



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:06 PM UTC

PDB ID : 9J0O / pdb_00009j0o
EMDB ID : EMD-61059
Title : Arrested elongation complex of mammalian RNA polymerase II with nucleosome (AEC1-nuc)
Authors : Naganuma, M.; Kujirai, T.; Ehara, H.; Uejima, T.; Ito, T.; Goto, M.; Aoki, M.; Henmi, M.; Miyamoto-Kohno, S.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2024-08-02
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

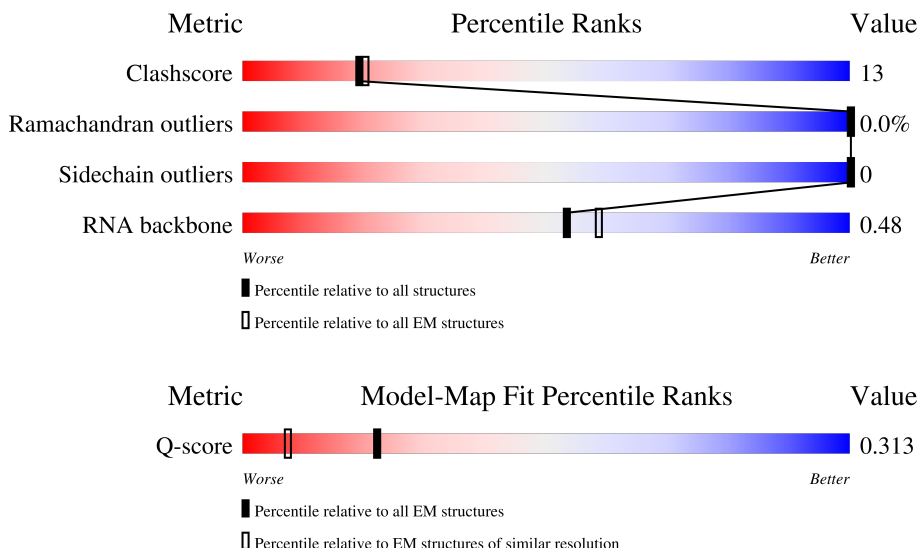
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1970	
2	B	1174	
3	C	271	

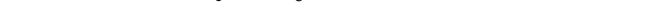
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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	Y	118	
14	Z	1107	
15	N	198	
16	P	16	
17	T	198	
18	a	136	
18	e	136	
19	b	103	
19	f	103	
20	c	130	
20	g	130	
21	d	126	
21	h	126	
22	U	528	
23	W	611	
24	V	580	

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Mol	Chain	Length	Quality of chain
25	X	404	 7% 91%

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59777 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
1	A	1395	Total	C	N	O	S	0	0
			11050	6952	1982	2047	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1121	Total	C	N	O	S	0	0
			8971	5679	1575	1653	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 13 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	SER	-	expression tag	UNP P63272

- Molecule 14 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	480	Total	C	N	O	S	0	0
			3837	2439	676	705	17		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1088	LYS	-	expression tag	UNP O00267
Z	1089	GLU	-	expression tag	UNP O00267
Z	1090	THR	-	expression tag	UNP O00267
Z	1091	ALA	-	expression tag	UNP O00267
Z	1092	ALA	-	expression tag	UNP O00267
Z	1093	ALA	-	expression tag	UNP O00267
Z	1094	LYS	-	expression tag	UNP O00267
Z	1095	PHE	-	expression tag	UNP O00267
Z	1096	GLU	-	expression tag	UNP O00267
Z	1097	ARG	-	expression tag	UNP O00267
Z	1098	GLN	-	expression tag	UNP O00267
Z	1099	HIS	-	expression tag	UNP O00267
Z	1100	MET	-	expression tag	UNP O00267
Z	1101	ASP	-	expression tag	UNP O00267
Z	1102	SER	-	expression tag	UNP O00267
Z	1103	SER	-	expression tag	UNP O00267
Z	1104	THR	-	expression tag	UNP O00267
Z	1105	SER	-	expression tag	UNP O00267
Z	1106	ALA	-	expression tag	UNP O00267
Z	1107	ALA	-	expression tag	UNP O00267

- Molecule 15 is a DNA chain called NON-TEMPLATE DNA (180-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	180	Total	C	N	O	P	0	0
			3706	1762	647	1117	180		

- Molecule 16 is a RNA chain called RNA (5'-R(P*AP*AP*UP*UP*AP*GP*CP*UP*CP*UP*UP*GP*UP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	16	Total	C	N	O	P	0	0
			335	150	52	117	16		

- Molecule 17 is a DNA chain called TEMPLATE DNA (191-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	191	Total	C	N	O	P	0	0
			3899	1848	756	1105	190		

- Molecule 18 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
18	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 20 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	c	103	Total	C	N	O	0	0
			796	502	155	139		
20	g	105	Total	C	N	O	0	0
			810	511	158	141		

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 22 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	183	Total	C	N	O	S	0	0
			1410	895	239	269	7		

- Molecule 23 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	543	Total	C	N	O	S	0	0
			4308	2753	721	810	24		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	591	GLY	-	expression tag	UNP Q8IXH7
W	592	SER	-	expression tag	UNP Q8IXH7
W	593	SER	-	expression tag	UNP Q8IXH7
W	594	GLY	-	expression tag	UNP Q8IXH7
W	595	SER	-	expression tag	UNP Q8IXH7
W	596	SER	-	expression tag	UNP Q8IXH7
W	597	GLY	-	expression tag	UNP Q8IXH7
W	598	LEU	-	expression tag	UNP Q8IXH7
W	599	GLU	-	expression tag	UNP Q8IXH7
W	600	VAL	-	expression tag	UNP Q8IXH7
W	601	LEU	-	expression tag	UNP Q8IXH7
W	602	PHE	-	expression tag	UNP Q8IXH7
W	603	GLN	-	expression tag	UNP Q8IXH7
W	604	GLY	-	expression tag	UNP Q8IXH7
W	605	PRO	-	expression tag	UNP Q8IXH7
W	606	HIS	-	expression tag	UNP Q8IXH7
W	607	HIS	-	expression tag	UNP Q8IXH7
W	608	HIS	-	expression tag	UNP Q8IXH7
W	609	HIS	-	expression tag	UNP Q8IXH7
W	610	HIS	-	expression tag	UNP Q8IXH7
W	611	HIS	-	expression tag	UNP Q8IXH7

- Molecule 24 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	548	Total	C	N	O	S	0	0
			4396	2818	749	804	25		

- Molecule 25 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	35	Total	C	N	O	S	0	0
			281	185	48	47	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-23	MET	-	initiating methionine	UNP P18615
X	-22	ASP	-	expression tag	UNP P18615
X	-21	TYR	-	expression tag	UNP P18615
X	-20	LYS	-	expression tag	UNP P18615
X	-19	ASP	-	expression tag	UNP P18615
X	-18	ASP	-	expression tag	UNP P18615
X	-17	ASP	-	expression tag	UNP P18615
X	-16	ASP	-	expression tag	UNP P18615
X	-15	LYS	-	expression tag	UNP P18615
X	-14	LEU	-	expression tag	UNP P18615
X	-13	GLU	-	expression tag	UNP P18615
X	-12	VAL	-	expression tag	UNP P18615
X	-11	LEU	-	expression tag	UNP P18615
X	-10	PHE	-	expression tag	UNP P18615
X	-9	GLN	-	expression tag	UNP P18615
X	-8	GLY	-	expression tag	UNP P18615
X	-7	PRO	-	expression tag	UNP P18615
X	-6	GLY	-	expression tag	UNP P18615
X	-5	SER	-	expression tag	UNP P18615
X	-4	SER	-	expression tag	UNP P18615
X	-3	GLY	-	expression tag	UNP P18615
X	-2	SER	-	expression tag	UNP P18615
X	-1	SER	-	expression tag	UNP P18615
X	0	GLY	-	expression tag	UNP P18615

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total 1	Zn 1	0
26	L	1	Total 1	Zn 1	0
26	Y	1	Total 1	Zn 1	0

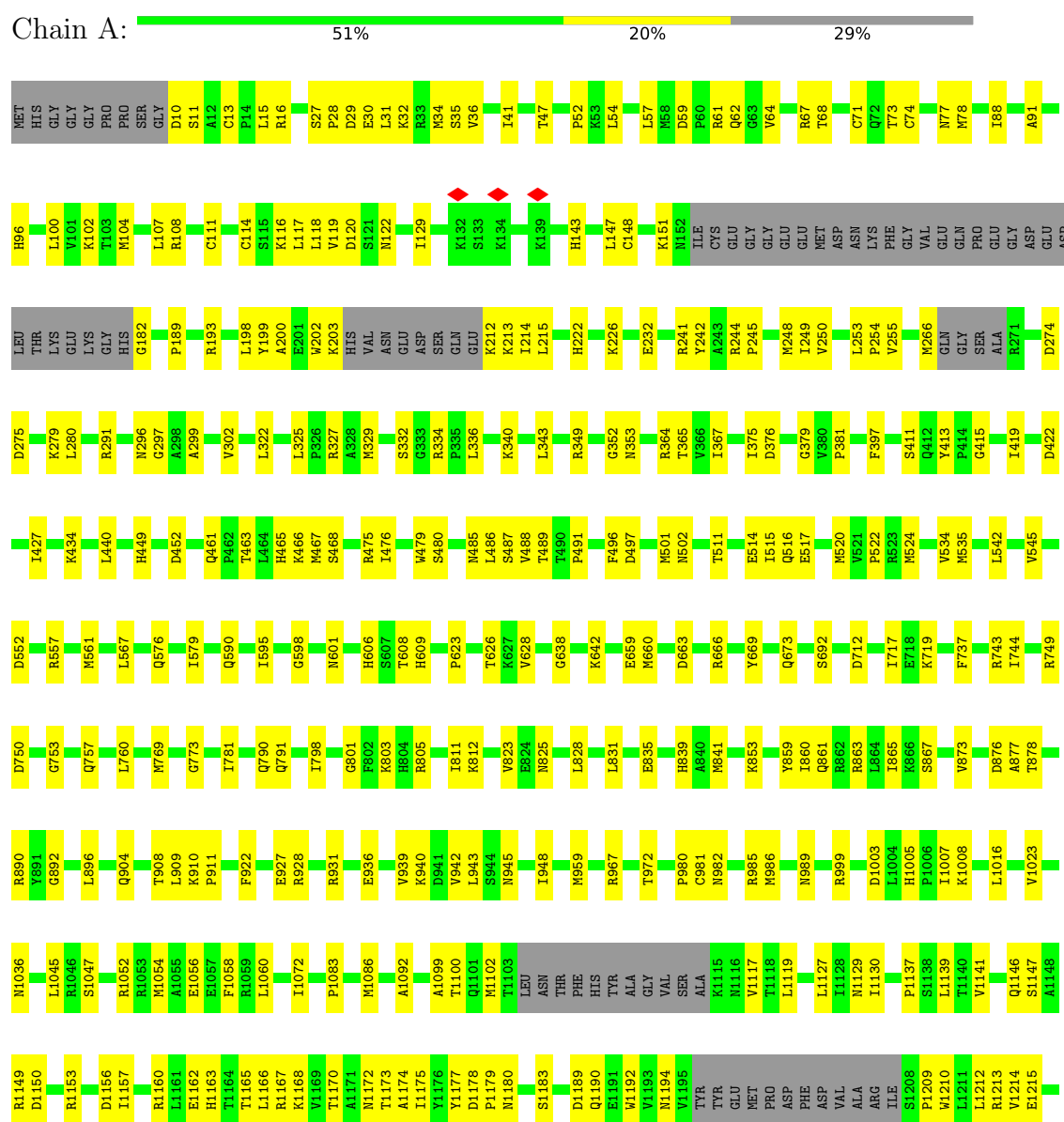
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

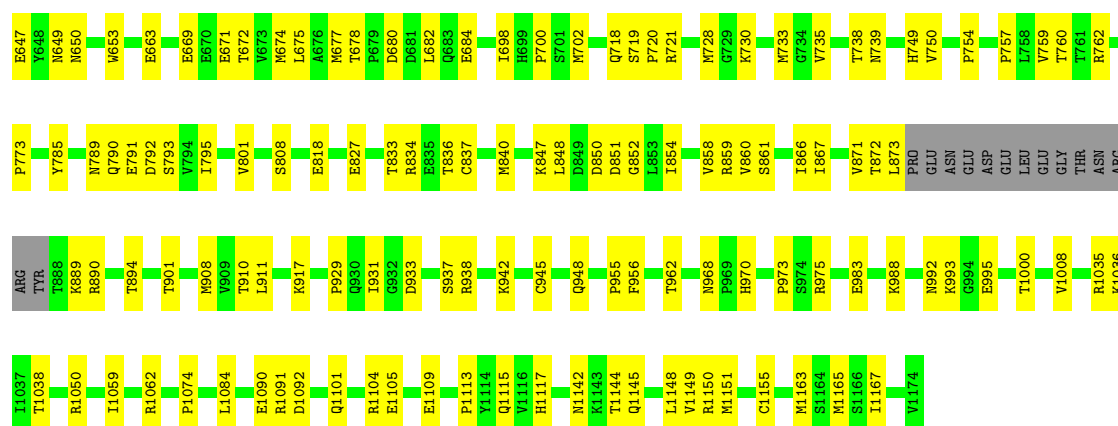
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



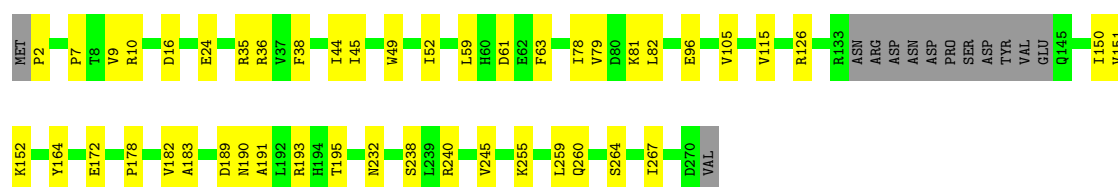
- Molecule 2: DNA-directed RNA polymerase subunit beta

L545	K361	ALA	P96	MET
S549	F364	LYS		TYR
M50		SER	GLU	ASP
	Y388	ALA	ARG	ALA
L553		T252	D102	GLU
A562	D394	R255		ASP
T565	R405	P261	P110	MET
K566	A406		M117	GLN
I567	M407	Q265		ASP
			L124	GLU
G571	L411	D281	Y125	ASP
G575	L412	R282	V126	ASP
I576	K413	T288	D127	ASP
H577		T289	I128	ASP
	I417		T131	E16
P580	Q420	P295		I17
		E296	L140	T18
L583	I423	N297		Y33
N584		N298	Q143	E36
N585	I435	E299	H144	K37
T586	L587	K300	Q145	G38
N588	I440	V301	K146	L39
K589	S441	X302		V40
L590		P303	K151	R41
	L448	V310	I152	Q42
R591		I311	P153	Q43
H592	D455		I154	V55
D595	Q456	V316	L163	
I596	K457			V59
	K458	F320	E176	
M603			C177	I65
R608	N471	S323		D66
E609	R472	K324	G189	L67
R610		G325	S190	GLN
E611	S477		E191	ALA
		T331		GLU
	L482		Q197	ALA
R623		K334		GLN
P624	L501		M200	HIS
L625	H502	K337		GLN
L626	N503	Y338	N203	SER
I627	T504	X339		GLY
V628	L505	K340	D212	GLU
E629		E341		VAL
K630	M508		S223	GLU
	V509	K345		GLU
L633		K346	T235	P81
L634	K524			
L635		L348	L240	L85
R636	M529	F349	A241	L86
K637	P538	H350	R242	K87
			GLY	F88
I640		S354	GLN	
	I541			I91
S646		F357		Y02



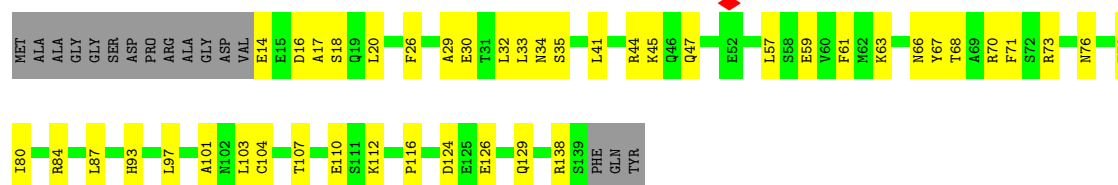
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 78% 17% 5%



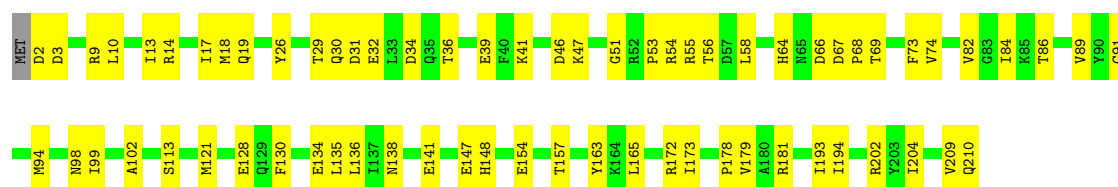
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 58% 31% 11%



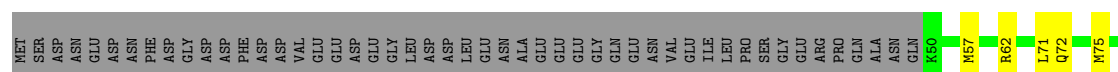
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 67% 32%



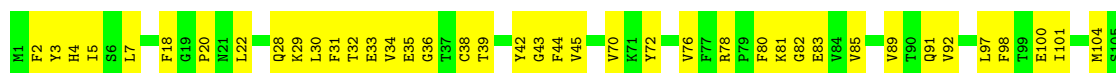
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 50% 11% 39%

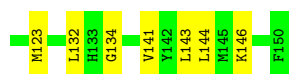




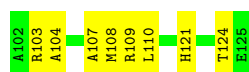
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



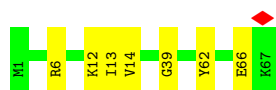
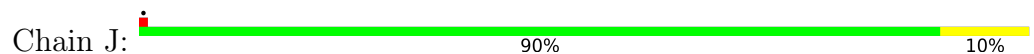
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



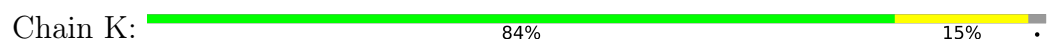
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



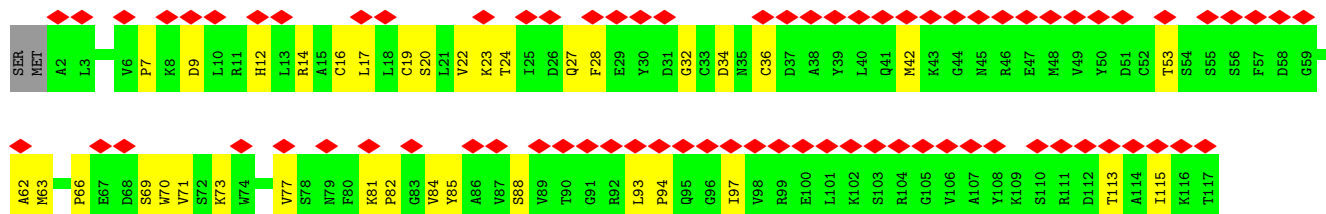
- Molecule 12: RPB12

Chain L: 



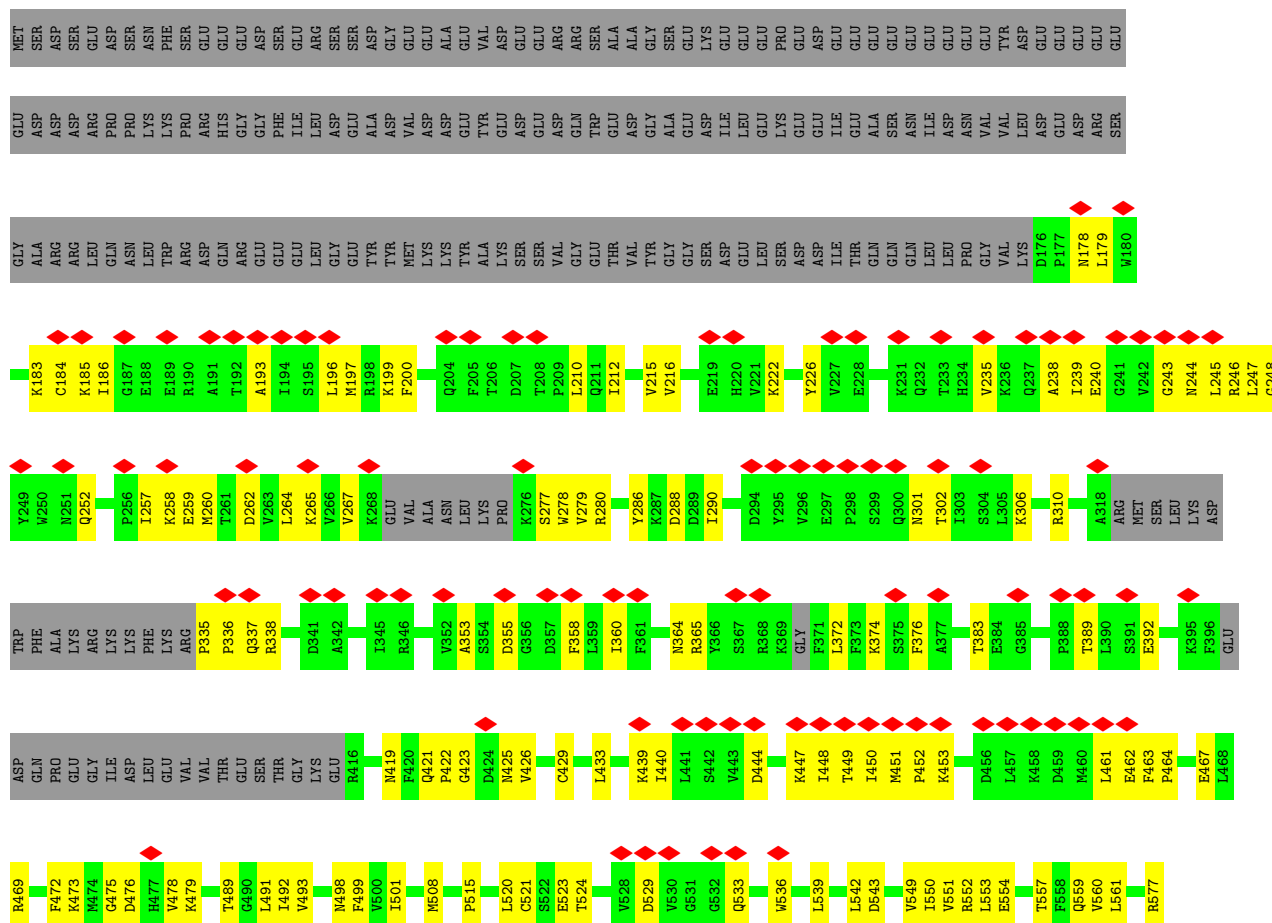
- Molecule 13: Transcription elongation factor SPT4

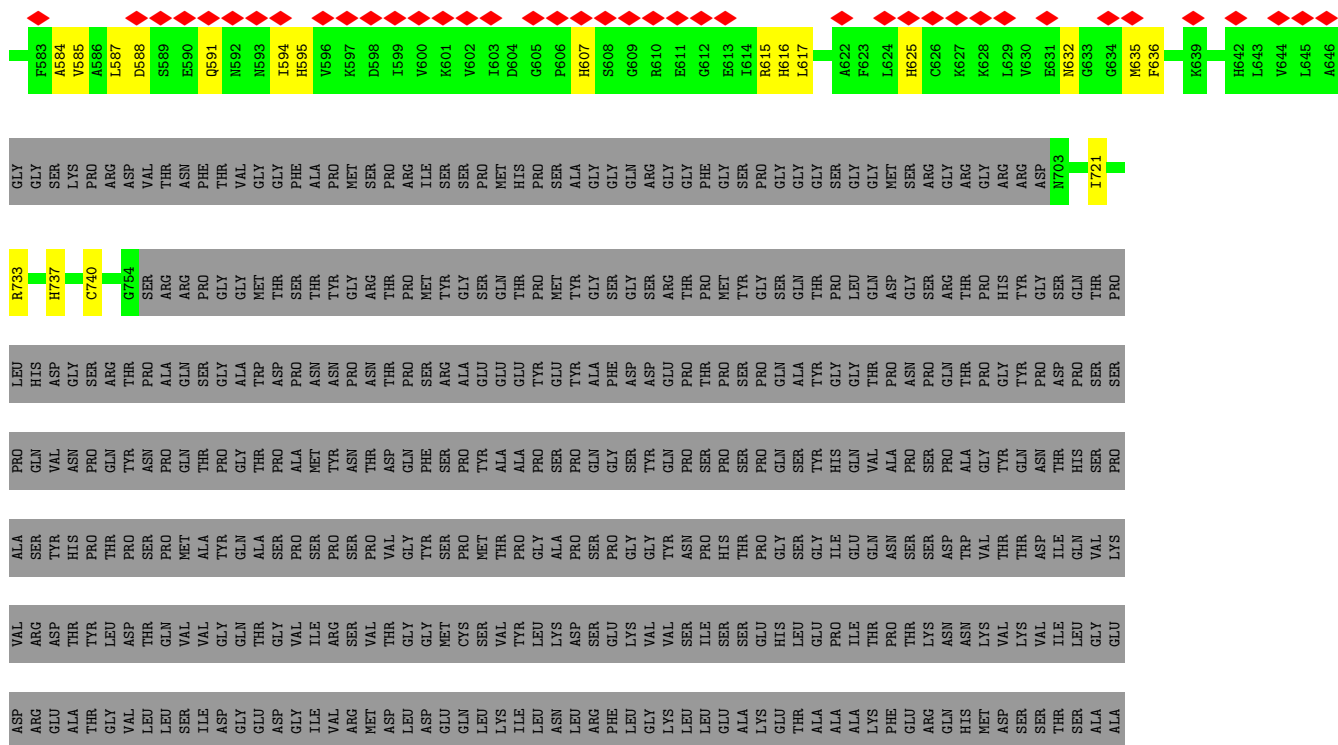
Chain Y: 



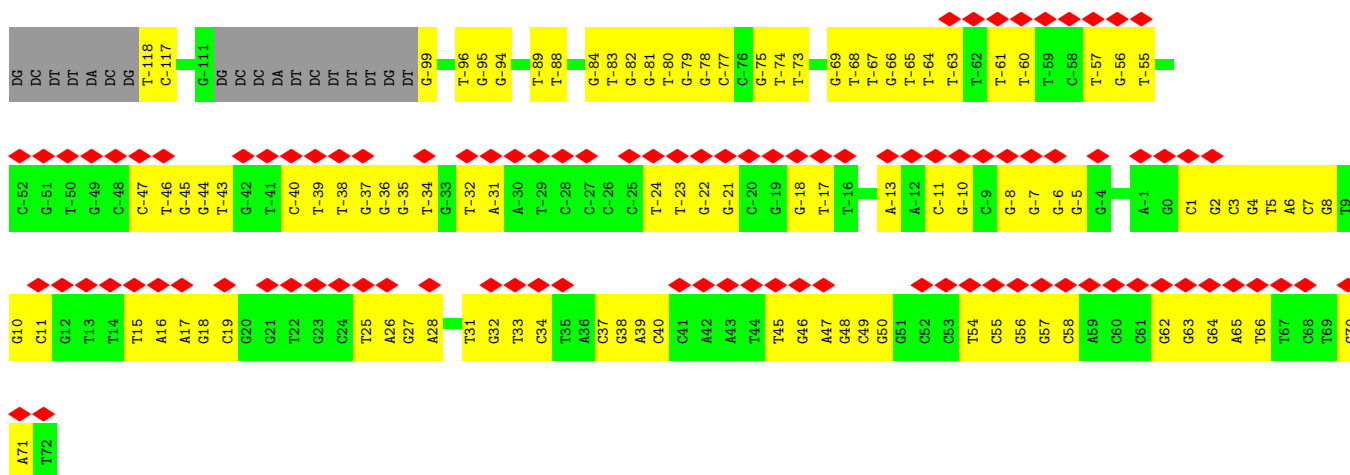
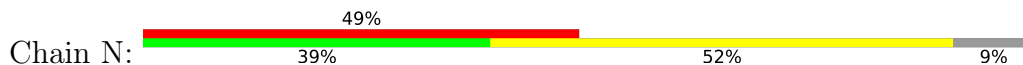
- Molecule 14: Transcription elongation factor SPT5

Chain Z: 

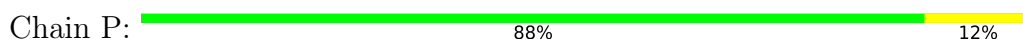




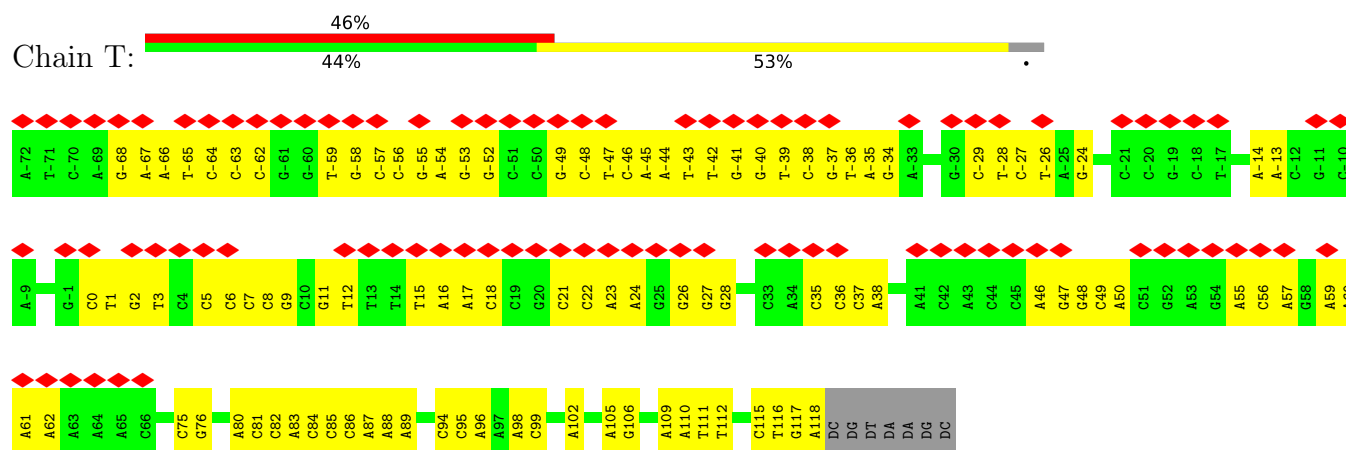
- Molecule 15: NON-TEMPLATE DNA (180-MER)



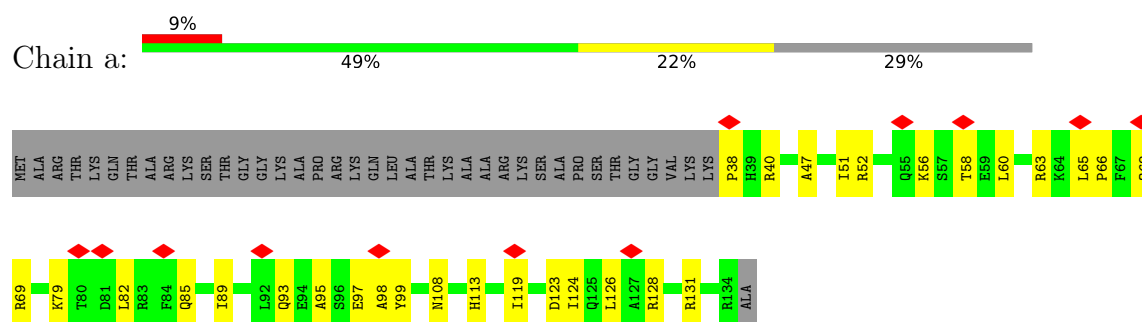
- Molecule 16: RNA (5'-R(P*AP*AP*UP*UP*AP*GP*CP*UP*CP*UP*UP*GP*UP*GP*UP*U)-3')



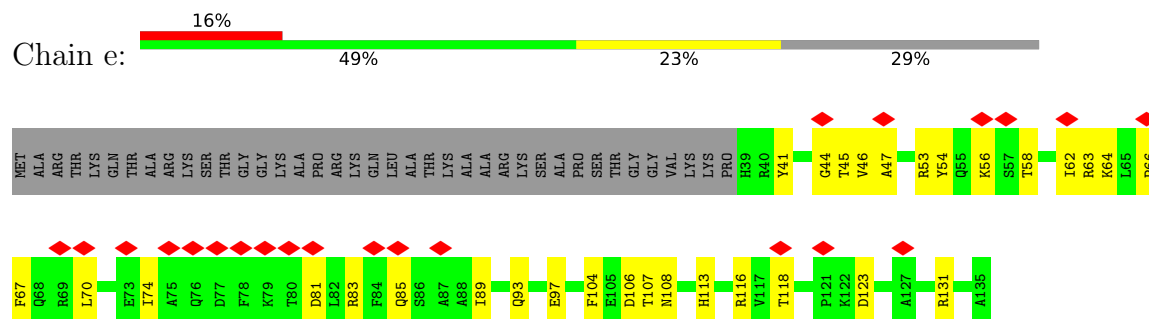
- Molecule 17: TEMPLATE DNA (191-MER)



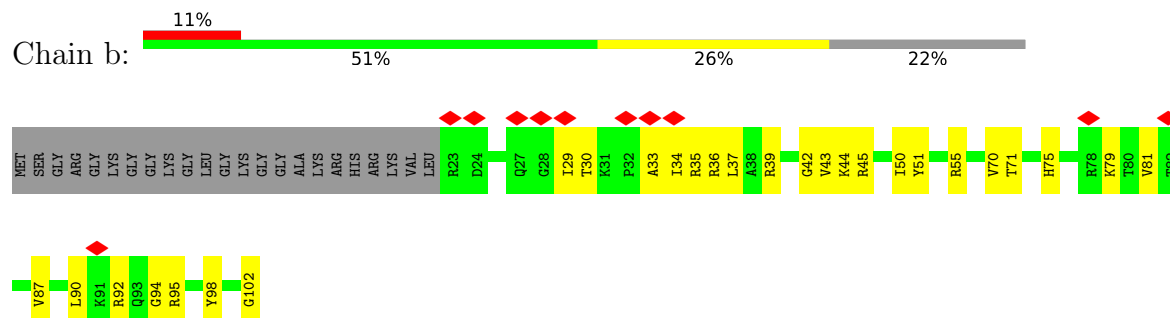
- Molecule 18: Histone H3.3



- Molecule 18: Histone H3.3

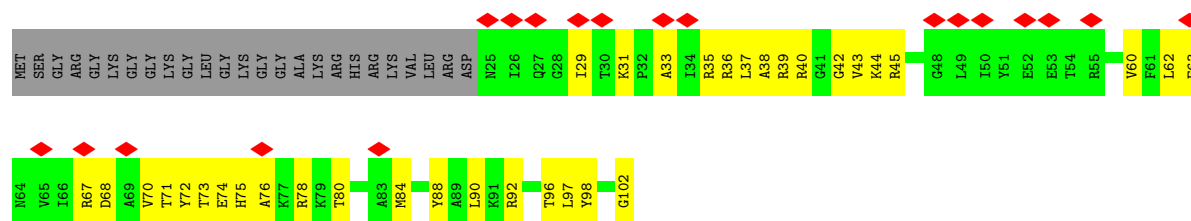


- Molecule 19: Histone H4

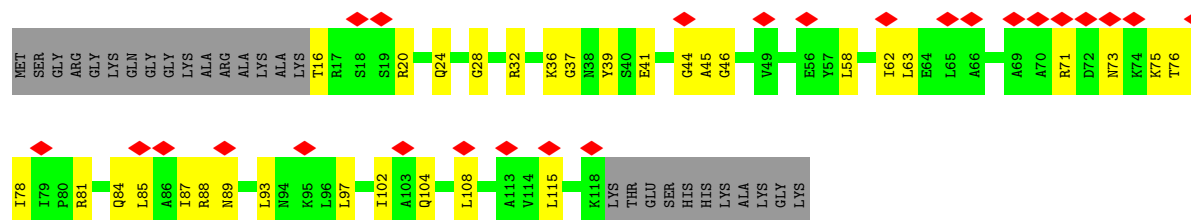


- Molecule 19: Histone H4

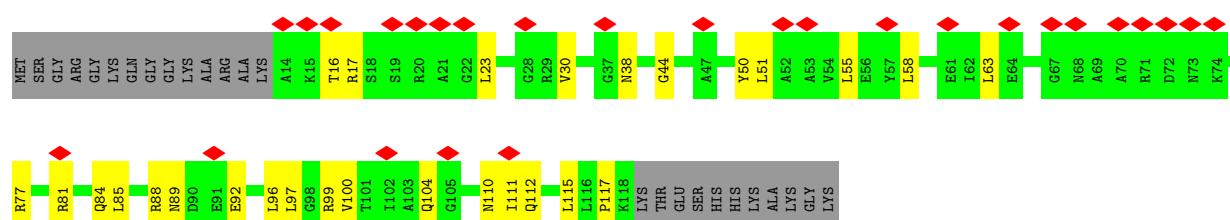




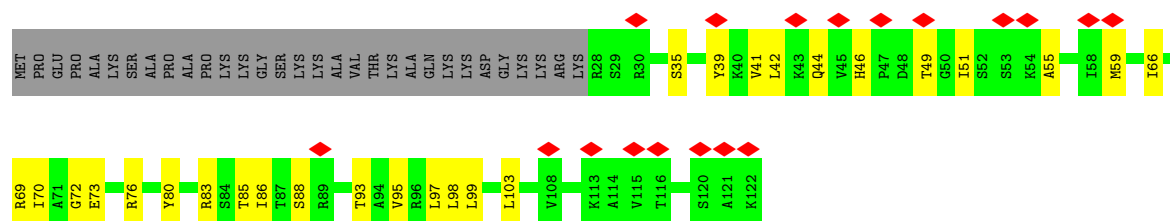
• Molecule 20: Histone H2A type 1-B/E



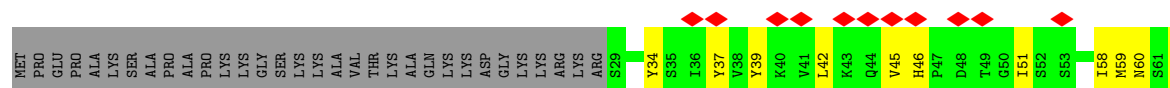
• Molecule 20: Histone H2A type 1-B/E

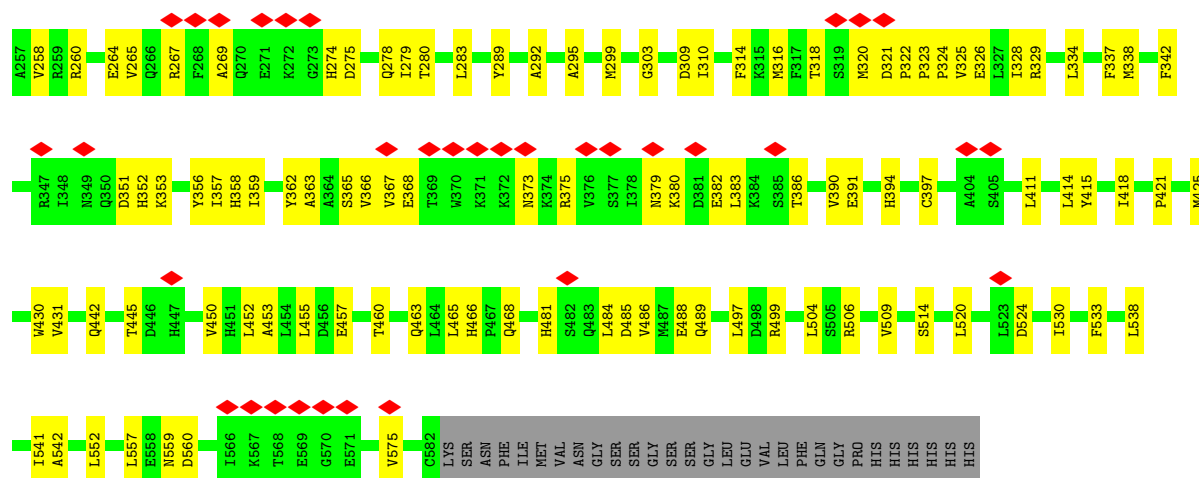


• Molecule 21: Histone H2B type 1-J

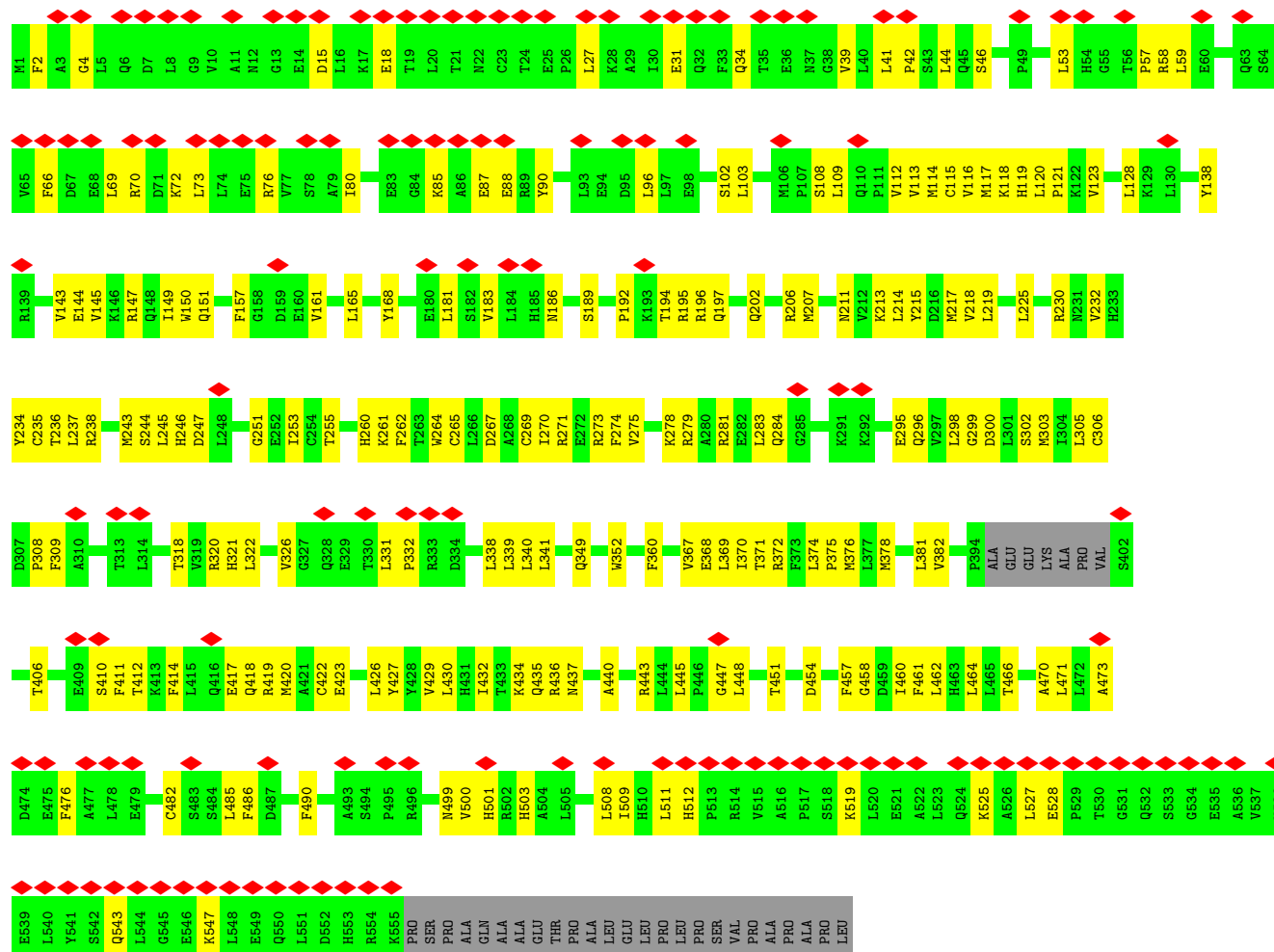


• Molecule 21: Histone H2B type 1-J

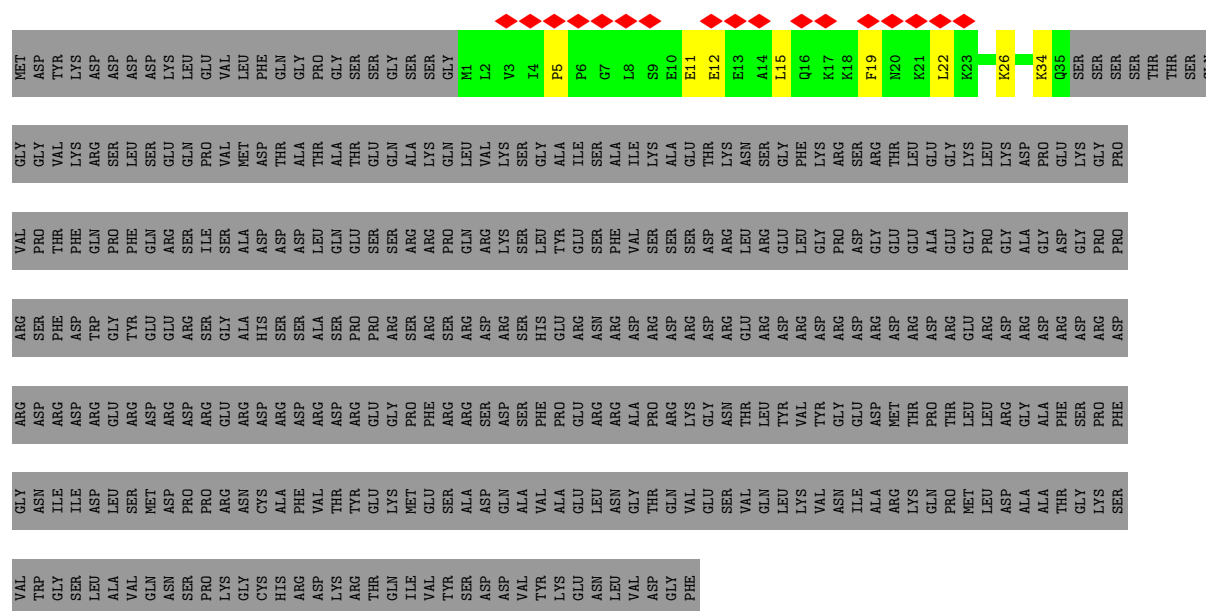




• Molecule 24: Negative elongation factor B



• Molecule 25: Negative elongation factor E



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24102	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.272, 1.272, 1.272	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.22	0/11248	0.36	0/15179
2	B	0.24	0/9149	0.38	0/12348
3	C	0.26	0/2115	0.36	0/2873
4	D	0.12	0/1017	0.34	0/1368
5	E	0.21	0/1751	0.38	0/2366
6	F	0.24	0/636	0.35	0/859
7	G	0.18	0/1364	0.41	0/1853
8	H	0.24	0/1219	0.39	0/1644
9	I	0.14	0/964	0.37	0/1305
10	J	0.26	0/542	0.40	1/730 (0.1%)
11	K	0.27	0/939	0.37	0/1271
12	L	0.23	0/395	0.44	0/524
13	Y	0.18	0/927	0.38	0/1250
14	Z	0.12	0/3903	0.33	0/5254
15	N	0.18	0/4147	0.37	0/6407
16	P	0.18	0/372	0.24	0/576
17	T	0.19	0/4384	0.34	0/6754
18	a	0.12	0/809	0.28	0/1085
18	e	0.11	0/807	0.30	0/1081
19	b	0.13	0/645	0.31	0/862
19	f	0.13	0/626	0.34	0/837
20	c	0.11	0/806	0.29	0/1089
20	g	0.12	0/820	0.32	0/1107
21	d	0.11	0/757	0.32	0/1015
21	h	0.11	0/736	0.29	0/990
22	U	0.13	0/1434	0.33	0/1948
23	W	0.13	0/4400	0.34	0/5977
24	V	0.13	0/4480	0.32	0/6049
25	X	0.12	0/283	0.27	0/372
All	All	0.19	0/61675	0.35	1/84973 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	14	VAL	N-CA-C	-6.36	106.93	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11050	0	11200	282	0
2	B	8971	0	9013	200	0
3	C	2072	0	2019	37	0
4	D	1004	0	980	37	0
5	E	1720	0	1737	53	0
6	F	626	0	657	13	0
7	G	1333	0	1321	53	0
8	H	1197	0	1156	35	0
9	I	942	0	871	31	0
10	J	533	0	553	4	0
11	K	920	0	942	14	0
12	L	389	0	393	16	0
13	Y	911	0	904	26	0
14	Z	3837	0	3895	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	3706	0	2041	107	0
16	P	335	0	169	0	0
17	T	3899	0	2128	98	0
18	a	797	0	835	29	0
18	e	796	0	832	31	0
19	b	638	0	676	33	0
19	f	619	0	659	35	0
20	c	796	0	848	35	0
20	g	810	0	866	24	0
21	d	746	0	771	26	0
21	h	725	0	745	29	0
22	U	1410	0	1455	58	0
23	W	4308	0	4306	157	0
24	V	4396	0	4491	173	0
25	X	281	0	330	8	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	Y	1	0	0	0	0
27	A	1	0	0	0	0
All	All	59777	0	56793	1472	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1472) 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)
23:W:149:MET:HE3	24:V:46:SER:HB2	1.41	1.02
15:N:-82:DG:H1	17:T:82:DC:H42	1.10	0.99
13:Y:63:MET:HE1	13:Y:69:SER:HB3	1.55	0.88
1:A:111:CYS:SG	1:A:114:CYS:HB3	2.14	0.86
15:N:-21:DG:N2	17:T:21:DC:O2	2.10	0.84
2:B:529:MET:HE2	2:B:702:MET:HG3	1.60	0.83
17:T:-44:DA:H3'	20:c:28:GLY:HA3	1.61	0.82
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.62	0.81
23:W:203:ARG:HG3	23:W:206:ARG:HH21	1.45	0.81
24:V:219:LEU:HD22	24:V:238:ARG:HE	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-95:DG:N2	17:T:95:DC:O2	2.13	0.80
7:G:101:ILE:HG13	7:G:104:MET:HB2	1.63	0.79
23:W:520:LEU:HD13	23:W:530:ILE:HG13	1.65	0.79
1:A:1243:LEU:HD21	1:A:1259:ILE:HG23	1.64	0.78
15:N:64:DG:N1	17:T:-64:DC:N3	2.28	0.77
2:B:859:ARG:NH1	2:B:860:VAL:O	2.17	0.77
22:U:127:LYS:HG3	23:W:213:LEU:HD23	1.65	0.77
20:c:115:LEU:HD11	18:e:108:ASN:HD21	1.49	0.76
23:W:425:MET:HE3	23:W:465:LEU:HD22	1.67	0.76
19:b:98:TYR:HB3	21:h:58:ILE:HG12	1.68	0.76
23:W:367:VAL:HB	23:W:379:ASN:HB3	1.66	0.76
15:N:-95:DG:N1	17:T:95:DC:N3	2.29	0.75
19:f:75:HIS:HB2	21:h:93:THR:HG21	1.67	0.75
5:E:67:ASP:OD1	24:V:279:ARG:NH2	2.20	0.75
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.67	0.75
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.68	0.75
23:W:148:GLN:NE2	24:V:42:PRO:O	2.20	0.75
24:V:417:GLU:HG3	24:V:418:GLN:HG3	1.68	0.75
4:D:80:ILE:HG22	4:D:84:ARG:HH11	1.51	0.74
15:N:63:DG:N2	17:T:-63:DC:O2	2.13	0.74
15:N:63:DG:N1	17:T:-63:DC:N3	2.28	0.74
22:U:142:GLN:OE1	23:W:468:GLN:NE2	2.20	0.73
23:W:97:LEU:HG	24:V:69:LEU:HB3	1.68	0.73
14:Z:549:VAL:HG11	14:Z:615:ARG:HH21	1.54	0.73
19:b:29:ILE:O	19:b:55:ARG:NH1	2.21	0.73
14:Z:355:ASP:HB2	14:Z:358:PHE:HB3	1.70	0.73
24:V:332:PRO:HB3	24:V:338:LEU:HD23	1.70	0.73
24:V:41:LEU:HB2	24:V:44:LEU:HB2	1.71	0.73
14:Z:529:ASP:HB3	14:Z:553:LEU:HD13	1.70	0.72
23:W:60:PRO:HD2	24:V:58:ARG:HD2	1.71	0.72
13:Y:71:VAL:HG23	14:Z:264:LEU:HD21	1.71	0.72
7:G:33:GLU:HG2	7:G:34:VAL:HG13	1.71	0.72
20:c:102:ILE:HG23	19:f:98:TYR:HB2	1.72	0.72
24:V:265:CYS:O	24:V:279:ARG:NH1	2.22	0.72
15:N:-23:DT:H2'	15:N:-22:DG:H8	1.55	0.72
1:A:487:SER:OG	1:A:673:GLN:NE2	2.23	0.72
15:N:62:DG:N2	17:T:-62:DC:O2	2.17	0.72
15:N:-47:DC:O2	17:T:47:DG:N2	2.18	0.71
23:W:51:PHE:O	23:W:86:ASN:ND2	2.22	0.71
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.23	0.71
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:GLN:NE2	1:A:791:GLN:O	2.20	0.71
4:D:29:ALA:HB1	7:G:3:TYR:HB3	1.72	0.71
2:B:298:MET:HA	2:B:301:VAL:HG12	1.73	0.70
22:U:89:TRP:NE1	23:W:196:GLN:O	2.24	0.70
2:B:1142:ASN:ND2	2:B:1145:GLN:OE1	2.24	0.70
24:V:275:VAL:HG11	24:V:341:LEU:HD21	1.71	0.70
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.74	0.70
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.74	0.70
19:b:39:ARG:NH1	19:b:44:LYS:O	2.25	0.69
15:N:64:DG:N2	17:T:-64:DC:O2	2.15	0.69
18:e:53:ARG:HA	18:e:56:LYS:HE3	1.75	0.69
22:U:29:ILE:HG12	22:U:59:GLY:HA3	1.73	0.69
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.24	0.69
24:V:151:GLN:HA	24:V:213:LYS:HG2	1.74	0.69
1:A:96:HIS:HB2	1:A:250:VAL:HG13	1.75	0.69
1:A:805:ARG:NH2	2:B:671:GLU:O	2.23	0.69
15:N:17:DA:H3'	18:a:65:LEU:HB3	1.75	0.69
1:A:118:LEU:HD12	1:A:148:CYS:HB3	1.75	0.69
14:Z:440:ILE:HG12	14:Z:450:ILE:HD11	1.75	0.69
18:e:108:ASN:ND2	19:f:42:GLY:O	2.26	0.69
1:A:332:SER:HB3	1:A:334:ARG:HG2	1.75	0.69
11:K:23:LYS:NZ	11:K:84:GLN:OE1	2.24	0.69
18:a:95:ALA:O	19:b:95:ARG:NH2	2.26	0.69
14:Z:533:GLN:O	14:Z:577:ARG:NH1	2.26	0.69
18:a:123:ASP:OD1	18:e:113:HIS:NE2	2.23	0.69
4:D:44:ARG:NH2	7:G:35:GLU:OE1	2.26	0.68
1:A:413:TYR:O	1:A:449:HIS:ND1	2.25	0.68
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	1.74	0.68
24:V:265:CYS:SG	24:V:279:ARG:NH1	2.66	0.68
1:A:411:SER:HB2	14:Z:733:ARG:HD3	1.74	0.68
2:B:88:PHE:HE2	2:B:412:LEU:HD21	1.59	0.68
9:I:104:ALA:HB1	9:I:107:ALA:HB3	1.74	0.68
13:Y:66:PRO:HD3	13:Y:82:PRO:HG3	1.76	0.68
20:g:23:LEU:HD11	21:h:114:ALA:HB1	1.75	0.68
22:U:38:ILE:HD13	22:U:41:ILE:HD12	1.74	0.68
2:B:649:ASN:OD1	2:B:650:ASN:N	2.25	0.68
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.27	0.68
1:A:753:GLY:O	1:A:757:GLN:HG2	1.94	0.67
2:B:240:LEU:HD12	2:B:255:ARG:HB3	1.76	0.67
1:A:719:LYS:NZ	23:W:445:THR:O	2.27	0.67
1:A:266:MET:HE3	2:B:890:ARG:HH12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.75	0.67
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.27	0.67
24:V:196:ARG:NH1	24:V:243:MET:SD	2.67	0.67
24:V:219:LEU:HD13	24:V:238:ARG:HH21	1.58	0.67
1:A:948:ILE:HD12	1:A:1007:ILE:HG21	1.76	0.67
14:Z:554:GLU:OE2	14:Z:559:GLN:NE2	2.27	0.66
18:a:128:ARG:HH21	18:a:131:ARG:HD2	1.60	0.66
20:c:24:GLN:OE1	21:d:44:GLN:NE2	2.27	0.66
22:U:181:LYS:NZ	22:U:185:THR:OG1	2.28	0.66
5:E:73:PHE:CD2	5:E:99:ILE:HD11	2.30	0.66
12:L:26:ASN:HD21	12:L:44:MET:HE1	1.61	0.66
14:Z:587:LEU:HD13	14:Z:591:GLN:HG3	1.78	0.66
20:g:85:LEU:O	20:g:89:ASN:ND2	2.28	0.66
14:Z:279:VAL:HG12	14:Z:383:THR:HA	1.77	0.66
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.78	0.66
24:V:189:SER:O	24:V:273:ARG:NH2	2.29	0.66
23:W:131:LYS:HB3	24:V:53:LEU:HD22	1.78	0.66
15:N:70:DG:H4'	18:e:41:TYR:HA	1.78	0.66
17:T:8:DC:OP1	19:f:39:ARG:NH2	2.28	0.66
14:Z:286:TYR:HE1	14:Z:310:ARG:H	1.44	0.65
2:B:282:ARG:NH2	9:I:21:ASN:OD1	2.29	0.65
7:G:82:GLY:N	7:G:147:ILE:O	2.27	0.65
15:N:-47:DC:H2''	15:N:-46:DT:C5	2.32	0.65
2:B:562:ALA:O	2:B:610:ARG:NH2	2.29	0.65
17:T:-24:DG:H5''	18:a:85:GLN:HG2	1.78	0.65
21:d:69:ARG:HB3	21:d:98:LEU:HD11	1.78	0.65
3:C:61:ASP:OD2	12:L:48:ARG:NH2	2.29	0.65
24:V:332:PRO:HD3	24:V:378:MET:HE1	1.78	0.65
4:D:76:ASN:O	4:D:79:THR:OG1	2.15	0.65
7:G:81:LYS:NZ	14:Z:476:ASP:OD1	2.29	0.65
14:Z:588:ASP:HB3	14:Z:594:ILE:HD13	1.78	0.65
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.14	0.65
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.78	0.65
13:Y:23:LYS:NZ	13:Y:32:GLY:O	2.30	0.64
1:A:860:ILE:HD13	1:A:863:ARG:HH21	1.61	0.64
24:V:196:ARG:O	24:V:202:GLN:NE2	2.31	0.64
5:E:2:ASP:OD1	5:E:3:ASP:N	2.29	0.64
24:V:269:CYS:SG	24:V:279:ARG:NH1	2.69	0.64
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.80	0.64
14:Z:280:ARG:NH2	14:Z:288:ASP:OD1	2.30	0.64
14:Z:447:LYS:NZ	14:Z:462:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:87:ILE:HA	20:c:93:LEU:HD23	1.79	0.64
18:e:116:ARG:NH2	18:e:123:ASP:OD2	2.30	0.64
19:f:39:ARG:NH1	19:f:43:VAL:O	2.30	0.64
19:f:92:ARG:HH22	21:h:98:LEU:HG	1.61	0.64
8:H:98:ARG:NE	8:H:100:GLU:OE1	2.29	0.64
14:Z:615:ARG:HH22	14:Z:635:MET:HG3	1.62	0.64
18:a:113:HIS:NE2	18:e:123:ASP:OD1	2.26	0.64
1:A:1286:ARG:HH21	9:I:54:TYR:HB2	1.62	0.64
2:B:388:TYR:OH	2:B:524:LYS:HE3	1.98	0.64
9:I:14:ILE:HG23	9:I:23:MET:HE1	1.78	0.64
2:B:295:PRO:HA	2:B:298:MET:HE3	1.80	0.64
2:B:388:TYR:H	2:B:504:THR:HG21	1.62	0.63
23:W:146:LEU:O	23:W:150:ILE:HG13	1.97	0.63
15:N:-47:DC:N3	17:T:47:DG:N1	2.31	0.63
23:W:100:TRP:HB3	24:V:76:ARG:HH12	1.62	0.63
24:V:147:ARG:O	24:V:211:ASN:ND2	2.30	0.63
6:F:100:ARG:NH2	6:F:121:ASP:O	2.30	0.63
15:N:-23:DT:H5'	18:e:83:ARG:HG3	1.80	0.63
1:A:1150:ASP:HB3	1:A:1153:ARG:HB2	1.81	0.63
17:T:23:DA:H2'	17:T:24:DA:C8	2.34	0.63
2:B:545:LEU:HD21	2:B:567:ILE:HG21	1.81	0.63
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.31	0.63
24:V:57:PRO:HB2	24:V:59:LEU:HG	1.81	0.63
14:Z:419:ASN:OD1	14:Z:421:GLN:NE2	2.32	0.63
17:T:8:DC:H5''	19:f:39:ARG:HH21	1.64	0.63
23:W:250:GLN:NE2	23:W:373:ASN:OD1	2.31	0.63
1:A:1179:PRO:HB3	9:I:33:ARG:HG2	1.79	0.63
7:G:120:ASP:HB2	7:G:127:CYS:H	1.63	0.63
23:W:504:LEU:HG	23:W:509:VAL:HG12	1.79	0.63
8:H:60:ILE:HD11	8:H:123:MET:HE1	1.80	0.62
24:V:372:ARG:HG3	25:X:11:GLU:HG3	1.80	0.62
20:c:87:ILE:HG21	20:c:97:LEU:HD12	1.79	0.62
1:A:1248:ASN:HB2	1:A:1256:VAL:HG22	1.82	0.62
15:N:-43:DT:H5''	20:g:16:THR:HA	1.80	0.62
2:B:347:MET:O	2:B:361:LYS:NZ	2.31	0.62
2:B:629:GLU:HB3	2:B:634:LEU:HD21	1.81	0.62
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.81	0.62
1:A:54:LEU:O	1:A:61:ARG:NH2	2.32	0.62
2:B:92:TYR:N	2:B:125:TYR:O	2.28	0.62
13:Y:7:PRO:HB3	13:Y:24:THR:HG23	1.81	0.62
24:V:103:LEU:HD22	24:V:109:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:ASN:HD21	1:A:1252:ALA:HB3	1.64	0.62
3:C:190:ASN:ND2	3:C:195:THR:O	2.30	0.62
19:b:33:ALA:HA	19:b:36:ARG:HE	1.64	0.62
23:W:59:GLU:OE2	24:V:59:LEU:N	2.33	0.62
1:A:598:GLY:HA3	1:A:660:MET:HE3	1.82	0.61
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.80	0.61
4:D:112:LYS:NZ	4:D:124:ASP:OD1	2.32	0.61
15:N:62:DG:N1	17:T:-62:DC:N3	2.33	0.61
13:Y:17:LEU:HB2	13:Y:93:LEU:HG	1.82	0.61
5:E:172:ARG:NH1	5:E:210:GLN:OE1	2.33	0.61
8:H:34:SER:O	22:U:15:ASN:ND2	2.34	0.61
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	1.81	0.61
2:B:827:GLU:HG2	2:B:871:VAL:HB	1.82	0.61
14:Z:248:GLY:O	14:Z:252:GLN:NE2	2.33	0.61
23:W:147:GLU:HA	23:W:150:ILE:HD12	1.81	0.61
1:A:381:PRO:HB3	1:A:480:SER:HA	1.82	0.61
1:A:461:GLN:HG3	17:T:102:DA:H2''	1.82	0.61
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.83	0.61
1:A:1165:THR:HG22	1:A:1168:LYS:HG2	1.81	0.61
14:Z:301:ASN:OD1	14:Z:302:THR:N	2.33	0.61
1:A:116:LYS:HD2	1:A:182:GLY:HA3	1.82	0.61
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.65	0.61
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.83	0.61
14:Z:478:VAL:HG21	14:Z:492:ILE:HG23	1.83	0.61
19:b:44:LYS:HD3	19:b:45:ARG:HG2	1.83	0.61
14:Z:306:LYS:HA	14:Z:372:LEU:O	1.99	0.61
1:A:803:LYS:O	1:A:812:LYS:NZ	2.33	0.61
1:A:1481:LYS:HA	7:G:20:PRO:HA	1.81	0.61
12:L:16:ILE:HD12	12:L:47:LYS:HD3	1.81	0.61
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.28	0.60
3:C:81:LYS:HZ3	3:C:126:ARG:HH22	1.49	0.60
5:E:69:THR:OG1	24:V:279:ARG:NE	2.33	0.60
19:f:39:ARG:NH2	19:f:44:LYS:O	2.34	0.60
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.83	0.60
17:T:88:DA:H2''	17:T:89:DA:C8	2.36	0.60
21:d:83:ARG:NH1	21:d:85:THR:O	2.34	0.60
19:f:38:ALA:HB1	19:f:43:VAL:HB	1.81	0.60
15:N:-23:DT:H2'	15:N:-22:DG:C8	2.35	0.60
17:T:-13:DA:H5''	19:b:30:THR:HG21	1.83	0.60
18:a:108:ASN:ND2	19:b:42:GLY:O	2.34	0.60
1:A:64:VAL:HG11	1:A:78:MET:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:ASP:OD1	5:E:32:GLU:N	2.34	0.60
24:V:445:LEU:HD21	24:V:485:LEU:HA	1.82	0.60
2:B:1144:THR:HG23	2:B:1145:GLN:OE1	2.01	0.60
22:U:57:LEU:O	22:U:60:THR:OG1	2.19	0.60
1:A:623:PRO:HA	8:H:27:ARG:HH21	1.66	0.60
1:A:717:ILE:HG12	1:A:737:PHE:HZ	1.66	0.60
7:G:36:GLY:HA2	7:G:45:VAL:O	2.02	0.60
24:V:454:ASP:HB3	24:V:457:PHE:HB2	1.84	0.60
1:A:59:ASP:HB3	1:A:62:GLN:HG3	1.84	0.60
1:A:927:GLU:HG3	1:A:943:LEU:HD11	1.84	0.60
14:Z:444:ASP:HB2	14:Z:448:ILE:HA	1.82	0.60
15:N:58:DC:OP1	20:c:77:ARG:N	2.35	0.60
23:W:69:TYR:OH	23:W:75:SER:O	2.20	0.60
2:B:354:SER:HG	2:B:357:CYS:HG	1.39	0.59
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.35	0.59
2:B:610:ARG:HD2	9:I:69:ILE:HD13	1.84	0.59
17:T:38:DA:H5''	20:g:44:GLY:HA2	1.83	0.59
24:V:181:LEU:HD13	24:V:466:THR:HB	1.84	0.59
2:B:872:THR:HA	2:B:889:LYS:HG3	1.84	0.59
24:V:275:VAL:HG13	24:V:279:ARG:HB2	1.83	0.59
1:A:535:MET:O	1:A:669:TYR:OH	2.20	0.59
1:A:606:HIS:HD2	1:A:608:THR:HG22	1.68	0.59
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.84	0.59
17:T:9:DG:H5''	18:e:46:VAL:HB	1.84	0.59
23:W:411:LEU:HD12	23:W:414:LEU:HD23	1.85	0.59
24:V:117:MET:HE2	24:V:145:VAL:HG11	1.85	0.59
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.36	0.59
2:B:608:ARG:HH12	9:I:100:HIS:CG	2.19	0.59
15:N:-24:DT:H2'	15:N:-23:DT:H71	1.84	0.59
17:T:95:DC:H2''	17:T:96:DA:C8	2.37	0.59
19:f:60:VAL:HA	19:f:63:GLU:HB2	1.85	0.59
15:N:38:DG:H5''	20:c:44:GLY:HA2	1.83	0.59
21:d:76:ARG:NH2	21:d:80:TYR:OH	2.35	0.59
13:Y:62:ALA:HB3	14:Z:215:VAL:HB	1.85	0.59
14:Z:290:ILE:HG13	14:Z:392:GLU:HG2	1.84	0.59
1:A:274:ASP:OD1	1:A:275:ASP:N	2.36	0.59
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.36	0.59
8:H:31:GLU:OE2	8:H:36:LYS:NZ	2.32	0.59
22:U:12:TRP:HE3	22:U:13:LEU:HD12	1.67	0.59
1:A:1178:ASP:OD1	1:A:1183:SER:OG	2.21	0.59
19:b:34:ILE:HB	19:b:51:TYR:HD1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.83	0.58
7:G:28:GLN:O	7:G:32:THR:HG23	2.03	0.58
1:A:972:THR:HG22	1:A:1320:ILE:HD13	1.84	0.58
8:H:2:ALA:O	8:H:84:ARG:NH2	2.37	0.58
18:a:52:ARG:HB3	18:a:56:LYS:HE2	1.86	0.58
23:W:67:LYS:HD2	24:V:27:LEU:HG	1.85	0.58
23:W:124:ILE:HD12	23:W:162:LEU:HD23	1.84	0.58
2:B:320:PHE:O	2:B:323:SER:OG	2.21	0.58
24:V:39:VAL:HG12	24:V:41:LEU:HG	1.85	0.58
14:Z:199:LYS:NZ	14:Z:240:GLU:O	2.23	0.58
20:c:84:GLN:HE21	20:c:88:ARG:HE	1.51	0.58
8:H:63:THR:HG21	8:H:68:GLY:HA2	1.84	0.58
13:Y:14:ARG:HB3	13:Y:53:THR:HB	1.84	0.58
14:Z:475:GLY:H	14:Z:492:ILE:HG13	1.67	0.58
24:V:235:CYS:SG	24:V:306:CYS:HB3	2.43	0.58
15:N:-57:DT:H2''	15:N:-56:DG:C8	2.39	0.58
1:A:825:ASN:ND2	1:A:835:GLU:OE2	2.35	0.58
5:E:194:ILE:HG12	5:E:204:ILE:HG12	1.85	0.58
1:A:1243:LEU:HD23	1:A:1244:ASN:N	2.19	0.58
2:B:354:SER:OG	2:B:357:CYS:SG	2.54	0.58
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.84	0.58
14:Z:425:ASN:H	14:Z:472:PHE:HE1	1.51	0.58
17:T:-40:DG:H2'	17:T:-39:DT:H71	1.86	0.58
19:b:35:ARG:NH2	19:b:39:ARG:HH21	2.02	0.58
1:A:896:LEU:HB2	1:A:1396:ARG:HH21	1.68	0.58
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.03	0.58
5:E:99:ILE:HG22	24:V:278:LYS:HZ1	1.69	0.58
1:A:104:MET:HG2	1:A:198:LEU:HD21	1.85	0.58
1:A:579:ILE:HG12	8:H:92:MET:HG2	1.85	0.58
2:B:18:THR:HG22	2:B:637:LYS:HG3	1.84	0.58
2:B:334:LYS:HG2	2:B:337:LYS:HE3	1.86	0.58
2:B:837:CYS:HB2	2:B:840:MET:HE3	1.86	0.58
3:C:78:ILE:HG22	3:C:82:LEU:HG	1.86	0.58
14:Z:184:CYS:SG	14:Z:185:LYS:N	2.77	0.58
15:N:45:DT:H2''	15:N:46:DG:C8	2.39	0.58
24:V:243:MET:HE3	24:V:264:TRP:HA	1.86	0.58
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.68	0.57
23:W:60:PRO:HD2	24:V:58:ARG:HH11	1.69	0.57
24:V:470:ALA:HA	24:V:511:LEU:HD21	1.86	0.57
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.86	0.57
22:U:34:THR:HG22	22:U:37:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:64:ASN:O	23:W:68:ARG:HG3	2.03	0.57
24:V:321:HIS:HB2	24:V:338:LEU:HD13	1.85	0.57
1:A:1213:ARG:HH12	1:A:1215:GLU:HB3	1.70	0.57
18:e:54:TYR:HB3	19:f:40:ARG:HE	1.68	0.57
2:B:759:VAL:HG11	2:B:983:GLU:HG3	1.85	0.57
18:e:44:GLY:HA2	18:e:47:ALA:HB3	1.86	0.57
2:B:508:MET:HE2	2:B:623:ARG:HG2	1.86	0.57
15:N:-118:DT:H2''	15:N:-117:DC:H5'	1.84	0.57
23:W:242:GLN:HB3	23:W:283:LEU:HD21	1.86	0.57
1:A:244:ARG:HE	1:A:245:PRO:HD2	1.68	0.57
2:B:789:ASN:O	2:B:968:ASN:HB2	2.05	0.57
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.39	0.57
9:I:81:THR:OG1	9:I:83:ASP:OD1	2.23	0.57
14:Z:365:ARG:HH12	14:Z:376:PHE:HZ	1.52	0.57
24:V:114:MET:HE3	24:V:114:MET:HA	1.86	0.57
1:A:91:ALA:HB2	1:A:291:ARG:HG3	1.87	0.57
5:E:26:TYR:HD1	5:E:64:HIS:HA	1.68	0.57
15:N:39:DA:H2''	15:N:40:DC:H5''	1.86	0.57
22:U:62:HIS:HA	23:W:278:GLN:HG2	1.87	0.57
23:W:209:LEU:HD11	23:W:245:MET:HE1	1.86	0.57
2:B:58:ILE:HD11	2:B:405:ARG:HG3	1.87	0.57
18:a:68:GLN:HG3	18:a:89:ILE:HD13	1.87	0.57
22:U:24:TRP:HA	23:W:235:GLU:HG2	1.87	0.57
23:W:97:LEU:HD13	24:V:76:ARG:HH21	1.70	0.57
24:V:509:ILE:O	24:V:512:HIS:ND1	2.35	0.57
9:I:108:MET:HA	9:I:108:MET:HE3	1.87	0.56
15:N:17:DA:H5''	18:a:66:PRO:HG3	1.87	0.56
1:A:365:THR:HG22	2:B:1059:ILE:HA	1.86	0.56
2:B:867:ILE:HB	2:B:894:THR:HG22	1.86	0.56
5:E:17:ILE:HG21	5:E:74:VAL:HG11	1.88	0.56
13:Y:23:LYS:HE2	13:Y:27:GLN:HB3	1.87	0.56
15:N:-68:DT:H2''	15:N:-67:DT:C5	2.39	0.56
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.87	0.56
2:B:1151:MET:HE3	2:B:1155:CYS:HB3	1.87	0.56
7:G:114:PRO:HD3	7:G:163:LEU:HB3	1.86	0.56
1:A:119:VAL:HG13	1:A:151:LYS:HZ2	1.71	0.56
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.85	0.56
1:A:606:HIS:CD2	1:A:608:THR:HG22	2.41	0.56
8:H:38:ASP:OD1	8:H:39:LEU:N	2.39	0.56
19:f:74:GLU:O	21:h:89:ARG:NH2	2.38	0.56
23:W:280:THR:HA	23:W:283:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:OD1	1:A:78:MET:N	2.38	0.56
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.71	0.56
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.30	0.56
24:V:308:PRO:HB3	24:V:460:ILE:HD11	1.88	0.56
17:T:75:DC:H2''	17:T:76:DG:N7	2.20	0.56
18:a:98:ALA:HB3	19:b:95:ARG:HH22	1.68	0.56
23:W:58:MET:HE2	23:W:90:VAL:HB	1.87	0.56
1:A:1261:ILE:O	1:A:1262:MET:HE2	2.05	0.56
1:A:1306:LYS:HE2	1:A:1308:TYR:HE1	1.70	0.56
2:B:191:GLU:OE1	2:B:472:ARG:NH1	2.38	0.56
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.88	0.56
14:Z:389:THR:OG1	14:Z:392:GLU:OE1	2.24	0.56
2:B:733:MET:HE2	2:B:749:HIS:HB3	1.88	0.56
1:A:31:LEU:HD11	1:A:254:PRO:HB3	1.88	0.56
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.70	0.56
23:W:357:ILE:HG21	23:W:391:GLU:HG3	1.87	0.56
2:B:929:PRO:O	2:B:948:GLN:NE2	2.38	0.56
17:T:84:DC:H2''	17:T:85:DC:H5'	1.88	0.56
18:e:104:PHE:HE2	19:f:37:LEU:HB3	1.70	0.56
1:A:296:ASN:OD1	1:A:297:GLY:N	2.37	0.55
7:G:114:PRO:HD2	7:G:163:LEU:HD23	1.88	0.55
15:N:-56:DG:H2''	15:N:-55:DT:C6	2.41	0.55
23:W:557:LEU:HD11	23:W:575:VAL:HB	1.88	0.55
1:A:1173:THR:HG23	1:A:1214:VAL:HG22	1.87	0.55
5:E:67:ASP:HB2	24:V:271:ARG:HH22	1.70	0.55
14:Z:196:LEU:HD23	14:Z:215:VAL:HG21	1.88	0.55
1:A:904:GLN:NE2	1:A:981:CYS:O	2.38	0.55
5:E:99:ILE:HG22	24:V:278:LYS:NZ	2.22	0.55
17:T:55:DA:H2''	17:T:56:DC:C5	2.42	0.55
1:A:576:GLN:O	1:A:590:GLN:NE2	2.39	0.55
5:E:30:GLN:NE2	5:E:34:ASP:OD2	2.39	0.55
17:T:-34:DG:H5'	21:d:85:THR:HB	1.87	0.55
18:e:106:ASP:OD2	18:e:131:ARG:NH2	2.36	0.55
24:V:299:GLY:O	24:V:302:SER:OG	2.17	0.55
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.39	0.55
2:B:789:ASN:HA	2:B:793:SER:HB3	1.88	0.55
13:Y:94:PRO:HD2	13:Y:97:ILE:HD12	1.88	0.55
14:Z:584:ALA:O	14:Z:595:HIS:ND1	2.38	0.55
15:N:1:DC:H2''	15:N:2:DG:C8	2.41	0.55
21:h:95:VAL:HG13	21:h:99:LEU:HD12	1.87	0.55
22:U:13:LEU:HD23	22:U:56:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:124:LEU:HD11	23:W:209:LEU:HB3	1.87	0.55
23:W:55:ASP:OD1	23:W:88:THR:HG22	2.06	0.55
24:V:382:VAL:HG13	25:X:22:LEU:HD22	1.87	0.55
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.18	0.55
17:T:-13:DA:OP1	19:b:36:ARG:NH2	2.40	0.55
21:h:34:TYR:HA	21:h:37:TYR:HD2	1.70	0.55
23:W:145:TRP:HB2	24:V:46:SER:OG	2.06	0.55
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.40	0.55
3:C:150:ILE:HG22	3:C:151:VAL:HG23	1.89	0.55
15:N:-13:DA:OP2	19:f:36:ARG:NH2	2.40	0.55
18:e:116:ARG:NH1	18:e:118:THR:O	2.40	0.55
24:V:128:LEU:HD13	24:V:149:ILE:HG22	1.88	0.55
1:A:863:ARG:HH12	1:A:1129:ASN:HD21	1.55	0.55
2:B:341:GLU:HG2	2:B:345:LYS:HE2	1.89	0.55
7:G:153:ASP:HA	14:Z:524:THR:HG23	1.89	0.55
20:g:110:ASN:ND2	20:g:112:GLN:OE1	2.31	0.55
22:U:17:LEU:HD21	22:U:32:LEU:HD12	1.88	0.55
2:B:509:VAL:HG11	2:B:524:LYS:HD2	1.89	0.55
5:E:98:ASN:CG	24:V:278:LYS:HG3	2.32	0.55
15:N:-89:DT:H1'	15:N:-88:DT:H5'	1.88	0.55
17:T:2:DG:H2'	17:T:3:DT:H71	1.87	0.55
20:c:63:LEU:HD13	21:d:42:LEU:HB2	1.88	0.55
21:h:75:SER:O	21:h:79:HIS:ND1	2.39	0.55
1:A:419:ILE:HD11	1:A:440:LEU:HB3	1.88	0.54
17:T:35:DC:H2''	17:T:36:DC:C5	2.41	0.54
2:B:565:THR:HA	2:B:610:ARG:HB3	1.88	0.54
17:T:98:DA:H2'	17:T:99:DC:C6	2.42	0.54
19:b:87:VAL:HG11	19:b:102:GLY:HA3	1.89	0.54
19:f:31:LYS:HE2	19:f:35:ARG:HD2	1.89	0.54
24:V:183:VAL:O	24:V:186:ASN:ND2	2.41	0.54
2:B:859:ARG:HB2	14:Z:737:HIS:CD2	2.43	0.54
20:c:104:GLN:HA	18:e:58:THR:HG21	1.89	0.54
22:U:61:LEU:HD22	23:W:279:ILE:HD13	1.89	0.54
22:U:120:ILE:HG13	23:W:206:ARG:HB2	1.88	0.54
1:A:1190:GLN:NE2	1:A:1248:ASN:OD1	2.41	0.54
2:B:626:LEU:HD13	2:B:698:ILE:HG12	1.89	0.54
4:D:80:ILE:HG22	4:D:84:ARG:NH1	2.21	0.54
24:V:436:ARG:HE	24:V:471:LEU:HD21	1.72	0.54
1:A:1036:ASN:OD1	5:E:202:ARG:NH1	2.39	0.54
3:C:190:ASN:O	3:C:193:ARG:NH1	2.40	0.54
20:c:32:ARG:HE	20:c:36:LYS:HE3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:482:CYS:HB3	24:V:519:LYS:HE2	1.90	0.54
1:A:1189:ASP:HA	1:A:1192:TRP:HZ3	1.72	0.54
4:D:73:ARG:HB3	4:D:138:ARG:HG2	1.89	0.54
17:T:-27:DC:H2''	17:T:-26:DT:C5	2.42	0.54
17:T:36:DC:H2''	17:T:37:DC:C5	2.43	0.54
1:A:1005:HIS:ND1	1:A:1007:ILE:HG12	2.22	0.54
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.41	0.54
2:B:646:ARG:O	2:B:647:GLU:HG2	2.08	0.54
4:D:34:ASN:O	4:D:68:THR:OG1	2.26	0.54
4:D:59:GLU:O	4:D:63:LYS:HG2	2.07	0.54
17:T:0:DC:H2'	17:T:1:DT:H71	1.90	0.54
1:A:352:GLY:O	1:A:353:ASN:ND2	2.41	0.54
1:A:909:LEU:C	1:A:911:PRO:HD3	2.32	0.54
17:T:15:DT:H2''	17:T:16:DA:N7	2.23	0.54
17:T:105:DA:H2'	17:T:106:DG:C8	2.42	0.54
2:B:298:MET:SD	9:I:14:ILE:HG13	2.48	0.54
19:f:75:HIS:NE2	21:h:77:LEU:HB3	2.23	0.54
14:Z:451:MET:O	14:Z:453:LYS:NZ	2.28	0.54
22:U:66:ARG:NH2	22:U:67:THR:OG1	2.41	0.54
2:B:625:LEU:HD13	2:B:675:LEU:HD11	1.89	0.53
12:L:22:CYS:SG	12:L:24:THR:OG1	2.60	0.53
22:U:123:GLU:OE1	23:W:206:ARG:HD2	2.08	0.53
2:B:635:LEU:HD21	2:B:640:ILE:HD11	1.89	0.53
20:c:46:GLY:HA3	21:d:88:SER:HB3	1.91	0.53
1:A:803:LYS:HB2	2:B:671:GLU:OE2	2.08	0.53
1:A:1163:HIS:NE2	1:A:1297:THR:HG22	2.23	0.53
14:Z:186:ILE:HG13	14:Z:222:LYS:HB3	1.89	0.53
15:N:27:DG:H2''	15:N:28:DA:N7	2.23	0.53
17:T:21:DC:H2'	17:T:22:DC:C6	2.44	0.53
20:g:50:TYR:HE1	21:h:111:GLY:HA3	1.72	0.53
10:J:12:LYS:NZ	10:J:39:GLY:O	2.40	0.53
2:B:331:THR:HG23	2:B:334:LYS:H	1.73	0.53
19:b:51:TYR:O	19:b:55:ARG:HG3	2.09	0.53
1:A:1003:ASP:OD1	1:A:1003:ASP:N	2.42	0.53
11:K:13:PHE:N	11:K:16:GLU:OE1	2.33	0.53
24:V:245:LEU:HD13	24:V:253:ILE:HG21	1.90	0.53
8:H:15:ILE:HG22	8:H:16:ASP:H	1.73	0.53
14:Z:199:LYS:NZ	14:Z:238:ALA:O	2.41	0.53
23:W:431:VAL:HG11	23:W:455:LEU:HD21	1.89	0.53
1:A:11:SER:OG	1:A:13:CYS:SG	2.62	0.53
24:V:432:ILE:HA	24:V:435:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:473:ALA:HB2	24:V:511:LEU:HD22	1.91	0.53
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.44	0.53
2:B:87:LYS:HD3	2:B:88:PHE:H	1.72	0.53
2:B:629:GLU:OE1	2:B:630:LYS:HG3	2.09	0.53
2:B:988:LYS:O	2:B:992:ASN:ND2	2.38	0.53
5:E:47:LYS:H	5:E:53:PRO:HG3	1.73	0.53
13:Y:20:SER:HB3	13:Y:85:TYR:CE1	2.44	0.53
15:N:-84:DG:H2''	15:N:-83:DT:H5'	1.90	0.53
23:W:241:ALA:O	23:W:245:MET:HG2	2.09	0.53
2:B:151:LYS:H	2:B:441:SER:HG	1.55	0.53
17:T:57:DA:H4'	20:g:77:ARG:HG3	1.90	0.53
22:U:175:ARG:HG2	23:W:453:ALA:HB1	1.90	0.53
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.45	0.52
17:T:47:DG:H2''	17:T:48:DG:C8	2.44	0.52
18:e:93:GLN:NE2	18:e:97:GLU:OE2	2.41	0.52
4:D:70:ARG:HG3	4:D:71:PHE:CD1	2.44	0.52
7:G:148:VAL:O	14:Z:475:GLY:HA3	2.08	0.52
13:Y:34:ASP:HB3	13:Y:81:LYS:HD2	1.91	0.52
22:U:124:LEU:HB3	23:W:248:LEU:HD11	1.90	0.52
24:V:270:ILE:O	24:V:273:ARG:NH1	2.42	0.52
24:V:349:GLN:NE2	24:V:423:GLU:OE1	2.42	0.52
20:g:55:LEU:HD23	20:g:58:LEU:HD12	1.92	0.52
1:A:642:LYS:HD2	1:A:773:GLY:HA3	1.91	0.52
14:Z:450:ILE:HG23	14:Z:452:PRO:HD3	1.91	0.52
15:N:-65:DT:H2''	15:N:-64:DT:H5''	1.91	0.52
15:N:49:DC:OP2	21:d:35:SER:OG	2.27	0.52
19:f:63:GLU:O	19:f:67:ARG:N	2.38	0.52
1:A:11:SER:OG	2:B:1117:HIS:NE2	2.40	0.52
1:A:769:MET:HE2	2:B:973:PRO:HG3	1.91	0.52
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.91	0.52
4:D:80:ILE:O	4:D:84:ARG:HG3	2.09	0.52
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.25	0.52
4:D:26:PHE:HD2	7:G:80:PHE:HZ	1.58	0.52
23:W:452:LEU:HB3	23:W:499:ARG:HD2	1.92	0.52
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.91	0.52
23:W:145:TRP:O	24:V:46:SER:OG	2.25	0.52
24:V:262:PHE:CE2	24:V:283:LEU:HD22	2.45	0.52
17:T:46:DA:H2''	17:T:47:DG:N7	2.25	0.52
22:U:164:GLN:HB2	23:W:542:ALA:HB3	1.92	0.52
23:W:353:LYS:HD2	23:W:394:HIS:CE1	2.44	0.52
23:W:380:LYS:HB3	23:W:383:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.92	0.52
2:B:859:ARG:HG2	14:Z:737:HIS:HA	1.91	0.52
19:b:92:ARG:NE	21:d:73:GLU:OE2	2.42	0.52
20:g:81:ARG:O	20:g:84:GLN:HG3	2.10	0.52
3:C:189:ASP:O	3:C:191:ALA:N	2.42	0.51
3:C:259:LEU:HD22	11:K:42:LEU:HD23	1.91	0.51
5:E:91:CYS:SG	5:E:121:MET:HE1	2.50	0.51
1:A:1288:ILE:O	1:A:1292:MET:HG3	2.09	0.51
2:B:834:ARG:HD3	2:B:840:MET:SD	2.50	0.51
7:G:44:PHE:HB2	7:G:157:ILE:HD11	1.90	0.51
22:U:22:GLU:O	22:U:55:LYS:NZ	2.32	0.51
23:W:149:MET:CE	24:V:46:SER:HB2	2.29	0.51
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.44	0.51
2:B:678:THR:H	2:B:682:LEU:HD13	1.75	0.51
2:B:1038:THR:HA	3:C:195:THR:HA	1.93	0.51
9:I:24:LEU:HG	9:I:37:TYR:HB3	1.93	0.51
23:W:120:LYS:HA	23:W:158:LEU:HD12	1.91	0.51
1:A:831:LEU:HB3	1:A:835:GLU:HG3	1.93	0.51
2:B:818:GLU:OE2	12:L:31:ARG:NH2	2.43	0.51
15:N:1:DC:H2''	15:N:2:DG:H8	1.74	0.51
17:T:-59:DT:H2''	17:T:-58:DG:H5''	1.93	0.51
20:c:37:GLY:HA3	20:c:39:TYR:CZ	2.46	0.51
23:W:96:LEU:O	23:W:100:TRP:HD1	1.93	0.51
1:A:811:ILE:HG22	2:B:674:MET:HE1	1.91	0.51
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.39	0.51
14:Z:364:ASN:O	14:Z:374:LYS:NZ	2.35	0.51
24:V:194:THR:HA	24:V:197:GLN:HG2	1.93	0.51
2:B:608:ARG:HH12	9:I:100:HIS:CD2	2.28	0.51
15:N:-7:DG:H2''	15:N:-6:DG:C8	2.45	0.51
17:T:-68:DG:H2''	17:T:-67:DA:H5''	1.92	0.51
20:c:84:GLN:HE21	20:c:88:ARG:NE	2.08	0.51
20:c:85:LEU:HD22	20:c:108:LEU:HD23	1.93	0.51
20:g:96:LEU:HD11	21:h:100:PRO:HD3	1.92	0.51
23:W:357:ILE:HD12	23:W:390:VAL:HG12	1.93	0.51
24:V:195:ARG:HH22	24:V:270:ILE:HG21	1.75	0.51
7:G:39:THR:HG23	7:G:42:TYR:H	1.75	0.51
17:T:22:DC:H2'	17:T:23:DA:C8	2.46	0.51
22:U:166:LYS:NZ	23:W:541:ILE:O	2.43	0.51
23:W:314:PHE:HB2	23:W:359:ILE:HD11	1.93	0.51
1:A:743:ARG:NH1	23:W:442:GLN:HA	2.26	0.51
1:A:1165:THR:OG1	1:A:1294:THR:O	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:7:PRO:HG3	13:Y:23:LYS:HA	1.92	0.51
19:f:72:TYR:O	19:f:76:ALA:N	2.43	0.51
2:B:850:ASP:OD1	2:B:850:ASP:N	2.43	0.51
15:N:58:DC:P	20:c:76:THR:H	2.33	0.51
1:A:189:PRO:HB2	1:A:200:ALA:HB1	1.93	0.51
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.93	0.51
2:B:587:LEU:HB3	2:B:603:MET:HE3	1.93	0.51
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.51
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.93	0.51
14:Z:178:ASN:OD1	14:Z:179:LEU:N	2.43	0.51
15:N:-74:DT:H2''	15:N:-73:DT:C6	2.46	0.51
19:b:102:GLY:OXT	21:h:64:ASN:ND2	2.44	0.51
23:W:100:TRP:CZ3	24:V:96:LEU:HD23	2.46	0.51
24:V:73:LEU:HD13	24:V:112:VAL:HG22	1.93	0.51
24:V:168:TYR:CE2	24:V:237:LEU:HB2	2.45	0.51
3:C:44:ILE:HD12	3:C:178:PRO:HB3	1.92	0.50
4:D:126:GLU:HA	4:D:129:GLN:HG2	1.92	0.50
7:G:100:GLU:HA	7:G:104:MET:O	2.11	0.50
9:I:64:GLU:O	9:I:68:ILE:HG12	2.11	0.50
13:Y:12:HIS:C	13:Y:14:ARG:HH12	2.20	0.50
1:A:41:ILE:HB	1:A:88:ILE:HG22	1.94	0.50
1:A:322:LEU:H	1:A:327:ARG:NH2	2.09	0.50
1:A:467:MET:HB3	1:A:491:PRO:HB3	1.93	0.50
2:B:680:ASP:O	2:B:684:GLU:HG2	2.11	0.50
13:Y:16:CYS:HA	13:Y:53:THR:HG22	1.92	0.50
14:Z:336:PRO:HD2	14:Z:338:ARG:HH22	1.76	0.50
14:Z:450:ILE:HG22	14:Z:463:PHE:H	1.76	0.50
1:A:1286:ARG:NH2	9:I:54:TYR:HB2	2.27	0.50
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.93	0.50
2:B:585:ASN:O	2:B:589:LYS:HG2	2.10	0.50
13:Y:22:VAL:HB	13:Y:84:VAL:HG13	1.93	0.50
15:N:-56:DG:H21	20:g:77:ARG:HH22	1.59	0.50
20:g:92:GLU:HB3	21:h:100:PRO:HG2	1.93	0.50
23:W:322:PRO:O	23:W:375:ARG:NH1	2.44	0.50
23:W:559:ASN:CG	23:W:560:ASP:H	2.20	0.50
24:V:85:LYS:NZ	24:V:87:GLU:HB2	2.26	0.50
4:D:63:LYS:HA	4:D:66:ASN:ND2	2.26	0.50
7:G:18:PHE:HA	7:G:22:LEU:HD13	1.92	0.50
7:G:43:GLY:HA3	7:G:78:ARG:HD3	1.94	0.50
17:T:17:DA:H5'	17:T:17:DA:C8	2.47	0.50
9:I:39:CYS:SG	9:I:40:ARG:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:GLU:N	1:A:1215:GLU:OE1	2.44	0.50
1:A:1301:ILE:HG23	1:A:1345:ARG:NH2	2.27	0.50
3:C:7:PRO:HA	3:C:24:GLU:O	2.11	0.50
15:N:-45:DG:H2''	15:N:-44:DG:C8	2.47	0.50
17:T:105:DA:H2'	17:T:106:DG:H8	1.76	0.50
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.94	0.50
14:Z:433:LEU:HD13	14:Z:461:LEU:HD13	1.94	0.50
17:T:83:DA:H2'	17:T:84:DC:C6	2.47	0.50
18:e:62:ILE:HG12	19:f:33:ALA:HB1	1.93	0.50
23:W:295:ALA:HB1	23:W:309:ASP:OD1	2.11	0.50
23:W:318:THR:HB	23:W:358:HIS:CE1	2.46	0.50
23:W:397:CYS:HB3	23:W:430:TRP:CD1	2.47	0.50
1:A:104:MET:HB3	1:A:108:ARG:HH12	1.76	0.50
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.92	0.50
2:B:550:MET:SD	2:B:575:GLY:HA3	2.50	0.50
2:B:847:LYS:HG2	2:B:854:ILE:HD11	1.94	0.50
7:G:97:LEU:HD23	7:G:108:ILE:HD13	1.93	0.50
8:H:36:LYS:NZ	22:U:16:LYS:HD2	2.26	0.50
22:U:144:LEU:HD12	22:U:148:ALA:HB1	1.94	0.50
23:W:415:TYR:HA	23:W:418:ILE:HG12	1.94	0.50
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.37	0.50
5:E:66:ASP:OD1	5:E:67:ASP:N	2.45	0.50
5:E:84:ILE:HD11	5:E:113:SER:HB2	1.94	0.50
8:H:60:ILE:HG23	8:H:141:VAL:HG13	1.94	0.50
14:Z:554:GLU:OE1	14:Z:557:THR:OG1	2.28	0.50
7:G:104:MET:HB3	7:G:106:CYS:SG	2.52	0.49
15:N:-79:DG:H8	15:N:-79:DG:OP2	1.95	0.49
17:T:111:DT:H2''	17:T:112:DT:C6	2.47	0.49
1:A:67:ARG:NH1	1:A:68:THR:H	2.09	0.49
1:A:485:ASN:O	1:A:488:VAL:HG22	2.11	0.49
1:A:863:ARG:HH12	1:A:1129:ASN:ND2	2.10	0.49
4:D:73:ARG:HG3	4:D:104:CYS:SG	2.52	0.49
13:Y:88:SER:OG	13:Y:113:THR:OG1	2.29	0.49
1:A:1189:ASP:HA	1:A:1192:TRP:CZ3	2.47	0.49
7:G:30:LEU:HD22	7:G:70:VAL:HG21	1.94	0.49
24:V:161:VAL:HG12	24:V:165:LEU:HG	1.92	0.49
5:E:9:ARG:HG3	5:E:136:LEU:HD21	1.93	0.49
13:Y:9:ASP:OD1	13:Y:9:ASP:N	2.46	0.49
15:N:-81:DG:H2'	15:N:-80:DT:O4'	2.12	0.49
20:c:44:GLY:N	21:d:86:ILE:O	2.30	0.49
22:U:137:LEU:O	23:W:260:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:481:HIS:O	23:W:489:GLN:NE2	2.45	0.49
24:V:372:ARG:HE	24:V:414:PHE:HZ	1.60	0.49
1:A:1166:LEU:HD23	1:A:1293:LEU:HA	1.94	0.49
1:A:1221:MET:HE1	1:A:1227:THR:HA	1.95	0.49
1:A:1313:GLN:OE1	1:A:1332:GLN:NE2	2.44	0.49
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.94	0.49
17:T:-49:DG:H2''	17:T:-48:DC:C5	2.47	0.49
21:d:55:ALA:O	21:d:59:MET:HG3	2.12	0.49
22:U:178:LEU:HD13	23:W:450:VAL:HG13	1.94	0.49
4:D:107:THR:HG23	4:D:110:GLU:H	1.76	0.49
24:V:422:CYS:SG	24:V:451:THR:HB	2.53	0.49
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.95	0.49
2:B:125:TYR:HB3	2:B:146:LYS:HA	1.94	0.49
8:H:8:ASP:OD1	8:H:34:SER:OG	2.31	0.49
17:T:88:DA:H2''	17:T:89:DA:H8	1.77	0.49
17:T:116:DT:H2''	17:T:117:DG:C8	2.48	0.49
19:f:68:ASP:O	19:f:71:THR:OG1	2.22	0.49
22:U:128:VAL:HA	23:W:213:LEU:HD21	1.94	0.49
24:V:331:LEU:HD11	25:X:12:GLU:HG3	1.95	0.49
15:N:-8:DG:H5'	15:N:-8:DG:C8	2.47	0.49
20:g:30:VAL:HG11	20:g:51:LEU:HD23	1.95	0.49
23:W:100:TRP:HH2	24:V:116:VAL:HG21	1.77	0.49
24:V:473:ALA:O	24:V:476:PHE:HB2	2.12	0.49
7:G:30:LEU:O	7:G:34:VAL:HG22	2.12	0.49
14:Z:212:ILE:HD11	14:Z:235:VAL:HA	1.95	0.49
17:T:22:DC:H2'	17:T:23:DA:H8	1.78	0.49
22:U:143:TYR:CD1	23:W:338:MET:HE1	2.48	0.49
23:W:238:TYR:HE1	23:W:265:VAL:HG12	1.78	0.49
24:V:376:MET:HE1	24:V:410:SER:OG	2.12	0.49
3:C:81:LYS:NZ	3:C:126:ARG:HH22	2.10	0.49
13:Y:36:CYS:CB	13:Y:42:MET:HE3	2.43	0.49
14:Z:278:TRP:HZ3	14:Z:392:GLU:HB3	1.78	0.49
15:N:65:DA:H1'	15:N:66:DT:H5'	1.93	0.49
1:A:422:ASP:OD1	1:A:422:ASP:N	2.45	0.48
3:C:59:LEU:HD13	3:C:63:PHE:CD2	2.48	0.48
6:F:72:GLN:HE21	7:G:18:PHE:HE2	1.61	0.48
14:Z:258:LYS:H	14:Z:258:LYS:HD2	1.78	0.48
17:T:-38:DC:H2''	17:T:-37:DG:OP2	2.13	0.48
1:A:367:ILE:HD13	1:A:501:MET:SD	2.52	0.48
2:B:265:GLN:HB2	2:B:324:ARG:HG2	1.94	0.48
14:Z:239:ILE:HD12	14:Z:245:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:607:HIS:CE1	14:Z:636:PHE:HB2	2.48	0.48
22:U:13:LEU:HD21	22:U:41:ILE:HG12	1.95	0.48
22:U:53:LYS:NZ	22:U:85:ASP:OD1	2.35	0.48
23:W:149:MET:HB3	23:W:155:TRP:HB3	1.93	0.48
1:A:364:ARG:HD2	2:B:1084:LEU:HD11	1.95	0.48
5:E:67:ASP:HB2	24:V:271:ARG:NH2	2.28	0.48
15:N:15:DT:H2''	15:N:16:DA:N7	2.29	0.48
15:N:38:DG:H5''	20:c:45:ALA:H	1.78	0.48
20:c:41:GLU:HB2	20:g:38:ASN:OD1	2.13	0.48
23:W:115:VAL:O	23:W:119:LEU:HG	2.13	0.48
2:B:177:CYS:SG	2:B:738:THR:OG1	2.65	0.48
6:F:71:LEU:O	6:F:75:MET:HG3	2.14	0.48
12:L:31:ARG:HA	12:L:31:ARG:NE	2.27	0.48
12:L:54:VAL:HB	14:Z:721:ILE:HG12	1.94	0.48
15:N:-78:DG:H2''	15:N:-77:DC:H5''	1.94	0.48
15:N:56:DG:H2''	15:N:57:DG:N7	2.29	0.48
21:h:108:VAL:O	21:h:112:THR:HG23	2.13	0.48
23:W:63:PHE:HZ	24:V:34:GLN:HE21	1.62	0.48
23:W:135:ILE:HA	23:W:138:GLU:HG2	1.95	0.48
24:V:232:VAL:HG23	24:V:308:PRO:HG3	1.95	0.48
24:V:318:THR:HG23	24:V:338:LEU:HD11	1.95	0.48
2:B:993:LYS:HE3	2:B:995:GLU:HG2	1.95	0.48
5:E:173:ILE:O	5:E:209:VAL:HA	2.14	0.48
15:N:-96:DT:H2''	15:N:-95:DG:C8	2.49	0.48
24:V:426:LEU:HB3	24:V:461:PHE:CD1	2.48	0.48
2:B:848:LEU:HD12	2:B:852:GLY:C	2.39	0.48
14:Z:550:ILE:HG12	14:Z:560:VAL:HG22	1.96	0.48
17:T:115:DC:C6	17:T:115:DC:H5'	2.49	0.48
2:B:88:PHE:CE2	2:B:412:LEU:HD21	2.45	0.48
2:B:1142:ASN:OD1	2:B:1145:GLN:N	2.36	0.48
13:Y:23:LYS:HB3	13:Y:28:PHE:CE2	2.49	0.48
14:Z:498:ASN:OD1	14:Z:499:PHE:N	2.47	0.48
17:T:15:DT:H2''	17:T:16:DA:C8	2.47	0.48
23:W:324:PRO:HB2	23:W:326:GLU:HG2	1.95	0.48
24:V:295:GLU:O	24:V:298:LEU:HB2	2.14	0.48
2:B:851:ASP:HB2	12:L:15:MET:SD	2.54	0.48
15:N:-95:DG:H2''	15:N:-94:DG:H5''	1.95	0.48
15:N:58:DC:OP1	20:c:76:THR:N	2.45	0.48
18:e:74:ILE:HG21	19:f:63:GLU:HG2	1.95	0.48
23:W:264:GLU:HA	23:W:267:ARG:HG2	1.95	0.48
1:A:47:THR:HG22	1:A:52:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:HE2	2:B:87:LYS:HA	1.96	0.48
2:B:85:LEU:HB2	2:B:131:THR:HB	1.96	0.48
4:D:30:GLU:HB2	7:G:4:HIS:HB3	1.96	0.48
5:E:58:LEU:HD23	5:E:58:LEU:H	1.78	0.48
9:I:88:LYS:NZ	9:I:121:HIS:HB2	2.29	0.48
18:a:58:THR:OG1	20:g:104:GLN:O	2.31	0.48
18:a:63:ARG:HG3	18:a:66:PRO:HG2	1.95	0.48
18:a:93:GLN:O	18:a:97:GLU:HG3	2.14	0.48
19:b:79:LYS:HA	19:b:79:LYS:HD3	1.61	0.48
1:A:241:ARG:NH2	1:A:242:TYR:OH	2.46	0.47
1:A:452:ASP:OD1	1:A:476:ILE:HG12	2.14	0.47
1:A:466:LYS:HG2	1:A:524:MET:HE1	1.95	0.47
1:A:1342:SER:HB3	1:A:1346:VAL:HG23	1.95	0.47
2:B:40:VAL:HG11	2:B:482:LEU:HD13	1.95	0.47
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.46	0.47
2:B:859:ARG:NH2	14:Z:740:CYS:HA	2.28	0.47
5:E:51:GLY:N	5:E:54:ARG:HH22	2.13	0.47
14:Z:479:LYS:HG3	14:Z:489:THR:HG22	1.96	0.47
15:N:-69:DG:H2''	15:N:-68:DT:H5'	1.96	0.47
2:B:88:PHE:CD1	2:B:128:ILE:HG12	2.50	0.47
2:B:110:PRO:HG2	2:B:163:LEU:HD13	1.95	0.47
2:B:529:MET:HE1	2:B:698:ILE:HD12	1.96	0.47
12:L:26:ASN:ND2	12:L:44:MET:HE1	2.26	0.47
15:N:63:DG:H5'	15:N:63:DG:H8	1.79	0.47
17:T:116:DT:H2''	17:T:117:DG:N7	2.29	0.47
24:V:214:LEU:HA	24:V:217:MET:HE3	1.94	0.47
24:V:376:MET:SD	24:V:411:PHE:HB2	2.54	0.47
1:A:117:LEU:HD23	1:A:120:ASP:HA	1.95	0.47
1:A:812:LYS:NZ	2:B:671:GLU:OE2	2.37	0.47
5:E:98:ASN:HB3	24:V:281:ARG:HD2	1.96	0.47
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.95	0.47
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.97	0.47
14:Z:549:VAL:HB	14:Z:635:MET:HE2	1.97	0.47
23:W:269:ALA:HB1	23:W:274:HIS:CG	2.50	0.47
1:A:945:ASN:HB3	1:A:948:ILE:HG12	1.95	0.47
2:B:626:LEU:HD23	2:B:633:LEU:HD23	1.95	0.47
3:C:255:LYS:HE3	11:K:42:LEU:HD11	1.97	0.47
5:E:36:THR:OG1	5:E:39:GLU:OE1	2.28	0.47
5:E:98:ASN:ND2	24:V:278:LYS:HG3	2.29	0.47
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.39	0.47
24:V:192:PRO:HG2	24:V:267:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:300:ASP:O	24:V:303:MET:HB3	2.13	0.47
24:V:339:LEU:HD11	24:V:370:ILE:HG21	1.95	0.47
1:A:322:LEU:H	1:A:327:ARG:HH21	1.63	0.47
1:A:1359:SER:O	1:A:1361:ASP:N	2.47	0.47
2:B:833:THR:HB	2:B:836:THR:HG22	1.95	0.47
4:D:34:ASN:OD1	4:D:35:SER:N	2.47	0.47
10:J:6:ARG:HG2	10:J:13:ILE:HD13	1.97	0.47
20:c:71:ARG:CZ	21:d:46:HIS:HD2	2.27	0.47
22:U:48:LEU:HD23	22:U:52:VAL:HG11	1.96	0.47
24:V:462:LEU:HB3	24:V:503:HIS:CD2	2.48	0.47
1:A:467:MET:HG2	1:A:534:VAL:HG21	1.97	0.47
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.96	0.47
3:C:81:LYS:HZ3	3:C:126:ARG:NH2	2.12	0.47
4:D:103:LEU:HD21	7:G:85:VAL:HA	1.96	0.47
23:W:155:TRP:CE3	23:W:158:LEU:HD13	2.49	0.47
23:W:328:ILE:HG12	23:W:363:ALA:HB2	1.96	0.47
24:V:143:VAL:HG11	24:V:206:ARG:HH22	1.78	0.47
24:V:150:TRP:HZ3	24:V:207:MET:HG3	1.79	0.47
1:A:29:ASP:OD1	1:A:30:GLU:N	2.46	0.47
1:A:1054:MET:SD	1:A:1058:PHE:HD2	2.38	0.47
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.47	0.47
2:B:917:LYS:HD3	12:L:31:ARG:HH12	1.78	0.47
3:C:45:ILE:HG13	3:C:79:VAL:HG12	1.95	0.47
7:G:38:CYS:HB2	7:G:44:PHE:CD2	2.49	0.47
7:G:98:PHE:HE1	14:Z:508:MET:HE2	1.79	0.47
14:Z:422:PRO:HA	14:Z:440:ILE:HB	1.96	0.47
14:Z:584:ALA:HB3	14:Z:617:LEU:HD23	1.96	0.47
15:N:-82:DG:H2''	15:N:-81:DG:C8	2.50	0.47
15:N:70:DG:OP1	18:e:45:THR:OG1	2.32	0.47
17:T:-57:DC:H2''	17:T:-56:DC:C4	2.50	0.47
17:T:21:DC:H2'	17:T:22:DC:H6	1.78	0.47
19:b:34:ILE:HA	19:b:37:LEU:HD12	1.96	0.47
20:c:81:ARG:HH22	18:e:56:LYS:HB2	1.80	0.47
21:d:42:LEU:O	21:d:46:HIS:N	2.47	0.47
23:W:520:LEU:HD22	23:W:530:ILE:HG21	1.95	0.47
24:V:66:PHE:CZ	24:V:108:SER:HB2	2.50	0.47
24:V:499:ASN:OD1	24:V:500:VAL:N	2.47	0.47
25:X:22:LEU:HD11	25:X:26:LYS:HE3	1.95	0.47
1:A:61:ARG:O	1:A:73:THR:OG1	2.26	0.47
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.35	0.47
1:A:1412:MET:HE3	1:A:1419:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.96	0.47
4:D:67:TYR:CE1	7:G:101:ILE:HG22	2.50	0.47
6:F:57:MET:HB2	6:F:123:LEU:CD1	2.45	0.47
18:e:107:THR:HG23	18:e:123:ASP:HB3	1.97	0.47
24:V:375:PRO:HA	25:X:15:LEU:HD22	1.97	0.47
24:V:412:THR:HG22	24:V:447:GLY:HA2	1.97	0.47
24:V:501:HIS:CD2	24:V:527:LEU:HD22	2.49	0.47
1:A:102:LYS:HB3	1:A:248:MET:HE1	1.97	0.47
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	2.15	0.47
1:A:873:VAL:HG12	1:A:1083:PRO:HA	1.97	0.47
5:E:154:GLU:O	5:E:157:THR:OG1	2.26	0.47
9:I:36:LEU:HB2	9:I:45:GLN:HE21	1.80	0.47
15:N:48:DG:H2''	15:N:49:DC:C5	2.50	0.47
17:T:-36:DT:H2''	17:T:-35:DA:N7	2.30	0.47
23:W:144:ALA:O	23:W:148:GLN:HG3	2.15	0.47
24:V:66:PHE:HZ	24:V:108:SER:HB2	1.80	0.47
24:V:85:LYS:HB3	24:V:88:GLU:HG2	1.96	0.47
24:V:236:THR:OG1	24:V:308:PRO:HD2	2.14	0.47
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.14	0.47
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.50	0.47
7:G:92:VAL:HG21	7:G:138:GLN:HA	1.96	0.47
9:I:49:ASP:N	9:I:49:ASP:OD2	2.47	0.47
15:N:-36:DG:H2''	15:N:-35:DG:N7	2.30	0.47
17:T:6:DC:H2''	17:T:7:DC:C5	2.50	0.47
17:T:11:DG:H2'	17:T:12:DT:H71	1.96	0.47
23:W:89:ALA:O	23:W:93:THR:OG1	2.15	0.47
23:W:150:ILE:O	23:W:156:ARG:NH1	2.48	0.47
24:V:225:LEU:HB3	24:V:234:TYR:CZ	2.50	0.47
1:A:117:LEU:N	1:A:232:GLU:OE2	2.48	0.46
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.97	0.46
1:A:839:HIS:HE1	2:B:719:SER:H	1.63	0.46
1:A:861:GLN:O	1:A:865:ILE:HG12	2.15	0.46
2:B:861:SER:HA	2:B:901:THR:HA	1.97	0.46
6:F:105:ILE:HG22	6:F:119:GLY:HA2	1.97	0.46
7:G:29:LYS:O	7:G:33:GLU:OE1	2.33	0.46
15:N:-40:DC:C6	15:N:-39:DT:H72	2.50	0.46
15:N:63:DG:H5'	15:N:63:DG:C8	2.50	0.46
18:a:51:ILE:HG12	19:b:39:ARG:HB3	1.98	0.46
18:a:79:LYS:HB3	18:a:82:LEU:HD11	1.96	0.46
18:e:70:LEU:HD21	19:f:29:ILE:HD11	1.96	0.46
22:U:14:HIS:HA	22:U:52:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.22	0.46
1:A:1177:TYR:HD2	9:I:35:LEU:HD13	1.81	0.46
1:A:1210:TRP:HH2	1:A:1281:ASP:HB3	1.79	0.46
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.97	0.46
2:B:848:LEU:HD23	2:B:848:LEU:H	1.80	0.46
7:G:109:SER:HB3	14:Z:493:VAL:HG11	1.97	0.46
14:Z:200:PHE:HD1	14:Z:210:LEU:HB2	1.80	0.46
18:a:119:ILE:HG12	19:b:43:VAL:HG11	1.97	0.46
22:U:72:LYS:HB2	22:U:101:PRO:HB3	1.98	0.46
23:W:87:TYR:OH	23:W:92:GLN:OE1	2.25	0.46
2:B:223:SER:OG	2:B:350:HIS:ND1	2.34	0.46
3:C:44:ILE:HD11	3:C:238:SER:HB3	1.97	0.46
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.46
15:N:15:DT:H2''	15:N:16:DA:C8	2.51	0.46
19:b:44:LYS:HE3	20:g:117:PRO:HG3	1.97	0.46
22:U:87:ASP:HB3	22:U:90:VAL:HG23	1.97	0.46
22:U:143:TYR:O	23:W:421:PRO:HB2	2.15	0.46
1:A:1156:ASP:OD1	1:A:1157:ILE:N	2.49	0.46
15:N:17:DA:OP1	18:a:69:ARG:NH2	2.48	0.46
17:T:-52:DG:OP1	21:d:39:TYR:OH	2.33	0.46
19:f:84:MET:HG2	19:f:88:TYR:CZ	2.51	0.46
23:W:365:SER:HB2	23:W:382:GLU:HB3	1.97	0.46
1:A:35:SER:OG	1:A:36:VAL:N	2.48	0.46
1:A:88:ILE:HG12	1:A:253:LEU:HB3	1.97	0.46
1:A:1234:LYS:HE2	1:A:1298:LEU:HA	1.96	0.46
2:B:538:PRO:HA	2:B:541:ILE:HD13	1.97	0.46
3:C:172:GLU:OE1	12:L:58:ARG:NH2	2.48	0.46
14:Z:257:ILE:O	14:Z:260:MET:HG2	2.15	0.46
19:b:34:ILE:HG21	19:b:51:TYR:HA	1.98	0.46
23:W:337:PHE:CZ	23:W:356:TYR:HB3	2.51	0.46
24:V:429:VAL:HG21	24:V:448:LEU:HD21	1.97	0.46
1:A:828:LEU:HD11	2:B:1008:VAL:HG21	1.97	0.46
1:A:1086:MET:HB3	1:A:1086:MET:HE3	1.76	0.46
2:B:124:LEU:HD22	2:B:152:ILE:HD11	1.98	0.46
2:B:566:LYS:HA	2:B:576:ILE:HD12	1.97	0.46
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.46	0.46
5:E:36:THR:N	5:E:39:GLU:OE2	2.46	0.46
7:G:151:ARG:HB2	14:Z:491:LEU:HD21	1.97	0.46
9:I:58:ILE:O	9:I:60:HIS:ND1	2.46	0.46
15:N:-43:DT:H3'	20:g:17:ARG:HG3	1.97	0.46
17:T:-45:DA:H2''	17:T:-44:DA:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:h:59:MET:HA	21:h:59:MET:HE2	1.98	0.46
23:W:48:LEU:HD22	23:W:82:LEU:HD12	1.97	0.46
23:W:248:LEU:HD13	23:W:258:VAL:HG21	1.97	0.46
23:W:353:LYS:O	23:W:357:ILE:HG12	2.15	0.46
1:A:59:ASP:OD2	1:A:61:ARG:NH2	2.43	0.46
1:A:1458:ILE:HD13	2:B:1091:ARG:HD2	1.97	0.46
2:B:55:VAL:O	2:B:58:ILE:HG22	2.16	0.46
2:B:937:SER:OG	2:B:938:ARG:N	2.49	0.46
4:D:44:ARG:NH1	4:D:57:LEU:HD23	2.30	0.46
12:L:37:ARG:HD2	12:L:37:ARG:N	2.31	0.46
19:f:76:ALA:O	19:f:78:ARG:HG3	2.15	0.46
20:g:97:LEU:HD11	21:h:62:PHE:CE1	2.51	0.46
23:W:87:TYR:HB3	24:V:2:PHE:HZ	1.80	0.46
24:V:196:ARG:HD2	24:V:244:SER:HB2	1.98	0.46
24:V:375:PRO:HA	24:V:378:MET:HE3	1.97	0.46
24:V:486:PHE:HA	24:V:490:PHE:HD2	1.79	0.46
1:A:199:TYR:CZ	1:A:213:LYS:HE3	2.51	0.46
1:A:199:TYR:HB3	1:A:215:LEU:HA	1.98	0.46
1:A:413:TYR:O	1:A:415:GLY:N	2.46	0.46
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.97	0.46
1:A:1130:ILE:HG23	1:A:1362:ILE:HD11	1.97	0.46
2:B:235:ILE:HD13	2:B:261:PRO:HD3	1.97	0.46
2:B:910:THR:OG1	2:B:911:LEU:N	2.47	0.46
15:N:-37:DG:H2''	15:N:-36:DG:C8	2.51	0.46
17:T:-54:DA:H4'	20:c:77:ARG:HH11	1.80	0.46
21:d:99:LEU:HD22	21:d:103:LEU:HD23	1.98	0.46
24:V:275:VAL:HG13	24:V:279:ARG:CB	2.46	0.46
1:A:212:LYS:HB3	1:A:214:ILE:HG23	1.98	0.46
1:A:609:HIS:HA	1:A:626:THR:HG21	1.98	0.46
1:A:839:HIS:CE1	2:B:719:SER:H	2.34	0.46
2:B:91:ILE:HD12	2:B:126:VAL:HB	1.97	0.46
15:N:-35:DG:H2'	15:N:-34:DT:H71	1.97	0.46
23:W:152:HIS:HB2	23:W:155:TRP:HD1	1.81	0.46
24:V:123:VAL:HB	24:V:128:LEU:HD21	1.98	0.46
1:A:927:GLU:HG2	1:A:931:ARG:HH12	1.81	0.46
5:E:14:ARG:O	5:E:18:MET:HG2	2.16	0.46
23:W:89:ALA:HB1	23:W:92:GLN:HB2	1.98	0.46
23:W:559:ASN:OD1	23:W:560:ASP:N	2.43	0.46
24:V:70:ARG:O	24:V:73:LEU:HG	2.16	0.46
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.49	0.45
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-23:DT:C2	15:N:-22:DG:C8	3.04	0.45
15:N:6:DA:H2''	15:N:7:DC:C5	2.51	0.45
24:V:113:VAL:O	24:V:117:MET:HG2	2.15	0.45
24:V:369:LEU:HD23	24:V:420:MET:HB3	1.99	0.45
1:A:15:LEU:HD11	2:B:1150:ARG:HG3	1.98	0.45
1:A:542:LEU:HA	1:A:545:VAL:HG12	1.99	0.45
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.98	0.45
4:D:26:PHE:CD2	7:G:80:PHE:HZ	2.35	0.45
14:Z:539:LEU:HA	14:Z:549:VAL:HG22	1.98	0.45
15:N:46:DG:H1'	15:N:47:DA:C5	2.50	0.45
23:W:485:ASP:OD1	23:W:486:VAL:N	2.50	0.45
1:A:325:LEU:O	1:A:327:ARG:NH1	2.50	0.45
2:B:92:TYR:HD1	2:B:146:LYS:HG3	1.82	0.45
8:H:8:ASP:OD2	8:H:32:SER:OG	2.27	0.45
8:H:59:VAL:O	8:H:144:LEU:HB2	2.17	0.45
20:g:88:ARG:NH2	20:g:100:VAL:O	2.50	0.45
1:A:982:ASN:O	1:A:986:MET:HG3	2.17	0.45
2:B:1109:GLU:HA	2:B:1113:PRO:HG3	1.99	0.45
10:J:66:GLU:HG3	12:L:18:ILE:HG21	1.98	0.45
15:N:-64:DT:C6	15:N:-63:DT:H72	2.52	0.45
17:T:-46:DC:H2''	17:T:-45:DA:N7	2.31	0.45
17:T:-14:DA:H4'	18:a:63:ARG:HH21	1.80	0.45
17:T:23:DA:H2'	17:T:24:DA:H8	1.80	0.45
19:f:90:LEU:HB3	19:f:96:THR:HA	1.99	0.45
23:W:146:LEU:HD11	23:W:175:THR:HG23	1.97	0.45
24:V:41:LEU:HD12	24:V:44:LEU:HD12	1.99	0.45
24:V:296:GLN:HA	24:V:360:PHE:CD1	2.51	0.45
1:A:104:MET:HB3	1:A:108:ARG:NH1	2.31	0.45
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.32	0.45
2:B:1144:THR:HG23	2:B:1145:GLN:CD	2.40	0.45
4:D:44:ARG:O	4:D:47:GLN:HG3	2.17	0.45
5:E:68:PRO:HD2	24:V:279:ARG:HH22	1.80	0.45
14:Z:549:VAL:C	14:Z:560:VAL:HG13	2.42	0.45
15:N:27:DG:C2	15:N:28:DA:C6	3.04	0.45
21:h:45:VAL:HG12	21:h:46:HIS:ND1	2.31	0.45
23:W:538:LEU:HD13	23:W:575:VAL:HG12	1.98	0.45
2:B:88:PHE:CE1	2:B:128:ILE:HG12	2.52	0.45
4:D:20:LEU:HD11	4:D:93:HIS:CG	2.52	0.45
17:T:-42:DT:OP2	20:c:20:ARG:NH2	2.49	0.45
20:g:50:TYR:CE1	21:h:111:GLY:HA3	2.49	0.45
21:h:34:TYR:HB3	21:h:37:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:138:PRO:HB2	22:U:140:GLU:HG2	1.98	0.45
24:V:260:HIS:CE1	24:V:261:LYS:HE3	2.51	0.45
2:B:96:PRO:HG3	2:B:154:ILE:HD13	1.99	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.98	0.45
4:D:32:LEU:HD21	7:G:4:HIS:HB2	1.99	0.45
5:E:69:THR:HB	24:V:278:LYS:HG2	1.98	0.45
9:I:30:LYS:HD3	9:I:30:LYS:N	2.32	0.45
14:Z:216:VAL:HB	14:Z:226:TYR:HB2	1.98	0.45
15:N:-80:DT:H2'	15:N:-79:DG:C8	2.52	0.45
15:N:70:DG:H2''	15:N:71:DA:C8	2.52	0.45
18:a:47:ALA:HB1	19:b:39:ARG:NH1	2.32	0.45
21:h:42:LEU:O	21:h:46:HIS:N	2.47	0.45
23:W:97:LEU:HD11	24:V:73:LEU:HB3	1.99	0.45
23:W:162:LEU:HB3	23:W:172:LEU:HD11	1.97	0.45
1:A:41:ILE:HG21	1:A:57:LEU:HD23	1.99	0.45
1:A:1157:ILE:HD13	1:A:1160:ARG:HH12	1.82	0.45
15:N:15:DT:H2''	15:N:16:DA:C5	2.51	0.45
19:b:75:HIS:HB2	21:d:93:THR:HG21	1.98	0.45
20:c:78:ILE:HD12	21:d:51:ILE:HG12	1.98	0.45
24:V:274:PHE:CD1	24:V:320:ARG:HD2	2.52	0.45
3:C:9:VAL:HG11	11:K:105:PHE:CD1	2.51	0.45
7:G:110:ARG:HA	7:G:113:ILE:HB	1.99	0.45
1:A:343:LEU:HA	1:A:349:ARG:H	1.81	0.45
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.17	0.45
3:C:35:ARG:HG3	3:C:182:VAL:HG11	1.99	0.45
4:D:44:ARG:HD3	4:D:61:PHE:CE1	2.51	0.45
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.30	0.45
14:Z:539:LEU:HB2	14:Z:616:HIS:CE1	2.52	0.45
14:Z:561:LEU:HD23	14:Z:635:MET:SD	2.56	0.45
15:N:-61:DT:H2''	15:N:-60:DT:H71	1.99	0.45
15:N:-18:DG:H2''	15:N:-17:DT:C5	2.52	0.45
15:N:25:DT:H2''	15:N:26:DA:N7	2.31	0.45
24:V:251:GLY:O	24:V:255:THR:OG1	2.22	0.45
1:A:487:SER:O	1:A:535:MET:HG2	2.17	0.44
2:B:407:MET:HB3	2:B:440:ILE:HD13	1.98	0.44
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.44	0.44
5:E:130:PHE:HB3	5:E:135:LEU:HD21	1.99	0.44
15:N:49:DC:H2''	15:N:50:DG:H8	1.83	0.44
17:T:8:DC:H2''	17:T:9:DG:C8	2.51	0.44
17:T:59:DA:H2''	17:T:60:DA:C8	2.52	0.44
17:T:117:DG:H2''	17:T:118:DA:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:N	1:A:10:ASP:OD1	2.49	0.44
1:A:119:VAL:HG21	1:A:147:LEU:HD23	1.98	0.44
3:C:81:LYS:HZ3	3:C:126:ARG:HH12	1.66	0.44
5:E:163:TYR:HB2	5:E:165:LEU:HD22	1.98	0.44
14:Z:353:ALA:HB3	14:Z:360:ILE:HB	2.00	0.44
14:Z:493:VAL:HB	14:Z:501:ILE:HG23	1.98	0.44
15:N:45:DT:H2''	15:N:46:DG:N7	2.31	0.44
18:e:85:GLN:O	18:e:89:ILE:HG13	2.17	0.44
21:h:99:LEU:HD22	21:h:103:LEU:HD23	1.98	0.44
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.45	0.44
2:B:36:GLU:HG3	2:B:37:LYS:HG3	1.99	0.44
17:T:5:DC:H2''	17:T:6:DC:C4	2.51	0.44
24:V:457:PHE:O	24:V:499:ASN:ND2	2.51	0.44
1:A:516:GLN:HA	1:A:520:MET:HG2	1.99	0.44
1:A:1484:MET:SD	1:A:1484:MET:N	2.91	0.44
2:B:790:GLN:HA	2:B:968:ASN:ND2	2.31	0.44
4:D:16:ASP:OD1	4:D:17:ALA:N	2.51	0.44
14:Z:464:PRO:HG2	14:Z:467:GLU:HB2	1.99	0.44
15:N:-99:DG:H5'	15:N:-99:DG:C8	2.53	0.44
17:T:49:DC:H2''	17:T:50:DA:C8	2.53	0.44
22:U:55:LYS:HA	22:U:55:LYS:HD3	1.82	0.44
1:A:16:ARG:O	2:B:1149:VAL:HG12	2.18	0.44
1:A:329:MET:HE2	1:A:329:MET:HB3	1.82	0.44
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	2.00	0.44
2:B:163:LEU:HD21	2:B:176:GLU:HG3	2.00	0.44
4:D:63:LYS:HA	4:D:63:LYS:HE3	1.99	0.44
9:I:60:HIS:HB3	9:I:103:ARG:NH1	2.33	0.44
14:Z:542:LEU:HD21	14:Z:560:VAL:HG11	1.99	0.44
21:d:72:GLY:O	21:d:76:ARG:HG3	2.18	0.44
22:U:138:PRO:HD3	23:W:256:SER:HB2	2.00	0.44
22:U:140:GLU:OE1	23:W:329:ARG:HB3	2.17	0.44
23:W:104:THR:HG22	24:V:80:ILE:HD11	1.98	0.44
24:V:367:VAL:HG21	25:X:5:PRO:HD3	1.98	0.44
1:A:514:GLU:CD	2:B:1101:GLN:HB2	2.42	0.44
1:A:1146:GLN:HA	1:A:1149:ARG:HH21	1.82	0.44
1:A:1218:ARG:NH2	1:A:1253:GLU:HA	2.32	0.44
2:B:448:LEU:HD23	2:B:448:LEU:HA	1.84	0.44
2:B:549:SER:OG	2:B:577:HIS:NE2	2.43	0.44
5:E:13:ILE:O	5:E:17:ILE:HG12	2.18	0.44
7:G:89:VAL:O	7:G:140:ASP:N	2.42	0.44
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:LEU:HB2	8:H:132:LEU:HD12	2.00	0.44
15:N:-34:DT:P	21:h:83:ARG:HE	2.39	0.44
17:T:-55:DG:H2''	17:T:-54:DA:N7	2.33	0.44
23:W:227:PHE:CZ	23:W:231:VAL:HG11	2.52	0.44
4:D:41:LEU:HD22	4:D:61:PHE:CE1	2.53	0.44
7:G:120:ASP:OD1	7:G:129:LYS:HG2	2.18	0.44
14:Z:193:ALA:O	14:Z:197:MET:HG3	2.18	0.44
14:Z:498:ASN:O	14:Z:515:PRO:HD3	2.18	0.44
15:N:-39:DT:H1'	15:N:-38:DT:H5''	2.00	0.44
15:N:55:DC:H2''	15:N:56:DG:N7	2.33	0.44
18:a:124:ILE:O	18:a:128:ARG:HG2	2.18	0.44
20:c:58:LEU:O	20:c:62:ILE:HG12	2.18	0.44
23:W:191:VAL:HA	23:W:204:VAL:HG11	1.99	0.44
24:V:246:HIS:ND1	24:V:260:HIS:HD2	2.15	0.44
24:V:275:VAL:CG1	24:V:341:LEU:HD21	2.43	0.44
24:V:543:GLN:O	24:V:547:LYS:HG2	2.18	0.44
1:A:1052:ARG:O	1:A:1056:GLU:HG2	2.18	0.44
2:B:801:VAL:HG13	2:B:929:PRO:HD2	2.00	0.44
2:B:1145:GLN:OE1	2:B:1145:GLN:N	2.51	0.44
4:D:44:ARG:HG3	4:D:47:GLN:HE21	1.83	0.44
5:E:141:GLU:N	5:E:141:GLU:OE1	2.51	0.44
14:Z:550:ILE:HG21	14:Z:553:LEU:HD23	1.99	0.44
15:N:54:DT:H6	15:N:54:DT:H2'	1.65	0.44
1:A:397:PHE:CZ	6:F:83:LEU:HD22	2.53	0.44
1:A:928:ARG:HE	8:H:106:THR:HB	1.83	0.44
15:N:38:DG:H5''	20:c:45:ALA:N	2.32	0.44
20:c:78:ILE:HB	21:d:51:ILE:HA	2.00	0.44
18:e:58:THR:HG22	18:e:58:THR:O	2.18	0.44
21:d:42:LEU:HD21	21:d:49:THR:O	2.18	0.44
19:f:68:ASP:HB3	19:f:72:TYR:CE2	2.52	0.44
19:f:97:LEU:O	19:f:102:GLY:HA3	2.18	0.44
21:h:87:THR:OG1	21:h:90:GLU:OE1	2.35	0.44
23:W:100:TRP:HB3	24:V:76:ARG:NH1	2.31	0.44
23:W:310:ILE:HG21	23:W:356:TYR:CD1	2.53	0.44
24:V:213:LYS:HG3	24:V:217:MET:HE2	2.00	0.44
14:Z:447:LYS:HG3	14:Z:449:THR:HG23	2.00	0.43
14:Z:536:TRP:HH2	14:Z:625:HIS:NE2	2.16	0.43
15:N:-6:DG:H2''	15:N:-5:DG:N7	2.33	0.43
21:h:39:TYR:HE1	21:h:51:ILE:HD11	1.82	0.43
1:A:798:ILE:HG23	1:A:841:MET:HE1	1.99	0.43
3:C:264:SER:HA	3:C:267:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:VAL:HG13	5:E:86:THR:HB	1.99	0.43
9:I:25:TYR:CE1	9:I:40:ARG:HG2	2.53	0.43
19:b:98:TYR:CD2	21:h:58:ILE:HG23	2.53	0.43
22:U:35:ALA:O	22:U:39:ASP:HB2	2.18	0.43
23:W:145:TRP:HA	23:W:148:GLN:HG3	1.98	0.43
1:A:561:MET:HG2	11:K:58:PHE:CD2	2.53	0.43
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	2.00	0.43
18:a:119:ILE:HG13	19:b:50:ILE:HG13	2.00	0.43
19:b:90:LEU:HB3	19:b:95:ARG:O	2.17	0.43
23:W:98:ALA:O	23:W:101:LEU:HG	2.18	0.43
24:V:267:ASP:HA	24:V:270:ILE:HD12	2.01	0.43
1:A:1235:ILE:HD13	1:A:1296:MET:HE2	1.99	0.43
1:A:1435:THR:O	1:A:1439:LEU:HD23	2.19	0.43
2:B:413:LYS:O	2:B:417:ILE:HG12	2.18	0.43
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.46	0.43
9:I:96:PHE:HD2	9:I:110:LEU:HD12	1.83	0.43
14:Z:472:PHE:CZ	14:Z:520:LEU:HB2	2.54	0.43
14:Z:543:ASP:N	14:Z:543:ASP:OD1	2.52	0.43
15:N:-46:DT:H2"	15:N:-45:DG:C8	2.53	0.43
22:U:22:GLU:HB2	22:U:24:TRP:HE3	1.82	0.43
22:U:92:MET:HE2	23:W:240:PHE:HB2	2.00	0.43
24:V:90:TYR:CD2	24:V:121:PRO:HG3	2.53	0.43
24:V:525:LYS:HA	24:V:528:GLU:OE1	2.18	0.43
1:A:214:ILE:HG13	1:A:214:ILE:O	2.17	0.43
1:A:496:PHE:HB2	2:B:791:GLU:O	2.19	0.43
1:A:936:GLU:HA	1:A:939:VAL:HG22	2.00	0.43
2:B:583:LEU:O	2:B:587:LEU:HD23	2.19	0.43
5:E:147:GLU:HB3	5:E:194:ILE:HB	2.00	0.43
7:G:91:GLN:HB3	7:G:98:PHE:HB2	1.99	0.43
14:Z:243:GLY:HA2	14:Z:246:ARG:HG2	2.01	0.43
14:Z:585:VAL:HA	14:Z:595:HIS:CE1	2.54	0.43
15:N:3:DC:H2"	15:N:4:DG:C8	2.54	0.43
17:T:-57:DC:H2"	17:T:-56:DC:C5	2.53	0.43
17:T:-43:DT:H5"	20:c:16:THR:HA	1.99	0.43
17:T:18:DC:OP1	18:e:64:LYS:HG2	2.18	0.43
22:U:156:LEU:HD11	23:W:463:GLN:HG3	2.01	0.43
1:A:712:ASP:HB3	1:A:744:ILE:HD13	1.99	0.43
1:A:853:LYS:NZ	1:A:1100:THR:O	2.48	0.43
2:B:595:ASP:OD1	2:B:596:ILE:N	2.47	0.43
5:E:128:GLU:OE1	5:E:128:GLU:N	2.52	0.43
14:Z:262:ASP:HA	14:Z:265:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:5:DC:H2''	17:T:6:DC:C5	2.53	0.43
21:h:60:ASN:O	21:h:64:ASN:ND2	2.51	0.43
23:W:63:PHE:CZ	24:V:31:GLU:HA	2.53	0.43
23:W:236:HIS:CE1	23:W:237:THR:HG23	2.54	0.43
24:V:284:GLN:HB2	24:V:340:LEU:HD22	1.99	0.43
24:V:326:VAL:HG21	24:V:381:LEU:HD23	2.01	0.43
24:V:445:LEU:HD12	24:V:448:LEU:HD12	2.01	0.43
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.59	0.43
13:Y:70:TRP:HA	13:Y:73:LYS:HE3	1.98	0.43
13:Y:77:VAL:HG11	13:Y:85:TYR:CE1	2.53	0.43
14:Z:423:GLY:HA2	14:Z:439:LYS:HE3	2.01	0.43
19:b:70:VAL:HG22	19:b:81:VAL:HG21	2.01	0.43
20:c:85:LEU:O	20:c:89:ASN:N	2.51	0.43
21:h:39:TYR:CE1	21:h:51:ILE:HD11	2.54	0.43
23:W:228:ALA:HA	23:W:231:VAL:HG22	1.99	0.43
23:W:557:LEU:HD23	23:W:557:LEU:O	2.19	0.43
24:V:120:LEU:HB2	24:V:123:VAL:HG22	2.00	0.43
1:A:222:HIS:O	1:A:226:LYS:HG3	2.18	0.43
1:A:867:SER:HB2	1:A:1414:ILE:HG23	2.01	0.43
1:A:986:MET:HE1	1:A:1072:ILE:HG12	2.00	0.43
2:B:455:ASP:OD1	2:B:456:GLN:N	2.52	0.43
2:B:649:ASN:CG	2:B:650:ASN:H	2.23	0.43
4:D:14:GLU:HA	14:Z:473:LYS:NZ	2.34	0.43
5:E:9:ARG:O	5:E:13:ILE:HG12	2.19	0.43
6:F:57:MET:HB2	6:F:123:LEU:HD13	2.00	0.43
14:Z:259:GLU:O	14:Z:262:ASP:HB3	2.19	0.43
13:Y:115:ILE:HB	14:Z:267:VAL:HG12	2.01	0.43
19:f:70:VAL:O	19:f:73:THR:HB	2.19	0.43
23:W:190:SER:O	23:W:193:THR:OG1	2.35	0.43
24:V:454:ASP:O	24:V:458:GLY:N	2.52	0.43
1:A:279:LYS:HD2	1:A:279:LYS:HA	1.86	0.43
1:A:1175:ILE:HG23	9:I:53:ILE:HB	1.99	0.43
1:A:1359:SER:C	1:A:1361:ASP:H	2.26	0.43
2:B:588:ARG:O	2:B:592:ARG:HD3	2.19	0.43
7:G:120:ASP:O	7:G:126:PRO:HA	2.19	0.43
8:H:143:LEU:HD12	8:H:143:LEU:HA	1.88	0.43
11:K:100:LEU:HD11	11:K:104:ARG:HE	1.84	0.43
13:Y:69:SER:OG	13:Y:71:VAL:HG12	2.18	0.43
14:Z:521:CYS:SG	14:Z:523:GLU:HG3	2.58	0.43
17:T:26:DG:H4'	17:T:27:DG:H5'	2.01	0.43
17:T:27:DG:H2''	17:T:28:DG:N7	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:292:ALA:HB2	23:W:316:MET:SD	2.59	0.43
23:W:325:VAL:HG22	23:W:329:ARG:HG2	2.00	0.43
24:V:115:CYS:HB3	24:V:119:HIS:CE1	2.54	0.43
24:V:432:ILE:HB	24:V:437:ASN:HB3	2.00	0.43
1:A:1321:ILE:HG13	1:A:1321:ILE:O	2.19	0.42
2:B:718:GLN:HG2	2:B:720:PRO:HD2	2.01	0.42
2:B:1104:ARG:HG3	2:B:1105:GLU:N	2.33	0.42
9:I:64:GLU:OE2	9:I:101:SER:OG	2.33	0.42
15:N:-34:DT:P	21:h:84:SER:H	2.42	0.42
15:N:-11:DC:C2	15:N:-10:DG:N7	2.87	0.42
19:f:84:MET:HG2	19:f:88:TYR:CE1	2.54	0.42
23:W:97:LEU:HD13	24:V:76:ARG:NH2	2.34	0.42
1:A:11:SER:HG	2:B:1117:HIS:HE2	1.64	0.42
1:A:511:THR:O	1:A:515:ILE:HG12	2.19	0.42
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.91	0.42
2:B:553:LEU:HB2	2:B:575:GLY:H	1.83	0.42
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.53	0.42
5:E:94:MET:SD	5:E:102:ALA:HB2	2.60	0.42
15:N:-67:DT:H2''	15:N:-66:DG:C8	2.54	0.42
17:T:86:DC:H2''	17:T:87:DA:H8	1.84	0.42
18:a:99:TYR:HB2	19:b:95:ARG:HH21	1.84	0.42
18:a:126:LEU:HG	18:e:113:HIS:HB2	1.99	0.42
20:g:63:LEU:HD13	21:h:42:LEU:HB2	2.00	0.42
22:U:24:TRP:HD1	23:W:274:HIS:CE1	2.37	0.42
23:W:299:MET:O	23:W:303:GLY:N	2.50	0.42
1:A:27:SER:OG	1:A:29:ASP:OD1	2.27	0.42
1:A:1162:GLU:HG3	1:A:1306:LYS:HA	2.01	0.42
1:A:1210:TRP:HE1	1:A:1261:ILE:HG22	1.84	0.42
1:A:1362:ILE:HG13	1:A:1363:VAL:N	2.34	0.42
2:B:968:ASN:OD1	2:B:970:HIS:ND1	2.51	0.42
15:N:37:DC:H2''	15:N:38:DG:N7	2.34	0.42
15:N:54:DT:H5'	15:N:54:DT:C6	2.54	0.42
21:d:97:LEU:HD23	21:d:97:LEU:HA	1.89	0.42
22:U:175:ARG:HH11	23:W:457:GLU:HA	1.83	0.42
1:A:486:LEU:O	1:A:489:THR:HG22	2.19	0.42
3:C:52:ILE:HD12	3:C:61:ASP:HB3	2.01	0.42
5:E:130:PHE:CD1	5:E:135:LEU:HD21	2.53	0.42
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.84	0.42
8:H:4:ILE:HD11	8:H:84:ARG:HE	1.84	0.42
8:H:5:LEU:HD22	8:H:134:GLY:HA3	2.02	0.42
12:L:50:LYS:HD3	12:L:50:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:277:SER:C	14:Z:278:TRP:HD1	2.27	0.42
15:N:-75:DG:H2''	15:N:-74:DT:C5	2.54	0.42
15:N:-32:DT:C2	15:N:-31:DA:N7	2.88	0.42
20:c:63:LEU:HD21	21:d:59:MET:HE1	2.01	0.42
22:U:92:MET:HE2	23:W:240:PHE:HD2	1.83	0.42
22:U:110:LEU:HB3	22:U:117:VAL:HG11	2.02	0.42
23:W:97:LEU:HD21	24:V:73:LEU:HD23	2.00	0.42
23:W:238:TYR:CE2	23:W:279:ILE:HG21	2.53	0.42
23:W:351:ASP:OD1	23:W:352:HIS:N	2.44	0.42
23:W:524:ASP:OD1	23:W:524:ASP:N	2.52	0.42
1:A:557:ARG:NH2	1:A:561:MET:HE1	2.34	0.42
1:A:1174:ALA:O	1:A:1212:LEU:HD12	2.19	0.42
1:A:1280:ASP:OD1	1:A:1280:ASP:N	2.52	0.42
4:D:87:LEU:HB3	4:D:97:LEU:HG	1.99	0.42
6:F:86:GLU:OE1	6:F:86:GLU:N	2.52	0.42
14:Z:200:PHE:HA	14:Z:210:LEU:HD13	2.00	0.42
15:N:4:DG:H2''	15:N:5:DT:C5	2.55	0.42
23:W:155:TRP:HE3	23:W:158:LEU:HD13	1.85	0.42
23:W:497:LEU:HD13	23:W:533:PHE:HB2	2.01	0.42
24:V:269:CYS:HG	24:V:279:ARG:NH1	2.16	0.42
1:A:129:ILE:HD13	1:A:143:HIS:HB3	2.02	0.42
1:A:1296:MET:HE3	1:A:1296:MET:HB3	1.87	0.42
2:B:455:ASP:HB3	2:B:458:LYS:HG3	2.01	0.42
3:C:16:ASP:OD1	3:C:240:ARG:NH2	2.32	0.42
6:F:86:GLU:HG2	6:F:92:ILE:HG12	2.02	0.42
14:Z:199:LYS:HG2	14:Z:210:LEU:HD11	2.01	0.42
17:T:-53:DG:H2''	17:T:-52:DG:C8	2.55	0.42
23:W:484:LEU:HD22	23:W:488:GLU:OE1	2.18	0.42
24:V:437:ASN:ND2	24:V:440:ALA:HB3	2.34	0.42
1:A:71:CYS:HB3	1:A:74:CYS:O	2.20	0.42
2:B:65:ILE:HD11	2:B:86:LEU:HD23	2.00	0.42
2:B:197:GLN:HB2	2:B:394:ASP:OD1	2.19	0.42
2:B:719:SER:OG	2:B:720:PRO:HD3	2.19	0.42
7:G:7:LEU:HB2	7:G:72:TYR:CZ	2.55	0.42
14:Z:260:MET:HE3	14:Z:260:MET:HB3	1.89	0.42
17:T:-47:DT:H2''	17:T:-46:DC:C5	2.55	0.42
17:T:-42:DT:H2''	17:T:-41:DG:C8	2.54	0.42
23:W:166:HIS:HB2	23:W:172:LEU:HD12	2.02	0.42
23:W:321:ASP:OD1	23:W:321:ASP:N	2.52	0.42
24:V:196:ARG:NH2	24:V:247:ASP:OD2	2.46	0.42
24:V:215:TYR:CZ	24:V:219:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:508:LEU:O	24:V:512:HIS:HB3	2.19	0.42
1:A:803:LYS:HE2	1:A:803:LYS:HB3	1.77	0.42
1:A:1117:VAL:HG23	1:A:1119:LEU:HG	2.01	0.42
1:A:1430:CYS:O	1:A:1435:THR:HG22	2.20	0.42
2:B:131:THR:HA	2:B:140:LEU:O	2.19	0.42
2:B:300:MET:O	2:B:303:PRO:HD2	2.20	0.42
2:B:728:MET:SD	2:B:942:LYS:HD3	2.60	0.42
15:N:-7:DG:H2''	15:N:-6:DG:N7	2.35	0.42
23:W:275:ASP:OD1	23:W:275:ASP:N	2.47	0.42
23:W:289:TYR:HE2	23:W:323:PRO:HA	1.84	0.42
24:V:382:VAL:HG21	25:X:19:PHE:CE1	2.55	0.42
1:A:379:GLY:HA2	1:A:475:ARG:O	2.19	0.42
1:A:1251:ASN:OD1	1:A:1251:ASN:N	2.53	0.42
2:B:288:ILE:HG22	2:B:289:ILE:HG13	2.01	0.42
2:B:325:GLY:HA3	2:B:338:TYR:CE1	2.55	0.42
2:B:609:GLU:O	2:B:611:GLU:N	2.52	0.42
5:E:10:LEU:HD23	5:E:13:ILE:HD11	2.02	0.42
9:I:88:LYS:HG3	9:I:89:CYS:N	2.35	0.42
17:T:61:DA:H2''	17:T:62:DA:H8	1.84	0.42
20:c:32:ARG:O	20:c:36:LYS:N	2.40	0.42
20:c:73:ASN:O	20:c:75:LYS:HG2	2.20	0.42
1:A:1146:GLN:HG2	1:A:1149:ARG:HH21	1.84	0.42
2:B:296:GLU:N	2:B:296:GLU:OE1	2.53	0.42
2:B:735:VAL:HA	2:B:750:VAL:HG23	2.01	0.42
2:B:859:ARG:HH22	2:B:901:THR:HB	1.84	0.42
2:B:908:MET:HE3	2:B:908:MET:HB3	1.89	0.42
2:B:1163:MET:HA	2:B:1167:ILE:O	2.20	0.42
14:Z:310:ARG:NH1	14:Z:335:PRO:O	2.53	0.42
15:N:-69:DG:H2'	15:N:-68:DT:H71	2.02	0.42
17:T:-36:DT:H2''	17:T:-35:DA:C5	2.55	0.42
18:a:60:LEU:HD21	20:g:104:GLN:HE22	1.85	0.42
18:a:98:ALA:HB3	19:b:95:ARG:NH2	2.34	0.42
23:W:123:LEU:HB2	23:W:158:LEU:HD11	2.02	0.42
23:W:320:MET:SD	23:W:320:MET:N	2.93	0.42
23:W:325:VAL:HB	23:W:368:GLU:CD	2.45	0.42
24:V:118:LYS:HE3	24:V:144:GLU:OE1	2.20	0.42
24:V:192:PRO:O	24:V:196:ARG:HG3	2.20	0.42
24:V:230:ARG:HG2	24:V:352:TRP:NE1	2.35	0.42
24:V:232:VAL:CG2	24:V:308:PRO:HG3	2.49	0.42
1:A:34:MET:HE2	1:A:34:MET:HB3	1.97	0.41
1:A:203:LYS:HE2	1:A:203:LYS:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLN:HG2	2:B:43:GLN:N	2.34	0.41
2:B:739:ASN:HB3	10:J:62:TYR:CZ	2.55	0.41
7:G:31:PHE:O	7:G:35:GLU:HB2	2.20	0.41
8:H:27:ARG:HD2	8:H:40:ILE:HG23	2.01	0.41
15:N:18:DG:H1'	15:N:19:DC:H5'	2.02	0.41
15:N:27:DG:H2''	15:N:28:DA:C8	2.55	0.41
23:W:100:TRP:O	23:W:104:THR:HG23	2.20	0.41
23:W:251:GLU:HB3	23:W:253:GLN:CD	2.45	0.41
23:W:342:PHE:O	23:W:430:TRP:HD1	2.02	0.41
24:V:76:ARG:O	24:V:80:ILE:HG12	2.20	0.41
1:A:28:PRO:O	1:A:32:LYS:HG2	2.20	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.87	0.41
1:A:940:LYS:HB3	1:A:940:LYS:HE2	1.81	0.41
1:A:1139:LEU:O	1:A:1337:GLU:HA	2.20	0.41
1:A:1440:MET:HE1	2:B:1165:MET:HG2	2.02	0.41
2:B:281:ASP:HB3	9:I:22:ASN:HA	2.03	0.41
2:B:348:LEU:HD21	2:B:364:PHE:CD1	2.56	0.41
8:H:67:ASP:OD1	8:H:67:ASP:N	2.53	0.41
8:H:91:VAL:HG22	8:H:144:LEU:HD23	2.01	0.41
8:H:106:THR:OG1	8:H:107:GLU:OE1	2.38	0.41
13:Y:16:CYS:HB3	13:Y:19:CYS:H	1.84	0.41
17:T:-66:DA:C8	17:T:-65:DT:H72	2.55	0.41
24:V:262:PHE:HZ	24:V:305:LEU:HD21	1.85	0.41
1:A:376:ASP:HB3	1:A:522:PRO:HD3	2.02	0.41
1:A:1319:LYS:HE3	1:A:1333:GLU:HG3	2.00	0.41
1:A:1342:SER:C	1:A:1344:MET:H	2.28	0.41
2:B:203:ASN:O	2:B:571:GLY:HA3	2.20	0.41
2:B:677:MET:HG3	2:B:700:PRO:HG3	2.02	0.41
8:H:30:CYS:HB2	8:H:39:LEU:HD23	2.01	0.41
17:T:-54:DA:H2''	17:T:-53:DG:C8	2.54	0.41
19:b:71:THR:HG21	21:d:97:LEU:HG	2.02	0.41
22:U:12:TRP:CE3	22:U:13:LEU:HD12	2.51	0.41
23:W:463:GLN:HA	23:W:466:HIS:NE2	2.36	0.41
24:V:322:LEU:HD21	24:V:374:LEU:HD22	2.03	0.41
1:A:479:TRP:HB2	2:B:931:ILE:HD11	2.02	0.41
1:A:1127:LEU:HD13	1:A:1382:LEU:HD12	2.02	0.41
2:B:501:LEU:HD12	2:B:505:LEU:HD12	2.01	0.41
2:B:854:ILE:HD11	2:B:858:VAL:HG11	2.02	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.85	0.41
15:N:-45:DG:C2	15:N:-44:DG:C6	3.09	0.41
17:T:-67:DA:H2''	17:T:-66:DA:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:94:GLY:O	20:g:99:ARG:HB3	2.20	0.41
22:U:43:LEU:H	22:U:43:LEU:HD23	1.85	0.41
24:V:72:LYS:O	24:V:76:ARG:HG3	2.20	0.41
24:V:349:GLN:HB3	24:V:419:ARG:HD3	2.02	0.41
24:V:464:LEU:HD23	24:V:464:LEU:HA	1.93	0.41
1:A:865:ILE:HD13	1:A:1092:ALA:CB	2.50	0.41
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	2.03	0.41
1:A:1167:ARG:HG3	1:A:1293:LEU:HG	2.02	0.41
2:B:33:TYR:HD1	2:B:653:TRP:CE2	2.38	0.41
2:B:143:GLN:HB3	2:B:145:GLN:HE22	1.86	0.41
2:B:721:ARG:HA	2:B:721:ARG:HD3	1.82	0.41
6:F:95:LYS:HE3	6:F:95:LYS:HB2	1.81	0.41
7:G:5:ILE:HD13	7:G:76:VAL:HG11	2.01	0.41
8:H:14:ASP:OD1	8:H:15:ILE:N	2.54	0.41
14:Z:440:ILE:HG23	14:Z:450:ILE:HG13	2.03	0.41
17:T:-29:DC:H2'	17:T:-28:DT:H71	2.02	0.41
17:T:80:DA:H2''	17:T:81:DC:C5	2.55	0.41
24:V:4:GLY:HA3	24:V:102:SER:O	2.20	0.41
24:V:214:LEU:O	24:V:218:VAL:HG23	2.20	0.41
24:V:236:THR:HG21	24:V:309:PHE:HE2	1.86	0.41
1:A:461:GLN:O	1:A:463:THR:N	2.51	0.41
1:A:1345:ARG:HH11	1:A:1345:ARG:HB2	1.85	0.41
2:B:873:LEU:HD23	2:B:890:ARG:HG2	2.03	0.41
7:G:80:PHE:HB2	7:G:83:GLU:OE1	2.20	0.41
7:G:92:VAL:HG22	7:G:97:LEU:HD12	2.01	0.41
15:N:33:DT:H2''	15:N:34:DC:H5''	2.02	0.41
22:U:60:THR:HA	22:U:63:LEU:HD13	2.02	0.41
23:W:101:LEU:HD22	23:W:111:VAL:HG11	2.03	0.41
23:W:185:GLN:HA	23:W:188:ILE:HD13	2.02	0.41
24:V:368:GLU:HA	24:V:371:THR:OG1	2.20	0.41
1:A:203:LYS:H	1:A:203:LYS:HG3	1.72	0.41
1:A:908:THR:HG23	1:A:1047:SER:HB2	2.02	0.41
6:F:86:GLU:H	6:F:86:GLU:CD	2.29	0.41
12:L:37:ARG:HD2	12:L:37:ARG:H	1.86	0.41
18:e:81:ASP:HA	18:e:83:ARG:NH1	2.36	0.41
19:f:39:ARG:HA	19:f:39:ARG:HD3	1.93	0.41
22:U:45:PHE:HB3	22:U:81:LEU:HD23	2.03	0.41
23:W:56:TYR:HD1	24:V:59:LEU:HD23	1.85	0.41
1:A:122:ASN:OD1	25:X:34:LYS:HG2	2.20	0.41
1:A:279:LYS:HD3	1:A:336:LEU:HD12	2.03	0.41
1:A:463:THR:HG23	1:A:468:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:ASN:OD1	1:A:1173:THR:N	2.53	0.41
4:D:45:LYS:HE2	4:D:61:PHE:HE2	1.86	0.41
5:E:86:THR:O	5:E:89:VAL:HG12	2.20	0.41
5:E:148:HIS:CD2	5:E:179:VAL:HG11	2.56	0.41
7:G:81:LYS:HG3	7:G:148:VAL:C	2.46	0.41
17:T:94:DC:H1'	17:T:95:DC:H5'	2.01	0.41
20:c:63:LEU:HD12	21:d:41:VAL:HG23	2.03	0.41
18:e:63:ARG:O	18:e:66:PRO:HD2	2.21	0.41
21:d:95:VAL:HG13	21:d:99:LEU:HD12	2.03	0.41
19:f:76:ALA:HB1	19:f:78:ARG:HE	1.86	0.41
24:V:406:THR:O	24:V:443:ARG:NH2	2.37	0.41
24:V:462:LEU:HD23	24:V:462:LEU:HA	1.94	0.41
1:A:749:ARG:HG3	1:A:750:ASP:N	2.35	0.41
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.03	0.41
1:A:1166:LEU:HG	1:A:1170:THR:OG1	2.21	0.41
1:A:1180:ASN:OD1	1:A:1183:SER:N	2.54	0.41
1:A:1209:PRO:HG2	1:A:1210:TRP:CE3	2.56	0.41
2:B:337:LYS:O	2:B:340:LYS:HG2	2.21	0.41
3:C:96:GLU:OE1	3:C:96:GLU:N	2.54	0.41
5:E:55:ARG:O	5:E:56:THR:OG1	2.26	0.41
7:G:110:ARG:HD3	7:G:128:TYR:CE1	2.56	0.41
7:G:166:ASP:N	7:G:166:ASP:OD1	2.53	0.41
14:Z:552:ARG:HA	14:Z:552:ARG:HD3	1.74	0.41
17:T:85:DC:H2''	17:T:86:DC:C5	2.56	0.41
19:b:33:ALA:HB2	19:b:36:ARG:HH21	1.86	0.41
18:e:83:ARG:HB2	19:f:80:THR:HA	2.03	0.41
21:d:66:ILE:O	21:d:70:ILE:HG13	2.20	0.41
23:W:195:CYS:O	23:W:201:PHE:HB2	2.21	0.41
23:W:362:TYR:HA	23:W:366:VAL:CG2	2.51	0.41
23:W:460:THR:HA	23:W:506:ARG:HD2	2.03	0.41
24:V:157:PHE:O	24:V:161:VAL:HG23	2.21	0.41
24:V:225:LEU:HB3	24:V:234:TYR:CE2	2.56	0.41
1:A:100:LEU:HD21	1:A:193:ARG:HD2	2.02	0.41
1:A:892:GLY:HA3	1:A:1396:ARG:HG2	2.02	0.41
1:A:939:VAL:HA	1:A:942:VAL:HG22	2.03	0.41
1:A:1405:MET:HE2	1:A:1405:MET:HB3	1.88	0.41
2:B:200:MET:HE3	2:B:200:MET:HB3	2.00	0.41
2:B:471:ASN:OD1	2:B:477:SER:OG	2.30	0.41
4:D:33:LEU:HD22	4:D:101:ALA:HB3	2.01	0.41
14:Z:426:VAL:HG11	14:Z:440:ILE:HD11	2.02	0.41
18:e:118:THR:OG1	19:f:45:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:138:TYR:OH	24:V:150:TRP:NE1	2.54	0.41
24:V:243:MET:HE2	24:V:264:TRP:CD1	2.56	0.41
24:V:427:TYR:HA	24:V:430:LEU:HD12	2.03	0.41
24:V:437:ASN:HD22	24:V:440:ALA:HB3	1.86	0.41
1:A:485:ASN:ND2	1:A:673:GLN:OE1	2.49	0.40
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	2.03	0.40
2:B:92:TYR:CD1	2:B:146:LYS:HG3	2.55	0.40
2:B:420:GLN:HA	2:B:423:ILE:HG12	2.02	0.40
2:B:762:ARG:HG3	2:B:1000:THR:OG1	2.21	0.40
2:B:931:ILE:HA	2:B:945:CYS:HB3	2.03	0.40
3:C:151:VAL:HG12	3:C:152:LYS:N	2.37	0.40
4:D:18:SER:HA	4:D:116:PRO:HG2	2.03	0.40
7:G:38:CYS:HB3	7:G:155:ASN:O	2.20	0.40
14:Z:310:ARG:NE	14:Z:337:GLN:HG3	2.35	0.40
15:N:-67:DT:H2"	15:N:-66:DG:N7	2.36	0.40
15:N:11:DC:OP1	18:a:38:PRO:HB3	2.21	0.40
15:N:31:DT:C2	15:N:32:DG:N7	2.89	0.40
17:T:8:DC:H5"	19:f:39:ARG:NH2	2.34	0.40
22:U:24:TRP:NE1	23:W:232:CYS:O	2.51	0.40
23:W:96:LEU:O	23:W:100:TRP:CD1	2.73	0.40
23:W:172:LEU:HD23	23:W:172:LEU:HA	1.95	0.40
23:W:334:LEU:HB3	23:W:338:MET:HE3	2.02	0.40
23:W:514:SER:HB2	23:W:552:LEU:HD21	2.02	0.40
24:V:15:ASP:O	24:V:18:GLU:HG3	2.21	0.40
1:A:488:VAL:HG12	1:A:535:MET:SD	2.62	0.40
1:A:743:ARG:CZ	23:W:442:GLN:HA	2.51	0.40
3:C:49:TRP:HB3	3:C:164:TYR:HB2	2.02	0.40
3:C:81:LYS:NZ	3:C:126:ARG:HH12	2.18	0.40
8:H:57:ARG:NH1	8:H:146:LYS:HZ3	2.19	0.40
13:Y:36:CYS:HB3	13:Y:42:MET:HE3	2.03	0.40
17:T:61:DA:H2"	17:T:62:DA:C8	2.56	0.40
22:U:89:TRP:HH2	23:W:201:PHE:CD2	2.39	0.40
23:W:63:PHE:CE1	24:V:31:GLU:HA	2.56	0.40
24:V:274:PHE:HB2	24:V:320:ARG:NH1	2.36	0.40
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.89	0.40
1:A:1212:LEU:HG	1:A:1214:VAL:HG23	2.04	0.40
2:B:956:PHE:HB3	2:B:962:THR:HG22	2.04	0.40
5:E:29:THR:OG1	5:E:31:ASP:OD1	2.33	0.40
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.21	0.40
8:H:106:THR:HG1	8:H:107:GLU:CD	2.29	0.40
14:Z:183:LYS:HB3	14:Z:247:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:8:DG:N2	18:a:40:ARG:HD3	2.36	0.40
17:T:109:DA:H2''	17:T:110:DA:H8	1.86	0.40
23:W:386:THR:O	23:W:390:VAL:HG23	2.22	0.40
1:A:497:ASP:OD2	2:B:942:LYS:NZ	2.54	0.40
1:A:863:ARG:HH12	1:A:1129:ASN:CG	2.28	0.40
1:A:999:ARG:NH1	8:H:103:GLU:OE2	2.53	0.40
5:E:73:PHE:CE2	5:E:99:ILE:HD11	2.55	0.40
7:G:2:PHE:HA	7:G:76:VAL:O	2.21	0.40
9:I:59:THR:HG23	9:I:61:GLU:H	1.86	0.40
14:Z:184:CYS:SG	14:Z:244:ASN:HB3	2.62	0.40
14:Z:429:CYS:SG	14:Z:469:ARG:HB2	2.61	0.40
14:Z:551:VAL:HG11	14:Z:632:ASN:HB3	2.04	0.40
17:T:7:DC:H2''	17:T:8:DC:C5	2.56	0.40
22:U:28:SER:O	22:U:32:LEU:HG	2.22	0.40
22:U:92:MET:HE2	23:W:240:PHE:CD2	2.56	0.40
22:U:96:ILE:HG23	22:U:106:LEU:HD22	2.03	0.40
24:V:183:VAL:HG11	24:V:434:LYS:HG3	2.04	0.40
24:V:462:LEU:HB3	24:V:503:HIS:CG	2.57	0.40
1:A:692:SER:OG	1:A:828:LEU:HD22	2.21	0.40
1:A:959:MET:HE3	1:A:959:MET:HB2	1.83	0.40
2:B:477:SER:HA	2:B:730:LYS:HG2	2.04	0.40
2:B:669:GLU:O	2:B:672:THR:HG22	2.21	0.40
4:D:14:GLU:HA	14:Z:473:LYS:HZ3	1.86	0.40
15:N:10:DG:H5'	18:a:40:ARG:HA	2.03	0.40
17:T:-47:DT:H1'	17:T:-46:DC:C2	2.57	0.40
18:e:67:PHE:CE1	19:f:62:LEU:HD11	2.57	0.40
20:g:111:ILE:HG23	20:g:115:LEU:HD12	2.03	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	1381/1970 (70%)	1298 (94%)	83 (6%)	0	100	100
2	B	1111/1174 (95%)	1042 (94%)	69 (6%)	0	100	100
3	C	254/271 (94%)	238 (94%)	16 (6%)	0	100	100
4	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	Y	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
14	Z	468/1107 (42%)	441 (94%)	27 (6%)	0	100	100
18	a	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
18	e	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
19	b	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
19	f	76/103 (74%)	72 (95%)	4 (5%)	0	100	100
20	c	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
20	g	103/130 (79%)	97 (94%)	6 (6%)	0	100	100
21	d	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
21	h	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
22	U	181/528 (34%)	178 (98%)	3 (2%)	0	100	100
23	W	541/611 (88%)	508 (94%)	32 (6%)	1 (0%)	43	71
24	V	544/580 (94%)	535 (98%)	9 (2%)	0	100	100
25	X	33/404 (8%)	33 (100%)	0	0	100	100
All	All	6418/8921 (72%)	6116 (95%)	301 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	W	191	VAL

5.3.2 Protein sidechains ⓘ

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	1229/1749 (70%)	1229 (100%)	0	100	100
2	B	985/1027 (96%)	985 (100%)	0	100	100
3	C	235/248 (95%)	235 (100%)	0	100	100
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	146/153 (95%)	146 (100%)	0	100	100
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	104/112 (93%)	104 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	Y	102/104 (98%)	102 (100%)	0	100	100
14	Z	423/955 (44%)	423 (100%)	0	100	100
18	a	83/110 (76%)	83 (100%)	0	100	100
18	e	82/110 (74%)	82 (100%)	0	100	100
19	b	65/79 (82%)	65 (100%)	0	100	100
19	f	63/79 (80%)	63 (100%)	0	100	100
20	c	82/100 (82%)	82 (100%)	0	100	100
20	g	83/100 (83%)	83 (100%)	0	100	100
21	d	81/105 (77%)	81 (100%)	0	100	100
21	h	79/105 (75%)	79 (100%)	0	100	100
22	U	158/451 (35%)	158 (100%)	0	100	100
23	W	479/530 (90%)	479 (100%)	0	100	100
24	V	491/515 (95%)	491 (100%)	0	100	100
25	X	31/351 (9%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5702/7760 (74%)	5702 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	273	GLN
1	A	330	GLN
1	A	387	ASN
1	A	412	GLN
1	A	461	GLN
1	A	465	HIS
1	A	502	ASN
1	A	507	GLN
1	A	662	HIS
1	A	783	GLN
1	A	1291	ASN
1	A	1310	HIS
2	B	111	ASN
2	B	145	GLN
2	B	197	GLN
2	B	642	GLN
2	B	716	HIS
3	C	66	HIS
3	C	265	HIS
4	D	66	ASN
6	F	72	GLN
8	H	131	ASN
9	I	45	GLN
10	J	52	HIS
13	Y	35	ASN
14	Z	418	HIS
14	Z	446	ASN
14	Z	632	ASN
14	Z	737	HIS
18	a	108	ASN
20	c	24	GLN
20	c	84	GLN
18	e	108	ASN
21	d	44	GLN

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Mol	Chain	Res	Type
19	f	27	GLN
20	g	24	GLN
20	g	68	ASN
20	g	89	ASN
20	g	104	GLN
21	h	44	GLN
21	h	64	ASN
22	U	62	HIS
23	W	126	HIS
23	W	148	GLN
23	W	250	GLN
23	W	350	GLN
23	W	358	HIS
24	V	22	ASN
24	V	296	GLN
24	V	431	HIS
24	V	437	ASN
25	X	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	2 (13%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	3	U
16	P	5	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

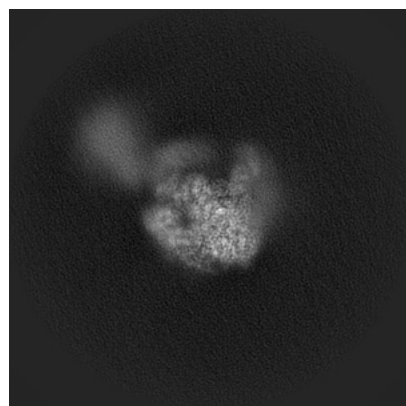
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61059. These allow visual inspection of the internal detail of the map and identification of artifacts.

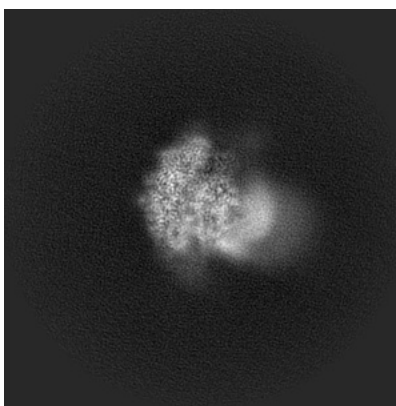
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

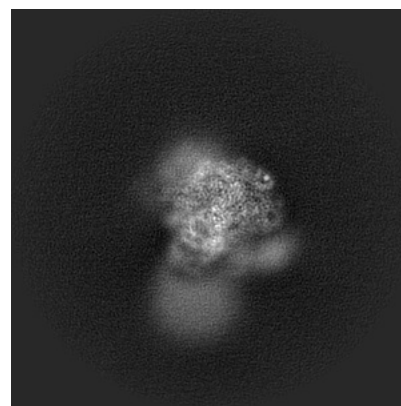
6.1.1 Primary map



X

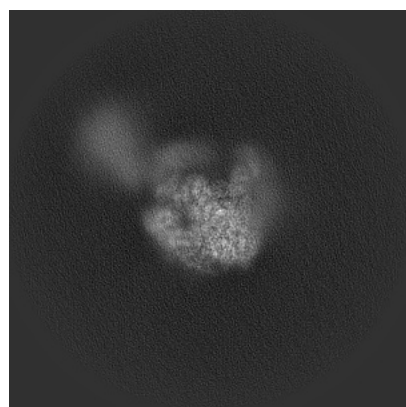


Y

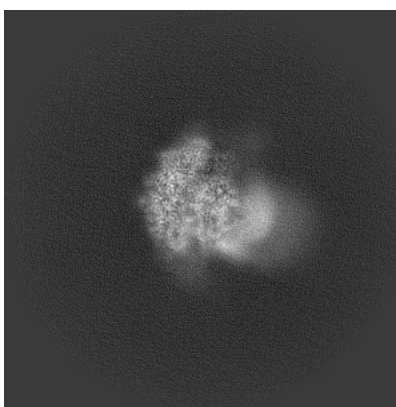


Z

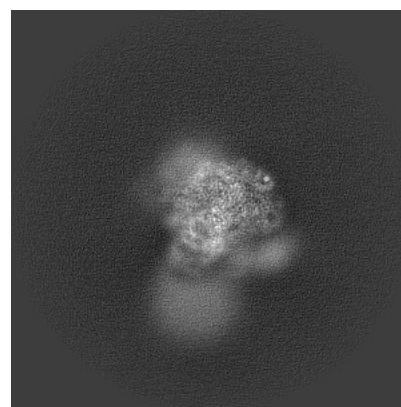
6.1.2 Raw map



X



Y

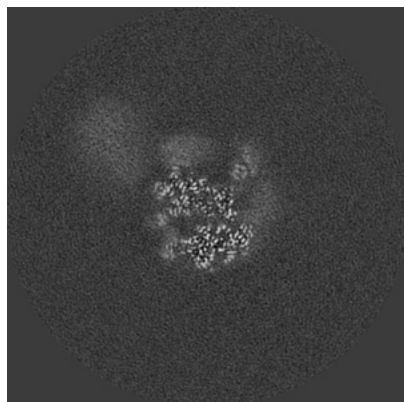


Z

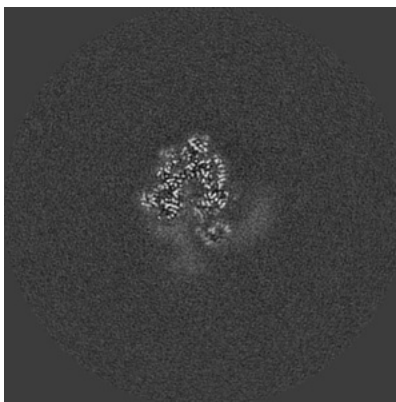
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

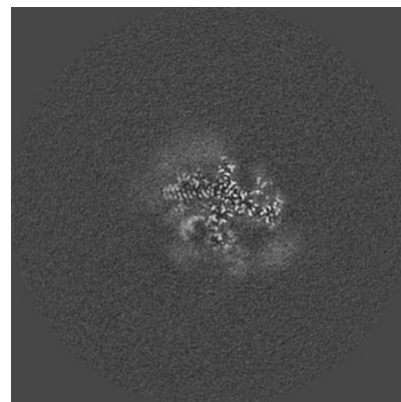
6.2.1 Primary map



X Index: 175

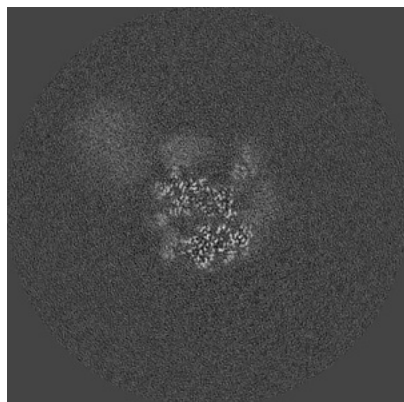


Y Index: 175

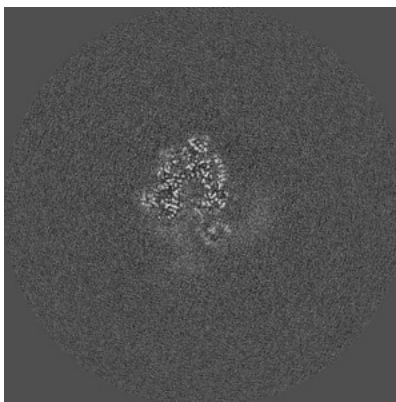


Z Index: 175

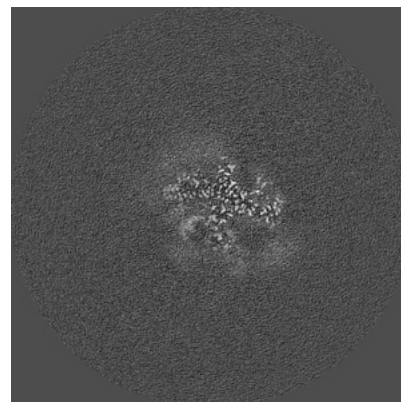
6.2.2 Raw map



X Index: 175



Y Index: 175

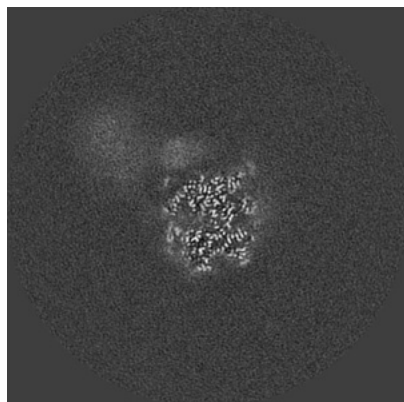


Z Index: 175

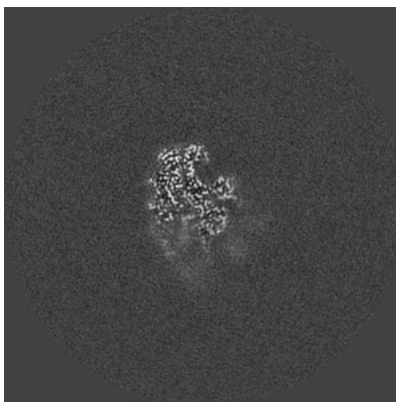
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

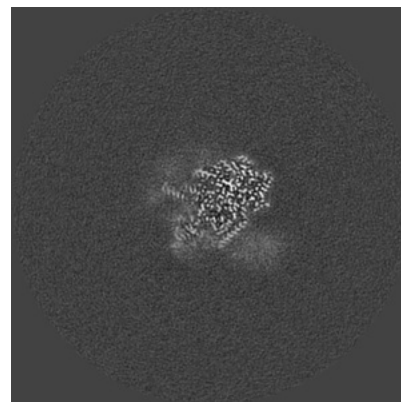
6.3.1 Primary map



X Index: 184

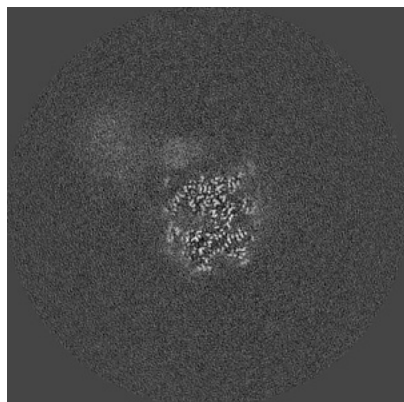


Y Index: 194

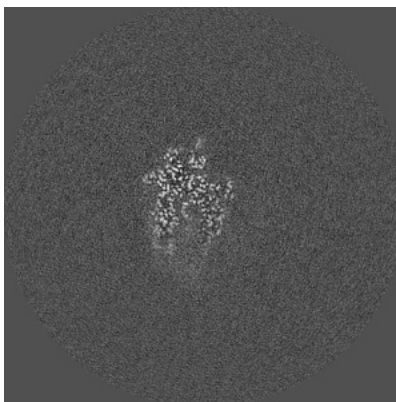


Z Index: 147

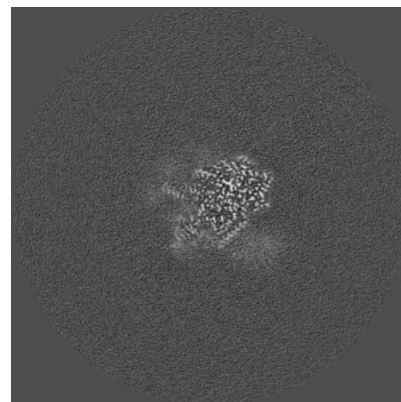
6.3.2 Raw map



X Index: 184



Y Index: 188

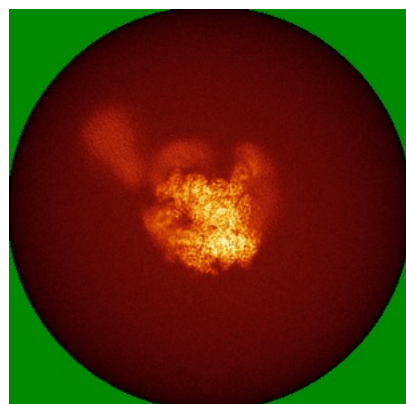


Z Index: 147

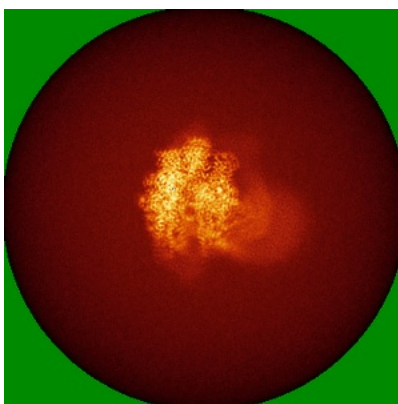
The images above show the largest variance slices of the map in three orthogonal directions.

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

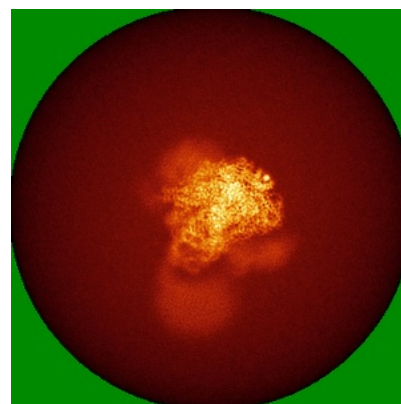
6.4.1 Primary map



X

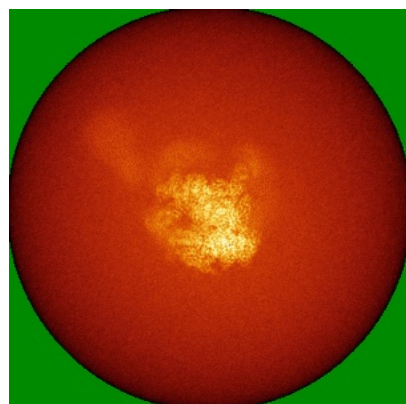


Y

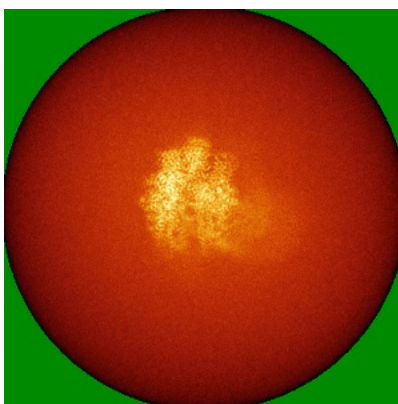


Z

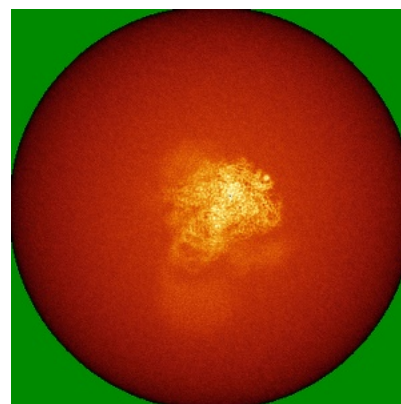
6.4.2 Raw map



X



Y

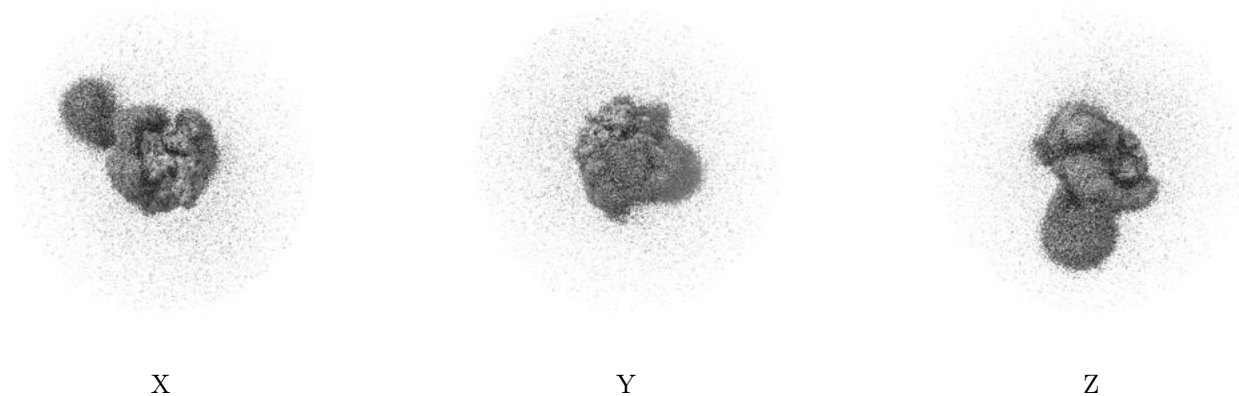


Z

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.

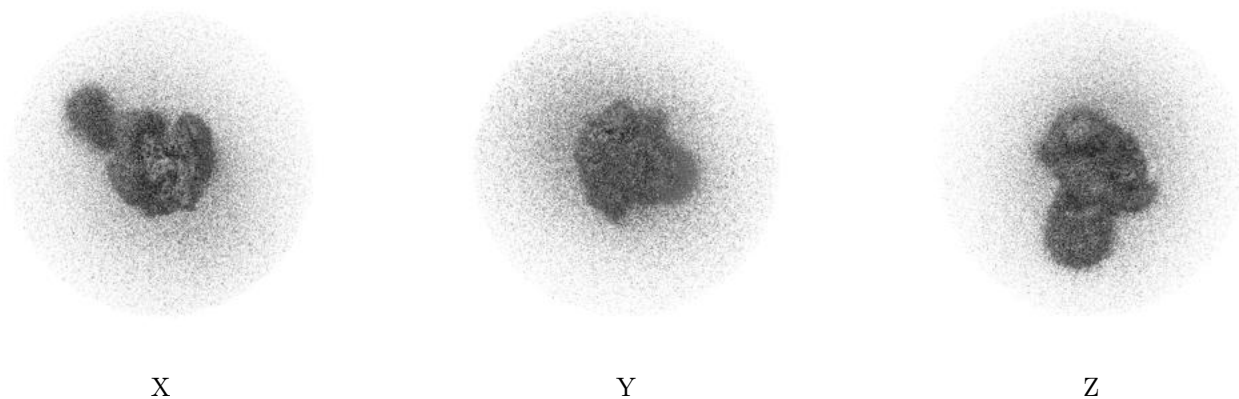
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

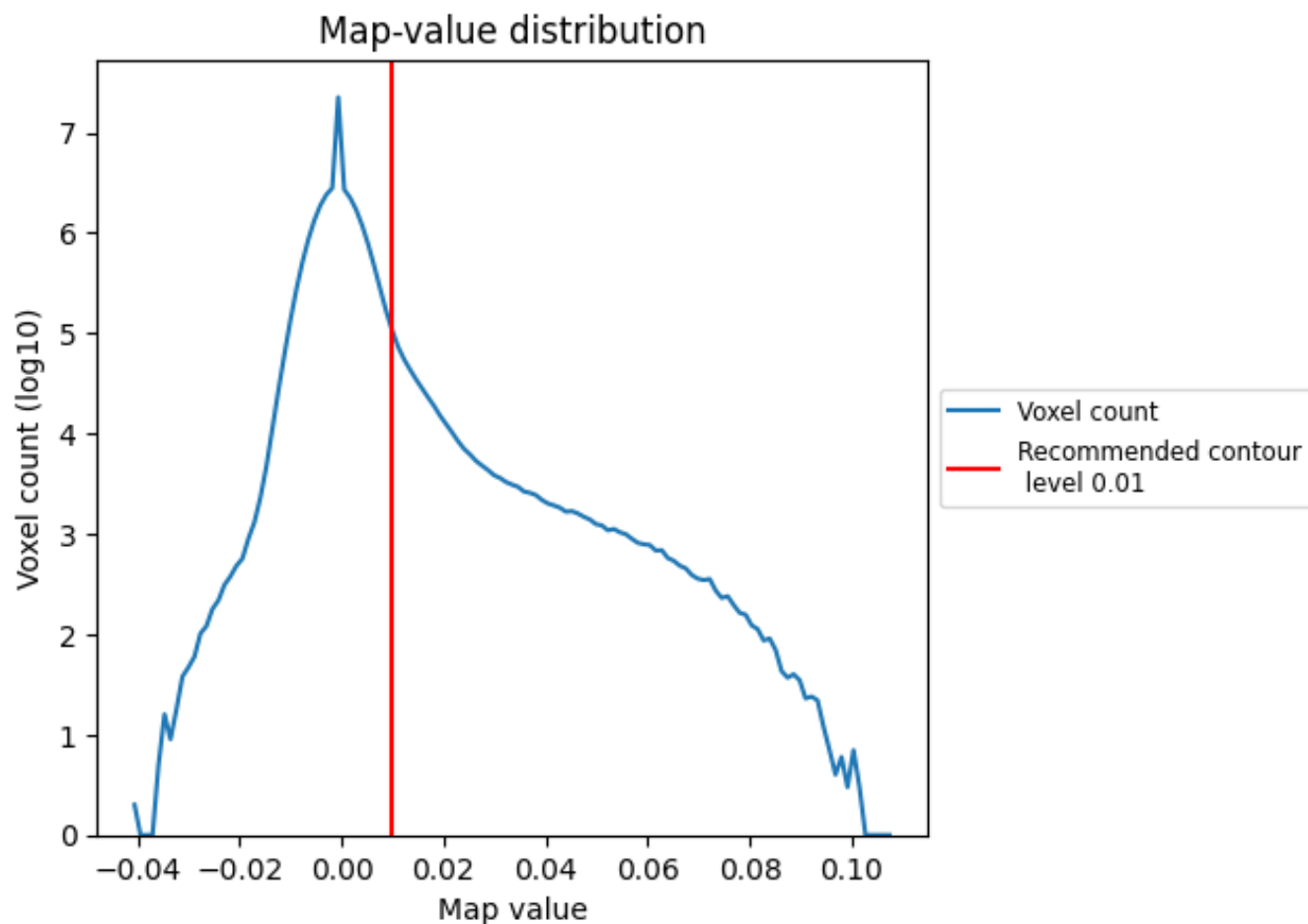
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

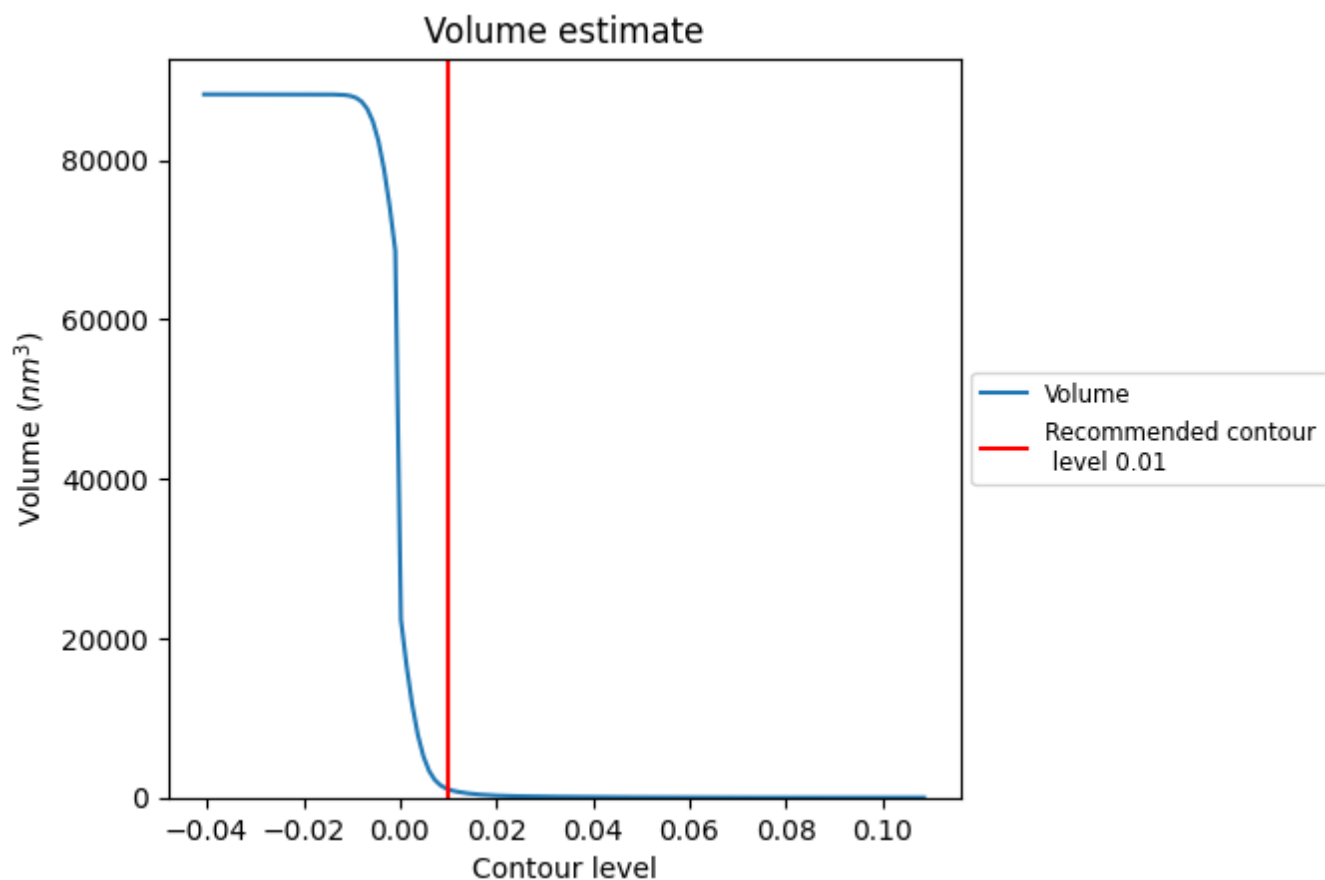
This section contains the results of statistical analysis of the map.

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.

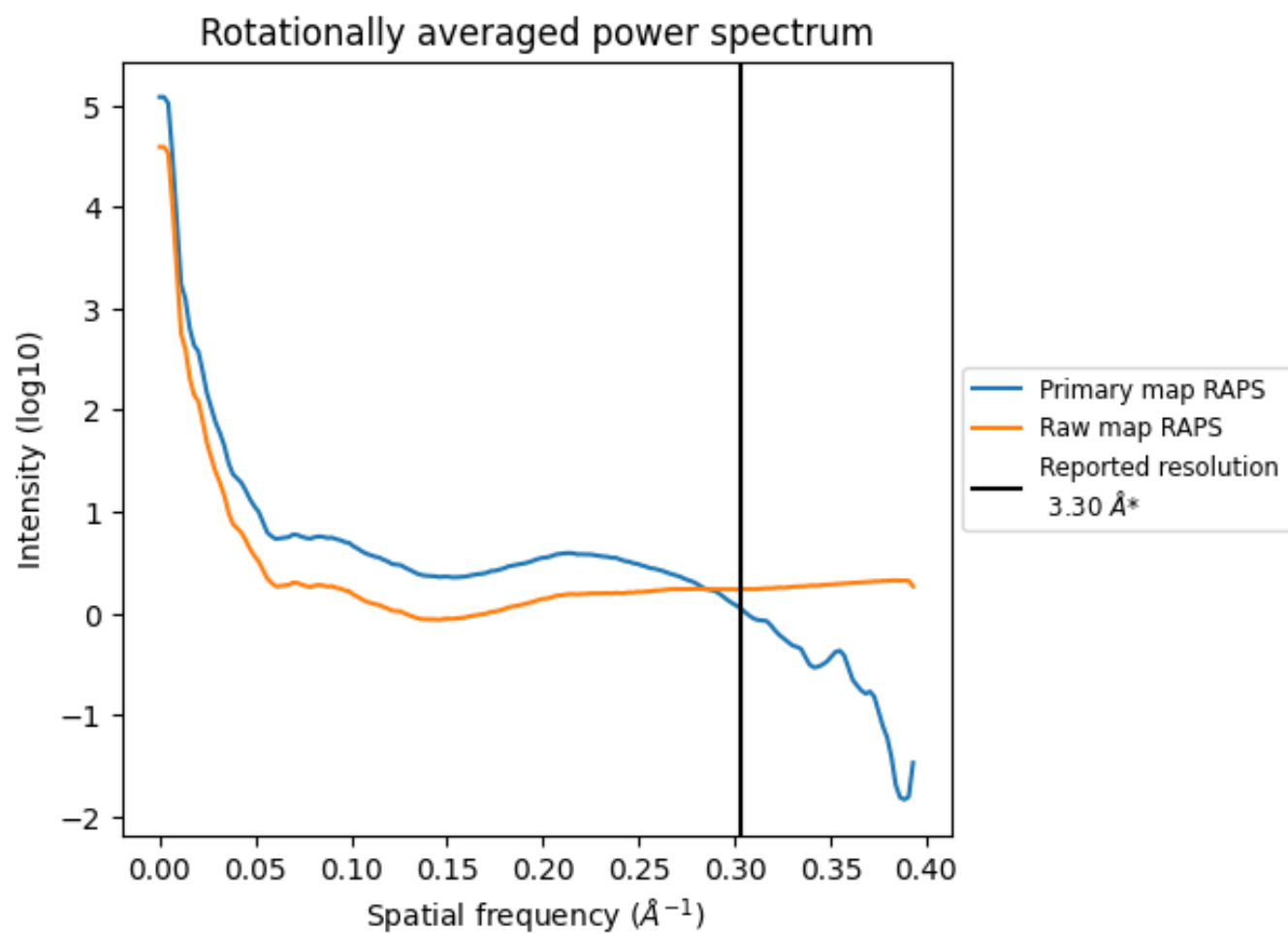
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1058 nm^3 ; this corresponds to an approximate mass of 956 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 ⓘ

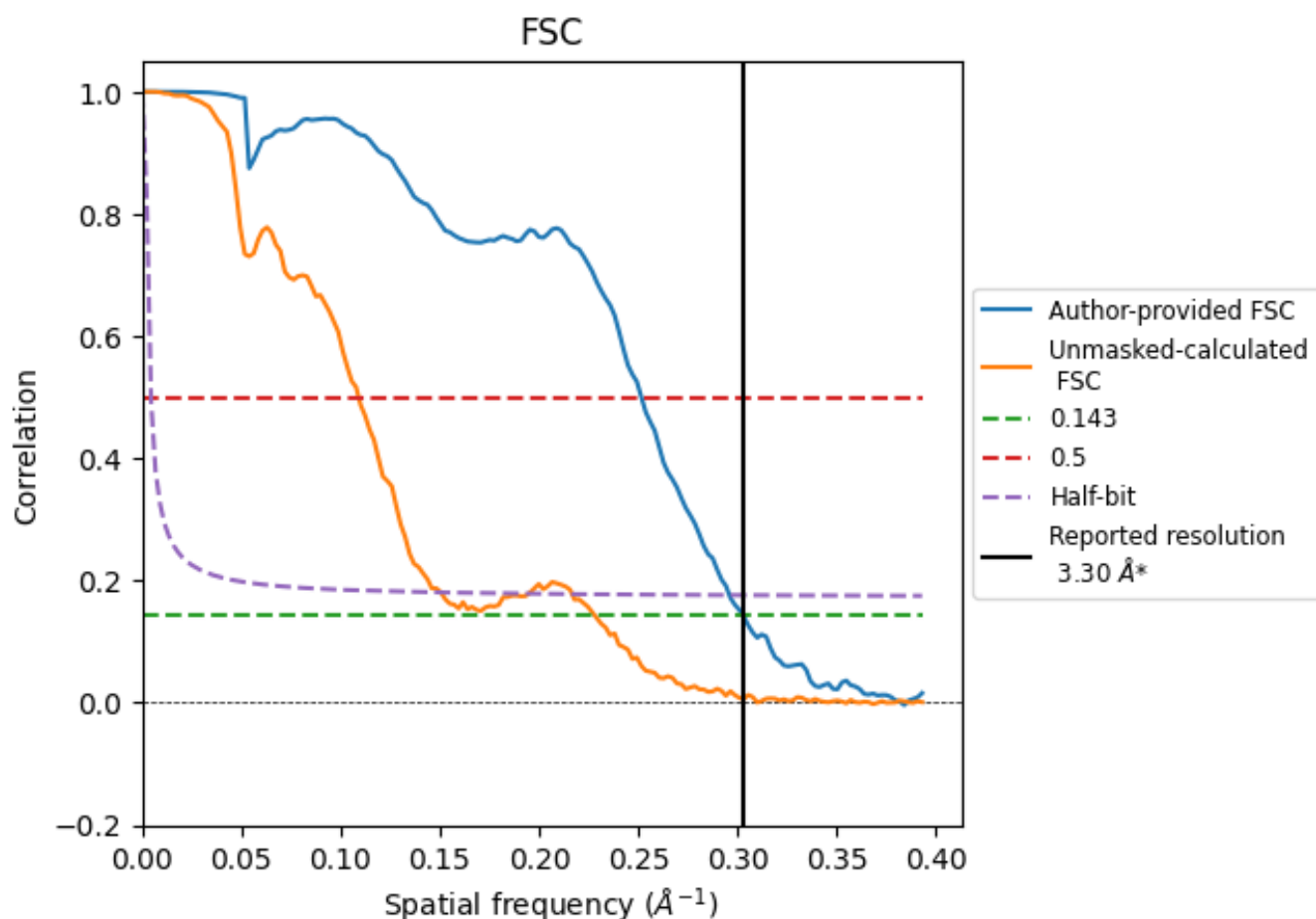


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

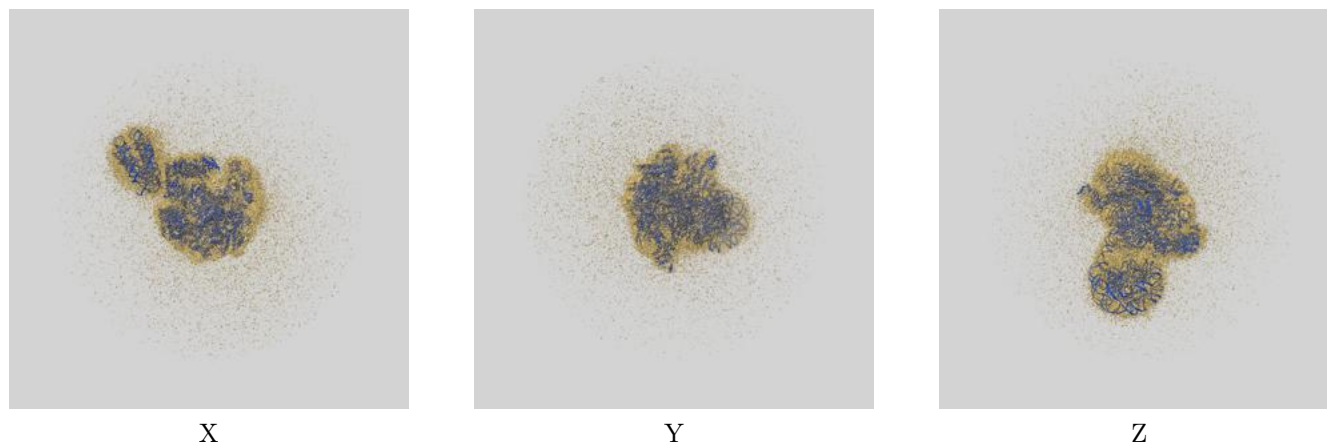
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.97	3.38
Unmasked-calculated*	4.39	9.17	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

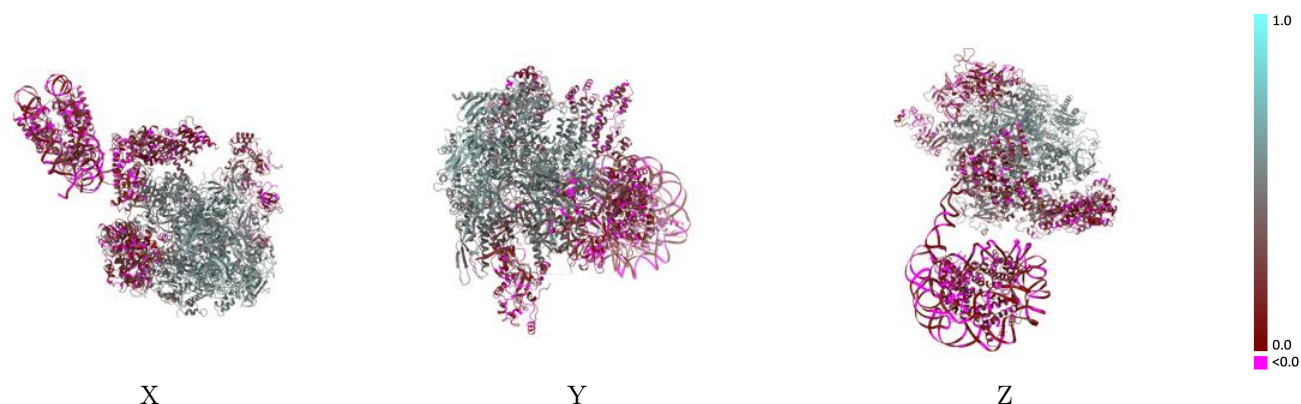
This section contains information regarding the fit between EMDB map EMD-61059 and PDB model 9J0O. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



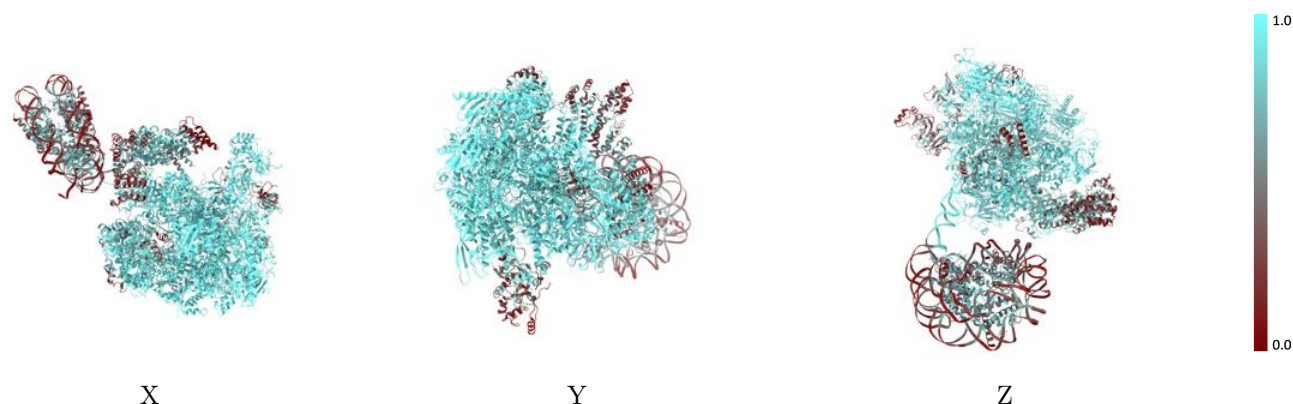
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



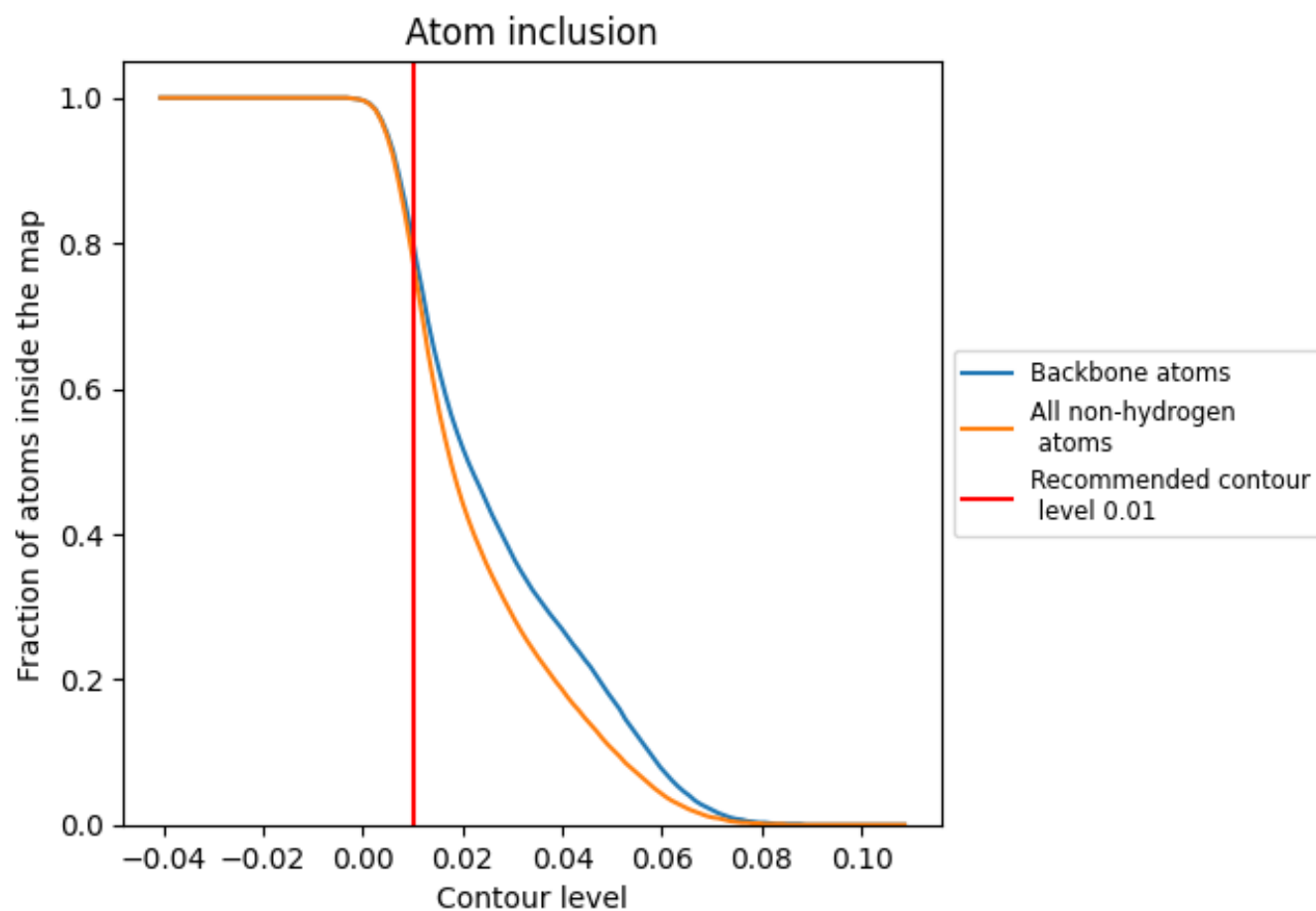
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.3130
A	 0.9750	 0.5000
B	 0.9780	 0.4970
C	 0.9910	 0.5420
D	 0.9500	 0.2010
E	 0.9760	 0.4770
F	 0.9870	 0.5350
G	 0.9600	 0.2810
H	 0.9820	 0.5170
I	 0.9430	 0.3490
J	 0.9870	 0.5520
K	 0.9900	 0.5420
L	 0.9840	 0.4710
N	 0.4420	 0.1010
P	 0.9220	 0.4290
T	 0.4810	 0.1190
U	 0.6740	 0.1610
V	 0.6330	 0.1330
W	 0.6410	 0.1780
X	 0.4340	 0.1040
Y	 0.2940	 0.0770
Z	 0.6000	 0.1750
a	 0.6720	 0.1070
b	 0.6650	 0.1180
c	 0.5990	 0.1060
d	 0.6270	 0.1070
e	 0.5940	 0.1420
f	 0.5610	 0.1150
g	 0.5830	 0.0940
h	 0.5340	 0.0760

