



## Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 02:28 PM JST

PDB ID : 9UZ9 / pdb\_00009uz9  
EMDB ID : EMD-64642  
Title : RNA polymerase II elongation complex stalled at SHL(-6) in the hexasome of the overlapping dinucleosome  
Authors : Chen, Z.; Ho, C.; Tanaka, H.; Kujirai, T.; Ogasawara, M.; Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.  
Deposited on : 2025-05-16  
Resolution : 6.74 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev133  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

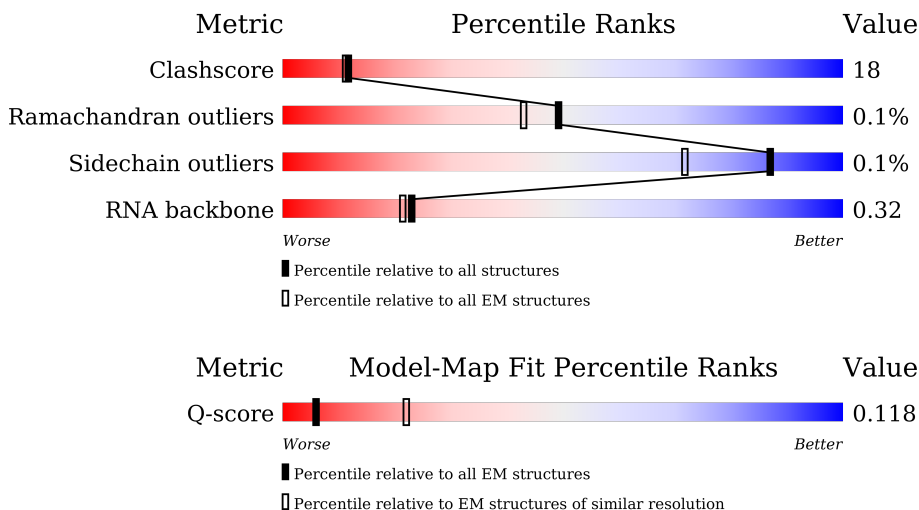
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.74 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	480 ( 6.24 - 7.24 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	

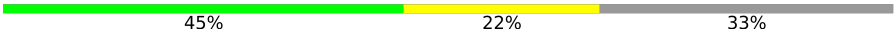
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Mol	Chain	Length	Quality of chain
4	D	186	61% 77% 6% 16%
5	E	214	63% 36%
6	F	155	33% 21% 46%
7	G	171	47% 74% 26%
8	H	145	66% 26% 8%
9	I	115	69% 28%
10	J	72	51% 40% 8%
11	K	118	66% 30%
12	L	72	42% 21% 38%
13	N	279	34% 63%
14	P	11	45% 36% 18%
15	T	279	46% 54%
16	a	139	52% 17% 32%
16	e	139	49% 19% 32%
16	k	139	35% 17% 47%
16	m	139	40% 29% 32%
17	b	106	47% 26% 26%
17	f	106	59% 14% 26%
17	l	106	37% 30% 33%
17	n	106	53% 21% 26%
18	c	133	53% 20% 26%
18	g	133	51% 22% 26%
18	o	133	57% 16% 27%
19	d	129	52% 18% 30%
19	h	129	53% 16% 31%

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Mol	Chain	Length	Quality of chain
19	p	129	 45% 22% 33%

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 52384 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1408	11095	6997	1935	2093	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1161	9261	5835	1636	1732	58	0	0

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	263	2098	1319	354	413	12	0	0

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	156	1210	753	210	245	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1740	1094	312	324	10	0	0

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a DNA chain called DNA (270-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	270	5497	2616	963	1648	270	0	0

- Molecule 14 is a RNA chain called RNA (5'-R(P\*UP\*GP\*UP\*GP\*UP\*UP\*UP\*GP\*GP\*G P\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	P	11	235	104	37	83	11	0	0

- Molecule 15 is a DNA chain called DNA (279-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	T	279	5752	2717	1114	1642	279	0	0

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	a	95	779	492	150	135	2	0	0
16	e	95	779	492	150	135	2	0	0
16	k	73	587	373	109	103	2	0	0
16	m	95	779	492	150	135	2	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243
k	-3	GLY	-	expression tag	UNP P84243
k	-2	SER	-	expression tag	UNP P84243
k	-1	HIS	-	expression tag	UNP P84243
m	-3	GLY	-	expression tag	UNP P84243
m	-2	SER	-	expression tag	UNP P84243
m	-1	HIS	-	expression tag	UNP P84243

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
17	l	71	Total	C	N	O	S	0	0
			568	357	113	97	1		
17	n	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
l	-3	GLY	-	expression tag	UNP P62805
l	-2	SER	-	expression tag	UNP P62805
l	-1	HIS	-	expression tag	UNP P62805
n	-3	GLY	-	expression tag	UNP P62805
n	-2	SER	-	expression tag	UNP P62805
n	-1	HIS	-	expression tag	UNP P62805

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	98	Total	C	N	O	0	0
			757	475	149	133		
18	g	98	Total	C	N	O	0	0
			757	475	149	133		
18	o	97	Total	C	N	O	0	0
			752	472	148	132		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
o	-3	GLY	-	expression tag	UNP P04908
o	-2	SER	-	expression tag	UNP P04908
o	-1	HIS	-	expression tag	UNP P04908

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	90	Total	C	N	O	S	0	0
			698	440	123	133	2		
19	h	89	Total	C	N	O	S	0	0
			689	435	122	130	2		
19	p	87	Total	C	N	O	S	0	0
			679	430	120	127	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
p	-3	GLY	-	expression tag	UNP P06899
p	-2	SER	-	expression tag	UNP P06899
p	-1	HIS	-	expression tag	UNP P06899

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

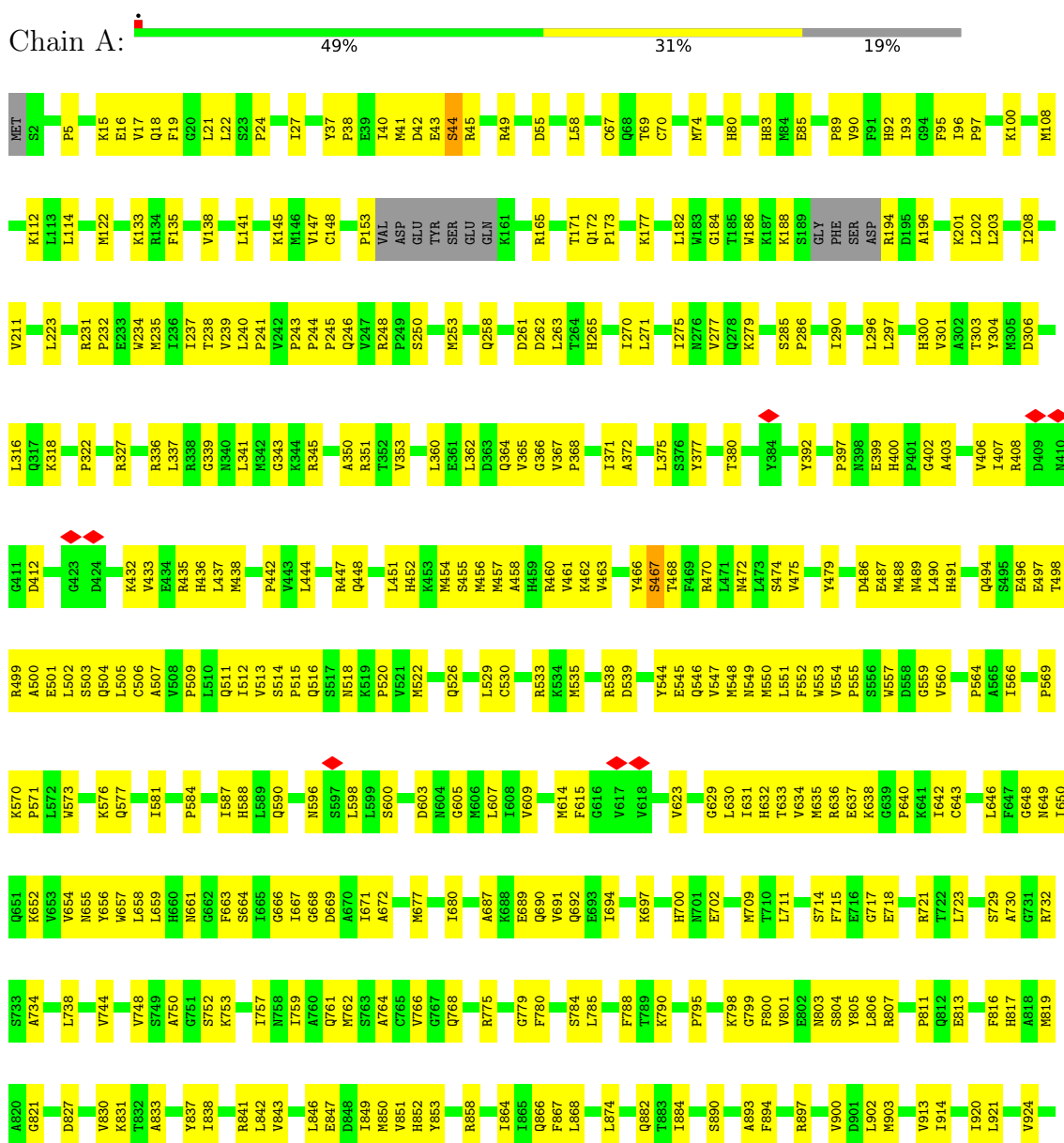
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0

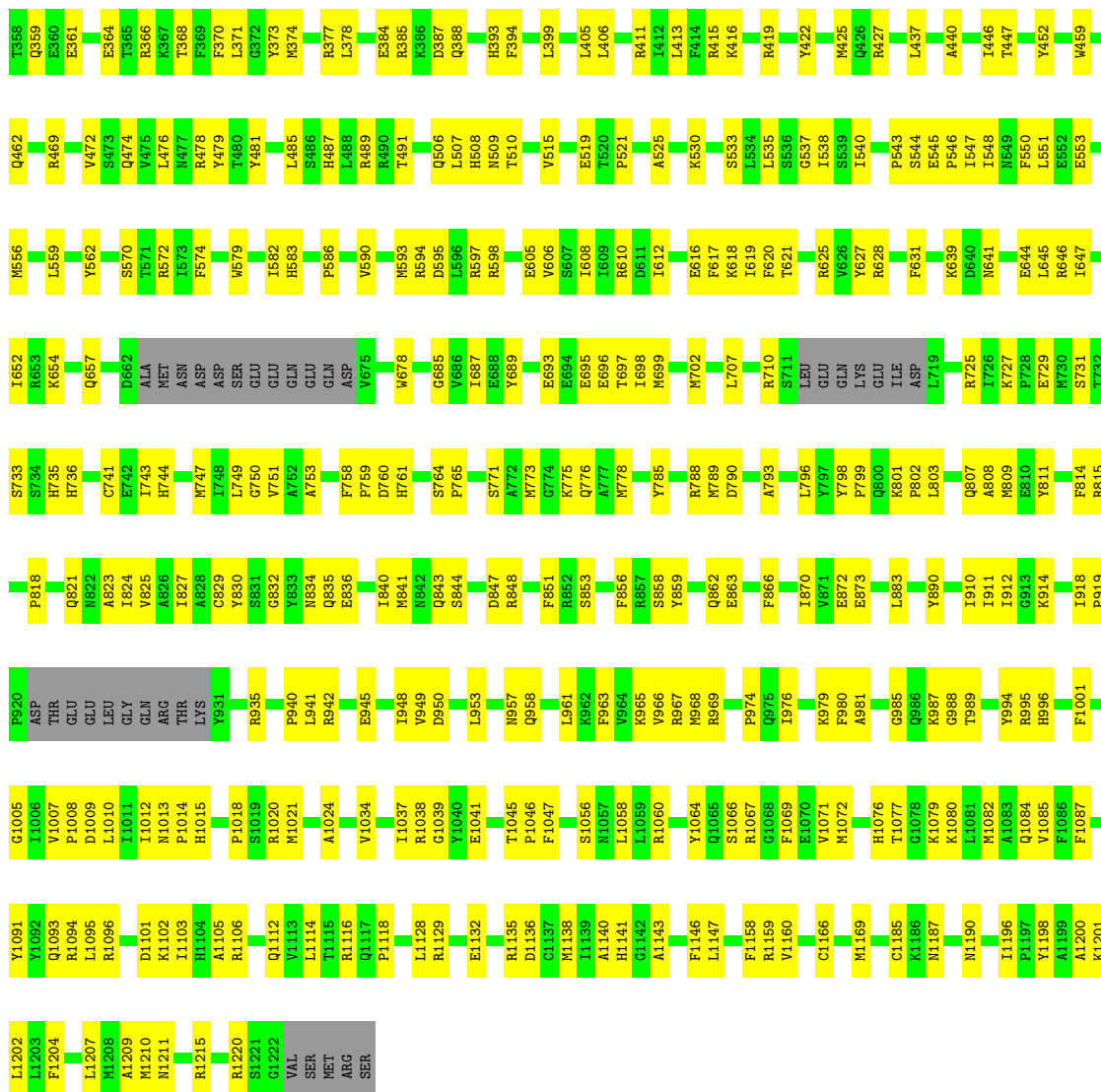
### 3 Residue-property plots

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.

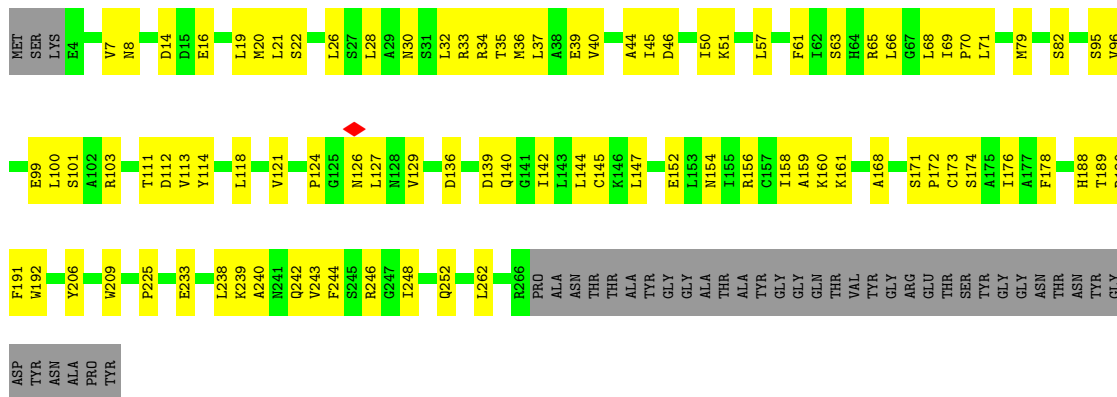
- Molecule 1: DNA-directed RNA polymerase subunit







● Molecule 3: RNA polymerase II third largest subunit B44, part of central core



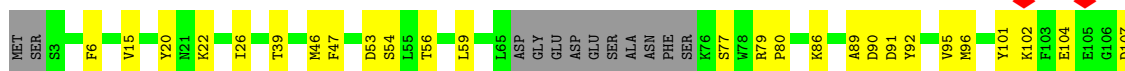
● Molecule 4: RNA polymerase II subunit B32





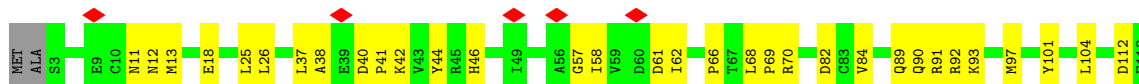
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 66% 26% 8%



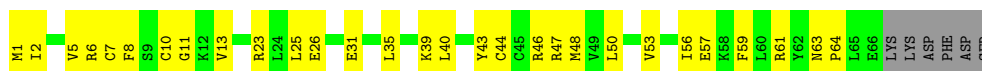
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 69% 28%



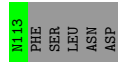
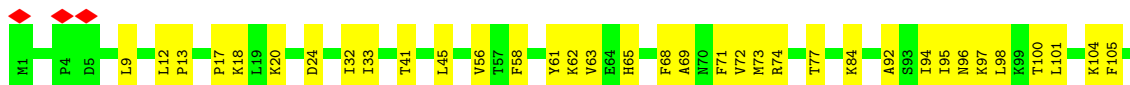
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 51% 40% 8%



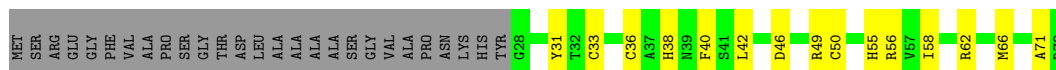
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 66% 30%



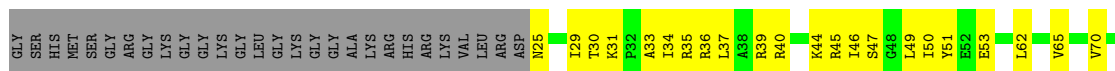
- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 42% 21% 38%

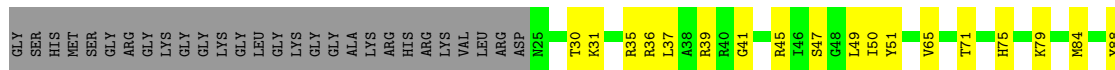




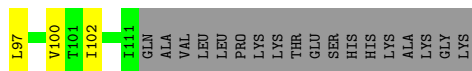




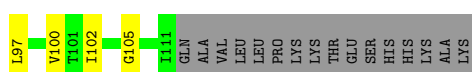
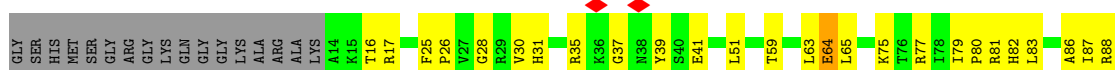
• Molecule 17: Histone H4



• Molecule 18: Histone H2A type 1-B/E



• Molecule 18: Histone H2A type 1-B/E

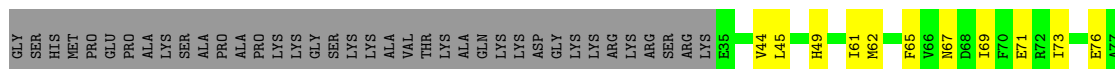


• Molecule 18: Histone H2A type 1-B/E

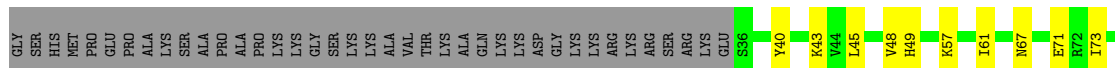


• Molecule 19: Histone H2B type 1-J

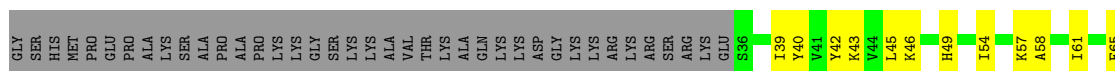




- Molecule 19: Histone H2B type 1-J



- Molecule 19: Histone H2B type 1-J



## 4 Experimental information

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	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.000666	Depositor
Map size ( $\text{\AA}$ )	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/11299	0.48	0/15266
2	B	0.21	0/9441	0.47	0/12732
3	C	0.24	0/2139	0.49	0/2895
4	D	0.15	0/1221	0.35	0/1648
5	E	0.22	0/1772	0.47	0/2385
6	F	0.18	0/687	0.48	0/931
7	G	0.22	0/1353	0.38	0/1837
8	H	0.19	0/1069	0.42	0/1444
9	I	0.14	0/934	0.39	0/1257
10	J	0.18	0/554	0.50	0/742
11	K	0.14	0/953	0.36	0/1291
12	L	0.12	0/365	0.35	0/484
13	N	0.54	0/6148	0.74	0/9479
14	P	0.63	0/261	0.82	0/405
15	T	0.57	0/6470	0.77	0/9987
16	a	0.34	0/790	0.49	0/1060
16	e	0.27	0/790	0.47	0/1060
16	k	0.33	0/594	0.59	0/797
16	m	0.31	0/790	0.53	0/1060
17	b	0.16	0/626	0.36	0/837
17	f	0.14	0/626	0.32	0/837
17	l	0.15	0/573	0.39	0/767
17	n	0.16	0/626	0.39	0/837
18	c	0.13	0/766	0.28	0/1033
18	g	0.21	0/766	0.36	0/1033
18	o	0.13	0/761	0.33	0/1026
19	d	0.14	0/709	0.33	0/955
19	h	0.14	0/700	0.33	0/943
19	p	0.14	0/690	0.33	0/930
All	All	0.33	0/54473	0.55	0/75958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11095	0	11132	472	0
2	B	9261	0	9265	385	0
3	C	2098	0	2059	79	0
4	D	1210	0	1205	9	0
5	E	1740	0	1754	61	0
6	F	677	0	693	34	0
7	G	1324	0	1342	28	0
8	H	1052	0	1050	30	0
9	I	917	0	869	30	0
10	J	545	0	561	35	0
11	K	932	0	944	27	0
12	L	359	0	359	13	0
13	N	5497	0	3045	288	0
14	P	235	0	116	5	0
15	T	5752	0	3115	178	0
16	a	779	0	814	21	0
16	e	779	0	814	21	0
16	k	587	0	615	26	0
16	m	779	0	814	41	0
17	b	619	0	659	27	0
17	f	619	0	659	14	0
17	l	568	0	614	27	0
17	n	619	0	659	21	0
18	c	757	0	802	26	0
18	g	757	0	802	26	0
18	o	752	0	797	16	0
19	d	698	0	710	20	0
19	h	689	0	704	16	0
19	p	679	0	698	24	0
20	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	52384	0	47670	1739	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 18.

All (1739) 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)
13:N:248:DC:H2''	13:N:249:DT:C7	1.16	1.59
13:N:115:DT:C2'	13:N:116:DT:H72	1.50	1.41
15:T:191:DT:H2''	15:T:192:DT:C7	1.52	1.37
13:N:248:DC:C2'	13:N:249:DT:H73	1.60	1.31
15:T:191:DT:C2'	15:T:192:DT:H73	1.60	1.30
13:N:69:DG:H2''	13:N:70:DT:C7	1.66	1.26
13:N:248:DC:C2'	13:N:249:DT:C7	2.13	1.26
13:N:235:DA:C2'	13:N:236:DT:H72	1.67	1.25
15:T:160:DT:H2''	15:T:161:DT:C7	1.69	1.22
13:N:235:DA:C2'	13:N:236:DT:C7	2.18	1.20
13:N:235:DA:H2''	13:N:236:DT:C7	1.73	1.18
15:T:160:DT:H2''	15:T:161:DT:H71	1.26	1.13
13:N:248:DC:H2''	13:N:249:DT:H71	1.21	1.11
13:N:69:DG:H2''	13:N:70:DT:H71	1.12	1.11
13:N:115:DT:C2'	13:N:116:DT:C7	2.29	1.11
13:N:235:DA:H2''	13:N:236:DT:H73	1.35	1.08
13:N:35:DG:H2'	13:N:36:DT:H72	1.34	1.07
13:N:163:DT:C6	13:N:164:DT:H72	1.89	1.07
13:N:115:DT:H2'	13:N:116:DT:H72	1.15	1.06
13:N:163:DT:N1	13:N:164:DT:H72	1.70	1.06
13:N:121:DC:H2''	13:N:122:DC:C5	1.91	1.04
13:N:96:DG:H2'	13:N:97:DT:H72	1.43	1.01
1:A:447:ARG:NH2	1:A:451:LEU:HB2	1.75	1.00
15:T:191:DT:O3'	15:T:192:DT:H71	1.62	0.99
13:N:115:DT:H2''	13:N:116:DT:C7	1.93	0.98
13:N:235:DA:N9	13:N:236:DT:H72	1.80	0.97
13:N:35:DG:C2'	13:N:36:DT:H72	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:NH2	1:A:451:LEU:CG	2.30	0.94
1:A:447:ARG:NH2	1:A:451:LEU:CB	2.30	0.94
1:A:447:ARG:HG2	1:A:455:SER:HB3	1.52	0.92
13:N:115:DT:H2''	13:N:116:DT:H72	1.51	0.92
2:B:764:SER:OG	2:B:765:PRO:HD3	1.70	0.92
13:N:235:DA:C1'	13:N:236:DT:H72	1.99	0.92
13:N:4:DT:H2''	13:N:5:DT:H71	1.49	0.91
13:N:69:DG:C2'	13:N:70:DT:H71	2.00	0.91
2:B:533:SER:HB2	2:B:628:ARG:HH12	1.33	0.91
1:A:447:ARG:HH22	1:A:451:LEU:HD12	1.36	0.90
13:N:35:DG:H2'	13:N:36:DT:C7	2.01	0.90
15:T:181:DG:H2''	15:T:182:DT:C7	2.00	0.90
13:N:115:DT:H2'	13:N:116:DT:C7	1.94	0.90
2:B:778:MET:HE1	2:B:853:SER:HA	1.53	0.89
13:N:235:DA:H2'	13:N:236:DT:H72	1.52	0.89
15:T:191:DT:C2'	15:T:192:DT:C7	2.30	0.87
2:B:627:TYR:HB2	2:B:689:TYR:HB3	1.56	0.87
1:A:1211:MET:HE1	1:A:1240:ILE:HG12	1.57	0.87
19:p:99:ARG:HH12	19:p:111:VAL:HG21	1.38	0.86
13:N:69:DG:C2'	13:N:70:DT:C7	2.53	0.86
2:B:556:MET:HG3	2:B:583:HIS:HB3	1.55	0.86
13:N:35:DG:C2'	13:N:36:DT:C7	2.54	0.85
13:N:60:DT:C6	13:N:61:DT:H72	2.11	0.85
15:T:19:DA:H2''	15:T:20:DC:C5	2.12	0.85
13:N:235:DA:C2'	13:N:236:DT:H73	1.98	0.85
1:A:343:GLY:HA2	2:B:1135:ARG:HH22	1.41	0.84
1:A:447:ARG:NH2	1:A:451:LEU:HG	1.92	0.84
1:A:790:LYS:H	9:I:69:PRO:HD3	1.42	0.84
13:N:235:DA:H2'	13:N:236:DT:C7	2.05	0.84
1:A:569:PRO:HD2	8:H:46:MET:HG3	1.60	0.84
15:T:152:DC:H2''	15:T:153:DT:H5'	1.60	0.84
15:T:108:DC:H2''	15:T:109:DT:H71	1.58	0.83
13:N:248:DC:H2''	13:N:249:DT:C5	2.14	0.82
13:N:248:DC:H2''	13:N:249:DT:H73	0.83	0.82
13:N:163:DT:H5''	18:c:16:THR:HA	1.61	0.82
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.62	0.81
13:N:121:DC:H2''	13:N:122:DC:H5	1.42	0.81
1:A:768:GLN:HA	1:A:800:PHE:HA	1.62	0.81
13:N:235:DA:C8	13:N:236:DT:H72	2.16	0.81
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.21	0.81
10:J:7:CYS:HB3	10:J:11:GLY:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:129:DG:H2''	13:N:130:DG:C8	2.16	0.80
13:N:217:DG:H2''	13:N:218:DT:H71	1.62	0.80
13:N:248:DC:C2'	13:N:249:DT:H71	1.97	0.80
1:A:843:VAL:O	1:A:847:GLU:HB3	1.81	0.80
1:A:516:GLN:HE22	1:A:1076:GLU:HB3	1.46	0.79
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.63	0.79
13:N:62:DG:H5''	18:o:16:THR:HA	1.64	0.79
15:T:160:DT:H2''	15:T:161:DT:C5	2.18	0.79
15:T:6:DA:C8	15:T:7:DT:H72	2.18	0.79
1:A:447:ARG:HH22	1:A:451:LEU:CD1	1.94	0.78
2:B:1072:MET:HE2	2:B:1085:VAL:HB	1.65	0.78
13:N:161:DA:H5''	18:c:32:ARG:HH12	1.47	0.78
17:b:34:ILE:HD11	17:b:55:ARG:HH21	1.48	0.78
1:A:447:ARG:HH21	1:A:451:LEU:CB	1.93	0.78
15:T:223:DG:H3'	19:p:39:ILE:HG13	1.65	0.78
13:N:246:DG:H2'	13:N:247:DT:H72	1.66	0.78
15:T:271:DA:H2''	15:T:272:DC:C5	2.19	0.78
13:N:206:DC:H2''	13:N:207:DT:H5''	1.67	0.77
1:A:694:ILE:HA	1:A:697:LYS:HZ3	1.51	0.76
5:E:19:LYS:HB3	5:E:34:MET:HE1	1.68	0.76
13:N:77:DT:H2''	13:N:78:DA:C5	2.21	0.76
15:T:191:DT:O3'	15:T:192:DT:C7	2.34	0.76
3:C:57:LEU:HD11	10:J:1:MET:HE1	1.68	0.76
9:I:25:LEU:HG	9:I:38:ALA:HB3	1.69	0.75
15:T:145:DT:H2''	15:T:146:DA:H5'	1.67	0.75
13:N:105:DG:H5'	13:N:105:DG:H8	1.50	0.75
16:k:117:VAL:HB	17:l:44:LYS:HD2	1.69	0.75
1:A:1316:LEU:HD11	1:A:1341:VAL:HB	1.68	0.75
13:N:246:DG:C2'	13:N:247:DT:H72	2.17	0.75
6:F:94:LEU:HD13	6:F:122:MET:HE1	1.67	0.75
13:N:33:DG:H2''	13:N:34:DT:H5'	1.68	0.75
13:N:161:DA:H2'	13:N:162:DA:C8	2.22	0.75
13:N:96:DG:C2'	13:N:97:DT:H72	2.16	0.74
1:A:672:ALA:HB3	1:A:677:MET:HE3	1.68	0.74
2:B:99:MET:HE1	2:B:111:TYR:HA	1.70	0.74
1:A:203:LEU:HB3	1:A:208:ILE:HD11	1.69	0.74
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.69	0.74
13:N:129:DG:H2''	13:N:130:DG:H8	1.51	0.74
1:A:201:LYS:HZ1	1:A:203:LEU:HD13	1.52	0.74
2:B:645:LEU:HD21	2:B:741:CYS:HB3	1.69	0.74
16:k:62:ILE:HD13	17:l:33:ALA:HB1	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:107:DC:H2''	13:N:108:DC:C5	2.22	0.74
15:T:191:DT:C3'	15:T:192:DT:H71	2.17	0.74
13:N:67:DT:H2''	13:N:68:DT:C5	2.23	0.73
15:T:8:DG:H3'	15:T:9:DT:H71	1.68	0.73
19:p:98:VAL:HG13	19:p:102:LEU:HD12	1.70	0.73
15:T:264:DC:H2'	15:T:265:DA:H8	1.54	0.73
2:B:950:ASP:HB2	2:B:969:ARG:HD2	1.70	0.73
2:B:1187:ASN:HD21	2:B:1190:ASN:HB2	1.54	0.73
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.71	0.73
15:T:6:DA:H2'	15:T:7:DT:C7	2.18	0.73
13:N:236:DT:N1	13:N:237:DT:H72	2.04	0.72
15:T:130:DC:H2''	15:T:131:DT:C5	2.24	0.72
13:N:109:DC:H2''	13:N:110:DC:C5	2.23	0.72
13:N:163:DT:C2'	13:N:164:DT:C7	2.66	0.72
1:A:709:MET:HE2	1:A:714:SER:HA	1.71	0.72
1:A:900:VAL:HG22	1:A:1031:ARG:HG3	1.71	0.72
1:A:452:HIS:HD2	1:A:1076:GLU:HG3	1.53	0.72
5:E:63:PRO:HB3	5:E:74:LEU:HD22	1.72	0.72
18:g:65:LEU:HB3	18:g:86:ALA:HB1	1.72	0.72
2:B:750:GLY:H	2:B:753:ALA:HB3	1.55	0.72
1:A:367:VAL:HG21	1:A:461:VAL:HG13	1.71	0.72
2:B:586:PRO:HG2	2:B:610:ARG:HH21	1.55	0.72
13:N:115:DT:C6	13:N:116:DT:H72	2.25	0.72
12:L:33:CYS:CB	12:L:36:CYS:SG	2.75	0.71
5:E:178:GLN:HA	5:E:214:LEU:HB2	1.69	0.71
13:N:210:DC:H2''	13:N:211:DC:C5	2.24	0.71
13:N:256:DA:C5	13:N:257:DC:N4	2.58	0.71
1:A:858:ARG:HG2	1:A:864:ILE:HG12	1.71	0.71
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.72	0.71
13:N:179:DC:H2''	13:N:180:DT:H71	1.72	0.71
1:A:248:ARG:HB3	1:A:263:LEU:HB2	1.71	0.71
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.54	0.71
13:N:86:DT:H2''	13:N:87:DT:C5	2.25	0.71
15:T:82:DG:C2'	15:T:83:DT:H72	2.20	0.71
1:A:447:ARG:HH22	1:A:451:LEU:CG	1.99	0.71
1:A:637:GLU:HG2	1:A:638:LYS:HG2	1.72	0.71
4:D:169:VAL:HG12	4:D:171:LEU:H	1.56	0.70
15:T:191:DT:C3'	15:T:192:DT:C7	2.69	0.70
8:H:102:LYS:HB3	8:H:114:TYR:HB2	1.72	0.70
1:A:962:LEU:HD11	1:A:1024:VAL:HG22	1.72	0.70
3:C:26:LEU:HD11	3:C:225:PRO:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:SER:HB2	1:A:258:GLN:HB2	1.72	0.70
1:A:533:ARG:HD2	1:A:750:ALA:HB2	1.71	0.70
2:B:985:GLY:HA2	2:B:987:LYS:HE2	1.73	0.70
2:B:229:ALA:HB2	2:B:378:LEU:HD13	1.72	0.70
15:T:191:DT:H1'	15:T:192:DT:C4	2.26	0.70
17:l:82:THR:HB	17:l:84:MET:HE3	1.74	0.70
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.74	0.70
3:C:51:LYS:HG2	12:L:66:MET:HE1	1.73	0.70
1:A:1023:LEU:HD11	1:A:1027:ARG:HE	1.57	0.70
13:N:115:DT:H2''	13:N:116:DT:C5	2.26	0.70
2:B:1001:PHE:HD2	2:B:1005:GLY:HA2	1.56	0.69
1:A:884:ILE:HG12	1:A:1023:LEU:HD13	1.74	0.69
6:F:128:ARG:HH21	6:F:153:VAL:H	1.40	0.69
1:A:1222:PHE:HB3	1:A:1226:LEU:HB3	1.75	0.69
3:C:66:LEU:HD12	3:C:69:ILE:HD12	1.73	0.69
15:T:108:DC:H2''	15:T:109:DT:C7	2.22	0.69
1:A:1120:VAL:HA	1:A:1330:THR:HG23	1.73	0.69
10:J:44:CYS:HA	10:J:47:ARG:HG2	1.75	0.69
2:B:594:ARG:HG3	2:B:597:ARG:HH21	1.58	0.69
13:N:96:DG:H2'	13:N:97:DT:C7	2.20	0.69
2:B:957:ASN:HB3	2:B:963:PHE:HB2	1.73	0.69
1:A:318:LYS:HD2	15:T:270:DC:N4	2.08	0.69
13:N:128:DG:H2''	13:N:129:DG:C8	2.27	0.69
13:N:163:DT:H2'	13:N:164:DT:C7	2.22	0.69
13:N:244:DT:H2'	13:N:245:DA:C8	2.27	0.69
18:g:75:LYS:HG2	18:g:82:HIS:HE1	1.56	0.68
8:H:39:THR:HB	8:H:123:CYS:HB3	1.76	0.68
1:A:882:GLN:HB3	1:A:1027:ARG:HH22	1.58	0.68
2:B:562:TYR:HD1	2:B:582:ILE:HD13	1.58	0.68
5:E:98:ARG:HA	5:E:101:GLU:HG2	1.74	0.68
13:N:185:DC:C2	13:N:186:DC:C5	2.81	0.68
15:T:160:DT:C2'	15:T:161:DT:H71	2.16	0.68
2:B:953:LEU:HB3	2:B:965:LYS:HB2	1.76	0.68
1:A:513:VAL:HA	1:A:520:PRO:HA	1.76	0.68
1:A:850:MET:HE2	1:A:1439:MET:HB3	1.76	0.68
2:B:66:ASN:HB3	2:B:69:ASP:H	1.59	0.68
1:A:1195:LEU:HD21	1:A:1270:MET:HE1	1.75	0.68
11:K:24:ASP:HB2	11:K:32:ILE:HG12	1.75	0.68
13:N:115:DT:C1'	13:N:116:DT:H72	2.21	0.68
15:T:130:DC:H2''	15:T:131:DT:C4	2.28	0.68
2:B:1116:ARG:HH22	2:B:1158:PHE:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:PRO:HD2	6:F:86:THR:HG21	1.75	0.67
13:N:161:DA:H2'	13:N:162:DA:H8	1.58	0.67
15:T:181:DG:H2''	15:T:182:DT:C5	2.30	0.67
15:T:219:DA:H2''	15:T:220:DA:H5'	1.76	0.67
1:A:21:LEU:HB2	1:A:234:TRP:HE3	1.60	0.67
2:B:58:LEU:HD12	2:B:425:MET:HG2	1.76	0.67
2:B:413:LEU:HB3	2:B:446:ILE:HG12	1.74	0.67
8:H:96:MET:HE1	8:H:120:LEU:HD22	1.76	0.67
15:T:82:DG:C8	15:T:83:DT:H72	2.29	0.67
6:F:85:LEU:HD13	6:F:90:ARG:HB3	1.77	0.67
10:J:56:ILE:HA	10:J:59:PHE:HD2	1.60	0.67
13:N:163:DT:C2	13:N:164:DT:C5	2.83	0.67
9:I:70:ARG:HA	9:I:84:VAL:HA	1.77	0.67
13:N:163:DT:H2'	13:N:164:DT:H73	1.77	0.67
15:T:6:DA:H2'	15:T:7:DT:H72	1.76	0.67
8:H:113:VAL:HB	8:H:124:LEU:HB3	1.76	0.66
2:B:789:MET:HG3	2:B:967:ARG:HD3	1.78	0.66
1:A:466:TYR:HB3	2:B:976:ILE:HB	1.77	0.66
1:A:1279:ILE:HG23	1:A:1318:GLU:HB3	1.78	0.66
2:B:204:ILE:HG23	2:B:491:THR:HA	1.77	0.66
2:B:829:CYS:HA	2:B:834:ASN:HD21	1.60	0.66
1:A:638:LYS:HB3	1:A:642:ILE:HD13	1.76	0.66
13:N:256:DA:C5	13:N:257:DC:C4	2.84	0.66
2:B:979:LYS:HZ3	2:B:987:LYS:HB3	1.60	0.66
3:C:70:PRO:HG3	10:J:13:VAL:HG21	1.77	0.66
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.78	0.66
1:A:920:ILE:HG13	1:A:921:LEU:HD12	1.76	0.66
2:B:337:ARG:HG2	2:B:340:LYS:HZ2	1.61	0.66
10:J:25:LEU:HD21	10:J:31:GLU:HG3	1.77	0.66
13:N:107:DC:H2''	13:N:108:DC:H5	1.61	0.66
18:o:97:LEU:HG	18:o:100:VAL:HB	1.78	0.66
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.79	0.65
2:B:77:ILE:HD11	2:B:119:MET:HB2	1.78	0.65
3:C:262:LEU:HD11	11:K:84:LYS:HG3	1.78	0.65
4:D:93:THR:HG21	4:D:102:VAL:HG21	1.78	0.65
15:T:152:DC:H2''	15:T:153:DT:C5'	2.26	0.65
1:A:666:GLY:HA3	2:B:1069:PHE:HZ	1.62	0.65
2:B:336:ILE:HG13	2:B:340:LYS:HE2	1.78	0.65
15:T:50:DT:H4'	16:e:83:ARG:HD3	1.77	0.65
1:A:1031:ARG:HB3	1:A:1032:ARG:HH21	1.60	0.65
5:E:27:TYR:HA	5:E:63:PRO:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HD22	1:A:581:ILE:HG21	1.79	0.65
17:b:26:ILE:HG13	17:b:55:ARG:HD3	1.79	0.65
17:l:73:THR:HG21	17:l:81:VAL:HG22	1.78	0.65
1:A:913:VAL:HG13	1:A:914:ILE:HG23	1.77	0.65
13:N:256:DA:C8	13:N:257:DC:C5	2.84	0.65
1:A:74:MET:HE1	1:A:246:GLN:HE21	1.62	0.65
13:N:85:DC:H1'	13:N:86:DT:H5'	1.79	0.65
17:f:67:ARG:HG2	19:h:99:ARG:HH12	1.61	0.65
13:N:122:DC:H4'	16:m:63:ARG:HD3	1.78	0.65
13:N:197:DA:H2''	13:N:198:DC:H5''	1.79	0.65
1:A:296:LEU:HG	1:A:300:HIS:CE1	2.32	0.64
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.78	0.64
13:N:96:DG:H2''	13:N:97:DT:H5''	1.79	0.64
19:h:73:ILE:HD13	19:h:101:LEU:HD12	1.79	0.64
2:B:802:PRO:HG2	2:B:809:MET:HE1	1.78	0.64
9:I:57:GLY:H	9:I:89:GLN:HG3	1.62	0.64
13:N:69:DG:H2''	13:N:70:DT:C5	2.30	0.64
1:A:526:GLN:HA	1:A:752:SER:HB2	1.78	0.64
1:A:607:LEU:HB3	1:A:614:MET:HE2	1.79	0.64
1:A:668:GLY:HA2	1:A:671:ILE:HD12	1.79	0.64
13:N:162:DA:H2'	13:N:163:DT:C6	2.31	0.64
15:T:264:DC:H2'	15:T:265:DA:C8	2.33	0.64
3:C:40:VAL:HB	3:C:172:PRO:HG3	1.78	0.64
18:c:59:THR:HG23	19:d:44:VAL:HG11	1.80	0.64
2:B:1080:LYS:HD2	3:C:188:HIS:CE1	2.33	0.64
7:G:152:THR:HA	7:G:157:ILE:HG22	1.80	0.64
1:A:882:GLN:HB2	1:A:958:LEU:HD12	1.80	0.64
1:A:811:PRO:HG2	2:B:702:MET:HE2	1.79	0.64
15:T:191:DT:H1'	15:T:192:DT:C5	2.32	0.64
2:B:208:ARG:HD3	2:B:469:ARG:HH22	1.63	0.63
13:N:163:DT:C2'	13:N:164:DT:H73	2.27	0.63
1:A:467:SER:HB3	2:B:1103:ILE:HD12	1.80	0.63
2:B:979:LYS:HA	2:B:989:THR:HA	1.80	0.63
1:A:842:LEU:HD21	1:A:1107:LEU:HD22	1.80	0.63
1:A:894:PHE:HA	1:A:897:ARG:HG2	1.81	0.63
3:C:111:THR:HB	3:C:147:LEU:HB2	1.80	0.63
13:N:67:DT:H2''	13:N:68:DT:C6	2.33	0.63
1:A:1148:VAL:HG23	1:A:1199:LEU:HD22	1.80	0.63
13:N:182:DG:H4'	16:a:83:ARG:HD3	1.80	0.63
15:T:28:DT:H2''	15:T:29:DG:C8	2.33	0.63
15:T:140:DG:H2''	15:T:141:DG:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:GLU:HG2	2:B:697:THR:HG23	1.80	0.63
2:B:1039:GLY:HA2	10:J:50:LEU:HD22	1.81	0.63
1:A:277:VAL:HG21	1:A:297:LEU:HD22	1.81	0.63
1:A:447:ARG:HH22	1:A:451:LEU:HB2	1.58	0.62
1:A:799:GLY:HA2	1:A:816:PHE:CD2	2.34	0.62
2:B:778:MET:HE2	2:B:796:LEU:HA	1.81	0.62
3:C:252:GLN:HG3	11:K:95:ILE:HD11	1.80	0.62
13:N:74:DC:H2'	13:N:75:DT:H71	1.81	0.62
1:A:55:ASP:HB3	1:A:58:LEU:HG	1.79	0.62
1:A:447:ARG:HH21	1:A:451:LEU:N	1.97	0.62
2:B:707:LEU:HD21	2:B:741:CYS:HB2	1.81	0.62
13:N:163:DT:C2'	13:N:164:DT:H72	2.28	0.62
1:A:1004:GLY:HA3	1:A:1009:ILE:HD13	1.81	0.62
1:A:1066:VAL:HA	1:A:1069:ILE:HG12	1.80	0.62
2:B:31:VAL:HG22	2:B:34:GLN:HB3	1.80	0.62
13:N:4:DT:H2''	13:N:5:DT:C7	2.26	0.62
13:N:249:DT:H71	13:N:249:DT:OP2	1.99	0.62
16:m:46:VAL:HA	16:m:49:ARG:HE	1.64	0.62
2:B:478:ARG:HH21	2:B:790:ASP:HB3	1.64	0.62
12:L:33:CYS:SG	12:L:50:CYS:CB	2.82	0.62
1:A:15:LYS:HB3	2:B:1220:ARG:HH22	1.65	0.62
3:C:51:LYS:HE3	3:C:156:ARG:HB2	1.80	0.62
5:E:60:LEU:HD11	5:E:76:THR:HB	1.81	0.62
5:E:172:SER:HA	5:E:176:ARG:HH22	1.65	0.62
15:T:56:DG:H2''	15:T:57:DT:H5'	1.82	0.62
15:T:82:DG:H2''	15:T:83:DT:C7	2.30	0.62
16:k:69:ARG:HH21	16:k:72:ARG:HE	1.46	0.62
10:J:44:CYS:O	10:J:48:MET:HG3	1.99	0.62
1:A:1295:PRO:HA	1:A:1301:TYR:HA	1.81	0.62
3:C:99:GLU:HB2	3:C:121:VAL:HG21	1.79	0.62
13:N:217:DG:C2'	13:N:218:DT:H71	2.30	0.62
1:A:838:ILE:HG12	1:A:841:ARG:HH21	1.65	0.61
5:E:45:ILE:HG13	5:E:57:MET:HE3	1.82	0.61
2:B:419:ARG:HH12	13:N:12:DG:H4'	1.63	0.61
15:T:31:DA:H5''	18:g:16:THR:HA	1.81	0.61
15:T:275:DA:H2''	15:T:276:DA:C8	2.35	0.61
1:A:1316:LEU:HD21	1:A:1341:VAL:HG21	1.80	0.61
5:E:192:GLY:HA2	5:E:212:ILE:HD11	1.82	0.61
1:A:526:GLN:HB3	2:B:1015:HIS:CD2	2.34	0.61
15:T:181:DG:H2''	15:T:182:DT:H73	1.80	0.61
1:A:1427:VAL:HG12	1:A:1439:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.81	0.61
13:N:43:DG:H1'	13:N:44:DT:H5'	1.83	0.61
13:N:60:DT:N1	13:N:61:DT:H72	2.16	0.61
13:N:171:DA:C2	15:T:110:DA:C2	2.89	0.61
2:B:1116:ARG:NH2	2:B:1198:TYR:HB2	2.15	0.61
16:m:46:VAL:HG22	16:m:49:ARG:HH21	1.66	0.61
1:A:345:ARG:HA	2:B:1129:ARG:HA	1.82	0.61
1:A:900:VAL:HG11	1:A:930:LEU:HD13	1.82	0.61
2:B:825:VAL:HG22	2:B:1010:LEU:HD11	1.82	0.61
3:C:206:TYR:HA	3:C:209:TRP:HD1	1.65	0.61
5:E:111:TYR:HE1	5:E:133:THR:HB	1.66	0.61
12:L:33:CYS:SG	12:L:50:CYS:HB2	2.39	0.61
2:B:229:ALA:HB3	2:B:247:ILE:HB	1.83	0.61
2:B:785:TYR:HA	2:B:788:ARG:HB2	1.82	0.61
13:N:222:DA:H2''	13:N:223:DA:C8	2.36	0.61
1:A:112:LYS:HB3	1:A:165:ARG:HH22	1.66	0.60
2:B:647:ILE:HD11	2:B:652:ILE:HD11	1.83	0.60
3:C:16:GLU:HB3	3:C:233:GLU:HG2	1.83	0.60
2:B:117:LEU:HB3	2:B:158:ILE:HG21	1.81	0.60
13:N:22:DT:H5'	13:N:22:DT:H6	1.65	0.60
16:k:86:SER:HA	16:k:89:ILE:HD12	1.83	0.60
1:A:1033:ILE:HG23	1:A:1039:LEU:HD13	1.83	0.60
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.82	0.60
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.84	0.60
7:G:91:VAL:HA	7:G:101:ALA:HA	1.83	0.60
9:I:92:ARG:HE	9:I:93:LYS:H	1.49	0.60
16:m:121:PRO:HG2	17:n:49:LEU:HB2	1.82	0.60
19:p:99:ARG:NH1	19:p:111:VAL:HG21	2.14	0.60
1:A:108:MET:H	1:A:172:GLN:HE22	1.49	0.60
2:B:1038:ARG:HH21	2:B:1058:LEU:HB3	1.66	0.60
3:C:65:ARG:HH22	10:J:2:ILE:HG13	1.66	0.60
13:N:151:DG:H2'	13:N:152:DC:C6	2.37	0.60
13:N:169:DG:N2	15:T:112:DG:C2	2.70	0.60
15:T:245:DC:H2'	15:T:246:DA:C8	2.35	0.60
18:c:42:ARG:HB2	19:d:88:THR:HG22	1.84	0.60
1:A:339:GLY:HA2	2:B:1129:ARG:HH22	1.66	0.60
19:p:40:TYR:HA	19:p:43:LYS:HD2	1.82	0.60
1:A:874:LEU:HA	1:A:1059:LEU:HA	1.84	0.60
8:H:104:GLU:HB3	8:H:112:LYS:HB3	1.83	0.60
13:N:260:DG:H2''	13:N:261:DT:C5	2.36	0.60
16:e:118:THR:HG22	17:f:45:ARG:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:ILE:HG12	3:C:142:ILE:HD13	1.84	0.60
16:e:49:ARG:HD3	16:e:52:ARG:HH21	1.67	0.60
1:A:1102:ARG:O	1:A:1106:ILE:HD12	2.00	0.59
2:B:175:LEU:HD13	2:B:183:MET:HE1	1.83	0.59
2:B:229:ALA:HB1	2:B:374:MET:HE3	1.84	0.59
2:B:1067:ARG:HG3	3:C:192:TRP:HZ3	1.67	0.59
1:A:403:ALA:HA	1:A:435:ARG:HA	1.83	0.59
1:A:588:HIS:HE1	1:A:609:VAL:HG13	1.66	0.59
5:E:197:ILE:HB	5:E:209:SER:HB3	1.84	0.59
19:d:79:ARG:HB2	19:d:83:TYR:CZ	2.37	0.59
1:A:42:ASP:HA	1:A:49:ARG:HG2	1.83	0.59
2:B:479:TYR:HB3	2:B:1096:ARG:HH21	1.65	0.59
2:B:776:GLN:HG2	2:B:1096:ARG:NH1	2.18	0.59
3:C:35:THR:HA	3:C:39:GLU:HG2	1.84	0.59
13:N:35:DG:H2''	13:N:36:DT:C6	2.37	0.59
13:N:115:DT:C6	13:N:116:DT:C7	2.86	0.59
1:A:93:ILE:HD12	1:A:96:ILE:HD11	1.85	0.59
1:A:634:VAL:HG13	1:A:635:MET:HE2	1.83	0.59
2:B:235:LEU:HG	2:B:242:ILE:HD11	1.84	0.59
2:B:639:LYS:NZ	2:B:641:ASN:HB2	2.18	0.59
13:N:207:DT:H5'	13:N:207:DT:H6	1.68	0.59
8:H:112:LYS:HZ3	8:H:123:CYS:HA	1.67	0.59
13:N:245:DA:H2''	13:N:246:DG:C8	2.37	0.59
16:a:62:ILE:HG23	17:b:29:ILE:HG23	1.84	0.59
17:f:92:ARG:HB3	19:h:79:ARG:HH22	1.68	0.59
1:A:41:MET:HB3	1:A:44:SER:H	1.68	0.59
1:A:1352:TYR:CE1	1:A:1371:MET:HE3	2.38	0.59
3:C:8:ASN:HB3	3:C:20:MET:HB3	1.83	0.59
13:N:113:DC:P	17:n:35:ARG:HH12	2.25	0.59
1:A:893:ALA:HB1	1:A:897:ARG:HH21	1.67	0.59
13:N:243:DC:C2'	13:N:244:DT:H71	2.33	0.59
1:A:1372:ALA:HA	1:A:1375:VAL:HG22	1.84	0.58
2:B:776:GLN:HB2	2:B:1095:LEU:HD22	1.84	0.58
7:G:153:ASP:C	7:G:155:ASN:H	2.11	0.58
15:T:270:DC:H2''	15:T:271:DA:C8	2.38	0.58
17:l:87:VAL:HG12	17:l:91:LYS:HE2	1.85	0.58
1:A:623:VAL:HG12	1:A:630:LEU:HD12	1.85	0.58
19:d:79:ARG:HE	19:d:83:TYR:HE2	1.51	0.58
2:B:883:LEU:HG	2:B:935:ARG:HA	1.84	0.58
13:N:163:DT:C2	13:N:164:DT:H72	2.38	0.58
15:T:124:DT:H2''	15:T:125:DC:H5'	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:HB2	2:B:120:GLU:HB3	1.84	0.58
2:B:31:VAL:HG21	2:B:192:GLY:HA3	1.85	0.58
2:B:336:ILE:HG12	2:B:340:LYS:HG3	1.85	0.58
1:A:500:ALA:O	1:A:504:GLN:HG2	2.03	0.58
1:A:648:GLY:O	1:A:652:LYS:HG2	2.04	0.58
2:B:182:LYS:HD3	10:J:63:ASN:HD21	1.69	0.58
19:d:78:SER:HA	19:d:89:ILE:HD11	1.86	0.58
2:B:259:ARG:HB3	2:B:305:MET:HE1	1.85	0.58
5:E:45:ILE:HG22	5:E:53:GLN:H	1.67	0.58
1:A:846:LEU:HD22	1:A:849:ILE:HD11	1.85	0.58
1:A:1119:THR:HB	1:A:1331:TYR:HB3	1.86	0.58
2:B:210:ALA:HB3	2:B:213:ILE:HD13	1.85	0.58
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.86	0.58
1:A:1155:TYR:HD1	9:I:41:PRO:HB2	1.68	0.58
2:B:272:ILE:HG21	2:B:326:ILE:HG22	1.85	0.58
2:B:631:PHE:HB3	2:B:645:LEU:HD22	1.86	0.58
2:B:699:MET:HE1	2:B:736:HIS:CD2	2.39	0.58
18:c:21:ALA:HB2	19:d:121:TYR:HB2	1.86	0.58
1:A:447:ARG:HH21	1:A:451:LEU:CG	2.13	0.58
1:A:999:LEU:HD13	1:A:1020:PHE:HD2	1.69	0.58
15:T:191:DT:H2''	15:T:192:DT:C5	2.35	0.58
1:A:19:PHE:HE2	1:A:1422:ASP:HB2	1.68	0.57
1:A:546:GLN:NE2	1:A:550:MET:HE3	2.19	0.57
2:B:574:PHE:HB2	2:B:618:LYS:HG2	1.84	0.57
13:N:35:DG:C8	13:N:36:DT:H72	2.39	0.57
15:T:160:DT:H2''	15:T:161:DT:H73	1.80	0.57
19:h:40:TYR:HA	19:h:43:LYS:HD2	1.86	0.57
13:N:185:DC:N3	13:N:186:DC:N4	2.52	0.57
18:g:87:ILE:HD13	18:g:97:LEU:HD12	1.86	0.57
17:l:47:SER:HB3	17:l:50:ILE:HG12	1.85	0.57
2:B:278:PHE:HB3	2:B:283:VAL:HG23	1.86	0.57
3:C:63:SER:HB3	12:L:71:ALA:HA	1.85	0.57
2:B:221:ALA:O	2:B:223:SER:N	2.37	0.57
5:E:16:ARG:HE	5:E:19:LYS:HE3	1.69	0.57
8:H:89:ALA:HB1	8:H:95:VAL:HG21	1.84	0.57
1:A:488:MET:HA	1:A:488:MET:HE2	1.87	0.57
1:A:544:TYR:HA	1:A:573:TRP:CH2	2.39	0.57
18:o:63:LEU:HD22	19:p:45:LEU:HD13	1.86	0.57
1:A:407:ILE:HB	1:A:432:LYS:HB2	1.87	0.57
13:N:235:DA:H2''	13:N:236:DT:C5	2.36	0.57
1:A:761:GLN:HB3	1:A:805:TYR:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LYS:HD2	9:I:68:LEU:HG	1.86	0.57
2:B:1056:SER:HB3	2:B:1067:ARG:NH2	2.19	0.57
15:T:131:DT:H6	15:T:131:DT:H5''	1.70	0.57
18:c:87:ILE:HD12	18:c:102:ILE:HD11	1.85	0.57
18:o:42:ARG:HB2	19:p:88:THR:HG22	1.86	0.57
1:A:838:ILE:HG12	1:A:841:ARG:NH2	2.20	0.57
15:T:241:DG:H2''	15:T:242:DA:C5	2.40	0.57
2:B:544:SER:O	2:B:548:ILE:HG12	2.04	0.57
2:B:1169:MET:HE1	2:B:1204:PHE:HB3	1.87	0.57
13:N:245:DA:H2''	13:N:246:DG:H8	1.69	0.57
1:A:1001:VAL:H	1:A:1013:GLN:HE22	1.53	0.57
3:C:101:SER:HA	3:C:154:ASN:HA	1.87	0.57
11:K:97:LYS:HZ3	11:K:101:LEU:HD13	1.70	0.57
15:T:100:DA:H2''	15:T:101:DG:C8	2.40	0.57
16:m:55:GLN:HG3	18:o:109:PRO:HA	1.85	0.57
2:B:180:LEU:HA	2:B:183:MET:HG2	1.87	0.56
13:N:121:DC:C2'	13:N:122:DC:C5	2.80	0.56
17:n:65:VAL:HA	17:n:93:GLN:HE22	1.69	0.56
1:A:17:VAL:HB	1:A:1422:ASP:HB3	1.87	0.56
1:A:122:MET:HE2	1:A:141:LEU:HB2	1.85	0.56
1:A:821:GLY:HA3	2:B:764:SER:OG	2.04	0.56
1:A:1199:LEU:HG	1:A:1240:ILE:HD11	1.87	0.56
2:B:710:ARG:HH22	2:B:727:LYS:H	1.53	0.56
12:L:33:CYS:HB3	12:L:38:HIS:H	1.71	0.56
13:N:96:DG:C2'	13:N:97:DT:C7	2.81	0.56
13:N:115:DT:H2''	13:N:116:DT:C6	2.40	0.56
13:N:236:DT:C6	13:N:237:DT:H72	2.39	0.56
15:T:273:DC:H2''	15:T:274:DA:C8	2.40	0.56
16:k:61:LEU:HD22	17:l:36:ARG:HD2	1.87	0.56
1:A:350:ALA:HB2	1:A:375:LEU:HD11	1.87	0.56
1:A:833:ALA:HA	15:T:260:DC:O4'	2.05	0.56
1:A:1424:CYS:HA	1:A:1429:GLU:HG2	1.87	0.56
2:B:384:GLU:HG2	9:I:91:ARG:HH21	1.69	0.56
2:B:570:SER:HB2	2:B:582:ILE:HB	1.86	0.56
15:T:111:DC:H2''	15:T:112:DG:N7	2.20	0.56
16:m:61:LEU:HD22	17:n:36:ARG:HD2	1.87	0.56
1:A:85:GLU:HA	1:A:239:VAL:HG23	1.87	0.56
1:A:1285:VAL:HG13	1:A:1311:THR:HG22	1.88	0.56
2:B:953:LEU:HD23	2:B:965:LYS:HD2	1.86	0.56
13:N:163:DT:C6	13:N:164:DT:C7	2.79	0.56
13:N:227:DC:H2''	13:N:228:DC:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:m:62:ILE:HD11	17:n:37:LEU:HD11	1.86	0.56
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.56
1:A:564:PRO:HA	1:A:573:TRP:CD1	2.41	0.56
3:C:96:VAL:HB	3:C:159:ALA:HB3	1.87	0.56
1:A:372:ALA:HA	1:A:437:LEU:HB3	1.87	0.56
1:A:730:ALA:HB1	1:A:764:ALA:HB1	1.88	0.56
2:B:387:ASP:HA	9:I:91:ARG:HD3	1.87	0.56
2:B:1160:VAL:HG11	2:B:1196:ILE:HG12	1.87	0.56
13:N:251:DC:H2''	13:N:252:DA:C8	2.41	0.56
15:T:53:DG:H2'	15:T:54:DC:C6	2.41	0.56
1:A:506:CYS:HA	2:B:1141:HIS:CE1	2.41	0.56
1:A:509:PRO:HB2	1:A:640:PRO:HB2	1.87	0.56
1:A:659:LEU:HD23	2:B:830:TYR:O	2.05	0.56
1:A:666:GLY:HA3	2:B:1069:PHE:CZ	2.39	0.56
1:A:1146:LYS:HD2	1:A:1271:LEU:HB3	1.88	0.56
13:N:35:DG:H2''	13:N:36:DT:C7	2.33	0.56
16:a:51:ILE:HG13	17:b:39:ARG:HD2	1.88	0.56
15:T:4:DG:H2''	15:T:5:DG:H5'	1.86	0.56
2:B:843:GLN:HE21	2:B:995:ARG:HA	1.71	0.56
3:C:44:ALA:HA	3:C:71:LEU:HD12	1.87	0.56
16:a:126:LEU:HD22	16:e:113:HIS:CG	2.40	0.56
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.88	0.55
1:A:817:HIS:CD2	2:B:764:SER:H	2.24	0.55
1:A:948:VAL:HG11	1:A:1019:LEU:HD21	1.87	0.55
2:B:617:PHE:HE1	2:B:619:ILE:HD11	1.71	0.55
2:B:949:VAL:HA	2:B:968:MET:HA	1.88	0.55
8:H:101:TYR:CE1	8:H:114:TYR:HB3	2.41	0.55
1:A:762:MET:HG3	2:B:1021:MET:HE1	1.87	0.55
1:A:943:PHE:O	1:A:947:ILE:HB	2.06	0.55
1:A:1259:GLU:HG2	1:A:1262:MET:HE3	1.89	0.55
10:J:23:ARG:O	10:J:26:GLU:HG2	2.06	0.55
13:N:206:DC:H2'	13:N:207:DT:H71	1.89	0.55
15:T:191:DT:H2''	15:T:192:DT:H73	0.66	0.55
1:A:497:GLU:O	1:A:501:GLU:HG3	2.05	0.55
1:A:697:LYS:HB2	1:A:702:GLU:HB2	1.88	0.55
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.88	0.55
9:I:12:ASN:C	9:I:13:MET:HE2	2.31	0.55
13:N:163:DT:C1'	13:N:164:DT:H72	2.36	0.55
15:T:181:DG:H2''	15:T:182:DT:H71	1.86	0.55
15:T:252:DA:H4'	15:T:253:DC:OP1	2.05	0.55
1:A:38:PRO:HG3	1:A:271:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:VAL:HG22	1:A:1054:GLN:HG3	1.87	0.55
2:B:213:ILE:O	2:B:215:GLN:HG3	2.06	0.55
2:B:279:ARG:HH11	2:B:317:GLN:HA	1.71	0.55
15:T:82:DG:C2'	15:T:83:DT:C7	2.85	0.55
16:k:126:LEU:O	16:k:130:ILE:HG12	2.07	0.55
13:N:69:DG:H2''	13:N:70:DT:H73	1.78	0.55
13:N:119:DA:H2''	13:N:120:DA:C8	2.40	0.55
13:N:212:DC:H2''	13:N:213:DC:C6	2.42	0.55
1:A:711:LEU:HG	9:I:97:MET:HE1	1.89	0.55
5:E:45:ILE:CG2	5:E:53:GLN:H	2.18	0.55
6:F:97:ARG:HH22	6:F:108:LEU:HD13	1.71	0.55
15:T:245:DC:H2'	15:T:246:DA:H8	1.70	0.55
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.88	0.55
13:N:129:DG:H1	15:T:151:DC:H42	1.53	0.55
2:B:1071:VAL:HG11	2:B:1080:LYS:HD3	1.89	0.55
13:N:11:DT:H4'	13:N:12:DG:OP1	2.06	0.55
13:N:143:DG:C8	13:N:144:DT:H72	2.42	0.55
13:N:171:DA:N1	15:T:110:DA:C2	2.74	0.55
13:N:235:DA:C4	13:N:236:DT:C4	2.95	0.55
16:e:49:ARG:HE	16:e:52:ARG:HE	1.54	0.55
16:m:64:LYS:NZ	16:m:68:GLN:HB2	2.21	0.55
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.87	0.55
2:B:176:ASP:O	2:B:179:ASP:N	2.40	0.55
13:N:58:DT:H2''	13:N:59:DT:C6	2.41	0.55
16:e:102:GLY:O	16:e:105:GLU:HG2	2.07	0.55
1:A:748:VAL:HG21	1:A:759:ILE:HD11	1.89	0.55
1:A:753:LYS:HE3	2:B:1020:ARG:HH12	1.71	0.55
3:C:50:ILE:HG23	12:L:62:ARG:HH21	1.72	0.55
3:C:82:SER:HB2	3:C:160:LYS:HB3	1.89	0.55
15:T:18:DG:H2''	15:T:19:DA:C8	2.41	0.55
1:A:590:GLN:HA	1:A:607:LEU:HD13	1.89	0.54
15:T:80:DA:H2''	15:T:81:DC:C5	2.42	0.54
1:A:924:VAL:HA	1:A:927:GLN:HB3	1.90	0.54
2:B:521:PRO:HB2	2:B:525:ALA:HB3	1.90	0.54
2:B:803:LEU:HD23	2:B:1041:GLU:HG2	1.87	0.54
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.89	0.54
1:A:1320:MET:HE1	1:A:1342:LEU:HD21	1.89	0.54
2:B:639:LYS:HZ2	2:B:641:ASN:HB2	1.72	0.54
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.89	0.54
15:T:174:DA:H2''	15:T:175:DC:H5'	1.89	0.54
1:A:669:ASP:HB3	1:A:744:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:179:DC:H2''	13:N:180:DT:C7	2.35	0.54
16:m:125:GLN:O	16:m:129:ARG:HG2	2.07	0.54
18:c:102:ILE:HG23	19:d:61:ILE:HD12	1.89	0.54
18:g:25:PHE:CZ	18:g:59:THR:HG21	2.42	0.54
13:N:256:DA:C2	15:T:25:DG:C2	2.96	0.54
18:g:25:PHE:HZ	18:g:59:THR:HG21	1.73	0.54
1:A:194:ARG:N	15:T:169:DG:H2'	2.22	0.54
1:A:458:ALA:HB2	1:A:502:LEU:HB3	1.90	0.54
1:A:656:TYR:CD1	1:A:659:LEU:HD12	2.43	0.54
2:B:160:LYS:H	2:B:447:THR:HG22	1.71	0.54
2:B:304:GLU:HG2	2:B:307:LYS:HE3	1.88	0.54
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.72	0.54
6:F:93:ILE:HG21	6:F:130:ILE:HD13	1.90	0.54
16:a:125:GLN:HG2	16:a:128:ARG:HH21	1.72	0.54
17:n:84:MET:HE3	17:n:88:TYR:CZ	2.43	0.54
18:o:64:GLU:HA	19:p:49:HIS:CE1	2.42	0.54
1:A:1168:ASP:OD1	1:A:1239:ILE:HG13	2.08	0.54
1:A:1231:SER:HB3	1:A:1239:ILE:HB	1.90	0.54
2:B:941:LEU:HD21	2:B:968:MET:HE2	1.89	0.54
7:G:46:VAL:HG12	7:G:47:THR:HG23	1.89	0.54
8:H:56:THR:HB	8:H:144:ARG:HB3	1.89	0.54
1:A:70:CYS:HB3	1:A:80:HIS:CE1	2.43	0.54
1:A:95:PHE:HE1	1:A:1417:ALA:HB2	1.73	0.54
1:A:1213:GLN:O	1:A:1217:LYS:HG2	2.08	0.54
2:B:203:LEU:HD21	2:B:405:LEU:HD12	1.89	0.54
2:B:612:ILE:HG21	9:I:61:ASP:HB2	1.90	0.54
19:d:76:GLU:HB3	19:d:97:ALA:HB1	1.90	0.54
1:A:153:PRO:HD3	1:A:165:ARG:HD2	1.88	0.54
2:B:597:ARG:NH1	2:B:608:ILE:H	2.06	0.54
8:H:54:SER:H	8:H:145:ARG:NH1	2.06	0.54
13:N:131:DG:H2''	13:N:132:DA:C8	2.42	0.54
13:N:248:DC:C3'	13:N:249:DT:H71	2.38	0.54
2:B:173:ARG:HG2	2:B:174:THR:HG23	1.90	0.53
2:B:515:VAL:HG11	2:B:530:LYS:HD3	1.90	0.53
8:H:53:ASP:HB3	8:H:145:ARG:HH12	1.71	0.53
11:K:9:LEU:HD23	11:K:69:ALA:HB2	1.91	0.53
15:T:6:DA:H2'	15:T:7:DT:H73	1.89	0.53
1:A:114:LEU:HB3	1:A:145:LYS:HG2	1.90	0.53
1:A:147:VAL:HG23	1:A:171:THR:HA	1.90	0.53
1:A:1400:LEU:HD12	1:A:1429:GLU:HG3	1.90	0.53
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:246:DG:C2'	13:N:247:DT:C7	2.86	0.53
18:c:97:LEU:HD22	18:c:100:VAL:HG21	1.90	0.53
2:B:641:ASN:HD21	2:B:646:ARG:HA	1.74	0.53
10:J:57:GLU:O	10:J:61:ARG:HG3	2.09	0.53
17:f:65:VAL:HA	17:f:93:GLN:HE22	1.73	0.53
1:A:397:PRO:HA	1:A:436:HIS:NE2	2.23	0.53
5:E:160:LYS:HD3	5:E:194:VAL:H	1.73	0.53
14:P:7:G:H2'	14:P:8:G:H8	1.73	0.53
15:T:276:DA:H2''	15:T:277:DC:C6	2.43	0.53
16:a:58:THR:HG21	18:g:81:ARG:HD3	1.91	0.53
16:m:104:PHE:HE2	17:n:37:LEU:HB3	1.73	0.53
1:A:588:HIS:CE1	1:A:609:VAL:HG13	2.43	0.53
1:A:1316:LEU:HD13	1:A:1337:GLU:HG2	1.90	0.53
5:E:52:PRO:HB2	5:E:54:ARG:HH22	1.74	0.53
15:T:185:DG:C5	15:T:186:DT:C4	2.97	0.53
15:T:206:DG:H2''	15:T:207:DC:H5'	1.89	0.53
1:A:962:LEU:HD22	1:A:1051:ILE:HG12	1.91	0.53
2:B:204:ILE:HG12	2:B:474:GLN:OE1	2.09	0.53
2:B:225:ILE:HD13	2:B:248:LYS:HB3	1.91	0.53
11:K:101:LEU:HD12	11:K:104:LYS:HE2	1.90	0.53
13:N:184:DA:H2''	13:N:185:DC:C6	2.44	0.53
16:k:126:LEU:HD22	16:m:113:HIS:CG	2.43	0.53
1:A:1081:MET:HE1	1:A:1099:GLY:HA2	1.91	0.53
7:G:116:PRO:HG2	7:G:119:LEU:HD12	1.90	0.53
13:N:211:DC:H1'	13:N:212:DC:H5'	1.90	0.53
1:A:914:ILE:HA	1:A:981:SER:H	1.73	0.53
2:B:413:LEU:HD13	2:B:446:ILE:HA	1.91	0.53
5:E:54:ARG:HD3	5:E:81:PHE:HB3	1.89	0.53
19:p:105:GLU:HB2	19:p:109:HIS:CE1	2.44	0.53
1:A:1056:GLN:HG3	6:F:84:TYR:CE2	2.44	0.53
1:A:1157:ASP:HB3	1:A:1243:ARG:HH12	1.74	0.53
17:f:92:ARG:HB3	19:h:79:ARG:NH2	2.23	0.53
2:B:1077:THR:HB	2:B:1079:LYS:HZ1	1.74	0.52
8:H:107:ASP:HB2	8:H:110:LYS:HB2	1.91	0.52
13:N:9:DT:H2''	13:N:10:DG:C8	2.44	0.52
13:N:143:DG:C2'	13:N:144:DT:H72	2.39	0.52
13:N:168:DC:H2''	13:N:169:DG:C8	2.44	0.52
15:T:271:DA:H2''	15:T:272:DC:C6	2.44	0.52
2:B:24:PHE:HD1	2:B:678:TRP:CE2	2.28	0.52
2:B:1080:LYS:HD2	3:C:188:HIS:HE1	1.74	0.52
5:E:155:LEU:HB3	5:E:159:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:70:LEU:HD21	17:b:26:ILE:HD12	1.91	0.52
17:b:35:ARG:O	17:b:39:ARG:HG2	2.09	0.52
16:e:49:ARG:HB3	16:e:53:ARG:HH21	1.74	0.52
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.90	0.52
2:B:519:GLU:HG3	2:B:775:LYS:HZ3	1.74	0.52
2:B:1001:PHE:C	2:B:1072:MET:HG3	2.35	0.52
13:N:236:DT:C2'	13:N:237:DT:H72	2.39	0.52
1:A:849:ILE:HD12	1:A:1067:GLY:HA3	1.91	0.52
2:B:1196:ILE:HD11	2:B:1201:LYS:HG2	1.90	0.52
3:C:136:ASP:H	3:C:139:ASP:HB2	1.75	0.52
13:N:60:DT:C2'	13:N:61:DT:C7	2.88	0.52
13:N:241:DC:H2''	13:N:242:DC:C5	2.44	0.52
15:T:101:DG:O5'	17:b:79:LYS:HD2	2.09	0.52
18:g:81:ARG:HA	18:g:105:GLY:HA2	1.92	0.52
2:B:759:PRO:HD2	2:B:1046:PRO:HG3	1.90	0.52
2:B:1056:SER:HB3	2:B:1067:ARG:HH22	1.74	0.52
13:N:105:DG:H5'	13:N:105:DG:C8	2.38	0.52
1:A:16:GLU:HB3	1:A:1421:LEU:HD11	1.91	0.52
1:A:529:LEU:HD23	1:A:752:SER:HB3	1.91	0.52
1:A:635:MET:CE	1:A:643:CYS:HB2	2.38	0.52
1:A:680:ILE:HG23	1:A:730:ALA:HB1	1.92	0.52
1:A:866:GLN:HE22	5:E:199:ARG:HH22	1.58	0.52
2:B:1077:THR:HB	2:B:1079:LYS:NZ	2.24	0.52
3:C:127:LEU:O	3:C:129:VAL:N	2.41	0.52
1:A:538:ARG:HA	1:A:576:LYS:HZ1	1.73	0.52
1:A:1120:VAL:HB	1:A:1309:LEU:HB2	1.90	0.52
2:B:452:TYR:CD1	15:T:269:DA:H5'	2.44	0.52
5:E:53:GLN:HB3	5:E:56:LEU:HD13	1.92	0.52
13:N:74:DC:H2''	13:N:75:DT:H5'	1.91	0.52
16:m:61:LEU:HD13	17:n:36:ARG:HB3	1.91	0.52
1:A:447:ARG:HH21	1:A:451:LEU:HG	1.69	0.52
1:A:539:ASP:HB2	8:H:22:LYS:HB2	1.92	0.52
2:B:1067:ARG:HG3	3:C:192:TRP:CZ3	2.44	0.52
3:C:103:ARG:HG3	3:C:152:GLU:HA	1.92	0.52
6:F:107:VAL:HG13	6:F:124:GLU:OE2	2.10	0.52
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.92	0.52
16:e:52:ARG:HD2	16:e:53:ARG:N	2.25	0.52
1:A:447:ARG:NH2	1:A:451:LEU:CD1	2.65	0.52
1:A:882:GLN:HB3	1:A:1027:ARG:NH2	2.24	0.52
2:B:288:GLU:HG3	9:I:11:ASN:HD21	1.75	0.52
7:G:114:LEU:HD13	7:G:162:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:96:DG:C8	13:N:97:DT:H72	2.45	0.52
18:g:63:LEU:HD22	19:h:45:LEU:HD13	1.92	0.52
2:B:1138:MET:HE2	2:B:1147:LEU:HB2	1.92	0.52
13:N:263:DA:H2''	13:N:264:DG:C8	2.44	0.52
16:k:78:PHE:HB3	17:l:70:VAL:HG21	1.92	0.52
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.91	0.51
1:A:406:VAL:HG22	1:A:433:VAL:HG22	1.93	0.51
2:B:76:GLU:HB3	2:B:122:SER:HB2	1.91	0.51
3:C:7:VAL:HG13	3:C:19:LEU:HD13	1.91	0.51
5:E:154:ARG:HA	5:E:195:VAL:HA	1.91	0.51
9:I:58:ILE:HA	9:I:62:ILE:HD12	1.92	0.51
1:A:67:CYS:SG	1:A:80:HIS:CD2	3.03	0.51
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.92	0.51
1:A:1353:LYS:O	1:A:1356:LEU:HG	2.10	0.51
1:A:435:ARG:HB2	1:A:438:MET:HE3	1.92	0.51
16:a:78:PHE:HB2	17:b:70:VAL:HG21	1.93	0.51
18:c:17:ARG:NH2	18:c:28:GLY:HA2	2.26	0.51
17:n:90:LEU:HB3	17:n:95:ARG:O	2.09	0.51
1:A:442:PRO:HG2	1:A:499:ARG:HG2	1.93	0.51
1:A:566:ILE:O	1:A:571:PRO:HA	2.11	0.51
1:A:1003:ARG:HH22	6:F:82:THR:HB	1.76	0.51
1:A:1056:GLN:HG3	6:F:84:TYR:HE2	1.75	0.51
2:B:645:LEU:HB3	2:B:647:ILE:HG22	1.92	0.51
2:B:776:GLN:HB3	2:B:1096:ARG:H	1.75	0.51
2:B:866:PHE:HE2	2:B:872:GLU:HG3	1.75	0.51
15:T:17:DT:H2''	15:T:18:DG:N7	2.25	0.51
16:a:84:PHE:HB3	16:a:89:ILE:HD11	1.93	0.51
16:e:108:ASN:O	16:e:112:ILE:HG12	2.10	0.51
18:o:44:GLY:HA3	19:p:90:THR:HG22	1.92	0.51
2:B:201:LYS:HD2	2:B:474:GLN:O	2.11	0.51
2:B:354:LEU:HD13	2:B:357:ILE:HD12	1.93	0.51
2:B:836:GLU:H	2:B:1013:ASN:HD22	1.58	0.51
10:J:63:ASN:HB2	10:J:64:PRO:HD2	1.93	0.51
13:N:102:DG:H3'	16:k:116:ARG:HD3	1.93	0.51
13:N:242:DC:H2''	13:N:243:DC:C6	2.46	0.51
16:e:120:MET:HG2	16:e:121:PRO:HD2	1.92	0.51
17:l:35:ARG:HG2	17:l:35:ARG:HH11	1.75	0.51
2:B:399:LEU:HD12	2:B:538:ILE:HD11	1.92	0.51
15:T:6:DA:C2'	15:T:7:DT:C7	2.87	0.51
18:g:87:ILE:HD12	18:g:102:ILE:HD11	1.92	0.51
19:p:42:TYR:O	19:p:46:LYS:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:O	1:A:279:LYS:HG2	2.10	0.51
2:B:1038:ARG:NH2	2:B:1058:LEU:HB3	2.26	0.51
9:I:44:TYR:CE2	9:I:46:HIS:HB2	2.45	0.51
13:N:172:DG:H2''	13:N:173:DA:C8	2.46	0.51
16:m:120:MET:HE3	16:m:122:LYS:HE2	1.92	0.51
1:A:1456:LEU:HD11	6:F:108:LEU:HD21	1.92	0.51
2:B:798:TYR:HA	10:J:1:MET:N	2.26	0.51
2:B:1014:PRO:O	2:B:1018:PRO:HD3	2.11	0.51
2:B:1037:ILE:HD13	10:J:43:TYR:HB3	1.91	0.51
2:B:1112:GLN:HG3	2:B:1114:LEU:H	1.76	0.51
4:D:101:VAL:HG13	7:G:105:PRO:HB3	1.93	0.51
13:N:86:DT:H2''	13:N:87:DT:C7	2.41	0.51
17:l:30:THR:O	17:l:34:ILE:HD12	2.11	0.51
16:m:129:ARG:HH21	16:m:133:GLU:C	2.19	0.51
1:A:368:PRO:HG2	1:A:371:ILE:HD12	1.93	0.51
11:K:95:ILE:HD12	11:K:98:LEU:HD21	1.93	0.51
13:N:159:DT:H3	15:T:121:DA:H61	1.59	0.51
13:N:235:DA:N9	13:N:236:DT:C7	2.66	0.51
1:A:70:CYS:HB3	1:A:80:HIS:HE1	1.75	0.50
2:B:996:HIS:CE1	3:C:37:LEU:HD22	2.45	0.50
5:E:176:ARG:HD2	5:E:214:LEU:HD21	1.92	0.50
16:e:84:PHE:HB3	16:e:89:ILE:HD11	1.93	0.50
19:p:99:ARG:HH21	19:p:107:ALA:HB1	1.76	0.50
1:A:512:ILE:HA	1:A:522:MET:HE2	1.92	0.50
1:A:1001:VAL:H	1:A:1013:GLN:NE2	2.09	0.50
2:B:695:GLU:HG3	2:B:698:ILE:HD11	1.94	0.50
3:C:34:ARG:HE	11:K:41:THR:HB	1.76	0.50
5:E:29:ILE:HB	5:E:34:MET:HE3	1.93	0.50
13:N:42:DG:H2''	13:N:43:DG:H5''	1.92	0.50
1:A:42:ASP:HB2	1:A:49:ARG:N	2.26	0.50
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.93	0.50
2:B:729:GLU:HG2	2:B:731:SER:HB3	1.93	0.50
2:B:796:LEU:HD11	2:B:851:PHE:HA	1.93	0.50
3:C:113:VAL:HG12	3:C:144:LEU:HD12	1.93	0.50
18:c:31:HIS:HB3	18:c:35:ARG:HH21	1.77	0.50
1:A:1122:LEU:HD21	1:A:1136:ILE:HG21	1.93	0.50
2:B:547:ILE:HG13	2:B:621:THR:HG21	1.94	0.50
17:b:75:HIS:CE1	19:d:93:GLU:HG3	2.46	0.50
18:g:97:LEU:HD22	18:g:100:VAL:HG21	1.93	0.50
16:m:52:ARG:HA	16:m:55:GLN:CD	2.36	0.50
17:n:71:THR:HG22	17:n:75:HIS:NE2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:SER:HB2	2:B:266:PRO:HG3	1.93	0.50
2:B:508:HIS:CE1	2:B:510:THR:HG23	2.46	0.50
2:B:1082:MET:HA	3:C:189:THR:HA	1.94	0.50
5:E:54:ARG:HB3	5:E:81:PHE:HB2	1.94	0.50
18:c:63:LEU:HD13	19:d:45:LEU:HB2	1.94	0.50
1:A:122:MET:HE1	1:A:138:VAL:HA	1.94	0.50
2:B:51:TRP:HE1	2:B:80:GLY:HA2	1.77	0.50
2:B:733:SER:HB3	2:B:736:HIS:CD2	2.46	0.50
6:F:133:VAL:HG22	6:F:147:GLY:HA2	1.93	0.50
17:b:34:ILE:HD11	17:b:55:ARG:NH2	2.23	0.50
1:A:37:TYR:HB3	1:A:49:ARG:CZ	2.41	0.50
2:B:799:PRO:C	2:B:818:PRO:HG2	2.37	0.50
3:C:244:PHE:O	3:C:248:ILE:HG12	2.11	0.50
4:D:169:VAL:HG13	4:D:171:LEU:HD23	1.92	0.50
13:N:60:DT:H2''	13:N:61:DT:C6	2.47	0.50
15:T:129:DC:H2''	15:T:130:DC:C5	2.46	0.50
15:T:251:DA:H2''	15:T:252:DA:O5'	2.12	0.50
1:A:400:HIS:CE1	1:A:463:VAL:HG21	2.47	0.50
3:C:114:TYR:HB3	3:C:140:GLN:O	2.12	0.50
5:E:175:PRO:HB2	5:E:211:ARG:HG2	1.93	0.50
15:T:82:DG:P	17:b:35:ARG:HH12	2.34	0.50
15:T:221:DA:H2''	15:T:222:DA:N7	2.27	0.50
17:l:31:LYS:HE3	17:l:51:TYR:CZ	2.47	0.50
16:m:64:LYS:HZ1	16:m:89:ILE:HG21	1.77	0.50
1:A:380:THR:HG21	6:F:102:SER:HB2	1.93	0.50
1:A:650:ILE:O	1:A:654:VAL:HG23	2.11	0.50
1:A:658:LEU:HD11	1:A:663:PHE:HB2	1.93	0.50
1:A:1211:MET:HG3	1:A:1230:TRP:HB2	1.93	0.50
1:A:1352:TYR:HB2	1:A:1375:VAL:HG11	1.94	0.50
2:B:279:ARG:NH1	2:B:317:GLN:HA	2.27	0.50
2:B:485:LEU:HB2	2:B:751:VAL:HG11	1.93	0.50
2:B:543:PRO:O	2:B:546:PRO:HD2	2.11	0.50
2:B:911:ILE:HG13	2:B:912:ILE:N	2.27	0.50
11:K:12:LEU:HD22	11:K:18:LYS:HB2	1.93	0.50
13:N:60:DT:C2	13:N:61:DT:C5	3.00	0.50
13:N:190:DT:H2''	13:N:191:DA:C8	2.47	0.50
18:g:64:GLU:HB3	19:h:48:VAL:HG21	1.92	0.50
16:m:102:GLY:O	16:m:105:GLU:HG2	2.12	0.50
2:B:572:ARG:H	2:B:616:GLU:HA	1.76	0.49
16:a:113:HIS:CG	16:e:126:LEU:HD22	2.47	0.49
1:A:42:ASP:HB2	1:A:49:ARG:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLU:HA	1:A:548:MET:HG2	1.94	0.49
2:B:437:LEU:HA	2:B:440:ALA:HB3	1.94	0.49
2:B:459:TRP:HB2	2:B:472:VAL:HG21	1.94	0.49
3:C:28:LEU:HD11	11:K:97:LYS:HD2	1.92	0.49
13:N:256:DA:N7	13:N:257:DC:N4	2.60	0.49
1:A:552:PHE:CE1	11:K:74:ARG:HB2	2.46	0.49
2:B:104:ALA:HA	2:B:109:LEU:HB2	1.94	0.49
2:B:178:VAL:HA	2:B:181:TYR:HD2	1.78	0.49
13:N:227:DC:H2''	13:N:228:DC:C5'	2.41	0.49
15:T:6:DA:N9	15:T:7:DT:H72	2.25	0.49
1:A:504:GLN:HB2	6:F:90:ARG:NH1	2.26	0.49
1:A:718:GLU:O	1:A:721:ARG:HG3	2.11	0.49
1:A:929:GLU:HB3	1:A:989:ILE:HD13	1.94	0.49
1:A:1193:TRP:CZ2	9:I:18:GLU:HB2	2.47	0.49
2:B:979:LYS:HE2	2:B:988:GLY:H	1.76	0.49
2:B:1034:VAL:O	2:B:1038:ARG:HG2	2.12	0.49
3:C:65:ARG:HD2	10:J:5:VAL:HG23	1.94	0.49
13:N:115:DT:N1	13:N:116:DT:H72	2.26	0.49
15:T:244:DA:H2''	15:T:245:DC:C5	2.48	0.49
16:k:102:GLY:HA2	16:k:105:GLU:CD	2.38	0.49
1:A:1354:GLU:O	1:A:1358:VAL:HG23	2.13	0.49
2:B:252:ARG:HG3	2:B:253:GLU:H	1.78	0.49
2:B:336:ILE:HG23	2:B:341:ARG:HB2	1.94	0.49
13:N:189:DT:H4'	13:N:190:DT:OP1	2.11	0.49
13:N:207:DT:H5'	13:N:207:DT:C6	2.45	0.49
17:l:35:ARG:O	17:l:39:ARG:HG2	2.13	0.49
16:m:120:MET:HG2	17:n:47:SER:HB2	1.94	0.49
1:A:95:PHE:CE1	1:A:1417:ALA:HB2	2.48	0.49
1:A:757:ILE:O	1:A:761:GLN:HG2	2.12	0.49
2:B:202:VAL:HG12	2:B:474:GLN:O	2.12	0.49
2:B:340:LYS:HA	2:B:343:GLN:HB3	1.95	0.49
13:N:45:DG:H2''	13:N:46:DC:H5'	1.94	0.49
13:N:256:DA:C8	13:N:257:DC:H5	2.30	0.49
1:A:515:PRO:HA	1:A:518:ASN:HA	1.95	0.49
1:A:1140:ILE:HD11	1:A:1322:VAL:HG11	1.95	0.49
2:B:890:TYR:CE2	2:B:910:ILE:HG13	2.47	0.49
5:E:3:ASP:HA	5:E:6:ARG:HE	1.78	0.49
7:G:19:GLY:O	7:G:22:MET:HE3	2.12	0.49
13:N:235:DA:C4	13:N:236:DT:C5	3.00	0.49
16:k:62:ILE:HD12	17:l:29:ILE:HG23	1.94	0.49
1:A:496:GLU:OE2	6:F:99:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:SER:HA	5:E:146:HIS:HA	1.94	0.49
3:C:242:GLN:O	3:C:246:ARG:HG2	2.12	0.49
13:N:159:DT:H2''	13:N:160:DC:C6	2.48	0.49
13:N:236:DT:C2	13:N:237:DT:H72	2.47	0.49
15:T:240:DG:H4'	15:T:241:DG:OP1	2.13	0.49
16:a:125:GLN:HA	16:a:128:ARG:HG2	1.93	0.49
1:A:516:GLN:NE2	1:A:1077:PRO:HD3	2.26	0.49
1:A:526:GLN:OE1	1:A:753:LYS:HB2	2.13	0.49
1:A:658:LEU:HD12	1:A:661:ASN:HB3	1.95	0.49
1:A:819:MET:HG2	2:B:507:LEU:HB3	1.93	0.49
2:B:304:GLU:O	2:B:307:LYS:HG2	2.13	0.49
2:B:996:HIS:HE1	3:C:37:LEU:HD22	1.77	0.49
13:N:256:DA:H2''	13:N:257:DC:H6	1.78	0.49
15:T:191:DT:C2'	15:T:192:DT:C5	2.94	0.49
15:T:233:DG:H2''	15:T:234:DG:N7	2.27	0.49
1:A:437:LEU:HD11	1:A:461:VAL:HG21	1.95	0.49
1:A:1011:GLU:HG3	1:A:1014:GLN:HE21	1.78	0.49
1:A:1279:ILE:HD12	1:A:1318:GLU:HG2	1.95	0.49
2:B:808:ALA:HA	2:B:811:TYR:CE2	2.47	0.49
1:A:526:GLN:HB3	2:B:1015:HIS:CG	2.48	0.48
1:A:775:ARG:CZ	1:A:798:LYS:HD3	2.43	0.48
2:B:308:PRO:HA	2:B:311:GLU:CD	2.38	0.48
2:B:427:ARG:HH22	15:T:273:DC:P	2.36	0.48
5:E:167:TYR:HB3	5:E:169:LEU:HG	1.96	0.48
13:N:46:DC:H2''	13:N:47:DC:C4	2.47	0.48
13:N:113:DC:H2''	13:N:114:DG:H5'	1.95	0.48
13:N:139:DC:H2''	13:N:140:DC:O4'	2.13	0.48
17:l:92:ARG:HG2	19:p:100:LEU:HD21	1.95	0.48
1:A:83:HIS:HA	1:A:241:PRO:HA	1.95	0.48
1:A:780:PHE:HE1	2:B:510:THR:HG22	1.78	0.48
2:B:323:LEU:HD13	2:B:342:ILE:HG23	1.94	0.48
2:B:1116:ARG:HD2	2:B:1116:ARG:O	2.13	0.48
14:P:2:U:H2'	14:P:3:G:C8	2.47	0.48
15:T:82:DG:N9	15:T:83:DT:H72	2.28	0.48
15:T:231:DA:H2''	15:T:232:DC:C2	2.47	0.48
18:c:79:ILE:HG12	18:c:82:HIS:ND1	2.28	0.48
1:A:22:LEU:HD12	2:B:1211:ASN:HA	1.94	0.48
1:A:40:ILE:HG22	1:A:41:MET:HE2	1.95	0.48
1:A:454:MET:SD	1:A:511:GLN:HB3	2.53	0.48
13:N:235:DA:H2''	13:N:236:DT:C6	2.47	0.48
13:N:250:DC:H2''	13:N:251:DC:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:271:DA:H2''	13:N:272:DC:C6	2.48	0.48
18:c:47:ALA:HB2	19:d:90:THR:HA	1.96	0.48
16:m:64:LYS:NZ	16:m:68:GLN:HE21	2.10	0.48
1:A:186:TRP:HB3	1:A:188:LYS:HG3	1.95	0.48
1:A:248:ARG:HB2	1:A:261:ASP:HB3	1.94	0.48
1:A:253:MET:CE	14:P:1:G:H1	2.26	0.48
1:A:362:LEU:HA	1:A:472:ASN:HB3	1.95	0.48
1:A:444:LEU:HD11	1:A:456:MET:HG2	1.94	0.48
1:A:656:TYR:HA	1:A:659:LEU:HD12	1.94	0.48
1:A:960:VAL:HG21	1:A:1055:PHE:N	2.28	0.48
5:E:164:LEU:HD22	5:E:169:LEU:HB2	1.94	0.48
13:N:214:DC:C2	13:N:215:DG:N7	2.81	0.48
15:T:179:DG:H4'	15:T:180:DC:OP1	2.13	0.48
15:T:278:DA:H2''	15:T:279:DC:C6	2.48	0.48
18:c:90:ASP:HB3	18:c:93:LEU:HB2	1.96	0.48
17:n:35:ARG:O	17:n:39:ARG:HG2	2.13	0.48
2:B:476:LEU:HA	2:B:487:HIS:CE1	2.48	0.48
2:B:547:ILE:O	2:B:551:LEU:HG	2.13	0.48
2:B:620:PHE:HE2	2:B:693:GLU:HG3	1.78	0.48
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.13	0.48
2:B:1072:MET:HE1	2:B:1087:PHE:HB2	1.95	0.48
3:C:174:SER:HB2	10:J:10:CYS:SG	2.53	0.48
13:N:63:DG:C8	13:N:63:DG:H5'	2.48	0.48
15:T:38:DG:H2''	15:T:39:DG:N7	2.28	0.48
17:f:47:SER:HB3	17:f:50:ILE:HG12	1.96	0.48
16:k:61:LEU:HD11	17:l:40:ARG:HG3	1.96	0.48
1:A:504:GLN:HE22	6:F:94:LEU:HB2	1.77	0.48
2:B:18:TRP:HZ2	2:B:1045:THR:HG21	1.78	0.48
2:B:263:ALA:HB2	2:B:274:ILE:HD13	1.95	0.48
2:B:550:PHE:O	2:B:553:GLU:HG2	2.13	0.48
13:N:69:DG:C2'	13:N:70:DT:H73	2.37	0.48
13:N:163:DT:H2'	13:N:164:DT:H72	1.92	0.48
15:T:6:DA:H2''	15:T:7:DT:C6	2.49	0.48
15:T:170:DG:H21	17:n:45:ARG:HH22	1.60	0.48
1:A:97:PRO:HG3	1:A:177:LYS:HE3	1.95	0.48
1:A:804:SER:H	1:A:807:ARG:HG2	1.77	0.48
2:B:590:VAL:HG21	2:B:610:ARG:HD2	1.96	0.48
15:T:27:DC:H2''	15:T:28:DT:C5	2.48	0.48
15:T:202:DT:H2''	15:T:203:DA:N7	2.29	0.48
15:T:230:DC:H2'	15:T:231:DA:O4'	2.14	0.48
18:c:25:PHE:HZ	18:c:59:THR:HG21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:f:72:TYR:OH	17:f:92:ARG:HD2	2.13	0.48
1:A:392:TYR:CG	1:A:438:MET:HE1	2.49	0.48
1:A:1140:ILE:O	1:A:1279:ILE:HG12	2.13	0.48
2:B:776:GLN:HG2	2:B:1096:ARG:HH11	1.79	0.48
2:B:823:ALA:HB1	2:B:1009:ASP:HB2	1.96	0.48
3:C:32:LEU:HD12	3:C:36:MET:HE3	1.96	0.48
6:F:79:ARG:HB3	6:F:146:TRP:CZ2	2.49	0.48
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.79	0.48
15:T:84:DG:H1'	15:T:85:DC:H5'	1.94	0.48
17:b:55:ARG:NH2	17:b:58:LEU:HD13	2.28	0.48
1:A:148:CYS:HB2	1:A:172:GLN:HE21	1.79	0.48
1:A:350:ALA:HB3	1:A:490:LEU:HB3	1.96	0.48
1:A:447:ARG:HH22	1:A:451:LEU:CB	2.12	0.48
1:A:816:PHE:HA	1:A:819:MET:CE	2.43	0.48
2:B:302:MET:HE3	2:B:385:ARG:CZ	2.42	0.48
2:B:462:GLN:HE22	15:T:269:DA:H4'	1.79	0.48
15:T:152:DC:H5'	16:m:83:ARG:HB2	1.94	0.48
17:b:70:VAL:HA	17:b:73:THR:HG22	1.96	0.48
18:g:97:LEU:HB3	18:g:100:VAL:HB	1.96	0.48
1:A:15:LYS:HB3	2:B:1220:ARG:NH2	2.27	0.48
1:A:108:MET:HE3	1:A:211:VAL:HG21	1.96	0.48
1:A:564:PRO:HB2	1:A:566:ILE:O	2.14	0.48
1:A:630:LEU:O	1:A:634:VAL:HG12	2.14	0.48
1:A:945:ARG:O	1:A:950:VAL:HA	2.14	0.48
1:A:1259:GLU:OE2	1:A:1263:LEU:HB2	2.13	0.48
1:A:1335:PHE:HA	1:A:1338:ILE:HD12	1.95	0.48
2:B:462:GLN:NE2	15:T:269:DA:H4'	2.29	0.48
2:B:535:LEU:HB2	2:B:628:ARG:HH21	1.79	0.48
3:C:206:TYR:HA	3:C:209:TRP:CD1	2.48	0.48
13:N:159:DT:H2''	13:N:160:DC:C5	2.49	0.48
13:N:256:DA:N9	13:N:257:DC:C5	2.82	0.48
13:N:262:DC:H2''	13:N:263:DA:C8	2.49	0.48
17:b:51:TYR:O	17:b:55:ARG:HG2	2.14	0.48
1:A:362:LEU:HD13	1:A:474:SER:HB2	1.95	0.47
1:A:535:MET:HG2	1:A:657:TRP:CE2	2.49	0.47
1:A:1436:LEU:HD22	7:G:63:PRO:HG2	1.95	0.47
2:B:479:TYR:CZ	2:B:1096:ARG:HG2	2.49	0.47
13:N:246:DG:H8	13:N:246:DG:H5'	1.78	0.47
15:T:191:DT:C1'	15:T:192:DT:C4	2.96	0.47
18:c:88:ARG:HA	18:c:94:ASN:OD1	2.14	0.47
1:A:351:ARG:NE	1:A:487:GLU:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ILE:HD13	2:B:117:LEU:HD13	1.95	0.47
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.96	0.47
8:H:86:LYS:HE3	8:H:90:ASP:OD2	2.13	0.47
13:N:246:DG:C8	13:N:247:DT:H72	2.49	0.47
15:T:177:DG:H2''	15:T:178:DC:C6	2.49	0.47
15:T:192:DT:H1'	15:T:193:DA:H5'	1.95	0.47
16:a:121:PRO:HG2	17:b:49:LEU:HD23	1.96	0.47
1:A:940:ASP:O	1:A:944:LEU:HG	2.15	0.47
1:A:1407:GLU:OE2	15:T:257:DC:H5''	2.14	0.47
2:B:58:LEU:O	2:B:74:ARG:HA	2.14	0.47
13:N:105:DG:H2'	13:N:106:DT:C6	2.49	0.47
13:N:243:DC:H2'	13:N:244:DT:H71	1.96	0.47
13:N:246:DG:C8	13:N:246:DG:H5'	2.50	0.47
19:p:57:LYS:O	19:p:61:ILE:HG12	2.14	0.47
1:A:231:ARG:HB2	1:A:234:TRP:CE2	2.49	0.47
1:A:1069:ILE:HG22	2:B:1140:ALA:HB1	1.97	0.47
2:B:99:MET:SD	2:B:104:ALA:HB2	2.54	0.47
2:B:422:TYR:HA	2:B:425:MET:HE2	1.97	0.47
1:A:596:ASN:HD21	1:A:605:GLY:HA3	1.80	0.47
1:A:1042:ASP:O	1:A:1045:GLU:HG3	2.14	0.47
9:I:84:VAL:O	9:I:101:TYR:HA	2.14	0.47
13:N:174:DC:H2''	13:N:175:DA:C8	2.50	0.47
1:A:341:LEU:HD11	2:B:1200:ALA:HA	1.96	0.47
2:B:87:PRO:HA	2:B:113:SER:HA	1.95	0.47
2:B:1138:MET:CE	2:B:1147:LEU:HB2	2.45	0.47
4:D:46:HIS:NE2	4:D:49:ILE:HD11	2.29	0.47
13:N:24:DG:H2'	13:N:25:DC:C6	2.50	0.47
13:N:185:DC:C2	13:N:186:DC:C4	3.03	0.47
13:N:256:DA:H2''	13:N:257:DC:C6	2.49	0.47
15:T:67:DG:H2''	15:T:68:DG:C8	2.50	0.47
15:T:222:DA:H1'	15:T:223:DG:C8	2.50	0.47
1:A:596:ASN:ND2	1:A:605:GLY:HA3	2.30	0.47
1:A:1195:LEU:HD22	1:A:1263:LEU:HD11	1.96	0.47
2:B:384:GLU:HG2	9:I:91:ARG:NH2	2.30	0.47
2:B:824:ILE:HB	2:B:1008:PRO:HA	1.95	0.47
6:F:107:VAL:HG12	6:F:109:VAL:H	1.79	0.47
13:N:126:DA:H61	15:T:154:DT:H3	1.63	0.47
13:N:152:DC:H4'	18:c:77:ARG:NH1	2.30	0.47
15:T:191:DT:O3'	15:T:192:DT:C5	2.67	0.47
16:a:54:TYR:HD2	17:b:39:ARG:HB2	1.80	0.47
17:l:76:ALA:HB1	17:l:78:ARG:HE	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:HA	1:A:506:CYS:HB2	1.97	0.47
1:A:1098:LEU:HD22	1:A:1358:VAL:HA	1.97	0.47
2:B:478:ARG:NH2	2:B:790:ASP:HB3	2.29	0.47
3:C:7:VAL:HG11	11:K:105:PHE:HD1	1.80	0.47
3:C:173:CYS:SG	3:C:243:VAL:HG11	2.54	0.47
11:K:61:TYR:HB3	11:K:73:MET:SD	2.55	0.47
13:N:151:DG:N2	15:T:130:DC:O2	2.48	0.47
13:N:174:DC:H2''	13:N:175:DA:H8	1.80	0.47
13:N:184:DA:H2''	13:N:185:DC:H6	1.79	0.47
13:N:243:DC:H2''	13:N:244:DT:H71	1.96	0.47
19:d:67:ASN:O	19:d:71:GLU:HG2	2.15	0.47
18:g:30:VAL:HG13	18:g:51:LEU:HD23	1.96	0.47
1:A:629:GLY:O	1:A:633:THR:HG23	2.14	0.47
1:A:813:GLU:HA	1:A:816:PHE:CD2	2.49	0.47
1:A:1031:ARG:O	1:A:1035:GLU:HB2	2.15	0.47
2:B:827:ILE:HG12	2:B:1012:ILE:HG12	1.96	0.47
13:N:217:DG:H2''	13:N:218:DT:C7	2.41	0.47
13:N:224:DC:C2	13:N:225:DC:C5	3.03	0.47
13:N:244:DT:H2'	13:N:245:DA:H8	1.79	0.47
15:T:27:DC:H2''	15:T:28:DT:C6	2.50	0.47
2:B:574:PHE:CZ	2:B:579:TRP:HB2	2.50	0.47
2:B:598:ARG:CZ	2:B:685:GLY:HA3	2.45	0.47
2:B:918:ILE:HD11	2:B:935:ARG:HB2	1.97	0.47
2:B:1001:PHE:HB3	2:B:1007:VAL:HG12	1.96	0.47
3:C:33:ARG:NH1	3:C:178:PHE:HD1	2.13	0.47
13:N:140:DC:O5'	13:N:140:DC:H6	1.98	0.47
13:N:235:DA:C1'	13:N:236:DT:C7	2.80	0.47
1:A:852:HIS:CG	6:F:139:PRO:HG3	2.49	0.46
2:B:840:ILE:O	2:B:1010:LEU:HA	2.15	0.46
2:B:1132:GLU:N	2:B:1135:ARG:HH21	2.13	0.46
3:C:100:LEU:HD12	3:C:118:LEU:HA	1.96	0.46
5:E:77:LEU:HD11	5:E:108:ILE:HB	1.96	0.46
7:G:50:ASP:O	7:G:54:ILE:HG13	2.16	0.46
15:T:44:DA:H2''	15:T:45:DT:OP2	2.13	0.46
15:T:245:DC:H2''	15:T:246:DA:O5'	2.14	0.46
16:a:78:PHE:CE1	17:b:67:ARG:HB2	2.50	0.46
1:A:723:LEU:HD11	1:A:795:PRO:HB3	1.97	0.46
1:A:1143:THR:HG23	1:A:1203:ARG:HH21	1.80	0.46
2:B:415:ARG:NH1	2:B:416:LYS:HA	2.30	0.46
13:N:60:DT:H2''	13:N:61:DT:H6	1.79	0.46
18:c:47:ALA:HB1	19:d:94:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:HA3	1:A:470:ARG:H	1.80	0.46
1:A:972:ILE:HG22	1:A:973:PHE:CD1	2.50	0.46
1:A:1338:ILE:HG23	1:A:1342:LEU:HB2	1.98	0.46
2:B:910:ILE:HD13	2:B:940:PRO:HB3	1.97	0.46
2:B:948:ILE:O	2:B:969:ARG:HD3	2.15	0.46
13:N:97:DT:H5''	13:N:97:DT:H6	1.81	0.46
13:N:115:DT:C4	13:N:116:DT:O4	2.69	0.46
16:m:45:THR:O	16:m:49:ARG:HG3	2.16	0.46
1:A:173:PRO:HG3	1:A:186:TRP:CD1	2.51	0.46
1:A:303:THR:HA	1:A:306:ASP:O	2.16	0.46
1:A:316:LEU:HA	1:A:322:PRO:HA	1.98	0.46
1:A:609:VAL:HG23	1:A:614:MET:HE1	1.96	0.46
1:A:959:PRO:HG2	1:A:1020:PHE:CD1	2.51	0.46
2:B:595:ASP:HA	2:B:598:ARG:HB3	1.96	0.46
2:B:631:PHE:CE1	2:B:687:ILE:HD11	2.51	0.46
2:B:1056:SER:HB2	2:B:1066:SER:HB2	1.97	0.46
13:N:51:DG:H2'	13:N:52:DC:C6	2.50	0.46
13:N:240:DT:H2''	13:N:241:DC:C5	2.51	0.46
15:T:182:DT:H4'	17:l:45:ARG:HG2	1.96	0.46
18:g:37:GLY:HA3	18:g:39:TYR:CE2	2.50	0.46
19:h:76:GLU:HB3	19:h:97:ALA:HB1	1.98	0.46
16:k:67:PHE:O	16:k:71:VAL:HG23	2.15	0.46
16:k:113:HIS:CG	16:m:126:LEU:HD22	2.50	0.46
1:A:253:MET:HE3	14:P:1:G:H1	1.81	0.46
3:C:171:SER:HB3	10:J:6:ARG:NH1	2.31	0.46
13:N:38:DT:H2''	13:N:39:DC:C6	2.50	0.46
13:N:260:DG:H2''	13:N:261:DT:C4	2.50	0.46
17:b:47:SER:HB3	17:b:50:ILE:HG12	1.96	0.46
17:b:55:ARG:C	17:b:59:LYS:HZ3	2.23	0.46
16:k:113:HIS:CE1	16:m:114:ALA:HB2	2.50	0.46
1:A:600:SER:OG	1:A:603:ASP:HA	2.15	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.55	0.46
2:B:606:VAL:HA	2:B:625:ARG:HH22	1.81	0.46
3:C:61:PHE:CE1	10:J:2:ILE:HD11	2.50	0.46
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.96	0.46
13:N:143:DG:N9	13:N:144:DT:H72	2.30	0.46
1:A:1153:GLU:HG3	1:A:1196:ARG:HH11	1.81	0.46
2:B:103:GLU:O	2:B:107:ARG:HB3	2.15	0.46
2:B:801:LYS:HE2	10:J:53:VAL:HG22	1.97	0.46
2:B:979:LYS:NZ	2:B:987:LYS:HB3	2.28	0.46
13:N:82:DC:P	16:k:84:PHE:H	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:178:DT:H2''	13:N:179:DC:C5	2.50	0.46
15:T:22:DC:H1'	15:T:23:DG:H5'	1.98	0.46
15:T:53:DG:H2'	15:T:54:DC:H6	1.81	0.46
15:T:89:DT:H2''	15:T:90:DA:C8	2.51	0.46
16:m:54:TYR:OH	17:n:36:ARG:HG2	2.15	0.46
17:n:92:ARG:HD3	17:n:92:ARG:N	2.31	0.46
18:o:79:ILE:HG12	18:o:82:HIS:CE1	2.51	0.46
2:B:265:LEU:O	2:B:268:VAL:HG22	2.16	0.46
2:B:1116:ARG:NH2	2:B:1158:PHE:HB2	2.28	0.46
3:C:242:GLN:HB3	3:C:246:ARG:NH2	2.31	0.46
10:J:39:LYS:HD2	10:J:39:LYS:O	2.16	0.46
11:K:12:LEU:HD12	11:K:13:PRO:HD2	1.98	0.46
1:A:375:LEU:HG	2:B:1105:ALA:HB1	1.98	0.46
1:A:498:THR:HB	2:B:1146:PHE:HD1	1.80	0.46
1:A:504:GLN:HB2	6:F:90:ARG:HH12	1.81	0.46
1:A:569:PRO:HG2	8:H:46:MET:HE3	1.98	0.46
1:A:1400:LEU:HB2	1:A:1429:GLU:HG3	1.97	0.46
2:B:176:ASP:O	2:B:177:GLU:C	2.59	0.46
11:K:17:PRO:HG2	11:K:20:LYS:HB2	1.96	0.46
13:N:93:DC:C2	13:N:94:DA:N7	2.84	0.46
15:T:79:DT:H2''	15:T:80:DA:C8	2.51	0.46
18:o:26:PRO:HG2	18:o:29:ARG:HB3	1.98	0.46
1:A:408:ARG:HD3	1:A:412:ASP:HB2	1.98	0.46
1:A:762:MET:HE3	2:B:1021:MET:SD	2.55	0.46
2:B:847:ASP:HB2	3:C:168:ALA:HB3	1.98	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD12	1.98	0.46
8:H:79:ARG:NH1	8:H:80:PRO:HD2	2.31	0.46
13:N:123:DG:H1	15:T:157:DC:H42	1.64	0.46
13:N:165:DG:C2	13:N:166:DG:C6	3.04	0.46
15:T:78:DG:C8	15:T:78:DG:H5'	2.50	0.46
15:T:113:DA:H2''	15:T:114:DC:H5''	1.97	0.46
16:m:50:GLU:O	16:m:54:TYR:CD2	2.69	0.46
18:o:37:GLY:HA3	18:o:39:TYR:CE2	2.51	0.46
1:A:262:ASP:HA	1:A:265:HIS:HB3	1.99	0.45
1:A:874:LEU:HD23	1:A:1059:LEU:HD23	1.98	0.45
3:C:45:ILE:HD12	3:C:66:LEU:HG	1.99	0.45
5:E:16:ARG:HH21	5:E:19:LYS:NZ	2.13	0.45
15:T:244:DA:H2''	15:T:245:DC:C6	2.51	0.45
15:T:255:DG:H3'	15:T:256:DC:H6	1.80	0.45
1:A:548:MET:HE3	11:K:58:PHE:CD1	2.51	0.45
1:A:554:VAL:HG13	1:A:649:ASN:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ILE:H	1:A:631:ILE:HD12	1.81	0.45
2:B:287:GLY:HA3	9:I:11:ASN:OD1	2.16	0.45
7:G:81:PRO:HG3	7:G:106:LEU:HD21	1.97	0.45
12:L:49:ARG:HA	12:L:56:ARG:HA	1.98	0.45
1:A:17:VAL:HG23	1:A:1424:CYS:SG	2.56	0.45
2:B:71:ILE:HA	2:B:127:ILE:HG22	1.97	0.45
3:C:79:MET:HE1	3:C:161:LYS:HB2	1.97	0.45
12:L:42:LEU:HD22	12:L:46:ASP:HB2	1.99	0.45
13:N:60:DT:C2'	13:N:61:DT:H72	2.46	0.45
15:T:6:DA:C2'	15:T:7:DT:H72	2.45	0.45
15:T:32:DG:H2'	15:T:33:DA:C8	2.52	0.45
15:T:117:DA:H4'	15:T:118:DT:OP1	2.16	0.45
15:T:129:DC:H2''	15:T:130:DC:C4	2.51	0.45
15:T:204:DG:H2''	15:T:205:DA:H8	1.81	0.45
18:c:84:GLN:NE2	18:c:102:ILE:HB	2.30	0.45
19:p:92:ARG:O	19:p:95:GLN:HG3	2.17	0.45
1:A:444:LEU:HD23	1:A:491:HIS:CD2	2.51	0.45
1:A:632:HIS:O	1:A:636:ARG:HG2	2.16	0.45
2:B:324:ASP:O	2:B:328:ARG:HG3	2.16	0.45
3:C:33:ARG:HB3	3:C:176:ILE:HG21	1.99	0.45
15:T:162:DA:H5''	17:n:30:THR:HG21	1.97	0.45
15:T:178:DC:H2''	15:T:179:DG:C8	2.50	0.45
16:a:120:MET:SD	16:a:122:LYS:HE2	2.57	0.45
17:b:38:ALA:HB1	17:b:43:VAL:HB	1.99	0.45
1:A:5:PRO:HG2	2:B:1159:ARG:NH2	2.32	0.45
1:A:364:GLN:HG2	1:A:460:ARG:HB3	1.97	0.45
1:A:408:ARG:HB2	1:A:412:ASP:HB2	1.98	0.45
2:B:252:ARG:HG3	2:B:253:GLU:N	2.31	0.45
13:N:143:DG:C2'	13:N:144:DT:C7	2.95	0.45
1:A:444:LEU:HD22	2:B:1146:PHE:CZ	2.52	0.45
1:A:505:LEU:HD21	6:F:91:ALA:HB2	1.97	0.45
1:A:830:VAL:HG12	1:A:831:LYS:HD3	1.98	0.45
1:A:1444:PHE:HZ	6:F:89:GLU:HA	1.80	0.45
2:B:36:ASP:CG	2:B:540:ILE:HD11	2.42	0.45
2:B:620:PHE:CE2	2:B:693:GLU:HG3	2.50	0.45
7:G:27:ARG:O	7:G:31:LEU:HG	2.16	0.45
13:N:77:DT:H2''	13:N:78:DA:N7	2.31	0.45
13:N:236:DT:C2'	13:N:237:DT:C7	2.95	0.45
19:h:78:SER:HA	19:h:89:ILE:HD11	1.99	0.45
1:A:58:LEU:HB3	1:A:245:PRO:HD3	1.99	0.45
2:B:476:LEU:HD12	2:B:487:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:PRO:O	2:B:590:VAL:HG13	2.17	0.45
2:B:699:MET:HE1	2:B:736:HIS:HB3	1.98	0.45
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.98	0.45
2:B:1084:GLN:HE22	3:C:190:ASP:C	2.25	0.45
6:F:103:MET:HE2	7:G:14:HIS:CE1	2.52	0.45
13:N:22:DT:H2''	13:N:23:DG:O5'	2.17	0.45
13:N:38:DT:H2''	13:N:39:DC:C5	2.51	0.45
13:N:256:DA:C6	13:N:257:DC:N4	2.84	0.45
15:T:158:DG:H2''	15:T:159:DG:C8	2.52	0.45
15:T:277:DC:H2''	15:T:278:DA:C8	2.52	0.45
17:b:54:THR:HA	17:b:57:VAL:HG22	1.97	0.45
1:A:114:LEU:HD22	1:A:148:CYS:HA	1.99	0.45
1:A:350:ALA:O	1:A:489:ASN:HA	2.17	0.45
1:A:655:ASN:O	1:A:659:LEU:HG	2.17	0.45
1:A:847:GLU:CG	1:A:1401:MET:HE1	2.47	0.45
2:B:182:LYS:CD	10:J:63:ASN:HD21	2.30	0.45
2:B:274:ILE:O	2:B:277:VAL:HG22	2.17	0.45
2:B:415:ARG:NH1	2:B:419:ARG:HE	2.15	0.45
2:B:749:LEU:HD21	2:B:759:PRO:HG3	1.98	0.45
5:E:42:ARG:O	5:E:46:CYS:HB2	2.17	0.45
13:N:208:DG:H2''	13:N:209:DT:C7	2.47	0.45
13:N:250:DC:H2''	13:N:251:DC:C5	2.52	0.45
15:T:6:DA:H2''	15:T:7:DT:H6	1.80	0.45
15:T:204:DG:H2''	15:T:205:DA:C8	2.52	0.45
1:A:244:PRO:HB2	1:A:246:GLN:OE1	2.17	0.45
1:A:1390:HIS:CD2	13:N:26:DC:H5'	2.52	0.45
2:B:71:ILE:HG13	2:B:127:ILE:HG22	1.98	0.45
2:B:275:VAL:O	2:B:279:ARG:HG3	2.17	0.45
2:B:590:VAL:HG11	2:B:610:ARG:HD2	1.99	0.45
2:B:760:ASP:HB3	2:B:1047:PHE:CZ	2.51	0.45
3:C:238:LEU:HD13	3:C:246:ARG:HD2	1.99	0.45
7:G:121:TYR:HB2	7:G:130:TYR:CZ	2.51	0.45
1:A:133:LYS:HA	1:A:133:LYS:HD2	1.75	0.45
2:B:47:GLN:HA	2:B:50:VAL:HG12	1.99	0.45
11:K:33:ILE:HG22	11:K:73:MET:HB3	1.99	0.45
16:a:50:GLU:HA	16:a:53:ARG:HE	1.82	0.45
16:e:79:LYS:HB3	16:e:82:LEU:HD11	1.98	0.45
1:A:90:VAL:HG21	1:A:301:VAL:HG11	1.97	0.44
1:A:858:ARG:NH1	6:F:139:PRO:HB2	2.31	0.44
1:A:1117:ALA:HA	1:A:1311:THR:O	2.18	0.44
2:B:103:GLU:HA	2:B:106:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ARG:N	3:C:33:ARG:HD3	2.30	0.44
16:e:86:SER:HA	16:e:89:ILE:HD12	1.98	0.44
18:g:75:LYS:HE3	18:g:77:ARG:HB2	1.97	0.44
1:A:1153:GLU:HG2	1:A:1196:ARG:HB3	1.99	0.44
3:C:171:SER:H	10:J:6:ARG:HH12	1.65	0.44
5:E:93:ARG:HH21	5:E:122:MET:HE2	1.82	0.44
13:N:256:DA:C4	13:N:257:DC:C5	3.06	0.44
18:c:64:GLU:HA	19:d:49:HIS:CD2	2.52	0.44
5:E:89:ILE:HD12	5:E:92:MET:HE3	1.99	0.44
12:L:50:CYS:HB3	12:L:55:HIS:H	1.82	0.44
13:N:196:DC:C4	13:N:197:DA:N6	2.86	0.44
19:h:57:LYS:O	19:h:61:ILE:HG12	2.17	0.44
18:o:50:TYR:OH	19:p:111:VAL:HG22	2.17	0.44
2:B:101:PRO:HG3	2:B:111:TYR:CZ	2.52	0.44
2:B:844:SER:HB3	2:B:848:ARG:NH1	2.32	0.44
2:B:1207:LEU:HA	2:B:1210:MET:HB3	2.00	0.44
13:N:11:DT:H2''	13:N:12:DG:O5'	2.17	0.44
13:N:100:DG:H21	17:l:45:ARG:NH2	2.15	0.44
1:A:114:LEU:HD11	1:A:172:GLN:HG3	1.99	0.44
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.52	0.44
3:C:30:ASN:O	3:C:30:ASN:ND2	2.50	0.44
18:c:25:PHE:CZ	18:c:59:THR:HG21	2.52	0.44
1:A:188:LYS:O	1:A:196:ALA:HB3	2.17	0.44
1:A:509:PRO:CB	1:A:640:PRO:HB2	2.47	0.44
1:A:516:GLN:HA	1:A:1073:SER:HB2	1.99	0.44
1:A:1316:LEU:HD22	1:A:1337:GLU:CG	2.47	0.44
1:A:1316:LEU:HD23	1:A:1317:ALA:H	1.82	0.44
2:B:218:LYS:HD3	2:B:227:HIS:NE2	2.33	0.44
5:E:136:GLU:O	5:E:140:VAL:HG23	2.17	0.44
13:N:188:DC:H2''	13:N:189:DT:C6	2.53	0.44
17:f:35:ARG:O	17:f:39:ARG:HG2	2.17	0.44
17:l:62:LEU:HA	17:l:65:VAL:HG22	1.98	0.44
18:o:57:TYR:OH	19:p:109:HIS:HB2	2.17	0.44
1:A:544:TYR:HA	1:A:573:TRP:HH2	1.80	0.44
1:A:555:PRO:HD3	1:A:652:LYS:HD2	1.99	0.44
2:B:388:GLN:HB3	9:I:91:ARG:HH12	1.82	0.44
2:B:631:PHE:CZ	2:B:743:ILE:HG23	2.53	0.44
2:B:733:SER:OG	9:I:70:ARG:HD3	2.18	0.44
2:B:758:PHE:HA	2:B:1046:PRO:HB3	2.00	0.44
2:B:841:MET:HE1	2:B:843:GLN:HA	1.99	0.44
2:B:863:GLU:HB2	2:B:961:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:PRO:HB2	5:E:54:ARG:HH12	1.81	0.44
11:K:63:VAL:HG22	11:K:71:PHE:HB3	1.99	0.44
13:N:57:DC:H2''	13:N:58:DT:C6	2.53	0.44
13:N:104:DT:H1'	13:N:105:DG:N7	2.32	0.44
13:N:246:DG:H2'	13:N:247:DT:C7	2.43	0.44
16:e:126:LEU:O	16:e:130:ILE:HG12	2.18	0.44
18:g:41:GLU:OE2	19:h:87:SER:HB2	2.17	0.44
1:A:270:ILE:HG12	1:A:300:HIS:HB3	2.00	0.44
13:N:6:DT:H2''	13:N:7:DG:C8	2.53	0.44
13:N:175:DA:C2	15:T:106:DG:C2	3.06	0.44
13:N:218:DT:H2''	13:N:219:DT:C6	2.53	0.44
15:T:131:DT:H5''	15:T:131:DT:C6	2.52	0.44
19:p:39:ILE:HG22	19:p:43:LYS:HE3	2.00	0.44
1:A:560:VAL:HG13	8:H:77:SER:HA	1.99	0.44
1:A:1335:PHE:O	1:A:1347:THR:HG23	2.17	0.44
2:B:12:ILE:HG13	2:B:16:ASP:HB2	2.00	0.44
2:B:174:THR:O	2:B:175:LEU:HB2	2.17	0.44
2:B:245:MET:HE3	2:B:354:LEU:HD23	1.99	0.44
2:B:639:LYS:HD2	2:B:641:ASN:H	1.83	0.44
2:B:735:HIS:H	9:I:70:ARG:NH1	2.16	0.44
5:E:14:SER:OG	5:E:140:VAL:HA	2.18	0.44
8:H:89:ALA:HA	8:H:142:LEU:HD23	2.00	0.44
9:I:82:ASP:OD2	9:I:104:LEU:HB2	2.18	0.44
10:J:35:LEU:HD22	10:J:40:LEU:HD12	1.99	0.44
10:J:47:ARG:CZ	10:J:48:MET:HE2	2.48	0.44
13:N:52:DC:H2'	13:N:53:DC:C6	2.53	0.44
15:T:150:DC:H1'	15:T:151:DC:H5'	2.00	0.44
17:b:25:ASN:O	17:b:25:ASN:ND2	2.50	0.44
16:e:51:ILE:HG13	17:f:39:ARG:HD2	2.00	0.44
17:n:31:LYS:HG3	17:n:51:TYR:CZ	2.53	0.44
19:p:54:ILE:HG13	19:p:58:ALA:HB3	1.99	0.44
1:A:365:VAL:C	1:A:462:LYS:HZ3	2.26	0.43
1:A:496:GLU:HA	1:A:499:ARG:HD3	2.00	0.43
1:A:960:VAL:HG21	1:A:1054:GLN:C	2.43	0.43
9:I:44:TYR:HE2	9:I:46:HIS:HB2	1.83	0.43
18:g:79:ILE:HG12	18:g:82:HIS:ND1	2.32	0.43
17:l:75:HIS:CE1	19:p:93:GLU:HG3	2.53	0.43
19:p:94:ILE:O	19:p:98:VAL:HG23	2.17	0.43
1:A:961:ASN:HD21	1:A:963:ARG:HH11	1.66	0.43
1:A:1009:ILE:HG12	5:E:166:ARG:NH2	2.33	0.43
1:A:1427:VAL:HA	1:A:1430:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:VAL:HB	2:B:594:ARG:HH12	1.83	0.43
10:J:56:ILE:HA	10:J:59:PHE:CD2	2.45	0.43
1:A:100:LYS:HD2	1:A:177:LYS:HB2	1.99	0.43
1:A:336:ARG:HD2	2:B:1202:LEU:HD23	1.99	0.43
1:A:362:LEU:CD1	1:A:474:SER:HB2	2.48	0.43
1:A:687:ALA:O	1:A:691:VAL:HG23	2.18	0.43
1:A:1317:ALA:HA	1:A:1320:MET:HE3	1.98	0.43
2:B:175:LEU:CD1	2:B:183:MET:HE1	2.46	0.43
2:B:252:ARG:HB3	2:B:255:LYS:CG	2.48	0.43
3:C:14:ASP:HA	3:C:239:LYS:HE2	2.00	0.43
11:K:72:VAL:HG22	11:K:73:MET:H	1.84	0.43
16:a:118:THR:HA	17:b:45:ARG:HB3	2.00	0.43
17:f:38:ALA:HB1	17:f:43:VAL:HB	2.00	0.43
16:k:104:PHE:CE2	17:l:37:LEU:HB3	2.53	0.43
16:m:79:LYS:HB3	16:m:82:LEU:HD11	2.00	0.43
1:A:1163:THR:HB	1:A:1172:VAL:HG21	2.00	0.43
2:B:14:THR:HG22	2:B:18:TRP:NE1	2.32	0.43
2:B:327:GLY:O	2:B:332:ALA:HB3	2.18	0.43
2:B:350:GLN:NE2	2:B:361:GLU:HG3	2.33	0.43
2:B:370:PHE:HD2	2:B:371:LEU:HD22	1.83	0.43
5:E:10:ARG:NH2	5:E:140:VAL:HG21	2.34	0.43
11:K:58:PHE:CE2	11:K:74:ARG:HD3	2.53	0.43
15:T:10:DA:C8	15:T:11:DT:C7	3.02	0.43
15:T:178:DC:H2''	15:T:179:DG:H8	1.83	0.43
15:T:185:DG:C2	15:T:186:DT:C2	3.06	0.43
16:k:72:ARG:HG2	16:k:84:PHE:CE2	2.53	0.43
1:A:43:GLU:C	1:A:45:ARG:N	2.76	0.43
1:A:513:VAL:HG22	1:A:520:PRO:HG3	2.00	0.43
2:B:605:GLU:HB2	2:B:627:TYR:CE2	2.53	0.43
2:B:980:PHE:CE1	2:B:1094:ARG:HB2	2.54	0.43
2:B:1076:HIS:HA	3:C:34:ARG:NH1	2.33	0.43
3:C:65:ARG:NH2	10:J:2:ILE:HG13	2.31	0.43
4:D:98:ALA:HA	7:G:36:GLY:HA3	2.00	0.43
5:E:38:LEU:O	5:E:42:ARG:HG3	2.18	0.43
18:g:26:PRO:HD3	19:h:40:TYR:CD1	2.54	0.43
16:k:99:TYR:CZ	16:k:103:LEU:HD11	2.54	0.43
19:p:76:GLU:O	19:p:80:LEU:HD23	2.19	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.43
1:A:351:ARG:HA	1:A:488:MET:O	2.18	0.43
1:A:377:TYR:HD1	1:A:494:GLN:HA	1.83	0.43
2:B:485:LEU:O	2:B:489:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:809:MET:HG2	2:B:815:ARG:HB3	1.99	0.43
5:E:102:LYS:HB2	5:E:104:PHE:CE2	2.53	0.43
8:H:89:ALA:HA	8:H:92:TYR:HD2	1.82	0.43
15:T:190:DT:H2''	15:T:191:DT:C5	2.53	0.43
16:m:57:SER:HB2	16:m:59:GLU:OE1	2.18	0.43
1:A:691:VAL:HG11	1:A:795:PRO:HG3	1.99	0.43
2:B:481:TYR:CE2	2:B:485:LEU:HD11	2.54	0.43
3:C:96:VAL:HG22	3:C:124:PRO:HD3	2.01	0.43
13:N:89:DA:H2''	13:N:90:DA:N7	2.34	0.43
13:N:264:DG:H5''	18:g:75:LYS:NZ	2.34	0.43
16:a:54:TYR:CZ	17:b:36:ARG:HG2	2.54	0.43
16:a:79:LYS:HB3	16:a:82:LEU:HD11	2.01	0.43
16:k:124:ILE:HG21	17:l:53:GLU:OE2	2.19	0.43
1:A:108:MET:H	1:A:172:GLN:NE2	2.17	0.43
1:A:549:ASN:O	1:A:553:TRP:HD1	2.02	0.43
1:A:700:HIS:CG	9:I:112:ASP:HB3	2.54	0.43
1:A:868:LEU:HD13	1:A:1002:LEU:HD21	2.00	0.43
1:A:966:ILE:HD11	1:A:1028:LEU:HD21	2.01	0.43
1:A:1141:GLU:OE2	1:A:1284:LYS:HD2	2.18	0.43
2:B:226:SER:HA	2:B:252:ARG:NH1	2.33	0.43
2:B:872:GLU:OE1	2:B:914:LYS:HD2	2.19	0.43
6:F:116:ASP:HB3	6:F:118:LEU:HD23	2.00	0.43
7:G:153:ASP:C	7:G:155:ASN:N	2.76	0.43
12:L:33:CYS:HB3	12:L:36:CYS:SG	2.49	0.43
13:N:92:DG:C4	13:N:93:DC:C5	3.07	0.43
13:N:269:DA:H5'	13:N:269:DA:C8	2.54	0.43
18:g:31:HIS:CD2	18:g:35:ARG:HE	2.36	0.43
1:A:766:VAL:HB	1:A:801:VAL:HB	2.00	0.43
1:A:890:SER:O	1:A:894:PHE:HD1	2.01	0.43
1:A:920:ILE:HG13	1:A:921:LEU:N	2.34	0.43
1:A:959:PRO:O	1:A:960:VAL:C	2.62	0.43
1:A:1065:MET:HB3	1:A:1068:VAL:HG12	2.00	0.43
1:A:1444:PHE:HB2	6:F:135:ARG:O	2.19	0.43
2:B:593:MET:HG3	2:B:608:ILE:HD13	2.01	0.43
13:N:198:DC:H2''	13:N:199:DG:C8	2.54	0.43
15:T:192:DT:C1'	15:T:193:DA:H5'	2.49	0.43
16:e:121:PRO:O	16:e:125:GLN:HG2	2.18	0.43
1:A:1061:HIS:O	1:A:1064:GLU:HG3	2.18	0.43
1:A:1065:MET:CE	1:A:1439:MET:HB2	2.49	0.43
2:B:214:VAL:HB	2:B:377:ARG:NH1	2.34	0.43
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:ARG:HH21	2:B:1198:TYR:HB2	1.81	0.43
11:K:92:ALA:O	11:K:95:ILE:HG22	2.19	0.43
15:T:200:DG:H2''	15:T:201:DC:C5	2.54	0.43
19:d:114:GLY:O	19:d:118:VAL:HG22	2.19	0.43
18:g:88:ARG:HA	18:g:88:ARG:HD3	1.80	0.43
18:o:59:THR:HA	18:o:62:ILE:HG22	2.00	0.43
1:A:43:GLU:HG2	1:A:45:ARG:HB2	2.00	0.42
1:A:530:CYS:O	1:A:533:ARG:HG2	2.19	0.42
1:A:538:ARG:HA	1:A:576:LYS:NZ	2.33	0.42
1:A:734:ALA:O	1:A:738:LEU:HG	2.18	0.42
1:A:784:SER:O	2:B:509:ASN:HB3	2.19	0.42
1:A:867:PHE:HE2	5:E:209:SER:HA	1.84	0.42
1:A:943:PHE:HD1	1:A:947:ILE:HD12	1.84	0.42
1:A:1449:ASP:HB2	6:F:133:VAL:HG23	2.00	0.42
2:B:848:ARG:HD3	10:J:7:CYS:O	2.19	0.42
2:B:1071:VAL:HG22	2:B:1084:GLN:CG	2.48	0.42
3:C:37:LEU:HD21	3:C:176:ILE:HG13	2.00	0.42
5:E:21:MET:HE1	5:E:134:PHE:CE2	2.54	0.42
5:E:122:MET:SD	5:E:126:VAL:HB	2.59	0.42
7:G:1:MET:O	7:G:79:TRP:HA	2.19	0.42
13:N:54:DG:C6	13:N:55:DC:N4	2.87	0.42
13:N:273:DA:C2	15:T:8:DG:C6	3.07	0.42
15:T:152:DC:H2'	15:T:153:DT:C6	2.53	0.42
15:T:174:DA:H2''	15:T:175:DC:C5'	2.49	0.42
18:c:83:LEU:HD22	19:d:62:MET:HE3	1.99	0.42
1:A:598:LEU:HB2	8:H:114:TYR:CZ	2.54	0.42
1:A:837:TYR:CE1	1:A:841:ARG:HD3	2.54	0.42
1:A:850:MET:HA	1:A:1065:MET:HE1	2.01	0.42
1:A:1149:THR:HA	1:A:1198:GLU:O	2.19	0.42
1:A:1428:SER:O	1:A:1432:MET:HE3	2.19	0.42
2:B:233:SER:O	2:B:241:LEU:HD12	2.19	0.42
2:B:364:GLU:O	2:B:368:THR:HG23	2.19	0.42
2:B:981:ALA:HB3	2:B:1093:GLN:HG3	2.01	0.42
5:E:87:VAL:HB	5:E:115:ILE:HA	2.00	0.42
12:L:38:HIS:ND1	12:L:40:PHE:HB3	2.34	0.42
13:N:100:DG:C5	13:N:101:DC:C4	3.08	0.42
16:m:52:ARG:HA	16:m:55:GLN:NE2	2.33	0.42
1:A:516:GLN:HE22	1:A:1077:PRO:HD3	1.84	0.42
1:A:853:TYR:CE2	6:F:136:ARG:HB3	2.54	0.42
1:A:1381:ARG:HH12	1:A:1395:ALA:HA	1.84	0.42
2:B:832:GLY:HA2	2:B:835:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASP:HA	3:C:145:CYS:O	2.20	0.42
6:F:116:ASP:O	6:F:120:ILE:HG13	2.19	0.42
8:H:53:ASP:HB3	8:H:145:ARG:NH1	2.34	0.42
11:K:62:LYS:O	11:K:71:PHE:HB2	2.19	0.42
11:K:96:ASN:O	11:K:100:THR:HG23	2.18	0.42
13:N:58:DT:H2''	13:N:59:DT:C5	2.54	0.42
13:N:169:DG:N2	15:T:112:DG:N2	2.66	0.42
13:N:178:DT:H2''	13:N:179:DC:C6	2.54	0.42
13:N:206:DC:C6	13:N:207:DT:H73	2.55	0.42
15:T:191:DT:C1'	15:T:192:DT:C5	3.02	0.42
17:b:55:ARG:HH22	17:b:58:LEU:HD13	1.84	0.42
16:e:57:SER:HB2	16:e:59:GLU:OE1	2.19	0.42
1:A:447:ARG:CG	1:A:455:SER:HB3	2.35	0.42
1:A:547:VAL:HG21	1:A:573:TRP:CE3	2.53	0.42
2:B:87:PRO:HB2	2:B:99:MET:HE3	2.00	0.42
2:B:481:TYR:O	2:B:485:LEU:HG	2.19	0.42
2:B:994:TYR:HA	2:B:995:ARG:NH1	2.35	0.42
4:D:23:GLU:HB3	7:G:82:PHE:HD2	1.84	0.42
5:E:111:TYR:CE1	5:E:115:ILE:HD11	2.54	0.42
13:N:96:DG:H2''	13:N:97:DT:C6	2.54	0.42
16:m:48:LEU:HB3	16:m:52:ARG:NH1	2.33	0.42
1:A:15:LYS:HD3	2:B:1220:ARG:HH12	1.84	0.42
1:A:1215:ALA:O	1:A:1218:ILE:HG22	2.20	0.42
2:B:814:PHE:CE1	2:B:818:PRO:HA	2.55	0.42
2:B:1101:ASP:OD1	2:B:1102:LYS:HG3	2.20	0.42
6:F:97:ARG:NH2	6:F:108:LEU:HD13	2.34	0.42
13:N:175:DA:N1	15:T:106:DG:N1	2.67	0.42
13:N:186:DC:H5'	13:N:186:DC:H6	1.84	0.42
16:e:68:GLN:HG2	16:e:72:ARG:HE	1.84	0.42
19:p:90:THR:O	19:p:94:ILE:HG12	2.20	0.42
1:A:24:PRO:HA	1:A:27:ILE:HD12	2.01	0.42
1:A:514:SER:OG	1:A:516:GLN:HG3	2.20	0.42
1:A:554:VAL:HG13	1:A:649:ASN:ND2	2.34	0.42
1:A:694:ILE:HD13	1:A:718:GLU:HG2	2.01	0.42
1:A:1043:ALA:O	1:A:1047:VAL:HG23	2.19	0.42
2:B:87:PRO:HG2	2:B:99:MET:O	2.19	0.42
12:L:31:TYR:HB3	12:L:58:ILE:HD12	2.00	0.42
13:N:199:DG:N2	15:T:82:DG:C2	2.88	0.42
13:N:214:DC:H2''	13:N:215:DG:H8	1.84	0.42
14:P:2:U:H2'	14:P:3:G:O4'	2.18	0.42
19:d:65:PHE:O	19:d:69:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:76:GLU:HA	19:d:79:ARG:HG2	2.02	0.42
16:m:65:LEU:HB3	16:m:69:ARG:NH1	2.35	0.42
16:m:101:VAL:HG13	17:n:41:GLY:HA2	2.02	0.42
1:A:501:GLU:OE1	2:B:1143:ALA:HB1	2.19	0.42
1:A:607:LEU:HD23	1:A:615:PHE:CZ	2.54	0.42
1:A:795:PRO:C	1:A:800:PHE:HB3	2.45	0.42
1:A:1289:LYS:HA	1:A:1306:LEU:O	2.20	0.42
2:B:279:ARG:HB3	2:B:284:VAL:HG12	2.00	0.42
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.55	0.42
2:B:821:GLN:HB2	2:B:851:PHE:CE2	2.55	0.42
2:B:858:SER:HA	2:B:966:VAL:O	2.19	0.42
5:E:152:HIS:CD2	5:E:197:ILE:HG12	2.54	0.42
10:J:8:PHE:HD2	10:J:48:MET:SD	2.42	0.42
15:T:219:DA:C2'	15:T:220:DA:H5'	2.48	0.42
16:k:61:LEU:HD13	17:l:36:ARG:HB3	2.01	0.42
16:m:46:VAL:HG22	16:m:49:ARG:NH2	2.32	0.42
16:m:65:LEU:HB2	16:m:66:PRO:HD3	2.02	0.42
1:A:689:GLU:HA	1:A:692:GLN:HG3	2.01	0.42
1:A:827:ASP:HA	1:A:831:LYS:NZ	2.34	0.42
1:A:843:VAL:HG11	2:B:1136:ASP:CG	2.44	0.42
2:B:308:PRO:HA	2:B:311:GLU:OE2	2.20	0.42
2:B:419:ARG:NH1	13:N:12:DG:H4'	2.33	0.42
2:B:798:TYR:HA	10:J:1:MET:H1	1.85	0.42
2:B:1084:GLN:NE2	3:C:191:PHE:HD1	2.17	0.42
3:C:7:VAL:HG22	3:C:21:LEU:HD13	2.01	0.42
5:E:92:MET:CE	5:E:122:MET:HG3	2.50	0.42
8:H:47:PHE:HZ	8:H:145:ARG:O	2.02	0.42
9:I:90:GLN:HG3	9:I:92:ARG:H	1.85	0.42
10:J:43:TYR:HA	10:J:46:ARG:HD3	2.02	0.42
13:N:10:DG:H4'	13:N:11:DT:OP1	2.19	0.42
13:N:62:DG:C2	13:N:63:DG:C5	3.07	0.42
15:T:82:DG:H2'	15:T:83:DT:H72	2.00	0.42
18:g:80:PRO:HA	18:g:83:LEU:HD12	2.00	0.42
17:l:49:LEU:HD23	17:l:49:LEU:O	2.19	0.42
1:A:337:LEU:HD12	1:A:1408:THR:HG21	2.01	0.42
1:A:504:GLN:CD	6:F:91:ALA:HA	2.45	0.42
1:A:974:HIS:CE1	1:A:976:ASP:HB2	2.55	0.42
1:A:1339:LEU:HA	1:A:1343:GLY:O	2.19	0.42
2:B:545:GLU:HB3	2:B:546:PRO:HD3	2.02	0.42
3:C:20:MET:HE1	3:C:22:SER:HB3	2.01	0.42
5:E:55:LYS:HA	5:E:58:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:51:DG:H2'	13:N:52:DC:H6	1.85	0.42
13:N:268:DT:H2''	13:N:269:DA:H5'	2.01	0.42
15:T:57:DT:H6	15:T:57:DT:H2'	1.76	0.42
15:T:112:DG:H2''	15:T:113:DA:C8	2.55	0.42
19:d:73:ILE:HD12	19:d:73:ILE:HA	1.89	0.42
1:A:533:ARG:CD	1:A:750:ALA:HB2	2.47	0.42
1:A:689:GLU:O	1:A:692:GLN:HG3	2.19	0.42
1:A:902:LEU:C	1:A:903:MET:HE2	2.45	0.42
1:A:1021:GLN:HB3	1:A:1025:ARG:NH1	2.35	0.42
2:B:177:GLU:HA	2:B:180:LEU:HD12	2.02	0.42
2:B:789:MET:HG3	2:B:967:ARG:HB2	2.01	0.42
3:C:68:LEU:HG	10:J:5:VAL:HB	2.02	0.42
13:N:146:DT:O2	15:T:135:DG:N2	2.53	0.42
13:N:190:DT:H2''	13:N:191:DA:N7	2.35	0.42
15:T:160:DT:C2'	15:T:161:DT:C7	2.65	0.42
17:f:75:HIS:CE1	19:h:92:ARG:HG2	2.55	0.42
16:k:70:LEU:HA	17:l:25:ASN:HB3	2.02	0.42
16:m:112:ILE:HD13	16:m:116:ARG:O	2.20	0.42
1:A:69:THR:HB	1:A:80:HIS:CD2	2.55	0.41
1:A:729:SER:O	1:A:732:ARG:HG3	2.19	0.41
2:B:981:ALA:HB1	2:B:987:LYS:NZ	2.35	0.41
4:D:141:GLU:HB3	4:D:163:LEU:HD21	2.02	0.41
5:E:92:MET:SD	5:E:92:MET:C	3.03	0.41
6:F:84:TYR:CD1	6:F:152:ILE:HB	2.55	0.41
8:H:91:ASP:O	8:H:144:ARG:HD3	2.20	0.41
13:N:163:DT:H2''	13:N:164:DT:H73	2.01	0.41
15:T:49:DC:H2''	15:T:50:DT:C6	2.55	0.41
15:T:276:DA:H2''	15:T:277:DC:C5	2.55	0.41
16:k:108:ASN:O	16:k:112:ILE:HG12	2.20	0.41
1:A:285:SER:HA	1:A:286:PRO:HD3	1.92	0.41
1:A:452:HIS:CD2	1:A:1076:GLU:HG3	2.41	0.41
1:A:457:MET:HB2	1:A:479:TYR:OH	2.20	0.41
1:A:503:SER:O	1:A:507:ALA:HB2	2.20	0.41
1:A:564:PRO:HB3	1:A:573:TRP:NE1	2.35	0.41
1:A:785:LEU:HD12	1:A:788:PHE:HE2	1.86	0.41
1:A:1102:ARG:HE	1:A:1106:ILE:CD1	2.33	0.41
1:A:1142:TYR:HB2	1:A:1279:ILE:C	2.45	0.41
2:B:18:TRP:CE2	2:B:807:GLN:HB2	2.55	0.41
2:B:49:LEU:HD13	2:B:411:ARG:HB2	2.02	0.41
2:B:863:GLU:OE2	2:B:873:GLU:HA	2.21	0.41
2:B:883:LEU:HD11	2:B:935:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:LEU:HD22	5:E:159:GLU:HB3	2.01	0.41
6:F:120:ILE:O	6:F:124:GLU:OE1	2.39	0.41
13:N:52:DC:H2''	13:N:53:DC:H5'	2.02	0.41
13:N:234:DG:H2''	13:N:235:DA:H8	1.85	0.41
15:T:96:DT:H2''	15:T:97:DG:H8	1.86	0.41
15:T:243:DA:H2'	15:T:244:DA:C8	2.54	0.41
19:h:67:ASN:O	19:h:71:GLU:OE1	2.37	0.41
1:A:243:PRO:HG2	1:A:248:ARG:NH1	2.35	0.41
1:A:557:TRP:CZ3	1:A:559:GLY:HA2	2.55	0.41
1:A:566:ILE:HG12	8:H:96:MET:HG2	2.02	0.41
1:A:694:ILE:HG22	1:A:715:PHE:CE1	2.55	0.41
1:A:965:ILE:HD12	1:A:1047:VAL:HG13	2.02	0.41
1:A:1028:LEU:HB3	1:A:1033:ILE:HD11	2.02	0.41
2:B:107:ARG:HH12	2:B:958:GLN:N	2.17	0.41
2:B:773:MET:HE2	2:B:1095:LEU:HD13	2.02	0.41
2:B:859:TYR:OH	2:B:942:ARG:HG3	2.20	0.41
2:B:994:TYR:HA	2:B:995:ARG:HH11	1.84	0.41
2:B:1060:ARG:HA	2:B:1064:TYR:O	2.21	0.41
5:E:134:PHE:CE1	5:E:185:ARG:HB3	2.55	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.01	0.41
13:N:234:DG:C6	13:N:235:DA:C6	3.08	0.41
17:b:61:PHE:O	17:b:65:VAL:HG23	2.20	0.41
17:b:71:THR:O	17:b:74:GLU:HG3	2.20	0.41
18:g:75:LYS:HE3	18:g:77:ARG:H	1.85	0.41
1:A:184:GLY:H	1:A:203:LEU:HD23	1.85	0.41
1:A:353:VAL:HA	1:A:486:ASP:O	2.20	0.41
2:B:366:ARG:HG3	2:B:559:LEU:HD13	2.02	0.41
2:B:399:LEU:HA	2:B:399:LEU:HD23	1.87	0.41
2:B:764:SER:OG	2:B:765:PRO:CD	2.56	0.41
2:B:870:ILE:HD13	2:B:919:PRO:HB3	2.02	0.41
3:C:239:LYS:HD2	3:C:240:ALA:H	1.85	0.41
5:E:189:LEU:HA	5:E:193:GLN:OE1	2.20	0.41
13:N:204:DC:P	16:a:120:MET:HE1	2.60	0.41
13:N:212:DC:H2''	13:N:213:DC:C5	2.55	0.41
16:a:57:SER:HB2	16:a:59:GLU:OE1	2.21	0.41
18:g:17:ARG:NH2	18:g:28:GLY:HA2	2.36	0.41
17:l:35:ARG:HG2	17:l:35:ARG:NH1	2.34	0.41
1:A:285:SER:OG	1:A:290:ILE:HD11	2.20	0.41
1:A:516:GLN:NE2	1:A:1076:GLU:HB3	2.26	0.41
1:A:535:MET:CE	1:A:654:VAL:HG22	2.50	0.41
1:A:634:VAL:HG13	1:A:635:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ILE:HD11	1:A:806:LEU:HD13	2.01	0.41
1:A:1100:VAL:N	1:A:1101:PRO:HD2	2.35	0.41
1:A:1400:LEU:HA	1:A:1403:CYS:SG	2.60	0.41
1:A:1453:LEU:HD22	7:G:22:MET:HE2	2.02	0.41
2:B:22:SER:HA	2:B:811:TYR:CE1	2.56	0.41
2:B:337:ARG:HG2	2:B:340:LYS:HG2	2.03	0.41
13:N:191:DA:H2''	13:N:192:DA:C8	2.55	0.41
13:N:227:DC:H2''	13:N:228:DC:O5'	2.20	0.41
15:T:90:DA:H1'	15:T:91:DA:C8	2.56	0.41
15:T:132:DG:H2''	15:T:133:DG:C8	2.56	0.41
16:m:82:LEU:HD23	17:n:79:LYS:HZ2	1.85	0.41
1:A:232:PRO:O	1:A:235:MET:HG2	2.21	0.41
1:A:360:LEU:HD11	1:A:470:ARG:HB3	2.02	0.41
1:A:402:GLY:H	1:A:438:MET:HE2	1.85	0.41
1:A:633:THR:O	1:A:637:GLU:OE1	2.38	0.41
1:A:847:GLU:HG2	1:A:1401:MET:HE1	2.03	0.41
1:A:1006:ASN:H	1:A:1009:ILE:HD12	1.85	0.41
1:A:1018:SER:HB2	5:E:204:SER:O	2.20	0.41
2:B:654:LYS:HA	2:B:657:GLN:HG2	2.02	0.41
3:C:57:LEU:CD1	10:J:1:MET:HE1	2.46	0.41
5:E:28:PHE:HB2	5:E:64:THR:CG2	2.50	0.41
13:N:245:DA:C2	15:T:36:DA:C2	3.09	0.41
18:c:97:LEU:HB3	18:c:100:VAL:HB	2.03	0.41
16:k:69:ARG:NH2	16:k:72:ARG:HE	2.15	0.41
2:B:252:ARG:HB3	2:B:255:LYS:HG3	2.02	0.41
2:B:506:GLN:HE21	2:B:508:HIS:HB2	1.86	0.41
2:B:974:PRO:HG3	2:B:1094:ARG:HH12	1.85	0.41
3:C:36:MET:HE2	3:C:36:MET:N	2.36	0.41
5:E:75:GLY:HA3	5:E:105:SER:HB2	2.01	0.41
8:H:59:LEU:HD11	8:H:122:MET:HE1	2.03	0.41
13:N:60:DT:H2'	13:N:61:DT:C7	2.51	0.41
13:N:163:DT:C2	13:N:164:DT:C7	3.02	0.41
13:N:218:DT:H2''	13:N:219:DT:C5	2.55	0.41
13:N:235:DA:C8	13:N:236:DT:C7	2.98	0.41
18:c:31:HIS:CG	18:c:35:ARG:HE	2.39	0.41
16:e:50:GLU:HA	16:e:53:ARG:HG2	2.01	0.41
17:f:35:ARG:HG2	17:f:46:ILE:HD12	2.03	0.41
16:m:58:THR:HG21	18:o:81:ARG:HD3	2.03	0.41
19:p:65:PHE:O	19:p:69:ILE:HG12	2.21	0.41
1:A:304:TYR:OH	2:B:1209:ALA:HB1	2.21	0.41
1:A:538:ARG:HB3	8:H:20:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PRO:HG2	1:A:587:ILE:HD11	2.03	0.41
2:B:519:GLU:HB2	2:B:771:SER:HB3	2.02	0.41
3:C:46:ASP:HB3	3:C:160:LYS:HB2	2.02	0.41
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.02	0.41
13:N:53:DC:H2''	13:N:54:DG:C8	2.55	0.41
13:N:163:DT:N1	13:N:164:DT:C7	2.61	0.41
16:m:50:GLU:HG3	17:n:39:ARG:HG3	2.03	0.41
1:A:92:HIS:HB2	1:A:237:ILE:HD11	2.03	0.41
1:A:362:LEU:HA	1:A:472:ASN:CB	2.51	0.41
1:A:535:MET:HG2	1:A:657:TRP:CD2	2.56	0.41
1:A:570:LYS:HA	1:A:571:PRO:HD3	1.97	0.41
1:A:709:MET:HE1	1:A:717:GLY:HA3	2.03	0.41
1:A:803:ASN:HA	1:A:807:ARG:HD3	2.01	0.41
1:A:851:VAL:HG12	1:A:1062:PRO:HA	2.02	0.41
1:A:1142:TYR:HB3	1:A:1282:ILE:O	2.20	0.41
1:A:1259:GLU:HG2	1:A:1262:MET:CE	2.50	0.41
1:A:1371:MET:O	1:A:1375:VAL:HG13	2.20	0.41
2:B:275:VAL:HG12	2:B:279:ARG:HE	1.86	0.41
2:B:393:HIS:O	2:B:394:PHE:C	2.63	0.41
2:B:590:VAL:HB	2:B:594:ARG:HH22	1.85	0.41
2:B:1138:MET:HE1	2:B:1147:LEU:HD22	2.03	0.41
3:C:70:PRO:HG3	10:J:13:VAL:CG2	2.50	0.41
3:C:126:ASN:O	3:C:127:LEU:C	2.64	0.41
5:E:82:CYS:HB2	5:E:109:PHE:CZ	2.55	0.41
7:G:30:LEU:HD22	7:G:72:VAL:HG11	2.03	0.41
13:N:37:DT:H5'	13:N:37:DT:C6	2.56	0.41
13:N:164:DT:H2''	13:N:165:DG:C8	2.56	0.41
15:T:139:DA:H2''	15:T:140:DG:O5'	2.21	0.41
15:T:145:DT:C2'	15:T:146:DA:H5'	2.46	0.41
15:T:223:DG:H2''	15:T:224:DA:H5'	2.03	0.41
18:c:71:ARG:HH12	19:d:49:HIS:HE1	1.68	0.41
17:f:75:HIS:NE2	19:h:93:GLU:HG3	2.36	0.41
16:m:47:ALA:HA	16:m:50:GLU:OE2	2.21	0.41
17:n:47:SER:HB3	17:n:50:ILE:HG12	2.03	0.41
18:o:79:ILE:HG12	18:o:82:HIS:ND1	2.36	0.41
1:A:182:LEU:O	1:A:202:LEU:HA	2.19	0.41
1:A:472:ASN:O	1:A:475:VAL:HG22	2.20	0.41
1:A:656:TYR:HD1	1:A:659:LEU:HD12	1.85	0.41
2:B:535:LEU:HD12	2:B:747:MET:HE2	2.03	0.41
2:B:631:PHE:HE1	2:B:687:ILE:HD11	1.86	0.41
2:B:641:ASN:OD1	2:B:644:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:MET:SD	9:I:66:PRO:HB2	2.61	0.41
2:B:942:ARG:HD2	2:B:945:GLU:CD	2.46	0.41
11:K:100:THR:O	11:K:104:LYS:HG2	2.21	0.41
13:N:33:DG:C2'	13:N:34:DT:H5'	2.44	0.41
15:T:171:DG:H3'	16:m:117:VAL:HG12	2.02	0.41
1:A:402:GLY:N	1:A:438:MET:HE2	2.36	0.40
1:A:444:LEU:HD21	1:A:456:MET:SD	2.60	0.40
1:A:646:LEU:O	1:A:650:ILE:HG22	2.21	0.40
1:A:1102:ARG:HH22	1:A:1113:ILE:HG21	1.86	0.40
2:B:16:ASP:O	2:B:20:VAL:HG23	2.21	0.40
2:B:214:VAL:HG21	2:B:373:TYR:HE2	1.87	0.40
2:B:776:GLN:HB3	2:B:1096:ARG:HG3	2.02	0.40
3:C:45:ILE:HA	3:C:159:ALA:HA	2.03	0.40
3:C:95:SER:HB2	3:C:158:ILE:HG23	2.02	0.40
7:G:91:VAL:HG12	7:G:101:ALA:HB2	2.03	0.40
8:H:54:SER:H	8:H:145:ARG:HH12	1.68	0.40
9:I:26:LEU:HD23	9:I:37:LEU:HD12	2.03	0.40
13:N:114:DG:C5	13:N:115:DT:C4	3.10	0.40
13:N:202:DC:H2''	13:N:203:DG:C8	2.55	0.40
15:T:242:DA:H1'	15:T:243:DA:C8	2.55	0.40
1:A:343:GLY:HA2	2:B:1135:ARG:NH2	2.21	0.40
1:A:466:TYR:CD2	2:B:976:ILE:HD12	2.56	0.40
2:B:323:LEU:HA	2:B:326:ILE:HG12	2.03	0.40
2:B:725:ARG:NH1	2:B:1047:PHE:HA	2.37	0.40
2:B:744:HIS:O	2:B:747:MET:HG3	2.21	0.40
2:B:851:PHE:CZ	2:B:980:PHE:HZ	2.39	0.40
2:B:1071:VAL:HG22	2:B:1084:GLN:HG3	2.03	0.40
13:N:90:DA:N6	15:T:189:DG:O6	2.54	0.40
13:N:166:DG:H1'	13:N:167:DT:H5'	2.03	0.40
13:N:175:DA:C2	13:N:176:DG:C6	3.09	0.40
18:g:64:GLU:HA	19:h:49:HIS:CE1	2.56	0.40
16:k:102:GLY:HA2	16:k:105:GLU:OE2	2.20	0.40
17:l:35:ARG:NH1	17:l:46:ILE:HD12	2.37	0.40
16:m:47:ALA:HA	16:m:50:GLU:CD	2.45	0.40
1:A:135:PHE:HE1	1:A:223:LEU:HD22	1.86	0.40
1:A:240:LEU:HD12	1:A:241:PRO:HD2	2.04	0.40
1:A:577:GLN:O	1:A:581:ILE:HG12	2.21	0.40
1:A:642:ILE:H	1:A:642:ILE:HD12	1.87	0.40
1:A:664:SER:HB2	2:B:1085:VAL:HG13	2.03	0.40
1:A:690:GLN:O	1:A:694:ILE:HG13	2.21	0.40
2:B:415:ARG:HH11	2:B:419:ARG:HE	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:836:GLU:H	2:B:1013:ASN:ND2	2.19	0.40
2:B:981:ALA:HB1	2:B:987:LYS:HZ2	1.86	0.40
5:E:60:LEU:HD12	5:E:77:LEU:O	2.20	0.40
7:G:126:SER:HA	7:G:127:PRO:HA	1.93	0.40
9:I:40:ASP:OD1	9:I:42:LYS:HG2	2.22	0.40
13:N:143:DG:H2'	13:N:144:DT:H72	2.03	0.40
15:T:10:DA:C2'	15:T:11:DT:H71	2.52	0.40
15:T:25:DG:C2	15:T:26:DC:C2	3.09	0.40
18:o:31:HIS:CD2	18:o:35:ARG:HE	2.39	0.40
1:A:1065:MET:O	1:A:1069:ILE:HG23	2.21	0.40
2:B:101:PRO:HG3	2:B:111:TYR:CE1	2.56	0.40
2:B:194:PHE:HZ	2:B:406:LEU:HD11	1.86	0.40
2:B:235:LEU:HD23	2:B:235:LEU:HA	1.96	0.40
2:B:355:PRO:HA	2:B:359:GLN:OE1	2.20	0.40
10:J:7:CYS:HB3	10:J:11:GLY:N	2.23	0.40
13:N:93:DC:H2''	13:N:94:DA:H8	1.86	0.40
13:N:117:DT:H6	13:N:117:DT:H2'	1.77	0.40
13:N:153:DT:C2	15:T:128:DG:N2	2.89	0.40
13:N:254:DG:N2	15:T:27:DC:O2	2.54	0.40
18:c:93:LEU:HD23	18:c:93:LEU:HA	1.94	0.40
16:e:70:LEU:HA	17:f:25:ASN:HB3	2.04	0.40
16:k:69:ARG:HH21	16:k:72:ARG:NE	2.15	0.40
1:A:837:TYR:CZ	1:A:841:ARG:HD3	2.57	0.40
1:A:1070:ALA:CB	1:A:1370:HIS:HB3	2.52	0.40
2:B:33:GLN:HG3	2:B:537:GLY:HA2	2.04	0.40
2:B:269:LYS:NZ	2:B:329:ARG:HA	2.36	0.40
2:B:574:PHE:O	2:B:618:LYS:HA	2.22	0.40
9:I:25:LEU:H	9:I:25:LEU:HD23	1.86	0.40
13:N:175:DA:C6	15:T:106:DG:N1	2.90	0.40
13:N:196:DC:H2''	13:N:197:DA:C8	2.57	0.40
15:T:152:DC:C5'	16:m:83:ARG:HB2	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1396/1743 (80%)	1324 (95%)	70 (5%)	2 (0%)	48	83
2	B	1151/1227 (94%)	1089 (95%)	61 (5%)	1 (0%)	48	83
3	C	261/304 (86%)	244 (94%)	17 (6%)	0	100	100
4	D	148/186 (80%)	143 (97%)	5 (3%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	59
8	H	129/145 (89%)	123 (95%)	6 (5%)	0	100	100
9	I	109/115 (95%)	101 (93%)	8 (7%)	0	100	100
10	J	64/72 (89%)	63 (98%)	1 (2%)	0	100	100
11	K	111/118 (94%)	103 (93%)	8 (7%)	0	100	100
12	L	43/72 (60%)	39 (91%)	4 (9%)	0	100	100
16	a	93/139 (67%)	93 (100%)	0	0	100	100
16	e	93/139 (67%)	90 (97%)	3 (3%)	0	100	100
16	k	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
16	m	93/139 (67%)	92 (99%)	1 (1%)	0	100	100
17	b	76/106 (72%)	76 (100%)	0	0	100	100
17	f	76/106 (72%)	76 (100%)	0	0	100	100
17	l	69/106 (65%)	68 (99%)	1 (1%)	0	100	100
17	n	76/106 (72%)	75 (99%)	1 (1%)	0	100	100
18	c	96/133 (72%)	95 (99%)	1 (1%)	0	100	100
18	g	96/133 (72%)	95 (99%)	1 (1%)	0	100	100
18	o	95/133 (71%)	95 (100%)	0	0	100	100
19	d	88/129 (68%)	87 (99%)	1 (1%)	0	100	100
19	h	87/129 (67%)	86 (99%)	1 (1%)	0	100	100
19	p	85/129 (66%)	84 (99%)	1 (1%)	0	100	100
All	All	5068/6288 (81%)	4857 (96%)	207 (4%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	154	VAL
1	A	467	SER
1	A	960	VAL
2	B	222	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1528 (80%)	1219 (100%)	4 (0%)	86	86
2	B	1016/1077 (94%)	1016 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	133/160 (83%)	133 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
16	a	81/112 (72%)	81 (100%)	0	100	100
16	e	81/112 (72%)	81 (100%)	0	100	100
16	k	61/112 (54%)	61 (100%)	0	100	100
16	m	81/112 (72%)	81 (100%)	0	100	100
17	b	63/81 (78%)	63 (100%)	0	100	100
17	f	63/81 (78%)	63 (100%)	0	100	100
17	l	59/81 (73%)	59 (100%)	0	100	100
17	n	63/81 (78%)	63 (100%)	0	100	100
18	c	77/102 (76%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	g	77/102 (76%)	76 (99%)	1 (1%)	61	74
18	o	77/102 (76%)	77 (100%)	0	100	100
19	d	76/107 (71%)	76 (100%)	0	100	100
19	h	75/107 (70%)	75 (100%)	0	100	100
19	p	74/107 (69%)	74 (100%)	0	100	100
All	All	4463/5380 (83%)	4458 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	399	GLU
1	A	448	GLN
1	A	468	THR
18	g	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	265	HIS
1	A	287	GLN
1	A	317	GLN
1	A	400	HIS
1	A	446	ASN
1	A	491	HIS
1	A	516	GLN
1	A	563	GLN
1	A	577	GLN
1	A	737	ASN
1	A	743	ASN
1	A	1261	GLN
2	B	97	HIS
2	B	157	HIS
2	B	215	GLN
2	B	506	GLN
2	B	656	GLN
2	B	996	HIS
2	B	1104	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	1141	HIS
2	B	1195	HIS
3	C	184	ASN
5	E	152	HIS
6	F	127	GLN
7	G	125	ASN
8	H	136	GLN
9	I	31	ASN
9	I	46	HIS
9	I	90	GLN
10	J	63	ASN
18	c	24	GLN
16	e	39	HIS
16	e	125	GLN
17	f	27	GLN
16	m	39	HIS
16	m	68	GLN
16	m	76	GLN
16	m	113	HIS
19	p	49	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/11 (90%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	1	G
14	P	3	G
14	P	5	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

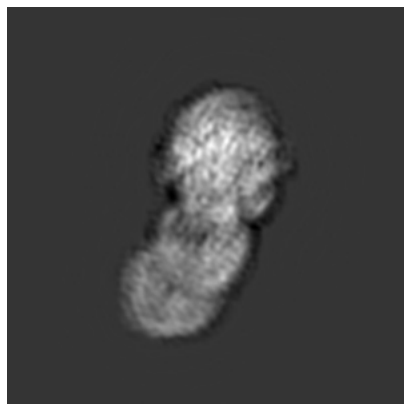
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64642. These allow visual inspection of the internal detail of the map and identification of artifacts.

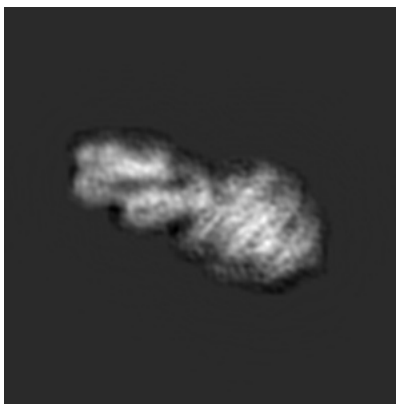
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

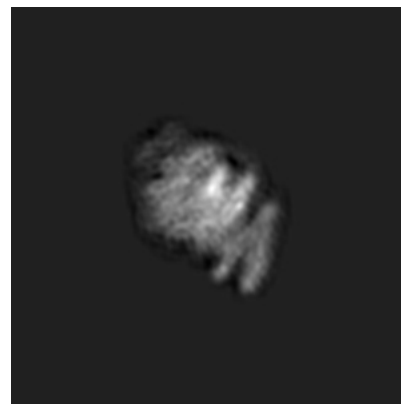
#### 6.1.1 Primary map



X

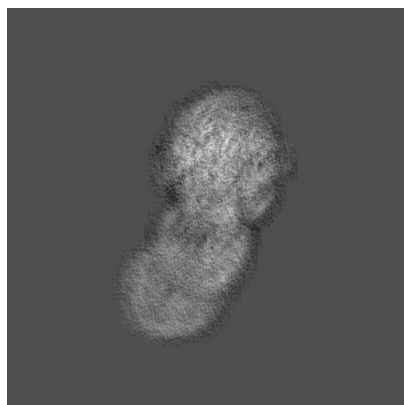


Y

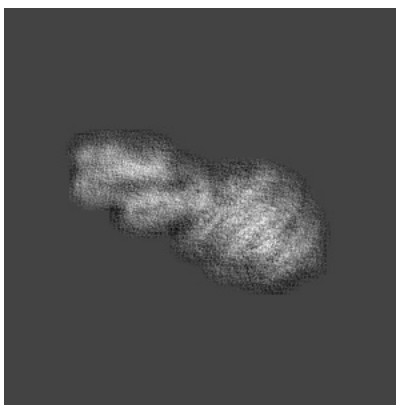


Z

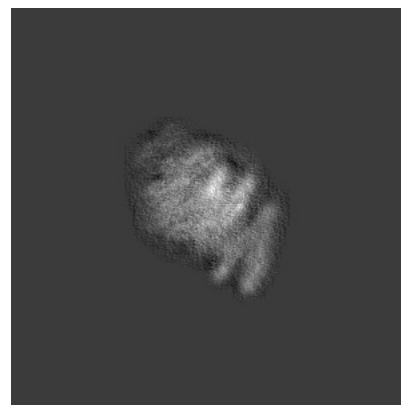
#### 6.1.2 Raw map



X



Y

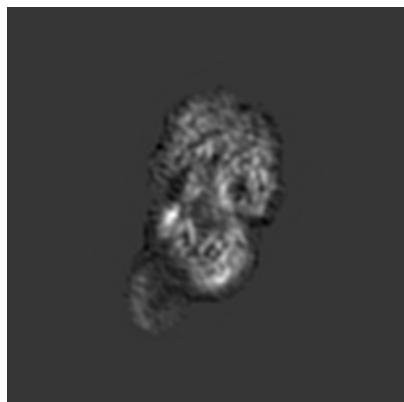


Z

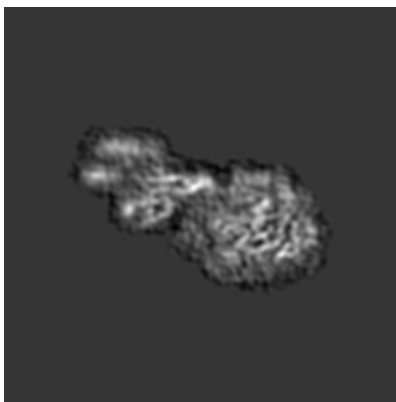
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

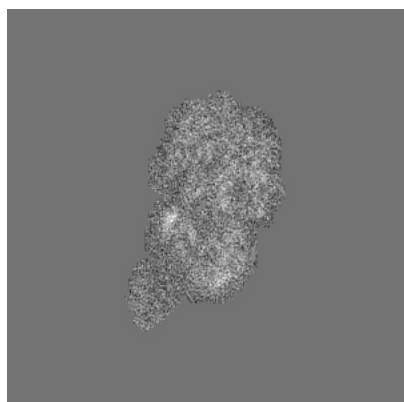


Y Index: 200

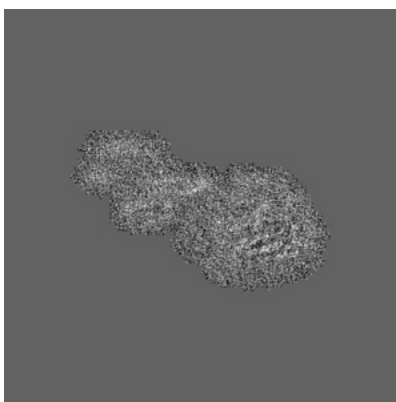


Z Index: 200

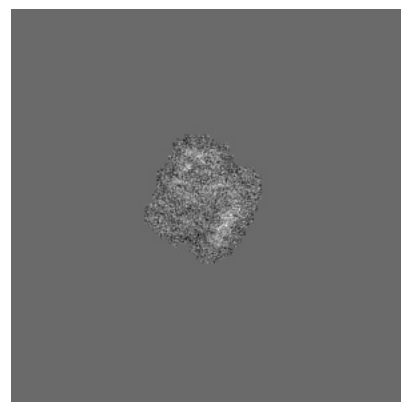
### 6.2.2 Raw map



X Index: 200



Y Index: 200

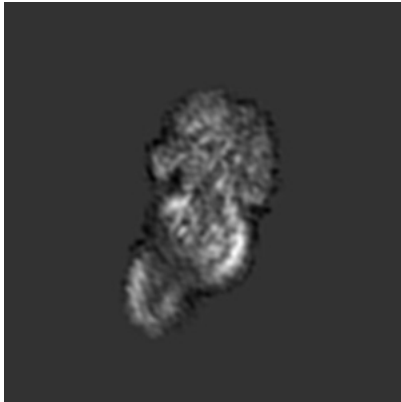


Z Index: 200

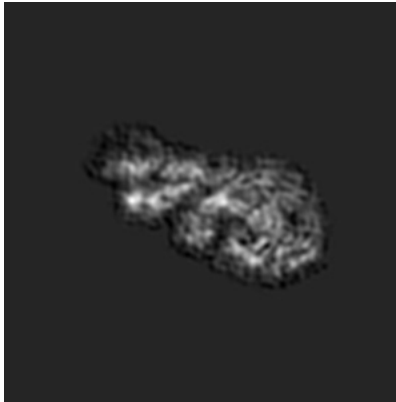
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

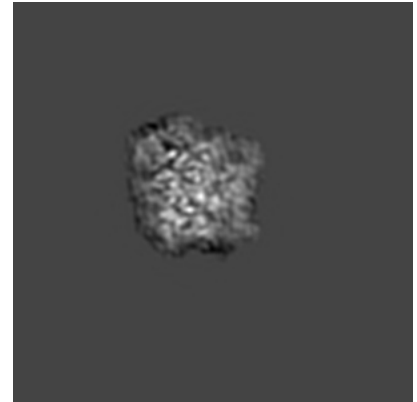
### 6.3.1 Primary map



X Index: 207

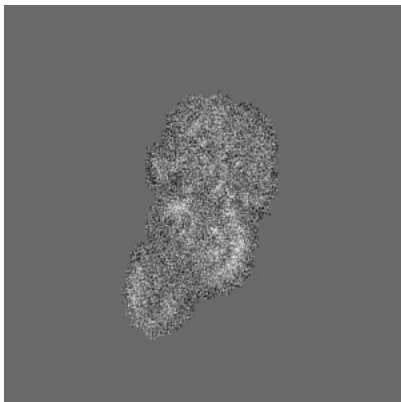


Y Index: 216

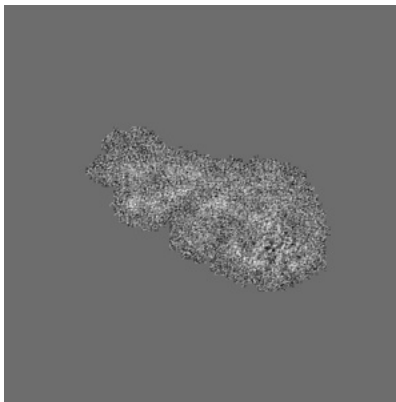


Z Index: 259

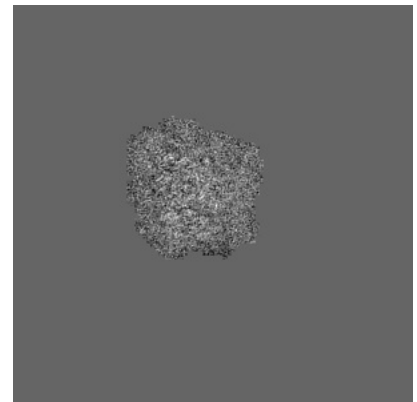
### 6.3.2 Raw map



X Index: 207



Y Index: 216

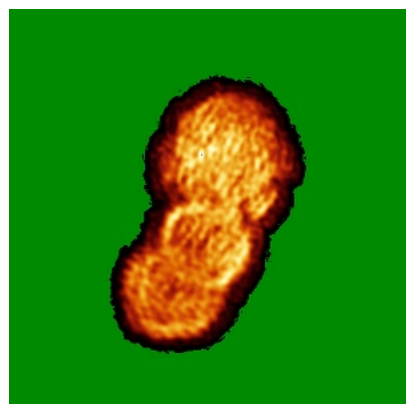


Z Index: 261

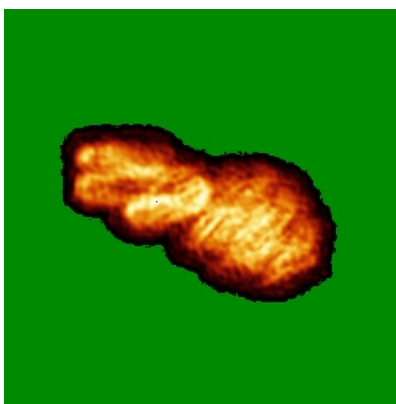
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

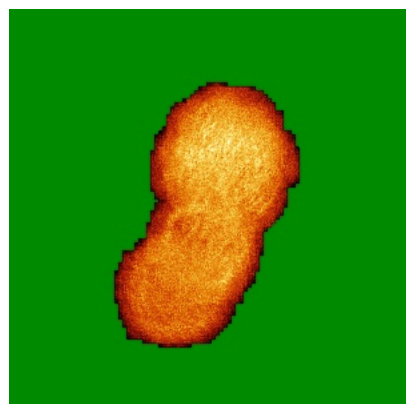


Y

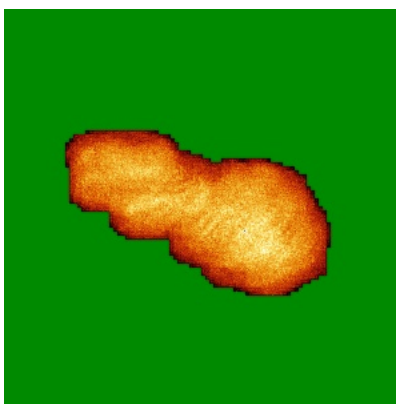


Z

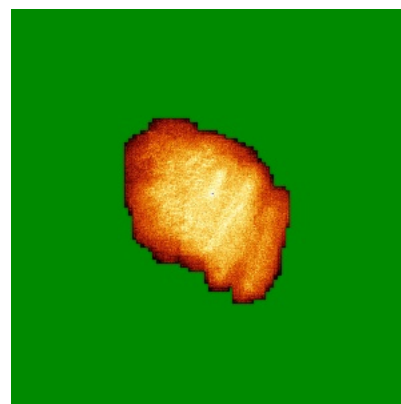
### 6.4.2 Raw map



X



Y

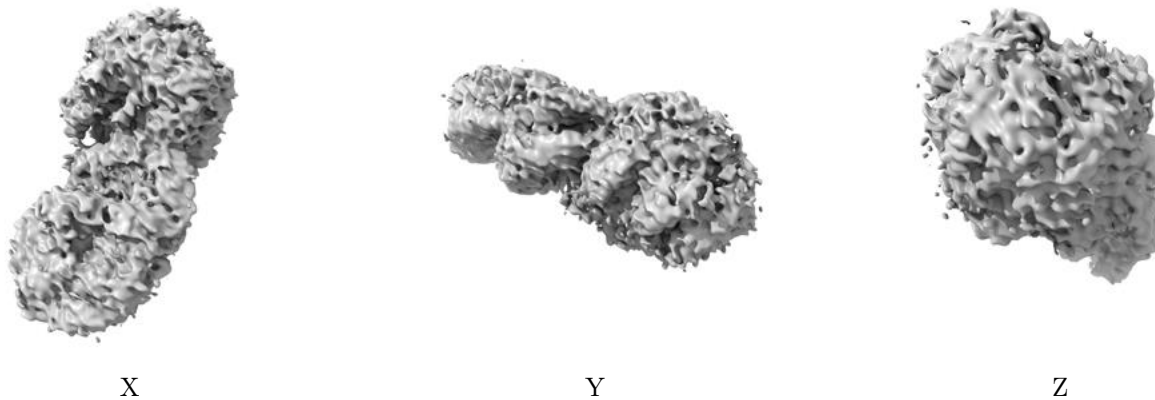


Z

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.

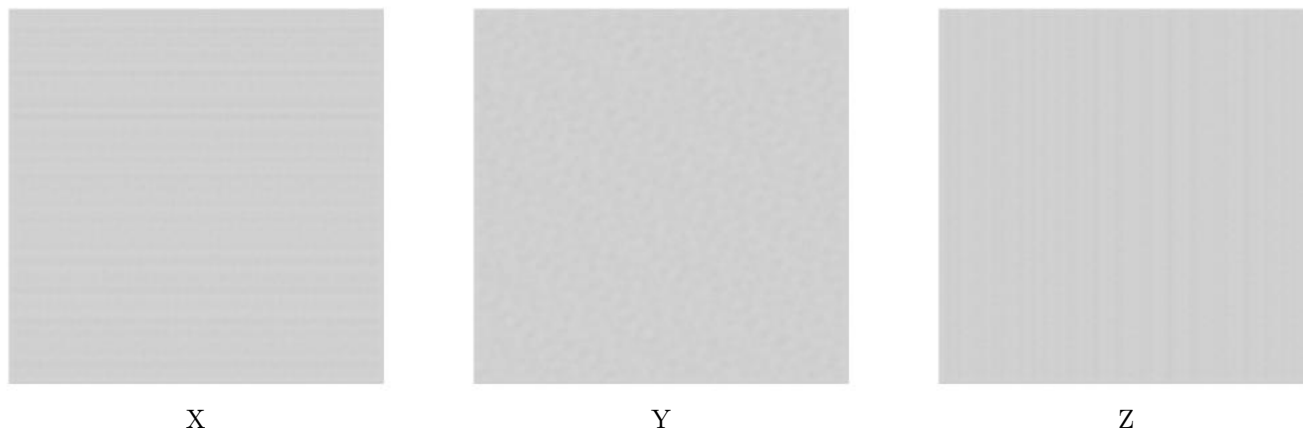
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.000666. 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



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

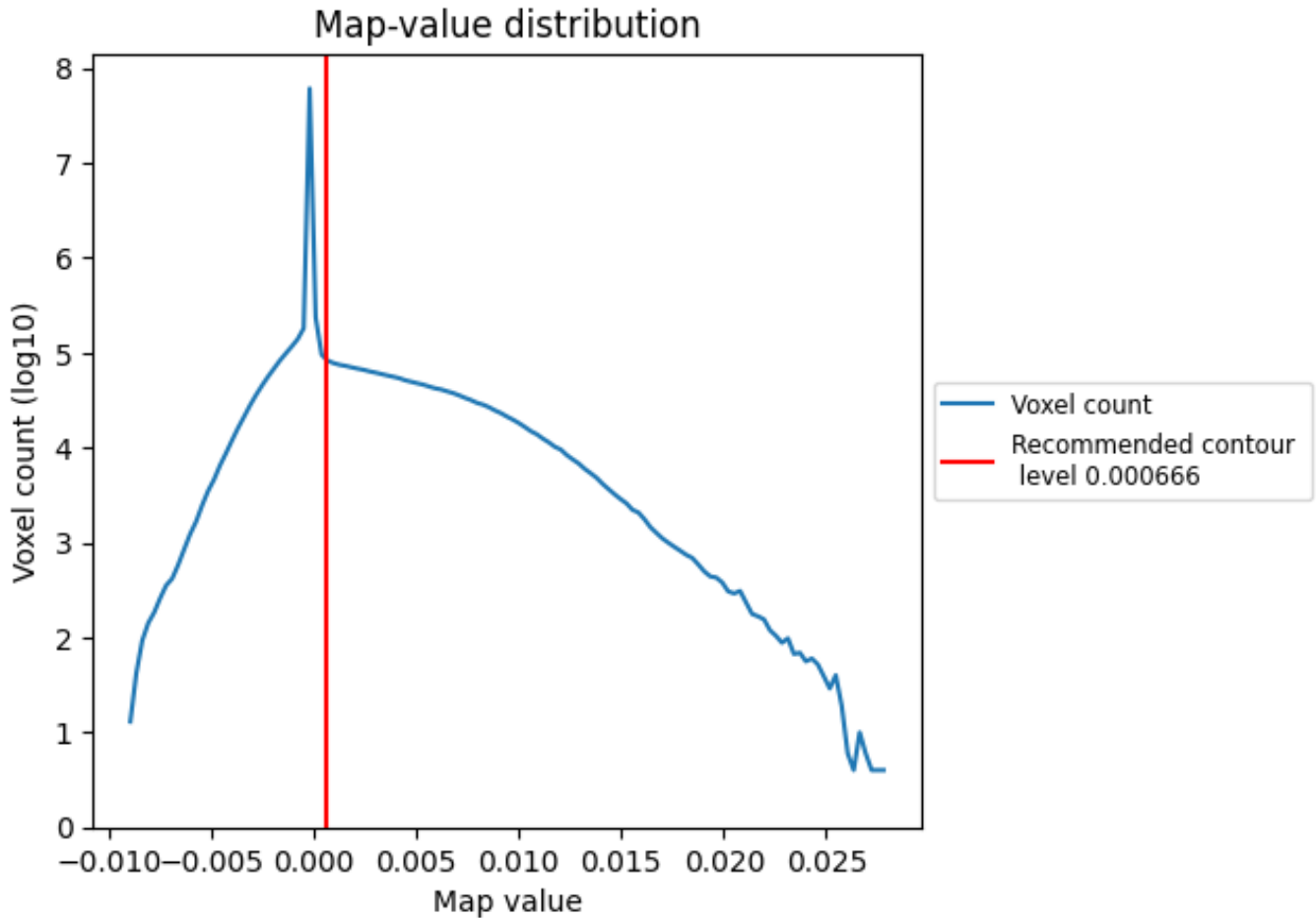
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

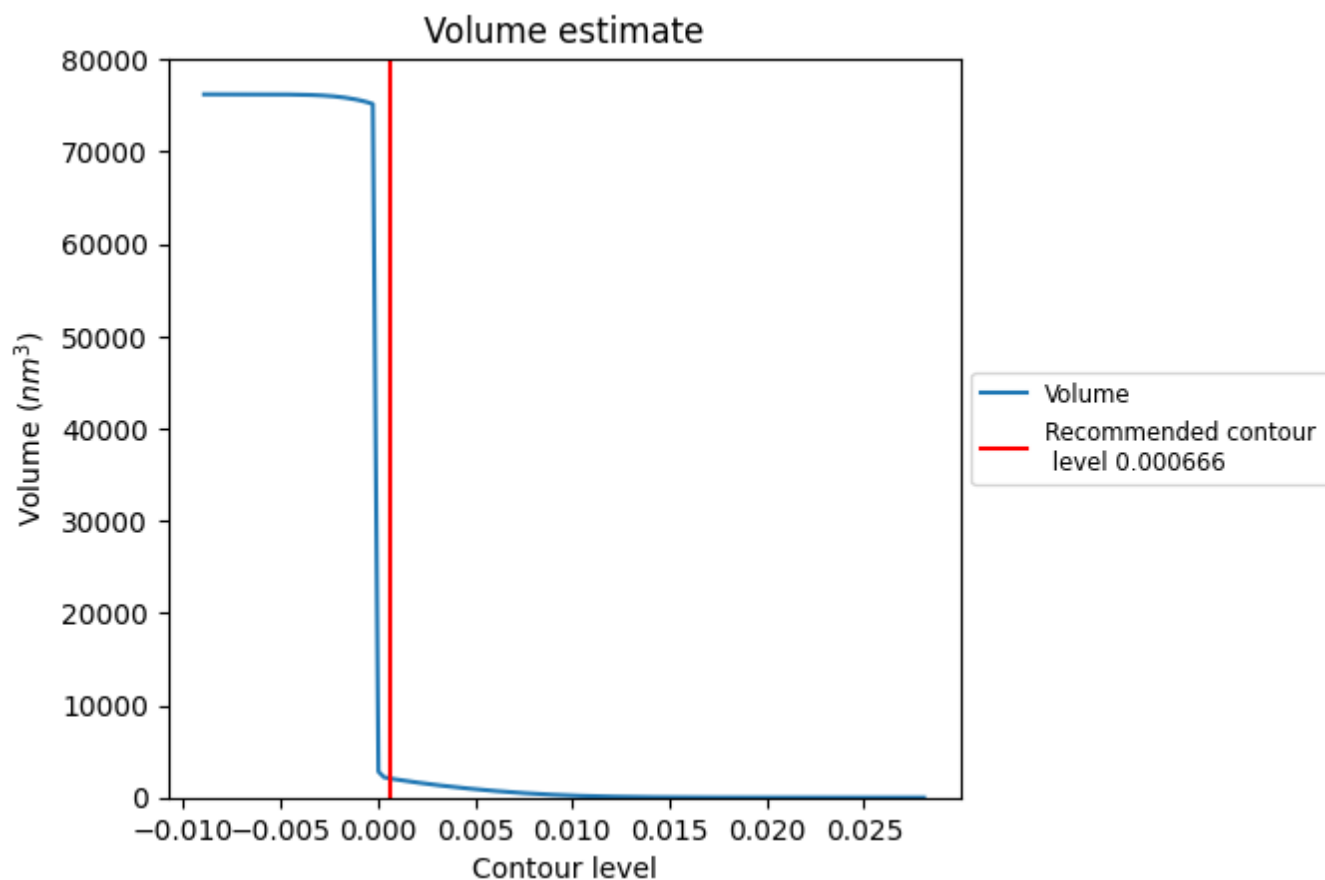
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

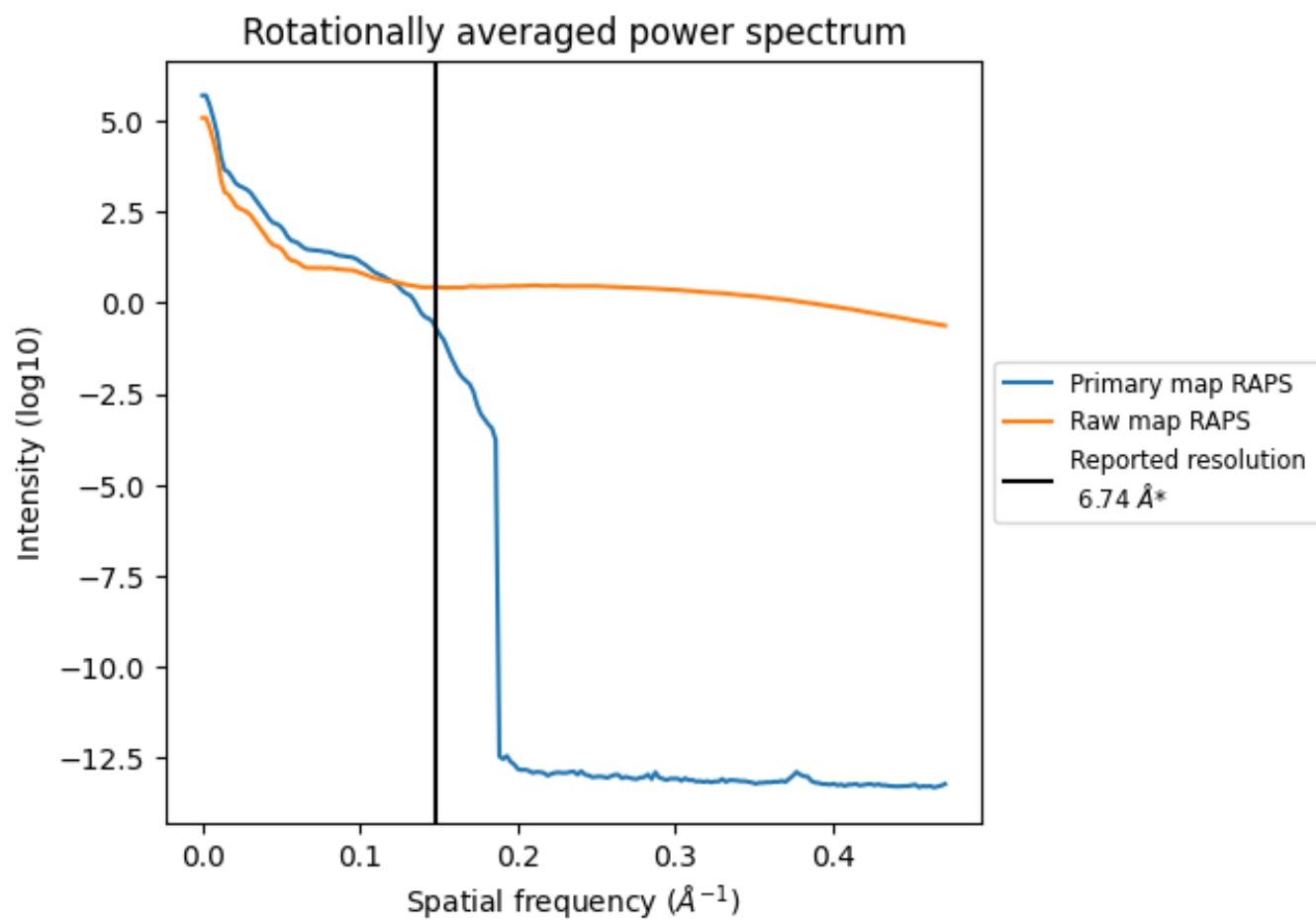
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2056  $\text{nm}^3$ ; this corresponds to an approximate mass of 1858 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](#)

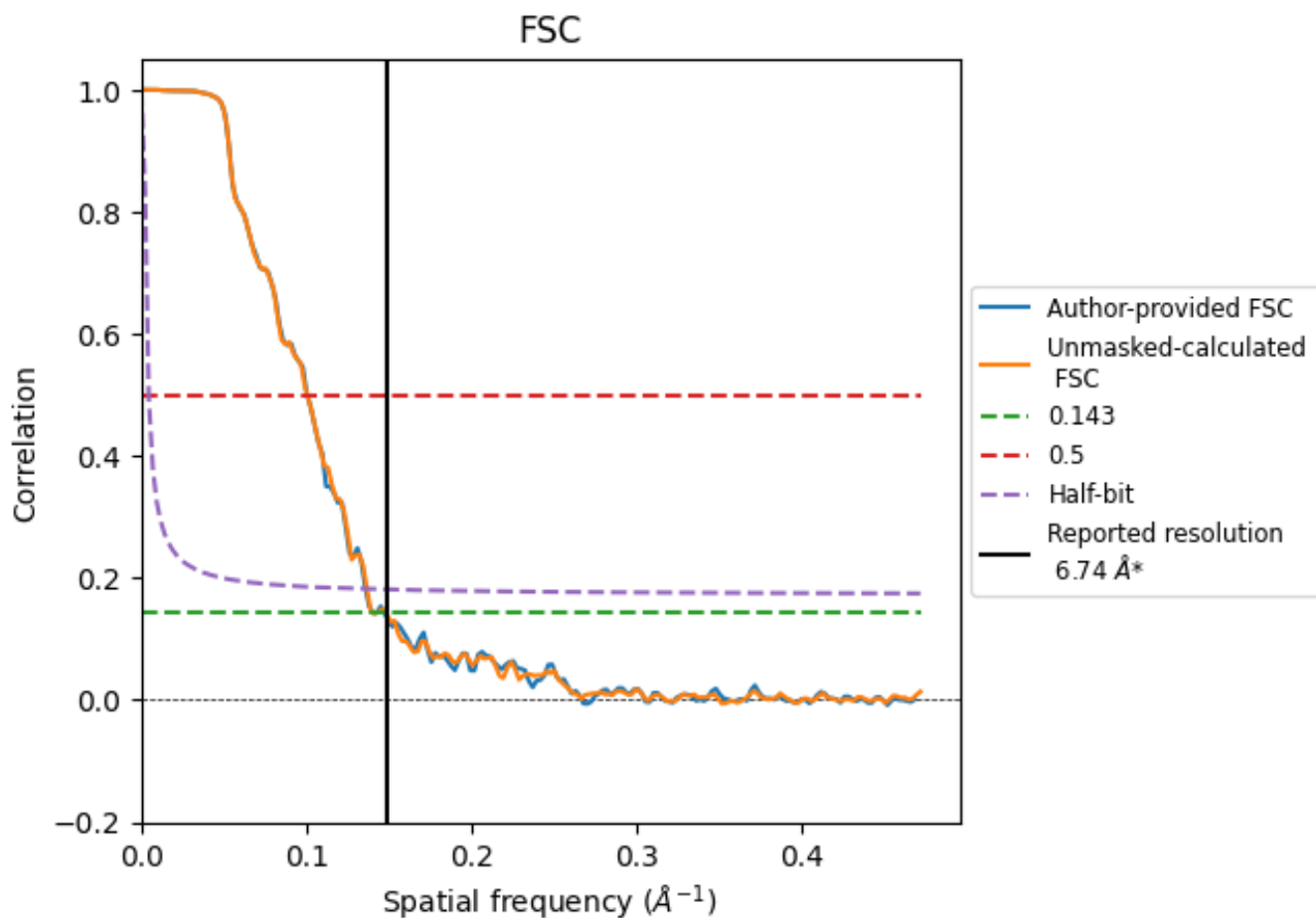


\*Reported resolution corresponds to spatial frequency of 0.148 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.148 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

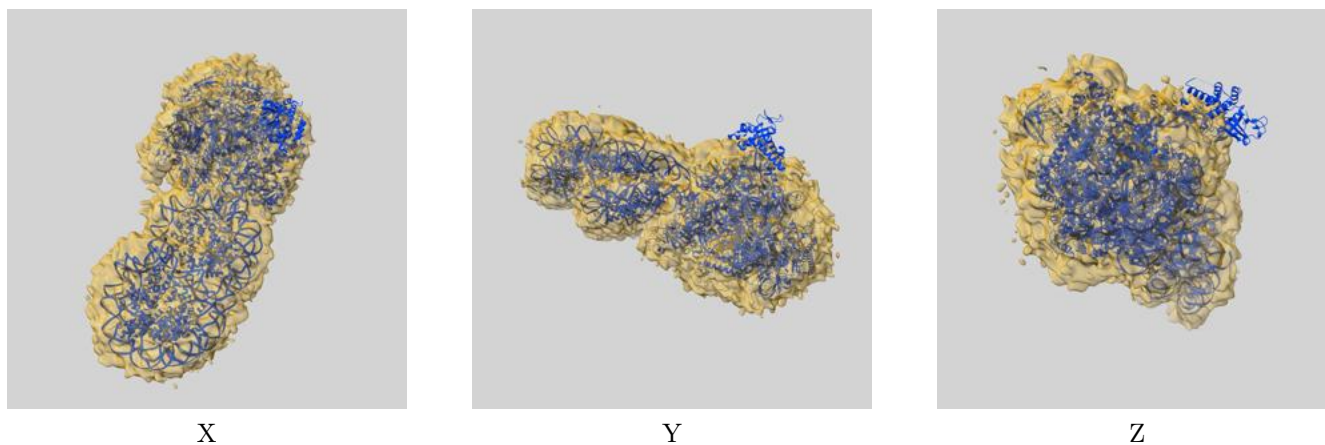
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.74	-	-
Author-provided FSC curve	7.13	9.95	7.36
Unmasked-calculated*	7.15	9.94	7.32

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

## 9 Map-model fit [i](#)

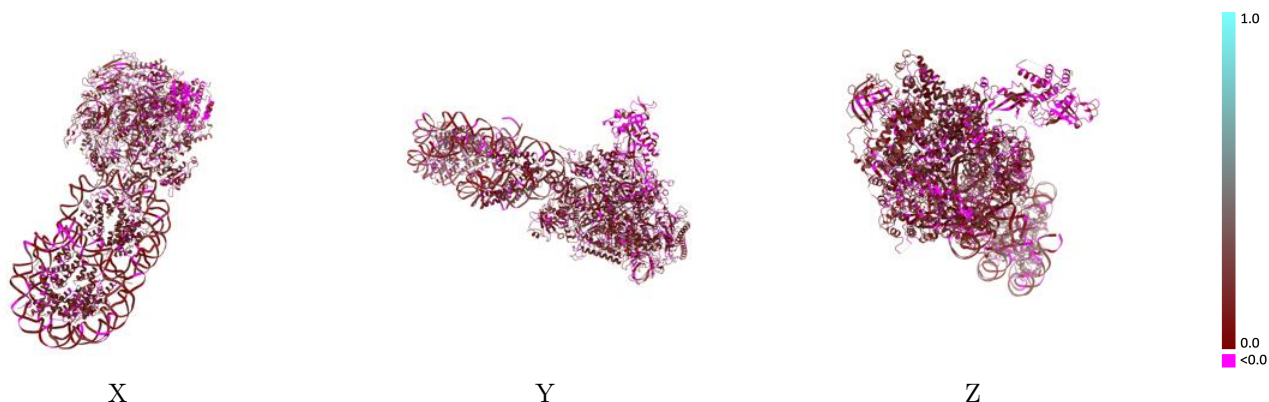
This section contains information regarding the fit between EMDB map EMD-64642 and PDB model 9UZ9. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



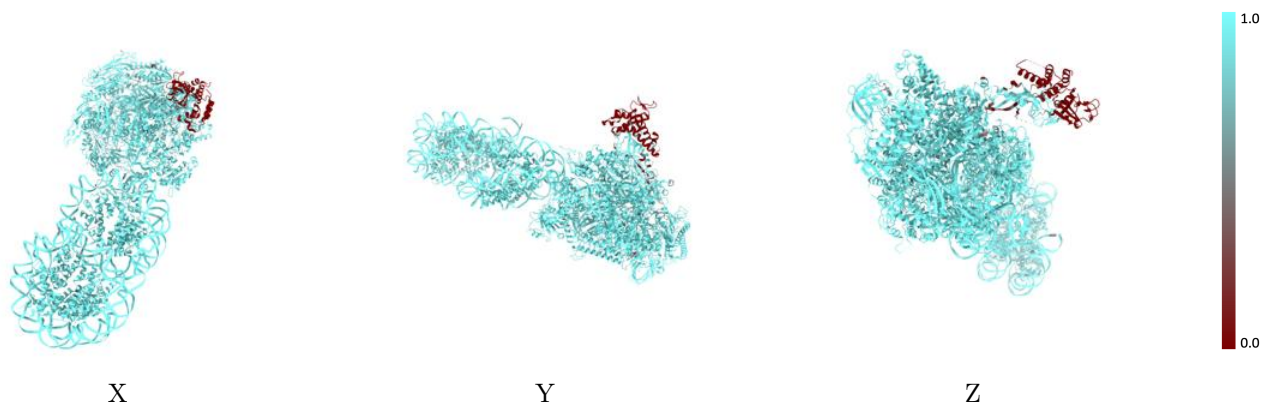
The images above show the 3D surface view of the map at the recommended contour level 0.000666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



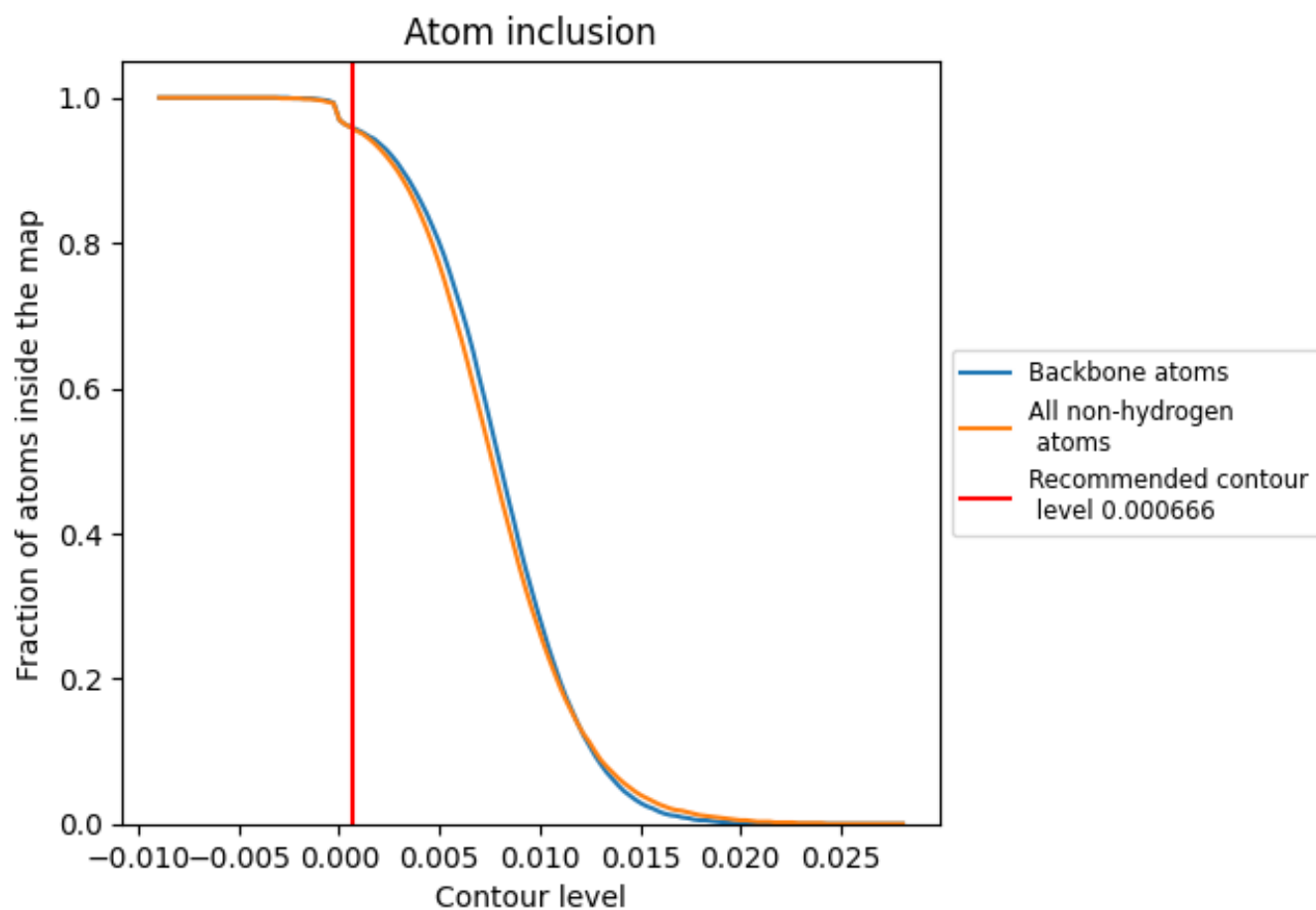
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.000666).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.000666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.1180
A	 0.9850	 0.1310
B	 0.9920	 0.1230
C	 0.9880	 0.1290
D	 0.2450	 0.0070
E	 0.9940	 0.1480
F	 0.9530	 0.1180
G	 0.5160	 0.0210
H	 0.9470	 0.1300
I	 0.9300	 0.0700
J	 0.9910	 0.1160
K	 0.9610	 0.1060
L	 0.9940	 0.1080
N	 0.9910	 0.1140
P	 1.0000	 0.1670
T	 0.9880	 0.1140
a	 1.0000	 0.1150
b	 0.9970	 0.1260
c	 0.9890	 0.1280
d	 0.9900	 0.1320
e	 1.0000	 0.1360
f	 1.0000	 0.0770
g	 0.9740	 0.1120
h	 1.0000	 0.1300
k	 1.0000	 0.1330
l	 0.9980	 0.1480
m	 0.9990	 0.1320
n	 1.0000	 0.1190
o	 0.9960	 0.1380
p	 0.9990	 0.1480

