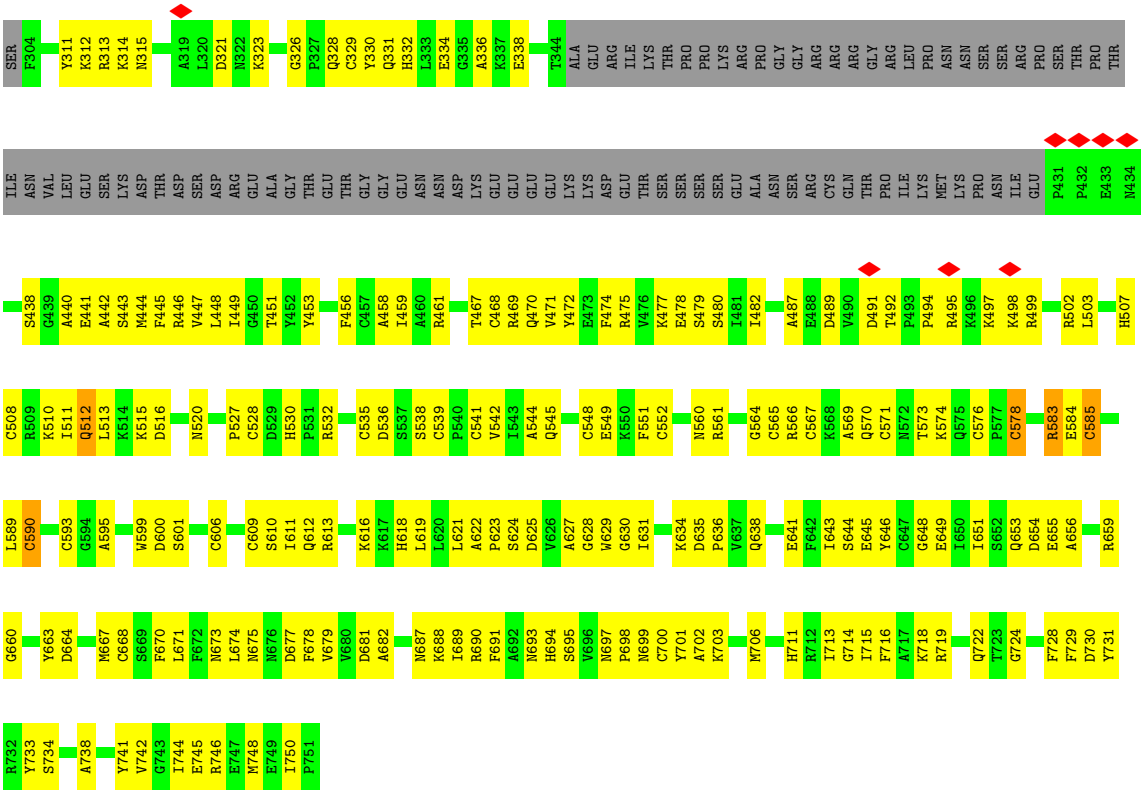




• Molecule 2: Histone-lysine N-methyltransferase EZH2

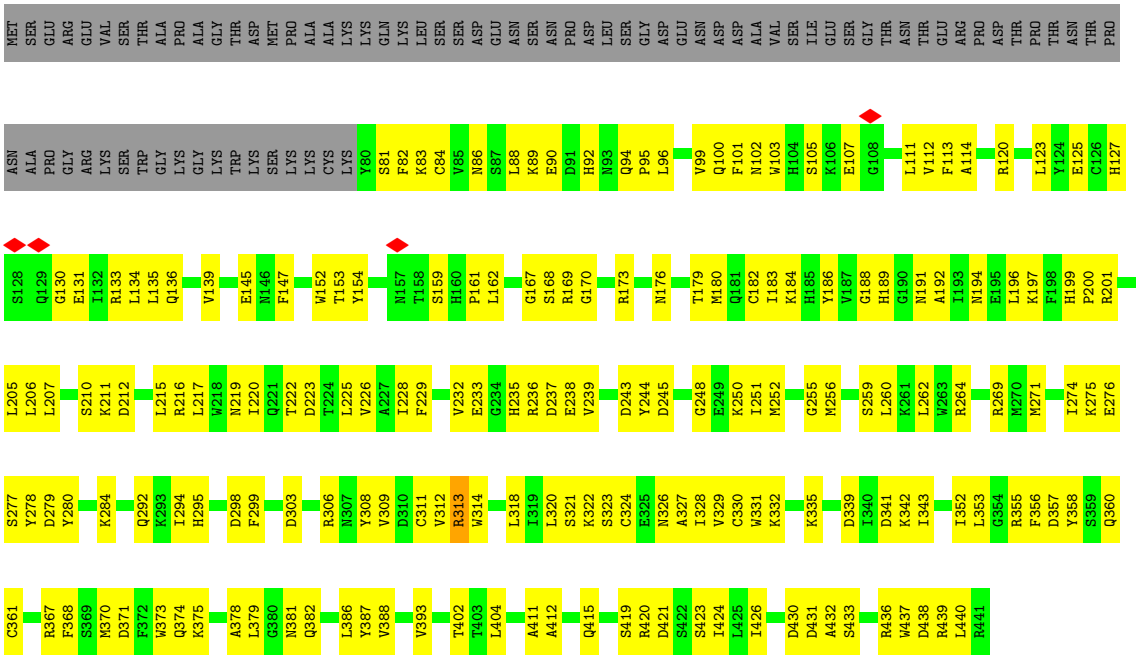
Chain I:





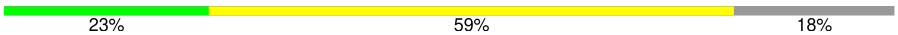
• Molecule 3: Polycomb protein EED

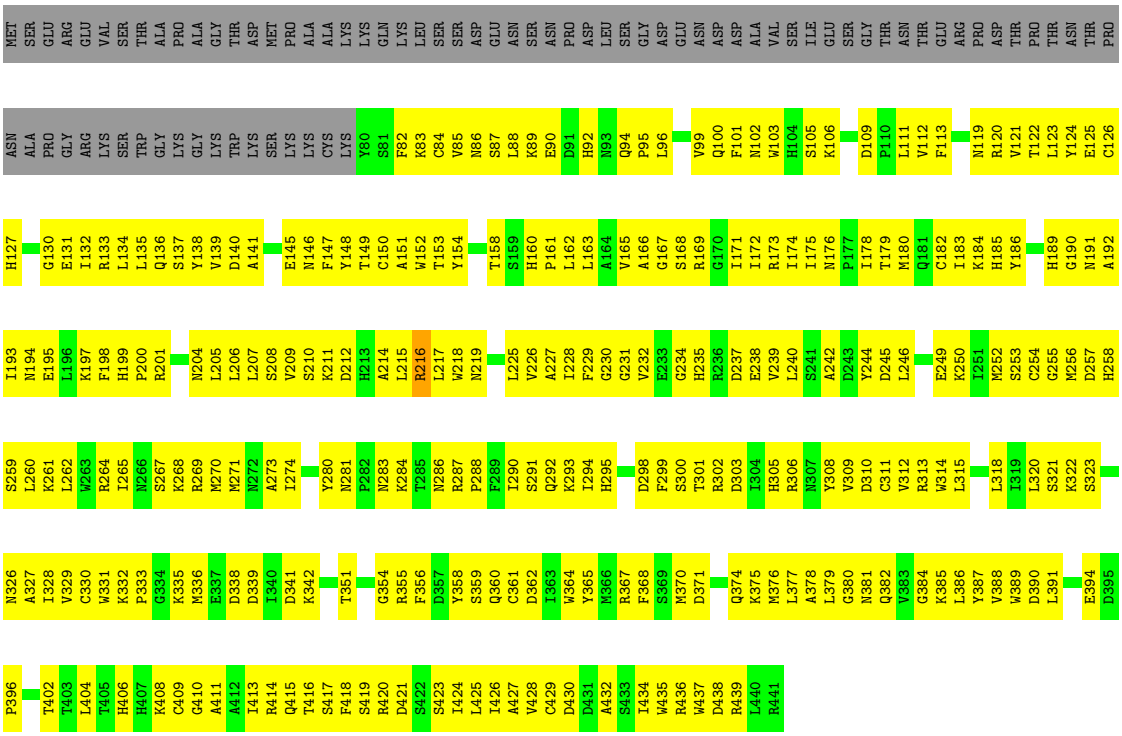
Chain F:



• Molecule 3: Polycomb protein EED

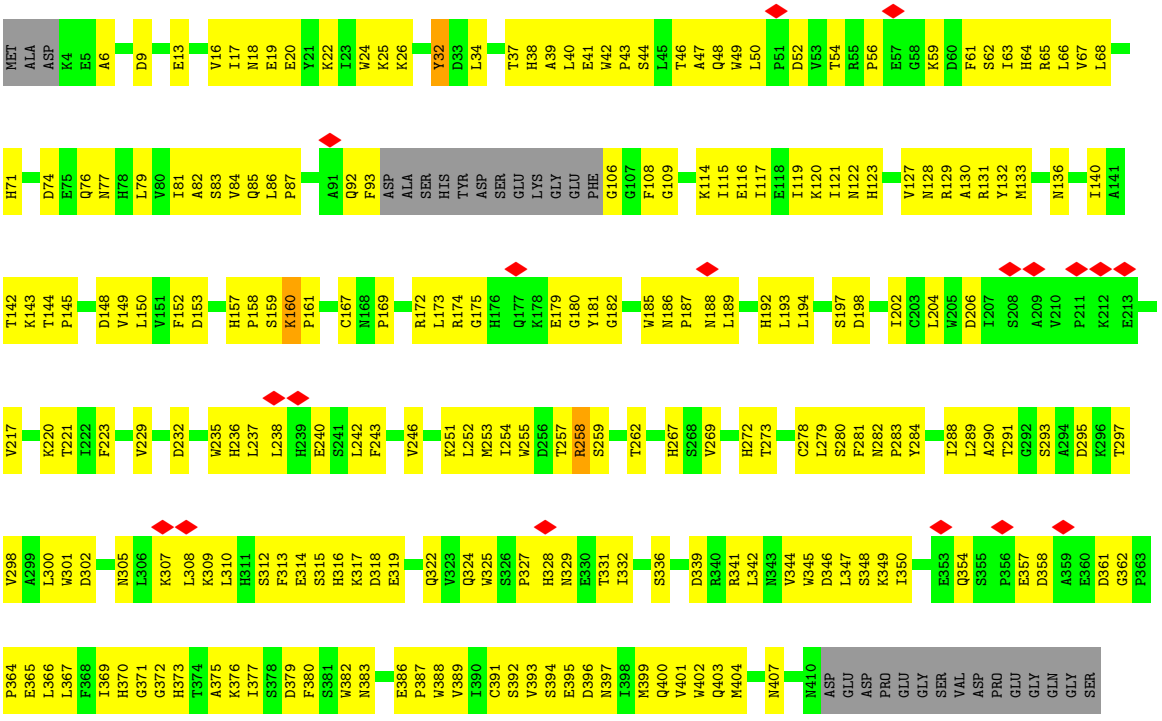
Chain K:





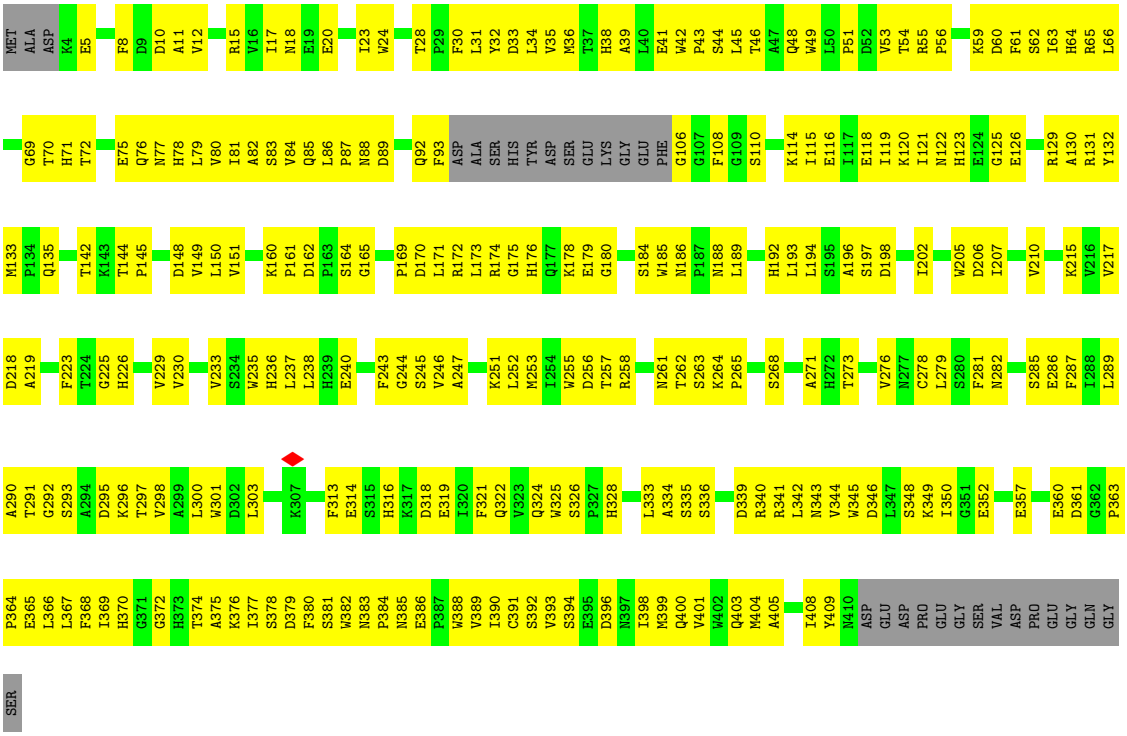
• Molecule 4: Histone-binding protein RBBP4

Chain L:



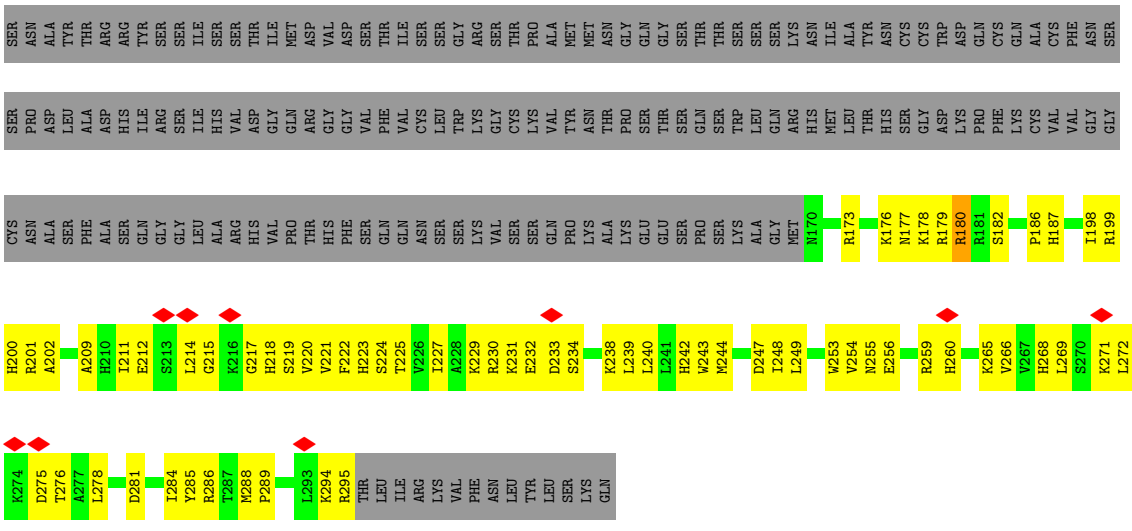
• Molecule 4: Histone-binding protein RBBP4

Chain O:



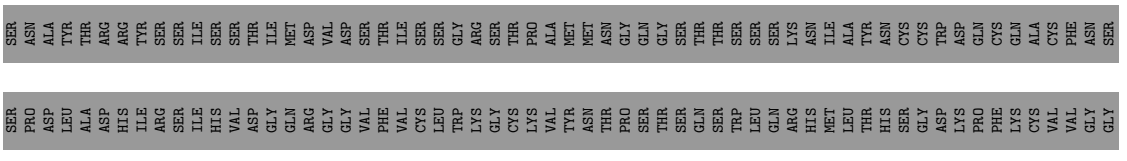
• Molecule 5: Zinc finger protein AEBP2

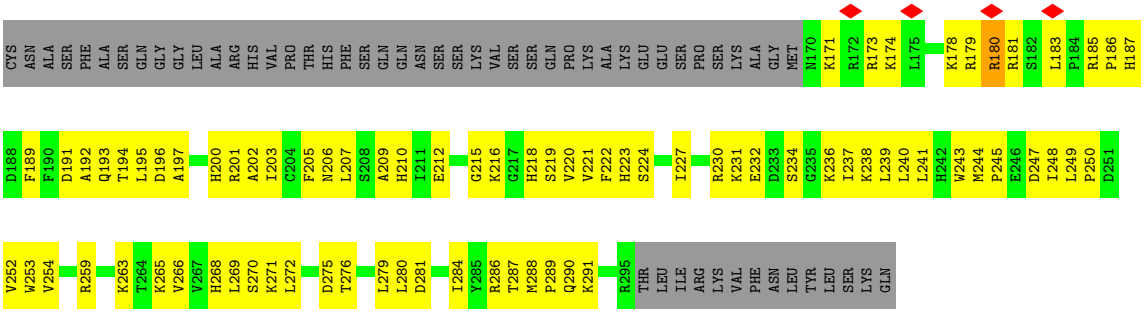
Chain M:



• Molecule 5: Zinc finger protein AEBP2

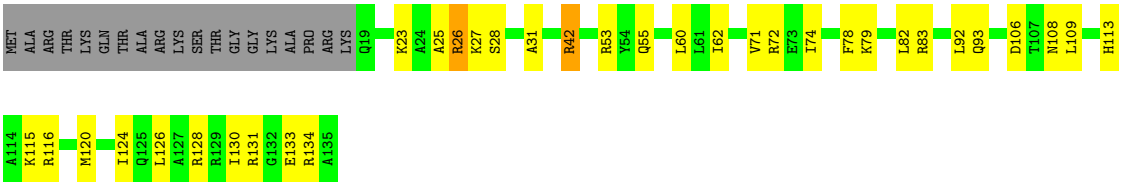
Chain Y:





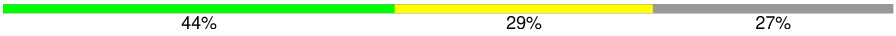
• Molecule 6: Histone H3.2

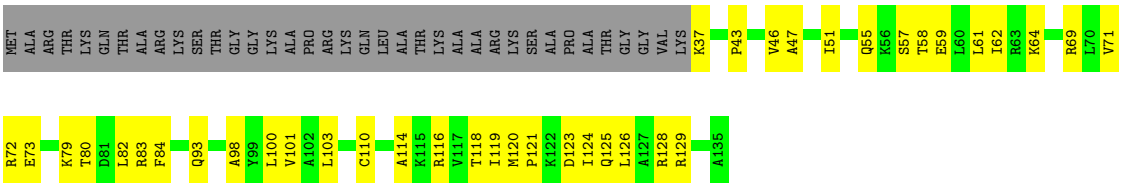
Chain A:



• Molecule 6: Histone H3.2

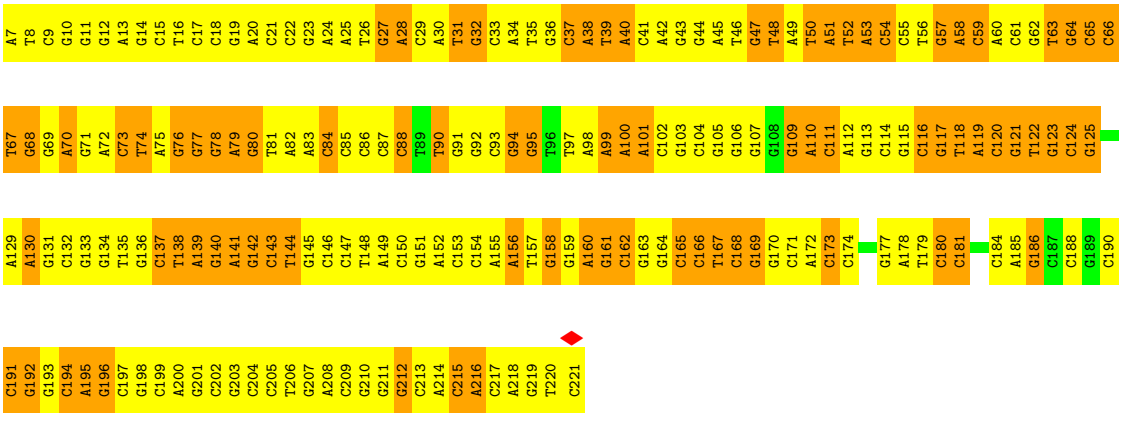
Chain W:





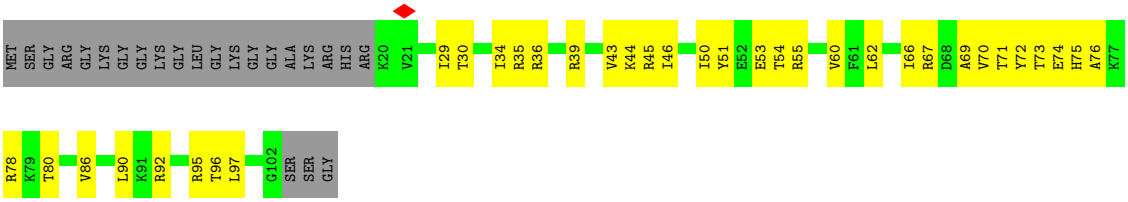
• Molecule 7: DNA (226-MER)

Chain H:



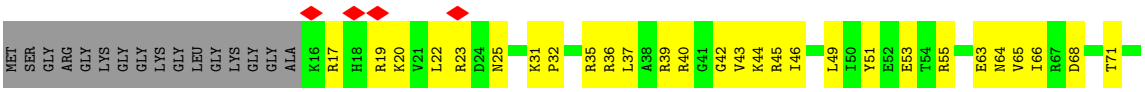
• Molecule 8: Histone H4

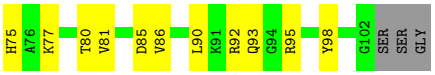
Chain J:



• Molecule 8: Histone H4

Chain X:



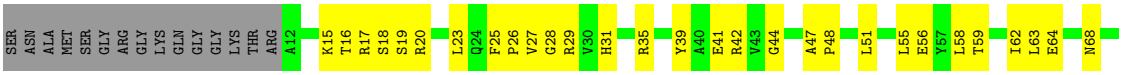


• Molecule 9: Histone H2A type 1

Chain R:

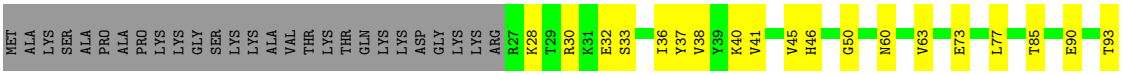
• Molecule 9: Histone H2A type 1

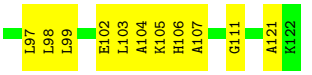
Chain U:



• Molecule 10: Histone H2B 1.1

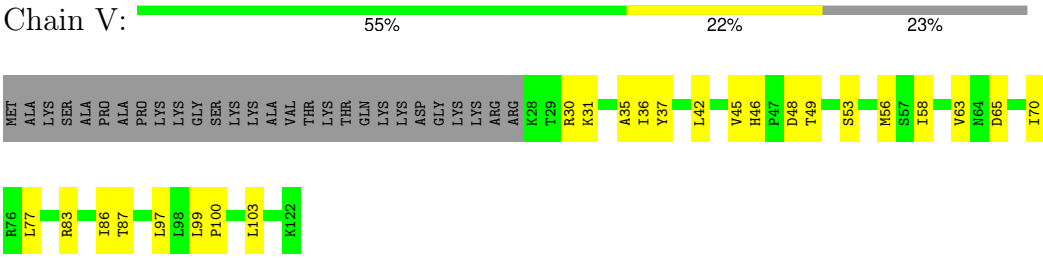
Chain S:





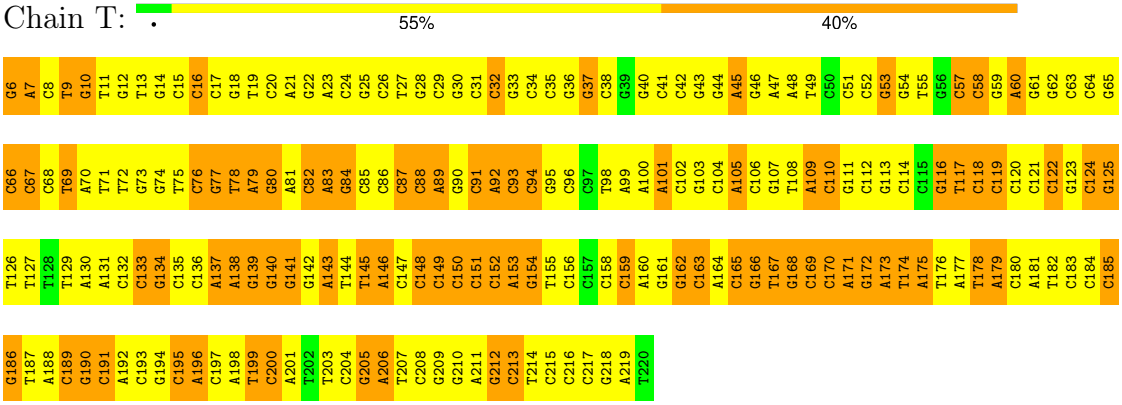
• Molecule 10: Histone H2B 1.1

Chain V:



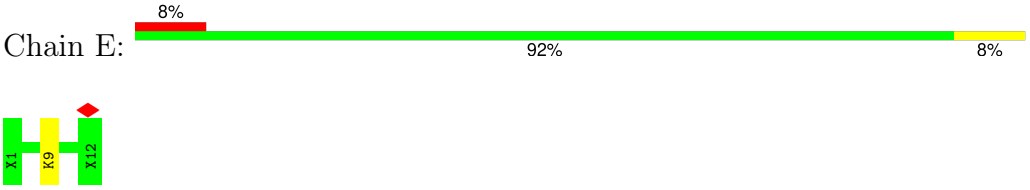
• Molecule 11: DNA (226-MER)

Chain T:



• Molecule 12: activating methylated peptide

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.3, 2.3, 2.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, SAH

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	B	0.29	0/3745	0.56	1/5035 (0.0%)
1	G	0.33	0/3745	0.57	2/5035 (0.0%)
2	C	0.26	0/4397	0.53	1/5923 (0.0%)
2	I	0.36	0/4971	0.65	7/6702 (0.1%)
3	F	0.24	0/3005	0.51	0/4070
3	K	0.32	0/3005	0.55	0/4070
4	L	0.27	0/3225	0.51	1/4394 (0.0%)
4	O	0.30	0/3225	0.51	0/4394
5	M	0.27	0/1070	0.59	1/1437 (0.1%)
5	Y	0.28	0/1070	0.56	0/1437
6	A	0.44	0/952	0.76	3/1276 (0.2%)
6	W	0.32	0/829	0.62	0/1111
7	H	0.76	2/4967 (0.0%)	1.74	324/7665 (4.2%)
8	J	0.37	0/668	0.65	1/894 (0.1%)
8	X	0.30	0/710	0.64	0/948
9	R	0.33	0/839	0.61	1/1132 (0.1%)
9	U	0.30	0/839	0.60	0/1132
10	S	0.31	0/763	0.55	0/1025
10	V	0.31	0/752	0.52	0/1011
11	T	0.79	6/4899 (0.1%)	1.73	300/7548 (4.0%)
All	All	0.45	8/47676 (0.0%)	0.97	642/66239 (1.0%)

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
1	B	0	2
4	L	0	1
6	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	3
11	T	0	5
All	All	0	12

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	54	DG	C2-N2	-6.61	1.27	1.34
11	T	124	DC	C4-N4	-6.57	1.28	1.33
11	T	53	DG	C2-N2	-5.49	1.29	1.34
7	H	178	DA	C5-C4	-5.21	1.35	1.38
11	T	48	DA	C5-C4	-5.21	1.35	1.38
11	T	52	DC	C4-N4	-5.18	1.29	1.33
11	T	124	DC	N3-C4	-5.17	1.30	1.33
7	H	107	DG	N9-C4	-5.08	1.33	1.38

All (642) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	93	DC	OP1-P-O3'	-34.70	28.85	105.20
11	T	167	DT	OP1-P-O3'	-34.42	29.47	105.20
11	T	76	DC	OP2-P-O3'	-33.34	31.85	105.20
7	H	85	DC	OP2-P-O3'	-32.65	33.37	105.20
7	H	94	DG	OP1-P-OP2	-14.47	97.90	119.60
11	T	168	DG	OP1-P-OP2	-13.53	99.30	119.60
2	I	502	ARG	NE-CZ-NH2	11.77	126.19	120.30
7	H	58	DA	OP1-P-O3'	11.35	130.16	105.20
11	T	104	DC	OP1-P-O3'	10.22	127.69	105.20
7	H	68	DG	OP1-P-O3'	10.18	127.60	105.20
7	H	59	DC	OP1-P-OP2	-9.88	104.79	119.60
11	T	109	DA	OP1-P-O3'	9.66	126.45	105.20
2	I	502	ARG	NE-CZ-NH1	-9.57	115.52	120.30
7	H	104	DC	OP1-P-O3'	9.49	126.08	105.20
11	T	93	DC	OP1-P-O3'	9.45	126.00	105.20
11	T	67	DC	OP1-P-O3'	9.31	125.69	105.20
11	T	133	DC	OP1-P-O3'	9.08	125.18	105.20
11	T	59	DG	OP1-P-OP2	-9.06	106.01	119.60
11	T	68	DC	OP1-P-OP2	-8.94	106.19	119.60
7	H	59	DC	OP1-P-O3'	8.93	124.85	105.20
7	H	161	DG	OP1-P-O3'	8.89	124.76	105.20
7	H	69	DG	OP1-P-OP2	-8.82	106.37	119.60
7	H	105	DG	OP1-P-OP2	-8.80	106.39	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	150	DC	OP1-P-O3'	8.74	124.44	105.20
11	T	48	DA	C5-C6-N1	8.72	122.06	117.70
11	T	119	DC	OP1-P-O3'	8.67	124.27	105.20
11	T	151	DC	OP1-P-OP2	-8.65	106.63	119.60
11	T	94	DC	OP1-P-OP2	-8.60	106.70	119.60
11	T	134	DG	OP1-P-OP2	-8.57	106.74	119.60
11	T	110	DC	OP1-P-OP2	-8.55	106.77	119.60
11	T	105	DA	OP1-P-OP2	-8.45	106.92	119.60
7	H	60	DA	OP1-P-OP2	-8.38	107.03	119.60
11	T	98	DT	OP1-P-O3'	8.37	123.61	105.20
11	T	120	DC	OP1-P-OP2	-8.28	107.19	119.60
2	C	623	PRO	CA-N-CD	-8.24	99.97	111.50
7	H	162	DC	OP1-P-OP2	-8.23	107.26	119.60
11	T	99	DA	OP1-P-OP2	-8.08	107.49	119.60
11	T	54	DG	N3-C2-N2	-8.07	114.25	119.90
7	H	185	DA	N1-C6-N6	-7.97	113.82	118.60
7	H	67	DT	OP1-P-O3'	7.96	122.72	105.20
7	H	163	DG	OP1-P-O3'	7.92	122.62	105.20
7	H	70	DA	OP1-P-OP2	-7.70	108.05	119.60
7	H	103	DG	OP1-P-OP2	-7.64	108.13	119.60
7	H	68	DG	OP1-P-OP2	-7.64	108.14	119.60
7	H	178	DA	C5-C6-N1	7.64	121.52	117.70
7	H	93	DC	OP1-P-OP2	-7.61	108.18	119.60
11	T	153	DA	OP1-P-OP2	-7.61	108.19	119.60
7	H	150	DC	OP1-P-OP2	-7.58	108.23	119.60
7	H	185	DA	C5-C6-N1	7.58	121.49	117.70
7	H	92	DG	OP1-P-O3'	7.53	121.77	105.20
11	T	83	DA	OP1-P-OP2	-7.49	108.36	119.60
7	H	88	DC	OP1-P-OP2	-7.49	108.37	119.60
7	H	149	DA	OP1-P-O3'	7.47	121.63	105.20
11	T	80	DG	OP1-P-OP2	-7.46	108.41	119.60
7	H	87	DC	OP1-P-O3'	7.45	121.58	105.20
7	H	172	DA	C5-C6-N1	7.43	121.41	117.70
7	H	93	DC	OP2-P-O3'	7.42	121.53	105.20
2	I	502	ARG	CD-NE-CZ	7.39	133.95	123.60
7	H	51	DA	OP1-P-OP2	-7.37	108.54	119.60
11	T	82	DC	OP1-P-O3'	7.36	121.39	105.20
11	T	109	DA	OP1-P-OP2	-7.36	108.57	119.60
2	I	590	CYS	CA-CB-SG	-7.35	100.77	114.00
11	T	152	DC	OP1-P-O3'	7.33	121.32	105.20
11	T	108	DT	OP1-P-O3'	7.30	121.25	105.20
7	H	48	DT	OP1-P-OP2	-7.29	108.67	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	164	DG	OP1-P-OP2	-7.26	108.70	119.60
11	T	57	DC	O4'-C4'-C3'	-7.21	101.61	104.50
7	H	80	DG	OP1-P-OP2	-7.21	108.79	119.60
7	H	79	DA	OP1-P-OP2	-7.14	108.89	119.60
7	H	55	DC	OP1-P-OP2	-7.12	108.92	119.60
11	T	160	DA	OP1-P-OP2	-7.10	108.95	119.60
11	T	183	DC	OP1-P-OP2	-7.10	108.95	119.60
11	T	118	DC	OP1-P-OP2	-7.08	108.98	119.60
7	H	100	DA	OP1-P-OP2	-7.05	109.02	119.60
7	H	119	DA	OP1-P-OP2	-7.05	109.02	119.60
11	T	163	DC	OP1-P-OP2	-7.02	109.07	119.60
7	H	49	DA	OP1-P-OP2	-7.00	109.10	119.60
11	T	184	DC	OP1-P-OP2	-7.00	109.10	119.60
7	H	102	DC	OP1-P-O3'	6.99	120.57	105.20
7	H	47	DG	OP1-P-OP2	-6.98	109.13	119.60
11	T	154	DG	OP1-P-OP2	-6.97	109.15	119.60
7	H	151	DG	OP1-P-OP2	-6.96	109.17	119.60
7	H	201	DG	OP1-P-OP2	-6.94	109.19	119.60
11	T	166	DG	OP1-P-OP2	-6.94	109.19	119.60
7	H	131	DG	OP1-P-OP2	-6.94	109.19	119.60
7	H	173	DC	C2-N3-C4	-6.94	116.43	119.90
7	H	156	DA	OP1-P-OP2	-6.93	109.20	119.60
7	H	142	DG	OP1-P-OP2	-6.92	109.21	119.60
7	H	159	DG	OP1-P-OP2	-6.92	109.22	119.60
7	H	82	DA	OP1-P-OP2	-6.91	109.23	119.60
7	H	43	DG	OP1-P-OP2	-6.90	109.25	119.60
11	T	28	DG	OP1-P-OP2	-6.90	109.25	119.60
7	H	58	DA	OP1-P-OP2	-6.89	109.26	119.60
11	T	136	DC	OP1-P-OP2	-6.88	109.28	119.60
7	H	139	DA	OP1-P-OP2	-6.88	109.28	119.60
11	T	47	DA	C5-C6-N1	6.88	121.14	117.70
11	T	149	DC	OP1-P-OP2	-6.88	109.28	119.60
7	H	61	DC	OP1-P-OP2	-6.87	109.29	119.60
11	T	77	DG	O5'-P-OP2	6.87	118.94	110.70
11	T	27	DT	OP1-P-OP2	-6.87	109.30	119.60
7	H	109	DG	OP1-P-OP2	-6.87	109.30	119.60
11	T	62	DG	OP1-P-OP2	-6.86	109.31	119.60
11	T	158	DC	OP1-P-OP2	-6.86	109.31	119.60
7	H	200	DA	OP1-P-OP2	-6.86	109.32	119.60
11	T	132	DC	OP1-P-OP2	-6.85	109.32	119.60
11	T	213	DC	OP1-P-OP2	-6.85	109.33	119.60
7	H	85	DC	OP1-P-OP2	-6.85	109.33	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	107	DG	OP1-P-OP2	-6.85	109.33	119.60
11	T	37	DG	OP1-P-OP2	-6.84	109.34	119.60
7	H	121	DG	OP1-P-OP2	-6.84	109.34	119.60
7	H	83	DA	OP1-P-OP2	-6.83	109.36	119.60
7	H	165	DC	OP1-P-OP2	-6.83	109.36	119.60
7	H	44	DG	OP1-P-OP2	-6.82	109.37	119.60
7	H	115	DG	OP1-P-OP2	-6.82	109.36	119.60
11	T	179	DA	OP1-P-OP2	-6.82	109.36	119.60
11	T	218	DG	OP1-P-OP2	-6.82	109.36	119.60
11	T	65	DG	OP1-P-OP2	-6.82	109.38	119.60
7	H	98	DA	OP1-P-OP2	-6.82	109.38	119.60
11	T	212	DG	OP1-P-OP2	-6.81	109.38	119.60
11	T	11	DT	OP1-P-OP2	-6.81	109.39	119.60
11	T	161	DG	OP1-P-OP2	-6.80	109.39	119.60
11	T	195	DC	OP1-P-OP2	-6.80	109.39	119.60
7	H	166	DC	OP1-P-OP2	-6.80	109.40	119.60
11	T	180	DC	OP1-P-OP2	-6.80	109.40	119.60
7	H	15	DC	OP1-P-OP2	-6.80	109.40	119.60
7	H	23	DG	OP1-P-OP2	-6.80	109.40	119.60
7	H	125	DG	OP1-P-OP2	-6.80	109.40	119.60
11	T	192	DA	OP1-P-OP2	-6.80	109.41	119.60
11	T	198	DA	OP1-P-OP2	-6.80	109.40	119.60
7	H	211	DG	OP1-P-OP2	-6.79	109.42	119.60
7	H	26	DT	OP1-P-OP2	-6.79	109.42	119.60
7	H	210	DG	OP1-P-OP2	-6.79	109.42	119.60
11	T	6	DG	OP1-P-OP2	-6.79	109.42	119.60
11	T	211	DA	OP1-P-OP2	-6.79	109.42	119.60
7	H	95	DG	OP1-P-OP2	-6.79	109.42	119.60
11	T	156	DC	OP1-P-OP2	-6.79	109.42	119.60
11	T	23	DA	OP1-P-OP2	-6.79	109.42	119.60
11	T	208	DC	OP1-P-OP2	-6.79	109.42	119.60
7	H	214	DA	OP1-P-OP2	-6.78	109.43	119.60
11	T	159	DC	OP1-P-O3'	6.78	120.12	105.20
7	H	32	DG	OP1-P-OP2	-6.78	109.43	119.60
7	H	37	DC	OP1-P-OP2	-6.78	109.43	119.60
11	T	14	DG	OP1-P-OP2	-6.78	109.43	119.60
7	H	27	DG	OP1-P-OP2	-6.78	109.43	119.60
7	H	29	DC	OP1-P-OP2	-6.78	109.43	119.60
7	H	218	DA	OP1-P-OP2	-6.78	109.43	119.60
11	T	181	DA	OP1-P-OP2	-6.78	109.43	119.60
7	H	28	DA	OP1-P-OP2	-6.78	109.43	119.60
11	T	205	DG	OP1-P-OP2	-6.78	109.44	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	13	DA	OP1-P-OP2	-6.78	109.44	119.60
11	T	18	DG	OP1-P-OP2	-6.78	109.44	119.60
7	H	194	DC	OP1-P-OP2	-6.77	109.44	119.60
7	H	19	DG	OP1-P-OP2	-6.77	109.44	119.60
7	H	202	DC	OP1-P-OP2	-6.77	109.44	119.60
11	T	206	DA	OP1-P-OP2	-6.77	109.44	119.60
7	H	40	DA	OP1-P-OP2	-6.77	109.45	119.60
7	H	134	DG	OP1-P-OP2	-6.77	109.44	119.60
7	H	137	DC	OP1-P-OP2	-6.77	109.45	119.60
7	H	203	DG	OP1-P-OP2	-6.77	109.45	119.60
11	T	16	DC	OP1-P-OP2	-6.77	109.45	119.60
7	H	217	DC	OP1-P-OP2	-6.77	109.45	119.60
11	T	204	DC	OP1-P-OP2	-6.77	109.45	119.60
11	T	209	DG	OP1-P-OP2	-6.77	109.45	119.60
7	H	16	DT	OP1-P-OP2	-6.76	109.45	119.60
7	H	133	DG	OP1-P-OP2	-6.76	109.45	119.60
7	H	143	DC	OP1-P-OP2	-6.76	109.45	119.60
11	T	45	DA	N1-C6-N6	-6.76	114.54	118.60
7	H	11	DG	OP1-P-OP2	-6.76	109.46	119.60
11	T	32	DC	OP1-P-OP2	-6.76	109.46	119.60
11	T	13	DT	OP1-P-OP2	-6.76	109.46	119.60
11	T	17	DC	OP1-P-OP2	-6.76	109.46	119.60
11	T	22	DG	OP1-P-OP2	-6.76	109.46	119.60
7	H	36	DG	OP1-P-OP2	-6.76	109.46	119.60
7	H	213	DC	OP1-P-OP2	-6.76	109.46	119.60
11	T	8	DC	OP1-P-OP2	-6.76	109.46	119.60
11	T	19	DT	OP1-P-OP2	-6.76	109.46	119.60
11	T	137	DA	OP1-P-OP2	-6.76	109.46	119.60
11	T	172	DG	OP1-P-OP2	-6.76	109.46	119.60
7	H	9	DC	OP1-P-OP2	-6.76	109.46	119.60
11	T	20	DC	OP1-P-OP2	-6.76	109.46	119.60
7	H	18	DC	OP1-P-OP2	-6.76	109.47	119.60
7	H	21	DC	OP1-P-OP2	-6.76	109.47	119.60
11	T	216	DC	OP1-P-OP2	-6.76	109.47	119.60
7	H	17	DC	OP1-P-OP2	-6.75	109.47	119.60
11	T	140	DG	OP1-P-OP2	-6.75	109.47	119.60
2	I	585	CYS	CA-CB-SG	-6.75	101.85	114.00
11	T	194	DG	OP1-P-OP2	-6.75	109.48	119.60
11	T	10	DG	OP1-P-OP2	-6.75	109.48	119.60
11	T	26	DC	OP1-P-OP2	-6.75	109.48	119.60
7	H	41	DC	OP1-P-OP2	-6.75	109.48	119.60
11	T	64	DC	OP1-P-OP2	-6.75	109.48	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	14	DG	OP1-P-OP2	-6.74	109.48	119.60
7	H	111	DC	OP1-P-OP2	-6.74	109.48	119.60
7	H	221	DC	OP1-P-OP2	-6.74	109.48	119.60
11	T	217	DC	OP1-P-OP2	-6.74	109.48	119.60
7	H	22	DC	OP1-P-OP2	-6.74	109.49	119.60
11	T	25	DG	OP1-P-OP2	-6.74	109.49	119.60
7	H	46	DT	OP1-P-OP2	-6.74	109.49	119.60
11	T	196	DA	OP1-P-OP2	-6.74	109.49	119.60
7	H	199	DC	OP1-P-OP2	-6.74	109.49	119.60
11	T	21	DA	OP1-P-OP2	-6.74	109.50	119.60
11	T	30	DG	OP1-P-OP2	-6.74	109.50	119.60
11	T	210	DG	OP1-P-OP2	-6.74	109.50	119.60
7	H	12	DG	OP1-P-OP2	-6.73	109.50	119.60
7	H	33	DC	OP1-P-OP2	-6.73	109.50	119.60
7	H	99	DA	OP1-P-OP2	-6.73	109.50	119.60
7	H	190	DC	OP1-P-OP2	-6.73	109.50	119.60
11	T	7	DA	OP1-P-OP2	-6.73	109.50	119.60
11	T	24	DC	OP1-P-OP2	-6.73	109.50	119.60
11	T	66	DC	OP1-P-OP2	-6.73	109.50	119.60
11	T	175	DA	OP1-P-OP2	-6.73	109.50	119.60
11	T	200	DC	OP1-P-OP2	-6.73	109.50	119.60
11	T	215	DC	OP1-P-OP2	-6.73	109.50	119.60
7	H	207	DG	OP1-P-OP2	-6.73	109.51	119.60
7	H	215	DC	OP1-P-OP2	-6.73	109.51	119.60
7	H	24	DA	OP1-P-OP2	-6.73	109.51	119.60
7	H	64	DG	OP1-P-OP2	-6.73	109.51	119.60
7	H	216	DA	OP1-P-OP2	-6.73	109.51	119.60
11	T	89	DA	OP1-P-OP2	-6.73	109.51	119.60
11	T	201	DA	OP1-P-OP2	-6.73	109.51	119.60
11	T	79	DA	OP1-P-O3'	6.73	120.00	105.20
11	T	95	DG	OP1-P-OP2	-6.73	109.51	119.60
11	T	74	DG	OP1-P-OP2	-6.72	109.51	119.60
11	T	96	DC	OP1-P-OP2	-6.72	109.51	119.60
7	H	20	DA	OP1-P-OP2	-6.72	109.52	119.60
7	H	104	DC	OP1-P-OP2	-6.72	109.52	119.60
11	T	29	DC	OP1-P-OP2	-6.72	109.52	119.60
7	H	209	DC	OP1-P-OP2	-6.72	109.53	119.60
7	H	212	DG	OP1-P-OP2	-6.72	109.53	119.60
11	T	116	DG	OP1-P-OP2	-6.72	109.53	119.60
7	H	193	DG	OP1-P-OP2	-6.71	109.53	119.60
11	T	123	DG	C5-C6-N1	6.71	114.86	111.50
7	H	42	DA	OP1-P-OP2	-6.71	109.53	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	129	DA	OP1-P-OP2	-6.71	109.53	119.60
11	T	36	DG	OP1-P-OP2	-6.71	109.53	119.60
7	H	25	DA	OP1-P-OP2	-6.71	109.54	119.60
11	T	104	DC	OP1-P-OP2	-6.70	109.54	119.60
11	T	167	DT	OP2-P-O3'	6.70	119.95	105.20
7	H	30	DA	OP1-P-OP2	-6.70	109.55	119.60
7	H	102	DC	OP1-P-OP2	-6.70	109.55	119.60
7	H	145	DG	OP1-P-OP2	-6.70	109.55	119.60
11	T	190	DG	OP1-P-OP2	-6.70	109.55	119.60
7	H	208	DA	OP1-P-OP2	-6.70	109.56	119.60
7	H	219	DG	OP1-P-OP2	-6.70	109.56	119.60
11	T	15	DC	OP1-P-OP2	-6.69	109.56	119.60
11	T	147	DC	OP1-P-OP2	-6.69	109.56	119.60
7	H	10	DG	OP1-P-OP2	-6.69	109.57	119.60
11	T	219	DA	OP1-P-OP2	-6.69	109.57	119.60
11	T	114	DC	OP1-P-OP2	-6.69	109.57	119.60
7	H	114	DC	OP1-P-OP2	-6.68	109.57	119.60
11	T	138	DA	OP1-P-OP2	-6.68	109.57	119.60
11	T	35	DC	OP1-P-OP2	-6.68	109.58	119.60
11	T	82	DC	OP1-P-OP2	-6.68	109.58	119.60
7	H	53	DA	OP1-P-OP2	-6.68	109.58	119.60
7	H	205	DC	OP1-P-OP2	-6.68	109.58	119.60
11	T	33	DG	OP1-P-OP2	-6.68	109.58	119.60
11	T	81	DA	OP1-P-OP2	-6.68	109.58	119.60
11	T	130	DA	OP1-P-OP2	-6.68	109.58	119.60
7	H	7	DA	OP1-P-OP2	-6.67	109.59	119.60
7	H	34	DA	OP1-P-OP2	-6.67	109.59	119.60
7	H	113	DG	OP1-P-OP2	-6.67	109.59	119.60
7	H	65	DC	OP1-P-OP2	-6.67	109.59	119.60
7	H	149	DA	OP1-P-OP2	-6.67	109.60	119.60
11	T	170	DC	OP1-P-OP2	-6.67	109.60	119.60
7	H	91	DG	OP1-P-OP2	-6.67	109.60	119.60
11	T	34	DC	OP1-P-OP2	-6.66	109.61	119.60
11	T	12	DG	OP1-P-OP2	-6.66	109.61	119.60
7	H	78	DG	OP1-P-OP2	-6.66	109.61	119.60
11	T	31	DC	OP1-P-OP2	-6.66	109.61	119.60
11	T	186	DG	OP1-P-OP2	-6.65	109.62	119.60
7	H	106	DG	C5-C6-N1	6.65	114.83	111.50
7	H	112	DA	OP1-P-OP2	-6.65	109.62	119.60
7	H	141	DA	OP1-P-OP2	-6.65	109.62	119.60
7	H	118	DT	OP1-P-O3'	6.65	119.83	105.20
7	H	38	DA	OP1-P-OP2	-6.65	109.63	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	73	DG	OP1-P-OP2	-6.64	109.64	119.60
7	H	196	DG	OP1-P-OP2	-6.64	109.64	119.60
7	H	168	DC	OP1-P-OP2	-6.64	109.64	119.60
11	T	84	DG	OP1-P-OP2	-6.64	109.64	119.60
7	H	71	DG	OP1-P-OP2	-6.64	109.64	119.60
7	H	54	DC	OP1-P-O3'	6.63	119.78	105.20
11	T	100	DA	OP1-P-OP2	-6.63	109.66	119.60
11	T	106	DC	OP1-P-OP2	-6.63	109.66	119.60
7	H	62	DG	OP1-P-OP2	-6.63	109.66	119.60
7	H	76	DG	OP1-P-OP2	-6.62	109.66	119.60
7	H	116	DC	OP1-P-OP2	-6.62	109.66	119.60
7	H	75	DA	OP1-P-OP2	-6.62	109.67	119.60
7	H	192	DG	OP1-P-OP2	-6.62	109.67	119.60
7	H	77	DG	OP1-P-OP2	-6.61	109.68	119.60
7	H	191	DC	OP1-P-OP2	-6.61	109.68	119.60
11	T	113	DG	OP1-P-OP2	-6.61	109.69	119.60
7	H	72	DA	OP1-P-OP2	-6.61	109.69	119.60
7	H	47	DG	OP1-P-O3'	6.61	119.73	105.20
7	H	117	DG	OP1-P-OP2	-6.60	109.70	119.60
11	T	191	DC	OP1-P-OP2	-6.60	109.70	119.60
7	H	195	DA	OP1-P-OP2	-6.60	109.70	119.60
11	T	177	DA	OP1-P-OP2	-6.60	109.71	119.60
11	T	188	DA	OP1-P-OP2	-6.59	109.71	119.60
7	H	132	DC	OP1-P-OP2	-6.59	109.71	119.60
7	H	140	DG	OP1-P-OP2	-6.59	109.71	119.60
7	H	130	DA	OP1-P-OP2	-6.59	109.71	119.60
7	H	155	DA	OP1-P-OP2	-6.59	109.72	119.60
11	T	139	DG	OP1-P-OP2	-6.57	109.74	119.60
11	T	146	DA	OP1-P-OP2	-6.57	109.74	119.60
11	T	103	DG	OP1-P-OP2	-6.57	109.75	119.60
11	T	159	DC	OP1-P-OP2	-6.57	109.75	119.60
7	H	45	DA	OP1-P-OP2	-6.56	109.75	119.60
7	H	66	DC	OP1-P-OP2	-6.56	109.76	119.60
11	T	63	DC	OP1-P-OP2	-6.55	109.77	119.60
11	T	85	DC	OP1-P-OP2	-6.55	109.78	119.60
7	H	73	DC	OP1-P-OP2	-6.54	109.79	119.60
7	H	197	DC	OP1-P-OP2	-6.54	109.79	119.60
7	H	50	DT	OP1-P-O3'	6.53	119.56	105.20
11	T	133	DC	OP1-P-OP2	-6.53	109.81	119.60
7	H	198	DG	OP1-P-OP2	-6.53	109.81	119.60
4	L	32	TYR	CB-CG-CD1	-6.52	117.09	121.00
11	T	124	DC	N3-C4-C5	6.51	124.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	147	DC	OP1-P-OP2	-6.51	109.83	119.60
7	H	153	DC	OP1-P-OP2	-6.51	109.84	119.60
11	T	48	DA	C4-C5-C6	-6.50	113.75	117.00
11	T	141	DG	OP1-P-OP2	-6.50	109.85	119.60
7	H	136	DG	OP1-P-OP2	-6.49	109.86	119.60
7	H	152	DA	OP1-P-OP2	-6.49	109.86	119.60
7	H	87	DC	OP1-P-OP2	-6.48	109.87	119.60
7	H	184	DC	N3-C4-C5	6.48	124.49	121.90
11	T	131	DA	OP1-P-OP2	-6.48	109.88	119.60
11	T	135	DC	OP1-P-OP2	-6.48	109.89	119.60
7	H	92	DG	OP1-P-OP2	-6.47	109.89	119.60
11	T	150	DC	OP1-P-OP2	-6.47	109.89	119.60
7	H	50	DT	OP1-P-OP2	-6.47	109.89	119.60
7	H	180	DC	N3-C2-O2	-6.46	117.38	121.90
11	T	143	DA	OP1-P-OP2	-6.46	109.91	119.60
11	T	93	DC	OP1-P-OP2	-6.46	109.91	119.60
11	T	70	DA	OP1-P-OP2	-6.45	109.92	119.60
7	H	101	DA	OP1-P-OP2	-6.45	109.93	119.60
11	T	79	DA	OP1-P-OP2	-6.45	109.93	119.60
11	T	153	DA	OP1-P-O3'	6.44	119.37	105.20
7	H	57	DG	OP1-P-OP2	-6.43	109.96	119.60
7	H	107	DG	O4'-C1'-C2'	6.43	111.04	105.90
11	T	76	DC	OP1-P-OP2	-6.43	109.96	119.60
7	H	120	DC	OP1-P-OP2	-6.42	109.97	119.60
7	H	124	DC	OP1-P-OP2	-6.41	109.98	119.60
7	H	154	DC	OP1-P-OP2	-6.41	109.98	119.60
11	T	92	DA	OP1-P-OP2	-6.41	109.99	119.60
11	T	45	DA	C5-C6-N1	6.40	120.90	117.70
7	H	178	DA	C4-C5-C6	-6.40	113.80	117.00
11	T	102	DC	OP1-P-OP2	-6.39	110.02	119.60
11	T	165	DC	OP1-P-OP2	-6.37	110.04	119.60
11	T	101	DA	OP1-P-OP2	-6.37	110.05	119.60
7	H	160	DA	OP1-P-OP2	-6.36	110.06	119.60
11	T	111	DG	OP1-P-OP2	-6.35	110.07	119.60
11	T	87	DC	OP1-P-OP2	-6.34	110.09	119.60
11	T	171	DA	OP1-P-OP2	-6.34	110.10	119.60
11	T	164	DA	OP1-P-OP2	-6.33	110.10	119.60
1	B	535	ARG	NE-CZ-NH2	6.33	123.46	120.30
11	T	142	DG	OP1-P-OP2	-6.31	110.13	119.60
11	T	119	DC	OP1-P-OP2	-6.31	110.13	119.60
11	T	162	DG	OP1-P-OP2	-6.29	110.16	119.60
7	H	123	DG	OP1-P-OP2	-6.29	110.16	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	112	DC	OP1-P-OP2	-6.27	110.19	119.60
11	T	121	DC	OP1-P-OP2	-6.26	110.20	119.60
11	T	69	DT	OP1-P-O3'	6.26	118.97	105.20
1	G	427	ARG	NE-CZ-NH2	6.25	123.43	120.30
7	H	163	DG	OP1-P-OP2	-6.24	110.24	119.60
7	H	81	DT	OP1-P-O3'	6.24	118.92	105.20
11	T	168	DG	O5'-P-OP1	-6.22	100.11	105.70
7	H	199	DC	OP1-P-O3'	6.21	118.86	105.20
7	H	43	DG	OP1-P-O3'	6.18	118.80	105.20
11	T	122	DC	C4'-C3'-C2'	-6.18	97.54	103.10
11	T	81	DA	OP1-P-O3'	6.17	118.76	105.20
7	H	164	DG	OP1-P-O3'	6.15	118.72	105.20
11	T	58	DC	N3-C2-O2	-6.14	117.60	121.90
11	T	174	DT	OP1-P-O3'	6.14	118.71	105.20
11	T	106	DC	OP1-P-O3'	6.14	118.70	105.20
11	T	61	DG	OP1-P-OP2	-6.12	110.43	119.60
7	H	155	DA	OP1-P-O3'	6.11	118.63	105.20
7	H	185	DA	C4-C5-C6	-6.09	113.96	117.00
6	A	42	ARG	NE-CZ-NH1	-6.07	117.26	120.30
7	H	64	DG	OP1-P-O3'	6.05	118.52	105.20
11	T	125	DG	OP1-P-OP2	-6.05	110.52	119.60
11	T	90	DG	OP1-P-OP2	-6.05	110.53	119.60
7	H	114	DC	OP1-P-O3'	6.03	118.47	105.20
11	T	35	DC	OP1-P-O3'	6.03	118.47	105.20
11	T	113	DG	OP1-P-O3'	6.02	118.45	105.20
7	H	130	DA	OP1-P-O3'	6.02	118.45	105.20
11	T	183	DC	OP1-P-O3'	6.02	118.44	105.20
11	T	179	DA	OP1-P-O3'	6.02	118.44	105.20
11	T	148	DC	OP1-P-O3'	6.01	118.43	105.20
11	T	165	DC	OP1-P-O3'	6.01	118.42	105.20
11	T	41	DC	N3-C2-O2	-6.00	117.70	121.90
7	H	173	DC	N3-C4-C5	5.99	124.30	121.90
7	H	138	DT	OP1-P-O3'	5.97	118.33	105.20
7	H	184	DC	N3-C2-O2	-5.96	117.73	121.90
7	H	158	DG	OP1-P-O3'	5.96	118.31	105.20
7	H	200	DA	OP1-P-O3'	5.95	118.30	105.20
7	H	45	DA	OP1-P-O3'	5.95	118.29	105.20
11	T	27	DT	OP1-P-O3'	5.95	118.28	105.20
7	H	142	DG	OP1-P-O3'	5.94	118.27	105.20
7	H	60	DA	OP1-P-O3'	5.93	118.25	105.20
7	H	124	DC	OP1-P-O3'	5.93	118.24	105.20
7	H	171	DC	N3-C2-O2	-5.93	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	63	DT	OP1-P-O3'	5.92	118.21	105.20
7	H	110	DA	OP1-P-OP2	-5.91	110.73	119.60
11	T	55	DT	C6-C5-C7	-5.90	119.36	122.90
7	H	97	DT	OP1-P-O3'	5.90	118.17	105.20
7	H	172	DA	N1-C6-N6	-5.89	115.06	118.60
7	H	136	DG	OP1-P-O3'	5.87	118.11	105.20
11	T	132	DC	OP1-P-O3'	5.86	118.10	105.20
11	T	88	DC	OP1-P-O3'	5.86	118.09	105.20
11	T	162	DG	OP1-P-O3'	5.85	118.08	105.20
7	H	39	DT	OP1-P-O3'	5.85	118.06	105.20
11	T	58	DC	N3-C4-C5	5.85	124.24	121.90
11	T	91	DC	OP1-P-OP2	-5.84	110.84	119.60
7	H	148	DT	OP1-P-O3'	5.84	118.05	105.20
7	H	193	DG	OP1-P-O3'	5.83	118.03	105.20
7	H	46	DT	OP1-P-O3'	5.82	118.01	105.20
1	G	486	ARG	NE-CZ-NH2	5.82	123.21	120.30
7	H	78	DG	OP1-P-O3'	5.81	117.98	105.20
11	T	176	DT	OP1-P-O3'	5.80	117.97	105.20
7	H	140	DG	OP1-P-O3'	5.79	117.94	105.20
7	H	11	DG	OP1-P-O3'	5.79	117.94	105.20
9	R	77	ARG	NE-CZ-NH2	5.79	123.19	120.30
11	T	28	DG	OP1-P-O3'	5.78	117.92	105.20
11	T	103	DG	OP1-P-O3'	5.78	117.92	105.20
11	T	199	DT	OP1-P-O3'	5.78	117.92	105.20
7	H	90	DT	OP1-P-O3'	5.77	117.89	105.20
7	H	27	DG	OP1-P-O3'	5.77	117.89	105.20
7	H	8	DT	OP1-P-O3'	5.76	117.87	105.20
11	T	139	DG	OP1-P-O3'	5.76	117.87	105.20
7	H	192	DG	OP1-P-O3'	5.75	117.86	105.20
7	H	103	DG	OP1-P-O3'	5.75	117.85	105.20
7	H	48	DT	OP1-P-O3'	5.75	117.84	105.20
11	T	64	DC	OP1-P-O3'	5.75	117.84	105.20
11	T	31	DC	OP1-P-O3'	5.74	117.83	105.20
11	T	51	DC	N1-C2-O2	5.74	122.34	118.90
11	T	10	DG	OP1-P-O3'	5.73	117.80	105.20
7	H	173	DC	N3-C2-O2	-5.72	117.89	121.90
11	T	42	DC	N3-C4-C5	5.72	124.19	121.90
11	T	189	DC	OP1-P-O3'	5.72	117.78	105.20
7	H	84	DC	OP1-P-O3'	5.72	117.78	105.20
7	H	42	DA	OP1-P-O3'	5.71	117.76	105.20
7	H	12	DG	OP1-P-O3'	5.71	117.75	105.20
7	H	31	DT	OP1-P-O3'	5.70	117.74	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	124	DC	N3-C4-N4	-5.70	114.01	118.00
7	H	132	DC	OP1-P-O3'	5.69	117.72	105.20
11	T	169	DC	OP1-P-O3'	5.69	117.72	105.20
7	H	61	DC	OP1-P-O3'	5.68	117.70	105.20
7	H	191	DC	OP1-P-O3'	5.68	117.69	105.20
7	H	26	DT	OP1-P-O3'	5.68	117.69	105.20
7	H	152	DA	OP1-P-O3'	5.66	117.66	105.20
7	H	217	DC	OP1-P-O3'	5.66	117.66	105.20
7	H	29	DC	OP1-P-O3'	5.66	117.65	105.20
11	T	182	DT	OP1-P-O3'	5.65	117.62	105.20
7	H	214	DA	OP1-P-O3'	5.65	117.62	105.20
7	H	82	DA	OP1-P-O3'	5.64	117.62	105.20
7	H	179	DT	C5-C6-N1	-5.64	120.32	123.70
7	H	178	DA	N1-C6-N6	-5.64	115.22	118.60
11	T	49	DT	C6-C5-C7	-5.64	119.52	122.90
11	T	185	DC	OP1-P-O3'	5.63	117.59	105.20
11	T	61	DG	OP1-P-O3'	5.63	117.58	105.20
7	H	101	DA	OP1-P-O3'	5.62	117.56	105.20
11	T	129	DT	OP1-P-O3'	5.62	117.55	105.20
11	T	195	DC	OP1-P-O3'	5.61	117.54	105.20
7	H	13	DA	OP1-P-O3'	5.61	117.53	105.20
11	T	17	DC	OP1-P-O3'	5.61	117.53	105.20
11	T	21	DA	OP1-P-O3'	5.61	117.53	105.20
11	T	29	DC	OP1-P-O3'	5.61	117.53	105.20
7	H	28	DA	OP1-P-O3'	5.60	117.52	105.20
11	T	23	DA	OP1-P-O3'	5.60	117.51	105.20
11	T	9	DT	OP1-P-O3'	5.59	117.51	105.20
7	H	14	DG	OP1-P-O3'	5.59	117.50	105.20
7	H	180	DC	N3-C4-C5	5.59	124.14	121.90
11	T	84	DG	OP1-P-O3'	5.59	117.50	105.20
11	T	160	DA	OP1-P-O3'	5.59	117.50	105.20
11	T	194	DG	OP1-P-O3'	5.59	117.50	105.20
7	H	76	DG	OP1-P-O3'	5.59	117.49	105.20
7	H	57	DG	OP1-P-O3'	5.59	117.49	105.20
11	T	173	DA	OP1-P-OP2	-5.58	111.22	119.60
7	H	99	DA	OP1-P-O3'	5.58	117.48	105.20
7	H	71	DG	OP1-P-O3'	5.58	117.47	105.20
11	T	6	DG	OP1-P-O3'	5.58	117.47	105.20
5	M	173	ARG	NE-CZ-NH2	5.57	123.09	120.30
7	H	15	DC	OP1-P-O3'	5.57	117.46	105.20
7	H	116	DC	OP1-P-O3'	5.57	117.44	105.20
7	H	41	DC	OP1-P-O3'	5.55	117.42	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	74	DT	OP1-P-O3'	5.55	117.42	105.20
7	H	32	DG	OP1-P-O3'	5.55	117.41	105.20
7	H	75	DA	OP1-P-O3'	5.55	117.41	105.20
11	T	25	DG	OP1-P-O3'	5.54	117.40	105.20
11	T	14	DG	OP1-P-O3'	5.54	117.39	105.20
7	H	181	DC	N3-C2-O2	-5.54	118.02	121.90
11	T	178	DT	OP1-P-O3'	5.54	117.38	105.20
7	H	10	DG	OP1-P-O3'	5.54	117.38	105.20
2	I	561	ARG	NE-CZ-NH2	5.53	123.07	120.30
7	H	16	DT	OP1-P-O3'	5.53	117.36	105.20
7	H	119	DA	OP1-P-O3'	5.53	117.36	105.20
7	H	190	DC	OP1-P-O3'	5.53	117.36	105.20
7	H	172	DA	C4-C5-C6	-5.53	114.24	117.00
7	H	220	DT	OP1-P-O3'	5.52	117.35	105.20
7	H	112	DA	OP1-P-O3'	5.52	117.34	105.20
11	T	190	DG	OP1-P-O3'	5.52	117.34	105.20
7	H	65	DC	OP1-P-O3'	5.52	117.34	105.20
7	H	218	DA	OP1-P-O3'	5.51	117.33	105.20
11	T	135	DC	OP1-P-O3'	5.51	117.33	105.20
6	A	42	ARG	NE-CZ-NH2	5.51	123.06	120.30
7	H	165	DC	OP1-P-O3'	5.51	117.32	105.20
11	T	136	DC	OP1-P-O3'	5.50	117.31	105.20
7	H	94	DG	OP1-P-O3'	5.50	117.31	105.20
7	H	208	DA	OP1-P-O3'	5.50	117.30	105.20
11	T	218	DG	OP1-P-O3'	5.50	117.30	105.20
7	H	111	DC	OP1-P-O3'	5.50	117.30	105.20
11	T	197	DC	OP1-P-O3'	5.50	117.30	105.20
7	H	86	DC	O5'-P-OP2	5.50	117.30	110.70
7	H	204	DC	OP1-P-O3'	5.50	117.29	105.20
11	T	105	DA	OP1-P-O3'	5.50	117.29	105.20
7	H	212	DG	OP1-P-O3'	5.49	117.28	105.20
7	H	215	DC	OP1-P-O3'	5.49	117.29	105.20
11	T	94	DC	OP1-P-O3'	5.49	117.28	105.20
7	H	180	DC	N1-C2-O2	5.49	122.19	118.90
7	H	17	DC	OP1-P-O3'	5.48	117.25	105.20
11	T	92	DA	OP1-P-O3'	5.48	117.25	105.20
11	T	63	DC	OP1-P-O3'	5.47	117.22	105.20
11	T	80	DG	OP1-P-O3'	5.46	117.22	105.20
11	T	20	DC	OP1-P-O3'	5.46	117.21	105.20
7	H	181	DC	N3-C4-C5	5.46	124.08	121.90
11	T	52	DC	N1-C2-O2	5.46	122.17	118.90
11	T	60	DA	OP1-P-OP2	-5.45	111.42	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	209	DG	OP1-P-O3'	5.45	117.18	105.20
7	H	21	DC	OP1-P-O3'	5.44	117.17	105.20
7	H	211	DG	OP1-P-O3'	5.44	117.17	105.20
11	T	138	DA	OP1-P-O3'	5.43	117.16	105.20
11	T	22	DG	OP1-P-O3'	5.43	117.14	105.20
7	H	201	DG	OP1-P-O3'	5.42	117.13	105.20
11	T	210	DG	OP1-P-O3'	5.42	117.13	105.20
7	H	184	DC	C2-N3-C4	-5.42	117.19	119.90
7	H	9	DC	OP1-P-O3'	5.42	117.12	105.20
7	H	141	DA	OP1-P-O3'	5.41	117.11	105.20
11	T	78	DT	OP2-P-O3'	5.41	117.11	105.20
7	H	202	DC	OP1-P-O3'	5.41	117.10	105.20
7	H	35	DT	OP1-P-O3'	5.40	117.09	105.20
7	H	120	DC	OP1-P-O3'	5.40	117.09	105.20
7	H	52	DT	OP1-P-O3'	5.40	117.08	105.20
7	H	194	DC	OP1-P-O3'	5.40	117.08	105.20
11	T	124	DC	N1-C2-O2	5.40	122.14	118.90
7	H	135	DT	OP1-P-O3'	5.40	117.07	105.20
11	T	52	DC	N3-C4-C5	5.40	124.06	121.90
11	T	155	DT	OP1-P-O3'	5.40	117.07	105.20
7	H	196	DG	OP1-P-O3'	5.39	117.07	105.20
11	T	208	DC	OP1-P-O3'	5.39	117.06	105.20
7	H	167	DT	OP1-P-O3'	5.39	117.06	105.20
7	H	213	DC	OP1-P-O3'	5.38	117.03	105.20
7	H	179	DT	C6-C5-C7	-5.38	119.67	122.90
11	T	149	DC	OP1-P-O3'	5.38	117.03	105.20
11	T	203	DT	OP1-P-O3'	5.37	117.02	105.20
7	H	25	DA	OP1-P-O3'	5.37	117.01	105.20
11	T	53	DG	N3-C2-N2	-5.37	116.14	119.90
7	H	113	DG	OP1-P-O3'	5.36	117.00	105.20
11	T	158	DC	OP1-P-O3'	5.36	116.99	105.20
7	H	122	DT	OP1-P-O3'	5.36	116.99	105.20
11	T	13	DT	OP1-P-O3'	5.35	116.97	105.20
11	T	11	DT	OP1-P-O3'	5.35	116.97	105.20
11	T	215	DC	OP1-P-O3'	5.35	116.97	105.20
7	H	24	DA	OP1-P-O3'	5.35	116.96	105.20
7	H	144	DT	OP1-P-O3'	5.34	116.95	105.20
11	T	51	DC	C5'-C4'-C3'	-5.34	104.48	114.10
11	T	112	DC	OP1-P-O3'	5.34	116.95	105.20
11	T	211	DA	OP1-P-O3'	5.33	116.94	105.20
11	T	54	DG	C6-N1-C2	-5.33	121.90	125.10
11	T	200	DC	OP1-P-O3'	5.33	116.93	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	212	DG	OP1-P-O3'	5.32	116.91	105.20
7	H	206	DT	OP1-P-O3'	5.31	116.89	105.20
11	T	24	DC	OP1-P-O3'	5.31	116.89	105.20
11	T	32	DC	OP1-P-O3'	5.31	116.88	105.20
11	T	83	DA	OP1-P-O3'	5.31	116.88	105.20
11	T	48	DA	N1-C6-N6	-5.31	115.42	118.60
7	H	23	DG	OP1-P-O3'	5.30	116.86	105.20
8	J	45	ARG	NE-CZ-NH2	5.30	122.95	120.30
7	H	216	DA	OP1-P-O3'	5.30	116.86	105.20
7	H	20	DA	OP1-P-O3'	5.30	116.86	105.20
7	H	186	DG	N1-C6-O6	-5.29	116.73	119.90
7	H	207	DG	OP1-P-O3'	5.29	116.83	105.20
11	T	18	DG	OP1-P-O3'	5.29	116.83	105.20
11	T	95	DG	OP1-P-O3'	5.29	116.83	105.20
11	T	193	DC	OP1-P-O3'	5.28	116.82	105.20
7	H	36	DG	OP1-P-O3'	5.28	116.82	105.20
11	T	207	DT	OP1-P-O3'	5.28	116.81	105.20
11	T	12	DG	OP1-P-O3'	5.27	116.80	105.20
11	T	187	DT	OP1-P-O3'	5.27	116.80	105.20
7	H	86	DC	OP1-P-O3'	5.27	116.80	105.20
11	T	58	DC	N1-C2-O2	5.27	122.06	118.90
7	H	197	DC	OP1-P-O3'	5.27	116.79	105.20
11	T	214	DT	OP1-P-O3'	5.27	116.78	105.20
7	H	153	DC	OP1-P-O3'	5.25	116.76	105.20
7	H	209	DC	OP1-P-O3'	5.25	116.76	105.20
11	T	7	DA	OP1-P-O3'	5.25	116.76	105.20
7	H	18	DC	OP1-P-O3'	5.25	116.75	105.20
7	H	91	DG	OP1-P-O3'	5.25	116.74	105.20
11	T	15	DC	OP1-P-O3'	5.24	116.74	105.20
2	I	583	ARG	NE-CZ-NH2	5.24	122.92	120.30
6	A	53	ARG	NE-CZ-NH2	5.24	122.92	120.30
11	T	55	DT	N3-C2-O2	-5.24	119.16	122.30
7	H	151	DG	OP1-P-O3'	5.23	116.71	105.20
7	H	195	DA	OP1-P-O3'	5.23	116.70	105.20
7	H	210	DG	OP1-P-O3'	5.22	116.68	105.20
11	T	26	DC	OP1-P-O3'	5.22	116.68	105.20
11	T	16	DC	OP1-P-O3'	5.21	116.67	105.20
11	T	102	DC	OP1-P-O3'	5.21	116.65	105.20
7	H	123	DG	OP1-P-O3'	5.20	116.65	105.20
11	T	191	DC	OP1-P-O3'	5.20	116.64	105.20
11	T	19	DT	OP1-P-O3'	5.19	116.62	105.20
7	H	40	DA	OP1-P-O3'	5.19	116.61	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	205	DG	OP1-P-O3'	5.18	116.59	105.20
7	H	146	DC	OP1-P-O3'	5.17	116.58	105.20
7	H	19	DG	OP1-P-O3'	5.17	116.58	105.20
11	T	120	DC	OP1-P-O3'	5.17	116.56	105.20
11	T	217	DC	OP1-P-O3'	5.15	116.53	105.20
11	T	53	DG	N1-C6-O6	-5.14	116.81	119.90
11	T	34	DC	OP1-P-O3'	5.12	116.47	105.20
7	H	22	DC	OP1-P-O3'	5.11	116.45	105.20
11	T	62	DG	OP1-P-O3'	5.11	116.45	105.20
11	T	140	DG	OP1-P-O3'	5.10	116.43	105.20
11	T	146	DA	OP1-P-O3'	5.09	116.41	105.20
7	H	33	DC	OP1-P-O3'	5.09	116.40	105.20
11	T	180	DC	OP1-P-O3'	5.09	116.40	105.20
11	T	73	DG	OP1-P-O3'	5.09	116.40	105.20
11	T	54	DG	N1-C2-N3	5.08	126.95	123.90
7	H	154	DC	OP1-P-O3'	5.08	116.37	105.20
11	T	91	DC	OP1-P-O3'	5.08	116.37	105.20
7	H	178	DA	C5-N7-C8	-5.06	101.37	103.90
7	H	79	DA	OP1-P-O3'	5.05	116.32	105.20
7	H	129	DA	OP1-P-O3'	5.05	116.32	105.20
11	T	117	DT	OP1-P-O3'	5.05	116.32	105.20
11	T	38	DC	C4'-C3'-C2'	-5.05	98.56	103.10
11	T	72	DT	OP1-P-O3'	5.05	116.30	105.20
11	T	38	DC	C1'-O4'-C4'	-5.04	105.06	110.10
11	T	204	DC	OP1-P-O3'	5.04	116.28	105.20
7	H	98	DA	OP1-P-O3'	5.02	116.25	105.20
11	T	45	DA	C4-C5-C6	-5.02	114.49	117.00
11	T	145	DT	OP1-P-O3'	5.01	116.22	105.20
7	H	177	DG	N1-C6-O6	-5.01	116.90	119.90
7	H	159	DG	OP1-P-O3'	5.00	116.21	105.20
7	H	188	DC	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	42	ARG	Sidechain
1	B	461	TYR	Sidechain
1	B	532	ARG	Sidechain
7	H	169	DG	Sidechain
7	H	173	DC	Sidechain
7	H	186	DG	Sidechain

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Mol	Chain	Res	Type	Group
4	L	32	TYR	Sidechain
11	T	122	DC	Sidechain
11	T	40	DG	Sidechain
11	T	43	DG	Sidechain
11	T	46	DG	Sidechain
11	T	57	DC	Sidechain

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	B	3665	0	3649	218	0
1	G	3665	0	3649	275	0
2	C	4304	0	4176	224	0
2	I	4863	0	4751	300	0
3	F	2930	0	2837	172	0
3	K	2930	0	2839	319	0
4	L	3139	0	2986	199	0
4	O	3139	0	2986	250	0
5	M	1047	0	1102	72	0
5	Y	1047	0	1102	87	0
6	A	939	0	995	35	0
6	W	817	0	858	44	0
7	H	4421	0	2399	95	0
8	J	661	0	709	32	0
8	X	702	0	755	43	0
9	R	829	0	887	41	0
9	U	829	0	887	54	0
10	S	752	0	775	33	0
10	V	741	0	762	30	0
11	T	4372	0	2392	87	0
12	E	67	0	32	3	0
13	C	26	0	19	1	0
13	I	26	0	19	4	0
All	All	45911	0	41566	2272	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 27.

All (2272) 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)
2:I:101:LEU:HB3	3:K:173:ARG:HH12	1.30	0.94
3:K:145:GLU:HG2	3:K:168:SER:HB2	1.50	0.93
1:G:450:CYS:HB3	1:G:455:LEU:H	1.37	0.89
3:K:147:PHE:HA	3:K:167:GLY:HA3	1.55	0.88
4:O:334:ALA:HB1	4:O:342:LEU:HD21	1.56	0.86
3:F:215:LEU:HB3	3:F:229:PHE:HB2	1.59	0.84
3:K:193:ILE:HD13	3:K:210:SER:HB3	1.59	0.84
1:G:626:PHE:HD1	1:G:631:GLN:HG2	1.43	0.83
4:O:32:TYR:HH	4:O:370:HIS:HD1	1.26	0.83
6:W:79:LYS:HG3	6:W:80:THR:H	1.44	0.83
2:I:646:TYR:HB3	2:I:713:ILE:HG23	1.60	0.83
2:I:129:HIS:HA	2:I:158:HIS:HB2	1.61	0.82
1:B:499:TYR:HA	4:L:18:ASN:HD21	1.42	0.82
1:G:521:LYS:HD3	1:G:577:GLN:HG3	1.62	0.82
1:B:105:LEU:HD23	5:M:269:LEU:HD12	1.62	0.82
3:K:197:LYS:HZ3	3:K:244:TYR:HB2	1.44	0.82
1:B:432:PHE:HB2	1:B:440:GLN:HB3	1.62	0.82
4:O:292:GLY:HA2	4:O:298:VAL:HA	1.60	0.82
3:F:216:ARG:HD2	3:F:225:LEU:HD11	1.61	0.81
1:B:626:PHE:HB3	1:B:631:GLN:HB3	1.63	0.81
2:C:586:ASP:HB3	2:C:589:LEU:HG	1.61	0.81
4:O:79:LEU:HB3	4:O:121:ILE:HB	1.61	0.80
1:B:478:TYR:H	1:B:547:GLU:HG3	1.46	0.80
2:I:289:CYS:HB2	2:I:297:HIS:HE1	1.46	0.80
4:L:188:ASN:HB2	4:L:240:GLU:HB3	1.63	0.80
1:B:319:MET:HB2	1:B:353:PRO:HB2	1.65	0.79
3:F:101:PHE:HE1	3:F:111:LEU:HB3	1.46	0.78
1:G:495:TYR:O	5:Y:185:ARG:NH1	2.17	0.78
2:C:60:TRP:NE1	3:F:105:SER:O	2.16	0.78
2:C:584:GLU:HG2	2:C:608:ASN:HD22	1.46	0.78
1:B:505:ASP:HA	1:B:508:ARG:HE	1.48	0.78
5:Y:185:ARG:HG3	5:Y:187:HIS:H	1.49	0.78
2:I:664:ASP:OD2	2:I:741:TYR:OH	2.02	0.77
2:I:331:GLN:O	2:I:469:ARG:NH1	2.17	0.77
1:G:187:LEU:HD21	1:G:205:GLN:HB3	1.65	0.77
7:H:84:DC:H42	11:T:143:DA:H61	1.32	0.77
2:I:694:HIS:CE1	2:I:730:ASP:HA	2.19	0.76
2:C:273:GLN:HE22	2:C:275:GLU:HB2	1.51	0.76
2:I:697:ASN:O	2:I:719:ARG:NH1	2.19	0.76
3:K:320:LEU:HD23	3:K:330:CYS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:77:ASN:ND2	4:O:125:GLY:O	2.17	0.76
1:B:645:GLN:HG3	1:B:649:LYS:HE3	1.66	0.76
2:C:699:ASN:ND2	2:C:726:GLU:O	2.19	0.76
1:G:654:ARG:HH11	2:I:444:MET:HE1	1.51	0.76
2:C:324:PRO:HA	2:C:329:CYS:HB3	1.68	0.75
4:L:122:ASN:HB2	4:L:167:CYS:HB3	1.68	0.75
1:G:443:GLU:O	1:G:445:ARG:NH2	2.19	0.75
2:C:674:LEU:H	2:C:679:VAL:HA	1.51	0.75
4:L:342:LEU:HB2	4:L:370:HIS:HB3	1.68	0.75
2:C:448:LEU:HB3	2:C:459:ILE:HG12	1.68	0.75
4:O:32:TYR:OH	4:O:370:HIS:ND1	2.20	0.75
5:M:227:ILE:HD11	5:M:242:HIS:HB2	1.68	0.74
3:F:360:GLN:HE22	3:F:382:GLN:HB3	1.52	0.74
4:L:253:MET:HE3	4:L:255:TRP:HE1	1.51	0.74
1:G:109:ILE:HG12	4:O:341:ARG:HH12	1.53	0.74
1:G:436:ASN:O	1:G:439:ARG:NH2	2.18	0.74
7:H:161:DG:OP1	10:S:37:TYR:OH	2.06	0.74
2:C:645:GLU:O	2:C:687:ASN:ND2	2.20	0.74
1:G:493:GLU:O	5:Y:185:ARG:NH2	2.21	0.74
2:I:329:CYS:HA	2:I:468:CYS:HB3	1.68	0.74
3:K:427:ALA:N	3:K:435:TRP:O	2.16	0.74
1:G:113:ARG:NH1	4:O:363:PRO:O	2.17	0.74
1:B:450:CYS:SG	1:B:471:HIS:NE2	2.60	0.74
4:O:298:VAL:HB	4:O:313:PHE:HB2	1.70	0.74
7:H:130:DA:OP1	6:W:69:ARG:NH1	2.21	0.73
3:K:191:ASN:N	3:K:212:ASP:OD1	2.19	0.73
1:G:251:LEU:HB3	1:G:253:ARG:HH22	1.52	0.73
1:G:629:ASP:O	1:G:633:ASN:ND2	2.21	0.73
3:K:312:VAL:HG22	3:K:321:SER:HA	1.69	0.73
8:J:29:ILE:HD12	8:J:34:ILE:HD11	1.70	0.73
1:G:526:THR:OG1	4:O:38:HIS:ND1	2.18	0.73
2:I:101:LEU:HB3	3:K:173:ARG:NH1	2.04	0.73
2:C:330:TYR:HE2	2:C:473:GLU:HG2	1.53	0.73
3:K:194:ASN:ND2	3:K:239:VAL:O	2.21	0.73
2:I:643:ILE:HB	2:I:715:ILE:HB	1.71	0.73
3:K:332:LYS:HD3	3:K:336:MET:HA	1.71	0.73
2:C:87:SER:HA	3:F:88:LEU:HA	1.69	0.72
10:S:73:GLU:OE1	8:X:92:ARG:NH1	2.22	0.72
1:G:663:MET:HG3	1:G:668:LEU:HD12	1.70	0.72
4:O:46:THR:HG21	4:O:129:ARG:HA	1.71	0.72
4:O:81:ILE:HB	4:O:119:ILE:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:403:GLN:NE2	4:O:404:MET:O	2.22	0.72
4:O:93:PHE:HB2	5:Y:171:LYS:HD3	1.69	0.72
2:C:698:PRO:O	2:C:719:ARG:NH1	2.22	0.72
3:K:119:ASN:HB2	3:K:140:ASP:HB3	1.72	0.72
2:I:682:ALA:O	2:I:690:ARG:NH1	2.22	0.72
2:C:174:LEU:HA	2:C:178:LEU:HB2	1.70	0.72
3:K:239:VAL:HA	3:K:255:GLY:HA3	1.71	0.72
4:L:40:LEU:HD21	4:L:399:MET:HB2	1.70	0.71
1:G:502:ASN:ND2	1:G:504:GLN:OE1	2.23	0.71
4:L:257:THR:HG22	4:L:258:ARG:H	1.55	0.71
7:H:121:DG:H5'	8:X:45:ARG:HD2	1.71	0.71
6:W:64:LYS:NZ	6:W:93:GLN:OE1	2.21	0.71
1:B:315:TYR:O	1:B:356:GLN:NE2	2.24	0.71
4:L:149:VAL:HB	4:L:173:LEU:HB2	1.72	0.71
7:H:120:DC:H4'	8:X:45:ARG:HE	1.55	0.71
2:I:289:CYS:HB2	2:I:297:HIS:CE1	2.26	0.71
2:I:61:LYS:O	3:K:106:LYS:NZ	2.24	0.71
1:G:510:PRO:HD3	3:K:185:HIS:CD2	2.24	0.71
3:K:189:HIS:HA	3:K:216:ARG:HH12	1.55	0.71
4:O:180:GLY:HA3	4:O:197:SER:HA	1.73	0.71
2:I:584:GLU:OE2	2:I:611:ILE:N	2.23	0.71
1:G:450:CYS:SG	1:G:453:CYS:N	2.63	0.71
5:Y:206:ASN:O	5:Y:210:HIS:N	2.21	0.71
9:U:112:GLN:HB2	9:U:115:LEU:HD23	1.73	0.71
5:Y:180:ARG:HG3	5:Y:183:LEU:HG	1.72	0.71
2:I:314:LYS:HE2	2:I:489:ASP:HB3	1.73	0.71
9:R:85:LEU:O	9:R:89:ASN:ND2	2.24	0.70
4:O:382:TRP:HB3	4:O:390:ILE:HG13	1.73	0.70
4:L:375:ALA:HB1	4:L:395:GLU:HG2	1.72	0.70
1:B:183:THR:OG1	1:B:211:LYS:O	2.09	0.70
3:K:194:ASN:ND2	3:K:238:GLU:OE2	2.24	0.70
3:K:330:CYS:SG	3:K:331:TRP:N	2.64	0.70
4:O:333:LEU:HB3	4:O:345:TRP:HB2	1.73	0.70
1:G:311:LEU:HD12	1:G:313:GLY:H	1.55	0.70
2:I:278:LEU:HB3	2:I:282:HIS:HE1	1.55	0.70
3:K:380:GLY:HA2	3:K:386:LEU:HA	1.73	0.70
4:O:56:PRO:HD2	4:O:62:SER:HA	1.73	0.70
1:B:360:ARG:NH2	1:B:362:THR:OG1	2.25	0.69
3:F:339:ASP:H	3:F:342:LYS:HE2	1.57	0.69
1:G:436:ASN:HA	1:G:439:ARG:HD2	1.73	0.69
1:B:590:GLU:HA	1:B:593:ARG:HE	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:622:ALA:O	2:C:630:GLY:N	2.24	0.69
6:A:72:ARG:NH1	7:H:90:DT:OP2	2.23	0.69
9:U:26:PRO:HG3	10:V:37:TYR:CE2	2.27	0.69
2:C:114:SER:HB3	3:F:232:VAL:HB	1.75	0.69
3:F:86:ASN:ND2	3:F:130:GLY:O	2.25	0.69
2:I:701:TYR:CD1	2:I:703:LYS:HE3	2.27	0.69
2:I:321:ASP:HB3	2:I:323:LYS:HE2	1.73	0.69
3:F:382:GLN:NE2	3:F:411:ALA:O	2.26	0.69
3:K:153:THR:HB	3:K:162:LEU:HB2	1.74	0.69
4:O:344:VAL:HG12	4:O:367:LEU:HB3	1.73	0.69
1:B:593:ARG:HG2	1:B:619:LEU:HD22	1.75	0.69
7:H:162:DC:H5"	10:S:30:ARG:HE	1.57	0.69
9:R:42:ARG:HB2	10:S:85:THR:HG22	1.73	0.69
6:W:83:ARG:HB2	8:X:80:THR:HG22	1.75	0.69
1:G:621:VAL:O	1:G:625:GLY:N	2.26	0.69
3:F:81:SER:HB3	3:F:440:LEU:HB2	1.74	0.69
8:J:51:TYR:HB3	8:J:55:ARG:HH22	1.57	0.69
2:I:693:ASN:OD1	13:I:801:SAH:N7	2.25	0.69
3:K:189:HIS:HA	3:K:216:ARG:NH1	2.08	0.69
2:C:242:GLU:HA	2:C:245:LYS:HD2	1.75	0.69
1:B:297:ALA:HB2	1:B:319:MET:HA	1.74	0.68
1:G:192:CYS:HA	1:G:246:LYS:H	1.58	0.68
1:G:603:PHE:O	1:G:611:LYS:NZ	2.24	0.68
2:I:656:ALA:O	2:I:660:GLY:N	2.21	0.68
3:K:312:VAL:O	3:K:313:ARG:NH2	2.27	0.68
3:K:360:GLN:OE1	3:K:385:LYS:NZ	2.20	0.68
1:B:311:LEU:O	1:B:315:TYR:OH	2.10	0.68
1:G:476:PHE:HA	1:G:489:VAL:HG12	1.74	0.68
1:G:672:MET:SD	1:G:673:SER:OG	2.49	0.68
1:G:252:PHE:HB2	1:G:297:ALA:HB3	1.75	0.68
1:G:563:ARG:NH2	2:I:623:PRO:O	2.26	0.68
1:B:162:THR:HG22	1:B:163:GLY:H	1.58	0.68
5:M:238:LYS:HB3	5:M:253:TRP:HB3	1.75	0.68
11:T:172:DG:OP1	9:U:77:ARG:NH1	2.26	0.68
2:I:229:SER:OG	2:I:230:MET:SD	2.50	0.68
3:K:184:LYS:HB3	3:K:186:TYR:CE2	2.29	0.68
4:L:187:PRO:HG3	4:L:237:LEU:HA	1.75	0.68
1:B:525:ILE:H	4:L:39:ALA:HB3	1.59	0.68
4:L:133:MET:SD	4:L:136:ASN:N	2.67	0.68
3:K:149:THR:O	3:K:166:ALA:N	2.26	0.68
5:Y:270:SER:OG	5:Y:271:LYS:NZ	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:HIS:HB3	1:B:158:GLN:HE22	1.59	0.68
4:O:130:ALA:O	4:O:131:ARG:NH2	2.27	0.68
4:O:290:ALA:HA	4:O:300:LEU:HA	1.76	0.67
4:O:349:LYS:HG2	4:O:364:PRO:HB2	1.76	0.67
9:R:84:GLN:HB2	9:R:102:ILE:HD11	1.74	0.67
1:B:526:THR:HG21	4:L:115:ILE:HD13	1.75	0.67
6:W:73:GLU:HG2	8:X:22:LEU:HB3	1.76	0.67
8:X:43:VAL:HG21	8:X:46:ILE:HD11	1.75	0.67
2:I:54:GLU:OE2	2:I:61:LYS:NZ	2.27	0.67
1:B:106:ILE:HD11	5:M:269:LEU:HB3	1.77	0.67
1:B:588:ASP:O	1:B:593:ARG:NH1	2.27	0.67
1:B:606:VAL:HB	1:B:611:LYS:HE3	1.77	0.67
1:G:628:ALA:HB3	1:G:631:GLN:HB2	1.76	0.67
1:B:192:CYS:SG	1:B:193:HIS:N	2.67	0.67
3:K:326:ASN:ND2	3:K:362:ASP:OD1	2.28	0.67
3:K:85:VAL:HB	3:K:436:ARG:HH11	1.57	0.67
5:Y:243:TRP:HB2	5:Y:248:ILE:HD13	1.76	0.67
1:B:600:ILE:HD11	1:B:618:ASN:HD22	1.59	0.67
3:K:209:VAL:HG22	3:K:215:LEU:HG	1.77	0.67
11:T:153:DA:OP2	9:U:35:ARG:NH1	2.28	0.67
10:V:73:GLU:N	10:V:73:GLU:OE1	2.28	0.67
2:I:45:ASN:ND2	3:K:315:LEU:O	2.24	0.67
2:C:122:VAL:HG21	2:C:684:ARG:HH12	1.59	0.67
2:C:565:CYS:H	2:C:589:LEU:HB3	1.59	0.67
2:I:675:ASN:OD1	2:I:678:PHE:N	2.28	0.67
4:L:133:MET:HB3	4:L:185:TRP:CD2	2.30	0.66
4:L:202:ILE:N	4:L:223:PHE:O	2.27	0.66
4:O:322:GLN:HG3	4:O:380:PHE:CE2	2.31	0.66
3:K:136:GLN:NE2	3:K:138:TYR:OH	2.28	0.66
4:O:122:ASN:ND2	4:O:165:GLY:O	2.28	0.66
1:G:522:ARG:NH1	4:O:396:ASP:O	2.29	0.66
2:I:273:GLN:HE21	2:I:276:GLN:HG3	1.60	0.66
2:I:448:LEU:O	2:I:451:THR:OG1	2.10	0.66
3:K:86:ASN:ND2	3:K:130:GLY:O	2.28	0.66
4:L:148:ASP:HB3	4:L:174:ARG:HE	1.60	0.66
1:B:295:PHE:N	1:B:320:GLN:O	2.29	0.66
2:I:17:LYS:HB2	2:I:222:LYS:HB3	1.77	0.66
1:B:142:GLU:HA	1:B:145:LYS:HE2	1.78	0.66
2:C:257:PRO:HG2	2:C:260:CYS:HB3	1.76	0.66
2:I:636:PRO:HB3	2:I:722:GLN:HA	1.78	0.66
2:I:700:CYS:HA	2:I:718:LYS:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:235:HIS:HD1	3:F:259:SER:HB2	1.60	0.66
4:O:253:MET:HE3	4:O:255:TRP:HZ2	1.60	0.66
2:C:703:LYS:O	2:C:714:GLY:N	2.29	0.66
4:L:66:LEU:HB2	4:L:82:ALA:HB3	1.78	0.66
2:I:104:VAL:HG23	3:K:169:ARG:HH12	1.61	0.66
4:O:61:PHE:HB3	4:O:108:PHE:HE1	1.61	0.66
4:O:79:LEU:N	4:O:121:ILE:O	2.23	0.66
5:Y:201:ARG:NH2	5:Y:281:ASP:OD1	2.28	0.66
4:L:22:LYS:HD2	4:L:26:LYS:HZ3	1.60	0.65
3:K:84:CYS:HB2	3:K:437:TRP:CE2	2.32	0.65
4:O:253:MET:HE3	4:O:255:TRP:CZ2	2.29	0.65
4:L:44:SER:HB3	4:L:393:VAL:HG21	1.77	0.65
2:I:571:CYS:HB3	2:I:585:CYS:SG	2.36	0.65
3:K:329:VAL:HB	3:K:355:ARG:HH11	1.61	0.65
1:G:121:ARG:NH2	4:O:360:GLU:OE2	2.29	0.65
2:I:98:LEU:HD23	3:K:139:VAL:HG11	1.78	0.65
1:G:430:TYR:HE2	1:G:444:ALA:HA	1.59	0.65
1:G:249:SER:OG	1:G:298:GLN:NE2	2.30	0.65
3:F:379:LEU:HB3	3:F:387:TYR:HB2	1.79	0.65
1:G:250:LEU:N	1:G:299:MET:O	2.27	0.65
4:O:379:ASP:O	4:O:393:VAL:N	2.25	0.65
1:B:467:LEU:HA	1:B:471:HIS:HD2	1.62	0.65
3:K:254:CYS:HB3	3:K:260:LEU:HD13	1.79	0.65
3:K:379:LEU:O	3:K:387:TYR:N	2.28	0.65
3:F:186:TYR:OH	3:F:220:ILE:O	2.14	0.65
2:I:748:MET:HG2	5:Y:178:LYS:HA	1.78	0.65
2:C:59:GLU:HB3	2:C:63:ARG:HH22	1.62	0.65
7:H:40:DA:N6	11:T:186:DG:O6	2.30	0.65
7:H:80:DG:OP2	10:V:83:ARG:NH1	2.29	0.65
5:Y:222:PHE:N	5:Y:265:LYS:O	2.30	0.65
2:I:329:CYS:H	2:I:332:HIS:CD2	2.15	0.65
3:K:100:GLN:HG3	3:K:151:ALA:HA	1.77	0.65
1:B:196:ARG:HD3	5:M:295:ARG:HH22	1.63	0.64
2:I:649:GLU:O	2:I:681:ASP:N	2.28	0.64
3:K:83:LYS:NZ	3:K:84:CYS:O	2.30	0.64
3:F:101:PHE:CE1	3:F:111:LEU:HB3	2.31	0.64
4:L:402:TRP:HZ3	4:L:404:MET:HB2	1.62	0.64
2:C:105:ALA:O	3:F:169:ARG:NH1	2.29	0.64
8:J:44:LYS:HB2	9:R:115:LEU:HD22	1.77	0.64
2:I:530:HIS:CE1	2:I:535:CYS:HA	2.33	0.64
3:K:124:TYR:HE1	3:K:134:LEU:HG	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:384:GLY:HA3	3:K:410:GLY:HA2	1.80	0.64
9:R:20:ARG:NH1	10:S:121:ALA:O	2.26	0.64
3:K:90:GLU:OE2	3:K:120:ARG:NH2	2.31	0.64
3:K:122:THR:HB	3:K:124:TYR:HE2	1.61	0.64
5:Y:231:LYS:HG3	5:Y:237:ILE:HG13	1.78	0.64
4:L:400:GLN:HE22	4:L:402:TRP:HB3	1.61	0.64
6:A:106:ASP:OD2	6:A:131:ARG:NH1	2.30	0.64
9:U:16:THR:O	9:U:19:SER:OG	2.15	0.64
3:K:381:ASN:N	3:K:385:LYS:O	2.31	0.64
4:O:188:ASN:HB2	4:O:240:GLU:HB3	1.79	0.64
3:K:237:ASP:HB3	3:K:257:ASP:HB3	1.80	0.64
4:O:223:PHE:HA	4:O:262:THR:HB	1.80	0.64
3:F:371:ASP:O	3:F:374:GLN:NE2	2.30	0.64
4:L:67:VAL:HG22	4:L:81:ILE:HD12	1.79	0.64
4:L:129:ARG:HG3	4:L:182:GLY:H	1.61	0.64
6:W:119:ILE:HG22	8:X:46:ILE:HA	1.79	0.64
1:G:251:LEU:HB3	1:G:253:ARG:NH2	2.13	0.64
1:G:621:VAL:HG13	1:G:626:PHE:HB2	1.79	0.64
3:K:262:LEU:O	3:K:298:ASP:N	2.31	0.64
4:O:24:TRP:O	4:O:28:THR:OG1	2.11	0.64
4:O:142:THR:O	4:O:150:LEU:N	2.31	0.64
1:G:428:ILE:HG22	1:G:487:ILE:HG22	1.80	0.64
4:O:298:VAL:O	4:O:313:PHE:N	2.30	0.64
1:B:451:PRO:HD2	1:B:467:LEU:HD11	1.80	0.64
5:M:243:TRP:HD1	5:M:248:ILE:HD12	1.63	0.64
7:H:50:DT:H2'	7:H:51:DA:C8	2.33	0.64
3:K:327:ALA:HB1	3:K:355:ARG:HH22	1.63	0.64
4:O:172:ARG:O	4:O:217:VAL:N	2.27	0.64
3:F:322:LYS:HB2	3:F:328:ILE:HG12	1.78	0.63
4:L:145:PRO:HA	4:L:179:GLU:HB3	1.79	0.63
5:M:218:HIS:O	5:M:268:HIS:ND1	2.29	0.63
1:G:522:ARG:HA	1:G:576:PRO:HG2	1.78	0.63
2:I:60:TRP:HE1	3:K:105:SER:H	1.44	0.63
5:Y:231:LYS:NZ	5:Y:232:GLU:O	2.28	0.63
2:C:529:ASP:HA	2:C:553:GLN:HB2	1.80	0.63
3:F:252:MET:HB2	3:F:314:TRP:CZ2	2.32	0.63
1:B:135:ASP:HA	1:B:138:LEU:HB2	1.79	0.63
9:R:17:ARG:NH1	11:T:71:DT:OP2	2.32	0.63
1:G:109:ILE:HG23	4:O:341:ARG:HH22	1.64	0.63
2:I:242:GLU:HA	2:I:245:LYS:HD2	1.80	0.63
3:K:208:SER:N	3:K:216:ARG:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:332:LYS:NZ	3:K:333:PRO:O	2.32	0.63
6:A:55:GLN:NE2	9:R:110:ASN:OD1	2.31	0.63
2:C:623:PRO:HA	2:C:629:TRP:HA	1.79	0.63
9:U:81:ARG:HD3	6:W:58:THR:HG21	1.80	0.63
4:O:61:PHE:HB2	4:O:85:GLN:HB3	1.81	0.63
1:B:448:LEU:HA	1:B:463:LEU:HD22	1.81	0.63
11:T:165:DC:H2"	11:T:166:DG:H5"	1.80	0.63
4:O:36:MET:N	4:O:401:VAL:O	2.31	0.63
4:O:185:TRP:CD2	4:O:193:LEU:HD12	2.33	0.63
4:L:318:ASP:HB2	4:L:339:ASP:HB3	1.79	0.63
5:M:224:SER:OG	5:M:259:ARG:NH1	2.25	0.63
1:G:557:TYR:HB2	5:Y:173:ARG:HH22	1.62	0.63
3:K:419:SER:N	3:K:424:ILE:O	2.30	0.63
1:B:589:PRO:HD3	2:C:117:GLN:HE21	1.64	0.63
7:H:88:DC:H42	11:T:139:DG:H1	1.47	0.63
2:I:86:THR:N	3:K:89:LYS:O	2.30	0.63
3:K:257:ASP:O	3:K:302:ARG:NE	2.31	0.63
4:O:174:ARG:HG3	4:O:218:ASP:HA	1.80	0.63
2:C:54:GLU:O	2:C:58:GLN:N	2.27	0.62
2:C:682:ALA:O	2:C:690:ARG:NH2	2.32	0.62
3:F:238:GLU:O	3:F:256:MET:N	2.27	0.62
3:K:84:CYS:HA	3:K:437:TRP:HA	1.81	0.62
3:K:427:ALA:O	3:K:435:TRP:N	2.27	0.62
5:Y:231:LYS:NZ	5:Y:234:SER:O	2.29	0.62
1:B:528:ILE:HB	1:B:557:TYR:HB3	1.81	0.62
9:R:55:LEU:HD22	10:S:63:VAL:HG13	1.81	0.62
2:I:693:ASN:HB3	2:I:728:PHE:CE1	2.33	0.62
2:C:85:VAL:HA	3:F:90:GLU:HA	1.81	0.62
2:C:122:VAL:N	2:C:650:ILE:O	2.32	0.62
2:C:694:HIS:ND1	2:C:729:PHE:O	2.32	0.62
6:A:23:LYS:HE2	6:A:26:ARG:HH12	1.64	0.62
2:I:43:SER:O	2:I:47:GLN:NE2	2.33	0.62
2:I:694:HIS:HE1	2:I:730:ASP:HA	1.65	0.62
1:B:526:THR:OG1	4:L:38:HIS:ND1	2.32	0.62
9:R:62:ILE:HD11	9:R:93:LEU:HD12	1.82	0.62
2:I:694:HIS:CE1	2:I:731:TYR:H	2.17	0.62
2:C:116:LEU:HD11	2:C:118:GLN:HE21	1.64	0.62
3:F:84:CYS:HB2	3:F:437:TRP:CE2	2.35	0.62
3:K:240:LEU:HD11	3:K:367:ARG:HH12	1.64	0.62
1:B:301:VAL:HG23	1:B:310:LEU:HD13	1.81	0.62
1:B:475:ILE:HG23	1:B:492:ASN:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:O	4:L:39:ALA:N	2.30	0.62
2:C:433:GLU:HG3	2:C:470:GLN:HG2	1.81	0.62
9:U:92:GLU:OE1	9:U:92:GLU:N	2.25	0.62
3:K:154:TYR:HA	3:K:161:PRO:HA	1.81	0.62
4:O:65:ARG:HA	4:O:83:SER:HA	1.81	0.62
2:C:623:PRO:O	2:C:623:PRO:HD2	1.99	0.62
5:Y:221:VAL:HG12	5:Y:266:VAL:HG22	1.82	0.62
1:B:646:LYS:HA	1:B:649:LYS:HD2	1.79	0.62
10:S:102:GLU:OE1	10:S:102:GLU:N	2.27	0.62
3:K:326:ASN:HA	3:K:358:TYR:CZ	2.35	0.62
3:K:365:TYR:O	3:K:414:ARG:NH2	2.26	0.62
2:C:326:GLY:N	2:C:457:CYS:SG	2.73	0.62
2:I:78:ARG:HE	5:Y:200:HIS:CE1	2.18	0.62
2:I:695:SER:HB2	2:I:728:PHE:HD2	1.65	0.62
2:I:701:TYR:HD1	2:I:703:LYS:HE3	1.63	0.62
3:K:427:ALA:HB3	3:K:435:TRP:HB2	1.81	0.62
4:O:198:ASP:HA	4:O:229:VAL:HG13	1.82	0.62
4:L:19:GLU:HA	4:L:22:LYS:HB3	1.80	0.62
5:M:198:ILE:O	5:M:202:ALA:N	2.30	0.62
1:B:316:GLU:HB3	5:M:229:LYS:HB2	1.81	0.61
3:F:386:LEU:HB3	3:F:404:LEU:HB2	1.81	0.61
4:L:298:VAL:O	4:L:313:PHE:N	2.33	0.61
11:T:153:DA:H2"	11:T:154:DG:C8	2.35	0.61
2:I:30:LYS:HD2	2:I:34:ARG:HE	1.65	0.61
3:K:189:HIS:HE2	3:K:216:ARG:HB2	1.63	0.61
2:C:322:ASN:HD21	2:C:336:ALA:HB3	1.66	0.61
4:L:62:SER:N	4:L:86:LEU:O	2.31	0.61
4:O:142:THR:HB	4:O:150:LEU:HB2	1.82	0.61
1:B:83:HIS:CD2	1:B:440:GLN:HB2	2.36	0.61
7:H:50:DT:H2'	7:H:51:DA:H8	1.65	0.61
1:G:509:GLN:OE1	3:K:185:HIS:N	2.33	0.61
1:G:581:VAL:HG13	3:K:287:ARG:HH11	1.65	0.61
2:C:106:SER:HB3	5:M:187:HIS:HB2	1.82	0.61
2:C:285:PHE:HA	2:C:292:TYR:HA	1.82	0.61
4:L:123:HIS:HE1	4:L:144:THR:HG22	1.63	0.61
3:K:269:ARG:HH11	3:K:292:GLN:HB3	1.65	0.61
4:O:89:ASP:O	4:O:92:GLN:NE2	2.32	0.61
1:B:575:ARG:NH1	3:F:280:TYR:OH	2.33	0.61
2:C:112:SER:OG	3:F:212:ASP:O	2.16	0.61
2:C:449:ILE:HD13	2:C:475:ARG:HD3	1.82	0.61
4:L:342:LEU:O	4:L:370:HIS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:ILE:H	1:G:444:ALA:HB2	1.64	0.61
2:I:497:LYS:HD2	2:I:498:LYS:HG3	1.83	0.61
3:K:226:VAL:HG12	3:K:227:ALA:H	1.65	0.61
1:B:113:ARG:NH1	4:L:366:LEU:O	2.33	0.61
3:F:378:ALA:HB1	3:F:386:LEU:HD11	1.82	0.61
6:A:83:ARG:HB2	8:J:80:THR:HG22	1.81	0.61
2:I:154:ASP:HB3	2:I:156:LYS:HE3	1.82	0.61
4:O:245:SER:HG	4:O:255:TRP:HE1	1.49	0.61
2:C:695:SER:OG	2:C:697:ASN:OD1	2.19	0.61
5:M:232:GLU:HG3	5:M:238:LYS:NZ	2.16	0.61
6:W:121:PRO:HG2	8:X:49:LEU:HD23	1.83	0.61
2:I:315:ASN:HD22	2:I:487:ALA:HB1	1.65	0.61
7:H:167:DT:H2"	7:H:168:DC:C5	2.36	0.61
11:T:126:DT:OP2	2:I:503:LEU:HD21	2.00	0.61
2:I:148:GLU:HA	2:I:151:LYS:HD2	1.81	0.61
4:O:48:GLN:OE1	4:O:381:SER:OG	2.19	0.61
4:L:83:SER:OG	4:L:116:GLU:O	2.14	0.61
2:I:541:CYS:O	2:I:545:GLN:N	2.33	0.61
1:B:511:GLY:O	1:B:515:SER:OG	2.19	0.61
3:F:327:ALA:HA	3:F:357:ASP:HA	1.82	0.61
4:L:293:SER:OG	4:L:297:THR:OG1	2.18	0.61
6:A:109:LEU:HD13	6:W:129:ARG:HD3	1.83	0.61
2:I:444:MET:HA	2:I:447:VAL:HB	1.82	0.61
6:A:62:ILE:O	6:A:93:GLN:NE2	2.33	0.60
9:R:65:LEU:HB3	9:R:86:ALA:HB1	1.82	0.60
2:I:27:ARG:HG3	2:I:30:LYS:HE3	1.81	0.60
2:I:36:ASP:HA	2:I:39:LYS:HE3	1.82	0.60
5:Y:207:LEU:O	5:Y:210:HIS:NE2	2.34	0.60
4:O:235:TRP:HA	4:O:243:PHE:HB3	1.83	0.60
4:L:34:LEU:HB2	4:L:403:GLN:HB3	1.82	0.60
5:Y:191:ASP:O	5:Y:194:THR:OG1	2.18	0.60
3:F:153:THR:HB	3:F:162:LEU:HB2	1.82	0.60
6:W:100:LEU:HD23	8:X:37:LEU:HD13	1.84	0.60
1:G:129:ARG:NH2	1:G:129:ARG:O	2.33	0.60
1:G:312:ASP:OD1	1:G:360:ARG:NH1	2.31	0.60
2:I:228:SER:HA	2:I:234:LYS:HB2	1.81	0.60
3:K:368:PHE:HA	3:K:379:LEU:HD13	1.82	0.60
1:B:112:HIS:N	4:L:361:ASP:OD2	2.35	0.60
1:B:503:PRO:HB2	1:B:564:LEU:HB2	1.84	0.60
11:T:172:DG:O5'	9:U:76:THR:OG1	2.20	0.60
1:G:112:HIS:N	4:O:361:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:176:ASN:HD21	3:K:178:ILE:HB	1.66	0.60
1:B:148:GLN:O	1:B:306:ARG:NH1	2.34	0.60
1:B:508:ARG:NH2	1:B:512:PHE:O	2.35	0.60
2:C:15:CYS:HA	2:C:18:ARG:HD2	1.83	0.60
3:F:147:PHE:HD1	3:F:167:GLY:HA3	1.67	0.60
4:L:46:THR:HG21	4:L:130:ALA:H	1.67	0.60
5:M:222:PHE:N	5:M:265:LYS:O	2.34	0.60
11:T:91:DC:P	6:W:72:ARG:HH12	2.25	0.60
11:T:162:DG:OP1	10:V:37:TYR:OH	2.13	0.60
8:X:85:ASP:OD1	8:X:86:VAL:N	2.34	0.60
2:I:108:PRO:HG2	2:I:629:TRP:CE2	2.37	0.60
3:K:126:CYS:HA	3:K:132:ILE:HA	1.82	0.60
3:K:189:HIS:NE2	3:K:216:ARG:HB2	2.17	0.60
1:B:103:ARG:NH2	5:M:284:ILE:O	2.34	0.60
1:B:116:THR:HG22	4:L:407:ASN:HD21	1.67	0.60
5:M:259:ARG:HE	5:M:260:HIS:H	1.49	0.60
2:I:178:LEU:HD11	2:I:240:LEU:HB3	1.83	0.60
4:O:205:TRP:HD1	4:O:217:VAL:HG12	1.67	0.60
5:Y:191:ASP:OD1	5:Y:192:ALA:N	2.35	0.60
1:B:430:TYR:O	1:B:442:THR:OG1	2.16	0.59
1:G:637:MET:HA	1:G:640:VAL:HG22	1.84	0.59
2:I:619:LEU:HD22	2:I:688:LYS:HB3	1.83	0.59
3:K:230:GLY:O	3:K:295:HIS:ND1	2.35	0.59
4:O:32:TYR:HH	4:O:370:HIS:CE1	2.19	0.59
4:O:230:VAL:HG12	4:O:247:ALA:HB2	1.84	0.59
1:B:431:GLN:HA	1:B:441:GLN:HA	1.83	0.59
8:X:90:LEU:HD12	8:X:95:ARG:HB2	1.83	0.59
4:O:125:GLY:HA3	4:O:145:PRO:HG2	1.84	0.59
2:I:47:GLN:HA	2:I:50:LEU:HD12	1.84	0.59
2:C:39:LYS:NZ	3:F:393:VAL:O	2.30	0.59
2:C:601:SER:O	2:C:613:ARG:NH2	2.36	0.59
2:I:326:GLY:O	2:I:332:HIS:NE2	2.35	0.59
2:I:442:ALA:O	2:I:446:ARG:NH2	2.35	0.59
3:K:237:ASP:OD1	3:K:238:GLU:N	2.28	0.59
1:B:191:VAL:HB	1:B:246:LYS:HB3	1.84	0.59
2:C:17:LYS:O	2:C:21:SER:N	2.34	0.59
5:M:201:ARG:NH2	5:M:281:ASP:OD1	2.28	0.59
3:K:130:GLY:HA2	3:K:436:ARG:HH12	1.67	0.59
3:K:371:ASP:CG	3:K:375:LYS:H	2.04	0.59
1:B:139:SER:HB2	4:L:308:LEU:HD21	1.85	0.59
1:B:628:ALA:HB3	1:B:631:GLN:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:TRP:HH2	3:F:107:GLU:HB2	1.68	0.59
9:R:118:LYS:NZ	9:R:119:CYS:SG	2.75	0.59
1:G:308:LEU:HG	1:G:310:LEU:H	1.67	0.59
1:G:529:LEU:HB2	4:O:35:VAL:HG11	1.85	0.59
1:B:196:ARG:NE	4:L:319:GLU:OE2	2.32	0.59
4:L:130:ALA:O	4:L:131:ARG:NH2	2.36	0.59
1:G:158:GLN:HG3	1:G:362:THR:N	2.18	0.59
3:K:191:ASN:HB2	3:K:211:LYS:HB3	1.83	0.59
4:O:370:HIS:CE1	4:O:372:GLY:H	2.20	0.59
1:B:88:GLN:HA	1:B:91:GLU:HB2	1.84	0.59
1:B:117:TYR:CD2	1:B:465:LYS:HE2	2.36	0.59
9:R:70:ALA:HA	9:R:82:HIS:CE1	2.38	0.59
2:I:631:ILE:HD11	2:I:691:PHE:HB2	1.84	0.59
6:A:60:LEU:HD13	6:A:93:GLN:NE2	2.17	0.59
1:G:238:GLU:HB3	1:G:241:ASN:HB2	1.85	0.59
4:O:142:THR:N	4:O:150:LEU:O	2.21	0.59
1:B:452:TRP:HB2	1:B:471:HIS:CE1	2.38	0.59
4:L:198:ASP:HA	4:L:229:VAL:HG13	1.85	0.59
4:L:290:ALA:HA	4:L:300:LEU:HA	1.84	0.59
1:G:530:VAL:HB	4:O:35:VAL:HB	1.84	0.59
3:K:321:SER:N	3:K:329:VAL:O	2.36	0.59
4:O:169:PRO:HG2	4:O:172:ARG:HD3	1.84	0.59
7:H:54:DC:H42	11:T:173:DA:H61	1.49	0.58
3:K:198:PHE:CD1	3:K:206:LEU:HB2	2.38	0.58
1:B:475:ILE:HD11	1:B:490:SER:HB3	1.85	0.58
2:C:321:ASP:HB3	2:C:337:LYS:HG2	1.85	0.58
2:C:443:SER:O	2:C:446:ARG:NH2	2.36	0.58
3:F:388:VAL:HB	3:F:402:THR:HB	1.85	0.58
1:G:115:LEU:HD13	1:G:117:TYR:HB2	1.83	0.58
3:K:259:SER:OG	3:K:300:SER:OG	2.22	0.58
2:C:82:GLU:HA	2:C:97:PRO:HA	1.84	0.58
4:L:65:ARG:HA	4:L:83:SER:HA	1.85	0.58
1:G:526:THR:HG23	4:O:38:HIS:HB2	1.84	0.58
3:K:381:ASN:HB3	3:K:385:LYS:HG3	1.84	0.58
5:Y:200:HIS:HA	5:Y:203:ILE:HB	1.86	0.58
2:C:637:VAL:HG13	2:C:641:GLU:HB2	1.85	0.58
9:U:79:ILE:H	9:U:82:HIS:HD2	1.50	0.58
3:K:122:THR:HB	3:K:124:TYR:CE2	2.39	0.58
3:K:249:GLU:O	3:K:265:ILE:N	2.34	0.58
4:O:276:VAL:HG22	4:O:293:SER:HA	1.84	0.58
1:B:87:LEU:HD21	1:B:440:GLN:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:GLU:HA	1:B:597:ILE:HB	1.85	0.58
3:F:412:ALA:HB3	3:F:430:ASP:HB2	1.84	0.58
1:G:502:ASN:HD21	1:G:504:GLN:HB3	1.68	0.58
5:Y:252:VAL:HG22	5:Y:253:TRP:H	1.67	0.58
5:Y:287:THR:HG22	5:Y:290:GLN:H	1.67	0.58
4:L:204:LEU:O	4:L:220:LYS:N	2.36	0.58
3:K:103:TRP:HA	3:K:420:ARG:HD2	1.84	0.58
4:O:194:LEU:HG	4:O:235:TRP:CE2	2.39	0.58
1:B:94:THR:HG23	1:B:452:TRP:HD1	1.69	0.58
1:B:528:ILE:HD13	1:B:557:TYR:HD2	1.69	0.58
4:L:327:PRO:HD3	4:L:382:TRP:CE2	2.39	0.58
7:H:158:DG:H22	11:T:69:DT:H3	1.50	0.58
2:I:102:ASN:ND2	3:K:182:CYS:O	2.37	0.58
2:I:491:ASP:O	2:I:495:ARG:NH2	2.36	0.58
3:K:217:LEU:HB3	3:K:226:VAL:HB	1.86	0.58
2:C:223:ILE:HG22	2:C:227:ILE:HG12	1.84	0.58
4:L:344:VAL:HG13	4:L:367:LEU:HB2	1.86	0.58
1:G:92:LYS:HB3	1:G:93:PRO:HD3	1.84	0.58
2:I:125:GLU:N	2:I:125:GLU:OE1	2.37	0.58
3:K:423:SER:HA	3:K:439:ARG:HB2	1.86	0.58
3:F:101:PHE:CG	3:F:419:SER:HA	2.39	0.58
4:L:24:TRP:CD1	4:L:372:GLY:HA3	2.39	0.58
1:G:629:ASP:HA	1:G:632:MET:HE2	1.84	0.58
1:G:657:MET:HA	1:G:660:LEU:HB2	1.86	0.58
2:I:701:TYR:N	2:I:716:PHE:O	2.24	0.58
3:K:146:ASN:O	3:K:168:SER:N	2.34	0.58
4:O:293:SER:OG	4:O:297:THR:OG1	2.20	0.58
1:B:597:ILE:HG12	1:B:615:LYS:HD3	1.85	0.57
2:C:546:ASN:O	2:C:560:ASN:ND2	2.35	0.57
2:C:673:ASN:HA	2:C:679:VAL:HG22	1.85	0.57
11:T:118:DC:H2"	11:T:119:DC:C2	2.39	0.57
9:U:110:ASN:O	6:W:55:GLN:NE2	2.31	0.57
5:Y:249:LEU:HG	5:Y:250:PRO:HD2	1.86	0.57
7:H:77:DG:N2	11:T:151:DC:O2	2.36	0.57
2:I:120:PHE:CD1	2:I:295:PHE:HB2	2.39	0.57
4:O:287:PHE:HA	4:O:303:LEU:HG	1.84	0.57
4:L:40:LEU:N	4:L:397:ASN:O	2.34	0.57
1:G:194:LYS:NZ	1:G:198:ASP:O	2.28	0.57
2:I:44:SER:O	2:I:48:LYS:NZ	2.30	0.57
2:C:172:VAL:HB	2:C:221:ASP:HA	1.86	0.57
3:F:217:LEU:HB3	3:F:226:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:109:DA:H5"	6:W:43:PRO:HG2	1.85	0.57
10:V:65:ASP:OD2	8:X:98:TYR:OH	2.20	0.57
2:I:655:GLU:O	2:I:659:ARG:N	2.34	0.57
4:O:173:LEU:HB3	4:O:205:TRP:CE2	2.39	0.57
3:F:303:ASP:O	3:F:306:ARG:NH2	2.37	0.57
4:L:315:SER:HB2	4:L:345:TRP:HH2	1.69	0.57
1:G:99:PHE:O	1:G:102:THR:OG1	2.22	0.57
1:G:468:LYS:HA	1:G:476:PHE:CD2	2.40	0.57
2:I:649:GLU:HB3	2:I:681:ASP:HB3	1.86	0.57
3:K:126:CYS:SG	3:K:127:HIS:N	2.78	0.57
1:B:654:ARG:N	2:C:265:ASP:OD1	2.36	0.57
2:C:567:CYS:O	2:C:592:THR:OG1	2.20	0.57
2:C:567:CYS:SG	2:C:577:PRO:HD2	2.44	0.57
4:L:192:HIS:HB3	4:L:204:LEU:HD11	1.85	0.57
4:L:313:PHE:HE1	4:L:365:GLU:HG3	1.69	0.57
4:L:399:MET:SD	4:L:401:VAL:HG23	2.44	0.57
10:S:77:LEU:HD23	8:X:75:HIS:ND1	2.19	0.57
2:I:494:PRO:HB3	2:I:499:ARG:HH11	1.70	0.57
10:S:90:GLU:OE1	10:S:90:GLU:N	2.25	0.57
6:W:57:SER:HB3	6:W:59:GLU:OE1	2.04	0.57
1:G:304:LYS:O	1:G:306:ARG:NH2	2.37	0.57
1:B:94:THR:O	1:B:98:ARG:N	2.35	0.57
2:C:617:LYS:HD2	2:C:633:ILE:HD11	1.86	0.57
3:F:424:ILE:HG23	3:F:436:ARG:HH21	1.69	0.57
1:G:565:TYR:HB2	1:G:574:LEU:HD23	1.87	0.57
2:I:670:PHE:HE1	2:I:690:ARG:HB2	1.70	0.57
4:O:11:ALA:O	4:O:15:ARG:NH2	2.34	0.57
1:B:204:ARG:HH12	1:B:245:VAL:HG21	1.69	0.57
2:C:638:GLN:HA	2:C:720:ALA:HA	1.87	0.57
5:M:273:PRO:O	5:M:276:THR:OG1	2.22	0.57
1:G:655:ASN:N	2:I:265:ASP:OD2	2.38	0.57
1:B:195:LYS:NZ	4:L:273:THR:O	2.34	0.57
2:C:321:ASP:O	2:C:337:LYS:NZ	2.36	0.57
3:F:176:ASN:HB3	3:F:179:THR:HB	1.87	0.57
4:L:180:GLY:HA3	4:L:197:SER:HA	1.87	0.57
4:L:223:PHE:HA	4:L:262:THR:HB	1.86	0.57
6:A:131:ARG:HG2	6:A:133:GLU:OE2	2.04	0.57
1:G:455:LEU:HD12	1:G:466:HIS:CE1	2.40	0.57
2:I:146:ILE:HA	2:I:149:LEU:HD12	1.86	0.57
2:I:663:TYR:O	2:I:668:CYS:N	2.37	0.57
2:C:694:HIS:HD1	2:C:730:ASP:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:28:LYS:HD2	11:T:144:DT:H5"	1.87	0.56
2:I:332:HIS:HB2	2:I:469:ARG:NH1	2.20	0.56
1:B:81:ALA:HB3	1:B:438:THR:HG22	1.85	0.56
1:B:430:TYR:CE2	1:B:451:PRO:HG3	2.39	0.56
4:L:284:TYR:OH	4:L:328:HIS:N	2.38	0.56
7:H:100:DA:H5"	8:J:30:THR:HG21	1.87	0.56
1:G:508:ARG:HE	1:G:513:ALA:HA	1.69	0.56
4:O:123:HIS:CE1	4:O:144:THR:HG22	2.39	0.56
1:B:478:TYR:HA	1:B:487:ILE:HD13	1.87	0.56
1:B:520:VAL:O	4:L:397:ASN:ND2	2.22	0.56
2:C:284:LEU:O	2:C:293:ASP:N	2.38	0.56
1:G:160:THR:HG22	1:G:358:THR:HG22	1.86	0.56
1:G:616:LEU:HD12	1:G:619:LEU:HD11	1.86	0.56
2:I:448:LEU:HB2	2:I:475:ARG:HH12	1.69	0.56
4:O:33:ASP:N	4:O:403:GLN:O	2.30	0.56
2:C:564:GLY:HA3	2:C:566:ARG:HH11	1.70	0.56
3:F:207:LEU:HD22	3:F:251:ILE:HD11	1.87	0.56
6:A:108:ASN:ND2	8:J:43:VAL:HA	2.20	0.56
11:T:86:DC:H2"	11:T:87:DC:C5	2.41	0.56
1:G:532:ARG:NH2	1:G:533:PRO:O	2.38	0.56
3:F:89:LYS:HA	3:F:433:SER:HA	1.87	0.56
3:F:436:ARG:NH2	3:F:438:ASP:OD1	2.39	0.56
3:K:193:ILE:HD12	3:K:208:SER:HB2	1.87	0.56
3:K:305:HIS:CD2	3:K:323:SER:HB2	2.40	0.56
4:O:174:ARG:O	4:O:205:TRP:NE1	2.38	0.56
4:O:408:ILE:HG13	4:O:409:TYR:HD1	1.70	0.56
1:B:162:THR:HB	1:B:356:GLN:HB3	1.87	0.56
1:B:166:HIS:N	1:B:216:ASN:OD1	2.37	0.56
2:C:104:VAL:O	5:M:187:HIS:NE2	2.37	0.56
9:U:87:VAL:HG23	9:U:88:ARG:HG2	1.88	0.56
1:G:134:VAL:O	1:G:138:LEU:N	2.32	0.56
3:K:354:GLY:HA2	3:K:396:PRO:HG3	1.87	0.56
3:K:387:TYR:HB3	3:K:389:TRP:CH2	2.41	0.56
1:B:521:LYS:HD3	1:B:577:GLN:HG3	1.86	0.56
2:C:286:CYS:SG	2:C:294:CYS:N	2.78	0.56
2:C:466:LYS:HB3	2:C:470:GLN:HB2	1.86	0.56
3:F:127:HIS:HB2	3:F:131:GLU:HB3	1.86	0.56
3:F:196:LEU:HD22	3:F:206:LEU:HD21	1.88	0.56
4:L:206:ASP:HB2	4:L:220:LYS:HD2	1.88	0.56
7:H:70:DA:OP1	9:U:17:ARG:N	2.27	0.56
7:H:165:DC:H2"	7:H:166:DC:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:699:ASN:O	2:I:718:LYS:N	2.37	0.56
4:O:151:VAL:HB	4:O:170:ASP:O	2.06	0.56
5:Y:185:ARG:HE	5:Y:186:PRO:HD2	1.69	0.56
6:W:61:LEU:HG	8:X:40:ARG:HH11	1.71	0.56
2:I:660:GLY:O	2:I:664:ASP:N	2.28	0.56
1:B:586:GLU:HG2	1:B:588:ASP:H	1.70	0.56
4:L:297:THR:HA	4:L:314:GLU:HA	1.88	0.56
6:A:92:LEU:HD22	8:J:86:VAL:HG11	1.88	0.56
9:U:17:ARG:NH1	9:U:28:GLY:HA2	2.20	0.56
2:I:622:ALA:O	2:I:630:GLY:N	2.39	0.56
3:K:262:LEU:HD21	3:K:299:PHE:HB3	1.87	0.56
2:C:86:THR:N	3:F:89:LYS:O	2.37	0.55
2:C:568:LYS:HG3	2:C:592:THR:HB	1.88	0.55
3:F:426:ILE:HG13	3:F:436:ARG:HG3	1.86	0.55
7:H:79:DA:H2"	7:H:80:DG:H5'	1.88	0.55
1:G:578:GLU:OE1	1:G:578:GLU:N	2.39	0.55
2:I:237:ALA:HA	2:I:240:LEU:HD13	1.87	0.55
3:K:112:VAL:HG22	3:K:125:GLU:HB2	1.87	0.55
3:F:318:LEU:HD11	3:F:353:LEU:HD21	1.87	0.55
11:T:178:DT:H2"	11:T:179:DA:C8	2.42	0.55
3:K:207:LEU:HA	3:K:217:LEU:HA	1.89	0.55
3:K:379:LEU:HD12	3:K:416:THR:HG21	1.87	0.55
4:O:65:ARG:HG2	4:O:83:SER:HB3	1.89	0.55
1:B:309:GLN:HE21	5:M:230:ARG:HH12	1.53	0.55
4:L:47:ALA:HA	4:L:68:LEU:HG	1.87	0.55
4:L:238:LEU:HD21	4:L:283:PRO:HA	1.88	0.55
5:M:180:ARG:HD3	5:M:182:SER:H	1.71	0.55
10:S:102:GLU:HA	10:S:105:LYS:HG2	1.89	0.55
2:I:444:MET:O	2:I:448:LEU:N	2.37	0.55
3:K:262:LEU:HG	3:K:299:PHE:O	2.06	0.55
4:O:298:VAL:N	4:O:313:PHE:O	2.38	0.55
2:C:105:ALA:HA	5:M:187:HIS:CE1	2.40	0.55
4:L:76:GLN:NE2	4:L:77:ASN:O	2.39	0.55
7:H:116:DC:H2"	7:H:117:DG:C8	2.42	0.55
1:G:430:TYR:HA	1:G:487:ILE:HG23	1.88	0.55
1:G:666:PHE:HB3	2:I:287:ARG:HE	1.72	0.55
2:I:108:PRO:HG2	2:I:629:TRP:CD2	2.41	0.55
3:K:245:ASP:OD2	3:K:250:LYS:N	2.39	0.55
6:A:27:LYS:HG2	2:I:731:TYR:HB3	1.86	0.55
1:G:510:PRO:HD3	3:K:185:HIS:HD2	1.71	0.55
1:G:525:ILE:HG12	1:G:562:ASN:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:215:LEU:O	3:K:228:ILE:HA	2.07	0.55
4:O:41:GLU:HG3	4:O:42:TRP:HD1	1.70	0.55
1:B:640:VAL:O	1:B:641:GLU:HG3	2.06	0.55
2:C:554:CYS:O	2:C:561:ARG:NH1	2.39	0.55
2:C:733:TYR:HB3	2:C:737:ASP:HB2	1.88	0.55
4:L:269:VAL:HG21	4:L:307:LYS:HA	1.87	0.55
3:K:123:LEU:O	3:K:135:LEU:HB2	2.07	0.55
3:F:311:CYS:SG	3:F:367:ARG:NE	2.68	0.55
8:X:51:TYR:O	8:X:55:ARG:HG3	2.07	0.55
1:G:103:ARG:O	1:G:107:ALA:N	2.28	0.55
1:G:512:PHE:O	1:G:515:SER:OG	2.17	0.55
1:G:622:MET:HB2	2:I:291:LYS:NZ	2.21	0.55
1:G:622:MET:HB2	2:I:291:LYS:HZ2	1.71	0.55
2:I:311:TYR:HE2	2:I:313:ARG:HB2	1.70	0.55
3:F:252:MET:HB2	3:F:314:TRP:HZ2	1.72	0.55
3:K:217:LEU:HD23	3:K:226:VAL:HG11	1.88	0.55
3:F:360:GLN:NE2	3:F:382:GLN:OE1	2.40	0.55
10:V:74:ALA:HB1	10:V:86:ILE:HD11	1.89	0.55
1:G:533:PRO:HB2	1:G:535:ARG:HG2	1.87	0.55
3:K:125:GLU:OE2	3:K:127:HIS:NE2	2.39	0.55
4:O:173:LEU:HD21	4:O:207:ILE:HD11	1.88	0.55
4:O:346:ASP:N	4:O:365:GLU:O	2.39	0.55
5:Y:196:ASP:OD1	5:Y:197:ALA:N	2.39	0.55
7:H:68:DG:OP1	10:V:30:ARG:NH2	2.40	0.55
9:U:26:PRO:HB3	9:U:29:ARG:HB2	1.89	0.55
1:G:111:LEU:HD11	4:O:369:ILE:HG12	1.89	0.55
1:G:465:LYS:HG2	1:G:469:LEU:HD23	1.89	0.55
3:K:153:THR:O	3:K:162:LEU:N	2.25	0.55
5:Y:224:SER:OG	5:Y:259:ARG:NH2	2.33	0.55
1:B:189:VAL:HG23	1:B:205:GLN:HB2	1.89	0.54
11:T:138:DA:H2"	11:T:139:DG:C8	2.41	0.54
11:T:167:DT:H2"	11:T:168:DG:H5"	1.89	0.54
11:T:172:DG:H2"	11:T:173:DA:C8	2.41	0.54
1:G:103:ARG:HA	5:Y:284:ILE:HG23	1.89	0.54
1:G:541:SER:HA	1:G:544:LEU:HB2	1.89	0.54
2:I:119:ASN:ND2	2:I:648:GLY:H	2.05	0.54
2:I:687:ASN:OD1	2:I:690:ARG:N	2.39	0.54
4:O:20:GLU:O	4:O:24:TRP:N	2.35	0.54
4:O:80:VAL:HG22	4:O:120:LYS:HG2	1.88	0.54
4:O:251:LYS:HA	4:O:271:ALA:H	1.72	0.54
3:F:328:ILE:O	3:F:356:PHE:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:256:GLU:HA	5:M:259:ARG:HB3	1.90	0.54
9:U:41:GLU:OE1	9:U:42:ARG:HG3	2.07	0.54
1:G:435:ASN:HB3	1:G:437:ASN:OD1	2.06	0.54
4:O:66:LEU:N	4:O:82:ALA:O	2.36	0.54
4:O:83:SER:OG	4:O:116:GLU:OE2	2.24	0.54
4:O:172:ARG:HG2	4:O:215:LYS:O	2.06	0.54
2:C:220:SER:OG	2:C:221:ASP:N	2.40	0.54
4:L:38:HIS:HB3	4:L:399:MET:HB3	1.88	0.54
5:M:255:ASN:OD1	5:M:256:GLU:N	2.40	0.54
1:G:126:ASN:ND2	1:G:128:LYS:HE2	2.22	0.54
1:G:318:ALA:HA	1:G:354:THR:HA	1.90	0.54
2:I:243:LYS:HA	2:I:246:GLU:HB2	1.87	0.54
3:K:411:ALA:HB3	3:K:429:CYS:SG	2.48	0.54
4:L:47:ALA:N	4:L:379:ASP:OD2	2.40	0.54
7:H:124:DC:H2"	7:H:125:DG:C8	2.42	0.54
7:H:157:DT:H2"	7:H:158:DG:C8	2.42	0.54
1:G:115:LEU:HB3	1:G:117:TYR:H	1.72	0.54
1:G:195:LYS:NZ	4:O:273:THR:O	2.41	0.54
4:L:375:ALA:HB2	4:L:396:ASP:HB2	1.89	0.54
7:H:66:DC:H2"	7:H:67:DT:C5	2.42	0.54
1:G:568:SER:HA	2:I:621:LEU:HD22	1.89	0.54
2:I:445:PHE:O	2:I:475:ARG:NH2	2.41	0.54
1:B:160:THR:HG22	1:B:230:LEU:HD13	1.90	0.54
2:I:706:MET:SD	2:I:711:HIS:ND1	2.81	0.54
3:K:198:PHE:HD1	3:K:206:LEU:HB2	1.72	0.54
4:O:60:ASP:OD2	4:O:92:GLN:NE2	2.41	0.54
4:O:346:ASP:N	4:O:367:LEU:HB2	2.22	0.54
1:B:312:ASP:HB2	1:B:361:TRP:CD1	2.42	0.54
2:C:107:VAL:H	3:F:169:ARG:HH11	1.55	0.54
3:F:211:LYS:HA	3:F:238:GLU:HG3	1.89	0.54
1:G:647:ILE:O	1:G:651:ASN:N	2.40	0.54
2:I:147:GLU:HA	2:I:150:ILE:HG22	1.90	0.54
3:K:368:PHE:CD2	3:K:377:LEU:HD11	2.43	0.54
5:Y:234:SER:OG	5:Y:236:LYS:NZ	2.29	0.54
3:F:382:GLN:HA	3:F:412:ALA:HA	1.89	0.54
4:L:316:HIS:CD2	4:L:318:ASP:H	2.25	0.54
1:G:158:GLN:HB2	1:G:360:ARG:HB2	1.89	0.54
3:K:172:ILE:HD11	3:K:193:ILE:HG13	1.89	0.54
4:O:245:SER:N	4:O:253:MET:O	2.37	0.54
2:C:112:SER:HB3	3:F:212:ASP:HB3	1.90	0.54
2:C:173:GLU:N	2:C:221:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:84:CYS:HA	3:F:437:TRP:HA	1.90	0.54
4:L:279:LEU:HA	4:L:291:THR:HG22	1.89	0.54
1:G:583:SER:O	2:I:688:LYS:NZ	2.36	0.54
1:G:644:GLY:O	1:G:648:ILE:N	2.33	0.54
2:I:601:SER:O	2:I:613:ARG:NH2	2.41	0.54
2:I:619:LEU:HD23	2:I:631:ILE:HG21	1.90	0.54
3:K:184:LYS:HB3	3:K:186:TYR:HE2	1.73	0.54
3:K:234:GLY:O	3:K:261:LYS:NZ	2.36	0.54
3:K:388:VAL:O	3:K:402:THR:HB	2.07	0.54
4:O:316:HIS:HD1	4:O:318:ASP:H	1.55	0.54
1:B:238:GLU:O	1:B:248:TYR:OH	2.25	0.54
2:C:176:ASN:O	2:C:180:GLN:N	2.42	0.54
2:C:322:ASN:HD22	2:C:337:LYS:HG3	1.73	0.54
4:L:38:HIS:O	4:L:399:MET:N	2.35	0.54
11:T:92:DA:H4'	8:X:17:ARG:HH12	1.73	0.54
1:G:296:VAL:O	1:G:320:GLN:N	2.41	0.54
1:G:315:TYR:HE1	5:Y:230:ARG:HD3	1.72	0.54
2:I:165:PHE:HE2	2:I:167:ASN:HB3	1.73	0.54
2:I:590:CYS:SG	2:I:593:CYS:SG	3.06	0.54
4:O:194:LEU:HG	4:O:235:TRP:CZ2	2.43	0.54
2:C:57:ASN:OD1	3:F:420:ARG:NH1	2.41	0.53
2:C:550:LYS:NZ	2:C:562:PHE:O	2.41	0.53
3:F:114:ALA:HA	3:F:123:LEU:HA	1.90	0.53
3:F:308:TYR:O	3:F:324:CYS:N	2.37	0.53
8:J:46:ILE:HG23	8:J:50:ILE:HG21	1.90	0.53
6:W:125:GLN:NE2	8:X:53:GLU:OE2	2.40	0.53
1:G:192:CYS:SG	1:G:193:HIS:N	2.81	0.53
3:K:152:TRP:HA	3:K:163:LEU:HG	1.90	0.53
4:O:340:ARG:HG2	4:O:376:LYS:HA	1.89	0.53
5:Y:216:LYS:HB2	5:Y:218:HIS:NE2	2.23	0.53
2:C:320:LEU:HD11	2:C:456:PHE:H	1.73	0.53
3:F:125:GLU:HB2	3:F:135:LEU:HD21	1.90	0.53
4:L:316:HIS:HD2	4:L:318:ASP:H	1.54	0.53
4:L:322:GLN:NE2	4:L:379:ASP:OD1	2.41	0.53
4:L:362:GLY:HA3	4:L:366:LEU:HD23	1.88	0.53
2:I:609:CYS:O	2:I:612:GLN:NE2	2.24	0.53
2:I:660:GLY:HA2	2:I:663:TYR:HB2	1.90	0.53
4:O:334:ALA:HA	4:O:343:ASN:O	2.09	0.53
1:B:113:ARG:NH2	4:L:362:GLY:O	2.41	0.53
2:C:466:LYS:HD2	2:C:474:PHE:HB2	1.90	0.53
3:F:130:GLY:HA2	3:F:436:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:124:ILE:HD11	8:J:50:ILE:HD11	1.90	0.53
1:G:619:LEU:O	1:G:623:LYS:N	2.37	0.53
1:B:473:ARG:HH12	4:L:19:GLU:HG2	1.72	0.53
2:C:746:ARG:HH12	5:M:178:LYS:HZ3	1.57	0.53
3:F:423:SER:HA	3:F:439:ARG:HB3	1.89	0.53
4:L:48:GLN:O	4:L:67:VAL:N	2.29	0.53
7:H:84:DC:N4	11:T:143:DA:H61	2.04	0.53
11:T:88:DC:H2"	11:T:89:DA:C8	2.44	0.53
1:G:453:CYS:HB3	1:G:466:HIS:CE1	2.43	0.53
2:I:112:SER:HB3	3:K:214:ALA:HB2	1.89	0.53
4:O:335:SER:C	4:O:342:LEU:HG	2.29	0.53
4:L:130:ALA:HB2	4:L:142:THR:HG23	1.90	0.53
11:T:173:DA:H2'	11:T:174:DT:O4'	2.09	0.53
1:G:657:MET:O	1:G:661:VAL:N	2.42	0.53
2:I:442:ALA:HA	2:I:445:PHE:CD2	2.43	0.53
3:K:92:HIS:CD2	3:K:94:GLN:HB2	2.44	0.53
1:B:166:HIS:CG	1:B:167:LYS:H	2.26	0.53
9:U:88:ARG:HB3	9:U:108:LEU:HD21	1.90	0.53
2:I:336:ALA:O	2:I:472:TYR:OH	2.21	0.53
2:I:541:CYS:SG	2:I:560:ASN:ND2	2.81	0.53
2:C:684:ARG:HG2	2:C:685:LYS:HG3	1.91	0.53
3:F:102:ASN:N	3:F:112:VAL:O	2.31	0.53
7:H:56:DT:H2"	7:H:57:DG:C8	2.44	0.53
1:G:652:LEU:HD13	2:I:265:ASP:HB2	1.91	0.53
2:I:467:THR:OG1	2:I:470:GLN:NE2	2.42	0.53
2:I:479:SER:HA	2:I:482:ILE:HG12	1.91	0.53
1:B:431:GLN:NE2	1:B:432:PHE:O	2.42	0.53
2:C:619:LEU:HD12	2:C:688:LYS:HB2	1.91	0.53
3:F:358:TYR:CE2	3:F:361:CYS:HB3	2.44	0.53
4:L:37:THR:HA	4:L:400:GLN:HA	1.91	0.53
5:M:211:ILE:O	5:M:217:GLY:N	2.34	0.53
1:G:605:ASP:HA	2:I:256:LEU:HA	1.90	0.53
2:I:289:CYS:HB3	2:I:294:CYS:SG	2.49	0.53
2:I:701:TYR:O	2:I:716:PHE:N	2.21	0.53
3:K:101:PHE:HE2	3:K:111:LEU:HD23	1.73	0.53
4:O:149:VAL:HB	4:O:173:LEU:HB2	1.91	0.53
4:O:293:SER:HG	4:O:297:THR:HG1	1.54	0.53
1:B:113:ARG:HA	1:B:121:ARG:HD2	1.90	0.53
2:C:324:PRO:HB3	2:C:331:GLN:HE21	1.74	0.53
4:L:350:ILE:HA	4:L:365:GLU:HB3	1.91	0.53
7:H:39:DT:H2"	7:H:40:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:ASP:HB2	1:G:309:GLN:HE21	1.72	0.53
1:G:596:THR:O	1:G:600:ILE:HG13	2.09	0.53
3:K:90:GLU:HG3	3:K:92:HIS:H	1.73	0.53
4:O:186:ASN:OD1	4:O:189:LEU:N	2.39	0.53
1:B:653:CYS:O	1:B:657:MET:HG2	2.09	0.53
2:C:704:VAL:HA	2:C:713:ILE:HA	1.91	0.53
4:L:56:PRO:HG2	4:L:59:LYS:HB2	1.91	0.53
4:L:253:MET:CE	4:L:255:TRP:HE1	2.20	0.53
2:I:750:ILE:HD11	5:Y:178:LYS:HE3	1.91	0.53
3:K:249:GLU:HA	3:K:265:ILE:HB	1.90	0.53
4:O:253:MET:HG3	4:O:268:SER:OG	2.09	0.53
1:B:567:HIS:CE1	1:B:574:LEU:HA	2.45	0.52
2:C:702:ALA:HB1	2:C:713:ILE:HD11	1.91	0.52
3:F:260:LEU:HG	3:F:331:TRP:HZ2	1.73	0.52
4:L:202:ILE:HB	4:L:223:PHE:HB2	1.92	0.52
9:U:59:THR:HA	9:U:62:ILE:HG22	1.91	0.52
1:G:535:ARG:HH12	4:O:30:PHE:C	2.12	0.52
3:K:270:MET:O	3:K:274:ILE:HG12	2.09	0.52
4:O:49:TRP:NE1	4:O:382:TRP:O	2.41	0.52
1:B:318:ALA:HA	1:B:354:THR:HA	1.92	0.52
3:F:101:PHE:O	3:F:152:TRP:NE1	2.40	0.52
9:U:47:ALA:HB2	10:V:87:THR:HA	1.90	0.52
6:W:114:ALA:O	6:W:116:ARG:HG3	2.09	0.52
4:O:408:ILE:HG13	4:O:409:TYR:CD1	2.45	0.52
2:C:96:ILE:HD12	3:F:134:LEU:HG	1.91	0.52
4:L:280:SER:HB2	4:L:325:TRP:CD1	2.44	0.52
1:G:314:GLU:HG3	5:Y:231:LYS:H	1.75	0.52
1:G:319:MET:SD	1:G:353:PRO:HB2	2.49	0.52
2:I:17:LYS:HB3	2:I:223:ILE:HG12	1.91	0.52
2:I:311:TYR:CE2	2:I:313:ARG:HB2	2.44	0.52
3:K:100:GLN:HB3	3:K:152:TRP:CD1	2.44	0.52
3:K:190:GLY:N	3:K:212:ASP:OD2	2.38	0.52
4:L:61:PHE:HB2	4:L:85:GLN:HB2	1.92	0.52
4:L:295:ASP:O	4:L:297:THR:HG23	2.09	0.52
5:M:218:HIS:HB2	5:M:268:HIS:CE1	2.44	0.52
8:X:64:ASN:HB3	8:X:93:GLN:HE22	1.74	0.52
2:I:329:CYS:H	2:I:332:HIS:HD2	1.54	0.52
3:K:101:PHE:CE2	3:K:111:LEU:HD23	2.45	0.52
3:K:119:ASN:ND2	3:K:140:ASP:O	2.42	0.52
1:B:430:TYR:CE2	1:B:444:ALA:HA	2.44	0.52
3:F:299:PHE:HB2	3:F:343:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:55:GLN:NE2	9:R:110:ASN:H	2.08	0.52
9:U:91:GLU:HA	9:U:94:ASN:HB3	1.92	0.52
1:G:452:TRP:HB3	1:G:471:HIS:CE1	2.44	0.52
1:G:557:TYR:N	5:Y:173:ARG:HH12	2.06	0.52
3:K:100:GLN:C	3:K:152:TRP:HE1	2.12	0.52
4:O:87:PRO:HB3	4:O:108:PHE:CD1	2.44	0.52
4:O:106:GLY:O	5:Y:173:ARG:NH2	2.43	0.52
4:O:257:THR:O	4:O:258:ARG:HG2	2.09	0.52
4:O:363:PRO:HG2	4:O:366:LEU:HB2	1.91	0.52
1:B:112:HIS:HA	1:B:115:LEU:HD13	1.91	0.52
2:C:119:ASN:HB3	2:C:650:ILE:HD11	1.90	0.52
2:C:530:HIS:NE2	2:C:535:CYS:SG	2.83	0.52
3:F:235:HIS:ND1	3:F:259:SER:HB2	2.23	0.52
7:H:52:DT:H2"	7:H:53:DA:C8	2.45	0.52
9:R:16:THR:HG23	9:R:19:SER:H	1.75	0.52
1:G:189:VAL:HG12	1:G:205:GLN:HG3	1.92	0.52
1:G:509:GLN:CD	3:K:185:HIS:H	2.12	0.52
1:G:567:HIS:CE1	3:K:288:PRO:HG3	2.44	0.52
1:G:584:GLU:HB2	2:I:688:LYS:NZ	2.24	0.52
2:I:507:HIS:O	2:I:511:ILE:HG12	2.10	0.52
3:K:82:PHE:CD2	3:K:439:ARG:HA	2.45	0.52
3:K:158:THR:HB	3:K:160:HIS:HD2	1.73	0.52
1:B:93:PRO:HB3	1:B:473:ARG:HD2	1.92	0.52
2:C:59:GLU:HA	2:C:62:GLN:HG2	1.90	0.52
3:F:320:LEU:HD23	3:F:330:CYS:HB2	1.92	0.52
5:M:232:GLU:HG3	5:M:238:LYS:HZ2	1.74	0.52
1:G:595:LYS:O	1:G:598:THR:OG1	2.25	0.52
1:G:662:SER:O	1:G:666:PHE:N	2.42	0.52
2:I:458:ALA:O	2:I:461:ARG:HG2	2.10	0.52
2:I:474:PHE:O	2:I:478:GLU:N	2.28	0.52
3:K:268:LYS:HA	3:K:271:MET:HB2	1.90	0.52
4:O:328:HIS:HE1	4:O:384:PRO:HA	1.75	0.52
1:B:230:LEU:HD21	1:B:360:ARG:HH11	1.75	0.52
1:B:242:SER:HA	1:B:245:VAL:HG22	1.91	0.52
2:C:620:LEU:HD11	2:C:634:LYS:HB2	1.92	0.52
3:F:176:ASN:O	3:F:180:MET:N	2.43	0.52
3:F:200:PRO:HG3	3:F:245:ASP:O	2.09	0.52
4:O:394:SER:OG	4:O:398:ILE:N	2.29	0.52
1:B:189:VAL:HA	1:B:205:GLN:HA	1.91	0.52
4:L:84:VAL:HG23	4:L:115:ILE:HG13	1.90	0.52
8:X:68:ASP:O	8:X:71:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:GLN:HE22	3:K:133:ARG:HA	1.74	0.52
2:I:128:LEU:HD22	2:I:150:ILE:HD13	1.91	0.52
2:C:20:LYS:NZ	2:C:180:GLN:OE1	2.43	0.52
2:C:116:LEU:HD11	2:C:118:GLN:NE2	2.25	0.52
3:F:103:TRP:HB3	3:F:420:ARG:HH21	1.75	0.52
3:F:262:LEU:HD23	3:F:343:ILE:HD11	1.92	0.52
3:F:271:MET:O	3:F:275:LYS:NZ	2.34	0.52
4:L:257:THR:HG22	4:L:258:ARG:N	2.24	0.52
8:J:92:ARG:HD2	10:V:97:LEU:HD23	1.92	0.52
11:T:126:DT:P	2:I:503:LEU:HD21	2.50	0.52
1:G:503:PRO:HB3	1:G:564:LEU:HB2	1.92	0.52
3:K:113:PHE:CE2	3:K:124:TYR:HB2	2.46	0.52
4:O:237:LEU:HG	4:O:281:PHE:HB2	1.92	0.52
4:O:344:VAL:HB	4:O:368:PHE:HB3	1.92	0.52
4:O:346:ASP:OD2	4:O:349:LYS:HB2	2.11	0.52
3:F:188:GLY:O	3:F:216:ARG:NH1	2.35	0.51
3:F:386:LEU:HD23	3:F:404:LEU:HD12	1.93	0.51
7:H:59:DC:OP2	10:V:53:SER:N	2.40	0.51
3:K:301:THR:OG1	3:K:303:ASP:OD1	2.20	0.51
4:O:205:TRP:CD1	4:O:217:VAL:HG12	2.45	0.51
1:B:244:MET:HA	4:L:273:THR:HG22	1.91	0.51
2:C:586:ASP:H	2:C:589:LEU:HD12	1.74	0.51
3:F:271:MET:HA	3:F:274:ILE:HD12	1.93	0.51
4:L:341:ARG:NH1	4:L:369:ILE:O	2.42	0.51
11:T:170:DC:H2"	11:T:171:DA:C8	2.45	0.51
1:G:676:LYS:O	1:G:679:THR:OG1	2.25	0.51
4:O:316:HIS:NE2	4:O:339:ASP:OD1	2.43	0.51
3:F:222:THR:HG21	3:F:278:TYR:HA	1.91	0.51
5:M:233:ASP:OD1	5:M:234:SER:N	2.43	0.51
6:A:27:LYS:HD2	2:I:729:PHE:HZ	1.74	0.51
9:R:64:GLU:HA	10:S:45:VAL:HG21	1.91	0.51
1:G:567:HIS:NE2	1:G:574:LEU:HA	2.25	0.51
3:K:89:LYS:NZ	3:K:90:GLU:O	2.42	0.51
5:Y:239:LEU:N	5:Y:254:VAL:O	2.32	0.51
1:B:430:TYR:N	1:B:442:THR:O	2.32	0.51
2:C:701:TYR:CZ	2:C:716:PHE:HB2	2.46	0.51
4:L:202:ILE:O	4:L:223:PHE:N	2.34	0.51
7:H:191:DC:O2	11:T:37:DG:N2	2.43	0.51
8:J:90:LEU:HD12	8:J:95:ARG:HB3	1.93	0.51
11:T:101:DA:OP2	8:X:36:ARG:NH2	2.41	0.51
9:U:115:LEU:HD12	8:X:44:LYS:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:440:ALA:O	2:I:443:SER:OG	2.19	0.51
2:C:694:HIS:HB3	13:C:801:SAH:HN61	1.75	0.51
11:T:82:DC:H2'	11:T:83:DA:C8	2.45	0.51
2:I:565:CYS:SG	2:I:590:CYS:HB2	2.51	0.51
4:O:36:MET:HE2	4:O:115:ILE:HD12	1.93	0.51
1:B:307:ARG:NH2	1:B:308:LEU:O	2.44	0.51
1:B:504:GLN:HE22	1:B:508:ARG:HB3	1.75	0.51
4:L:185:TRP:CD2	4:L:193:LEU:HD12	2.45	0.51
4:L:186:ASN:ND2	4:L:189:LEU:HB2	2.26	0.51
6:A:116:ARG:NH2	6:A:120:MET:HG2	2.26	0.51
7:H:137:DC:H2"	7:H:138:DT:C5	2.46	0.51
1:G:100:LEU:HD23	1:G:103:ARG:HE	1.75	0.51
1:G:523:THR:HG23	1:G:576:PRO:HB3	1.92	0.51
3:K:311:CYS:HB3	3:K:368:PHE:CD1	2.45	0.51
2:C:321:ASP:H	2:C:323:LYS:NZ	2.09	0.51
4:L:172:ARG:O	4:L:217:VAL:N	2.39	0.51
7:H:84:DC:H42	11:T:143:DA:N6	2.07	0.51
7:H:194:DC:H2"	7:H:195:DA:C8	2.46	0.51
10:S:36:ILE:HG13	10:S:37:TYR:CD1	2.46	0.51
2:I:286:CYS:HB3	2:I:294:CYS:SG	2.51	0.51
2:I:670:PHE:CE1	2:I:690:ARG:HB2	2.44	0.51
2:C:284:LEU:HB3	2:C:292:TYR:HD2	1.76	0.51
4:L:50:LEU:HB3	4:L:52:ASP:OD1	2.10	0.51
7:H:77:DG:H2"	7:H:78:DG:N7	2.26	0.51
2:I:27:ARG:O	2:I:30:LYS:HG3	2.10	0.51
3:K:269:ARG:NH1	3:K:293:LYS:H	2.08	0.51
3:K:428:VAL:HG22	3:K:434:ILE:HG22	1.93	0.51
4:O:15:ARG:HG3	5:Y:189:PHE:CE2	2.46	0.51
4:O:43:PRO:HG2	4:O:71:HIS:HB3	1.92	0.51
4:O:151:VAL:HG23	4:O:172:ARG:HA	1.93	0.51
1:B:627:ILE:HA	2:C:290:PHE:CZ	2.45	0.51
2:C:662:VAL:HA	2:C:665:LYS:HE2	1.93	0.51
1:B:124:ARG:CZ	4:L:354:GLN:HA	2.41	0.51
4:L:71:HIS:CE1	5:M:294:LYS:HE3	2.46	0.51
4:L:322:GLN:HB3	4:L:336:SER:HB3	1.93	0.51
4:O:64:HIS:O	4:O:84:VAL:N	2.36	0.51
4:O:386:GLU:HB3	4:O:389:VAL:HG12	1.93	0.51
1:B:534:LYS:HB2	4:L:93:PHE:HB3	1.92	0.50
2:C:240:LEU:HA	2:C:243:LYS:HD2	1.92	0.50
3:K:328:ILE:HB	3:K:356:PHE:O	2.11	0.50
4:O:185:TRP:CE2	4:O:193:LEU:HD12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HH22	1:B:130:LYS:HE2	1.75	0.50
1:B:314:GLU:HB3	5:M:231:LYS:HB3	1.93	0.50
1:B:450:CYS:HG	1:B:471:HIS:HE2	1.59	0.50
3:F:89:LYS:HG3	3:F:433:SER:HB3	1.93	0.50
7:H:122:DT:P	6:W:46:VAL:HB	2.51	0.50
1:G:96:ILE:O	1:G:100:LEU:HG	2.11	0.50
1:G:450:CYS:HB3	1:G:455:LEU:N	2.18	0.50
2:I:54:GLU:HA	2:I:57:ASN:HB3	1.93	0.50
2:I:224:PHE:HA	2:I:227:ILE:HD12	1.93	0.50
3:K:226:VAL:HG12	3:K:227:ALA:N	2.25	0.50
3:K:370:MET:SD	3:K:374:GLN:HG3	2.50	0.50
2:C:23:TYR:CD2	2:C:175:VAL:HG22	2.46	0.50
3:F:264:ARG:HD2	3:F:298:ASP:OD2	2.11	0.50
3:F:328:ILE:N	3:F:356:PHE:O	2.37	0.50
4:L:79:LEU:N	4:L:121:ILE:O	2.44	0.50
4:L:300:LEU:HG	4:L:310:LEU:HB2	1.93	0.50
4:L:387:PRO:HG2	4:L:388:TRP:CD1	2.47	0.50
11:T:152:DC:H5"	9:U:44:GLY:HA2	1.92	0.50
2:I:649:GLU:N	2:I:681:ASP:O	2.43	0.50
3:K:231:GLY:HA3	3:K:295:HIS:CE1	2.47	0.50
3:K:376:MET:HA	3:K:390:ASP:HA	1.93	0.50
1:B:590:GLU:OE1	1:B:590:GLU:N	2.43	0.50
2:C:621:LEU:HD11	2:C:629:TRP:HE3	1.75	0.50
9:U:74:LYS:O	9:U:74:LYS:HD3	2.11	0.50
6:W:84:PHE:CD1	8:X:81:VAL:HB	2.46	0.50
1:B:317:VAL:HG23	1:B:319:MET:HE3	1.94	0.50
2:C:619:LEU:HD13	2:C:631:ILE:HG21	1.94	0.50
3:F:173:ARG:NH2	3:F:184:LYS:O	2.44	0.50
9:R:24:GLN:NE2	10:S:40:LYS:HE3	2.27	0.50
9:U:26:PRO:HG3	10:V:37:TYR:HE2	1.75	0.50
1:G:473:ARG:HG3	1:G:495:TYR:CD2	2.46	0.50
2:I:45:ASN:O	2:I:49:ILE:HG12	2.12	0.50
2:I:445:PHE:HA	2:I:475:ARG:NH1	2.26	0.50
3:K:120:ARG:HA	3:K:139:VAL:HA	1.94	0.50
3:K:216:ARG:CD	3:K:228:ILE:HG12	2.42	0.50
3:K:260:LEU:O	3:K:300:SER:HA	2.11	0.50
4:O:43:PRO:O	4:O:71:HIS:N	2.43	0.50
4:O:350:ILE:HA	4:O:365:GLU:HB3	1.93	0.50
3:F:99:VAL:H	3:F:415:GLN:HG2	1.77	0.50
3:F:235:HIS:CE1	3:F:255:GLY:H	2.30	0.50
8:J:35:ARG:O	8:J:39:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:26:PRO:CB	9:U:29:ARG:HB2	2.42	0.50
2:I:66:GLN:NE2	2:I:67:PRO:O	2.38	0.50
2:I:448:LEU:HD13	2:I:451:THR:HG21	1.94	0.50
2:C:681:ASP:OD2	2:C:684:ARG:NH2	2.45	0.50
3:F:216:ARG:HD3	3:F:228:ILE:HD12	1.94	0.50
9:U:115:LEU:O	8:X:44:LYS:HD2	2.11	0.50
1:G:158:GLN:HE22	1:G:232:VAL:HG13	1.77	0.50
3:K:378:ALA:HA	3:K:388:VAL:HA	1.94	0.50
1:B:244:MET:SD	1:B:244:MET:N	2.85	0.50
1:B:458:ARG:NE	4:L:357:GLU:OE2	2.45	0.50
2:C:79:GLY:C	5:M:199:ARG:HH12	2.15	0.50
3:F:264:ARG:HH12	3:F:343:ILE:HG12	1.77	0.50
4:L:289:LEU:O	4:L:301:TRP:N	2.41	0.50
7:H:100:DA:H2"	7:H:101:DA:C8	2.47	0.50
9:U:16:THR:HG23	9:U:19:SER:H	1.76	0.50
10:V:100:PRO:HD2	10:V:103:LEU:HD12	1.94	0.50
6:W:62:ILE:HD11	8:X:37:LEU:HD11	1.94	0.50
1:G:121:ARG:NE	4:O:357:GLU:HB3	2.26	0.50
3:K:127:HIS:CD2	3:K:133:ARG:HD3	2.47	0.50
3:K:176:ASN:O	3:K:180:MET:N	2.42	0.50
3:K:269:ARG:CZ	3:K:294:ILE:HG13	2.41	0.50
4:O:56:PRO:HD3	4:O:63:ILE:HG13	1.94	0.50
1:B:647:ILE:O	1:B:651:ASN:N	2.44	0.49
4:L:63:ILE:HA	4:L:85:GLN:HA	1.92	0.49
4:L:329:ASN:HB3	4:L:332:ILE:HD13	1.93	0.49
9:R:31:HIS:O	9:R:35:ARG:HG3	2.12	0.49
1:G:597:ILE:HA	1:G:600:ILE:HD12	1.94	0.49
1:G:611:LYS:O	1:G:615:LYS:HG3	2.12	0.49
2:I:332:HIS:HB2	2:I:469:ARG:HH11	1.77	0.49
3:K:99:VAL:HG22	3:K:415:GLN:HB3	1.92	0.49
3:K:194:ASN:HB2	3:K:240:LEU:HG	1.94	0.49
1:B:478:TYR:N	1:B:547:GLU:HG3	2.23	0.49
1:B:658:LEU:HA	1:B:661:VAL:HG12	1.93	0.49
1:B:678:VAL:HG21	2:C:462:LEU:HD21	1.92	0.49
3:F:328:ILE:HG13	3:F:358:TYR:CE1	2.47	0.49
4:L:6:ALA:HA	4:L:9:ASP:HB2	1.93	0.49
5:M:268:HIS:HB3	5:M:271:LYS:HE2	1.94	0.49
1:G:607:ASN:HB2	1:G:610:GLU:OE2	2.12	0.49
2:I:150:ILE:O	2:I:154:ASP:N	2.44	0.49
2:I:165:PHE:CE2	2:I:167:ASN:HB3	2.47	0.49
2:I:456:PHE:HA	2:I:459:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:651:ILE:HD11	2:I:671:LEU:HD11	1.94	0.49
2:I:745:GLU:OE1	2:I:745:GLU:N	2.45	0.49
3:K:87:SER:OG	3:K:434:ILE:O	2.18	0.49
3:K:150:CYS:HA	3:K:165:VAL:HA	1.95	0.49
5:Y:241:LEU:HD11	5:Y:254:VAL:HG22	1.94	0.49
5:Y:270:SER:HG	5:Y:271:LYS:HZ2	1.59	0.49
5:Y:275:ASP:OD1	5:Y:276:THR:N	2.45	0.49
3:F:96:LEU:HG	3:F:432:ALA:HA	1.94	0.49
4:L:43:PRO:HB3	4:L:395:GLU:HA	1.95	0.49
7:H:118:DT:H2"	7:H:119:DA:N7	2.28	0.49
8:J:44:LYS:CB	9:R:115:LEU:HD22	2.41	0.49
1:G:563:ARG:NH1	2:I:625:ASP:OD1	2.45	0.49
1:G:610:GLU:OE1	1:G:610:GLU:N	2.36	0.49
2:I:510:LYS:HA	2:I:513:LEU:HG	1.95	0.49
3:K:119:ASN:HA	3:K:147:PHE:HD2	1.77	0.49
4:O:39:ALA:HA	4:O:398:ILE:HD13	1.95	0.49
5:Y:259:ARG:HG3	5:Y:263:LYS:NZ	2.27	0.49
2:C:86:THR:O	3:F:89:LYS:N	2.36	0.49
2:C:599:TRP:HA	2:C:613:ARG:CZ	2.42	0.49
6:A:25:ALA:C	6:A:26:ARG:HD3	2.33	0.49
2:I:150:ILE:HG13	2:I:155:GLY:HA2	1.94	0.49
2:I:328:GLN:HG2	2:I:469:ARG:HE	1.77	0.49
8:J:72:TYR:CE1	10:V:97:LEU:HD21	2.48	0.49
9:U:78:ILE:HG23	9:U:82:HIS:HB2	1.94	0.49
9:U:81:ARG:NH2	9:U:85:LEU:HG	2.27	0.49
2:I:674:LEU:HD22	2:I:678:PHE:HB2	1.95	0.49
4:O:279:LEU:HD11	4:O:289:LEU:HD11	1.94	0.49
4:O:293:SER:N	4:O:297:THR:O	2.45	0.49
3:F:194:ASN:ND2	3:F:239:VAL:O	2.46	0.49
7:H:51:DA:H2'	7:H:52:DT:H71	1.95	0.49
1:G:111:LEU:HD21	4:O:369:ILE:HG13	1.95	0.49
1:G:137:MET:O	1:G:141:VAL:HG23	2.12	0.49
3:K:120:ARG:HG2	3:K:139:VAL:HG23	1.94	0.49
5:Y:269:LEU:HA	5:Y:272:LEU:HD23	1.95	0.49
1:B:453:CYS:SG	1:B:466:HIS:NE2	2.75	0.49
2:C:636:PRO:HB3	2:C:722:GLN:HA	1.94	0.49
3:F:313:ARG:HB2	3:F:320:LEU:HB2	1.94	0.49
4:L:144:THR:HG21	4:L:150:LEU:HG	1.95	0.49
7:H:174:DC:H42	11:T:53:DG:H1	1.61	0.49
1:G:187:LEU:HD23	1:G:188:LEU:N	2.27	0.49
1:G:521:LYS:HB2	4:O:42:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:653:CYS:SG	1:G:654:ARG:N	2.86	0.49
3:K:312:VAL:HG13	3:K:320:LEU:O	2.11	0.49
4:O:328:HIS:CE1	4:O:385:ASN:H	2.30	0.49
5:Y:272:LEU:HD12	5:Y:276:THR:HG21	1.93	0.49
1:B:93:PRO:O	1:B:97:TYR:N	2.33	0.49
2:C:45:ASN:OD1	2:C:46:ARG:N	2.45	0.49
5:M:215:GLY:HA3	5:M:219:SER:O	2.11	0.49
9:R:81:ARG:HG2	9:R:85:LEU:HD23	1.94	0.49
1:G:137:MET:HA	1:G:140:LYS:HE3	1.94	0.49
1:G:556:THR:OG1	5:Y:173:ARG:NH1	2.41	0.49
2:I:66:GLN:HG2	3:K:160:HIS:ND1	2.28	0.49
2:I:746:ARG:HD2	5:Y:179:ARG:O	2.12	0.49
3:K:253:SER:OG	3:K:261:LYS:O	2.27	0.49
1:B:105:LEU:HD21	5:M:268:HIS:HE1	1.78	0.49
1:B:586:GLU:OE2	2:C:117:GLN:NE2	2.46	0.49
6:A:79:LYS:HB3	6:A:82:LEU:HD21	1.95	0.49
7:H:117:DG:H2"	7:H:118:DT:C5	2.48	0.49
11:T:169:DC:H2"	11:T:170:DC:C5	2.47	0.49
2:I:315:ASN:ND2	2:I:487:ALA:HB1	2.28	0.49
2:I:663:TYR:HB3	2:I:668:CYS:O	2.12	0.49
4:O:41:GLU:HG3	4:O:42:TRP:CD1	2.48	0.49
4:O:120:LYS:HB3	4:O:161:PRO:HB3	1.94	0.49
4:O:251:LYS:HE2	4:O:268:SER:HB3	1.94	0.49
4:O:367:LEU:HD23	4:O:368:PHE:HB2	1.95	0.49
1:B:113:ARG:HD3	4:L:361:ASP:HB3	1.95	0.49
7:H:56:DT:H2"	7:H:57:DG:N7	2.27	0.49
9:U:39:TYR:O	10:V:75:SER:OG	2.23	0.49
6:W:79:LYS:HG2	6:W:82:LEU:HD21	1.94	0.49
1:G:428:ILE:H	1:G:444:ALA:CB	2.26	0.49
2:I:120:PHE:CE1	2:I:295:PHE:HB2	2.48	0.49
2:I:593:CYS:SG	2:I:606:CYS:HB2	2.53	0.49
3:K:380:GLY:HA3	3:K:413:ILE:HG21	1.95	0.49
5:Y:202:ALA:O	5:Y:206:ASN:N	2.37	0.49
2:C:670:PHE:HD2	2:C:683:THR:HG23	1.78	0.48
3:F:92:HIS:CD2	3:F:94:GLN:HB3	2.48	0.48
3:F:326:ASN:HA	3:F:358:TYR:CE2	2.48	0.48
4:L:349:LYS:HG2	4:L:364:PRO:HB2	1.95	0.48
9:R:79:ILE:HG22	9:R:81:ARG:H	1.78	0.48
2:I:571:CYS:CB	2:I:585:CYS:SG	3.01	0.48
2:I:654:ASP:N	2:I:654:ASP:OD1	2.44	0.48
3:K:339:ASP:H	3:K:342:LYS:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:184:SER:C	4:O:193:LEU:HG	2.34	0.48
5:Y:227:ILE:HB	5:Y:240:LEU:HD23	1.94	0.48
3:F:243:ASP:OD2	3:F:314:TRP:N	2.47	0.48
6:A:128:ARG:HH12	8:J:60:VAL:HG11	1.78	0.48
11:T:153:DA:OP1	9:U:35:ARG:NH2	2.46	0.48
1:G:83:HIS:NE2	1:G:439:ARG:O	2.42	0.48
1:G:157:LEU:HD11	1:G:359:LEU:HG	1.94	0.48
3:K:153:THR:HA	3:K:198:PHE:HE2	1.78	0.48
3:K:183:ILE:HG13	3:K:184:LYS:HD3	1.95	0.48
3:K:217:LEU:O	3:K:226:VAL:N	2.40	0.48
3:K:287:ARG:HD2	3:K:290:ILE:HD11	1.95	0.48
4:O:56:PRO:HG2	4:O:59:LYS:HB2	1.95	0.48
4:O:399:MET:HE2	4:O:399:MET:HA	1.94	0.48
1:B:104:ASN:ND2	1:B:109:ILE:HG13	2.28	0.48
1:B:118:MET:SD	1:B:462:SER:HB2	2.54	0.48
1:B:479:VAL:N	1:B:486:ARG:O	2.30	0.48
2:C:107:VAL:HG22	3:F:169:ARG:HH11	1.78	0.48
4:L:324:GLN:NE2	4:L:380:PHE:O	2.46	0.48
9:U:15:LYS:HD2	9:U:20:ARG:HH11	1.79	0.48
2:I:645:GLU:HA	2:I:714:GLY:HA2	1.96	0.48
3:K:186:TYR:HB3	3:K:218:TRP:CZ3	2.47	0.48
3:K:339:ASP:HB3	3:K:342:LYS:HD3	1.95	0.48
5:Y:185:ARG:NE	5:Y:186:PRO:HD2	2.28	0.48
1:B:467:LEU:HD13	1:B:471:HIS:CD2	2.48	0.48
1:B:600:ILE:HB	1:B:615:LYS:HE3	1.94	0.48
6:A:71:VAL:HG23	8:J:66:ILE:HD11	1.95	0.48
8:J:70:VAL:O	8:J:73:THR:OG1	2.21	0.48
9:U:88:ARG:HG3	9:U:108:LEU:HD11	1.96	0.48
1:G:234:SER:OG	1:G:235:ASN:N	2.47	0.48
2:I:88:ASP:H	3:K:88:LEU:HA	1.77	0.48
2:I:700:CYS:HA	2:I:718:LYS:N	2.27	0.48
3:K:204:ASN:O	3:K:219:ASN:HA	2.13	0.48
3:K:215:LEU:HD22	3:K:229:PHE:HB2	1.94	0.48
3:K:311:CYS:HB2	3:K:322:LYS:HD2	1.96	0.48
1:B:87:LEU:O	1:B:91:GLU:N	2.41	0.48
1:B:492:ASN:HB3	1:B:495:TYR:HB2	1.93	0.48
4:L:120:LYS:N	4:L:159:SER:O	2.44	0.48
1:G:85:LEU:O	1:G:88:GLN:HG3	2.13	0.48
1:G:198:ASP:N	1:G:198:ASP:OD1	2.45	0.48
3:K:281:ASN:HD21	3:K:283:ASN:HB2	1.79	0.48
1:B:150:SER:HA	1:B:308:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PHE:CZ	1:B:231:ALA:HB2	2.48	0.48
1:B:478:TYR:HB3	1:B:547:GLU:HG3	1.95	0.48
2:C:436:GLU:O	2:C:465:THR:OG1	2.29	0.48
3:F:360:GLN:NE2	3:F:382:GLN:HB3	2.23	0.48
4:L:6:ALA:HB1	5:M:286:ARG:HH12	1.79	0.48
5:M:180:ARG:HD3	5:M:182:SER:N	2.28	0.48
6:A:72:ARG:HH12	7:H:90:DT:P	2.34	0.48
8:J:86:VAL:O	8:J:90:LEU:HD23	2.13	0.48
9:U:114:VAL:HG23	9:U:115:LEU:HD22	1.96	0.48
2:I:438:SER:N	2:I:441:GLU:OE1	2.25	0.48
2:I:695:SER:HB3	2:I:698:PRO:HB3	1.94	0.48
4:O:162:ASP:OD2	4:O:164:SER:HB3	2.13	0.48
4:O:324:GLN:HB3	4:O:382:TRP:CH2	2.49	0.48
2:C:273:GLN:NE2	2:C:275:GLU:HB2	2.25	0.48
3:F:373:TRP:HB3	3:F:375:LYS:HE3	1.96	0.48
4:L:120:LYS:HB3	4:L:161:PRO:HG3	1.95	0.48
7:H:77:DG:H2"	7:H:78:DG:C5	2.49	0.48
8:J:34:ILE:HG21	8:J:54:THR:HG21	1.96	0.48
9:U:64:GLU:O	9:U:68:ASN:N	2.40	0.48
1:G:526:THR:HA	4:O:38:HIS:HA	1.95	0.48
1:G:637:MET:N	1:G:637:MET:SD	2.80	0.48
2:I:512:GLN:HA	2:I:516:ASP:HB2	1.96	0.48
2:I:634:LYS:NZ	2:I:635:ASP:OD1	2.30	0.48
3:K:106:LYS:HB2	3:K:109:ASP:OD2	2.14	0.48
3:K:367:ARG:O	3:K:416:THR:OG1	2.21	0.48
1:B:479:VAL:HB	1:B:486:ARG:HB3	1.96	0.48
2:C:46:ARG:HH11	2:C:50:LEU:HD21	1.79	0.48
2:C:448:LEU:HD13	2:C:459:ILE:HA	1.94	0.48
4:L:153:ASP:H	4:L:157:HIS:HD2	1.60	0.48
5:M:221:VAL:HA	5:M:266:VAL:HA	1.96	0.48
7:H:76:DG:H2"	7:H:77:DG:C8	2.49	0.48
10:S:90:GLU:HA	10:S:93:THR:HG22	1.95	0.48
1:G:610:GLU:O	1:G:613:VAL:HG12	2.13	0.48
1:B:121:ARG:HB3	4:L:358:ASP:OD1	2.14	0.48
1:B:359:LEU:HD23	1:B:360:ARG:N	2.29	0.48
2:C:320:LEU:HB2	2:C:323:LYS:HD2	1.96	0.48
3:F:250:LYS:HG2	3:F:264:ARG:HA	1.96	0.48
3:F:250:LYS:HG2	3:F:264:ARG:HG3	1.96	0.48
3:F:269:ARG:HH11	3:F:292:GLN:HB3	1.79	0.48
4:L:64:HIS:O	4:L:84:VAL:N	2.42	0.48
8:X:92:ARG:O	8:X:92:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:46:ARG:O	2:I:50:LEU:N	2.42	0.48
2:I:89:LEU:HD11	3:K:86:ASN:HA	1.96	0.48
2:I:150:ILE:HD12	2:I:153:TYR:HB2	1.94	0.48
4:O:24:TRP:CE2	4:O:372:GLY:HA3	2.48	0.48
1:B:315:TYR:HE2	1:B:359:LEU:HB2	1.78	0.48
2:C:122:VAL:HB	2:C:651:ILE:HG22	1.96	0.48
2:C:640:ASN:N	2:C:717:ALA:O	2.34	0.48
3:F:311:CYS:HB2	3:F:322:LYS:HB3	1.95	0.48
4:L:342:LEU:HD12	4:L:370:HIS:HD2	1.79	0.48
8:J:76:ALA:HB3	8:J:78:ARG:HG2	1.96	0.48
1:G:567:HIS:CE1	1:G:574:LEU:HA	2.49	0.48
2:I:159:GLY:O	3:K:306:ARG:NH2	2.47	0.48
2:I:469:ARG:C	2:I:471:VAL:H	2.16	0.48
3:K:96:LEU:HG	3:K:432:ALA:HA	1.95	0.48
3:K:249:GLU:OE1	3:K:249:GLU:N	2.47	0.48
1:B:94:THR:HG23	1:B:452:TRP:CD1	2.49	0.47
1:B:631:GLN:O	1:B:635:ALA:N	2.47	0.47
2:C:434:ASN:HB2	2:C:466:LYS:HE2	1.96	0.47
4:L:174:ARG:N	4:L:217:VAL:O	2.47	0.47
4:L:185:TRP:CE2	4:L:193:LEU:HD12	2.49	0.47
7:H:56:DT:O2	11:T:172:DG:N2	2.46	0.47
1:G:475:ILE:HG23	1:G:492:ASN:HA	1.95	0.47
1:G:671:ILE:HA	1:G:674:ILE:HD12	1.94	0.47
2:I:170:ILE:HD12	2:I:170:ILE:H	1.79	0.47
5:Y:206:ASN:ND2	5:Y:212:GLU:HB2	2.29	0.47
1:B:309:GLN:NE2	5:M:230:ARG:HH12	2.12	0.47
1:B:496:ASP:HA	5:M:186:PRO:HG3	1.96	0.47
2:C:65:ILE:HG23	3:F:161:PRO:HG3	1.96	0.47
10:V:35:ALA:HA	10:V:56:MET:SD	2.54	0.47
1:G:115:LEU:C	1:G:117:TYR:H	2.16	0.47
2:I:549:GLU:HG3	2:I:551:PHE:H	1.79	0.47
2:I:590:CYS:HB3	2:I:595:ALA:HB2	1.95	0.47
2:I:750:ILE:HG23	5:Y:174:LYS:HE2	1.95	0.47
3:K:174:ILE:N	3:K:182:CYS:SG	2.87	0.47
3:K:265:ILE:O	3:K:267:SER:N	2.47	0.47
4:O:48:GLN:HE21	4:O:131:ARG:CZ	2.28	0.47
2:C:29:LEU:HD22	2:C:33:ARG:HH11	1.79	0.47
3:F:233:GLU:HB3	3:F:295:HIS:O	2.14	0.47
5:M:221:VAL:HG23	5:M:266:VAL:HG22	1.95	0.47
7:H:99:DA:H2"	7:H:100:DA:C8	2.49	0.47
9:R:93:LEU:HD22	10:S:103:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:79:LYS:HG3	6:W:80:THR:N	2.21	0.47
2:I:59:GLU:HA	2:I:62:GLN:HG2	1.96	0.47
2:I:573:THR:HG22	2:I:574:LYS:H	1.79	0.47
3:K:293:LYS:HB3	3:K:295:HIS:NE2	2.30	0.47
3:K:419:SER:HB3	3:K:424:ILE:HB	1.96	0.47
4:O:261:ASN:HB2	4:O:264:LYS:HG2	1.96	0.47
2:C:327:PRO:O	2:C:328:GLN:NE2	2.47	0.47
2:C:593:CYS:SG	2:C:606:CYS:HB2	2.54	0.47
3:F:229:PHE:HE1	3:F:294:ILE:HD13	1.79	0.47
3:F:386:LEU:O	3:F:404:LEU:N	2.47	0.47
4:L:272:HIS:HD2	4:L:293:SER:HB3	1.80	0.47
9:U:91:GLU:OE1	9:U:91:GLU:N	2.43	0.47
1:G:572:LEU:HD11	3:K:225:LEU:HD23	1.94	0.47
2:I:65:ILE:HD11	3:K:161:PRO:HB3	1.96	0.47
2:I:449:ILE:HD12	2:I:453:TYR:HA	1.96	0.47
2:I:616:LYS:HZ2	2:I:644:SER:HB3	1.79	0.47
2:C:339:PHE:HA	2:C:342:ALA:HB3	1.96	0.47
2:C:687:ASN:HD21	2:C:689:ILE:HG22	1.80	0.47
3:F:90:GLU:HG2	3:F:432:ALA:HB1	1.96	0.47
1:G:519:PRO:HG2	4:O:72:THR:C	2.34	0.47
1:G:666:PHE:HB2	1:G:668:LEU:HG	1.95	0.47
3:K:305:HIS:HD2	3:K:309:VAL:HB	1.79	0.47
3:K:359:SER:O	3:K:381:ASN:ND2	2.47	0.47
4:O:28:THR:HG23	4:O:32:TYR:CE1	2.50	0.47
3:F:308:TYR:HB2	3:F:324:CYS:SG	2.54	0.47
5:M:281:ASP:HB3	5:M:284:ILE:HG13	1.97	0.47
3:K:375:LYS:O	3:K:391:LEU:N	2.48	0.47
4:O:133:MET:HB2	4:O:185:TRP:CE2	2.50	0.47
1:B:91:GLU:HA	1:B:94:THR:HB	1.96	0.47
1:B:521:LYS:NZ	1:B:576:PRO:O	2.44	0.47
2:C:643:ILE:HB	2:C:715:ILE:HB	1.97	0.47
4:L:74:ASP:OD1	4:L:74:ASP:N	2.47	0.47
4:L:148:ASP:HA	4:L:174:ARG:HG3	1.96	0.47
4:L:282:ASN:HB2	4:L:288:ILE:HB	1.95	0.47
4:L:341:ARG:HE	4:L:369:ILE:HG13	1.79	0.47
4:L:373:HIS:CG	4:L:377:ILE:HD13	2.50	0.47
5:M:222:PHE:HB3	5:M:243:TRP:CE3	2.49	0.47
7:H:119:DA:H1'	7:H:120:DC:C2	2.49	0.47
7:H:196:DG:N2	11:T:32:DC:O2	2.48	0.47
10:V:48:ASP:OD1	10:V:48:ASP:N	2.47	0.47
6:W:47:ALA:O	6:W:51:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:SER:HA	1:G:300:THR:HA	1.95	0.47
1:G:451:PRO:HB2	1:G:452:TRP:CE3	2.49	0.47
1:G:626:PHE:CD1	1:G:631:GLN:HG2	2.35	0.47
2:I:624:SER:N	2:I:628:GLY:O	2.31	0.47
3:K:121:VAL:O	3:K:137:SER:HB3	2.14	0.47
3:K:258:HIS:HB2	3:K:302:ARG:HE	1.80	0.47
5:Y:205:PHE:HE1	5:Y:280:LEU:HB2	1.80	0.47
2:C:339:PHE:O	2:C:343:LEU:N	2.36	0.47
2:C:624:SER:N	2:C:628:GLY:O	2.46	0.47
3:F:332:LYS:NZ	3:F:335:LYS:O	2.48	0.47
4:L:331:THR:HA	4:L:347:LEU:HB2	1.96	0.47
9:R:32:ARG:NH2	10:S:32:GLU:OE2	2.47	0.47
11:T:79:DA:C6	11:T:80:DG:C6	3.02	0.47
6:W:103:LEU:HD21	6:W:124:ILE:HG13	1.96	0.47
1:G:508:ARG:HH11	1:G:514:PHE:N	2.13	0.47
2:I:58:GLN:O	2:I:62:GLN:HG2	2.14	0.47
3:K:101:PHE:CD1	3:K:113:PHE:HB3	2.50	0.47
3:K:287:ARG:HD3	3:K:288:PRO:HD2	1.96	0.47
4:O:225:GLY:HA2	4:O:263:SER:O	2.15	0.47
5:Y:289:PRO:O	5:Y:290:GLN:HG2	2.15	0.47
1:B:607:ASN:ND2	2:C:261:THR:O	2.47	0.47
2:C:71:LEU:HG	3:F:136:GLN:NE2	2.30	0.47
5:M:225:THR:N	5:M:242:HIS:O	2.35	0.47
7:H:180:DC:H1’	7:H:181:DC:C6	2.50	0.47
2:I:18:ARG:HE	2:I:230:MET:HE1	1.79	0.47
2:I:54:GLU:O	2:I:58:GLN:N	2.44	0.47
4:O:54:THR:O	4:O:62:SER:OG	2.31	0.47
4:O:72:THR:HG21	4:O:75:GLU:O	2.14	0.47
2:C:321:ASP:H	2:C:323:LYS:HZ3	1.63	0.47
11:T:124:DC:H2”	11:T:125:DG:C8	2.50	0.47
1:G:204:ARG:HD3	1:G:204:ARG:H	1.80	0.47
1:G:528:ILE:HG13	4:O:36:MET:HG2	1.96	0.47
2:I:745:GLU:OE2	5:Y:181:ARG:NH2	2.48	0.47
3:K:183:ILE:C	3:K:184:LYS:HD3	2.35	0.47
4:O:55:ARG:NH2	4:O:88:ASN:OD1	2.48	0.47
5:Y:222:PHE:CE1	5:Y:245:PRO:HG2	2.50	0.47
1:B:161:PHE:CE2	1:B:211:LYS:HB3	2.49	0.46
2:C:20:LYS:HA	2:C:23:TYR:CD2	2.50	0.46
2:C:46:ARG:HH12	3:F:375:LYS:HG2	1.79	0.46
2:C:173:GLU:O	2:C:177:ALA:N	2.48	0.46
3:F:100:GLN:HG3	3:F:152:TRP:NE1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:243:TRP:HB2	5:M:248:ILE:HG21	1.97	0.46
7:H:57:DG:H2"	7:H:58:DA:H8	1.80	0.46
6:W:103:LEU:HD11	6:W:128:ARG:HH12	1.80	0.46
2:I:731:TYR:HB3	2:I:733:TYR:CE1	2.49	0.46
3:K:329:VAL:HG23	3:K:354:GLY:O	2.15	0.46
4:O:336:SER:HB2	4:O:342:LEU:HB2	1.97	0.46
4:O:391:CYS:HA	4:O:400:GLN:O	2.14	0.46
1:B:430:TYR:HB2	1:B:442:THR:OG1	2.16	0.46
1:B:643:TYR:HA	1:B:646:LYS:HD3	1.98	0.46
3:F:276:GLU:HA	3:F:279:ASP:HB3	1.97	0.46
4:L:54:THR:HG23	4:L:65:ARG:HH12	1.79	0.46
7:H:120:DC:H4'	8:X:45:ARG:NE	2.25	0.46
6:W:121:PRO:HB3	8:X:53:GLU:OE1	2.16	0.46
1:G:655:ASN:HA	1:G:658:LEU:HD12	1.97	0.46
1:G:671:ILE:H	1:G:671:ILE:HD12	1.80	0.46
2:I:100:THR:HG21	5:Y:193:GLN:HB3	1.96	0.46
2:I:296:LEU:HD23	2:I:296:LEU:H	1.81	0.46
2:I:527:PRO:HA	2:I:552:CYS:SG	2.54	0.46
2:I:564:GLY:HA2	2:I:589:LEU:HD12	1.97	0.46
2:I:742:VAL:HG12	13:I:801:SAH:C8	2.45	0.46
3:K:250:LYS:HE2	3:K:314:TRP:HH2	1.80	0.46
4:O:36:MET:HB3	4:O:401:VAL:HB	1.96	0.46
4:L:309:LYS:HD3	4:L:312:SER:HB3	1.97	0.46
4:L:386:GLU:HB3	4:L:389:VAL:HG12	1.96	0.46
6:W:121:PRO:HA	6:W:124:ILE:HG22	1.97	0.46
1:G:93:PRO:HA	1:G:96:ILE:HD12	1.97	0.46
1:G:430:TYR:HB2	1:G:442:THR:OG1	2.16	0.46
1:G:450:CYS:HG	1:G:466:HIS:HE2	1.63	0.46
3:K:394:GLU:OE1	3:K:394:GLU:N	2.41	0.46
4:O:173:LEU:HD22	4:O:205:TRP:CG	2.51	0.46
2:C:57:ASN:HA	2:C:60:TRP:HB3	1.97	0.46
2:C:548:CYS:HB2	2:C:560:ASN:HB3	1.98	0.46
3:F:279:ASP:OD1	3:F:284:LYS:NZ	2.48	0.46
4:L:232:ASP:HB3	4:L:246:VAL:HB	1.97	0.46
9:R:31:HIS:ND1	9:R:48:PRO:HG3	2.29	0.46
11:T:185:DC:H2"	11:T:186:DG:C8	2.51	0.46
1:G:305:ASN:O	1:G:307:ARG:NH2	2.48	0.46
3:K:103:TRP:O	3:K:420:ARG:NH2	2.48	0.46
3:K:269:ARG:NH2	3:K:294:ILE:HG13	2.30	0.46
3:K:379:LEU:HG	3:K:380:GLY:O	2.15	0.46
4:O:49:TRP:CD2	4:O:383:ASN:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:233:VAL:HG12	4:O:245:SER:HA	1.96	0.46
5:Y:259:ARG:NH2	5:Y:263:LYS:HD3	2.30	0.46
1:B:230:LEU:HD11	1:B:360:ARG:HE	1.80	0.46
1:B:571:CYS:HB3	2:C:629:TRP:CZ3	2.50	0.46
1:B:576:PRO:HA	1:B:579:MET:SD	2.55	0.46
2:C:109:ILE:HD12	3:F:191:ASN:HA	1.98	0.46
3:F:154:TYR:HA	3:F:161:PRO:HA	1.96	0.46
5:M:230:ARG:HG2	5:M:238:LYS:HE2	1.98	0.46
5:M:278:LEU:HD21	5:M:285:TYR:H	1.81	0.46
11:T:163:DC:OP2	10:V:36:ILE:HD13	2.16	0.46
1:G:100:LEU:HB3	1:G:104:ASN:OD1	2.16	0.46
1:G:192:CYS:O	1:G:246:LYS:NZ	2.37	0.46
4:O:70:THR:HG22	4:O:77:ASN:OD1	2.14	0.46
4:O:176:HIS:CE1	4:O:196:ALA:HA	2.50	0.46
4:O:189:LEU:HB3	4:O:192:HIS:ND1	2.31	0.46
2:C:445:PHE:HE2	2:C:475:ARG:HD2	1.81	0.46
7:H:88:DC:N4	11:T:139:DG:H1	2.13	0.46
9:R:87:VAL:HG21	9:R:97:LEU:HD12	1.98	0.46
1:G:211:LYS:HB2	1:G:211:LYS:HE2	1.80	0.46
1:G:618:ASN:HD22	2:I:291:LYS:HE3	1.81	0.46
2:I:30:LYS:O	2:I:34:ARG:HG3	2.16	0.46
2:I:46:ARG:CZ	2:I:50:LEU:HD21	2.46	0.46
2:I:128:LEU:O	2:I:129:HIS:ND1	2.49	0.46
2:I:334:GLU:O	2:I:338:GLU:HG2	2.15	0.46
4:O:133:MET:SD	4:O:135:GLN:HB2	2.56	0.46
4:O:388:TRP:HB3	4:O:404:MET:SD	2.55	0.46
5:Y:215:GLY:HA3	5:Y:219:SER:O	2.16	0.46
1:B:477:ASN:HB3	1:B:488:ASP:O	2.16	0.46
2:C:106:SER:H	5:M:187:HIS:CD2	2.34	0.46
3:F:101:PHE:CD2	3:F:113:PHE:HB3	2.51	0.46
3:F:329:VAL:HB	3:F:355:ARG:NH1	2.30	0.46
4:L:87:PRO:HB3	4:L:108:PHE:CD2	2.51	0.46
4:L:173:LEU:HA	4:L:217:VAL:HB	1.98	0.46
5:M:239:LEU:H	5:M:254:VAL:H	1.63	0.46
6:W:119:ILE:HG21	8:X:46:ILE:HD13	1.98	0.46
1:G:218:ASP:OD1	1:G:218:ASP:N	2.47	0.46
1:G:568:SER:HB3	2:I:621:LEU:HB2	1.97	0.46
1:G:582:ASP:OD1	1:G:582:ASP:N	2.49	0.46
1:G:610:GLU:HA	1:G:613:VAL:HG12	1.98	0.46
2:I:541:CYS:HA	2:I:544:ALA:HB3	1.98	0.46
3:K:100:GLN:HB3	3:K:152:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:262:LEU:HD12	3:K:298:ASP:HB2	1.97	0.46
3:K:281:ASN:ND2	3:K:283:ASN:HB2	2.30	0.46
3:K:418:PHE:CD1	3:K:425:LEU:HD12	2.50	0.46
1:B:429:PHE:HB3	1:B:441:GLN:OE1	2.16	0.46
2:C:262:PRO:HD2	2:C:270:LYS:HE2	1.97	0.46
2:C:625:ASP:OD1	2:C:625:ASP:N	2.49	0.46
4:L:24:TRP:NE1	4:L:372:GLY:HA3	2.30	0.46
4:L:371:GLY:HA2	4:L:373:HIS:CD2	2.50	0.46
10:S:104:ALA:HA	10:S:107:ALA:HB3	1.97	0.46
3:K:140:ASP:OD1	3:K:141:ALA:N	2.49	0.46
3:K:261:LYS:HA	3:K:300:SER:HB2	1.98	0.46
4:O:15:ARG:HA	5:Y:189:PHE:HE2	1.79	0.46
1:B:250:LEU:HD23	1:B:301:VAL:HB	1.98	0.46
2:C:83:CYS:SG	2:C:98:LEU:HD21	2.56	0.46
9:R:57:TYR:CE2	10:S:106:HIS:HB2	2.51	0.46
11:T:167:DT:H1'	11:T:168:DG:O4'	2.16	0.46
9:U:25:PHE:HZ	9:U:59:THR:HG21	1.81	0.46
9:U:63:LEU:HD21	10:V:42:LEU:HB2	1.98	0.46
1:G:192:CYS:SG	1:G:245:VAL:HG12	2.56	0.46
1:G:655:ASN:O	1:G:658:LEU:HB2	2.16	0.46
2:I:515:LYS:HB3	2:I:545:GLN:NE2	2.31	0.46
2:I:664:ASP:C	2:I:667:MET:H	2.19	0.46
3:K:86:ASN:OD1	3:K:87:SER:N	2.49	0.46
2:C:289:CYS:HB3	2:C:294:CYS:SG	2.56	0.46
2:C:437:TRP:HE1	2:C:466:LYS:CD	2.29	0.46
2:C:554:CYS:HB3	2:C:558:CYS:HB3	1.53	0.46
4:L:194:LEU:HG	4:L:235:TRP:CE2	2.51	0.46
4:L:402:TRP:CZ3	4:L:404:MET:HB2	2.47	0.46
7:H:109:DG:H1'	7:H:110:DA:H5'	1.99	0.46
11:T:170:DC:H2"	11:T:171:DA:C4	2.51	0.46
1:G:624:HIS:HB2	1:G:626:PHE:CE2	2.50	0.46
2:I:565:CYS:HA	2:I:578:CYS:SG	2.56	0.46
4:O:60:ASP:N	4:O:60:ASP:OD1	2.49	0.46
4:O:175:GLY:HA3	4:O:219:ALA:HB2	1.98	0.46
4:O:186:ASN:N	4:O:192:HIS:O	2.44	0.46
4:O:193:LEU:HA	4:O:235:TRP:HE1	1.80	0.46
4:O:349:LYS:HB3	4:O:365:GLU:HA	1.97	0.46
5:Y:248:ILE:HD12	5:Y:248:ILE:H	1.81	0.46
2:C:171:PHE:HA	2:C:174:LEU:HD13	1.98	0.45
7:H:53:DA:H2"	7:H:54:DC:H5"	1.98	0.45
11:T:44:DG:H3'	2:I:569:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:126:DT:H2"	11:T:127:DT:H5'	1.97	0.45
1:G:109:ILE:HD12	4:O:23:ILE:HG21	1.98	0.45
2:I:330:TYR:HD1	2:I:331:GLN:HG2	1.80	0.45
3:K:124:TYR:CD1	3:K:134:LEU:HA	2.51	0.45
3:K:152:TRP:CD2	3:K:163:LEU:HD12	2.50	0.45
3:K:193:ILE:HA	3:K:210:SER:HA	1.97	0.45
3:K:368:PHE:CA	3:K:379:LEU:HD13	2.46	0.45
3:K:387:TYR:HD1	3:K:389:TRP:CZ2	2.35	0.45
4:O:53:VAL:HG21	4:O:64:HIS:CE1	2.51	0.45
4:O:172:ARG:N	4:O:215:LYS:O	2.49	0.45
4:O:193:LEU:CA	4:O:235:TRP:HE1	2.29	0.45
1:B:525:ILE:HA	1:B:560:GLY:HA3	1.98	0.45
2:C:649:GLU:N	2:C:681:ASP:O	2.38	0.45
3:F:183:ILE:O	3:F:183:ILE:HG13	2.17	0.45
3:F:312:VAL:HA	3:F:321:SER:HA	1.97	0.45
4:L:392:SER:O	4:L:399:MET:HA	2.16	0.45
6:A:79:LYS:HD2	8:J:74:GLU:OE2	2.17	0.45
8:J:66:ILE:HA	8:J:69:ALA:HB3	1.98	0.45
3:K:417:SER:O	3:K:425:LEU:HG	2.16	0.45
1:B:121:ARG:NH2	4:L:357:GLU:O	2.50	0.45
2:C:94:GLN:HE22	3:F:133:ARG:HA	1.82	0.45
2:C:435:VAL:HG22	2:C:466:LYS:HG2	1.97	0.45
4:L:341:ARG:HA	4:L:371:GLY:HA3	1.96	0.45
7:H:70:DA:H5"	9:U:16:THR:HA	1.98	0.45
7:H:118:DT:H2"	7:H:119:DA:C8	2.51	0.45
11:T:137:DA:H2"	11:T:138:DA:OP2	2.16	0.45
11:T:212:DG:H2"	11:T:213:DC:H5'	1.98	0.45
9:U:51:LEU:HD13	10:V:70:ILE:HG21	1.98	0.45
1:G:92:LYS:HA	1:G:95:GLN:HE21	1.80	0.45
1:G:639:PHE:CE1	1:G:643:TYR:HB2	2.52	0.45
2:I:87:SER:OG	2:I:91:PHE:HB2	2.17	0.45
3:K:95:PRO:HA	3:K:430:ASP:O	2.16	0.45
3:K:381:ASN:O	3:K:413:ILE:HG22	2.16	0.45
1:B:304:LYS:HB3	1:B:304:LYS:HE2	1.76	0.45
7:H:27:DG:H2"	7:H:28:DA:C8	2.51	0.45
7:H:195:DA:H2"	7:H:196:DG:C8	2.51	0.45
1:G:93:PRO:HB3	1:G:473:ARG:HD2	1.97	0.45
1:G:186:VAL:HG23	1:G:250:LEU:HD21	1.99	0.45
1:G:618:ASN:O	2:I:291:LYS:NZ	2.31	0.45
2:I:82:GLU:HA	2:I:97:PRO:HA	1.98	0.45
2:I:94:GLN:NE2	3:K:131:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:PHE:HA	4:O:86:LEU:O	2.17	0.45
1:B:113:ARG:HG3	1:B:122:ASN:HD21	1.81	0.45
2:C:564:GLY:HA3	2:C:589:LEU:HD22	1.98	0.45
3:F:199:HIS:CE1	3:F:201:ARG:HB2	2.52	0.45
7:H:67:DT:O4	11:T:159:DC:N4	2.50	0.45
6:W:124:ILE:HG12	6:W:128:ARG:HH11	1.82	0.45
1:G:617:TRP:HA	1:G:639:PHE:CE2	2.52	0.45
3:K:140:ASP:HB2	3:K:147:PHE:HE2	1.82	0.45
4:O:186:ASN:HD21	4:O:240:GLU:HB2	1.81	0.45
4:O:189:LEU:HG	4:O:240:GLU:OE1	2.16	0.45
5:Y:268:HIS:HB3	5:Y:271:LYS:HZ3	1.82	0.45
2:C:705:MET:O	2:C:706:MET:HE2	2.16	0.45
3:F:323:SER:O	3:F:358:TYR:OH	2.35	0.45
7:H:212:DG:N2	11:T:16:DC:O2	2.50	0.45
6:W:73:GLU:HG3	8:X:25:ASN:OD1	2.16	0.45
1:G:83:HIS:CD2	1:G:440:GLN:HB2	2.51	0.45
1:G:475:ILE:N	1:G:490:SER:O	2.47	0.45
3:K:195:GLU:HG2	3:K:242:ALA:HB3	1.98	0.45
3:K:252:MET:HG2	3:K:314:TRP:NE1	2.32	0.45
1:B:516:ARG:HH11	5:M:288:MET:HE3	1.80	0.45
1:B:617:TRP:CD2	1:B:620:HIS:HE1	2.34	0.45
2:C:227:ILE:HA	2:C:230:MET:CE	2.47	0.45
1:G:238:GLU:OE1	1:G:241:ASN:ND2	2.50	0.45
1:G:618:ASN:HD21	2:I:292:TYR:H	1.65	0.45
3:K:102:ASN:HB2	3:K:152:TRP:CH2	2.52	0.45
3:K:148:TYR:N	3:K:166:ALA:O	2.42	0.45
3:K:169:ARG:HB3	3:K:171:ILE:CD1	2.47	0.45
4:O:202:ILE:HB	4:O:223:PHE:CD1	2.52	0.45
4:O:405:ALA:O	4:O:408:ILE:HG12	2.17	0.45
5:Y:216:LYS:HB2	5:Y:218:HIS:CD2	2.52	0.45
1:B:250:LEU:HB2	1:B:299:MET:SD	2.57	0.45
1:B:575:ARG:NH1	3:F:280:TYR:HH	2.13	0.45
2:C:647:CYS:HB2	2:C:687:ASN:HB3	1.98	0.45
4:L:49:TRP:HA	4:L:66:LEU:HD13	1.98	0.45
1:G:242:SER:HA	1:G:245:VAL:HG22	1.99	0.45
1:G:251:LEU:HD22	1:G:298:GLN:HG2	1.98	0.45
3:K:281:ASN:N	3:K:284:LYS:HD3	2.31	0.45
5:Y:209:ALA:HB1	5:Y:220:VAL:HG22	1.99	0.45
5:Y:275:ASP:O	5:Y:279:LEU:HG	2.17	0.45
3:F:199:HIS:NE2	3:F:248:GLY:HA3	2.31	0.45
3:F:251:ILE:O	3:F:262:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:195:DA:H61	11:T:32:DC:H42	1.64	0.45
11:T:149:DC:H2"	11:T:150:DC:C5	2.52	0.45
1:G:516:ARG:NH1	5:Y:288:MET:O	2.50	0.45
2:I:330:TYR:CD1	2:I:331:GLN:HG2	2.52	0.45
3:K:195:GLU:HB2	3:K:240:LEU:O	2.17	0.45
3:K:227:ALA:N	3:K:291:SER:OG	2.50	0.45
5:Y:230:ARG:O	5:Y:238:LYS:N	2.37	0.45
1:B:83:HIS:HD2	1:B:440:GLN:HB2	1.78	0.45
1:B:532:ARG:HG3	4:L:92:GLN:HB2	1.99	0.45
2:C:649:GLU:O	2:C:681:ASP:N	2.34	0.45
7:H:31:DT:H2"	7:H:32:DG:C8	2.51	0.45
7:H:122:DT:H2"	7:H:123:DG:H8	1.82	0.45
9:U:55:LEU:HD22	10:V:63:VAL:HG23	1.99	0.45
1:G:115:LEU:HD11	1:G:465:LYS:NZ	2.32	0.45
1:G:311:LEU:H	1:G:315:TYR:HH	1.65	0.45
1:G:578:GLU:HB3	3:K:286:ASN:HB2	1.98	0.45
3:K:138:TYR:OH	3:K:180:MET:HG2	2.16	0.45
3:K:264:ARG:N	3:K:298:ASP:OD2	2.50	0.45
3:K:421:ASP:OD1	3:K:421:ASP:N	2.50	0.45
3:K:426:ILE:HD11	3:K:434:ILE:HB	1.99	0.45
4:O:346:ASP:OD1	4:O:348:SER:OG	2.29	0.45
2:C:338:GLU:O	2:C:342:ALA:N	2.44	0.44
2:C:475:ARG:NH2	2:C:478:GLU:OE1	2.50	0.44
2:C:685:LYS:HD3	3:F:232:VAL:HG21	1.97	0.44
3:F:111:LEU:HD21	3:F:420:ARG:HB3	1.98	0.44
4:L:81:ILE:HB	4:L:119:ILE:HD12	1.99	0.44
4:L:85:GLN:HE21	4:L:114:LYS:HD3	1.82	0.44
6:A:78:PHE:CE2	8:J:67:ARG:HB2	2.53	0.44
1:G:608:GLU:OE1	1:G:608:GLU:N	2.45	0.44
2:I:228:SER:HB3	2:I:236:THR:HA	1.99	0.44
2:I:584:GLU:OE2	2:I:610:SER:N	2.50	0.44
2:I:675:ASN:CG	2:I:677:ASP:H	2.21	0.44
3:K:87:SER:O	3:K:88:LEU:HD23	2.17	0.44
3:K:189:HIS:NE2	3:K:208:SER:OG	2.44	0.44
3:K:226:VAL:CG1	3:K:227:ALA:H	2.29	0.44
3:K:326:ASN:HA	3:K:358:TYR:CE2	2.52	0.44
3:K:389:TRP:HE1	3:K:402:THR:H	1.64	0.44
5:Y:280:LEU:HD12	5:Y:281:ASP:HB3	1.99	0.44
1:B:157:LEU:O	1:B:233:SER:HB3	2.17	0.44
1:B:640:VAL:HB	1:B:680:LYS:HE2	1.98	0.44
3:F:370:MET:HE3	3:F:371:ASP:OD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:246:VAL:HG22	4:L:252:LEU:HB2	1.98	0.44
11:T:133:DC:H4'	11:T:134:DG:OP1	2.17	0.44
3:K:225:LEU:HD12	3:K:226:VAL:H	1.83	0.44
3:K:335:LYS:N	3:K:338:ASP:OD2	2.33	0.44
3:K:418:PHE:HA	3:K:425:LEU:HA	1.98	0.44
1:B:100:LEU:HA	1:B:103:ARG:HB3	1.99	0.44
1:B:151:HIS:CE1	1:B:361:TRP:HB3	2.53	0.44
1:B:159:LEU:HA	1:B:359:LEU:HA	1.98	0.44
4:L:82:ALA:HA	4:L:117:ILE:HG12	1.99	0.44
4:L:257:THR:O	4:L:258:ARG:HD3	2.18	0.44
5:M:211:ILE:HD11	5:M:269:LEU:HD11	2.00	0.44
11:T:205:DG:H2"	11:T:206:DA:C8	2.52	0.44
8:X:19:ARG:O	8:X:20:LYS:HD2	2.17	0.44
1:G:163:GLY:HA2	1:G:217:PRO:HG2	2.00	0.44
1:G:505:ASP:OD1	1:G:508:ARG:NH1	2.50	0.44
1:G:643:TYR:O	1:G:647:ILE:HG12	2.17	0.44
3:K:245:ASP:CG	3:K:250:LYS:H	2.20	0.44
3:K:385:LYS:HZ2	3:K:387:TYR:HE2	1.66	0.44
1:B:600:ILE:HD11	1:B:618:ASN:ND2	2.30	0.44
2:C:165:PHE:HB2	2:C:224:PHE:HE1	1.82	0.44
3:F:205:LEU:HD13	3:F:219:ASN:HA	1.99	0.44
4:L:49:TRP:HB2	4:L:383:ASN:HB3	1.99	0.44
5:M:209:ALA:HB1	5:M:220:VAL:HG23	2.00	0.44
9:R:64:GLU:HG3	10:S:45:VAL:HG21	1.99	0.44
11:T:195:DC:H2"	11:T:196:DA:C8	2.51	0.44
9:U:100:VAL:HG21	8:X:98:TYR:CE2	2.52	0.44
8:X:31:LYS:HE3	8:X:51:TYR:HE2	1.82	0.44
1:G:161:PHE:HD2	1:G:229:SER:HB2	1.82	0.44
2:I:599:TRP:HA	2:I:613:ARG:HH11	1.82	0.44
3:K:109:ASP:O	3:K:111:LEU:HD12	2.18	0.44
3:K:368:PHE:CE2	3:K:377:LEU:HD11	2.53	0.44
4:O:44:SER:OG	4:O:69:GLY:N	2.47	0.44
4:O:374:THR:OG1	4:O:375:ALA:N	2.51	0.44
1:B:111:LEU:HG	4:L:369:ILE:HG22	1.99	0.44
2:C:593:CYS:O	2:C:605:SER:OG	2.36	0.44
3:F:86:ASN:HB3	3:F:436:ARG:HB3	2.00	0.44
4:L:150:LEU:HB3	4:L:152:PHE:HE1	1.81	0.44
4:L:254:ILE:HB	4:L:267:HIS:HB2	2.00	0.44
4:L:316:HIS:CD2	4:L:317:LYS:H	2.34	0.44
7:H:121:DG:O6	11:T:105:DA:N6	2.50	0.44
7:H:156:DA:C8	7:H:157:DT:H72	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:57:TYR:CZ	10:S:106:HIS:HB2	2.53	0.44
11:T:78:DT:H2"	11:T:79:DA:N7	2.32	0.44
1:G:504:GLN:HE22	1:G:508:ARG:HH21	1.65	0.44
1:G:621:VAL:HG13	1:G:626:PHE:HD2	1.83	0.44
2:I:497:LYS:HD2	2:I:498:LYS:N	2.33	0.44
3:K:270:MET:HA	3:K:273:ALA:HB3	2.00	0.44
4:O:178:LYS:HD2	4:O:198:ASP:HB3	2.00	0.44
1:B:212:GLN:HG3	1:B:212:GLN:O	2.18	0.44
1:B:234:SER:OG	1:B:235:ASN:N	2.50	0.44
1:B:319:MET:N	1:B:353:PRO:O	2.51	0.44
1:B:516:ARG:HH12	5:M:289:PRO:HA	1.81	0.44
3:F:206:LEU:HB3	3:F:220:ILE:HD11	2.00	0.44
4:L:22:LYS:NZ	4:L:25:LYS:HE3	2.33	0.44
7:H:57:DG:H2"	7:H:58:DA:C8	2.53	0.44
9:R:97:LEU:HB3	9:R:100:VAL:HB	2.00	0.44
8:X:65:VAL:HG21	8:X:90:LEU:HD22	1.99	0.44
1:G:109:ILE:HA	4:O:341:ARG:NH2	2.33	0.44
2:I:56:LEU:HD23	2:I:59:GLU:OE2	2.17	0.44
3:K:358:TYR:HE2	3:K:361:CYS:HB3	1.81	0.44
4:O:278:CYS:O	4:O:291:THR:HG23	2.16	0.44
5:Y:231:LYS:HG2	5:Y:232:GLU:N	2.33	0.44
2:C:168:ASP:O	2:C:172:VAL:HG23	2.18	0.44
4:L:13:GLU:HG3	4:L:17:ILE:HG23	2.00	0.44
4:L:342:LEU:HD12	4:L:370:HIS:CD2	2.52	0.44
11:T:174:DT:H2'	11:T:175:DA:C8	2.52	0.44
8:X:17:ARG:O	8:X:17:ARG:NE	2.34	0.44
1:G:109:ILE:HG12	4:O:341:ARG:NH1	2.26	0.44
1:G:192:CYS:C	1:G:246:LYS:HG3	2.38	0.44
1:G:359:LEU:HD21	1:G:361:TRP:NE1	2.32	0.44
1:G:577:GLN:OE1	1:G:577:GLN:N	2.44	0.44
2:I:25:ARG:O	2:I:28:GLN:HG2	2.17	0.44
2:I:172:VAL:HG22	2:I:247:LEU:HD21	2.00	0.44
2:I:226:ALA:HB1	2:I:230:MET:HE1	1.99	0.44
2:I:236:THR:HG22	2:I:239:GLU:HG3	1.98	0.44
2:I:285:PHE:HA	2:I:292:TYR:HA	2.00	0.44
3:K:245:ASP:OD1	3:K:245:ASP:N	2.51	0.44
4:O:246:VAL:HG22	4:O:252:LEU:CB	2.48	0.44
4:O:335:SER:HA	4:O:380:PHE:CE2	2.53	0.44
1:B:516:ARG:NH1	5:M:288:MET:O	2.51	0.44
2:C:16:ARG:HB3	2:C:179:GLY:HA2	1.99	0.44
2:C:174:LEU:HG	2:C:178:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:LYS:HE2	2:C:294:CYS:HA	2.00	0.44
2:C:313:ARG:NH2	2:C:314:LYS:O	2.51	0.44
3:F:90:GLU:HG3	3:F:92:HIS:CE1	2.53	0.44
3:F:329:VAL:CG2	3:F:352:ILE:HD11	2.48	0.44
4:L:85:GLN:HE21	4:L:114:LYS:HA	1.83	0.44
1:G:490:SER:OG	1:G:491:ILE:N	2.50	0.44
1:G:561:HIS:CE1	2:I:724:GLY:H	2.36	0.44
2:I:94:GLN:CD	3:K:134:LEU:H	2.22	0.44
3:K:205:LEU:HA	3:K:218:TRP:O	2.17	0.44
3:K:364:TRP:CE3	3:K:365:TYR:HB2	2.53	0.44
4:O:314:GLU:OE1	4:O:314:GLU:N	2.51	0.44
1:B:603:PHE:O	1:B:611:LYS:NZ	2.37	0.44
2:C:687:ASN:ND2	2:C:689:ILE:HG22	2.32	0.44
3:F:262:LEU:O	3:F:298:ASP:N	2.38	0.44
4:L:383:ASN:OD1	4:L:386:GLU:HB2	2.18	0.44
7:H:137:DC:O2	7:H:138:DT:N3	2.50	0.44
1:G:592:LEU:HA	1:G:595:LYS:HG2	2.00	0.44
2:I:137:GLU:HG2	2:I:138:VAL:HG23	1.99	0.44
2:I:296:LEU:HG	2:I:297:HIS:CE1	2.53	0.44
2:I:734:SER:O	2:I:738:ALA:N	2.45	0.44
2:I:742:VAL:HA	13:I:801:SAH:C4	2.48	0.44
3:K:217:LEU:O	3:K:225:LEU:HD12	2.18	0.44
3:K:305:HIS:CG	3:K:323:SER:HB2	2.53	0.44
3:K:318:LEU:HD12	3:K:330:CYS:SG	2.57	0.44
4:O:131:ARG:HD3	4:O:131:ARG:HA	1.78	0.44
2:C:604:VAL:HG11	2:C:613:ARG:NH1	2.33	0.43
2:C:674:LEU:HD23	2:C:678:PHE:HB2	2.00	0.43
3:F:424:ILE:HD12	3:F:436:ARG:NH2	2.33	0.43
11:T:189:DC:H2”	11:T:190:DG:C8	2.53	0.43
6:W:103:LEU:HD11	6:W:128:ARG:NH1	2.33	0.43
1:G:315:TYR:CE2	1:G:359:LEU:HB2	2.53	0.43
2:I:567:CYS:SG	2:I:576:CYS:SG	3.16	0.43
2:I:627:ALA:HB3	2:I:693:ASN:HD21	1.83	0.43
3:K:122:THR:HA	3:K:137:SER:HB3	1.99	0.43
4:O:295:ASP:O	4:O:297:THR:HG23	2.17	0.43
4:O:318:ASP:HB2	4:O:339:ASP:HB3	2.00	0.43
5:Y:191:ASP:OD2	5:Y:193:GLN:NE2	2.51	0.43
1:B:98:ARG:HG3	1:B:101:ARG:NH1	2.33	0.43
1:B:615:LYS:O	1:B:619:LEU:HG	2.18	0.43
2:C:549:GLU:N	2:C:552:CYS:SG	2.90	0.43
8:J:97:LEU:HD13	9:R:101:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:50:TYR:CE1	10:S:111:GLY:HA3	2.53	0.43
9:R:67:GLY:HA3	10:S:46:HIS:CE1	2.53	0.43
9:U:75:LYS:NZ	9:U:79:ILE:HD13	2.33	0.43
2:I:444:MET:HB3	2:I:448:LEU:HD23	2.00	0.43
3:K:377:LEU:O	3:K:389:TRP:N	2.35	0.43
4:O:194:LEU:HB3	4:O:233:VAL:HG23	2.00	0.43
5:Y:202:ALA:HA	5:Y:205:PHE:HB3	2.00	0.43
1:B:156:HIS:HB3	1:B:158:GLN:NE2	2.30	0.43
3:F:192:ALA:HB3	3:F:211:LYS:NZ	2.33	0.43
4:L:204:LEU:N	4:L:221:THR:O	2.48	0.43
3:K:176:ASN:ND2	3:K:179:THR:OG1	2.50	0.43
3:K:206:LEU:C	3:K:217:LEU:HD12	2.38	0.43
4:O:60:ASP:O	4:O:88:ASN:N	2.45	0.43
4:O:70:THR:HB	4:O:78:HIS:H	1.83	0.43
4:O:81:ILE:HD12	4:O:119:ILE:HG21	2.00	0.43
4:O:226:HIS:N	4:O:253:MET:HE1	2.33	0.43
4:O:364:PRO:HG2	4:O:365:GLU:OE1	2.18	0.43
2:C:568:LYS:HE3	2:C:568:LYS:HB2	1.88	0.43
2:C:624:SER:OG	2:C:629:TRP:O	2.32	0.43
2:C:646:TYR:HE1	2:C:682:ALA:HB3	1.84	0.43
4:L:49:TRP:NE1	4:L:391:CYS:SG	2.91	0.43
9:R:26:PRO:HD3	10:S:37:TYR:CD2	2.53	0.43
11:T:153:DA:P	9:U:35:ARG:HH12	2.41	0.43
1:G:241:ASN:O	1:G:245:VAL:HG22	2.18	0.43
2:I:698:PRO:HG3	2:I:729:PHE:HA	2.01	0.43
3:K:310:ASP:OD1	3:K:310:ASP:N	2.52	0.43
4:O:33:ASP:OD2	4:O:405:ALA:HA	2.19	0.43
4:O:194:LEU:HD23	4:O:194:LEU:HA	1.90	0.43
1:B:187:LEU:HB2	1:B:251:LEU:HB2	1.99	0.43
1:B:516:ARG:NH1	5:M:288:MET:HG3	2.34	0.43
1:B:654:ARG:NH2	2:C:264:ILE:O	2.51	0.43
1:B:671:ILE:O	1:B:674:ILE:HG12	2.17	0.43
2:C:706:MET:HE1	2:C:711:HIS:ND1	2.33	0.43
3:F:103:TRP:HB3	3:F:420:ARG:NH2	2.32	0.43
5:M:199:ARG:HD2	5:M:200:HIS:N	2.34	0.43
8:J:92:ARG:CZ	8:J:92:ARG:HB3	2.47	0.43
9:U:26:PRO:HG3	10:V:37:TYR:CD2	2.54	0.43
2:I:313:ARG:HD2	2:I:313:ARG:HA	1.74	0.43
2:I:643:ILE:N	2:I:715:ILE:O	2.52	0.43
3:K:92:HIS:CD2	3:K:94:GLN:H	2.37	0.43
3:K:96:LEU:HD23	3:K:96:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:126:CYS:CB	3:K:132:ILE:HG12	2.48	0.43
3:K:152:TRP:CE3	3:K:163:LEU:HD12	2.53	0.43
4:O:5:GLU:HA	4:O:8:PHE:HB3	2.00	0.43
2:C:71:LEU:N	3:F:136:GLN:OE1	2.52	0.43
2:C:285:PHE:HE2	2:C:287:ARG:HG2	1.84	0.43
2:C:446:ARG:HD3	2:C:446:ARG:H	1.84	0.43
4:L:38:HIS:HD2	4:L:40:LEU:HD23	1.83	0.43
4:L:128:ASN:HB2	4:L:143:LYS:HB3	2.01	0.43
4:L:174:ARG:HG2	4:L:175:GLY:H	1.84	0.43
4:L:281:PHE:HD2	4:L:289:LEU:HD13	1.83	0.43
4:L:301:TRP:NE1	4:L:309:LYS:HB2	2.33	0.43
8:J:29:ILE:O	8:J:29:ILE:HG13	2.19	0.43
1:G:92:LYS:HA	5:Y:195:LEU:HD11	2.01	0.43
1:G:643:TYR:HA	1:G:646:LYS:HG3	2.00	0.43
2:I:84:SER:OG	2:I:94:GLN:O	2.24	0.43
2:I:145:PHE:O	2:I:149:LEU:HG	2.19	0.43
2:I:510:LYS:H	2:I:510:LYS:HG3	1.58	0.43
2:I:651:ILE:HG13	2:I:679:VAL:HG13	2.00	0.43
3:K:134:LEU:O	3:K:135:LEU:HD23	2.19	0.43
3:K:195:GLU:HB3	3:K:209:VAL:HB	2.01	0.43
3:K:358:TYR:CE2	3:K:361:CYS:HB3	2.52	0.43
4:O:10:ASP:CG	5:Y:286:ARG:HH11	2.22	0.43
4:O:376:LYS:HZ3	4:O:378:SER:HB3	1.83	0.43
2:C:109:ILE:HG23	3:F:191:ASN:HA	2.00	0.43
2:C:703:LYS:HD3	2:C:703:LYS:HA	1.80	0.43
4:L:127:VAL:HG13	4:L:142:THR:HG23	2.01	0.43
4:L:236:HIS:ND1	4:L:242:LEU:HB3	2.34	0.43
4:L:331:THR:OG1	4:L:346:ASP:OD1	2.33	0.43
6:A:71:VAL:HA	6:A:74:ILE:HG22	2.01	0.43
9:R:32:ARG:HH22	10:S:32:GLU:CD	2.22	0.43
11:T:139:DG:H2"	11:T:140:DG:C8	2.54	0.43
6:W:79:LYS:CG	6:W:82:LEU:HD21	2.49	0.43
1:G:158:GLN:O	1:G:360:ARG:N	2.44	0.43
1:G:566:PHE:CD1	1:G:573:PRO:HA	2.53	0.43
1:G:591:TRP:CZ3	3:K:232:VAL:HG21	2.52	0.43
3:K:205:LEU:HB3	3:K:217:LEU:HD11	1.98	0.43
3:K:425:LEU:O	3:K:437:TRP:N	2.49	0.43
5:Y:232:GLU:HG3	5:Y:236:LYS:HE2	2.01	0.43
1:B:600:ILE:O	1:B:611:LYS:HE2	2.19	0.43
4:L:152:PHE:HE2	4:L:167:CYS:HB2	1.84	0.43
4:L:375:ALA:HB3	4:L:394:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:239:LEU:N	5:M:254:VAL:O	2.52	0.43
7:H:142:DG:N2	11:T:86:DC:O2	2.51	0.43
6:W:118:THR:HA	8:X:45:ARG:HB2	2.01	0.43
1:G:126:ASN:OD1	1:G:128:LYS:HG2	2.18	0.43
1:G:146:GLY:O	1:G:148:GLN:NE2	2.52	0.43
1:G:468:LYS:HA	1:G:476:PHE:CE2	2.54	0.43
2:I:285:PHE:HB2	2:I:292:TYR:CE2	2.53	0.43
3:K:238:GLU:HB3	3:K:256:MET:HB2	2.00	0.43
4:O:17:ILE:HA	4:O:20:GLU:CD	2.39	0.43
4:O:51:PRO:HB3	4:O:132:TYR:CZ	2.53	0.43
4:O:76:GLN:NE2	4:O:123:HIS:O	2.49	0.43
4:O:313:PHE:HB3	4:O:345:TRP:CZ2	2.54	0.43
4:O:380:PHE:HA	4:O:392:SER:HA	2.01	0.43
3:F:271:MET:O	3:F:275:LYS:HG2	2.19	0.43
4:L:50:LEU:HD12	4:L:65:ARG:HB3	2.00	0.43
7:H:141:DA:H2"	7:H:142:DG:C8	2.54	0.43
7:H:144:DT:O2	11:T:84:DG:N2	2.52	0.43
7:H:169:DG:H1	11:T:58:DC:H42	1.66	0.43
7:H:215:DC:H2"	7:H:216:DA:C8	2.54	0.43
9:R:88:ARG:NH1	9:R:100:VAL:O	2.52	0.43
1:G:97:TYR:CD1	1:G:100:LEU:HD12	2.53	0.43
2:I:281:PHE:O	2:I:285:PHE:N	2.51	0.43
2:I:638:GLN:N	2:I:641:GLU:OE1	2.38	0.43
3:K:246:LEU:HD12	3:K:246:LEU:HA	1.82	0.43
4:O:45:LEU:HA	4:O:393:VAL:HG11	2.01	0.43
4:O:54:THR:OG1	4:O:63:ILE:HB	2.18	0.43
5:Y:241:LEU:HD11	5:Y:254:VAL:HG13	2.01	0.43
5:Y:245:PRO:HD2	5:Y:248:ILE:HD11	2.00	0.43
5:Y:247:ASP:HB3	5:Y:279:LEU:HD13	2.01	0.43
5:Y:270:SER:HG	5:Y:271:LYS:NZ	2.16	0.43
1:B:161:PHE:HD2	1:B:229:SER:HB2	1.83	0.43
1:B:499:TYR:HA	4:L:18:ASN:ND2	2.23	0.43
2:C:48:LYS:O	2:C:52:ARG:HG2	2.19	0.43
2:C:165:PHE:HE1	2:C:243:LYS:HB3	1.83	0.43
2:C:585:CYS:H	2:C:608:ASN:HB3	1.83	0.43
6:A:115:LYS:HE2	6:A:115:LYS:HA	2.00	0.43
6:A:124:ILE:HD12	8:J:53:GLU:HG2	2.00	0.43
7:H:137:DC:H2"	7:H:138:DT:C6	2.54	0.43
8:J:75:HIS:CD2	10:V:77:LEU:HD21	2.54	0.43
1:G:158:GLN:HB2	1:G:360:ARG:CB	2.49	0.43
2:I:46:ARG:HD3	2:I:50:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:86:THR:O	3:K:89:LYS:N	2.43	0.43
2:I:631:ILE:HG12	2:I:691:PHE:C	2.39	0.43
2:I:744:ILE:HB	13:I:801:SAH:N1	2.34	0.43
3:K:406:HIS:CD2	3:K:408:LYS:HB2	2.54	0.43
3:K:423:SER:OG	3:K:424:ILE:HG12	2.18	0.43
4:O:38:HIS:CG	4:O:39:ALA:N	2.86	0.43
4:O:148:ASP:OD1	4:O:149:VAL:N	2.52	0.43
4:O:244:GLY:HA2	4:O:255:TRP:HD1	1.84	0.43
4:O:377:ILE:HD13	4:O:394:SER:HA	2.00	0.43
2:C:27:ARG:HH22	2:C:165:PHE:HA	1.84	0.42
2:C:621:LEU:HD21	2:C:629:TRP:CZ3	2.54	0.42
4:L:106:GLY:N	4:L:109:GLY:O	2.51	0.42
4:L:130:ALA:HA	4:L:142:THR:HA	2.01	0.42
5:M:214:LEU:HD12	5:M:221:VAL:HG11	2.01	0.42
5:M:275:ASP:OD1	5:M:276:THR:N	2.52	0.42
10:S:45:VAL:HG22	10:S:46:HIS:CE1	2.54	0.42
11:T:9:DT:H2"	11:T:10:DG:C8	2.54	0.42
1:G:166:HIS:CD2	1:G:353:PRO:HG3	2.54	0.42
2:I:89:LEU:HB2	2:I:91:PHE:HD1	1.84	0.42
2:I:257:PRO:HB2	2:I:259:GLU:OE1	2.18	0.42
3:K:88:LEU:HD12	3:K:434:ILE:HD11	2.01	0.42
3:K:127:HIS:N	3:K:131:GLU:O	2.51	0.42
3:K:252:MET:HE1	3:K:262:LEU:HB2	2.01	0.42
3:K:303:ASP:OD1	3:K:303:ASP:N	2.50	0.42
3:K:361:CYS:HB2	3:K:381:ASN:ND2	2.34	0.42
1:B:307:ARG:NH1	1:B:309:GLN:HA	2.34	0.42
7:H:37:DC:H2"	7:H:38:DA:H8	1.84	0.42
9:U:31:HIS:HB2	9:U:48:PRO:HG3	2.01	0.42
1:G:600:ILE:HG22	1:G:611:LYS:HD3	2.00	0.42
2:I:100:THR:OG1	2:I:101:LEU:N	2.49	0.42
2:I:286:CYS:SG	2:I:288:ARG:HB3	2.59	0.42
2:I:330:TYR:HA	2:I:472:TYR:CD2	2.54	0.42
2:I:532:ARG:HA	2:I:532:ARG:NH2	2.34	0.42
4:O:64:HIS:CE1	4:O:86:LEU:HD21	2.54	0.42
5:Y:259:ARG:HG3	5:Y:263:LYS:HZ2	1.84	0.42
1:B:566:PHE:HA	1:B:573:PRO:HA	2.01	0.42
1:B:617:TRP:O	1:B:620:HIS:CE1	2.72	0.42
2:C:731:TYR:HB3	2:C:733:TYR:CZ	2.55	0.42
4:L:370:HIS:CD2	4:L:371:GLY:H	2.36	0.42
5:M:212:GLU:HA	5:M:217:GLY:H	1.84	0.42
7:H:110:DA:H1'	7:H:111:DC:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:120:DC:C5'	8:X:45:ARG:HH11	2.32	0.42
7:H:143:DC:OP1	10:V:31:LYS:NZ	2.43	0.42
8:X:63:GLU:HA	8:X:66:ILE:HG22	2.00	0.42
1:G:161:PHE:CD2	1:G:229:SER:HB2	2.55	0.42
1:G:508:ARG:NE	1:G:512:PHE:O	2.52	0.42
2:I:84:SER:OG	2:I:93:THR:HG22	2.18	0.42
2:I:275:GLU:O	2:I:279:HIS:N	2.52	0.42
3:K:198:PHE:HA	3:K:205:LEU:O	2.19	0.42
3:K:199:HIS:CG	3:K:200:PRO:HD2	2.55	0.42
3:K:258:HIS:HE2	3:K:308:TYR:HD1	1.65	0.42
2:C:320:LEU:HG	2:C:455:ASN:HA	2.01	0.42
3:F:371:ASP:CG	3:F:375:LYS:H	2.23	0.42
11:T:6:DG:H2"	11:T:7:DA:C8	2.53	0.42
11:T:116:DG:H2"	11:T:117:DT:H72	2.01	0.42
6:W:121:PRO:O	6:W:124:ILE:HG22	2.20	0.42
1:G:151:HIS:HB2	1:G:361:TRP:CD2	2.54	0.42
1:G:583:SER:HA	2:I:618:HIS:CE1	2.54	0.42
1:G:645:GLN:HA	1:G:648:ILE:HB	2.01	0.42
3:K:124:TYR:HD1	3:K:134:LEU:HA	1.84	0.42
4:O:319:GLU:OE2	4:O:321:PHE:HB3	2.19	0.42
1:B:105:LEU:HD21	5:M:268:HIS:CE1	2.53	0.42
1:B:186:VAL:HA	1:B:252:PHE:HA	2.02	0.42
2:C:46:ARG:O	2:C:50:LEU:HG	2.19	0.42
2:C:238:GLU:HA	2:C:241:LYS:HD2	2.01	0.42
3:F:82:PHE:O	3:F:83:LYS:HE2	2.19	0.42
3:F:153:THR:O	3:F:162:LEU:N	2.27	0.42
3:F:173:ARG:HB3	3:F:182:CYS:SG	2.59	0.42
5:M:223:HIS:HB2	5:M:244:MET:HG2	2.02	0.42
5:M:230:ARG:HH11	5:M:238:LYS:HG2	1.85	0.42
8:J:96:THR:CG2	9:R:100:VAL:HG22	2.49	0.42
9:R:62:ILE:HD13	9:R:62:ILE:HA	1.90	0.42
11:T:190:DG:H2"	11:T:191:DC:C6	2.54	0.42
6:W:98:ALA:HA	6:W:101:VAL:HG12	2.01	0.42
1:G:590:GLU:O	1:G:593:ARG:HG2	2.20	0.42
3:K:406:HIS:NE2	3:K:408:LYS:HB2	2.34	0.42
3:K:409:CYS:HB2	3:K:435:TRP:CE2	2.55	0.42
4:O:173:LEU:HD23	4:O:217:VAL:HB	2.01	0.42
4:O:238:LEU:HD12	4:O:286:GLU:HA	2.01	0.42
5:Y:230:ARG:HE	5:Y:238:LYS:HB2	1.85	0.42
1:B:521:LYS:HB2	4:L:42:TRP:CZ2	2.55	0.42
1:B:629:ASP:O	1:B:633:ASN:ND2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:ARG:O	3:F:159:SER:OG	2.28	0.42
2:C:675:ASN:OD1	2:C:678:PHE:N	2.50	0.42
6:A:28:SER:HB3	2:I:673:ASN:HD22	1.84	0.42
7:H:141:DA:C6	7:H:142:DG:C6	3.07	0.42
7:H:191:DC:H2"	7:H:192:DG:C8	2.54	0.42
9:U:18:SER:HB2	9:U:23:LEU:O	2.20	0.42
9:U:76:THR:O	10:V:49:THR:OG1	2.18	0.42
1:G:135:ASP:OD1	1:G:136:ASP:N	2.50	0.42
2:I:146:ILE:O	2:I:149:LEU:HB2	2.19	0.42
2:I:289:CYS:O	2:I:291:LYS:HG3	2.20	0.42
2:I:530:HIS:CE1	2:I:539:CYS:HG	2.35	0.42
2:I:674:LEU:HB3	2:I:678:PHE:O	2.20	0.42
4:O:78:HIS:O	4:O:80:VAL:HG23	2.19	0.42
4:O:256:ASP:OD1	4:O:257:THR:N	2.53	0.42
5:Y:248:ILE:HG22	5:Y:249:LEU:N	2.34	0.42
1:B:478:TYR:H	1:B:547:GLU:CG	2.24	0.42
1:B:617:TRP:HA	1:B:620:HIS:CE1	2.55	0.42
1:B:656:PHE:O	1:B:660:LEU:N	2.47	0.42
3:F:189:HIS:CE1	3:F:210:SER:HB3	2.54	0.42
4:L:40:LEU:C	4:L:397:ASN:HB3	2.39	0.42
6:A:27:LYS:HA	2:I:733:TYR:HE1	1.84	0.42
6:A:113:HIS:CD2	6:W:126:LEU:HD13	2.54	0.42
8:J:67:ARG:O	8:J:71:THR:HG23	2.20	0.42
1:G:97:TYR:HD1	1:G:100:LEU:HD12	1.83	0.42
1:G:115:LEU:HD21	1:G:465:LYS:HZ1	1.85	0.42
1:G:465:LYS:HE2	1:G:469:LEU:HG	2.02	0.42
1:G:595:LYS:HE2	1:G:595:LYS:HB2	1.88	0.42
2:I:178:LEU:HD13	2:I:241:LYS:HD2	2.02	0.42
3:K:235:HIS:ND1	3:K:257:ASP:OD2	2.47	0.42
4:O:31:LEU:HD23	4:O:31:LEU:HA	1.78	0.42
4:O:49:TRP:HA	4:O:66:LEU:HD13	2.01	0.42
4:O:324:GLN:NE2	4:O:325:TRP:H	2.18	0.42
5:Y:280:LEU:HD11	5:Y:284:ILE:HG13	2.01	0.42
1:B:86:PHE:CE1	1:B:434:TYR:HB2	2.54	0.42
1:B:241:ASN:O	1:B:245:VAL:HG22	2.20	0.42
1:B:522:ARG:HB2	4:L:397:ASN:HD22	1.85	0.42
1:B:524:PRO:HA	4:L:39:ALA:O	2.20	0.42
1:B:648:ILE:HG12	1:B:681:LEU:HD13	2.02	0.42
2:C:525:TYR:OH	2:C:551:PHE:HB2	2.19	0.42
3:F:170:GLY:HA3	3:F:189:HIS:HB3	2.02	0.42
3:F:431:ASP:N	3:F:431:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:278:CYS:O	4:L:291:THR:HB	2.20	0.42
10:S:38:VAL:HA	10:S:41:VAL:HG12	2.01	0.42
10:S:93:THR:O	10:S:97:LEU:HD23	2.20	0.42
9:U:58:LEU:HD12	10:V:99:LEU:HD21	2.00	0.42
1:G:166:HIS:O	1:G:216:ASN:ND2	2.52	0.42
4:O:145:PRO:HA	4:O:179:GLU:OE1	2.19	0.42
4:O:316:HIS:ND1	4:O:318:ASP:O	2.53	0.42
4:O:352:GLU:O	4:O:364:PRO:HG3	2.20	0.42
5:Y:223:HIS:HB2	5:Y:244:MET:HG3	2.01	0.42
1:B:188:LEU:HD12	1:B:249:SER:O	2.20	0.42
1:B:192:CYS:HA	1:B:246:LYS:H	1.84	0.42
2:C:521:HIS:CG	2:C:522:VAL:H	2.38	0.42
3:F:313:ARG:CZ	3:F:368:PHE:HZ	2.33	0.42
7:H:63:DT:C4	7:H:64:DG:C6	3.08	0.42
1:G:98:ARG:HG3	1:G:101:ARG:NH1	2.34	0.42
1:G:607:ASN:ND2	2:I:261:THR:O	2.29	0.42
2:I:120:PHE:HB3	2:I:649:GLU:OE1	2.20	0.42
3:K:176:ASN:ND2	3:K:179:THR:H	2.17	0.42
4:O:12:VAL:O	4:O:15:ARG:HB2	2.20	0.42
5:Y:202:ALA:HB1	5:Y:212:GLU:OE2	2.20	0.42
5:Y:230:ARG:HB3	5:Y:253:TRP:CZ3	2.55	0.42
1:B:428:ILE:HA	1:B:485:ALA:O	2.20	0.42
2:C:438:SER:OG	2:C:441:GLU:OE1	2.38	0.42
3:F:82:PHE:CE1	3:F:439:ARG:HB2	2.55	0.42
3:F:381:ASN:ND2	3:F:387:TYR:OH	2.53	0.42
4:L:132:TYR:HA	4:L:140:ILE:HA	2.01	0.42
7:H:70:DA:OP2	9:U:17:ARG:NH2	2.52	0.42
10:V:58:ILE:HG23	8:X:98:TYR:HB3	2.02	0.42
1:G:191:VAL:HG12	1:G:246:LYS:HD2	2.01	0.42
1:G:658:LEU:O	1:G:661:VAL:HB	2.20	0.42
4:O:253:MET:HG2	4:O:265:PRO:HB3	2.02	0.42
1:B:83:HIS:CE1	1:B:438:THR:HB	2.55	0.41
1:B:522:ARG:O	4:L:41:GLU:HA	2.19	0.41
2:C:467:THR:O	2:C:471:VAL:HG23	2.20	0.41
3:F:92:HIS:HB3	3:F:120:ARG:NH2	2.35	0.41
3:F:196:LEU:HB3	3:F:206:LEU:HD11	2.02	0.41
4:L:169:PRO:O	4:L:172:ARG:NE	2.53	0.41
5:M:240:LEU:HB2	5:M:253:TRP:CE2	2.55	0.41
7:H:116:DC:H2"	7:H:117:DG:H8	1.85	0.41
9:R:77:ARG:HA	10:S:50:GLY:O	2.20	0.41
11:T:75:DT:H2"	11:T:76:DC:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ARG:HG3	1:G:101:ARG:CZ	2.50	0.41
1:G:222:THR:OG1	1:G:223:LYS:N	2.53	0.41
1:G:312:ASP:HA	1:G:359:LEU:HD22	2.00	0.41
1:G:610:GLU:C	1:G:614:MET:HE1	2.40	0.41
2:I:223:ILE:O	2:I:227:ILE:HG13	2.20	0.41
3:K:148:TYR:HE1	3:K:168:SER:HG	1.67	0.41
3:K:169:ARG:HB3	3:K:171:ILE:HD12	2.03	0.41
3:K:238:GLU:O	3:K:256:MET:N	2.52	0.41
3:K:424:ILE:HG23	3:K:438:ASP:OD1	2.20	0.41
4:O:279:LEU:HD11	4:O:281:PHE:HE1	1.85	0.41
1:B:195:LYS:HA	1:B:195:LYS:HD3	1.89	0.41
5:M:247:ASP:OD1	5:M:247:ASP:N	2.53	0.41
6:A:126:LEU:O	6:A:130:ILE:HG12	2.20	0.41
11:T:148:DC:H2”	11:T:149:DC:C5	2.55	0.41
10:V:36:ILE:H	10:V:36:ILE:HD12	1.84	0.41
6:W:51:ILE:HD12	8:X:42:GLY:HA2	2.01	0.41
8:X:77:LYS:HD3	8:X:77:LYS:HA	1.87	0.41
1:G:144:MET:HA	1:G:147:GLU:HB2	2.02	0.41
1:G:540:MET:O	1:G:544:LEU:HG	2.20	0.41
2:I:110:MET:HG2	2:I:111:TYR:O	2.20	0.41
3:K:160:HIS:HB3	3:K:178:ILE:HD13	2.02	0.41
3:K:327:ALA:HB1	3:K:355:ARG:HH12	1.85	0.41
4:O:118:GLU:HG2	4:O:119:ILE:HG13	2.02	0.41
1:B:230:LEU:HD21	1:B:360:ARG:NH1	2.34	0.41
1:B:596:THR:HA	1:B:599:GLN:HB3	2.02	0.41
2:C:46:ARG:HD2	2:C:46:ARG:HA	1.83	0.41
2:C:572:ASN:CG	2:C:607:LYS:HB2	2.41	0.41
2:C:748:MET:HG2	5:M:177:ASN:HD22	1.84	0.41
4:L:158:PRO:HB2	4:L:160:LYS:HG3	2.02	0.41
7:H:100:DA:P	8:J:36:ARG:HH22	2.43	0.41
10:S:105:LYS:HA	10:S:105:LYS:HE3	2.03	0.41
11:T:76:DC:H2”	11:T:77:DG:C8	2.55	0.41
11:T:145:DT:H2”	11:T:146:DA:H8	1.85	0.41
6:W:71:VAL:HG22	6:W:84:PHE:HE2	1.86	0.41
8:X:35:ARG:O	8:X:39:ARG:HG2	2.20	0.41
1:G:525:ILE:HG23	1:G:559:SER:O	2.21	0.41
1:G:620:HIS:CG	1:G:639:PHE:HD2	2.38	0.41
1:G:672:MET:SD	1:G:673:SER:N	2.93	0.41
2:I:102:ASN:ND2	3:K:173:ARG:HH11	2.18	0.41
2:I:138:VAL:HG12	2:I:142:ASP:OD1	2.20	0.41
2:I:259:GLU:HG2	2:I:261:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:343:ASN:HD22	4:O:369:ILE:HD12	1.84	0.41
1:B:136:ASP:HB2	4:L:302:ASP:OD2	2.21	0.41
1:B:571:CYS:HB3	2:C:629:TRP:HZ3	1.85	0.41
2:C:222:LYS:HE2	2:C:222:LYS:HB2	1.91	0.41
2:C:555:SER:OG	2:C:556:SER:N	2.52	0.41
3:F:145:GLU:HB2	3:F:168:SER:HB2	2.02	0.41
3:F:197:LYS:HD3	3:F:244:TYR:HD2	1.85	0.41
4:L:16:VAL:HG12	4:L:20:GLU:OE1	2.21	0.41
4:L:150:LEU:HB3	4:L:152:PHE:CE1	2.55	0.41
4:L:223:PHE:CE2	4:L:259:SER:HB2	2.56	0.41
1:G:525:ILE:H	4:O:39:ALA:HB3	1.85	0.41
2:I:128:LEU:HD23	2:I:157:VAL:HG23	2.02	0.41
2:I:239:GLU:HA	2:I:242:GLU:HG2	2.02	0.41
2:I:539:CYS:HB3	2:I:542:VAL:HB	2.03	0.41
3:K:192:ALA:O	3:K:211:LYS:N	2.41	0.41
4:O:61:PHE:HB3	4:O:108:PHE:CE1	2.48	0.41
4:O:62:SER:O	4:O:85:GLN:HA	2.19	0.41
2:C:279:HIS:HA	2:C:282:HIS:HB3	2.02	0.41
6:A:23:LYS:NZ	2:I:653:GLN:HB3	2.36	0.41
7:H:139:DA:C6	7:H:140:DG:C2	3.08	0.41
8:J:62:LEU:HD23	8:J:62:LEU:O	2.20	0.41
9:R:26:PRO:HB3	10:S:37:TYR:CE2	2.56	0.41
1:G:127:ILE:HG13	1:G:127:ILE:O	2.20	0.41
2:I:17:LYS:HZ3	2:I:220:SER:N	2.17	0.41
2:I:36:ASP:N	2:I:36:ASP:OD1	2.52	0.41
2:I:508:CYS:HA	2:I:511:ILE:HB	2.03	0.41
2:I:702:ALA:O	2:I:703:LYS:HE2	2.20	0.41
4:O:38:HIS:NE2	4:O:39:ALA:O	2.54	0.41
4:O:326:SER:HA	4:O:382:TRP:NE1	2.36	0.41
4:O:326:SER:HA	4:O:382:TRP:HE1	1.85	0.41
2:C:119:ASN:HA	2:C:648:GLY:O	2.21	0.41
2:C:528:CYS:SG	2:C:552:CYS:HB3	2.60	0.41
3:F:130:GLY:HA2	3:F:436:ARG:HH11	1.83	0.41
3:F:421:ASP:OD1	3:F:421:ASP:N	2.49	0.41
6:A:128:ARG:HD3	6:A:134:ARG:HH21	1.86	0.41
11:T:66:DC:H2”	11:T:67:DC:C5	2.55	0.41
1:G:568:SER:OG	1:G:584:GLU:OE1	2.26	0.41
1:G:634:HIS:O	1:G:638:LEU:HD23	2.20	0.41
2:I:280:SER:O	2:I:283:THR:OG1	2.36	0.41
2:I:600:ASP:OD1	2:I:601:SER:N	2.54	0.41
3:K:130:GLY:HA2	3:K:436:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:148:TYR:HD2	3:K:365:TYR:OH	2.03	0.41
3:K:176:ASN:ND2	3:K:178:ILE:HB	2.32	0.41
3:K:193:ILE:CD1	3:K:208:SER:HB2	2.50	0.41
3:K:370:MET:HG2	3:K:391:LEU:HD11	2.02	0.41
4:O:206:ASP:O	4:O:210:VAL:HG23	2.21	0.41
4:O:271:ALA:HA	4:O:301:TRP:CZ2	2.56	0.41
5:Y:269:LEU:HD12	5:Y:270:SER:N	2.35	0.41
1:B:150:SER:HB2	1:B:237:PHE:CZ	2.56	0.41
2:C:100:THR:HA	3:F:139:VAL:O	2.20	0.41
4:L:236:HIS:H	4:L:243:PHE:HA	1.85	0.41
4:L:331:THR:OG1	4:L:348:SER:N	2.53	0.41
4:L:370:HIS:CG	4:L:371:GLY:H	2.39	0.41
7:H:169:DG:H1'	7:H:170:DG:C5	2.55	0.41
10:S:98:LEU:HB3	10:S:99:LEU:HD12	2.02	0.41
11:T:86:DC:H2"	11:T:87:DC:C4	2.56	0.41
11:T:140:DG:C6	11:T:141:DG:C6	3.08	0.41
6:W:120:MET:O	6:W:123:ASP:HB2	2.20	0.41
12:E:9:M3L:HM11	3:K:148:TYR:CE2	2.55	0.41
1:G:249:SER:OG	1:G:299:MET:O	2.33	0.41
1:G:566:PHE:HB2	2:I:621:LEU:O	2.21	0.41
3:K:175:ILE:HG13	3:K:182:CYS:N	2.36	0.41
3:K:355:ARG:H	3:K:396:PRO:CB	2.33	0.41
5:Y:209:ALA:O	5:Y:220:VAL:HG13	2.20	0.41
2:C:122:VAL:HG21	2:C:684:ARG:NH1	2.29	0.41
2:C:571:CYS:HA	2:C:576:CYS:SG	2.61	0.41
2:C:621:LEU:HA	2:C:631:ILE:HD13	2.03	0.41
2:C:731:TYR:HB3	2:C:733:TYR:CE1	2.56	0.41
3:F:95:PRO:HA	3:F:430:ASP:O	2.21	0.41
6:A:31:ALA:HB3	2:I:520:ASN:HD22	1.85	0.41
6:A:126:LEU:HD11	6:W:110:CYS:HA	2.02	0.41
9:R:84:GLN:HA	9:R:87:VAL:HG12	2.02	0.41
11:T:45:DA:H5"	2:I:567:CYS:HA	2.02	0.41
11:T:110:DC:H6	11:T:110:DC:H2'	1.73	0.41
9:U:64:GLU:HG3	10:V:46:HIS:HE1	1.86	0.41
9:U:95:LYS:NZ	10:V:100:PRO:HG3	2.35	0.41
10:V:45:VAL:HG12	10:V:46:HIS:ND1	2.36	0.41
1:G:239:PRO:HA	1:G:242:SER:OG	2.21	0.41
1:G:247:SER:H	1:G:304:LYS:NZ	2.18	0.41
1:G:607:ASN:OD1	2:I:262:PRO:HA	2.21	0.41
2:I:477:LYS:O	2:I:480:SER:OG	2.23	0.41
3:K:258:HIS:CD2	3:K:308:TYR:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:264:ARG:HH11	3:K:341:ASP:HA	1.85	0.41
4:O:12:VAL:HG12	5:Y:194:THR:HG22	2.01	0.41
4:O:286:GLU:O	4:O:303:LEU:HD11	2.21	0.41
1:B:191:VAL:O	1:B:246:LYS:N	2.53	0.41
1:B:428:ILE:HG22	1:B:429:PHE:N	2.35	0.41
1:B:504:GLN:HA	1:B:507:HIS:HB2	2.03	0.41
1:B:628:ALA:H	1:B:631:GLN:NE2	2.19	0.41
1:B:632:MET:SD	1:B:668:LEU:HD13	2.61	0.41
2:C:82:GLU:HG2	2:C:97:PRO:HB3	2.03	0.41
2:C:90:ASP:OD1	2:C:90:ASP:N	2.54	0.41
2:C:102:ASN:OD1	3:F:173:ARG:NH1	2.54	0.41
2:C:444:MET:N	2:C:444:MET:SD	2.94	0.41
3:F:92:HIS:HD2	3:F:94:GLN:HB3	1.85	0.41
3:F:237:ASP:HB3	3:F:256:MET:HB3	2.03	0.41
3:F:309:VAL:HA	3:F:323:SER:HA	2.01	0.41
3:F:318:LEU:HD13	3:F:332:LYS:HB3	2.03	0.41
3:F:358:TYR:HE2	3:F:361:CYS:HB3	1.86	0.41
4:L:48:GLN:OE1	4:L:49:TRP:N	2.54	0.41
4:L:257:THR:C	4:L:258:ARG:HD3	2.41	0.41
5:M:249:LEU:HD23	5:M:249:LEU:H	1.86	0.41
7:H:54:DC:N4	11:T:173:DA:H61	2.18	0.41
11:T:117:DT:C2	11:T:118:DC:C2	3.09	0.41
11:T:152:DC:H2"	11:T:153:DA:H8	1.86	0.41
11:T:213:DC:H6	11:T:213:DC:H2'	1.74	0.41
9:U:25:PHE:O	9:U:27:VAL:N	2.54	0.41
9:U:81:ARG:HD3	6:W:58:THR:CG2	2.50	0.41
8:X:31:LYS:HE3	8:X:51:TYR:CE2	2.56	0.41
1:G:183:THR:HA	1:G:213:VAL:H	1.86	0.41
1:G:311:LEU:HD12	1:G:313:GLY:N	2.30	0.41
1:G:595:LYS:HG3	1:G:596:THR:N	2.36	0.41
2:I:86:THR:HA	2:I:93:THR:HG23	2.03	0.41
2:I:442:ALA:HB1	2:I:446:ARG:HH12	1.86	0.41
2:I:471:VAL:O	2:I:475:ARG:N	2.31	0.41
2:I:528:CYS:SG	2:I:548:CYS:HA	2.60	0.41
2:I:536:ASP:OD2	2:I:538:SER:OG	2.26	0.41
3:K:252:MET:HE1	3:K:262:LEU:HD22	2.02	0.41
3:K:280:TYR:CG	3:K:281:ASN:N	2.88	0.41
3:K:326:ASN:HB3	3:K:358:TYR:O	2.21	0.41
3:K:332:LYS:HE2	3:K:332:LYS:HB2	1.83	0.41
3:K:381:ASN:OD1	3:K:382:GLN:N	2.54	0.41
3:K:404:LEU:HD23	3:K:437:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:171:LEU:H	4:O:215:LYS:HA	1.85	0.41
4:O:322:GLN:NE2	4:O:379:ASP:OD1	2.54	0.41
3:F:250:LYS:NZ	3:F:341:ASP:OD1	2.51	0.41
4:L:181:TYR:OH	5:M:295:ARG:HB2	2.21	0.41
4:L:305:ASN:HB3	4:L:308:LEU:HB3	2.02	0.41
11:T:93:DC:H4'	11:T:94:DC:OP1	2.20	0.41
9:U:23:LEU:HD22	9:U:56:GLU:OE1	2.21	0.41
1:G:458:ARG:C	1:G:459:LYS:HD3	2.41	0.41
1:G:614:MET:HG3	2:I:292:TYR:CD1	2.55	0.41
1:G:637:MET:HG2	1:G:638:LEU:HD22	2.03	0.41
2:I:81:ARG:HB2	2:I:98:LEU:HD22	2.03	0.41
2:I:128:LEU:HD13	2:I:150:ILE:HD13	2.02	0.41
3:K:102:ASN:HB2	3:K:152:TRP:CZ2	2.56	0.41
3:K:211:LYS:HA	3:K:238:GLU:OE1	2.20	0.41
3:K:367:ARG:HD3	3:K:415:GLN:NE2	2.36	0.41
4:O:71:HIS:ND1	4:O:126:GLU:HB3	2.35	0.41
4:O:110:SER:H	4:O:114:LYS:NZ	2.19	0.41
4:O:236:HIS:HE1	4:O:238:LEU:HB2	1.86	0.41
4:O:296:LYS:HB3	4:O:316:HIS:O	2.21	0.41
2:C:528:CYS:HB2	2:C:540:PRO:HD2	2.03	0.40
2:C:652:SER:OG	2:C:654:ASP:OD1	2.22	0.40
4:L:47:ALA:N	4:L:131:ARG:HH12	2.19	0.40
5:M:178:LYS:C	5:M:179:ARG:HD3	2.42	0.40
6:A:109:LEU:CD1	6:W:129:ARG:HD3	2.49	0.40
9:R:70:ALA:HA	9:R:82:HIS:NE2	2.35	0.40
12:E:9:M3L:HM31	3:K:148:TYR:HE2	1.86	0.40
1:G:105:LEU:HB3	5:Y:269:LEU:HD11	2.02	0.40
1:G:140:LYS:HA	1:G:143:LYS:HG2	2.03	0.40
1:G:312:ASP:HA	1:G:359:LEU:HB3	2.03	0.40
1:G:502:ASN:ND2	1:G:504:GLN:HB3	2.35	0.40
1:G:528:ILE:HG23	4:O:35:VAL:O	2.21	0.40
2:I:166:ILE:HG21	2:I:174:LEU:HD21	2.02	0.40
2:I:314:LYS:HE3	2:I:314:LYS:HB2	1.95	0.40
2:I:631:ILE:HG21	2:I:689:ILE:HD12	2.03	0.40
3:K:281:ASN:HB3	3:K:284:LYS:HG3	2.03	0.40
3:K:281:ASN:H	3:K:284:LYS:HD3	1.86	0.40
4:O:34:LEU:HD23	4:O:403:GLN:HB3	2.03	0.40
4:O:336:SER:HB2	4:O:342:LEU:HD12	2.03	0.40
1:B:196:ARG:CZ	5:M:295:ARG:HH12	2.33	0.40
5:M:218:HIS:HB2	5:M:268:HIS:HE1	1.86	0.40
7:H:63:DT:H2'	7:H:64:DG:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:94:DG:H3'	7:H:95:DG:C8	2.57	0.40
10:S:33:SER:OG	10:S:60:ASN:ND2	2.55	0.40
1:G:445:ARG:O	1:G:446:ASP:HB3	2.21	0.40
3:K:82:PHE:HB2	3:K:404:LEU:HD21	2.03	0.40
3:K:151:ALA:O	3:K:163:LEU:HG	2.21	0.40
4:O:282:ASN:HB3	4:O:285:SER:O	2.21	0.40
1:B:508:ARG:CZ	1:B:514:PHE:H	2.35	0.40
1:B:565:TYR:HE2	2:C:632:PHE:CG	2.39	0.40
2:C:17:LYS:HD3	2:C:181:TYR:HA	2.03	0.40
2:C:65:ILE:HG21	3:F:105:SER:HA	2.03	0.40
2:C:621:LEU:HD11	2:C:629:TRP:CE3	2.55	0.40
3:F:274:ILE:O	3:F:277:SER:OG	2.21	0.40
3:F:313:ARG:HH22	3:F:322:LYS:N	2.19	0.40
5:M:259:ARG:O	5:M:260:HIS:CG	2.75	0.40
7:H:160:DA:C6	7:H:161:DG:C6	3.09	0.40
9:R:16:THR:HA	11:T:71:DT:H5"	2.01	0.40
6:W:64:LYS:HA	6:W:64:LYS:HE3	2.03	0.40
12:E:9:M3L:HM11	3:K:148:TYR:HE2	1.87	0.40
1:G:498:SER:O	4:O:18:ASN:ND2	2.43	0.40
1:G:616:LEU:HD12	1:G:616:LEU:HA	1.90	0.40
3:K:150:CYS:HB3	3:K:165:VAL:HG13	2.04	0.40
3:K:269:ARG:HH11	3:K:293:LYS:H	1.69	0.40
3:K:360:GLN:C	3:K:381:ASN:HD21	2.24	0.40
4:O:282:ASN:CG	4:O:285:SER:H	2.24	0.40
1:B:299:MET:HE3	1:B:310:LEU:HD21	2.02	0.40
2:C:260:CYS:SG	2:C:261:THR:N	2.93	0.40
2:C:629:TRP:N	2:C:629:TRP:CD1	2.90	0.40
3:F:96:LEU:HD23	3:F:96:LEU:HA	1.98	0.40
4:L:82:ALA:HA	4:L:117:ILE:HG23	2.04	0.40
4:L:341:ARG:HB3	4:L:369:ILE:HD11	2.02	0.40
7:H:122:DT:H3'	6:W:46:VAL:HG21	2.03	0.40
7:H:167:DT:H3	11:T:60:DA:H61	1.68	0.40
8:X:31:LYS:N	8:X:32:PRO:HD2	2.37	0.40
1:G:81:ALA:N	1:G:438:THR:HB	2.36	0.40
1:G:662:SER:HB2	1:G:666:PHE:CE2	2.56	0.40
1:G:675:ASP:OD1	2:I:461:ARG:NH1	2.55	0.40
2:I:675:ASN:HD21	2:I:677:ASP:HB2	1.86	0.40
3:K:211:LYS:HA	3:K:238:GLU:OE2	2.22	0.40
3:K:335:LYS:HA	3:K:351:THR:OG1	2.20	0.40
4:O:282:ASN:HB2	4:O:325:TRP:HZ3	1.87	0.40
4:O:325:TRP:CD1	4:O:325:TRP:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:566:ARG:NH1	2:C:589:LEU:O	2.54	0.40
3:F:186:TYR:CE1	3:F:223:ASP:HA	2.56	0.40
3:F:323:SER:OG	3:F:324:CYS:N	2.55	0.40
4:L:50:LEU:HG	4:L:67:VAL:HG23	2.02	0.40
5:M:272:LEU:HA	5:M:273:PRO:HD3	1.96	0.40
7:H:47:DG:C2	7:H:48:DT:C2	3.09	0.40
7:H:65:DC:H2"	7:H:66:DC:C5	2.56	0.40
7:H:73:DC:H2'	7:H:74:DT:C6	2.56	0.40
11:T:199:DT:H2"	11:T:200:DC:C5	2.56	0.40
1:G:152:SER:HB2	1:G:156:HIS:HD2	1.87	0.40
1:G:322:MET:N	1:G:322:MET:SD	2.95	0.40
1:G:509:GLN:NE2	3:K:185:HIS:H	2.19	0.40
2:I:46:ARG:HH21	2:I:50:LEU:HD11	1.85	0.40
2:I:52:ARG:HB3	3:K:246:LEU:HD23	2.02	0.40
2:I:120:PHE:HD1	2:I:295:PHE:HB2	1.84	0.40
2:I:278:LEU:HD23	2:I:281:PHE:CD1	2.56	0.40
2:I:469:ARG:O	2:I:470:GLN:HB2	2.22	0.40
3:K:258:HIS:O	3:K:302:ARG:HA	2.22	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	B	427/619 (69%)	396 (93%)	31 (7%)	0	100	100
1	G	427/619 (69%)	384 (90%)	42 (10%)	1 (0%)	44	78
2	C	524/753 (70%)	481 (92%)	43 (8%)	0	100	100
2	I	597/753 (79%)	534 (89%)	61 (10%)	2 (0%)	37	73
3	F	360/441 (82%)	334 (93%)	26 (7%)	0	100	100
3	K	360/441 (82%)	313 (87%)	47 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	391/425 (92%)	370 (95%)	21 (5%)	0	100	100
4	O	391/425 (92%)	362 (93%)	29 (7%)	0	100	100
5	M	124/303 (41%)	110 (89%)	13 (10%)	1 (1%)	16	55
5	Y	124/303 (41%)	106 (86%)	18 (14%)	0	100	100
6	A	115/136 (85%)	107 (93%)	8 (7%)	0	100	100
6	W	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
8	J	81/106 (76%)	80 (99%)	1 (1%)	0	100	100
8	X	85/106 (80%)	81 (95%)	4 (5%)	0	100	100
9	R	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
9	U	106/133 (80%)	102 (96%)	4 (4%)	0	100	100
10	S	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
10	V	93/123 (76%)	90 (97%)	3 (3%)	0	100	100
All	All	4502/6078 (74%)	4138 (92%)	360 (8%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	566	ARG
1	G	480	TYR
5	M	176	LYS
2	I	492	THR

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	B	415/575 (72%)	409 (99%)	6 (1%)	62	75
1	G	415/575 (72%)	412 (99%)	3 (1%)	81	87
2	C	478/672 (71%)	473 (99%)	5 (1%)	73	82
2	I	539/672 (80%)	533 (99%)	6 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	324/392 (83%)	322 (99%)	2 (1%)	84 88
3	K	324/392 (83%)	322 (99%)	2 (1%)	84 88
4	L	351/375 (94%)	347 (99%)	4 (1%)	70 80
4	O	351/375 (94%)	350 (100%)	1 (0%)	91 92
5	M	117/271 (43%)	116 (99%)	1 (1%)	75 83
5	Y	117/271 (43%)	115 (98%)	2 (2%)	56 72
6	A	97/111 (87%)	96 (99%)	1 (1%)	73 82
6	W	86/111 (78%)	85 (99%)	1 (1%)	67 79
8	J	68/81 (84%)	68 (100%)	0	100 100
8	X	72/81 (89%)	71 (99%)	1 (1%)	62 75
9	R	85/104 (82%)	84 (99%)	1 (1%)	67 79
9	U	85/104 (82%)	85 (100%)	0	100 100
10	S	81/103 (79%)	81 (100%)	0	100 100
10	V	80/103 (78%)	80 (100%)	0	100 100
All	All	4085/5368 (76%)	4049 (99%)	36 (1%)	74 83

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	124	ARG
1	B	129	ARG
1	B	204	ARG
1	B	439	ARG
1	B	465	LYS
1	B	535	ARG
2	C	313	ARG
2	C	446	ARG
2	C	583	ARG
2	C	658	ARG
2	C	684	ARG
3	F	236	ARG
3	F	313	ARG
4	L	160	LYS
4	L	251	LYS
4	L	258	ARG
4	L	376	LYS
5	M	180	ARG

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Mol	Chain	Res	Type
6	A	26	ARG
9	R	32	ARG
6	W	37	LYS
8	X	23	ARG
1	G	129	ARG
1	G	204	ARG
1	G	445	ARG
2	I	30	LYS
2	I	312	LYS
2	I	512	GLN
2	I	570	GLN
2	I	578	CYS
2	I	583	ARG
3	K	201	ARG
3	K	216	ARG
4	O	160	LYS
5	Y	180	ARG
5	Y	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	104	ASN
1	B	158	GLN
1	B	205	GLN
1	B	309	GLN
1	B	504	GLN
1	B	527	HIS
1	B	561	HIS
1	B	620	HIS
1	B	631	GLN
2	C	117	GLN
2	C	176	ASN
2	C	309	ASN
2	C	322	ASN
2	C	328	GLN
2	C	331	GLN
2	C	520	ASN
2	C	521	HIS
2	C	608	ASN
2	C	653	GLN

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Mol	Chain	Res	Type
3	F	92	HIS
4	L	18	ASN
4	L	76	GLN
4	L	85	GLN
4	L	122	ASN
4	L	272	HIS
4	L	316	HIS
4	L	370	HIS
4	L	400	GLN
5	M	177	ASN
5	M	283	ASN
6	A	55	GLN
6	A	108	ASN
8	J	93	GLN
9	R	24	GLN
10	S	60	ASN
10	S	79	HIS
9	U	82	HIS
10	V	44	GLN
6	W	68	GLN
8	X	93	GLN
1	G	95	GLN
1	G	120	HIS
1	G	166	HIS
1	G	298	GLN
1	G	517	ASN
1	G	527	HIS
1	G	633	ASN
2	I	47	GLN
2	I	58	GLN
2	I	102	ASN
2	I	273	GLN
2	I	282	HIS
2	I	297	HIS
2	I	470	GLN
2	I	520	ASN
2	I	546	ASN
2	I	598	HIS
2	I	618	HIS
3	K	94	GLN
3	K	136	GLN
3	K	219	ASN

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Mol	Chain	Res	Type
3	K	292	GLN
3	K	374	GLN
4	O	64	HIS
4	O	168	ASN
4	O	200	HIS
4	O	239	HIS
4	O	250	GLN
4	O	324	GLN
4	O	328	HIS
4	O	410	ASN
5	Y	200	HIS
5	Y	223	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
12	M3L	E	9	12	10,11,12	0.55	0	9,14,16	0.58	0

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
12	M3L	E	9	12	-	6/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	9	M3L	CD-CE-NZ-CM1
12	E	9	M3L	CD-CE-NZ-CM3
12	E	9	M3L	CD-CE-NZ-CM2
12	E	9	M3L	CG-CD-CE-NZ
12	E	9	M3L	CE-CD-CG-CB
12	E	9	M3L	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	9	M3L	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
13	SAH	I	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.95	3 (13%)
13	SAH	C	801	-	23,28,28	1.28	3 (13%)	22,40,40	1.88	4 (18%)

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
13	SAH	I	801	-	-	3/11/31/31	0/3/3/3
13	SAH	C	801	-	-	2/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	801	SAH	C2-N3	4.20	1.38	1.32
13	I	801	SAH	C2-N3	4.01	1.38	1.32
13	C	801	SAH	C2-N1	2.55	1.38	1.33
13	I	801	SAH	C2-N1	2.38	1.38	1.33
13	I	801	SAH	OXT-C	-2.34	1.23	1.30
13	C	801	SAH	OXT-C	-2.23	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	801	SAH	N3-C2-N1	-6.39	120.00	128.67
13	C	801	SAH	N3-C2-N1	-6.24	120.20	128.67
13	I	801	SAH	C5'-SD-CG	-4.52	88.85	102.26
13	C	801	SAH	C5'-SD-CG	-3.98	90.46	102.26
13	I	801	SAH	OXT-C-O	-2.81	117.71	124.08
13	C	801	SAH	OXT-C-O	-2.69	117.98	124.08
13	C	801	SAH	C4'-O4'-C1'	2.09	111.84	109.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	I	801	SAH	O4'-C4'-C5'-SD
13	I	801	SAH	C3'-C4'-C5'-SD
13	C	801	SAH	CA-CB-CG-SD
13	I	801	SAH	C-CA-CB-CG
13	C	801	SAH	CB-CG-SD-C5'

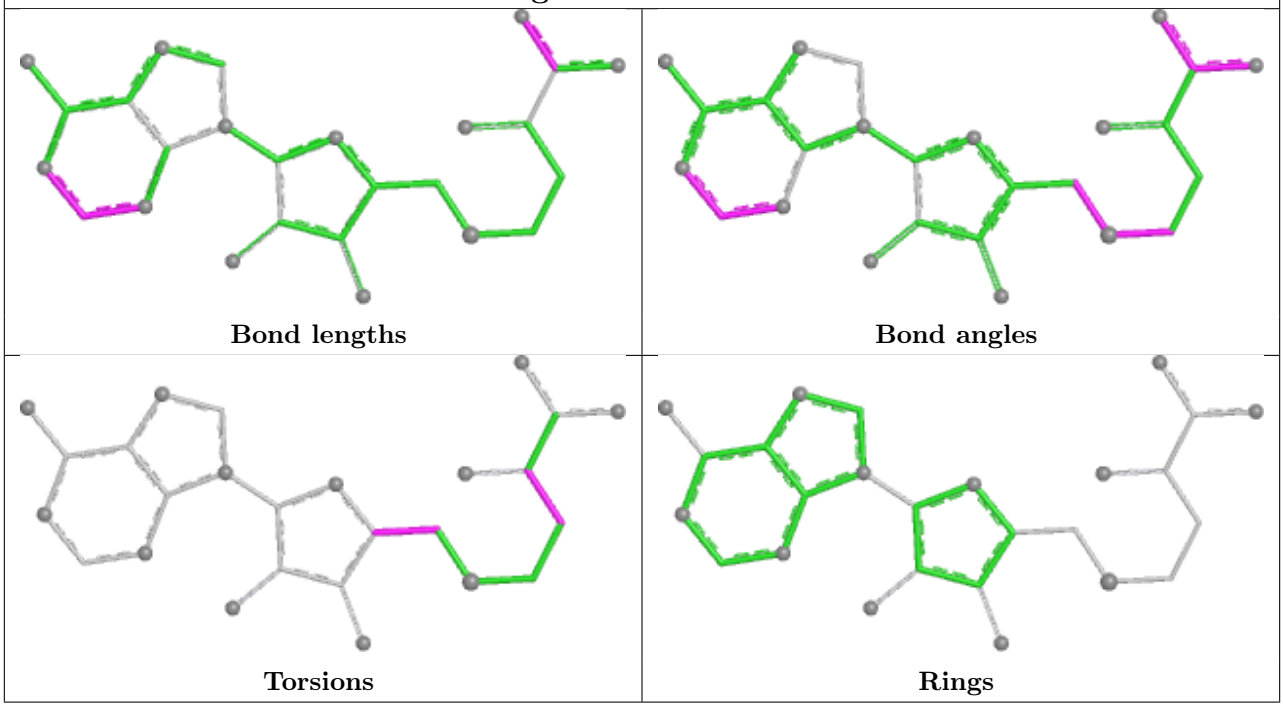
There are no ring outliers.

2 monomers are involved in 5 short contacts:

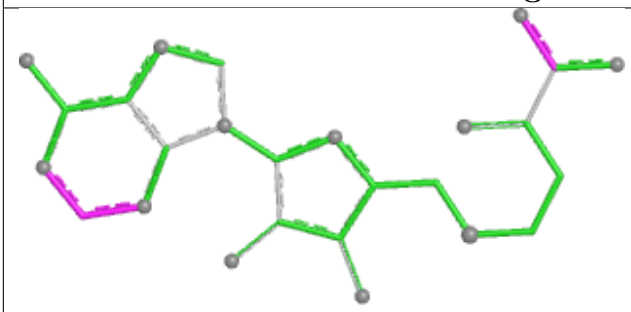
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	801	SAH	4	0
13	C	801	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

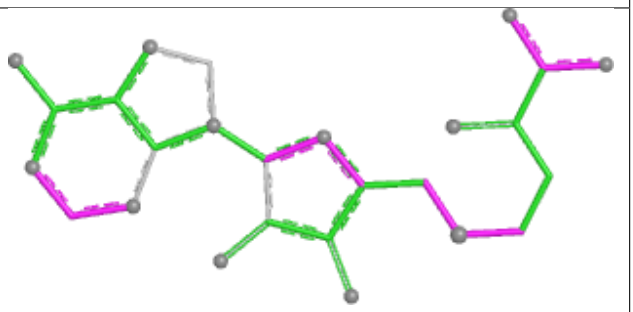
Ligand SAH I 801



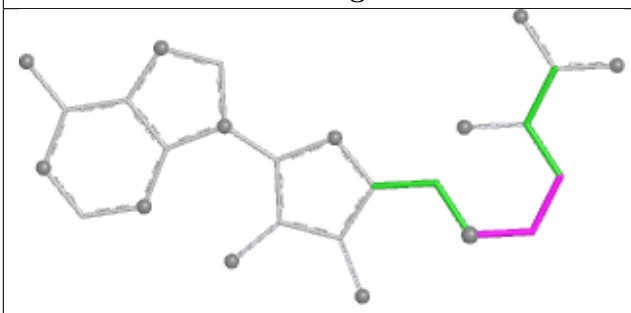
Ligand SAH C 801



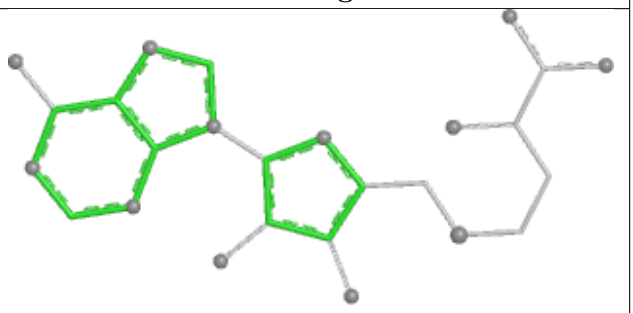
Bond lengths



Bond angles



Torsions



Rings

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.

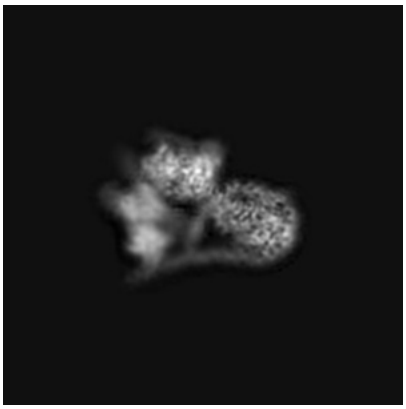
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41110. These allow visual inspection of the internal detail of the map and identification of artifacts.

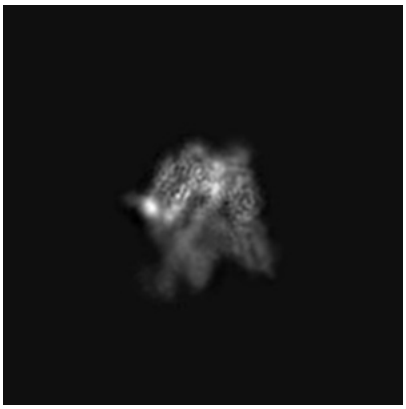
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

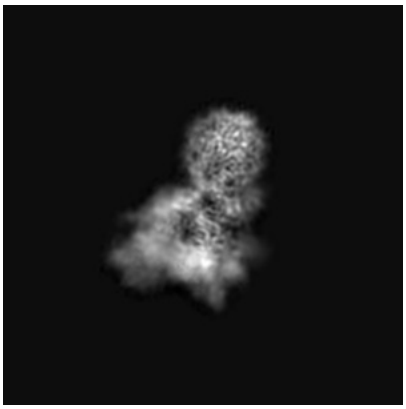
6.1.1 Primary map



X

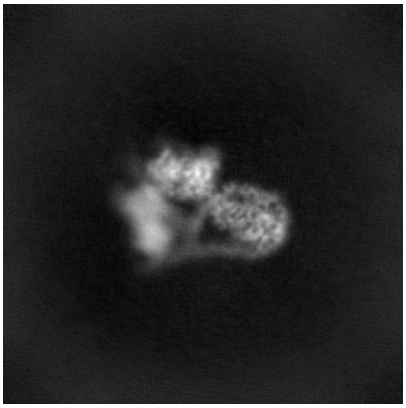


Y

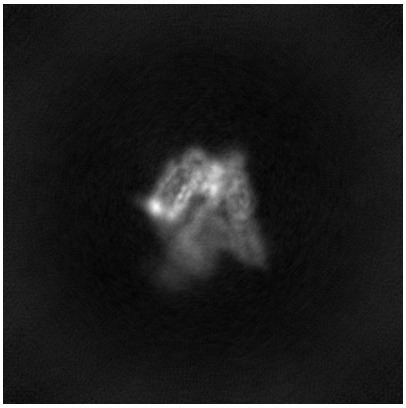


Z

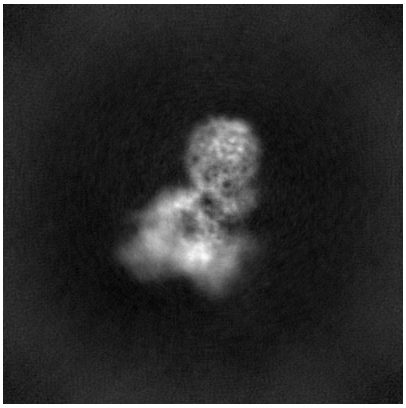
6.1.2 Raw map



X



Y

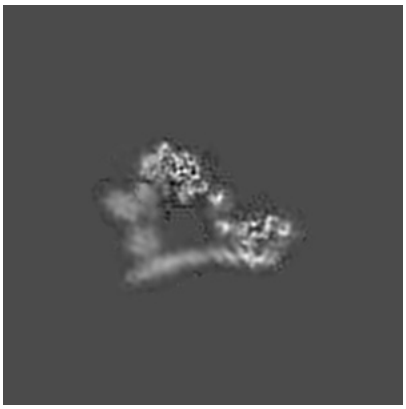


Z

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

6.2 Central slices (i)

6.2.1 Primary map

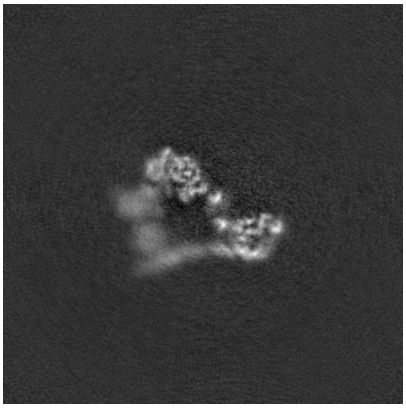


X Index: 100

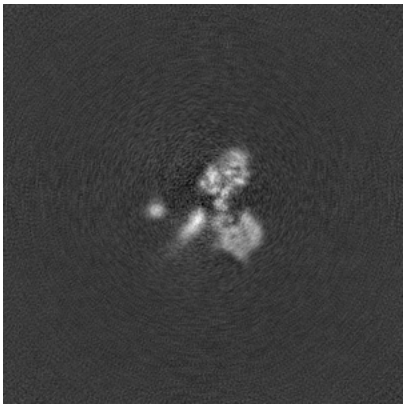
Y Index: 100

Z Index: 100

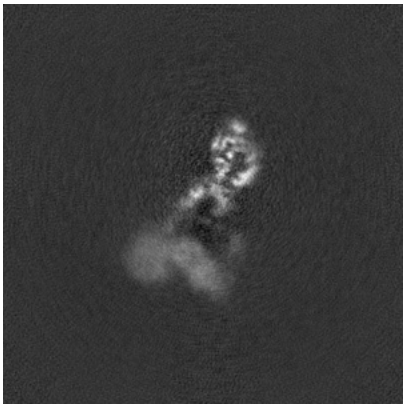
6.2.2 Raw map



X Index: 165



Y Index: 165

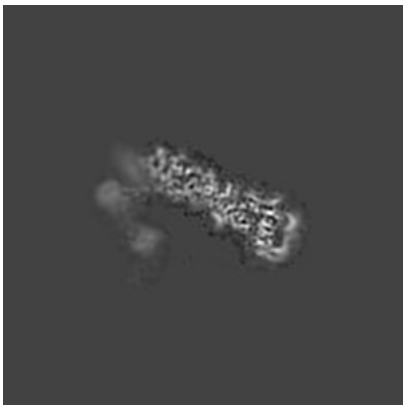


Z Index: 165

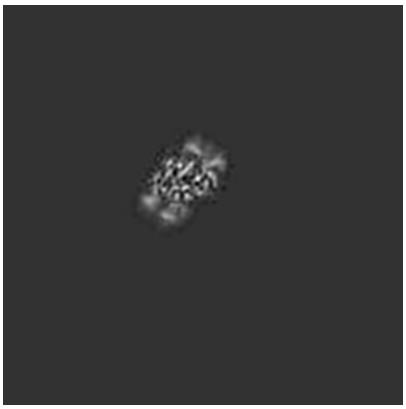
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

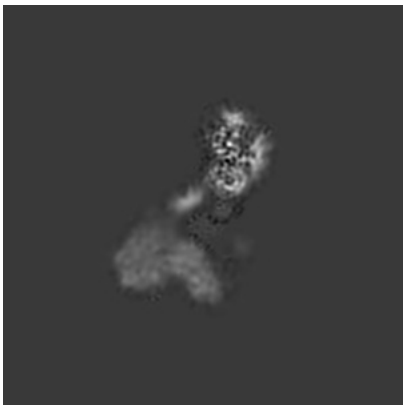
6.3.1 Primary map



X Index: 108

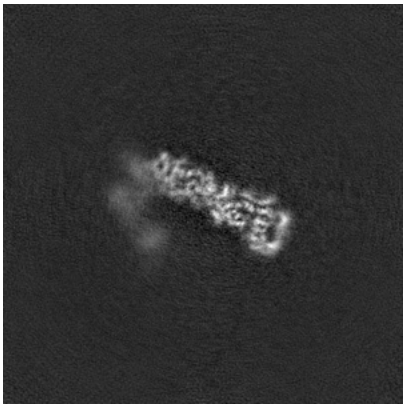


Y Index: 130

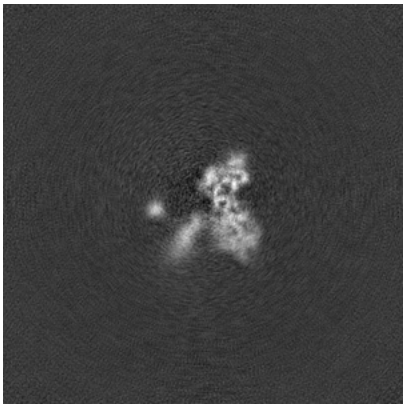


Z Index: 97

6.3.2 Raw map



X Index: 177



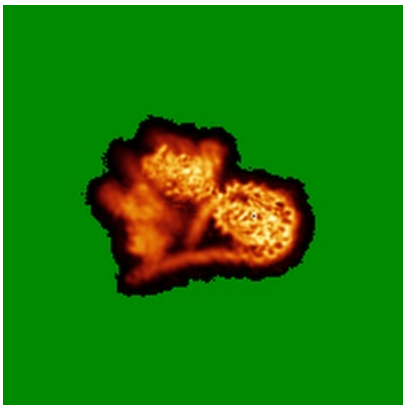
Y Index: 161

Z Index: 160

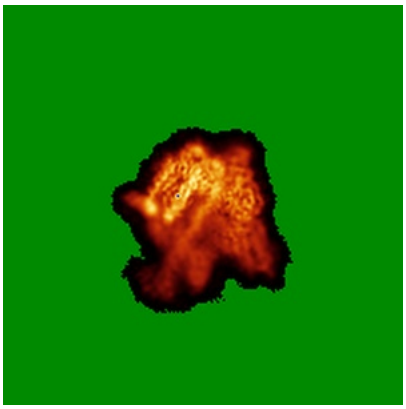
The images above show the largest variance slices of the map in three orthogonal directions.

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

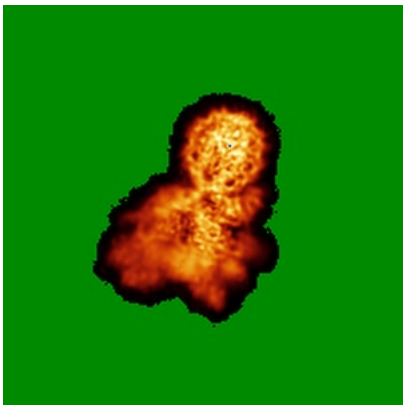
6.4.1 Primary map



X

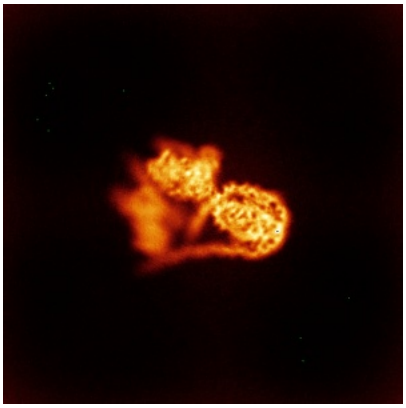


Y

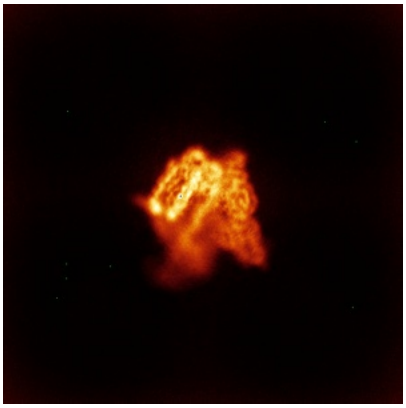


Z

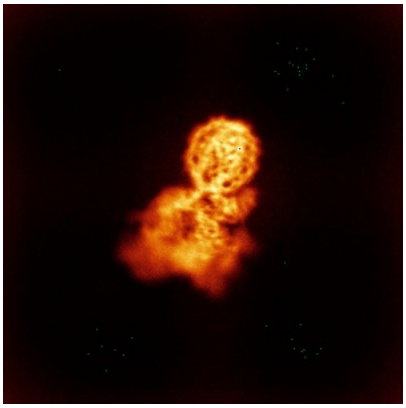
6.4.2 Raw map



X



Y

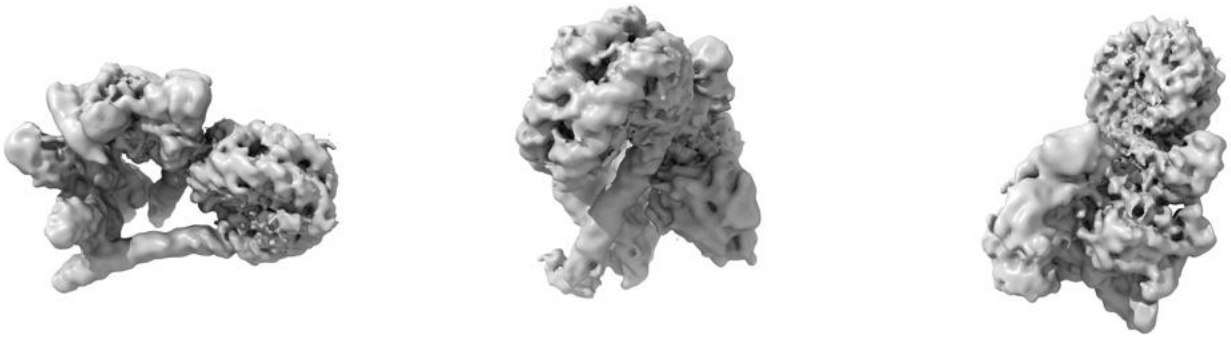


Z

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 0.02. 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.

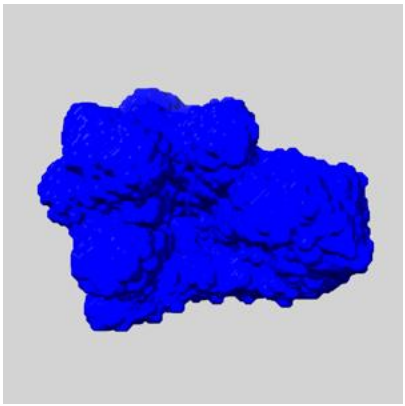
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

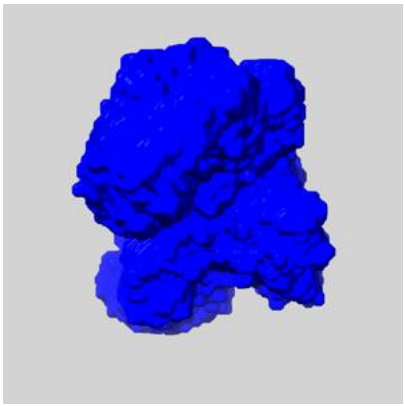
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

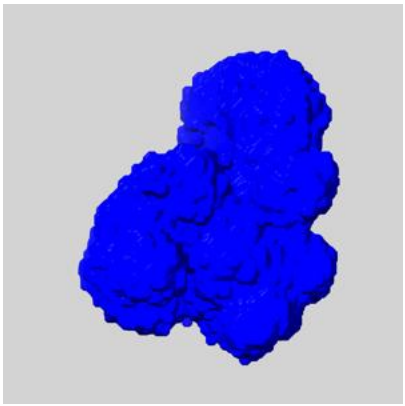
6.6.1 emd_41110_msk_1.map



X



Y

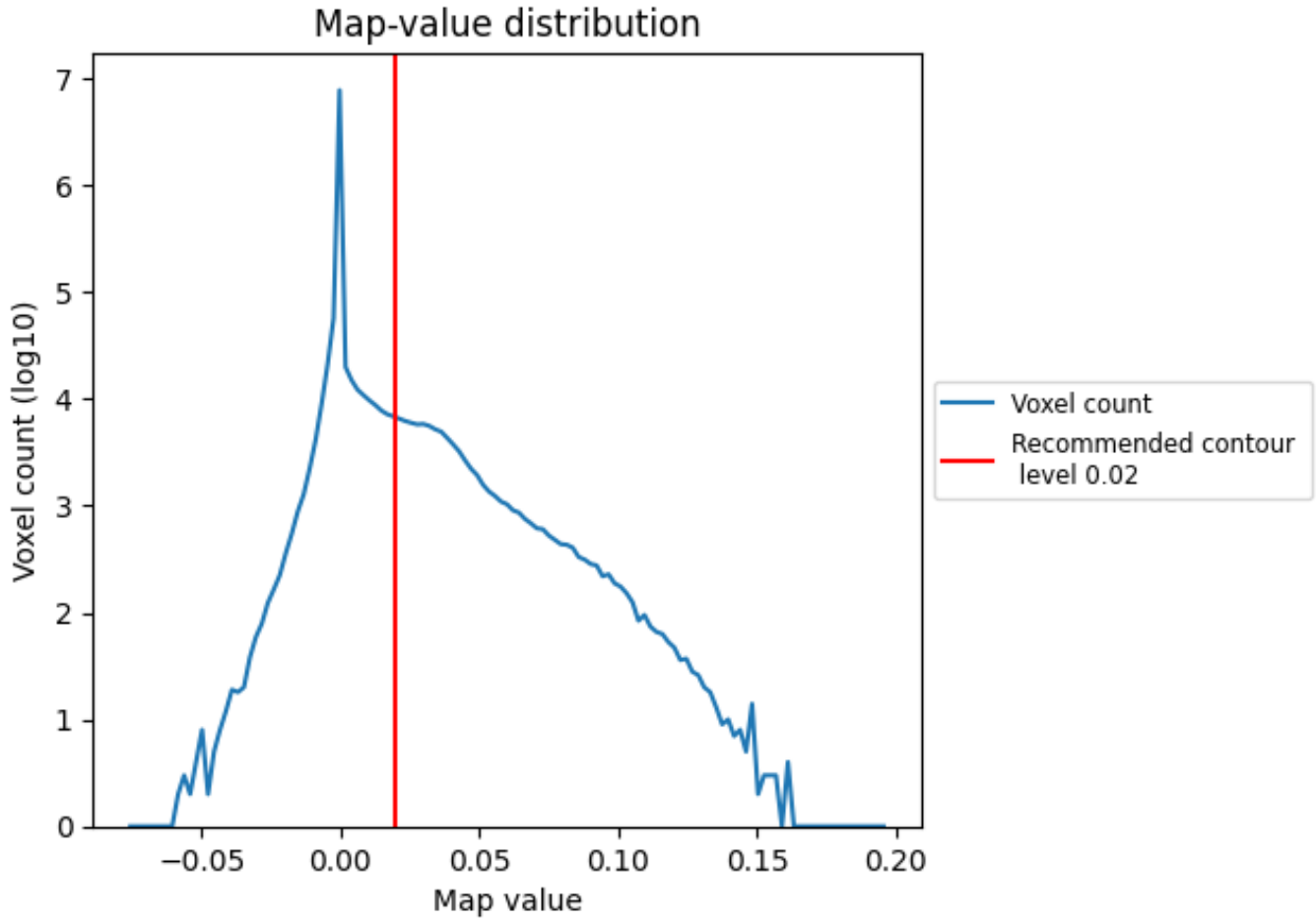


Z

7 Map analysis

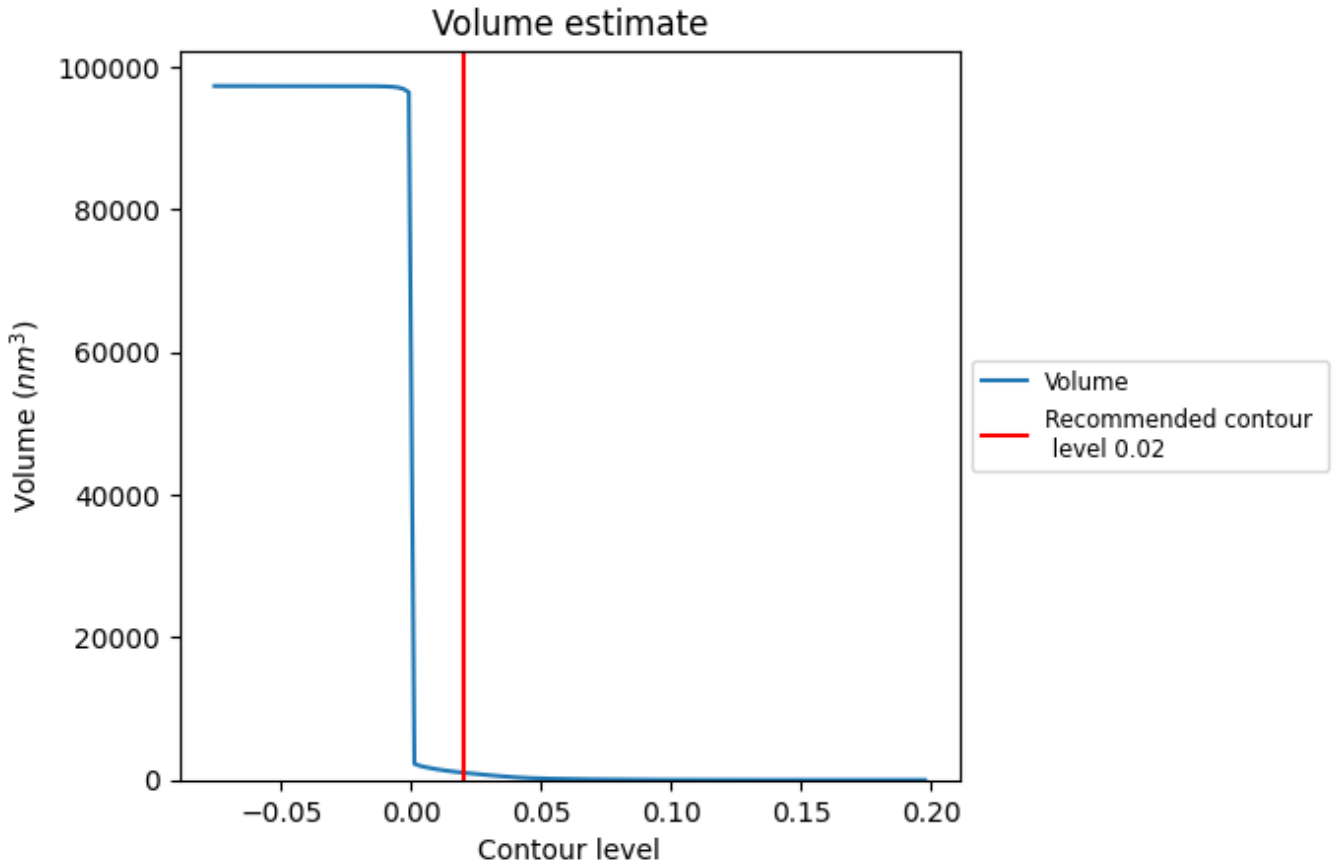
This section contains the results of statistical analysis of the map.

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.

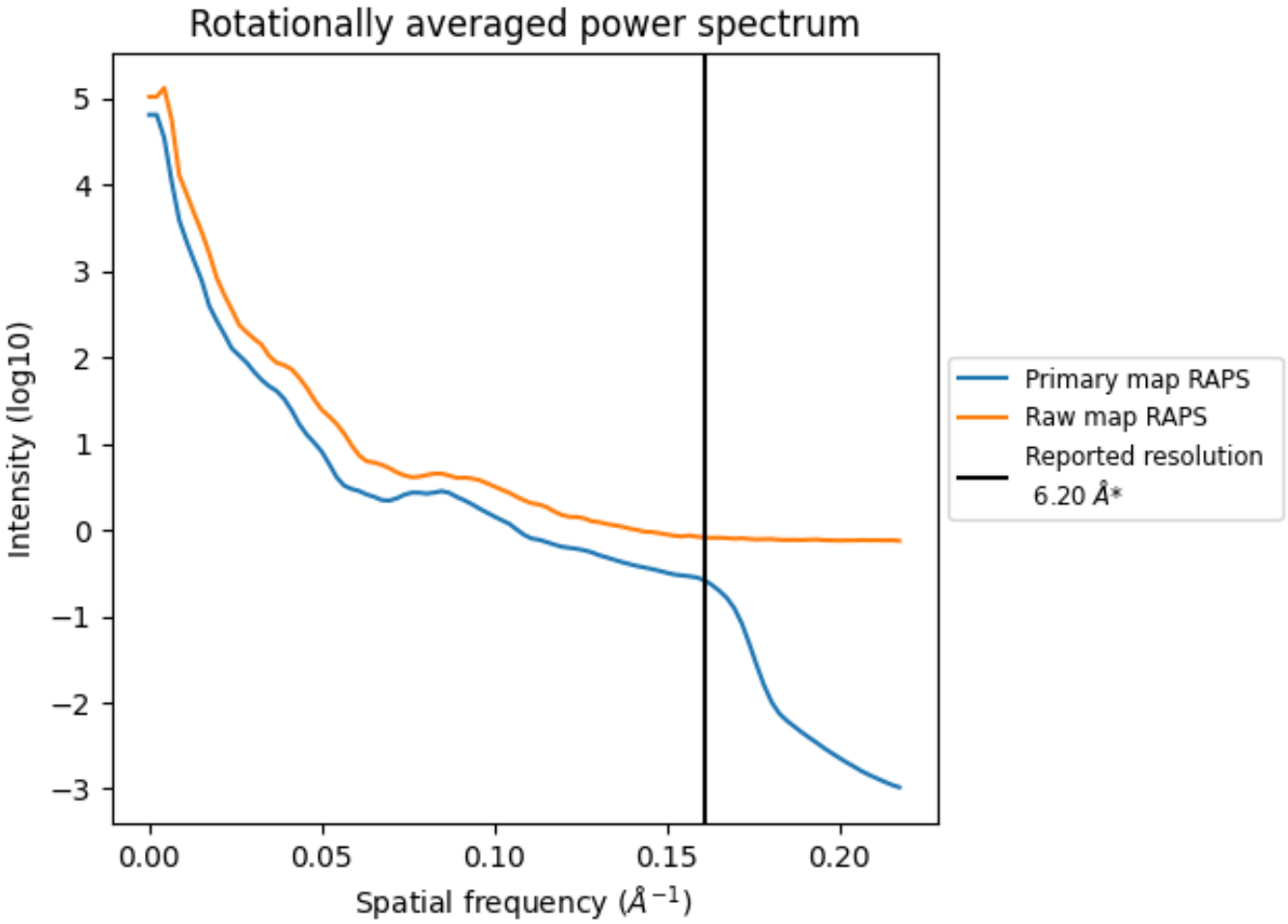
7.2 Volume estimate



The volume at the recommended contour level is 1023 nm^3; this corresponds to an approximate mass of 924 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)

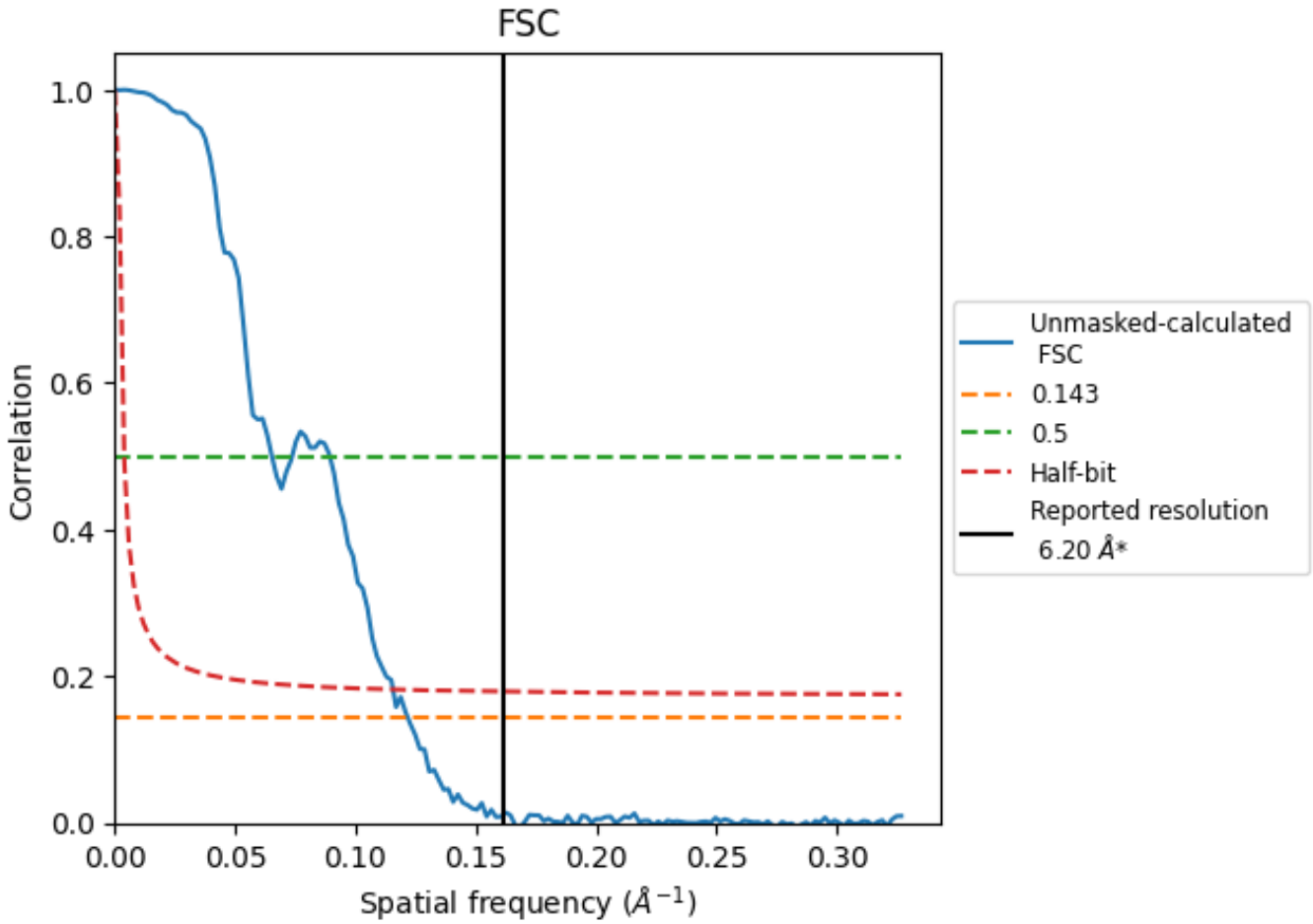


*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

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 0.161 Å^{-1}

8.2 Resolution estimates (i)

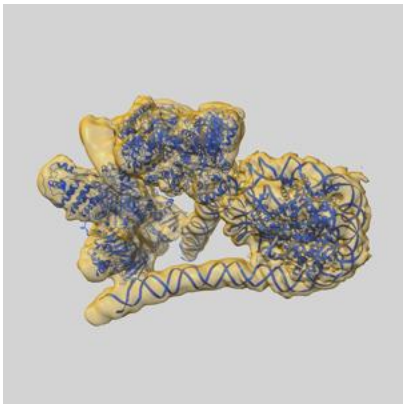
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.21	15.34	8.65

*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 8.21 differs from the reported value 6.2 by more than 10 %

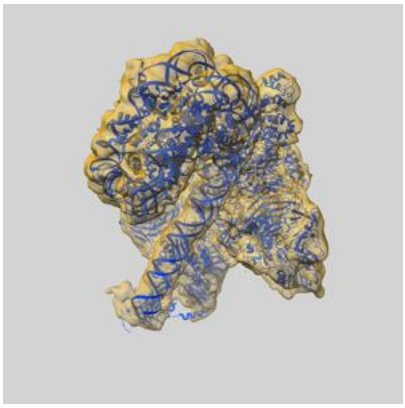
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41110 and PDB model 8T9G. Per-residue inclusion information can be found in section 3 on page 9.

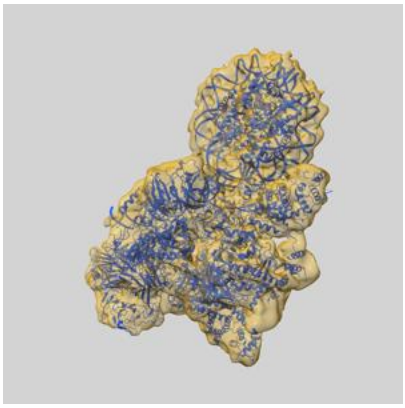
9.1 Map-model overlay



X



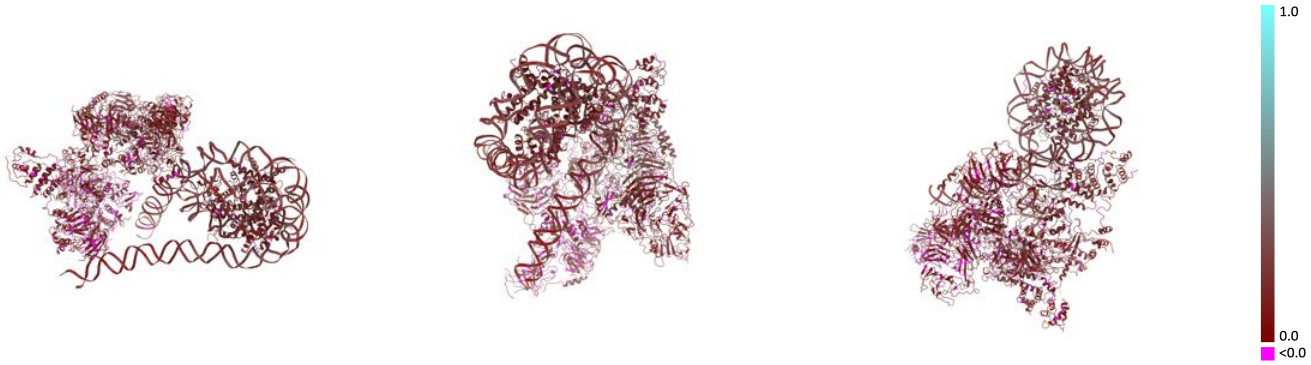
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

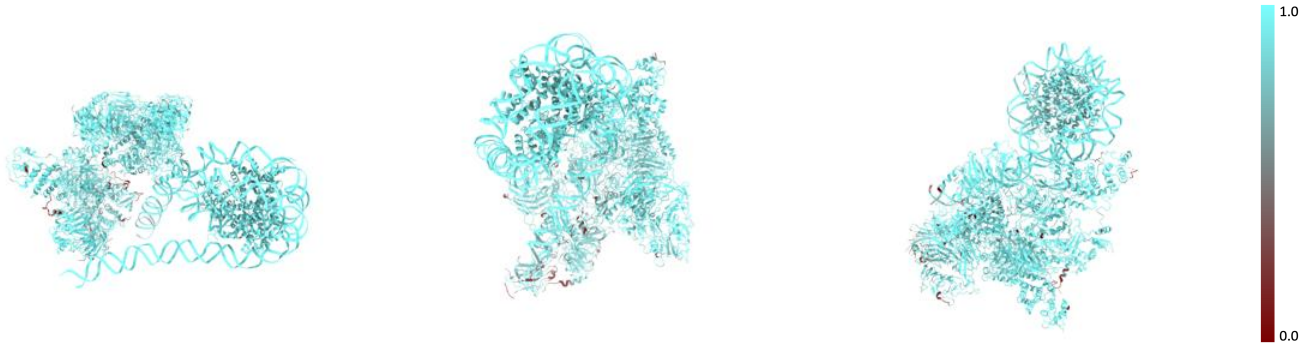
9.2 Q-score mapped to coordinate model (i)



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.

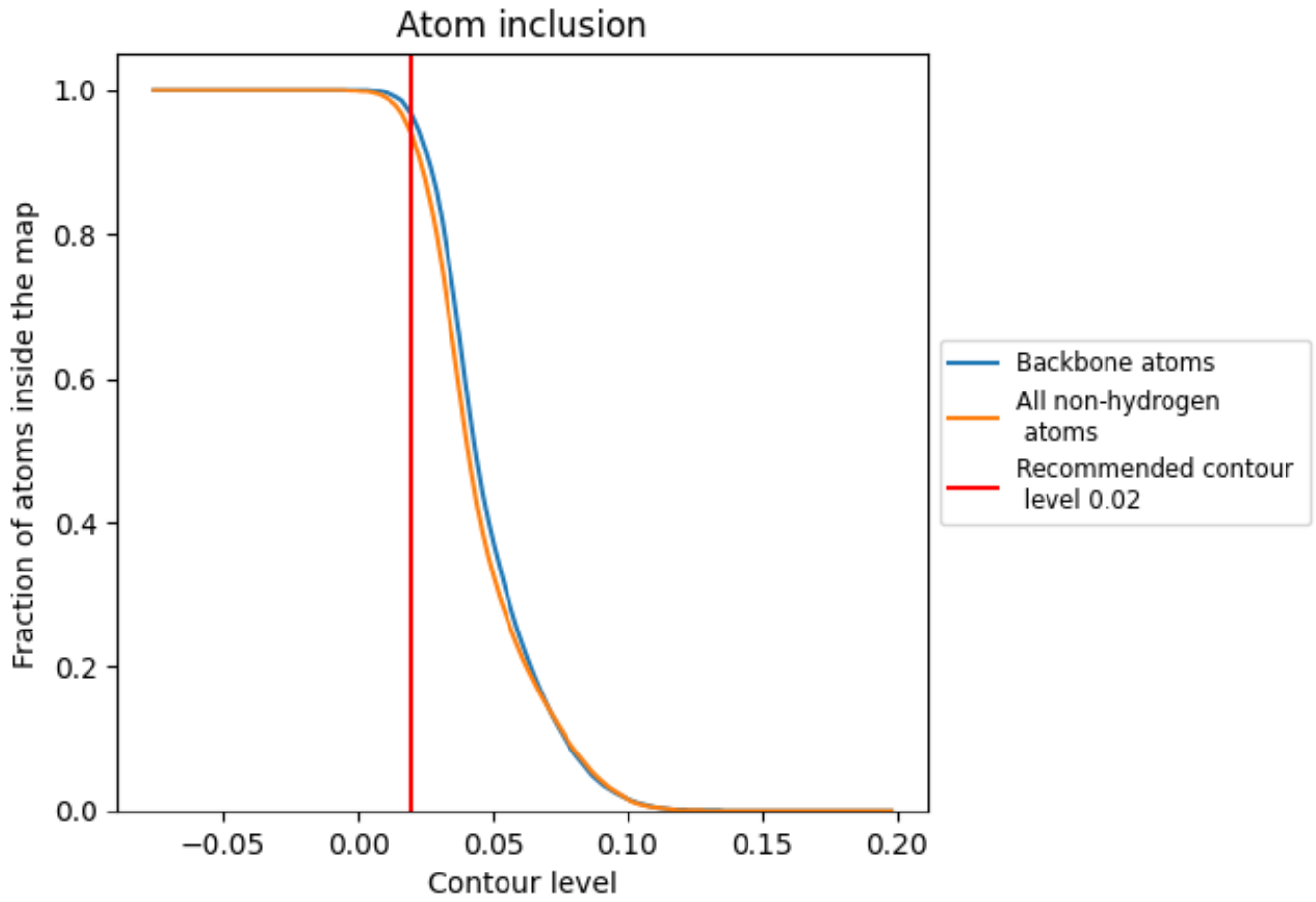
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.1630
A	0.9420	0.1900
B	0.8110	0.1060
C	0.9280	0.1220
E	0.8510	0.1660
F	0.9740	0.0960
G	0.9310	0.1730
H	0.9840	0.2140
I	0.9480	0.1860
J	0.9070	0.1960
K	0.9640	0.1930
L	0.9200	0.1010
M	0.8820	0.1030
O	0.9700	0.1480
R	0.9400	0.2140
S	0.9360	0.1920
T	0.9820	0.2120
U	0.9420	0.1980
V	0.9320	0.1990
W	0.9400	0.1780
X	0.8780	0.1710
Y	0.9050	0.1640