



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:54 PM UTC

PDB ID : 9EH1 / pdb_00009eh1
EMDB ID : EMD-48043
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-SETD2-nucleosome, 20 bp upstream
Authors : Markert, J.; Farnung, L.
Deposited on : 2024-11-21
Resolution : 3.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

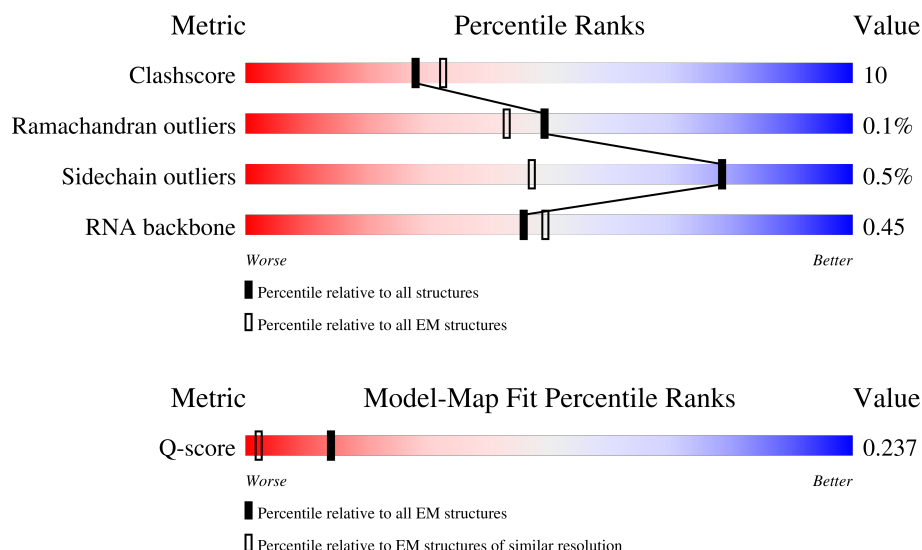
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1544	 72% 20% 8%
2	B	1159	 78% 19% .
3	C	269	 75% 21% .

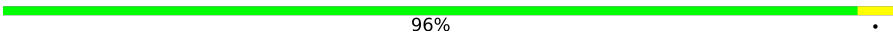
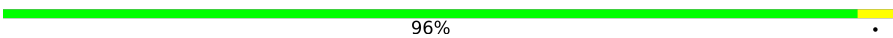
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Mol	Chain	Length	Quality of chain
4	D	126	
5	E	209	
6	F	78	
7	G	171	
8	H	149	
9	I	116	
10	J	66	
11	K	115	
12	L	47	
13	M	1002	
14	N	170	
15	O	132	
16	P	11	
17	Q	890	
18	R	248	
19	S	170	
20	T	181	
21	U	125	
22	V	244	
23	W	300	
24	X	43	
25	Y	116	
26	Z	510	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	78	 96% .
28	f	78	 96% .
29	c	130	 77% . 20%
29	g	130	 75% . 21%
30	d	123	 73% . 25%
30	h	123	 69% . 28%
31	l	589	 37% 7% 55% .

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 72243 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	1426	Total	C	N	O	P	0	0
			11255	7074	2014	2095	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1122	Total	C	N	O	S	0	0
			8980	5684	1576	1656	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 RNA polymerase Rpb4/RPC9 core domain-containing protein.

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 polymerases I, II, and III subunit RPABC2.

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 subunit.

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 polymerase I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	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 RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	N	O	S	0	0
			4883	2708	1072	1096	7		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	170	Total	C	N	O	P	0	0
			3474	1651	626	1027	170		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	132	Total	C	N	O	S	0	0
			1046	663	181	196	6		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	11	Total	C	N	O	P	0	0
			233	105	42	75	11		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			7226	4579	1264	1352	31		

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	N	O	S	0	0
			1836	1152	340	337	7		

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	161	Total	C	N	O	0	0
			657	334	161	162		

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	181	Total	C	N	O	P	0	0
			3725	1765	701	1078	181		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	125	Total	C	N	O	S	0	0
			856	538	151	166	1		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	244	Total	C	N	O	S	0	0
			1703	1061	305	333	4		

- Molecule 23 is a protein called Superkiller complex protein 8, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	43	Total	C	N	O	0	0
			353	220	69	64		

- Molecule 25 is a protein called Transcription elongation factor SPT4.

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

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	510	Total	C	N	O	P	S	0	0
			4025	2552	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	101	Total	C	N	O	S	0	0
			823	520	157	142	4		
27	e	94	Total	C	N	O	S	0	0
			776	491	149	133	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
28	f	78	Total	C	N	O	S	0	0
			622	393	120	108	1		

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	104	Total	C	N	O		0	0
			800	504	156	140			
29	g	103	Total	C	N	O		0	0
			795	501	155	139			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	92	Total	C	N	O	S	0	0
			721	454	129	136	2		
30	h	89	Total	C	N	O	S	0	0
			694	438	122	132	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	3	MET	-	initiating methionine	UNP P02281
d	32	THR	SER	engineered mutation	UNP P02281
h	3	MET	-	initiating methionine	UNP P02281
h	32	THR	SER	engineered mutation	UNP P02281

- Molecule 31 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	263	Total	C	N	O	S	0	0
			2149	1329	393	406	21		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	C	1	Total	Zn	0
			1	1	
32	I	2	Total	Zn	0
			2	2	
32	J	1	Total	Zn	0
			1	1	
32	L	1	Total	Zn	0
			1	1	
32	Y	1	Total	Zn	0
			1	1	

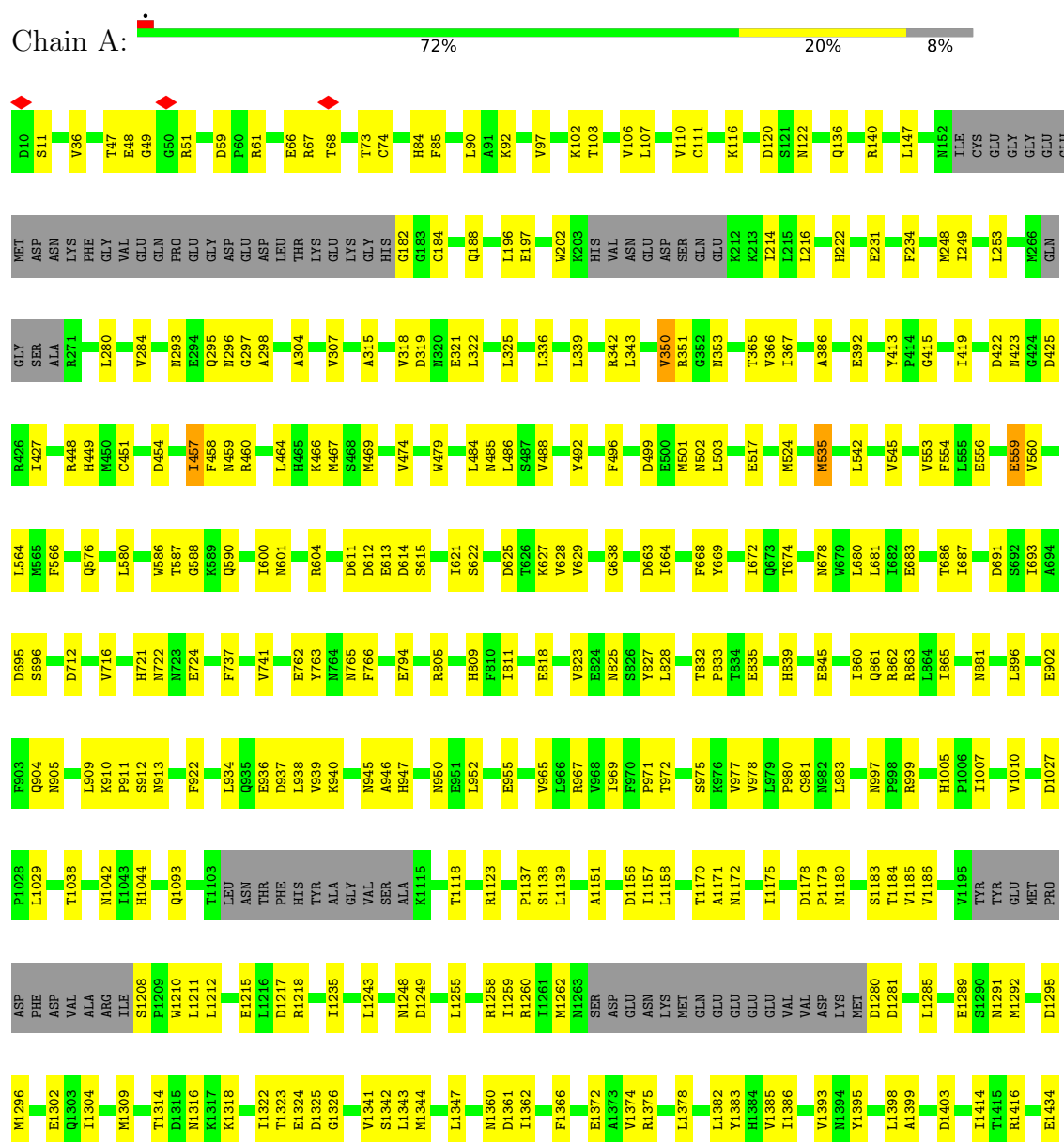
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

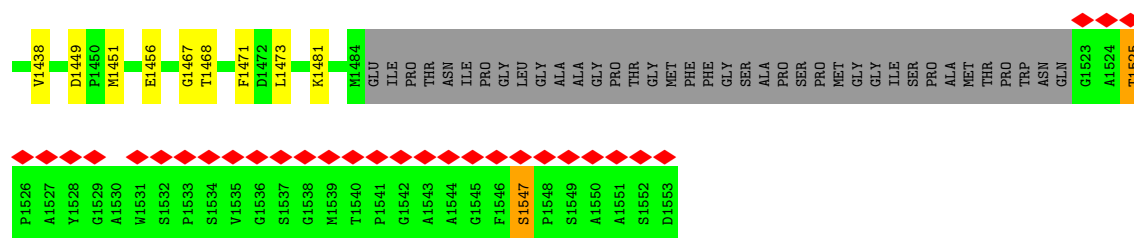
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

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.

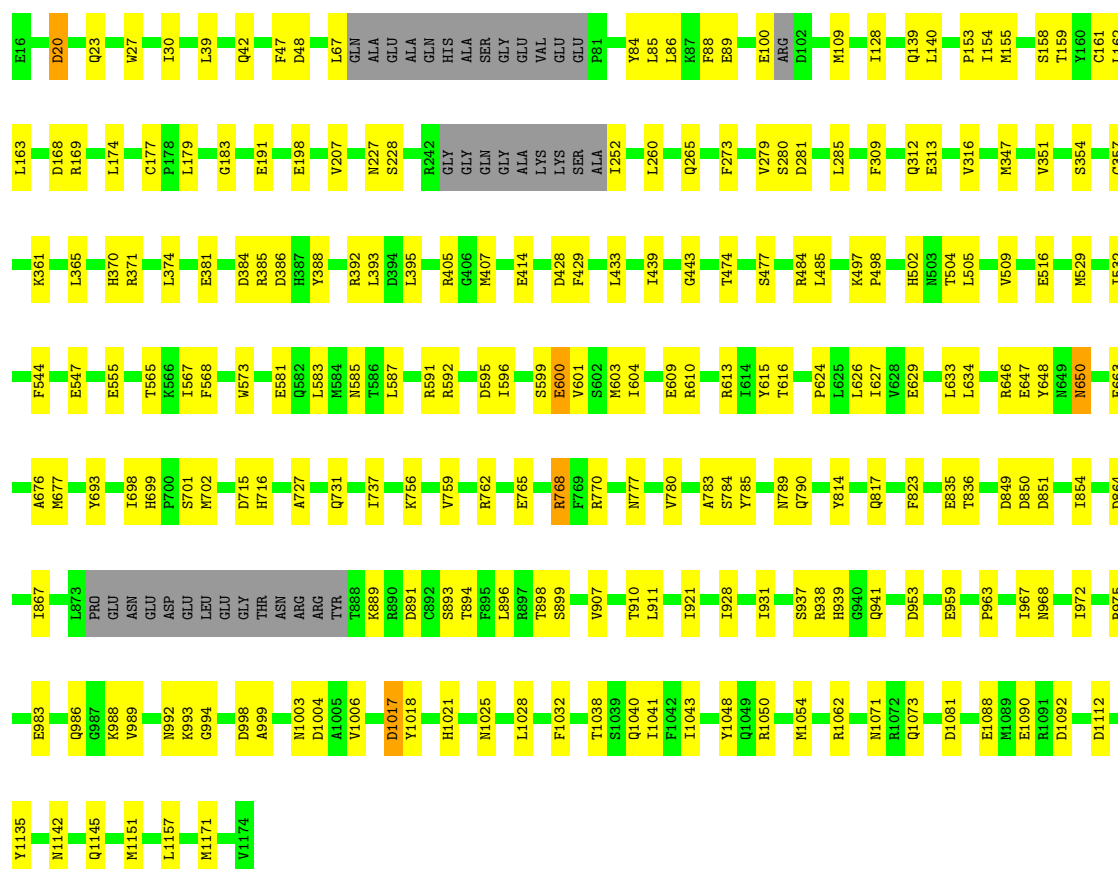
• Molecule 1: DNA-directed RNA polymerase subunit





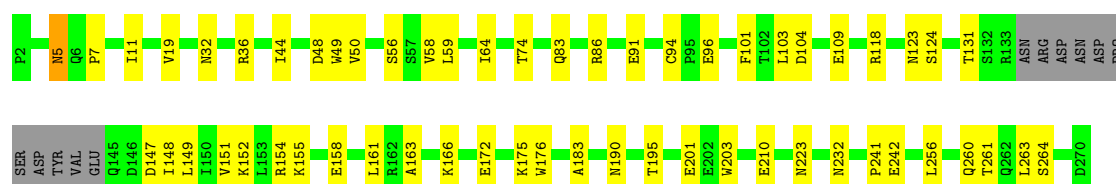
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 78% 19%

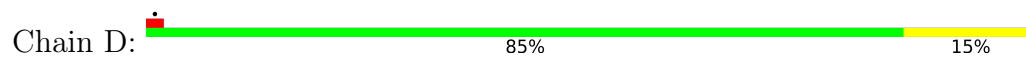


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

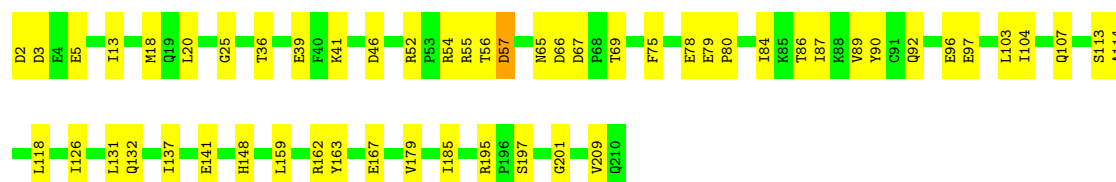
Chain C: 75% 21%



• Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein



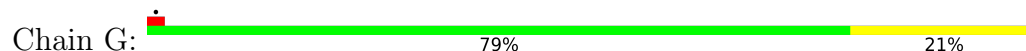
- Molecule 5: DNA-directed RNA polymerase II subunit E



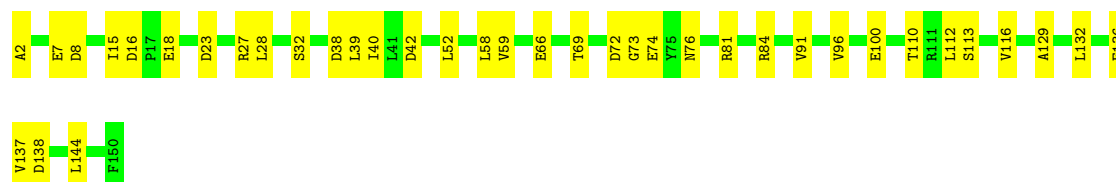
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerase subunit

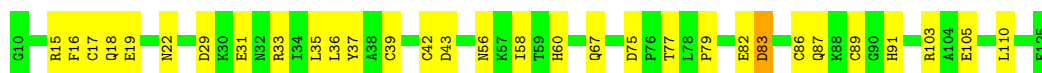


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

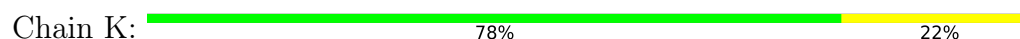




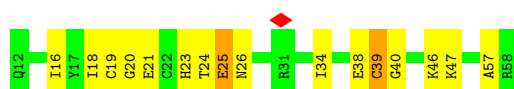
- Molecule 10: DNA-directed RNA polymerase I, II, and III subunit RPABC5



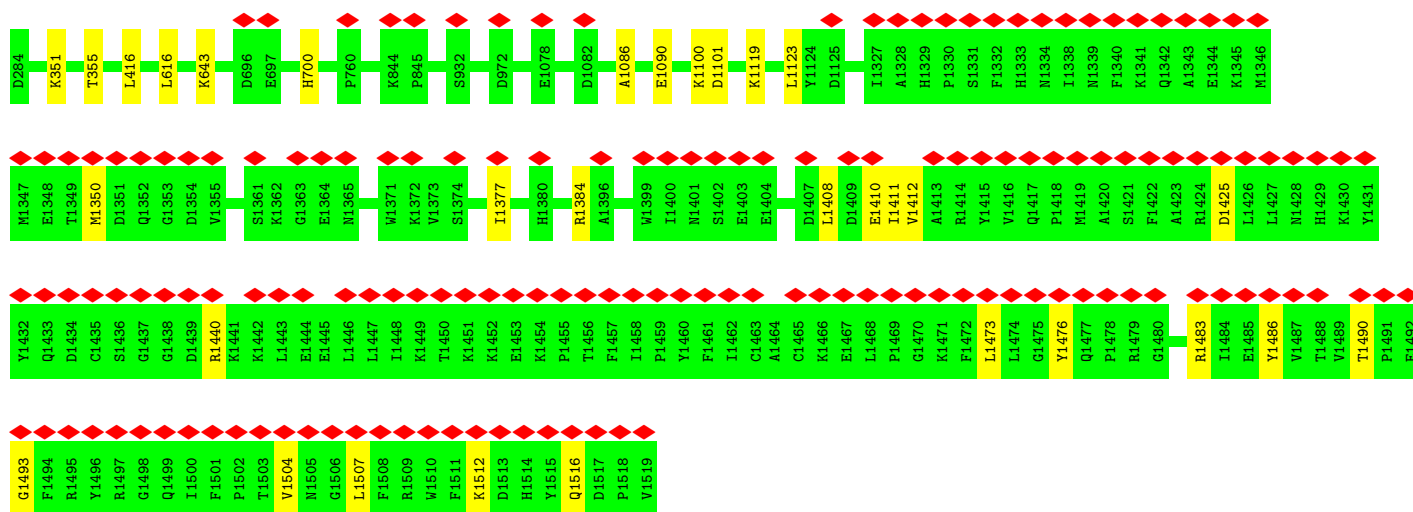
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



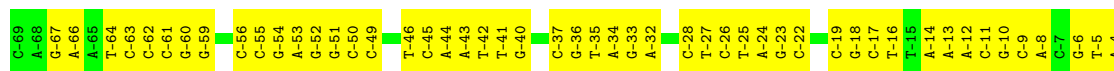
- Molecule 12: RNA polymerase II subunit K

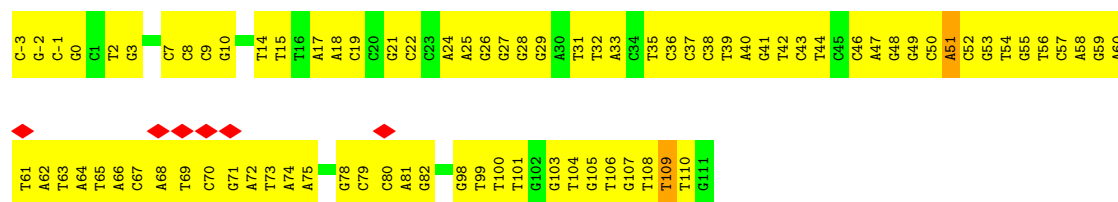


- Molecule 13: Transcription elongation factor SPT6

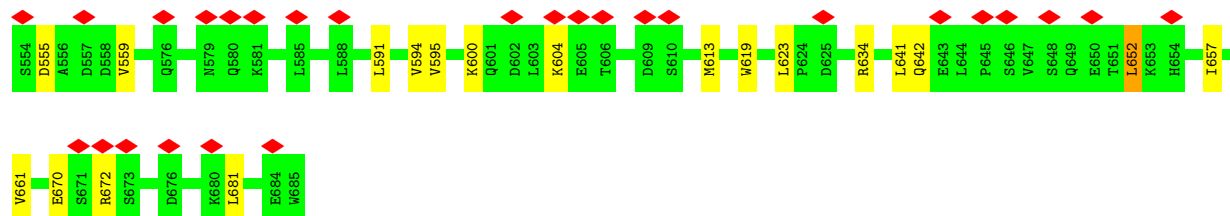
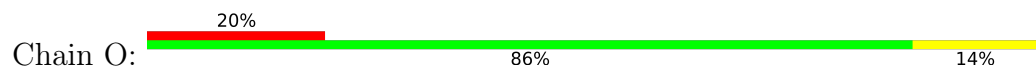


- Molecule 14: Non-template DNA

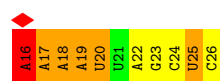




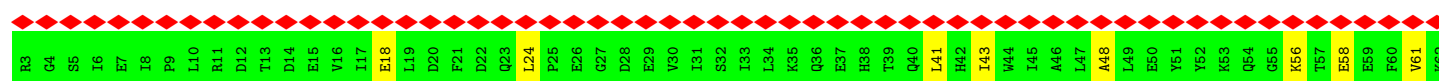
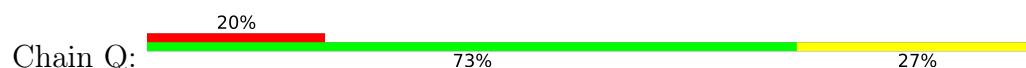
• Molecule 15: Protein IWS1 homolog

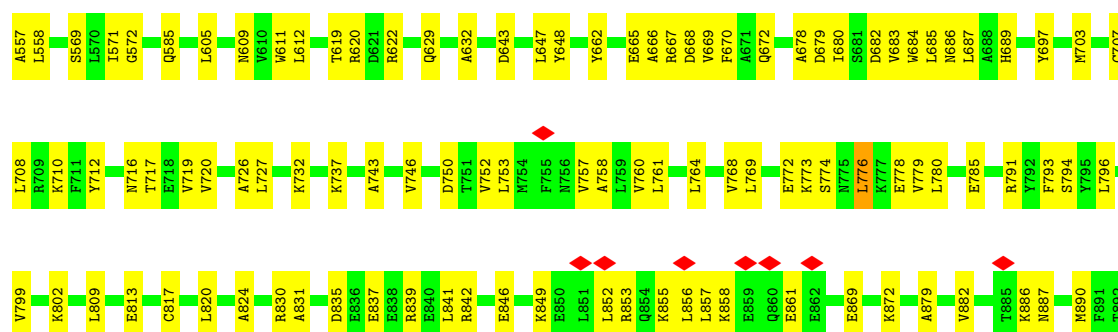


• Molecule 16: RNA

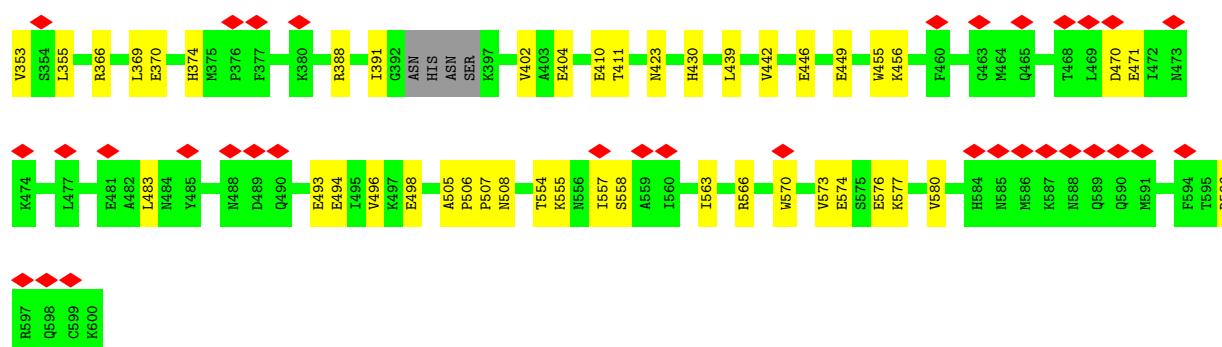
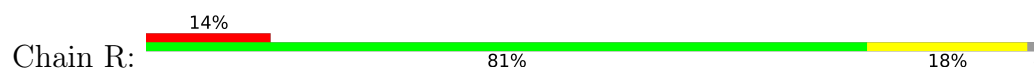


• Molecule 17: RNA polymerase-associated protein CTR9 homolog





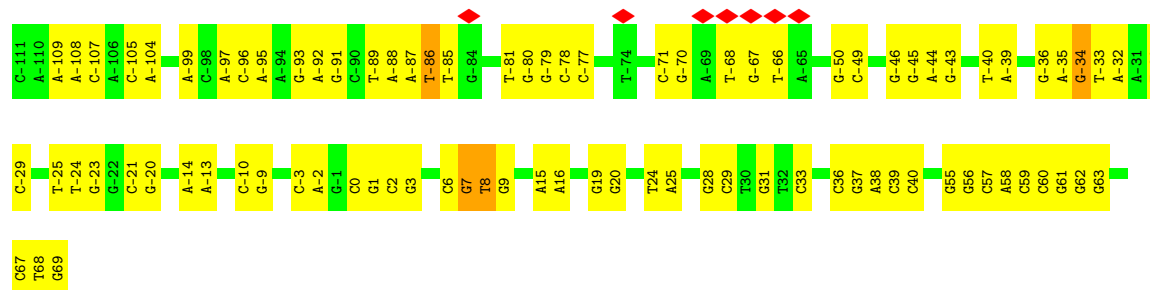
- Molecule 18: RNA polymerase-associated protein RTF1 homolog



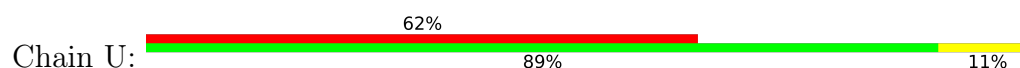
- Molecule 19: Transcription elongation factor A protein 1

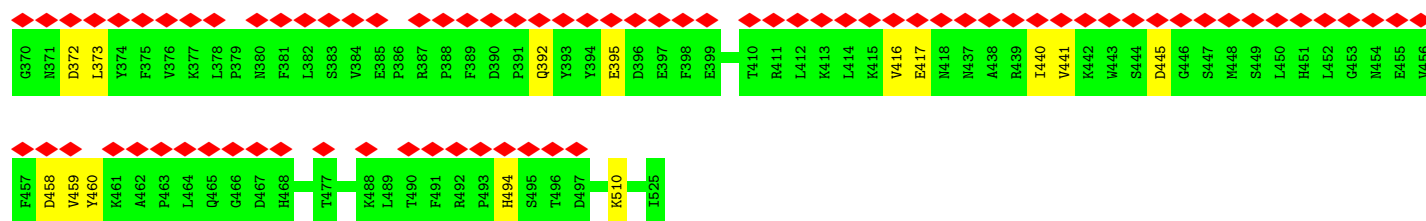


- Molecule 20: Template DNA

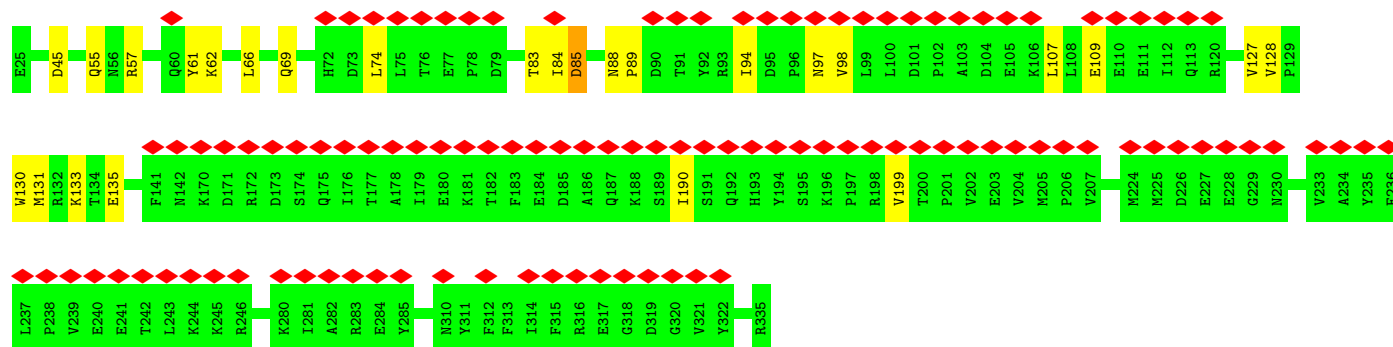
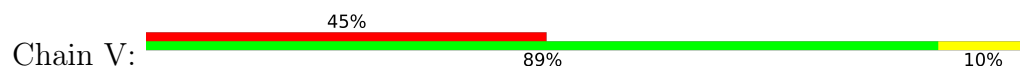


- Molecule 21: RNA polymerase-associated protein LEO1

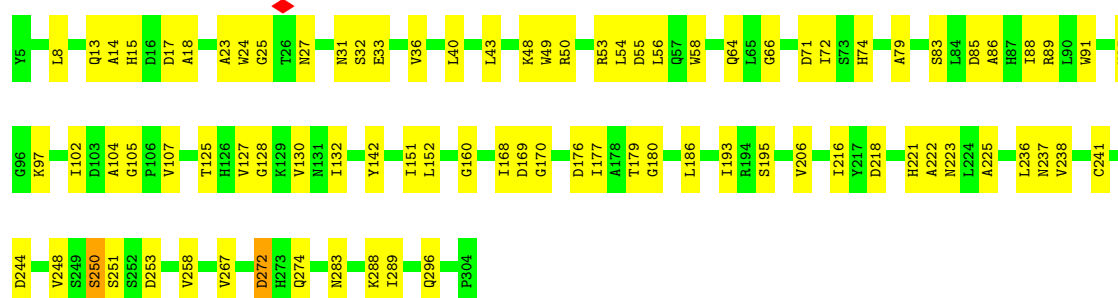




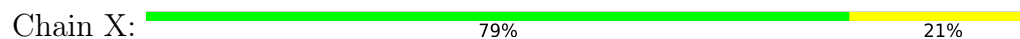
- Molecule 22: RNA polymerase II-associated factor 1 homolog



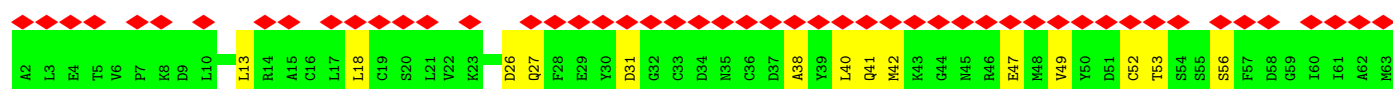
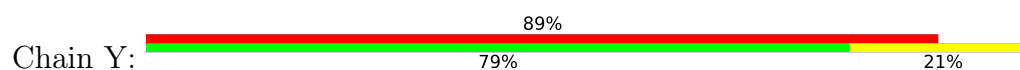
- Molecule 23: Superskiller complex protein 8, N-terminally processed

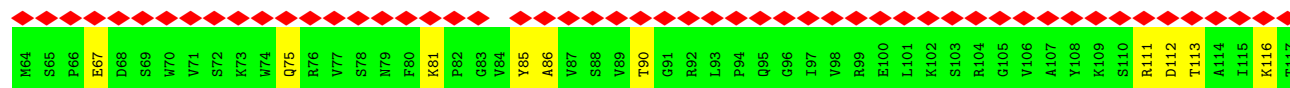


- Molecule 24: Parafibromin

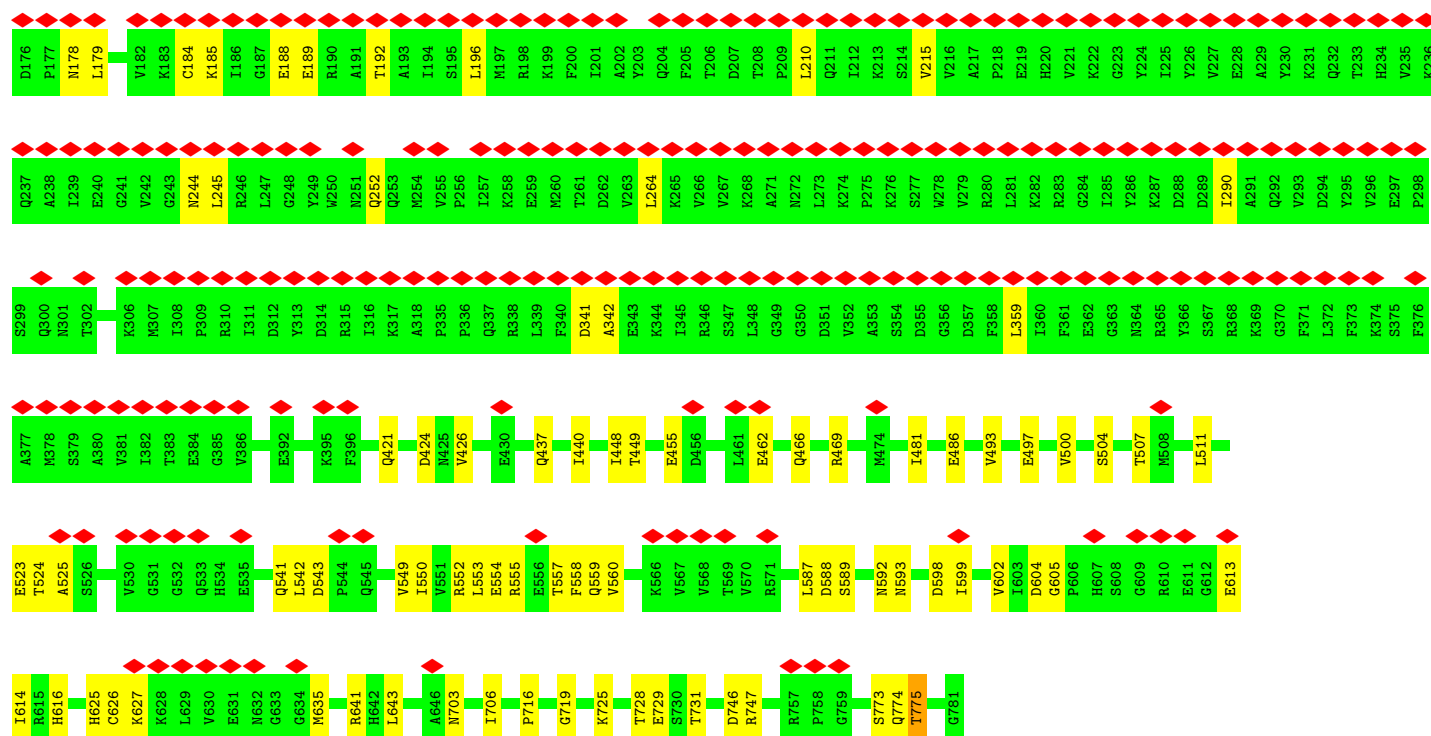
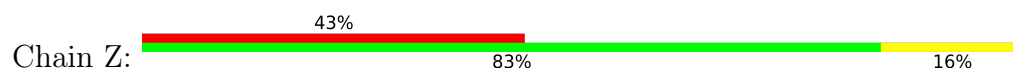


- Molecule 25: Transcription elongation factor SPT4

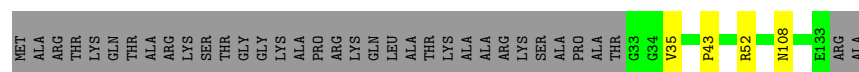




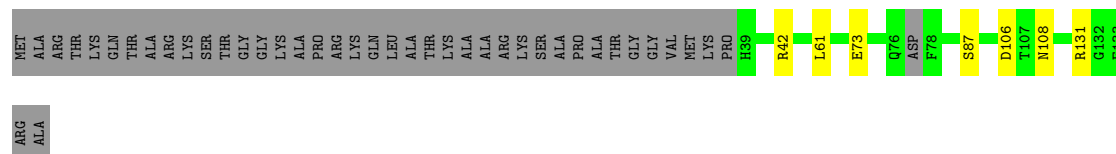
• Molecule 26: Transcription elongation factor SPT5



• Molecule 27: Histone H3



• Molecule 27: Histone H3



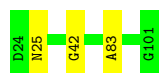
• Molecule 28: Histone H4





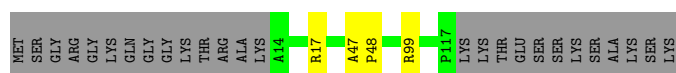
- Molecule 28: Histone H4

Chain f: 96%



- Molecule 29: Histone H2A type 1

Chain c: 77% 20%



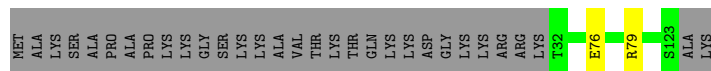
- Molecule 29: Histone H2A type 1

Chain g: 75% 21%



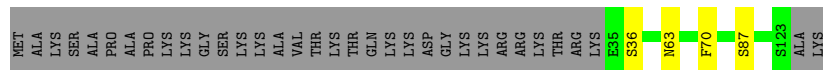
- Molecule 30: Histone H2B 1.1

Chain d: 73% 25%



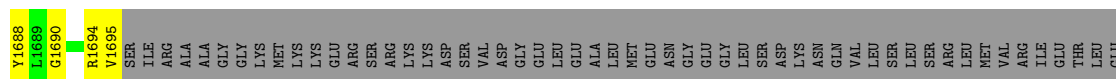
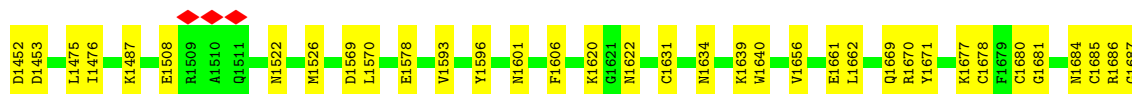
- Molecule 30: Histone H2B 1.1

Chain h: 69% 28%



- Molecule 31: Histone-lysine N-methyltransferase SETD2

Chain l: 37% 7% 55%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121657	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.541	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	550.0, 550.0, 550.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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, TPO, SEP, 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	0/11437	0.32	0/15433
2	B	0.24	0/9158	0.33	0/12360
3	C	0.29	0/2115	0.35	0/2873
4	D	0.17	0/1017	0.25	0/1368
5	E	0.22	0/1751	0.31	0/2366
6	F	0.26	0/636	0.31	0/859
7	G	0.17	0/1364	0.27	0/1853
8	H	0.26	0/1219	0.35	0/1644
9	I	0.23	0/964	0.31	0/1305
10	J	0.28	0/533	0.35	0/719
11	K	0.26	0/939	0.32	0/1271
12	L	0.27	0/403	0.32	0/536
13	M	0.11	0/4944	0.23	0/6387
14	N	0.37	0/3891	0.99	3/5999 (0.1%)
15	O	0.12	0/1062	0.23	0/1428
16	P	0.58	0/260	1.53	3/402 (0.7%)
17	Q	0.16	0/7365	0.30	0/9927
18	R	0.11	0/1866	0.24	0/2519
19	S	0.13	0/659	0.18	0/827
20	T	0.37	0/4184	0.98	8/6458 (0.1%)
21	U	0.13	0/870	0.24	0/1183
22	V	0.13	0/1728	0.31	0/2357
23	W	0.16	0/2392	0.28	0/3257
24	X	0.17	0/356	0.28	0/478
25	Y	0.11	0/927	0.21	0/1250
26	Z	0.10	0/4084	0.22	0/5498
27	a	0.21	0/835	0.33	0/1120
27	e	0.23	0/786	0.35	0/1053
28	b	0.21	0/629	0.34	0/843
28	f	0.21	0/629	0.32	0/843
29	c	0.20	0/810	0.30	0/1095
29	g	0.22	0/805	0.31	0/1088

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	0.24	0/732	0.33	0/986
30	h	0.24	0/705	0.35	0/951
31	l	0.14	0/2189	0.31	0/2930
All	All	0.22	0/74244	0.46	14/101466 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	109	DT	OP1-P-O3'	-21.64	43.08	108.00
20	T	-86	DT	OP1-P-O3'	7.08	129.24	108.00
16	P	16	A	N9-C1'-C2'	6.78	124.17	114.00
20	T	-99	DA	OP1-P-O3'	6.68	128.03	108.00
20	T	-34	DG	OP2-P-O3'	6.53	127.58	108.00
20	T	7	DG	OP2-P-O3'	6.49	127.46	108.00
20	T	31	DG	OP2-P-O3'	6.12	126.35	108.00
14	N	98	DG	OP1-P-O3'	5.83	125.49	108.00
16	P	20	U	N1-C1'-C2'	5.69	120.53	112.00
20	T	33	DC	OP2-P-O3'	5.65	124.95	108.00
20	T	-46	DG	OP1-P-O3'	5.47	124.40	108.00
14	N	51	DA	OP1-P-O3'	5.05	123.15	108.00
20	T	8	DT	OP1-P-OP2	-5.03	104.91	120.00
16	P	25	U	C3'-C2'-C1'	5.01	106.31	101.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	0	11374	234	0
2	B	8980	0	9019	179	0
3	C	2072	0	2020	53	0
4	D	1004	0	980	16	0
5	E	1720	0	1737	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	626	0	657	13	0
7	G	1333	0	1321	29	0
8	H	1197	0	1156	26	0
9	I	942	0	872	28	0
10	J	524	0	541	16	0
11	K	920	0	942	22	0
12	L	397	0	405	17	0
13	M	4883	0	2550	22	0
14	N	3474	0	1914	157	0
15	O	1046	0	1096	11	0
16	P	233	0	119	11	0
17	Q	7226	0	7169	186	0
18	R	1836	0	1699	31	0
19	S	657	0	199	5	0
20	T	3725	0	2030	86	0
21	U	856	0	680	11	0
22	V	1703	0	1426	26	0
23	W	2333	0	2246	55	0
24	X	353	0	371	7	0
25	Y	911	0	907	17	0
26	Z	4025	0	4041	62	0
27	a	823	0	864	7	0
27	e	776	0	815	6	0
28	b	622	0	660	3	0
28	f	622	0	660	3	0
29	c	800	0	851	3	0
29	g	795	0	846	4	0
30	d	721	0	742	1	0
30	h	694	0	709	3	0
31	l	2149	0	2089	30	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
All	All	72243	0	65707	1313	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 10.

All (1313) 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)
17:Q:276:ALA:HB1	17:Q:288:VAL:HG23	1.30	1.12
17:Q:353:TYR:OH	22:V:57:ARG:O	1.79	1.00
3:C:36:ARG:NH1	11:K:41:THR:OG1	1.99	0.95
31:l:1677:LYS:HA	31:l:1688:TYR:HA	1.49	0.95
17:Q:534:TYR:OH	17:Q:556:GLU:OE1	1.87	0.92
27:a:108:ASN:ND2	28:b:42:GLY:O	2.03	0.92
5:E:67:ASP:OD1	5:E:69:THR:OG1	1.91	0.89
2:B:790:GLN:O	2:B:968:ASN:ND2	2.06	0.89
12:L:25:GLU:N	12:L:25:GLU:OE1	2.07	0.88
20:T:9:DG:OP1	31:l:1639:LYS:NZ	2.06	0.88
2:B:891:ASP:OD1	2:B:893:SER:OG	1.92	0.87
1:A:140:ARG:NH2	1:A:234:PHE:O	2.09	0.86
1:A:559:GLU:N	1:A:559:GLU:OE1	2.09	0.85
5:E:141:GLU:N	5:E:141:GLU:OE1	2.09	0.85
1:A:116:LYS:NZ	1:A:182:GLY:O	2.10	0.85
1:A:535:MET:O	1:A:669:TYR:OH	1.93	0.84
17:Q:605:LEU:O	17:Q:609:ASN:ND2	2.09	0.84
1:A:818:GLU:OE1	1:A:818:GLU:N	2.10	0.84
3:C:242:GLU:OE1	3:C:242:GLU:N	2.11	0.83
12:L:39:CYS:SG	12:L:40:GLY:N	2.51	0.83
17:Q:776:LEU:O	17:Q:779:VAL:HG22	1.78	0.83
2:B:600:GLU:N	2:B:600:GLU:OE1	2.12	0.83
1:A:1324:GLU:N	1:A:1324:GLU:OE1	2.11	0.83
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.09	0.82
8:H:38:ASP:OD1	8:H:39:LEU:N	2.11	0.82
17:Q:799:VAL:O	17:Q:802:LYS:NZ	2.12	0.82
7:G:139:GLN:OE1	7:G:139:GLN:N	2.13	0.82
2:B:817:GLN:N	2:B:817:GLN:OE1	2.13	0.81
25:Y:38:ALA:O	25:Y:41:GLN:NE2	2.14	0.81
5:E:55:ARG:O	5:E:56:THR:OG1	1.98	0.81
8:H:18:GLU:N	8:H:18:GLU:OE1	2.14	0.80
9:I:31:GLU:N	9:I:31:GLU:OE1	2.15	0.80
1:A:556:GLU:OE1	1:A:556:GLU:N	2.14	0.80
18:R:388:ARG:NH1	18:R:446:GLU:O	2.14	0.80
2:B:191:GLU:OE1	2:B:191:GLU:N	2.15	0.80
2:B:676:ALA:HB2	2:B:693:TYR:CD1	2.17	0.80
2:B:1004:ASP:OD1	18:R:596:ARG:NH2	2.15	0.80
5:E:78:GLU:OE1	5:E:78:GLU:N	2.15	0.80
17:Q:384:LEU:HD13	17:Q:397:ALA:HB2	1.62	0.79
26:Z:523:GLU:N	26:Z:523:GLU:OE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:TYR:CZ	2:B:505:LEU:HD21	2.19	0.78
12:L:38:GLU:O	12:L:40:GLY:N	2.17	0.78
2:B:992:ASN:O	10:J:46:ARG:NH1	2.17	0.78
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.17	0.77
31:I:1631:CYS:SG	31:I:1685:CYS:HA	2.25	0.77
4:D:76:ASN:O	4:D:79:THR:OG1	2.01	0.77
5:E:36:THR:N	5:E:39:GLU:OE2	2.17	0.77
17:Q:333:THR:HG21	17:Q:347:LEU:HD12	1.65	0.77
1:A:946:ALA:O	1:A:950:ASN:ND2	2.18	0.77
1:A:184:CYS:SG	15:O:600:LYS:NZ	2.57	0.77
2:B:23:GLN:N	2:B:23:GLN:OE1	2.18	0.77
23:W:251:SER:OG	23:W:253:ASP:OD1	2.03	0.76
26:Z:541:GLN:NE2	26:Z:543:ASP:O	2.18	0.76
5:E:5:GLU:N	5:E:5:GLU:OE1	2.18	0.76
2:B:699:HIS:ND1	2:B:701:SER:OG	2.19	0.76
14:N:53:DG:H2'	14:N:54:DT:H71	1.67	0.76
1:A:971:PRO:O	1:A:972:THR:OG1	2.02	0.75
2:B:381:GLU:OE1	2:B:381:GLU:N	2.19	0.75
1:A:479:TRP:HB2	2:B:931:ILE:HD11	1.69	0.75
4:D:59:GLU:N	4:D:59:GLU:OE1	2.19	0.75
1:A:862:ARG:NH1	2:B:1088:GLU:OE1	2.19	0.75
1:A:1137:PRO:HB2	1:A:1341:VAL:HG23	1.69	0.75
1:A:936:GLU:N	1:A:936:GLU:OE1	2.19	0.75
2:B:100:GLU:N	2:B:100:GLU:OE1	2.20	0.74
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.68	0.74
17:Q:276:ALA:CB	17:Q:288:VAL:HG23	2.16	0.74
1:A:448:ARG:NH1	1:A:451:CYS:SG	2.60	0.74
1:A:805:ARG:NH1	9:I:77:THR:OG1	2.20	0.74
3:C:210:GLU:N	3:C:210:GLU:OE1	2.21	0.74
5:E:167:GLU:N	5:E:167:GLU:OE1	2.21	0.74
14:N:-11:DC:H2''	14:N:-10:DG:C8	2.23	0.73
25:Y:56:SER:OG	25:Y:90:THR:OG1	2.04	0.73
26:Z:469:ARG:NH2	26:Z:497:GLU:O	2.20	0.73
13:M:616:LEU:N	13:M:643:LYS:O	2.21	0.73
1:A:47:THR:OG1	1:A:51:ARG:O	2.07	0.73
5:E:96:GLU:OE1	5:E:96:GLU:N	2.22	0.73
17:Q:768:VAL:HG21	17:Q:778:GLU:HG3	1.70	0.73
4:D:96:GLU:N	4:D:96:GLU:OE1	2.21	0.73
25:Y:49:VAL:O	25:Y:53:THR:OG1	2.04	0.72
5:E:2:ASP:OD1	5:E:3:ASP:N	2.22	0.72
1:A:1027:ASP:OD1	1:A:1029:LEU:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:GLU:N	5:E:79:GLU:OE1	2.22	0.72
12:L:38:GLU:OE1	12:L:38:GLU:N	2.22	0.72
23:W:40:LEU:HD12	23:W:66:GLY:HA3	1.72	0.72
23:W:24:TRP:NE1	23:W:32:SER:O	2.22	0.72
26:Z:729:GLU:N	26:Z:729:GLU:OE1	2.22	0.72
1:A:695:ASP:O	1:A:696:SER:OG	2.05	0.71
2:B:228:SER:O	2:B:405:ARG:NH1	2.23	0.71
3:C:175:LYS:NZ	12:L:57:ALA:O	2.19	0.71
11:K:77:THR:OG1	11:K:81:TYR:O	2.05	0.71
1:A:945:ASN:OD1	1:A:947:HIS:N	2.22	0.71
3:C:109:GLU:OE1	3:C:109:GLU:N	2.22	0.71
8:H:136:GLU:N	8:H:136:GLU:OE1	2.22	0.71
1:A:1481:LYS:O	13:M:1384:ARG:NH1	2.22	0.71
1:A:423:ASN:ND2	1:A:425:ASP:OD1	2.24	0.71
20:T:-67:DG:H3'	20:T:-66:DT:H72	1.71	0.71
27:e:108:ASN:ND2	28:f:42:GLY:O	2.24	0.71
1:A:910:LYS:NZ	19:S:264:GLY:O	2.24	0.71
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.72	0.71
14:N:-42:DT:OP2	29:c:17:ARG:NH2	2.19	0.70
2:B:42:GLN:N	2:B:42:GLN:OE1	2.23	0.70
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.24	0.70
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.08	0.70
5:E:39:GLU:N	5:E:39:GLU:OE1	2.23	0.70
23:W:206:VAL:HG11	23:W:238:VAL:HG21	1.73	0.70
23:W:236:LEU:N	23:W:250:SER:O	2.25	0.70
14:N:-42:DT:H2'	14:N:-41:DT:H71	1.73	0.70
2:B:516:GLU:N	2:B:516:GLU:OE1	2.25	0.70
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.24	0.70
6:F:112:ASP:OD1	6:F:113:GLY:N	2.25	0.70
17:Q:743:ALA:O	17:Q:746:VAL:HG22	1.92	0.69
17:Q:18:GLU:N	17:Q:18:GLU:OE1	2.25	0.69
1:A:687:ILE:HD11	1:A:766:PHE:CZ	2.27	0.69
25:Y:56:SER:HG	25:Y:90:THR:HG1	1.33	0.69
14:N:-26:DC:H2''	14:N:-25:DT:H71	1.75	0.69
26:Z:455:GLU:OE1	26:Z:455:GLU:N	2.26	0.69
20:T:-81:DT:OP1	20:T:-81:DT:H71	1.92	0.69
17:Q:94:VAL:HG23	17:Q:140:LEU:HD11	1.74	0.69
6:F:86:GLU:N	6:F:86:GLU:OE1	2.26	0.69
1:A:48:GLU:OE1	1:A:48:GLU:N	2.25	0.69
1:A:1212:LEU:HD11	1:A:1285:LEU:HD13	1.74	0.69
12:L:21:GLU:OE1	12:L:21:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:DC:H2''	14:N:47:DA:C8	2.28	0.69
17:Q:500:SER:OG	17:Q:523:ILE:HD11	1.93	0.69
20:T:-24:DT:C2	20:T:-23:DG:C8	2.81	0.69
2:B:650:ASN:N	2:B:650:ASN:OD1	2.25	0.69
1:A:296:ASN:OD1	1:A:297:GLY:N	2.27	0.68
17:Q:167:LEU:HD21	17:Q:189:ALA:HB2	1.73	0.68
17:Q:620:ARG:NH2	17:Q:629:GLN:OE1	2.26	0.68
23:W:95:ASN:O	23:W:97:LYS:NZ	2.26	0.68
9:I:87:GLN:OE1	9:I:87:GLN:N	2.26	0.68
11:K:93:ASP:OD1	11:K:94:LEU:N	2.27	0.68
17:Q:95:GLN:NE2	22:V:84:ILE:O	2.26	0.68
1:A:576:GLN:O	1:A:590:GLN:NE2	2.26	0.68
1:A:1217:ASP:OD1	1:A:1218:ARG:N	2.26	0.68
1:A:1342:SER:O	1:A:1344:MET:N	2.27	0.68
17:Q:313:ALA:HB2	17:Q:328:TYR:CB	2.23	0.68
18:R:554:THR:O	18:R:558:SER:OG	2.12	0.68
17:Q:371:TYR:OH	22:V:69:GLN:NE2	2.27	0.68
23:W:53:ARG:NH1	23:W:54:LEU:O	2.26	0.68
9:I:82:GLU:OE1	9:I:82:GLU:N	2.27	0.67
17:Q:65:GLU:OE2	17:Q:93:TYR:OH	2.11	0.67
1:A:231:GLU:OE1	1:A:231:GLU:N	2.27	0.67
17:Q:237:GLY:HA2	22:V:74:LEU:HD21	1.76	0.67
20:T:67:DC:H2'	20:T:68:DT:H71	1.76	0.67
10:J:31:GLU:OE2	22:V:133:LYS:NZ	2.27	0.67
17:Q:454:LEU:HD21	17:Q:476:ALA:HB3	1.75	0.67
17:Q:750:ASP:OD1	17:Q:752:VAL:N	2.27	0.67
1:A:1172:ASN:N	1:A:1215:GLU:OE2	2.27	0.67
5:E:84:ILE:HD11	5:E:113:SER:O	1.95	0.67
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.67	0.67
17:Q:768:VAL:HG21	17:Q:778:GLU:CG	2.24	0.67
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.24	0.67
3:C:118:ARG:NH1	3:C:147:ASP:OD2	2.28	0.67
4:D:70:ARG:NH1	7:G:88:VAL:HG21	2.10	0.67
8:H:137:VAL:HG22	8:H:138:ASP:OD1	1.94	0.67
20:T:-87:DA:H2''	20:T:-86:DT:H72	1.77	0.67
20:T:-34:DG:H2''	20:T:-33:DT:H72	1.77	0.66
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.77	0.66
5:E:97:GLU:N	5:E:97:GLU:OE1	2.28	0.66
8:H:66:GLU:N	8:H:66:GLU:OE1	2.27	0.66
14:N:-52:DG:H2''	14:N:-51:DG:C8	2.31	0.66
26:Z:554:GLU:OE2	26:Z:559:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLU:OE1	1:A:724:GLU:N	2.29	0.66
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.31	0.66
9:I:67:GLN:N	9:I:67:GLN:OE1	2.27	0.66
17:Q:406:GLU:N	17:Q:406:GLU:OE1	2.29	0.66
1:A:197:GLU:N	1:A:197:GLU:OE1	2.28	0.66
17:Q:401:LEU:HD22	17:Q:418:LEU:HG	1.76	0.66
2:B:609:GLU:N	2:B:609:GLU:OE1	2.29	0.65
11:K:17:LYS:O	11:K:36:ASN:ND2	2.29	0.65
17:Q:708:LEU:HD21	17:Q:719:VAL:HG21	1.78	0.65
21:U:372:ASP:OD1	21:U:373:LEU:N	2.29	0.65
1:A:1456:GLU:N	1:A:1456:GLU:OE1	2.27	0.65
17:Q:286:SER:O	17:Q:290:HIS:ND1	2.29	0.65
18:R:366:ARG:NH2	26:Z:773:SER:OG	2.29	0.65
31:I:1678:CYS:N	31:I:1687:GLY:O	2.27	0.65
1:A:66:GLU:N	1:A:66:GLU:OE1	2.29	0.65
1:A:825:ASN:ND2	1:A:835:GLU:OE2	2.29	0.65
4:D:62:MET:O	4:D:66:ASN:ND2	2.30	0.65
3:C:58:VAL:HG11	10:J:59:LEU:HB3	1.78	0.65
3:C:86:ARG:NH1	26:Z:716:PRO:O	2.29	0.65
17:Q:776:LEU:HD22	17:Q:831:ALA:HA	1.78	0.65
17:Q:842:ARG:O	17:Q:846:GLU:HG2	1.97	0.65
23:W:64:GLN:OE1	23:W:89:ARG:NH2	2.30	0.65
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.28	0.65
7:G:110:ARG:NH1	7:G:114:PRO:O	2.30	0.65
9:I:19:GLU:N	9:I:19:GLU:OE1	2.30	0.65
14:N:-33:DG:H1'	14:N:-32:DA:C8	2.31	0.65
23:W:71:ASP:OD1	23:W:72:ILE:N	2.30	0.65
1:A:466:LYS:N	1:A:1093:GLN:OE1	2.30	0.64
17:Q:276:ALA:HB1	17:Q:288:VAL:CG2	2.18	0.64
7:G:10:GLU:N	7:G:10:GLU:OE1	2.31	0.64
1:A:902:GLU:OE1	1:A:902:GLU:N	2.30	0.64
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.31	0.64
23:W:176:ASP:O	23:W:180:GLY:N	2.30	0.64
2:B:384:ASP:OD1	2:B:385:ARG:N	2.30	0.64
12:L:25:GLU:O	12:L:26:ASN:ND2	2.31	0.64
13:M:1440:ARG:NH1	13:M:1486:TYR:OH	2.31	0.64
1:A:321:GLU:C	1:A:322:LEU:HD22	2.23	0.64
23:W:258:VAL:O	23:W:267:VAL:HG22	1.98	0.64
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.13	0.64
8:H:110:THR:O	8:H:129:ALA:N	2.31	0.64
1:A:353:ASN:ND2	2:B:1073:GLN:OE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:728:THR:OG1	26:Z:731:THR:O	2.10	0.63
31:l:1669:GLN:N	31:l:1690:GLY:HA2	2.13	0.63
8:H:72:ASP:OD1	8:H:73:GLY:N	2.32	0.63
17:Q:856:LEU:HD23	17:Q:857:LEU:HD22	1.81	0.63
23:W:272:ASP:O	23:W:274:GLN:NE2	2.31	0.63
23:W:195:SER:OG	23:W:236:LEU:O	2.17	0.63
26:Z:462:GLU:N	26:Z:462:GLU:OE1	2.32	0.63
26:Z:598:ASP:OD1	26:Z:599:ILE:N	2.31	0.63
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	1.99	0.63
10:J:44:CYS:O	10:J:47:ARG:NH1	2.32	0.63
1:A:103:THR:HG22	1:A:248:MET:HE3	1.81	0.63
1:A:613:GLU:OE2	1:A:622:SER:OG	2.11	0.63
17:Q:313:ALA:HB2	17:Q:328:TYR:HB3	1.81	0.63
2:B:555:GLU:OE1	2:B:555:GLU:N	2.32	0.63
27:e:106:ASP:OD2	27:e:131:ARG:NH2	2.32	0.63
2:B:388:TYR:H	2:B:504:THR:HG21	1.63	0.63
1:A:222:HIS:ND1	1:A:249:ILE:HD11	2.14	0.62
1:A:454:ASP:O	1:A:474:VAL:HG23	1.99	0.62
1:A:1180:ASN:O	1:A:1183:SER:OG	2.12	0.62
17:Q:682:ASP:O	17:Q:686:ASN:ND2	2.31	0.62
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.31	0.62
26:Z:504:SER:OG	26:Z:507:THR:O	2.16	0.62
2:B:650:ASN:H	21:U:460:TYR:HH	1.47	0.62
3:C:64:ILE:CD1	3:C:151:VAL:HG11	2.30	0.62
1:A:479:TRP:CB	2:B:931:ILE:HD11	2.30	0.62
1:A:524:MET:HA	1:A:524:MET:HE2	1.79	0.62
17:Q:668:ASP:OD1	17:Q:669:VAL:N	2.33	0.62
15:O:555:ASP:O	15:O:559:VAL:HG23	2.00	0.62
1:A:61:ARG:O	1:A:73:THR:OG1	2.15	0.62
1:A:459:ASN:OD1	1:A:460:ARG:N	2.33	0.62
1:A:1361:ASP:OD1	1:A:1362:ILE:N	2.33	0.62
3:C:86:ARG:NH2	3:C:172:GLU:OE2	2.33	0.62
20:T:-109:DA:C4	20:T:-108:DA:N7	2.68	0.62
18:R:411:THR:OG1	18:R:423:ASN:O	2.17	0.62
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.31	0.62
7:G:22:LEU:O	7:G:26:VAL:HG23	1.99	0.62
30:d:76:GLU:OE1	30:d:79:ARG:NH1	2.32	0.62
3:C:123:ASN:OD1	3:C:124:SER:N	2.33	0.62
1:A:295:GLN:O	15:O:672:ARG:NH1	2.33	0.61
2:B:867:ILE:HG22	2:B:894:THR:HG22	1.81	0.61
1:A:11:SER:O	2:B:1135:TYR:OH	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:494:GLU:N	18:R:494:GLU:OE1	2.31	0.61
1:A:674:THR:O	1:A:678:ASN:ND2	2.32	0.61
3:C:149:LEU:HD21	3:C:152:LYS:NZ	2.15	0.61
2:B:959:GLU:N	2:B:959:GLU:OE1	2.33	0.61
8:H:40:ILE:HG22	8:H:40:ILE:O	2.00	0.61
26:Z:604:ASP:OD1	26:Z:605:GLY:N	2.33	0.61
2:B:155:MET:HE2	2:B:183:GLY:HA2	1.82	0.61
2:B:835:GLU:N	2:B:835:GLU:OE1	2.33	0.61
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.82	0.61
11:K:84:GLN:N	11:K:84:GLN:OE1	2.34	0.61
25:Y:47:GLU:N	25:Y:47:GLU:OE1	2.34	0.61
17:Q:41:LEU:HD23	17:Q:81:ASP:HB3	1.83	0.61
3:C:59:LEU:HD12	3:C:151:VAL:HG12	1.82	0.60
20:T:57:DC:H2''	20:T:58:DA:C8	2.35	0.60
1:A:904:GLN:NE2	1:A:981:CYS:O	2.33	0.60
26:Z:437:GLN:OE1	26:Z:437:GLN:N	2.34	0.60
4:D:44:ARG:NH2	7:G:35:GLU:OE2	2.33	0.60
7:G:49:THR:OG1	7:G:73:LYS:O	2.18	0.60
7:G:141:ASP:OD2	7:G:143:ILE:HD11	2.02	0.60
20:T:69:DG:OP1	27:e:42:ARG:N	2.32	0.60
17:Q:386:ALA:HB1	17:Q:394:ARG:HG2	1.84	0.60
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.28	0.60
7:G:116:GLU:N	7:G:116:GLU:OE1	2.32	0.60
23:W:27:ASN:ND2	23:W:74:HIS:O	2.34	0.60
26:Z:775:TPO:O1P	26:Z:775:TPO:N	2.32	0.60
1:A:492:TYR:CD2	1:A:501:MET:HE1	2.36	0.60
1:A:762:GLU:OE1	1:A:762:GLU:N	2.30	0.60
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.36	0.60
23:W:248:VAL:HG11	23:W:289:ILE:HD13	1.83	0.60
1:A:621:ILE:HG23	1:A:621:ILE:O	2.02	0.60
14:N:103:DG:C2'	14:N:104:DT:H71	2.31	0.60
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.83	0.60
26:Z:602:VAL:HG22	26:Z:643:LEU:CD2	2.32	0.59
26:Z:729:GLU:O	26:Z:747:ARG:NH2	2.35	0.59
17:Q:285:TYR:HA	17:Q:288:VAL:HG12	1.84	0.59
25:Y:81:LYS:O	25:Y:85:TYR:OH	2.14	0.59
26:Z:613:GLU:N	26:Z:625:HIS:O	2.35	0.59
27:e:87:SER:OG	28:f:83:ALA:HB2	2.01	0.59
2:B:89:GLU:OE1	2:B:89:GLU:N	2.34	0.59
14:N:38:DC:H2''	14:N:39:DT:C6	2.37	0.59
20:T:-67:DG:H3'	20:T:-66:DT:C7	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-1:DC:H2''	14:N:0:DG:C8	2.37	0.59
1:A:1449:ASP:OD1	1:A:1451:MET:N	2.33	0.59
16:P:18:A:O2'	16:P:19:A:P	2.59	0.59
20:T:-89:DT:H2'	20:T:-88:DA:H8	1.66	0.59
23:W:33:GLU:O	23:W:49:TRP:N	2.34	0.59
23:W:125:THR:CG2	23:W:127:VAL:HG22	2.32	0.59
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.33	0.59
14:N:-17:DC:H2'	14:N:-16:DT:H72	1.84	0.59
2:B:281:ASP:OD1	2:B:285:LEU:HD13	2.02	0.59
17:Q:672:GLN:OE1	17:Q:672:GLN:N	2.35	0.59
2:B:849:ASP:OD2	12:L:46:LYS:NZ	2.32	0.59
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.35	0.59
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.84	0.59
1:A:120:ASP:O	1:A:122:ASN:N	2.36	0.58
2:B:198:GLU:N	2:B:198:GLU:OE1	2.36	0.58
2:B:756:LYS:NZ	22:V:135:GLU:O	2.36	0.58
4:D:59:GLU:OE2	4:D:60:VAL:HG23	2.03	0.58
20:T:15:DA:H1'	20:T:16:DA:C8	2.38	0.58
2:B:699:HIS:CE1	2:B:701:SER:HG	2.19	0.58
14:N:17:DA:H1'	14:N:18:DA:C8	2.39	0.58
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.36	0.58
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.39	0.58
17:Q:423:GLU:OE1	24:X:231:TRP:NE1	2.35	0.58
23:W:86:ALA:O	23:W:104:ALA:N	2.36	0.58
1:A:488:VAL:O	1:A:488:VAL:HG12	2.04	0.58
9:I:86:CYS:SG	9:I:87:GLN:N	2.77	0.58
14:N:-26:DC:H2''	14:N:-25:DT:C7	2.33	0.58
17:Q:313:ALA:HB2	17:Q:328:TYR:HB2	1.85	0.58
17:Q:612:LEU:HD23	17:Q:612:LEU:O	2.04	0.58
31:I:1680:CYS:SG	31:I:1681:GLY:N	2.76	0.58
1:A:1525:TPO:O	1:A:1525:TPO:O3P	2.22	0.58
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.86	0.58
14:N:-13:DA:H2''	14:N:-12:DA:H8	1.69	0.57
26:Z:426:VAL:HG13	26:Z:440:ILE:HD11	1.85	0.57
2:B:867:ILE:CG2	2:B:894:THR:HG22	2.34	0.57
1:A:683:GLU:O	2:B:1038:THR:OG1	2.20	0.57
26:Z:613:GLU:O	26:Z:625:HIS:N	2.35	0.57
31:I:1669:GLN:H	31:I:1690:GLY:HA2	1.68	0.57
17:Q:392:GLU:N	17:Q:392:GLU:OE1	2.37	0.57
1:A:90:LEU:HD21	1:A:92:LYS:O	2.04	0.57
14:N:9:DC:H2''	14:N:10:DG:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:81:DA:H2''	14:N:82:DG:C8	2.40	0.57
3:C:7:PRO:O	11:K:104:ARG:NH1	2.38	0.57
17:Q:443:GLU:OE1	17:Q:443:GLU:N	2.38	0.57
17:Q:774:SER:O	17:Q:830:ARG:NH1	2.37	0.57
23:W:17:ASP:OD1	23:W:18:ALA:N	2.38	0.57
8:H:74:GLU:OE2	8:H:76:ASN:ND2	2.38	0.57
17:Q:670:PHE:HB3	17:Q:687:LEU:HD21	1.87	0.57
18:R:410:GLU:OE2	18:R:423:ASN:ND2	2.38	0.57
20:T:-93:DG:H2'	20:T:-92:DA:O4'	2.05	0.57
23:W:31:ASN:OD1	23:W:32:SER:N	2.37	0.57
1:A:59:ASP:OD1	1:A:61:ARG:N	2.38	0.57
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.40	0.57
23:W:160:GLY:C	23:W:177:ILE:HD11	2.30	0.57
15:O:657:ILE:O	15:O:661:VAL:HG23	2.05	0.56
17:Q:386:ALA:HB1	17:Q:394:ARG:CG	2.35	0.56
25:Y:26:ASP:OD1	25:Y:27:GLN:N	2.38	0.56
31:I:1593:VAL:HG11	31:I:1671:TYR:OH	2.04	0.56
1:A:1262:MET:SD	1:A:1262:MET:N	2.78	0.56
3:C:190:ASN:ND2	3:C:195:THR:O	2.36	0.56
6:F:98:LYS:NZ	6:F:127:ASP:O	2.38	0.56
1:A:280:LEU:O	1:A:284:VAL:HG23	2.05	0.56
2:B:227:ASN:ND2	2:B:227:ASN:O	2.38	0.56
3:C:5:ASN:OD1	3:C:5:ASN:N	2.38	0.56
10:J:8:PHE:H	10:J:48:MET:HE3	1.68	0.56
1:A:1318:LYS:NZ	19:S:293:GLU:O	2.37	0.56
2:B:998:ASP:OD1	2:B:999:ALA:N	2.38	0.56
4:D:107:THR:HG23	4:D:110:GLU:H	1.71	0.56
8:H:2:ALA:O	8:H:84:ARG:NH2	2.37	0.56
25:Y:75:GLN:NE2	25:Y:86:ALA:O	2.39	0.56
2:B:30:ILE:HD11	2:B:698:ILE:HG21	1.87	0.56
2:B:313:GLU:HG3	2:B:316:VAL:HG12	1.88	0.56
6:F:90:LEU:HD23	6:F:90:LEU:O	2.06	0.56
14:N:24:DA:H2''	14:N:25:DA:C8	2.41	0.56
17:Q:384:LEU:CD1	17:Q:397:ALA:HB2	2.35	0.56
23:W:218:ASP:N	23:W:223:ASN:O	2.35	0.56
2:B:484:ARG:C	2:B:485:LEU:HD12	2.31	0.56
2:B:581:GLU:O	2:B:585:ASN:ND2	2.39	0.56
14:N:-19:DC:H2''	14:N:-18:DG:C8	2.41	0.56
14:N:9:DC:H2''	14:N:10:DG:H8	1.70	0.55
14:N:51:DA:C2	14:N:52:DC:C2	2.94	0.55
23:W:272:ASP:OD1	23:W:272:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:18:LEU:O	25:Y:111:ARG:NE	2.38	0.55
2:B:1028:LEU:HD12	2:B:1041:ILE:HG13	1.88	0.55
14:N:99:DT:H2'	14:N:100:DT:H6	1.70	0.55
5:E:55:ARG:C	5:E:56:THR:HG1	2.08	0.55
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.35	0.55
1:A:458:PHE:CD2	1:A:501:MET:HE2	2.41	0.55
1:A:484:LEU:N	1:A:484:LEU:HD23	2.21	0.55
14:N:42:DT:H2''	14:N:43:DC:C6	2.41	0.55
7:G:109:SER:CB	26:Z:493:VAL:HG11	2.37	0.55
11:K:100:LEU:HD21	11:K:104:ARG:NE	2.21	0.55
23:W:128:GLY:O	23:W:151:ILE:HD11	2.06	0.55
26:Z:588:ASP:OD1	26:Z:592:ASN:N	2.38	0.55
2:B:650:ASN:N	21:U:460:TYR:HH	2.05	0.55
17:Q:386:ALA:HB2	17:Q:393:LYS:CB	2.37	0.55
26:Z:592:ASN:OD1	26:Z:593:ASN:N	2.39	0.55
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.88	0.55
3:C:201:GLU:OE1	3:C:201:GLU:N	2.34	0.55
17:Q:239:ALA:HA	17:Q:257:LEU:HD13	1.88	0.55
17:Q:373:ASN:ND2	22:V:66:LEU:HD12	2.22	0.55
1:A:67:ARG:O	1:A:68:THR:OG1	2.17	0.55
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.88	0.55
14:N:-53:DA:C2	14:N:-52:DG:C4	2.95	0.55
2:B:601:VAL:HG22	2:B:616:THR:HG22	1.89	0.55
17:Q:189:ALA:HB1	17:Q:200:VAL:HG12	1.89	0.55
20:T:-10:DC:H2''	20:T:-9:DG:C8	2.42	0.55
23:W:237:ASN:OD1	23:W:238:VAL:N	2.39	0.55
2:B:155:MET:O	2:B:158:SER:OG	2.23	0.54
3:C:11:ILE:N	3:C:11:ILE:HD12	2.22	0.54
8:H:91:VAL:HG13	8:H:144:LEU:HD23	1.89	0.54
11:K:36:ASN:OD1	11:K:70:LYS:NZ	2.40	0.54
25:Y:112:ASP:OD2	25:Y:116:LYS:NZ	2.40	0.54
16:P:19:A:O2'	16:P:20:U:H5'	2.07	0.54
17:Q:143:ASP:N	17:Q:143:ASP:OD1	2.40	0.54
17:Q:401:LEU:CD1	17:Q:421:ILE:HD12	2.38	0.54
1:A:74:CYS:SG	1:A:84:HIS:CE1	3.01	0.54
2:B:407:MET:HE1	2:B:443:GLY:C	2.32	0.54
2:B:626:LEU:N	2:B:626:LEU:HD12	2.23	0.54
8:H:58:LEU:HD23	8:H:59:VAL:N	2.22	0.54
15:O:634:ARG:NH1	15:O:670:GLU:OE2	2.40	0.54
10:J:7:CYS:HA	10:J:48:MET:HE3	1.89	0.54
14:N:51:DA:H8	14:N:51:DA:OP1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:110:ILE:CD1	17:Q:140:LEU:HD13	2.37	0.54
23:W:186:LEU:HD11	23:W:222:ALA:HB1	1.88	0.54
26:Z:542:LEU:HD21	26:Z:560:VAL:HG21	1.89	0.54
16:P:19:A:C2	20:T:-85:DT:O2	2.61	0.54
17:Q:401:LEU:HD12	17:Q:421:ILE:HD12	1.90	0.54
20:T:-87:DA:C2'	20:T:-86:DT:H72	2.38	0.54
14:N:37:DC:H1'	14:N:38:DC:C5	2.43	0.54
14:N:65:DT:C2	14:N:66:DA:C8	2.95	0.54
14:N:28:DG:H1'	14:N:29:DG:C8	2.43	0.54
17:Q:764:LEU:C	17:Q:764:LEU:HD23	2.33	0.54
1:A:1302:GLU:O	1:A:1304:ILE:N	2.37	0.54
2:B:139:GLN:OE1	2:B:139:GLN:N	2.40	0.54
17:Q:401:LEU:HD21	17:Q:417:GLU:HB2	1.89	0.54
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.36	0.54
17:Q:753:LEU:O	17:Q:757:VAL:HG13	2.08	0.54
25:Y:40:LEU:HD23	25:Y:40:LEU:O	2.08	0.54
1:A:627:LYS:O	1:A:629:VAL:HG23	2.08	0.53
3:C:19:VAL:HG23	3:C:241:PRO:CG	2.37	0.53
14:N:-35:DT:O3'	14:N:-34:DA:C8	2.61	0.53
16:P:22:A:H2'	16:P:23:G:H8	1.73	0.53
20:T:-81:DT:C2	20:T:-80:DG:C8	2.96	0.53
25:Y:52:CYS:SG	25:Y:53:THR:N	2.81	0.53
1:A:427:ILE:N	1:A:427:ILE:HD12	2.23	0.53
14:N:54:DT:C2	14:N:55:DG:C8	2.96	0.53
21:U:445:ASP:OD2	22:V:199:VAL:HG21	2.07	0.53
26:Z:481:ILE:N	26:Z:481:ILE:HD12	2.22	0.53
14:N:7:DC:H1'	14:N:8:DC:C6	2.44	0.53
23:W:13:GLN:NE2	23:W:15:HIS:O	2.42	0.53
26:Z:466:GLN:OE1	26:Z:466:GLN:N	2.41	0.53
17:Q:123:ILE:O	17:Q:124:ILE:HD13	2.09	0.53
17:Q:189:ALA:HB1	17:Q:200:VAL:CG1	2.39	0.53
1:A:1179:PRO:O	9:I:33:ARG:NH2	2.41	0.53
14:N:99:DT:H2'	14:N:100:DT:C6	2.43	0.53
18:R:402:VAL:O	18:R:430:HIS:ND1	2.40	0.53
20:T:-92:DA:C2	20:T:-91:DG:C5	2.96	0.53
22:V:45:ASP:HB3	24:X:232:ARG:HE	1.73	0.53
1:A:1259:ILE:HD12	1:A:1259:ILE:N	2.23	0.53
7:G:101:ILE:HD12	7:G:101:ILE:N	2.24	0.53
20:T:-33:DT:C2'	20:T:-32:DA:C8	2.92	0.53
2:B:1003:ASN:OD1	2:B:1006:VAL:HG23	2.09	0.53
17:Q:166:LEU:HD12	17:Q:166:LEU:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:426:ASP:OD1	17:Q:429:GLY:N	2.41	0.53
23:W:176:ASP:OD2	23:W:179:THR:HG22	2.08	0.53
31:L:1681:GLY:HA2	31:L:1685:CYS:HB2	1.91	0.53
13:M:1516:GLN:N	13:M:1516:GLN:OE1	2.42	0.53
20:T:37:DG:H2''	20:T:38:DA:H8	1.74	0.53
26:Z:550:ILE:HD13	26:Z:558:PHE:HB3	1.91	0.53
1:A:36:VAL:HG12	1:A:85:PHE:O	2.09	0.53
14:N:-45:DC:H1'	14:N:-44:DA:C8	2.44	0.53
14:N:-5:DT:H1'	14:N:-4:DA:C8	2.44	0.53
18:R:493:GLU:OE1	18:R:493:GLU:N	2.41	0.53
26:Z:626:CYS:SG	26:Z:627:LYS:N	2.82	0.53
1:A:1547:SEP:O2P	13:M:1512:LYS:NZ	2.39	0.52
14:N:-37:DC:H2''	14:N:-36:DG:C8	2.43	0.52
14:N:-25:DT:H4'	14:N:-24:DA:OP1	2.09	0.52
14:N:68:DA:H2'	14:N:69:DT:H72	1.90	0.52
18:R:449:GLU:OE1	18:R:449:GLU:N	2.40	0.52
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.22	0.52
2:B:595:ASP:C	2:B:596:ILE:HD12	2.34	0.52
14:N:74:DA:H1'	14:N:75:DA:N7	2.24	0.52
17:Q:237:GLY:CA	22:V:74:LEU:HD21	2.37	0.52
17:Q:336:ALA:HB1	17:Q:339:SER:OG	2.09	0.52
20:T:59:DC:C2	20:T:60:DC:C5	2.98	0.52
2:B:727:ALA:O	2:B:731:GLN:NE2	2.41	0.52
9:I:103:ARG:NH2	9:I:105:GLU:OE2	2.43	0.52
14:N:55:DG:H2'	14:N:56:DT:H71	1.92	0.52
17:Q:69:ILE:H	17:Q:69:ILE:HD12	1.74	0.52
17:Q:201:ARG:HH12	17:Q:227:LEU:HD13	1.75	0.52
17:Q:697:TYR:OH	17:Q:726:ALA:O	2.17	0.52
2:B:941:GLN:OE1	2:B:975:ARG:NH1	2.42	0.52
13:M:1410:GLU:N	13:M:1410:GLU:OE1	2.42	0.52
14:N:-6:DG:H2''	14:N:-5:DT:C6	2.45	0.52
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.91	0.52
1:A:913:ASN:ND2	1:A:1325:ASP:O	2.43	0.52
14:N:8:DC:H2''	14:N:9:DC:C6	2.45	0.52
14:N:32:DT:H2''	14:N:33:DA:C8	2.45	0.52
26:Z:500:VAL:HG23	26:Z:500:VAL:O	2.09	0.52
2:B:312:GLN:N	2:B:312:GLN:OE1	2.42	0.52
8:H:27:ARG:C	8:H:28:LEU:HD22	2.35	0.52
14:N:18:DA:C4	14:N:19:DC:C6	2.98	0.52
20:T:-89:DT:H2'	20:T:-88:DA:C8	2.44	0.52
26:Z:746:ASP:OD1	26:Z:747:ARG:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:ILE:N	4:D:115:ILE:HD12	2.25	0.52
5:E:84:ILE:HD11	5:E:113:SER:C	2.35	0.52
14:N:106:DT:C2	14:N:107:DG:C8	2.98	0.52
20:T:-109:DA:C2	20:T:-108:DA:C5	2.97	0.52
20:T:7:DG:H2'	20:T:8:DT:C7	2.40	0.52
5:E:57:ASP:N	5:E:57:ASP:OD1	2.42	0.52
20:T:-97:DA:H2''	20:T:-96:DC:H6	1.74	0.52
2:B:836:THR:OG1	2:B:889:LYS:NZ	2.30	0.52
21:U:458:ASP:OD1	21:U:459:VAL:N	2.43	0.52
1:A:367:ILE:HD11	1:A:499:ASP:HB2	1.92	0.51
1:A:614:ASP:OD1	1:A:615:SER:N	2.42	0.51
2:B:474:THR:O	2:B:477:SER:OG	2.22	0.51
2:B:759:VAL:HG21	2:B:983:GLU:HG3	1.92	0.51
2:B:780:VAL:HG21	2:B:1048:TYR:CE1	2.45	0.51
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.92	0.51
17:Q:619:THR:HG22	17:Q:622:ARG:CZ	2.40	0.51
18:R:470:ASP:OD1	18:R:471:GLU:N	2.43	0.51
26:Z:424:ASP:HB2	26:Z:440:ILE:HD12	1.91	0.51
1:A:485:ASN:OD1	1:A:486:LEU:N	2.44	0.51
1:A:1171:ALA:HB3	1:A:1215:GLU:OE2	2.10	0.51
14:N:-13:DA:H2''	14:N:-12:DA:C8	2.45	0.51
18:R:404:GLU:N	18:R:404:GLU:OE1	2.43	0.51
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.43	0.51
3:C:49:TRP:NE1	26:Z:719:GLY:O	2.43	0.51
3:C:161:LEU:HD12	3:C:161:LEU:C	2.35	0.51
6:F:61:GLU:O	6:F:65:VAL:HG23	2.10	0.51
14:N:-3:DC:H1'	14:N:-2:DG:C8	2.45	0.51
17:Q:68:ARG:HE	17:Q:89:LEU:HD12	1.75	0.51
20:T:-44:DA:C2	20:T:-43:DG:C5	2.98	0.51
26:Z:550:ILE:HD11	26:Z:552:ARG:O	2.10	0.51
14:N:61:DT:C2	14:N:62:DA:C8	2.99	0.51
17:Q:679:ASP:O	17:Q:680:ILE:HD13	2.10	0.51
17:Q:768:VAL:HG22	17:Q:768:VAL:O	2.11	0.51
20:T:-81:DT:OP1	20:T:-81:DT:C6	2.64	0.51
2:B:347:MET:O	2:B:361:LYS:NZ	2.40	0.51
14:N:74:DA:H1'	14:N:75:DA:C8	2.45	0.51
20:T:36:DC:H2''	20:T:37:DG:C8	2.45	0.51
20:T:55:DG:N2	20:T:56:DG:N2	2.58	0.51
22:V:88:ASN:N	22:V:89:PRO:CD	2.74	0.51
2:B:583:LEU:O	2:B:587:LEU:HD23	2.11	0.51
2:B:1050:ARG:NH2	2:B:1054:MET:SD	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:17:DA:H1'	14:N:18:DA:N7	2.25	0.51
17:Q:534:TYR:HD2	17:Q:557:ALA:HB2	1.76	0.51
26:Z:602:VAL:HG22	26:Z:643:LEU:HD23	1.93	0.51
27:a:52:ARG:NH1	31:l:1522:ASN:OD1	2.39	0.51
1:A:386:ALA:O	1:A:449:HIS:ND1	2.44	0.51
1:A:1156:ASP:OD1	1:A:1157:ILE:N	2.44	0.51
13:M:1350:MET:HE2	13:M:1350:MET:HA	1.92	0.51
14:N:26:DG:H1'	14:N:27:DG:C8	2.46	0.51
20:T:-25:DT:H2'	20:T:-24:DT:H72	1.92	0.51
2:B:502:HIS:ND1	2:B:504:THR:HG22	2.26	0.51
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.44	0.51
13:M:1086:ALA:O	13:M:1090:GLU:N	2.35	0.51
13:M:1100:LYS:O	31:l:2028:LYS:N	2.38	0.51
17:Q:437:ALA:O	17:Q:440:ILE:HG22	2.11	0.51
23:W:132:ILE:HG21	23:W:142:TYR:CZ	2.46	0.51
1:A:611:ASP:OD1	1:A:612:ASP:N	2.43	0.51
14:N:49:DG:H2''	14:N:50:DC:C5	2.46	0.50
18:R:353:VAL:O	18:R:456:LYS:NZ	2.41	0.50
20:T:-14:DA:H2''	20:T:-13:DA:H8	1.77	0.50
1:A:1208:SER:OG	1:A:1210:TRP:CE2	2.64	0.50
14:N:2:DT:H2''	14:N:3:DG:C8	2.46	0.50
14:N:107:DG:H2'	14:N:108:DT:H71	1.92	0.50
1:A:315:ALA:O	1:A:319:ASP:N	2.41	0.50
1:A:419:ILE:HG23	1:A:419:ILE:O	2.11	0.50
1:A:712:ASP:O	1:A:716:VAL:HG23	2.11	0.50
9:I:83:ASP:N	9:I:83:ASP:OD1	2.41	0.50
14:N:-44:DA:H1'	14:N:-43:DA:C8	2.46	0.50
20:T:-40:DT:H2''	20:T:-39:DA:C8	2.46	0.50
26:Z:554:GLU:OE1	26:Z:557:THR:OG1	2.28	0.50
1:A:686:THR:OG1	1:A:687:ILE:N	2.44	0.50
1:A:1123:ARG:CG	1:A:1385:VAL:HG11	2.41	0.50
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.94	0.50
26:Z:421:GLN:N	26:Z:421:GLN:OE1	2.44	0.50
1:A:111:CYS:N	1:A:116:LYS:O	2.40	0.50
14:N:59:DG:H2''	14:N:60:DA:C8	2.47	0.50
17:Q:272:LEU:HB2	17:Q:295:ALA:HB2	1.94	0.50
17:Q:776:LEU:HD22	17:Q:831:ALA:CA	2.40	0.50
21:U:392:GLN:OE1	21:U:392:GLN:N	2.45	0.50
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.42	0.50
3:C:103:LEU:HD23	3:C:104:ASP:N	2.26	0.50
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:63:DT:C2	14:N:64:DA:C8	3.00	0.50
17:Q:506:LEU:O	17:Q:510:MET:N	2.45	0.50
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.44	0.50
16:P:22:A:H2'	16:P:23:G:C8	2.46	0.50
20:T:57:DC:C2'	20:T:58:DA:C8	2.94	0.50
2:B:988:LYS:O	2:B:992:ASN:ND2	2.45	0.50
4:D:70:ARG:HH12	7:G:88:VAL:HG21	1.76	0.50
7:G:138:GLN:N	7:G:138:GLN:OE1	2.45	0.50
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.94	0.49
2:B:252:ILE:HD12	2:B:252:ILE:N	2.27	0.49
11:K:11:LEU:O	11:K:37:LYS:NZ	2.42	0.49
13:M:1377:ILE:N	13:M:1377:ILE:HD12	2.27	0.49
14:N:-35:DT:H2''	14:N:-34:DA:N7	2.27	0.49
1:A:937:ASP:OD1	1:A:937:ASP:N	2.45	0.49
2:B:20:ASP:N	2:B:20:ASP:OD1	2.43	0.49
2:B:626:LEU:HD11	2:B:698:ILE:HG12	1.94	0.49
2:B:47:PHE:HB2	2:B:155:MET:SD	2.52	0.49
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.93	0.49
17:Q:190:LEU:O	17:Q:193:ASN:ND2	2.45	0.49
17:Q:204:MET:HE1	22:V:107:LEU:HD13	1.94	0.49
18:R:366:ARG:NH2	26:Z:775:TPO:O2P	2.46	0.49
1:A:464:LEU:O	1:A:861:GLN:NE2	2.42	0.49
1:A:1211:LEU:C	1:A:1211:LEU:HD12	2.38	0.49
1:A:1291:ASN:OD1	1:A:1292:MET:N	2.46	0.49
17:Q:612:LEU:HD23	17:Q:612:LEU:C	2.37	0.49
17:Q:678:ALA:O	17:Q:684:TRP:NE1	2.45	0.49
20:T:-97:DA:H2''	20:T:-96:DC:C6	2.47	0.49
26:Z:587:LEU:H	26:Z:587:LEU:HD23	1.77	0.49
5:E:13:ILE:HD11	5:E:132:GLN:HB2	1.95	0.49
11:K:45:ILE:HD12	11:K:94:LEU:HD21	1.95	0.49
12:L:18:ILE:N	12:L:18:ILE:HD12	2.28	0.49
14:N:39:DT:H1'	14:N:40:DA:C8	2.47	0.49
17:Q:887:ASN:HA	17:Q:890:MET:HG2	1.95	0.49
22:V:61:TYR:N	22:V:62:LYS:HA	2.28	0.49
23:W:48:LYS:N	23:W:55:ASP:O	2.42	0.49
23:W:107:VAL:HG22	23:W:107:VAL:O	2.11	0.49
2:B:39:LEU:HD12	2:B:39:LEU:N	2.28	0.49
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.47	0.49
3:C:154:ARG:NH1	10:J:60:LEU:O	2.35	0.49
26:Z:553:LEU:N	26:Z:553:LEU:HD12	2.27	0.49
2:B:161:CYS:SG	2:B:162:LEU:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:132:ASP:O	13:M:416:LEU:CA	2.61	0.49
9:I:39:CYS:SG	9:I:42:CYS:N	2.82	0.49
14:N:-62:DC:H2''	14:N:-61:DC:C6	2.48	0.49
2:B:85:LEU:HD12	2:B:85:LEU:N	2.28	0.49
14:N:14:DT:H2'	14:N:15:DT:H72	1.95	0.49
14:N:47:DA:C6	14:N:48:DG:C6	3.01	0.49
14:N:73:DT:C2	14:N:74:DA:C8	3.00	0.49
22:V:84:ILE:O	22:V:84:ILE:HG23	2.13	0.49
2:B:814:TYR:OH	2:B:896:LEU:HD12	2.13	0.49
5:E:148:HIS:CD2	5:E:179:VAL:HG11	2.48	0.49
8:H:58:LEU:HD23	8:H:58:LEU:C	2.38	0.49
13:M:1101:ASP:O	31:I:2025:ILE:HG22	2.13	0.49
17:Q:737:LYS:HZ2	17:Q:764:LEU:HD13	1.77	0.49
24:X:233:THR:O	24:X:236:THR:OG1	2.26	0.49
1:A:1212:LEU:N	1:A:1212:LEU:HD12	2.28	0.48
2:B:989:VAL:HG12	22:V:131:MET:HE1	1.95	0.48
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.45	0.48
14:N:-62:DC:C2	20:T:63:DG:N2	2.81	0.48
14:N:99:DT:H3'	14:N:100:DT:H71	1.94	0.48
1:A:560:VAL:O	1:A:564:LEU:HD23	2.14	0.48
14:N:31:DT:H2'	14:N:32:DT:H71	1.95	0.48
17:Q:769:LEU:HD13	17:Q:824:ALA:HB2	1.94	0.48
23:W:79:ALA:O	23:W:91:TRP:O	2.31	0.48
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.42	0.48
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.46	0.48
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.45	0.48
3:C:148:ILE:N	3:C:148:ILE:HD12	2.29	0.48
4:D:39:MET:SD	4:D:40:LEU:N	2.87	0.48
14:N:26:DG:O3'	14:N:27:DG:H8	1.96	0.48
26:Z:184:CYS:SG	26:Z:185:LYS:N	2.87	0.48
1:A:587:THR:HG22	1:A:588:GLY:N	2.27	0.48
1:A:737:PHE:O	1:A:741:VAL:HG23	2.13	0.48
1:A:860:ILE:HD13	1:A:863:ARG:NH2	2.28	0.48
2:B:395:LEU:HD21	2:B:532:ILE:HD13	1.95	0.48
2:B:634:LEU:HD22	2:B:634:LEU:N	2.28	0.48
17:Q:708:LEU:HD11	17:Q:719:VAL:HG21	1.94	0.48
17:Q:793:PHE:HA	17:Q:796:LEU:HD21	1.95	0.48
26:Z:290:ILE:N	26:Z:290:ILE:HD12	2.29	0.48
1:A:604:ARG:O	1:A:628:VAL:N	2.47	0.48
1:A:909:LEU:C	1:A:911:PRO:HD3	2.39	0.48
2:B:309:PHE:O	2:B:312:GLN:NE2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:PHE:HB2	2:B:613:ARG:HG2	1.94	0.48
2:B:1017:ASP:OD1	2:B:1017:ASP:N	2.45	0.48
7:G:30:LEU:O	7:G:34:VAL:HG22	2.12	0.48
17:Q:852:LEU:HD12	17:Q:852:LEU:C	2.39	0.48
20:T:39:DC:C2	20:T:40:DC:C5	3.01	0.48
22:V:109:GLU:OE1	22:V:109:GLU:N	2.43	0.48
23:W:169:ASP:OD1	23:W:169:ASP:N	2.45	0.48
1:A:196:LEU:HD12	1:A:196:LEU:N	2.28	0.48
1:A:983:LEU:HD12	1:A:1044:HIS:CE1	2.49	0.48
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.14	0.48
1:A:1414:ILE:O	1:A:1414:ILE:HG22	2.13	0.48
18:R:374:HIS:ND1	18:R:498:GLU:OE1	2.41	0.48
21:U:395:GLU:N	21:U:395:GLU:OE1	2.46	0.48
26:Z:192:THR:OG1	26:Z:244:ASN:ND2	2.46	0.48
2:B:937:SER:OG	2:B:938:ARG:N	2.44	0.48
14:N:103:DG:H2'	14:N:104:DT:H71	1.94	0.48
17:Q:737:LYS:HE3	17:Q:760:VAL:HG22	1.96	0.48
20:T:-80:DG:H2''	20:T:-79:DG:C8	2.48	0.48
20:T:-25:DT:H2'	20:T:-24:DT:C7	2.43	0.48
5:E:20:LEU:C	5:E:20:LEU:HD23	2.38	0.48
14:N:-9:DC:H2''	14:N:-8:DA:H8	1.78	0.48
18:R:577:LYS:HA	18:R:580:VAL:HG22	1.96	0.48
20:T:-71:DC:C2	20:T:-70:DG:C8	3.02	0.48
2:B:633:LEU:HD12	2:B:633:LEU:N	2.29	0.48
6:F:80:MET:N	6:F:96:GLU:OE2	2.38	0.48
7:G:54:ILE:HD13	7:G:70:VAL:HG23	1.96	0.48
7:G:101:ILE:N	7:G:104:MET:O	2.47	0.48
16:P:18:A:O2'	16:P:19:A:O5'	2.31	0.48
26:Z:341:ASP:OD1	26:Z:342:ALA:N	2.47	0.48
2:B:898:THR:O	2:B:899:SER:OG	2.26	0.48
3:C:50:VAL:HG22	3:C:163:ALA:HB2	1.95	0.48
7:G:108:ILE:N	7:G:108:ILE:HD12	2.29	0.48
11:K:24:ASP:OD1	11:K:25:THR:N	2.43	0.48
14:N:-56:DC:H2''	14:N:-55:DC:C5	2.49	0.48
17:Q:776:LEU:N	17:Q:776:LEU:HD23	2.28	0.48
17:Q:856:LEU:CD2	17:Q:857:LEU:HD22	2.43	0.48
22:V:127:VAL:HG23	22:V:128:VAL:N	2.29	0.48
1:A:293:ASN:O	1:A:298:ALA:N	2.44	0.47
1:A:560:VAL:HG21	1:A:586:TRP:CG	2.49	0.47
1:A:1473:LEU:N	1:A:1473:LEU:HD12	2.28	0.47
2:B:568:PHE:CE2	2:B:573:TRP:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-11:DC:C2'	14:N:-10:DG:C8	2.96	0.47
17:Q:86:LEU:HG	17:Q:120:ALA:HB2	1.96	0.47
17:Q:662:TYR:O	17:Q:666:ALA:N	2.46	0.47
2:B:814:TYR:N	2:B:921:ILE:O	2.47	0.47
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.14	0.47
14:N:56:DT:H2''	14:N:57:DC:C6	2.49	0.47
17:Q:341:VAL:HG21	17:Q:367:VAL:HG13	1.95	0.47
20:T:19:DG:C4	20:T:20:DG:C8	3.03	0.47
9:I:110:LEU:N	9:I:110:LEU:HD22	2.29	0.47
12:L:18:ILE:HD11	12:L:47:LYS:HB2	1.96	0.47
20:T:24:DT:O3'	20:T:25:DA:C8	2.67	0.47
23:W:25:GLY:N	23:W:72:ILE:HD12	2.30	0.47
1:A:422:ASP:OD1	1:A:423:ASN:N	2.48	0.47
2:B:646:ARG:C	2:B:648:TYR:H	2.22	0.47
5:E:114:ALA:O	5:E:118:LEU:HD13	2.14	0.47
20:T:-88:DA:H2'	20:T:-87:DA:C8	2.50	0.47
20:T:37:DG:H2''	20:T:38:DA:C8	2.48	0.47
21:U:441:VAL:HG11	22:V:190:ILE:CD1	2.45	0.47
31:I:1452:ASP:OD1	31:I:1453:ASP:N	2.48	0.47
1:A:1318:LYS:NZ	19:S:292:ASN:O	2.48	0.47
14:N:109:DT:H2'	14:N:110:DT:H71	1.96	0.47
17:Q:471:LYS:O	17:Q:475:LEU:HD23	2.14	0.47
26:Z:189:GLU:N	26:Z:189:GLU:OE1	2.46	0.47
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.22	0.47
5:E:126:ILE:HD12	5:E:126:ILE:N	2.29	0.47
20:T:-25:DT:H2''	20:T:-24:DT:C6	2.50	0.47
20:T:-21:DC:C2	20:T:-20:DG:C8	3.03	0.47
1:A:977:VAL:HG22	1:A:978:VAL:N	2.30	0.47
2:B:529:MET:HB2	2:B:702:MET:CG	2.44	0.47
2:B:850:ASP:OD1	2:B:851:ASP:N	2.48	0.47
3:C:91:GLU:N	3:C:91:GLU:OE1	2.48	0.47
3:C:149:LEU:HD21	3:C:152:LYS:HZ2	1.79	0.47
14:N:35:DT:H2''	14:N:36:DC:C6	2.48	0.47
14:N:39:DT:O3'	14:N:40:DA:H8	1.98	0.47
14:N:80:DC:C2	14:N:81:DA:N7	2.82	0.47
23:W:56:LEU:HD11	23:W:58:TRP:O	2.14	0.47
14:N:27:DG:H2''	14:N:28:DG:C8	2.50	0.47
14:N:104:DT:H2''	14:N:105:DG:H8	1.80	0.47
17:Q:239:ALA:HB2	17:Q:257:LEU:HB3	1.96	0.47
18:R:439:LEU:O	18:R:442:VAL:HG12	2.15	0.47
20:T:-108:DA:H2'	20:T:-107:DC:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:94:ILE:HD12	22:V:94:ILE:H	1.80	0.47
17:Q:384:LEU:HD22	17:Q:397:ALA:CB	2.45	0.47
22:V:127:VAL:HG23	22:V:128:VAL:H	1.79	0.47
26:Z:589:SER:OG	26:Z:641:ARG:O	2.11	0.47
1:A:1158:LEU:C	1:A:1158:LEU:HD23	2.40	0.47
2:B:140:LEU:HD23	2:B:140:LEU:H	1.80	0.47
7:G:147:ILE:HD12	7:G:147:ILE:N	2.29	0.47
13:M:351:LYS:O	13:M:355:THR:N	2.44	0.47
14:N:-42:DT:C2'	14:N:-41:DT:H71	2.43	0.47
23:W:248:VAL:HG12	23:W:258:VAL:HG22	1.96	0.47
2:B:67:LEU:HD12	2:B:84:TYR:OH	2.16	0.46
2:B:699:HIS:CE1	2:B:701:SER:OG	2.67	0.46
17:Q:43:ILE:HD12	17:Q:43:ILE:H	1.80	0.46
17:Q:94:VAL:HG21	17:Q:136:CYS:SG	2.55	0.46
17:Q:395:ASP:OD1	17:Q:395:ASP:N	2.48	0.46
20:T:61:DG:H2''	20:T:62:DG:C8	2.50	0.46
1:A:1434:GLU:O	1:A:1438:VAL:HG22	2.15	0.46
3:C:50:VAL:HG22	3:C:163:ALA:CB	2.46	0.46
3:C:131:THR:HG22	3:C:147:ASP:OD1	2.15	0.46
5:E:148:HIS:NE2	5:E:179:VAL:HG11	2.30	0.46
14:N:18:DA:C4	14:N:19:DC:C5	3.03	0.46
14:N:64:DA:H2'	14:N:65:DT:H72	1.96	0.46
17:Q:326:PHE:HA	17:Q:350:MET:HG2	1.97	0.46
17:Q:423:GLU:OE2	24:X:229:ARG:NH2	2.48	0.46
20:T:-3:DC:H2''	20:T:-2:DA:C8	2.51	0.46
20:T:28:DG:H2''	20:T:29:DC:C6	2.50	0.46
2:B:207:VAL:HG21	2:B:371:ARG:HG2	1.97	0.46
2:B:279:VAL:HG13	2:B:280:SER:N	2.29	0.46
8:H:96:VAL:HA	8:H:116:VAL:HA	1.96	0.46
9:I:29:ASP:O	9:I:33:ARG:N	2.48	0.46
17:Q:80:LYS:O	17:Q:84:THR:HG23	2.15	0.46
17:Q:163:ILE:HG21	17:Q:189:ALA:HA	1.97	0.46
17:Q:289:GLN:O	17:Q:293:LEU:HD23	2.15	0.46
17:Q:439:ARG:O	17:Q:443:GLU:OE2	2.34	0.46
17:Q:855:LYS:O	17:Q:858:LYS:HG3	2.15	0.46
26:Z:188:GLU:N	26:Z:188:GLU:OE1	2.49	0.46
4:D:114:LEU:C	4:D:115:ILE:HD12	2.41	0.46
5:E:66:ASP:OD1	5:E:67:ASP:N	2.48	0.46
14:N:80:DC:C2	14:N:81:DA:C8	3.04	0.46
17:Q:386:ALA:HB2	17:Q:393:LYS:HB3	1.96	0.46
2:B:285:LEU:HD22	9:I:16:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:MET:SD	2:B:603:MET:N	2.89	0.46
5:E:84:ILE:HA	5:E:87:ILE:HG12	1.98	0.46
9:I:35:LEU:C	9:I:36:LEU:HD22	2.40	0.46
14:N:32:DT:C2'	14:N:33:DA:C8	2.98	0.46
14:N:60:DA:C8	14:N:61:DT:H72	2.50	0.46
14:N:72:DA:C2'	14:N:73:DT:H72	2.46	0.46
20:T:7:DG:H2'	20:T:8:DT:H72	1.96	0.46
20:T:38:DA:H2''	20:T:39:DC:H6	1.81	0.46
2:B:567:ILE:N	2:B:567:ILE:HD12	2.29	0.46
3:C:83:GLN:N	3:C:83:GLN:OE1	2.48	0.46
9:I:42:CYS:SG	9:I:43:ASP:N	2.89	0.46
17:Q:611:TRP:HD1	17:Q:632:ALA:HB2	1.81	0.46
17:Q:708:LEU:HD23	17:Q:712:TYR:OH	2.16	0.46
20:T:58:DA:H2''	20:T:59:DC:H6	1.79	0.46
22:V:94:ILE:HG22	22:V:94:ILE:O	2.16	0.46
23:W:170:GLY:HA2	23:W:193:ILE:HG13	1.97	0.46
1:A:1151:ALA:HB1	1:A:1309:MET:HE1	1.98	0.46
1:A:1280:ASP:OD1	1:A:1281:ASP:N	2.49	0.46
17:Q:879:ALA:O	17:Q:882:VAL:HG12	2.16	0.46
18:R:483:LEU:C	18:R:483:LEU:HD23	2.41	0.46
31:L:1578:GLU:O	31:L:1622:ASN:ND2	2.48	0.46
1:A:90:LEU:HD23	1:A:90:LEU:O	2.15	0.46
1:A:881:ASN:OD1	1:A:881:ASN:N	2.49	0.46
1:A:1175:ILE:HD11	1:A:1285:LEU:HD12	1.97	0.46
1:A:1243:LEU:N	1:A:1243:LEU:HD12	2.30	0.46
2:B:911:LEU:HD21	12:L:34:ILE:HD13	1.96	0.46
13:M:1119:LYS:O	13:M:1123:LEU:N	2.49	0.46
17:Q:94:VAL:CG2	17:Q:140:LEU:HD11	2.43	0.46
20:T:-79:DG:H2''	20:T:-78:DC:H6	1.80	0.46
31:L:1670:ARG:HD2	31:L:1694:ARG:HA	1.98	0.46
1:A:460:ARG:NH2	16:P:26:C:O2'	2.48	0.46
2:B:759:VAL:HG23	2:B:759:VAL:O	2.14	0.46
12:L:24:THR:OG1	12:L:38:GLU:OE2	2.30	0.46
14:N:17:DA:O3'	14:N:18:DA:H8	1.99	0.46
14:N:104:DT:H2''	14:N:105:DG:C8	2.51	0.46
20:T:-109:DA:H2''	20:T:-108:DA:H8	1.81	0.46
23:W:66:GLY:O	23:W:83:SER:OG	2.30	0.46
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.47	0.46
2:B:433:LEU:HD22	2:B:433:LEU:N	2.31	0.46
2:B:592:ARG:CZ	2:B:627:ILE:HD13	2.46	0.46
12:L:16:ILE:HD11	12:L:25:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-46:DT:H2''	14:N:-45:DC:C6	2.50	0.46
14:N:59:DG:H2''	14:N:60:DA:H8	1.80	0.46
14:N:66:DA:H2''	14:N:67:DC:C6	2.51	0.46
17:Q:302:GLU:HA	17:Q:305:GLN:HG2	1.98	0.46
21:U:440:ILE:HD12	21:U:440:ILE:N	2.30	0.46
1:A:997:ASN:O	1:A:999:ARG:N	2.44	0.45
2:B:428:ASP:OD1	2:B:429:PHE:N	2.50	0.45
5:E:103:LEU:C	5:E:103:LEU:HD23	2.40	0.45
5:E:131:LEU:N	5:E:131:LEU:HD12	2.31	0.45
17:Q:493:ASN:O	17:Q:497:VAL:HG23	2.15	0.45
1:A:809:HIS:CE1	2:B:677:MET:SD	3.09	0.45
1:A:912:SER:O	1:A:913:ASN:C	2.59	0.45
14:N:-41:DT:H2''	14:N:-40:DG:C8	2.51	0.45
17:Q:155:VAL:HG11	17:Q:165:ALA:HB1	1.97	0.45
17:Q:716:ASN:OD1	17:Q:717:THR:N	2.49	0.45
22:V:97:ASN:ND2	22:V:98:VAL:O	2.49	0.45
23:W:160:GLY:CA	23:W:177:ILE:HD11	2.46	0.45
26:Z:196:LEU:CD2	26:Z:215:VAL:HG11	2.46	0.45
1:A:553:VAL:C	1:A:554:PHE:CD1	2.95	0.45
3:C:58:VAL:HG12	3:C:58:VAL:O	2.15	0.45
11:K:93:ASP:OD1	11:K:93:ASP:C	2.60	0.45
11:K:100:LEU:HD23	11:K:100:LEU:C	2.42	0.45
14:N:39:DT:H2''	14:N:40:DA:N7	2.31	0.45
17:Q:86:LEU:HD23	17:Q:120:ALA:HA	1.97	0.45
17:Q:448:ASP:OD1	17:Q:449:VAL:N	2.49	0.45
19:S:177:TYR:O	19:S:181:ARG:N	2.35	0.45
4:D:92:LEU:N	4:D:92:LEU:HD12	2.31	0.45
14:N:-17:DC:H2'	14:N:-16:DT:C7	2.45	0.45
15:O:591:LEU:O	15:O:595:VAL:HG23	2.17	0.45
17:Q:401:LEU:HA	17:Q:404:VAL:HG22	1.98	0.45
17:Q:791:ARG:O	17:Q:794:SER:OG	2.27	0.45
23:W:241:CYS:O	23:W:244:ASP:N	2.43	0.45
2:B:544:PHE:O	2:B:547:GLU:HG3	2.16	0.45
5:E:107:GLN:OE1	5:E:132:GLN:NE2	2.49	0.45
14:N:-41:DT:H2''	14:N:-40:DG:H8	1.81	0.45
14:N:68:DA:H2'	14:N:69:DT:C7	2.47	0.45
17:Q:166:LEU:HD13	17:Q:188:LYS:HE3	1.98	0.45
17:Q:572:GLY:O	17:Q:585:GLN:NE2	2.50	0.45
20:T:-33:DT:H2''	20:T:-32:DA:C8	2.52	0.45
20:T:2:DC:H2''	20:T:3:DG:C8	2.51	0.45
26:Z:486:GLU:OE2	26:Z:555:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:497:GLU:OE1	26:Z:497:GLU:N	2.44	0.45
14:N:47:DA:C4	14:N:48:DG:N7	2.84	0.45
17:Q:48:ALA:HB2	17:Q:63:LEU:HD11	1.98	0.45
17:Q:215:GLU:OE1	17:Q:215:GLU:N	2.40	0.45
17:Q:768:VAL:HG21	17:Q:778:GLU:HG2	1.99	0.45
1:A:1183:SER:O	1:A:1184:THR:OG1	2.35	0.45
1:A:1378:LEU:O	1:A:1378:LEU:HD23	2.16	0.45
9:I:105:GLU:OE1	9:I:105:GLU:N	2.42	0.45
16:P:16:A:O2'	16:P:17:A:OP2	2.29	0.45
17:Q:302:GLU:N	17:Q:302:GLU:OE1	2.48	0.45
17:Q:680:ILE:O	17:Q:683:VAL:HG22	2.16	0.45
18:R:574:GLU:HA	18:R:577:LYS:HG2	1.98	0.45
2:B:986:GLN:NE2	2:B:998:ASP:O	2.43	0.45
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.49	0.45
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.82	0.45
11:K:38:GLU:HA	11:K:38:GLU:OE1	2.17	0.45
14:N:-14:DA:OP2	31:l:1487:LYS:NZ	2.46	0.45
14:N:71:DG:H2''	14:N:72:DA:C8	2.52	0.45
31:l:1634:ASN:ND2	31:l:1661:GLU:O	2.46	0.45
1:A:1210:TRP:CD1	1:A:1285:LEU:HD11	2.51	0.45
2:B:963:PRO:HG3	2:B:1043:ILE:HD12	1.98	0.45
14:N:21:DG:H2''	14:N:22:DC:C6	2.52	0.45
14:N:46:DC:H2''	14:N:47:DA:H8	1.77	0.45
17:Q:869:GLU:O	17:Q:872:LYS:HG2	2.17	0.45
20:T:-68:DT:C2	20:T:-67:DG:C8	3.05	0.45
20:T:0:DC:H2''	20:T:1:DG:C8	2.52	0.45
29:g:51:LEU:HD21	30:h:70:PHE:CD1	2.52	0.45
4:D:31:THR:HG22	7:G:3:TYR:CE2	2.52	0.45
13:M:1490:THR:N	13:M:1493:GLY:O	2.50	0.45
14:N:71:DG:H2''	14:N:72:DA:H8	1.81	0.45
20:T:6:DC:H2''	20:T:7:DG:C8	2.51	0.45
1:A:1211:LEU:C	1:A:1212:LEU:HD12	2.42	0.44
14:N:74:DA:C2	14:N:75:DA:C6	3.04	0.44
17:Q:534:TYR:CD2	17:Q:557:ALA:HB2	2.51	0.44
17:Q:737:LYS:HZ1	17:Q:761:LEU:HA	1.81	0.44
20:T:-68:DT:H2''	20:T:-67:DG:O5'	2.17	0.44
23:W:130:VAL:HG22	23:W:151:ILE:HG13	1.99	0.44
1:A:663:ASP:OD1	1:A:664:ILE:N	2.50	0.44
1:A:1255:LEU:N	1:A:1255:LEU:HD12	2.32	0.44
1:A:1386:ILE:HG12	1:A:1393:VAL:HG21	1.99	0.44
2:B:1006:VAL:HG22	22:V:130:TRP:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:ARG:NH1	9:I:37:TYR:CZ	2.86	0.44
14:N:28:DG:H1'	14:N:29:DG:N7	2.33	0.44
14:N:74:DA:N3	14:N:75:DA:C5	2.85	0.44
17:Q:24:LEU:HD11	17:Q:56:LYS:NZ	2.32	0.44
17:Q:135:ALA:HB1	17:Q:152:PHE:CD2	2.53	0.44
17:Q:538:GLY:HA3	17:Q:554:PHE:CE1	2.52	0.44
17:Q:538:GLY:O	17:Q:550:ALA:HB2	2.18	0.44
18:R:391:ILE:HD12	18:R:391:ILE:N	2.32	0.44
25:Y:67:GLU:OE1	25:Y:67:GLU:N	2.41	0.44
31:I:1526:MET:HA	31:I:1640:TRP:CZ3	2.53	0.44
1:A:253:LEU:HD23	1:A:253:LEU:C	2.41	0.44
1:A:681:LEU:HD23	2:B:785:TYR:O	2.16	0.44
1:A:687:ILE:HD13	2:B:972:ILE:HB	1.98	0.44
1:A:721:HIS:CG	9:I:110:LEU:HD21	2.52	0.44
1:A:832:THR:HG23	1:A:833:PRO:HD2	1.98	0.44
2:B:48:ASP:OD2	2:B:159:THR:HG21	2.18	0.44
2:B:265:GLN:N	2:B:265:GLN:OE1	2.49	0.44
2:B:370:HIS:NE2	2:B:374:LEU:HD11	2.32	0.44
3:C:56:SER:OG	3:C:158:GLU:N	2.43	0.44
9:I:58:ILE:HD12	9:I:58:ILE:N	2.33	0.44
14:N:-5:DT:H1'	14:N:-4:DA:N7	2.31	0.44
17:Q:643:ASP:OD2	24:X:239:GLN:NE2	2.49	0.44
21:U:416:VAL:HG13	21:U:417:GLU:N	2.32	0.44
1:A:350:VAL:HG23	1:A:351:ARG:H	1.82	0.44
1:A:1366:PHE:CB	1:A:1374:VAL:HG21	2.47	0.44
2:B:497:LYS:N	2:B:498:PRO:CD	2.81	0.44
3:C:74:THR:HG23	3:C:74:THR:O	2.17	0.44
14:N:-44:DA:C2	14:N:-43:DA:C6	3.04	0.44
16:P:24:C:O2'	16:P:25:U:H5'	2.18	0.44
17:Q:809:LEU:HD12	17:Q:809:LEU:N	2.33	0.44
19:S:291:CYS:N	19:S:296:ASN:O	2.48	0.44
20:T:-44:DA:C2	20:T:-43:DG:C6	3.06	0.44
1:A:457:ILE:HD11	1:A:469:MET:C	2.43	0.44
2:B:1157:LEU:O	2:B:1157:LEU:HD23	2.18	0.44
11:K:97:GLU:OE1	11:K:98:LEU:N	2.51	0.44
20:T:-50:DG:H2''	20:T:-49:DC:C6	2.53	0.44
29:c:99:ARG:NE	29:c:99:ARG:HA	2.33	0.44
2:B:604:ILE:N	2:B:604:ILE:HD12	2.32	0.44
2:B:1038:THR:HA	3:C:195:THR:HA	1.99	0.44
3:C:256:LEU:HD23	11:K:42:LEU:HD11	1.98	0.44
14:N:43:DC:C2	14:N:44:DT:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:425:THR:O	17:Q:426:ASP:C	2.60	0.44
18:R:507:PRO:HA	18:R:508:ASN:HA	1.77	0.44
20:T:-96:DC:H2'	20:T:-95:DA:C8	2.52	0.44
1:A:1248:ASN:OD1	1:A:1249:ASP:N	2.51	0.44
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.53	0.44
14:N:100:DT:H2'	14:N:101:DT:C6	2.53	0.44
22:V:55:GLN:OE1	22:V:57:ARG:NE	2.47	0.44
26:Z:448:ILE:O	26:Z:449:THR:OG1	2.30	0.44
1:A:600:ILE:HG22	1:A:601:ASN:N	2.33	0.44
14:N:68:DA:C8	14:N:69:DT:H72	2.52	0.44
27:a:35:VAL:HG22	31:l:1606:PHE:CB	2.48	0.44
31:l:1569:ASP:OD1	31:l:1570:LEU:N	2.51	0.44
2:B:163:LEU:HD22	2:B:163:LEU:N	2.33	0.44
7:G:141:ASP:OD1	7:G:142:GLU:N	2.51	0.44
14:N:39:DT:H1'	14:N:40:DA:N7	2.33	0.44
17:Q:427:ILE:HG13	17:Q:460:LEU:HD22	2.00	0.44
18:R:355:LEU:HD12	18:R:355:LEU:N	2.33	0.44
23:W:186:LEU:HD12	23:W:186:LEU:N	2.33	0.44
28:b:98:TYR:CE2	29:g:100:VAL:HG11	2.53	0.44
31:l:1596:TYR:OH	31:l:1601:ASN:ND2	2.50	0.44
1:A:102:LYS:O	1:A:106:VAL:HG23	2.18	0.43
1:A:1123:ARG:HG2	1:A:1385:VAL:HG11	1.98	0.43
14:N:2:DT:C2'	14:N:3:DG:C8	3.01	0.43
17:Q:647:LEU:HD11	17:Q:648:TYR:CE1	2.53	0.43
26:Z:703:ASN:N	26:Z:706:ILE:HD12	2.32	0.43
1:A:542:LEU:O	1:A:545:VAL:HG12	2.18	0.43
3:C:19:VAL:HG23	3:C:241:PRO:HG2	1.99	0.43
4:D:87:LEU:O	4:D:87:LEU:HD23	2.18	0.43
14:N:69:DT:C4	14:N:70:DC:C4	3.06	0.43
17:Q:772:GLU:HA	17:Q:773:LYS:HB2	1.98	0.43
25:Y:13:LEU:HD23	25:Y:13:LEU:H	1.84	0.43
29:g:31:HIS:CE1	29:g:35:ARG:HE	2.36	0.43
1:A:107:LEU:HD23	1:A:107:LEU:O	2.17	0.43
2:B:140:LEU:HD23	2:B:140:LEU:N	2.33	0.43
3:C:148:ILE:HD12	3:C:148:ILE:H	1.83	0.43
9:I:17:CYS:SG	9:I:18:GLN:N	2.91	0.43
14:N:-60:DG:H2''	14:N:-59:DG:C8	2.53	0.43
14:N:-24:DA:H2''	14:N:-23:DG:H8	1.83	0.43
17:Q:727:LEU:HB3	17:Q:732:LYS:HB3	2.01	0.43
17:Q:839:ARG:HA	17:Q:842:ARG:NH1	2.33	0.43
23:W:23:ALA:N	23:W:36:VAL:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:216:ILE:O	23:W:225:ALA:HB3	2.18	0.43
26:Z:245:LEU:HD22	26:Z:245:LEU:N	2.34	0.43
30:h:36:SER:HB2	30:h:63:ASN:OD1	2.18	0.43
31:l:1656:VAL:HG11	31:l:1662:LEU:HD21	1.99	0.43
1:A:110:VAL:HG22	1:A:111:CYS:N	2.33	0.43
8:H:69:THR:HG1	8:H:81:ARG:HH22	1.61	0.43
8:H:91:VAL:CG1	8:H:144:LEU:HD23	2.49	0.43
14:N:-5:DT:O2	14:N:-4:DA:C4	2.71	0.43
17:Q:83:MET:HE3	17:Q:124:ILE:HB	1.99	0.43
1:A:97:VAL:CG1	1:A:318:VAL:HG23	2.48	0.43
1:A:325:LEU:HD22	1:A:325:LEU:N	2.34	0.43
2:B:351:VAL:HG21	2:B:361:LYS:HG2	1.99	0.43
7:G:85:VAL:HG22	7:G:147:ILE:HD11	2.01	0.43
14:N:-35:DT:C2	14:N:-34:DA:C6	3.06	0.43
14:N:-34:DA:C5	14:N:-33:DG:C6	3.07	0.43
14:N:47:DA:H2''	14:N:48:DG:H8	1.84	0.43
20:T:-33:DT:H2'	20:T:-32:DA:C8	2.54	0.43
1:A:955:GLU:OE1	1:A:1010:VAL:HG22	2.19	0.43
5:E:52:ARG:O	5:E:54:ARG:N	2.49	0.43
7:G:76:VAL:HG22	7:G:77:PHE:N	2.32	0.43
14:N:40:DA:C2	14:N:41:DG:C4	3.07	0.43
14:N:79:DC:H2''	14:N:80:DC:C6	2.52	0.43
15:O:594:VAL:HG11	15:O:619:TRP:CH2	2.54	0.43
20:T:-109:DA:C6	20:T:-108:DA:N6	2.86	0.43
26:Z:549:VAL:HG11	26:Z:635:MET:CE	2.48	0.43
1:A:936:GLU:O	1:A:939:VAL:HG22	2.19	0.43
5:E:159:LEU:HD12	5:E:163:TYR:HD2	1.83	0.43
5:E:197:SER:O	5:E:201:GLY:N	2.52	0.43
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.18	0.43
13:M:1411:ILE:HG23	13:M:1412:VAL:N	2.33	0.43
17:Q:333:THR:HG21	17:Q:347:LEU:CD1	2.44	0.43
2:B:27:TRP:CD1	2:B:762:ARG:HE	2.36	0.43
2:B:756:LYS:O	2:B:777:ASN:ND2	2.39	0.43
5:E:185:ILE:HD12	5:E:209:VAL:HG21	2.00	0.43
6:F:53:THR:OG1	6:F:118:TRP:NE1	2.52	0.43
8:H:8:ASP:OD2	8:H:32:SER:OG	2.33	0.43
12:L:16:ILE:HD11	12:L:25:GLU:HB3	2.00	0.43
20:T:-97:DA:C4	20:T:-96:DC:C5	3.06	0.43
26:Z:511:LEU:C	26:Z:511:LEU:HD23	2.44	0.43
1:A:413:TYR:O	1:A:449:HIS:CD2	2.71	0.43
2:B:27:TRP:CG	2:B:762:ARG:HE	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:854:ILE:O	2:B:907:VAL:HG21	2.19	0.43
8:H:15:ILE:HG22	8:H:28:LEU:HD13	2.01	0.43
8:H:52:LEU:HD12	8:H:52:LEU:N	2.34	0.43
8:H:100:GLU:O	8:H:113:SER:N	2.52	0.43
13:M:1425:ASP:OD2	13:M:1504:VAL:HG11	2.19	0.43
14:N:42:DT:C2'	14:N:43:DC:C6	3.02	0.43
16:P:18:A:O2'	16:P:19:A:OP1	2.36	0.43
17:Q:758:ALA:HB1	17:Q:793:PHE:CE1	2.54	0.43
26:Z:252:GLN:OE1	26:Z:252:GLN:N	2.52	0.43
27:a:35:VAL:HG22	31:l:1606:PHE:HB2	2.01	0.43
31:l:1684:ASN:O	31:l:1685:CYS:C	2.60	0.43
1:A:560:VAL:HG21	1:A:586:TRP:CD2	2.54	0.43
13:M:616:LEU:O	13:M:643:LYS:N	2.39	0.43
14:N:-64:DT:H2''	14:N:-63:DC:C6	2.54	0.43
14:N:-54:DG:H1'	14:N:-53:DA:C8	2.53	0.43
17:Q:68:ARG:HE	17:Q:86:LEU:HD13	1.84	0.43
17:Q:163:ILE:HB	17:Q:164:PRO:HD3	2.01	0.43
17:Q:166:LEU:HD13	17:Q:188:LYS:CE	2.49	0.43
17:Q:269:PRO:HB3	17:Q:295:ALA:O	2.19	0.43
17:Q:687:LEU:HB2	17:Q:703:MET:HE1	1.99	0.43
17:Q:858:LYS:HA	17:Q:861:GLU:HG3	2.00	0.43
20:T:-78:DC:H2''	20:T:-77:DC:C6	2.54	0.43
23:W:85:ASP:OD2	23:W:89:ARG:NH1	2.39	0.43
26:Z:178:ASN:OD1	26:Z:179:LEU:N	2.51	0.43
2:B:109:MET:HE2	2:B:174:LEU:HD13	2.00	0.42
3:C:48:ASP:OD2	3:C:166:LYS:HD2	2.18	0.42
9:I:16:PHE:HA	9:I:22:ASN:O	2.19	0.42
14:N:-50:DC:H2''	14:N:-49:DC:C6	2.54	0.42
17:Q:73:LEU:C	17:Q:73:LEU:HD23	2.44	0.42
17:Q:92:TYR:HA	17:Q:95:GLN:HB2	2.01	0.42
1:A:216:LEU:N	1:A:216:LEU:HD22	2.34	0.42
1:A:467:MET:SD	1:A:524:MET:HB3	2.59	0.42
1:A:1235:ILE:HD12	1:A:1296:MET:HE2	2.01	0.42
1:A:1258:ARG:C	1:A:1259:ILE:HD12	2.44	0.42
2:B:260:LEU:HD12	2:B:260:LEU:N	2.34	0.42
2:B:646:ARG:O	2:B:647:GLU:HB3	2.19	0.42
14:N:100:DT:H2'	14:N:101:DT:H6	1.84	0.42
15:O:613:MET:HE2	15:O:652:LEU:HD12	2.00	0.42
15:O:642:GLN:HG3	15:O:681:LEU:HD21	2.02	0.42
20:T:-35:DA:OP1	30:h:87:SER:N	2.52	0.42
20:T:6:DC:H4'	28:b:45:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG22	1:A:366:VAL:N	2.34	0.42
1:A:484:LEU:HD21	1:A:496:PHE:CE1	2.54	0.42
1:A:484:LEU:HD21	1:A:496:PHE:HE1	1.85	0.42
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.52	0.42
1:A:1138:SER:O	1:A:1360:ASN:HB3	2.20	0.42
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.19	0.42
11:K:81:TYR:OH	11:K:89:ASN:ND2	2.42	0.42
14:N:-19:DC:C2'	14:N:-18:DG:C8	3.03	0.42
14:N:43:DC:C6	14:N:44:DT:H71	2.54	0.42
23:W:152:LEU:HD12	23:W:168:ILE:HA	2.00	0.42
31:l:1476:ILE:HB	31:l:1620:LYS:HB3	2.00	0.42
2:B:384:ASP:OD1	2:B:386:ASP:N	2.39	0.42
7:G:12:LEU:N	7:G:12:LEU:HD12	2.35	0.42
7:G:60:GLN:NE2	7:G:67:LEU:HD22	2.35	0.42
17:Q:65:GLU:HA	17:Q:89:LEU:HD11	2.00	0.42
17:Q:524:LEU:HD11	17:Q:537:LEU:HD12	2.00	0.42
20:T:38:DA:C4	20:T:39:DC:C5	3.07	0.42
29:c:47:ALA:N	29:c:48:PRO:HD2	2.35	0.42
1:A:486:LEU:HD21	2:B:790:GLN:HB2	2.01	0.42
9:I:60:HIS:O	9:I:60:HIS:ND1	2.50	0.42
17:Q:427:ILE:HD13	17:Q:464:LEU:HD21	2.01	0.42
17:Q:569:SER:OG	24:X:234:ARG:NH1	2.53	0.42
17:Q:849:LYS:O	17:Q:852:LEU:HG	2.20	0.42
25:Y:40:LEU:HD22	25:Y:42:MET:HB2	2.02	0.42
1:A:794:GLU:N	1:A:845:GLU:OE2	2.38	0.42
1:A:1138:SER:C	1:A:1139:LEU:HD12	2.45	0.42
1:A:1323:THR:O	1:A:1326:GLY:N	2.53	0.42
3:C:103:LEU:HD23	3:C:103:LEU:C	2.44	0.42
18:R:369:LEU:C	18:R:369:LEU:HD12	2.44	0.42
26:Z:524:THR:HG22	26:Z:525:ALA:N	2.35	0.42
1:A:1211:LEU:HD23	1:A:1260:ARG:NH2	2.35	0.42
1:A:1322:ILE:N	1:A:1322:ILE:HD12	2.34	0.42
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.29	0.42
6:F:118:TRP:HB3	6:F:123:LEU:HD22	2.01	0.42
10:J:14:VAL:HG22	10:J:14:VAL:O	2.20	0.42
12:L:19:CYS:SG	12:L:20:GLY:N	2.93	0.42
14:N:-44:DA:N3	14:N:-43:DA:C5	2.87	0.42
23:W:125:THR:HG22	23:W:127:VAL:HG22	2.01	0.42
27:a:35:VAL:HG13	31:l:1606:PHE:HB3	2.01	0.42
1:A:910:LYS:N	1:A:911:PRO:HD3	2.35	0.42
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:OG1	2:B:911:LEU:N	2.52	0.42
17:Q:380:ILE:HB	17:Q:400:HIS:CE1	2.55	0.42
20:T:-87:DA:H2''	20:T:-86:DT:C7	2.49	0.42
20:T:-24:DT:N3	20:T:-23:DG:N7	2.68	0.42
23:W:8:LEU:HD13	23:W:288:LYS:HE3	2.02	0.42
31:l:1475:LEU:H	31:l:1475:LEU:HD23	1.85	0.42
2:B:273:PHE:CE1	2:B:365:LEU:HD23	2.55	0.42
5:E:25:GLY:O	5:E:65:ASN:HB2	2.19	0.42
14:N:-23:DG:H2''	14:N:-22:DC:H6	1.84	0.42
17:Q:454:LEU:HD11	17:Q:473:TYR:CD1	2.54	0.42
17:Q:719:VAL:HG23	17:Q:720:VAL:N	2.34	0.42
17:Q:835:ASP:OD2	17:Q:839:ARG:NH2	2.53	0.42
20:T:-86:DT:H5'	20:T:-86:DT:C6	2.54	0.42
23:W:14:ALA:N	23:W:296:GLN:O	2.47	0.42
1:A:503:LEU:C	1:A:503:LEU:HD23	2.44	0.42
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.54	0.42
1:A:934:LEU:N	1:A:934:LEU:HD12	2.35	0.42
1:A:937:ASP:C	1:A:938:LEU:HD12	2.45	0.42
1:A:1235:ILE:HA	1:A:1296:MET:HE2	2.02	0.42
1:A:1382:LEU:CD2	1:A:1398:LEU:HD22	2.50	0.42
2:B:86:LEU:HD11	2:B:128:ILE:HD11	2.01	0.42
5:E:159:LEU:HD12	5:E:163:TYR:CD2	2.55	0.42
5:E:162:ARG:C	5:E:162:ARG:HD3	2.44	0.42
17:Q:95:GLN:OE1	22:V:83:THR:OG1	2.37	0.42
17:Q:351:TYR:HB3	17:Q:356:ASP:O	2.19	0.42
17:Q:764:LEU:HD22	17:Q:785:GLU:OE1	2.20	0.42
17:Q:852:LEU:HD12	17:Q:853:ARG:N	2.35	0.42
25:Y:27:GLN:O	25:Y:31:ASP:N	2.52	0.42
1:A:486:LEU:N	1:A:486:LEU:HD12	2.35	0.41
1:A:1170:THR:HG22	1:A:1171:ALA:N	2.35	0.41
2:B:393:LEU:HD11	2:B:485:LEU:HD23	2.02	0.41
3:C:48:ASP:HB3	3:C:166:LYS:HG2	2.01	0.41
14:N:-1:DC:C2'	14:N:0:DG:C8	3.03	0.41
14:N:47:DA:C2	14:N:48:DG:C4	3.08	0.41
14:N:57:DC:C2	14:N:58:DA:N7	2.88	0.41
17:Q:837:GLU:O	17:Q:841:LEU:HG	2.20	0.41
18:R:493:GLU:O	18:R:496:VAL:HG22	2.20	0.41
20:T:-36:DG:H2''	20:T:-35:DA:C8	2.55	0.41
20:T:19:DG:C4	20:T:20:DG:N7	2.88	0.41
1:A:1383:TYR:HA	1:A:1386:ILE:HG22	2.02	0.41
2:B:354:SER:OG	2:B:357:CYS:SG	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:MET:CG	2:B:624:PRO:HD2	2.48	0.41
2:B:715:ASP:OD1	2:B:716:HIS:CD2	2.73	0.41
2:B:928:ILE:HD12	2:B:928:ILE:H	1.85	0.41
11:K:100:LEU:HD21	11:K:104:ARG:CZ	2.50	0.41
14:N:-43:DA:C8	14:N:-42:DT:H72	2.55	0.41
14:N:-5:DT:O3'	14:N:-4:DA:C8	2.73	0.41
17:Q:685:LEU:O	17:Q:689:HIS:ND1	2.53	0.41
29:g:99:ARG:HA	29:g:99:ARG:NE	2.35	0.41
31:l:1631:CYS:SG	31:l:1686:ARG:N	2.82	0.41
1:A:336:LEU:N	1:A:336:LEU:HD22	2.34	0.41
1:A:680:LEU:HD21	2:B:784:SER:OG	2.19	0.41
1:A:695:ASP:C	1:A:696:SER:HG	2.17	0.41
1:A:811:ILE:HD11	9:I:79:PRO:N	2.36	0.41
1:A:1184:THR:O	1:A:1185:VAL:C	2.63	0.41
13:M:1473:LEU:HD23	13:M:1473:LEU:C	2.46	0.41
14:N:-28:DC:C2	14:N:-27:DT:C5	3.08	0.41
14:N:50:DC:H1'	14:N:51:DA:P	2.60	0.41
17:Q:793:PHE:HA	17:Q:796:LEU:CD2	2.49	0.41
18:R:369:LEU:HD12	18:R:370:GLU:N	2.34	0.41
23:W:283:ASN:HB2	23:W:288:LYS:HB2	2.02	0.41
25:Y:113:THR:HG22	25:Y:113:THR:O	2.19	0.41
1:A:580:LEU:N	1:A:580:LEU:HD12	2.35	0.41
5:E:86:THR:O	5:E:89:VAL:HG12	2.20	0.41
11:K:32:LEU:N	11:K:32:LEU:HD12	2.35	0.41
14:N:-12:DA:C2	14:N:-11:DC:C2	3.08	0.41
16:P:16:A:H4'	16:P:17:A:O5'	2.20	0.41
17:Q:858:LYS:O	17:Q:861:GLU:HG3	2.20	0.41
18:R:505:ALA:N	18:R:506:PRO:HD2	2.36	0.41
1:A:343:LEU:HD12	1:A:343:LEU:C	2.46	0.41
1:A:1416:ARG:NH2	20:T:-97:DA:N3	2.69	0.41
2:B:88:PHE:O	2:B:89:GLU:HB3	2.19	0.41
2:B:168:ASP:OD1	2:B:169:ARG:N	2.54	0.41
2:B:565:THR:HA	2:B:610:ARG:HB3	2.03	0.41
3:C:101:PHE:N	3:C:163:ALA:O	2.49	0.41
7:G:107:PHE:C	7:G:108:ILE:HD12	2.45	0.41
14:N:57:DC:C2	14:N:58:DA:C8	3.08	0.41
14:N:62:DA:H2'	14:N:63:DT:H72	2.02	0.41
17:Q:272:LEU:CB	17:Q:295:ALA:HB2	2.51	0.41
17:Q:757:VAL:HG23	17:Q:758:ALA:N	2.35	0.41
18:R:563:ILE:HA	18:R:566:ARG:HG2	2.02	0.41
23:W:88:ILE:O	23:W:102:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:210:LEU:HD12	26:Z:210:LEU:N	2.35	0.41
1:A:1347:LEU:HB2	5:E:137:ILE:HD13	2.03	0.41
2:B:823:PHE:CD1	14:N:78:DG:OP2	2.74	0.41
10:J:1:MET:O	10:J:56:ILE:HB	2.20	0.41
14:N:-4:DA:C5'	27:a:43:PRO:HG2	2.50	0.41
14:N:51:DA:OP1	14:N:51:DA:C8	2.73	0.41
14:N:53:DG:C2'	14:N:54:DT:H71	2.44	0.41
17:Q:710:LYS:HB2	17:Q:712:TYR:CD1	2.55	0.41
17:Q:717:THR:O	17:Q:720:VAL:HG22	2.19	0.41
18:R:404:GLU:OE2	18:R:455:TRP:NE1	2.51	0.41
1:A:339:LEU:O	1:A:342:ARG:HB3	2.21	0.41
2:B:392:ARG:C	2:B:393:LEU:HD22	2.45	0.41
2:B:864:ASP:OD1	26:Z:725:LYS:NZ	2.53	0.41
3:C:154:ARG:O	3:C:155:LYS:C	2.64	0.41
5:E:80:PRO:HA	5:E:107:GLN:HB2	2.02	0.41
14:N:-12:DA:C4	14:N:-11:DC:C5	3.09	0.41
14:N:58:DA:C6	14:N:59:DG:C6	3.09	0.41
17:Q:558:LEU:HD22	17:Q:571:ILE:HG13	2.02	0.41
20:T:-109:DA:N3	20:T:-108:DA:C8	2.89	0.41
20:T:-105:DC:H2''	20:T:-104:DA:C8	2.56	0.41
20:T:-86:DT:H6	20:T:-86:DT:H2'	1.77	0.41
20:T:-44:DA:N1	20:T:-43:DG:C6	2.89	0.41
20:T:-30:DT:H2''	20:T:-29:DC:C6	2.56	0.41
23:W:218:ASP:O	23:W:222:ALA:HA	2.19	0.41
27:e:61:LEU:N	27:e:61:LEU:HD22	2.35	0.41
31:l:1669:GLN:NE2	31:l:1695:VAL:HG21	2.36	0.41
1:A:147:LEU:HD23	1:A:147:LEU:C	2.45	0.41
1:A:625:ASP:OD1	1:A:638:GLY:N	2.54	0.41
1:A:722:ASN:C	1:A:724:GLU:OE1	2.63	0.41
1:A:1123:ARG:HG3	1:A:1385:VAL:HG11	2.03	0.41
1:A:1468:THR:O	6:F:64:ARG:NH1	2.54	0.41
2:B:1071:ASN:OD1	2:B:1071:ASN:O	2.39	0.41
4:D:60:VAL:O	4:D:63:LYS:HG2	2.21	0.41
14:N:-61:DC:C2	14:N:-60:DG:C8	3.09	0.41
14:N:99:DT:H4'	14:N:100:DT:OP1	2.21	0.41
20:T:-81:DT:OP1	20:T:-81:DT:H6	2.03	0.41
1:A:202:TRP:HH2	1:A:214:ILE:HD11	1.86	0.41
1:A:304:ALA:O	1:A:307:VAL:HG22	2.21	0.41
1:A:459:ASN:O	1:A:502:ASN:N	2.54	0.41
1:A:965:VAL:O	1:A:969:ILE:HG12	2.20	0.41
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:VAL:HG23	1:A:1186:VAL:HG13	2.03	0.41
2:B:153:PRO:C	2:B:154:ILE:HD12	2.46	0.41
2:B:599:SER:OG	2:B:600:GLU:OE1	2.34	0.41
3:C:261:THR:O	3:C:264:SER:OG	2.35	0.41
5:E:103:LEU:HD23	5:E:104:ILE:N	2.36	0.41
10:J:13:ILE:HD12	10:J:13:ILE:N	2.36	0.41
12:L:25:GLU:OE1	12:L:25:GLU:CA	2.69	0.41
13:M:1476:TYR:OH	13:M:1483:ARG:NH1	2.53	0.41
14:N:-33:DG:H1'	14:N:-32:DA:N7	2.36	0.41
17:Q:163:ILE:O	17:Q:166:LEU:HG	2.21	0.41
17:Q:468:GLY:O	17:Q:472:LYS:HG2	2.21	0.41
17:Q:886:LYS:O	17:Q:890:MET:HG2	2.21	0.41
20:T:-33:DT:C4	20:T:-32:DA:N6	2.89	0.41
22:V:85:ASP:HB3	22:V:88:ASN:OD1	2.20	0.41
23:W:48:LYS:HG2	23:W:50:ARG:CZ	2.51	0.41
24:X:256:VAL:HG13	24:X:257:LYS:N	2.36	0.41
26:Z:614:ILE:HD11	26:Z:616:HIS:O	2.20	0.41
1:A:136:GLN:OE1	1:A:136:GLN:N	2.54	0.41
2:B:285:LEU:HD22	9:I:16:PHE:CZ	2.56	0.41
2:B:1021:HIS:CD2	3:C:203:TRP:CE2	3.09	0.41
3:C:223:ASN:OD1	3:C:223:ASN:N	2.54	0.41
3:C:260:GLN:HB2	11:K:91:ILE:HG21	2.03	0.41
5:E:75:PHE:CD2	5:E:90:TYR:CD1	3.08	0.41
6:F:97:LEU:HB2	6:F:102:ILE:HD11	2.03	0.41
7:G:145:LEU:HD12	7:G:145:LEU:C	2.46	0.41
8:H:15:ILE:O	8:H:16:ASP:C	2.63	0.41
9:I:89:CYS:SG	9:I:91:HIS:HB2	2.61	0.41
10:J:25:LEU:HB3	18:R:563:ILE:HD11	2.02	0.41
14:N:47:DA:C4	14:N:48:DG:C8	3.10	0.41
15:O:613:MET:HE1	15:O:641:LEU:HD22	2.03	0.41
17:Q:431:LEU:HD11	17:Q:464:LEU:HD11	2.03	0.41
18:R:555:LYS:O	18:R:557:ILE:N	2.48	0.41
27:e:73:GLU:OE1	28:f:25:ASN:ND2	2.54	0.41
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.94	0.40
2:B:1071:ASN:O	2:B:1073:GLN:N	2.52	0.40
10:J:64:PRO:O	12:L:23:HIS:CE1	2.74	0.40
11:K:31:CYS:C	11:K:32:LEU:HD12	2.46	0.40
14:N:18:DA:C5	14:N:19:DC:C5	3.09	0.40
14:N:49:DG:H1'	14:N:50:DC:C6	2.56	0.40
17:Q:80:LYS:O	17:Q:83:MET:HG3	2.20	0.40
17:Q:85:CYS:O	17:Q:88:THR:OG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:132:LEU:HD23	17:Q:132:LEU:C	2.46	0.40
18:R:570:TRP:HA	18:R:573:VAL:HG22	2.02	0.40
1:A:1325:ASP:OD1	1:A:1326:GLY:N	2.54	0.40
7:G:67:LEU:HD23	7:G:67:LEU:H	1.86	0.40
14:N:68:DA:H2''	14:N:69:DT:C6	2.56	0.40
17:Q:58:GLU:O	17:Q:61:VAL:HG12	2.21	0.40
23:W:221:HIS:ND1	23:W:223:ASN:OD1	2.54	0.40
31:l:1508:GLU:N	31:l:1508:GLU:OE1	2.54	0.40
1:A:49:GLY:O	1:A:51:ARG:N	2.52	0.40
1:A:939:VAL:HG23	1:A:940:LYS:N	2.36	0.40
2:B:505:LEU:HD22	2:B:509:VAL:CG2	2.51	0.40
2:B:789:ASN:O	2:B:968:ASN:HB2	2.22	0.40
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.22	0.40
3:C:263:LEU:HB2	11:K:19:ILE:HD13	2.04	0.40
13:M:1408:LEU:H	13:M:1408:LEU:HD23	1.87	0.40
13:M:1507:LEU:O	13:M:1507:LEU:HD23	2.22	0.40
14:N:-67:DG:H1'	14:N:-66:DA:C8	2.56	0.40
14:N:-11:DC:H2''	14:N:-10:DG:H8	1.78	0.40
14:N:69:DT:C4	14:N:70:DC:N4	2.89	0.40
17:Q:662:TYR:HB3	17:Q:665:GLU:HB2	2.02	0.40
20:T:-45:DG:C4	20:T:-44:DA:C8	3.09	0.40
20:T:8:DT:H5'	27:a:43:PRO:HA	2.03	0.40
21:U:459:VAL:HG23	21:U:494:HIS:C	2.46	0.40
1:A:413:TYR:O	1:A:415:GLY:N	2.54	0.40
1:A:905:ASN:HA	1:A:975:SER:O	2.22	0.40
2:B:1025:ASN:OD1	2:B:1025:ASN:N	2.54	0.40
5:E:92:GLN:O	5:E:96:GLU:OE1	2.39	0.40
14:N:58:DA:C2	14:N:59:DG:C4	3.10	0.40
17:Q:772:GLU:HA	17:Q:773:LYS:CB	2.52	0.40
26:Z:359:LEU:N	26:Z:359:LEU:HD12	2.37	0.40
1:A:1395:TYR:CZ	1:A:1399:ALA:HB2	2.57	0.40
1:A:1471:PHE:HB2	6:F:107:ARG:O	2.21	0.40
2:B:30:ILE:CD1	2:B:698:ILE:HG21	2.50	0.40
2:B:179:LEU:HD22	2:B:768:ARG:CD	2.49	0.40
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.61	0.40
3:C:94:CYS:SG	3:C:96:GLU:N	2.89	0.40
14:N:-51:DG:H2''	14:N:-50:DC:H6	1.86	0.40
14:N:-46:DT:H6	14:N:-46:DT:H5''	1.85	0.40
15:O:623:LEU:HD22	15:O:623:LEU:N	2.36	0.40
17:Q:131:LEU:HD12	17:Q:158:GLN:HE21	1.86	0.40
17:Q:351:TYR:HB2	17:Q:360:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:86:ALA:HB1	23:W:105:GLY:HA2	2.03	0.40
26:Z:264:LEU:HD12	26:Z:264:LEU:C	2.47	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	1408/1544 (91%)	1295 (92%)	112 (8%)	1 (0%)	48	78
2	B	1112/1159 (96%)	1024 (92%)	88 (8%)	0	100	100
3	C	254/269 (94%)	228 (90%)	26 (10%)	0	100	100
4	D	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
5	E	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
6	F	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
7	G	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
8	H	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
9	I	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
10	J	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
11	K	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
12	L	45/47 (96%)	41 (91%)	3 (7%)	1 (2%)	5	24
13	M	976/1002 (97%)	937 (96%)	38 (4%)	1 (0%)	48	78
15	O	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
17	Q	888/890 (100%)	851 (96%)	37 (4%)	0	100	100
18	R	240/248 (97%)	233 (97%)	7 (3%)	0	100	100
19	S	157/170 (92%)	154 (98%)	3 (2%)	0	100	100
21	U	117/125 (94%)	105 (90%)	11 (9%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	V	234/244 (96%)	219 (94%)	15 (6%)	0	100	100
23	W	298/300 (99%)	288 (97%)	10 (3%)	0	100	100
24	X	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
25	Y	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
26	Z	497/510 (98%)	474 (95%)	22 (4%)	1 (0%)	43	73
27	a	99/136 (73%)	98 (99%)	1 (1%)	0	100	100
27	e	90/136 (66%)	90 (100%)	0	0	100	100
28	b	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
28	f	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
29	c	102/130 (78%)	101 (99%)	1 (1%)	0	100	100
29	g	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
30	d	90/123 (73%)	90 (100%)	0	0	100	100
30	h	87/123 (71%)	85 (98%)	2 (2%)	0	100	100
31	l	259/589 (44%)	237 (92%)	22 (8%)	0	100	100
All	All	8505/9352 (91%)	8024 (94%)	476 (6%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	39	CYS
13	M	700	HIS
1	A	1343	LEU
21	U	510	LYS
26	Z	774	GLN

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	1245/1341 (93%)	1240 (100%)	5 (0%)	84	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	986/1013 (97%)	981 (100%)	5 (0%)	81	85
3	C	235/246 (96%)	234 (100%)	1 (0%)	84	86
4	D	109/116 (94%)	109 (100%)	0	100	100
5	E	191/191 (100%)	189 (99%)	2 (1%)	68	79
6	F	68/68 (100%)	68 (100%)	0	100	100
7	G	146/152 (96%)	146 (100%)	0	100	100
8	H	130/130 (100%)	130 (100%)	0	100	100
9	I	104/104 (100%)	102 (98%)	2 (2%)	50	73
10	J	55/55 (100%)	55 (100%)	0	100	100
11	K	104/104 (100%)	104 (100%)	0	100	100
12	L	44/44 (100%)	43 (98%)	1 (2%)	44	70
13	M	196/894 (22%)	196 (100%)	0	100	100
15	O	118/118 (100%)	116 (98%)	2 (2%)	53	74
17	Q	761/763 (100%)	751 (99%)	10 (1%)	61	77
18	R	170/222 (77%)	169 (99%)	1 (1%)	78	83
19	S	4/148 (3%)	4 (100%)	0	100	100
21	U	65/112 (58%)	65 (100%)	0	100	100
22	V	144/227 (63%)	143 (99%)	1 (1%)	76	82
23	W	255/255 (100%)	252 (99%)	3 (1%)	63	78
24	X	40/40 (100%)	40 (100%)	0	100	100
25	Y	102/102 (100%)	102 (100%)	0	100	100
26	Z	435/444 (98%)	435 (100%)	0	100	100
27	a	87/111 (78%)	87 (100%)	0	100	100
27	e	82/111 (74%)	82 (100%)	0	100	100
28	b	64/64 (100%)	64 (100%)	0	100	100
28	f	64/64 (100%)	64 (100%)	0	100	100
29	c	82/102 (80%)	82 (100%)	0	100	100
29	g	82/102 (80%)	82 (100%)	0	100	100
30	d	79/103 (77%)	79 (100%)	0	100	100
30	h	76/103 (74%)	76 (100%)	0	100	100
31	l	235/534 (44%)	233 (99%)	2 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6558/8183 (80%)	6523 (100%)	35 (0%)	78	85

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	VAL
1	A	457	ILE
1	A	535	MET
1	A	559	GLU
1	A	1289	GLU
2	B	20	ASP
2	B	600	GLU
2	B	650	ASN
2	B	768	ARG
2	B	1017	ASP
3	C	5	ASN
5	E	18	MET
5	E	57	ASP
9	I	56	ASN
9	I	83	ASP
12	L	25	GLU
15	O	604	LYS
15	O	652	LEU
17	Q	377	THR
17	Q	535	LEU
17	Q	552	ASP
17	Q	667	ARG
17	Q	707	CYS
17	Q	776	LEU
17	Q	780	LEU
17	Q	813	GLU
17	Q	817	CYS
17	Q	820	LEU
18	R	576	GLU
22	V	85	ASP
23	W	43	LEU
23	W	250	SER
23	W	272	ASP
31	l	2031	THR
31	l	2038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	372	ASN
1	A	449	HIS
1	A	529	GLN
1	A	539	GLN
1	A	700	GLN
1	A	711	GLN
1	A	791	GLN
1	A	950	ASN
1	A	1044	HIS
1	A	1417	HIS
1	A	1457	ASN
1	A	1462	GLN
2	B	197	GLN
2	B	227	ASN
2	B	582	GLN
2	B	716	HIS
2	B	725	GLN
2	B	1071	ASN
3	C	111	GLN
5	E	65	ASN
5	E	168	ASN
7	G	9	HIS
9	I	32	ASN
12	L	13	GLN
12	L	26	ASN
13	M	1505	ASN
17	Q	38	HIS
17	Q	40	GLN
17	Q	105	ASN
17	Q	151	GLN
17	Q	212	ASN
17	Q	268	ASN
17	Q	373	ASN
17	Q	391	GLN
17	Q	407	GLN
17	Q	490	HIS
17	Q	527	HIS
17	Q	559	GLN
17	Q	585	GLN
17	Q	609	ASN
17	Q	617	GLN

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Mol	Chain	Res	Type
17	Q	628	HIS
17	Q	651	ASN
17	Q	714	HIS
17	Q	775	ASN
17	Q	825	GLN
17	Q	860	GLN
18	R	571	ASN
22	V	69	GLN
23	W	27	ASN
23	W	268	HIS
23	W	273	HIS
25	Y	12	HIS
26	Z	244	ASN
26	Z	272	ASN
26	Z	446	ASN
26	Z	559	GLN
28	b	93	GLN
29	c	24	GLN
30	d	109	HIS
29	g	82	HIS
31	l	1667	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/11 (100%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	17	A
16	P	19	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	16	A
16	P	18	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	TPO	Z	775	26	8,10,11	1.12	0	10,14,16	1.95	1 (10%)
1	TPO	A	1525	1	8,10,11	1.11	0	10,14,16	2.14	1 (10%)
1	SEP	A	1547	1	8,9,10	1.61	1 (12%)	7,12,14	1.39	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	TPO	Z	775	26	-	1/9/11/13	-
1	TPO	A	1525	1	-	0/9/11/13	-
1	SEP	A	1547	1	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.53	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-6.11	106.73	123.33
26	Z	775	TPO	P-OG1-CB	-5.44	108.55	123.33
1	A	1547	SEP	OG-CB-CA	3.05	111.12	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	Z	775	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Z	775	TPO	2	0
1	A	1525	TPO	1	0
1	A	1547	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	12
26	Z	5
22	V	4
21	U	3

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Mol	Chain	Number of breaks
14	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	1287:MET	C	1327:ILE	N	44.24
1	Z	646:ALA	C	703:ASN	N	38.49
1	V	142:ASN	C	170:LYS	N	36.57
1	N	83:DT	O3'	95:DT	P	32.16
1	M	477:LYS	C	538:LYS	N	29.12
1	U	497:ASP	C	505:SER	N	26.85
1	M	430:ALA	C	440:ILE	N	17.11
1	Z	318:ALA	C	335:PRO	N	16.58
1	Z	396:PHE	C	416:ARG	N	16.32
1	M	763:GLN	C	775:GLN	N	13.15
1	V	207:VAL	C	217:SER	N	12.87
1	V	299:GLU	C	310:ASN	N	12.67
1	V	113:GLN	C	120:ARG	N	11.80
1	M	1384:ARG	C	1396:ALA	N	10.99
1	Z	268:LYS	C	271:ALA	N	10.43
1	U	399:GLU	C	406:GLU	N	10.26
1	U	418:ASN	C	437:ASN	N	8.33
1	Z	767:ARG	C	771:TYR	N	6.21
1	M	815:THR	C	824:GLU	N	6.07
1	M	1334:ASN	C	1338:ILE	N	5.65
1	M	332:LEU	C	349:SER	N	5.15
1	M	572:ASP	C	580:THR	N	4.90
1	M	1039:THR	C	1051:GLU	N	4.81
1	M	932:SER	C	935:GLU	N	4.53
1	M	675:GLY	C	684:THR	N	3.34

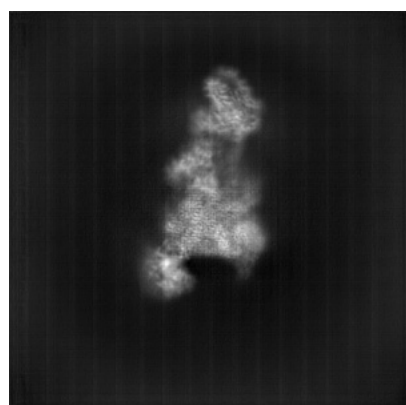
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48043. These allow visual inspection of the internal detail of the map and identification of artifacts.

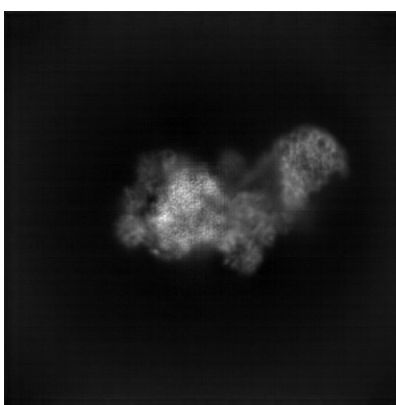
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

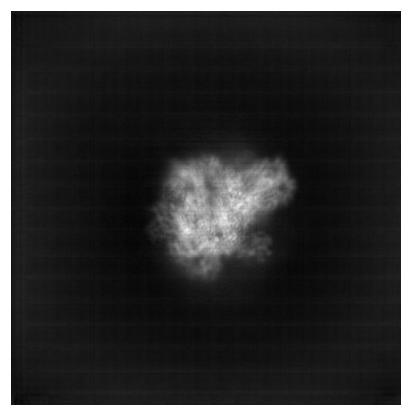
6.1.1 Primary map



X



Y

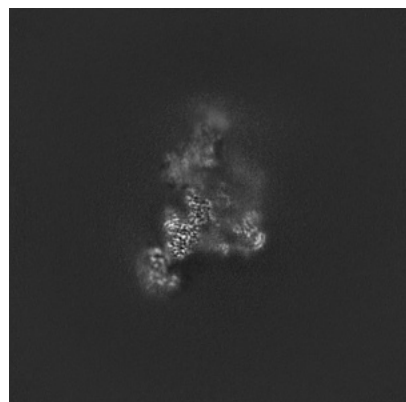


Z

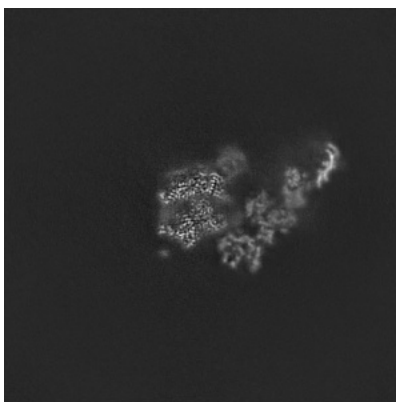
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

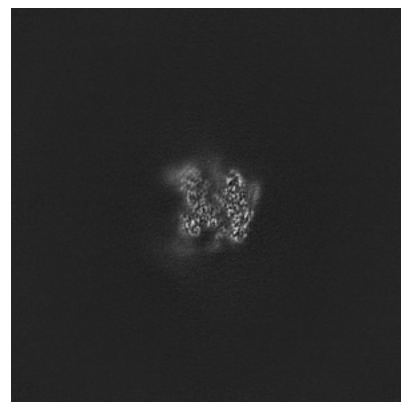
6.2.1 Primary map



X Index: 250



Y Index: 250

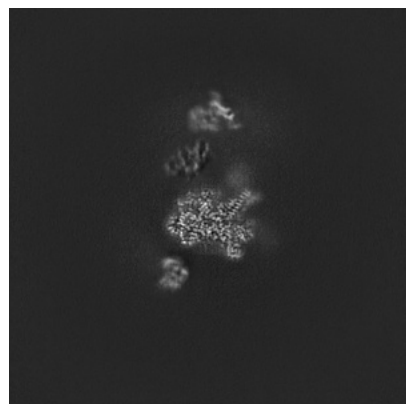


Z Index: 250

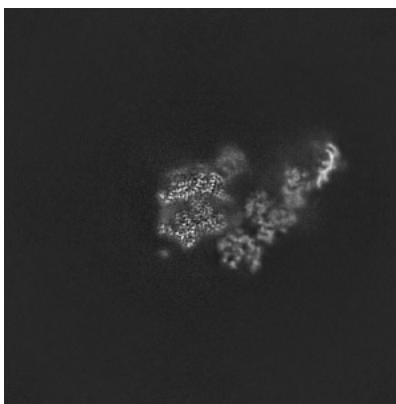
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

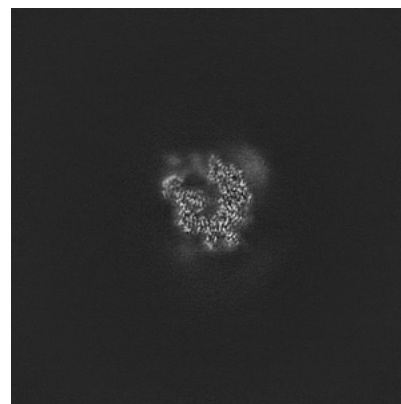
6.3.1 Primary map



X Index: 273



Y Index: 251

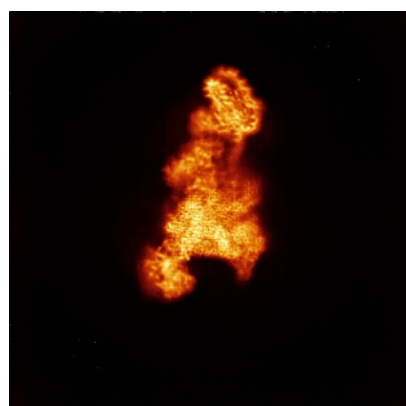


Z Index: 219

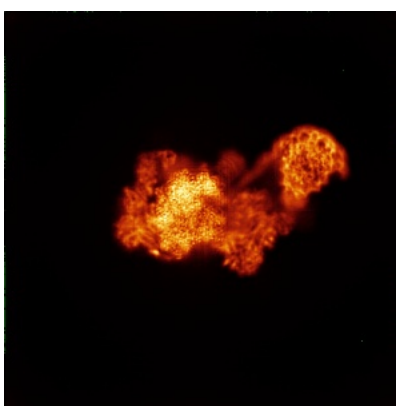
The images above show the largest variance slices of the map in three orthogonal directions.

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

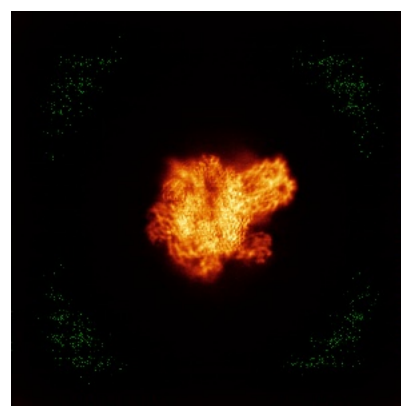
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

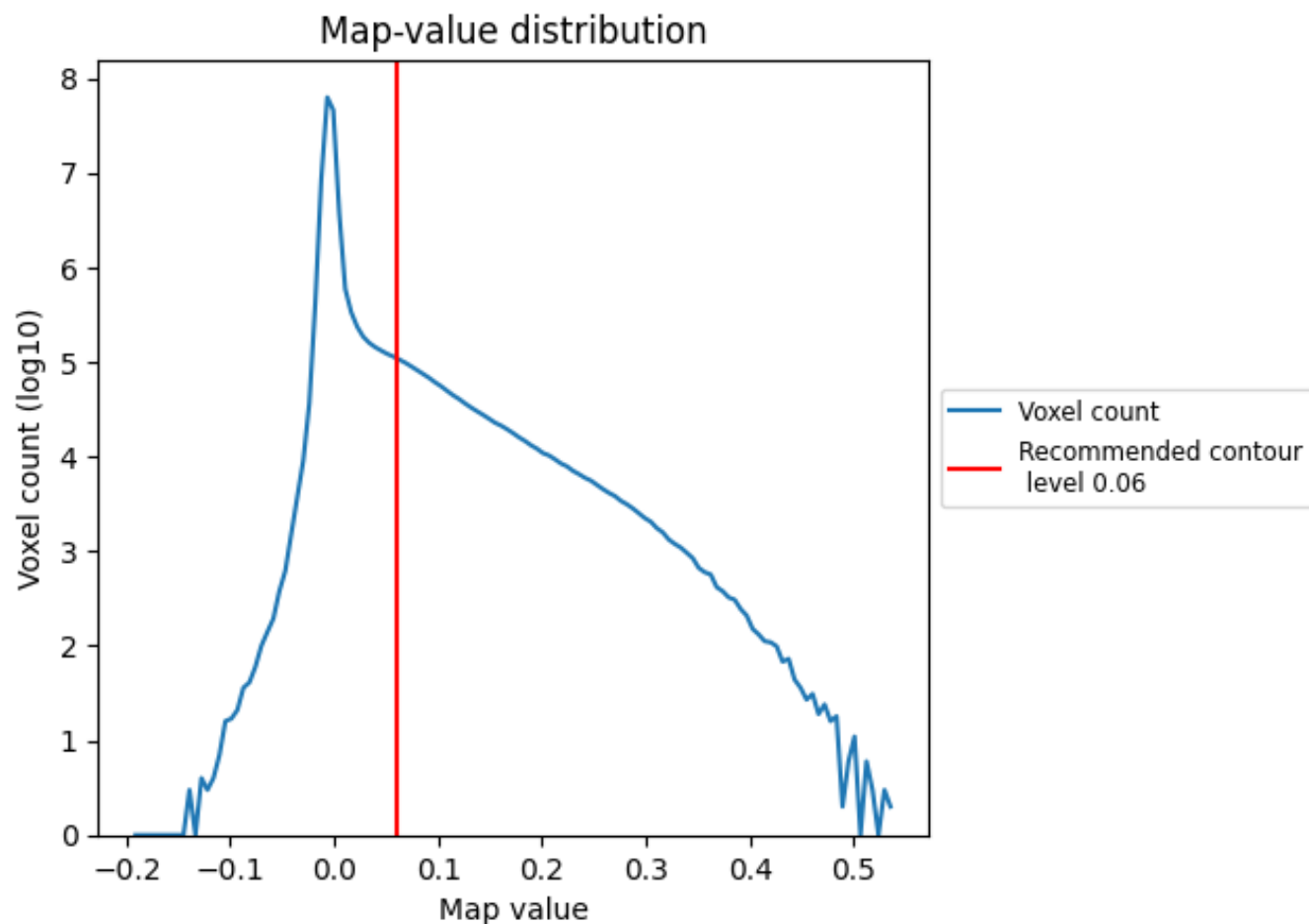
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

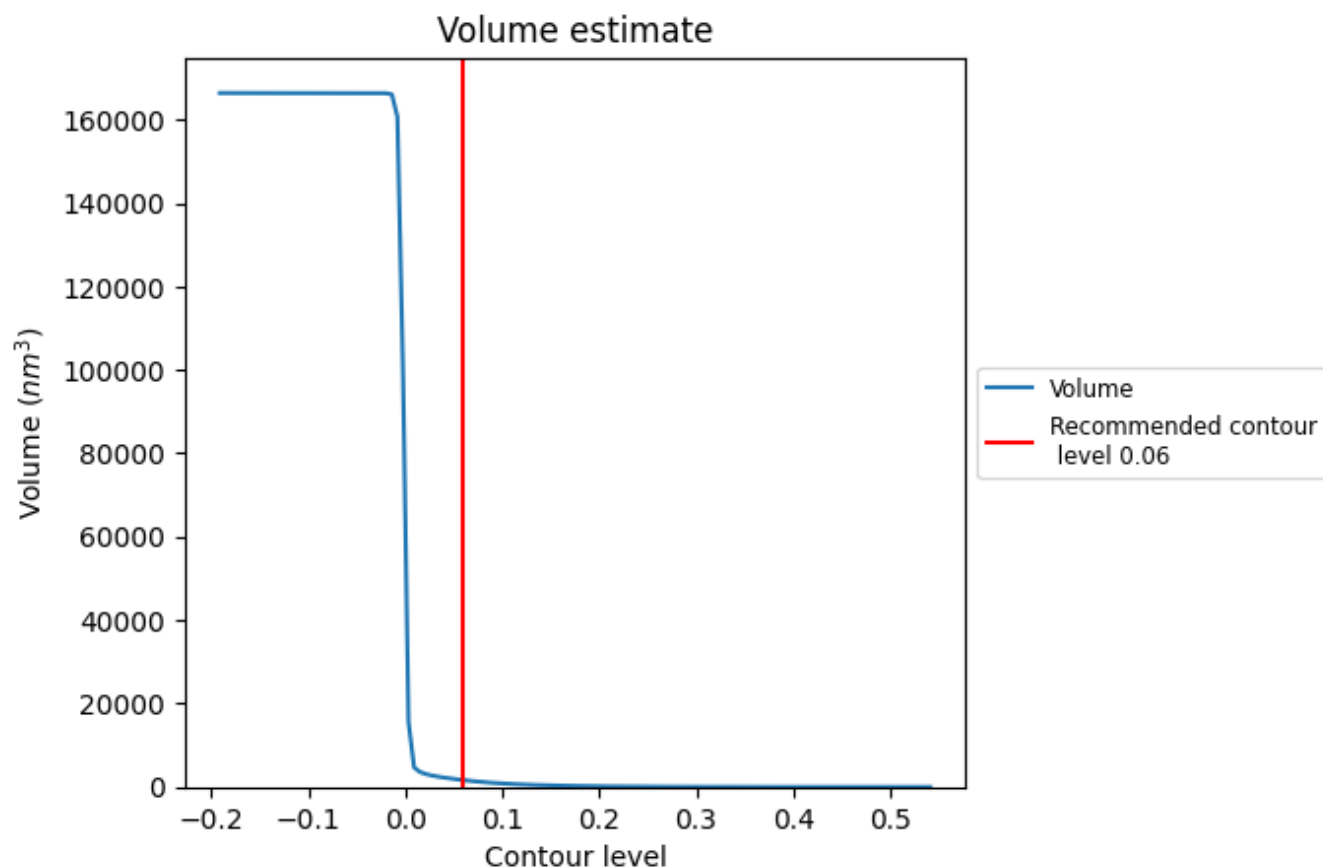
This section contains the results of statistical analysis of the map.

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.

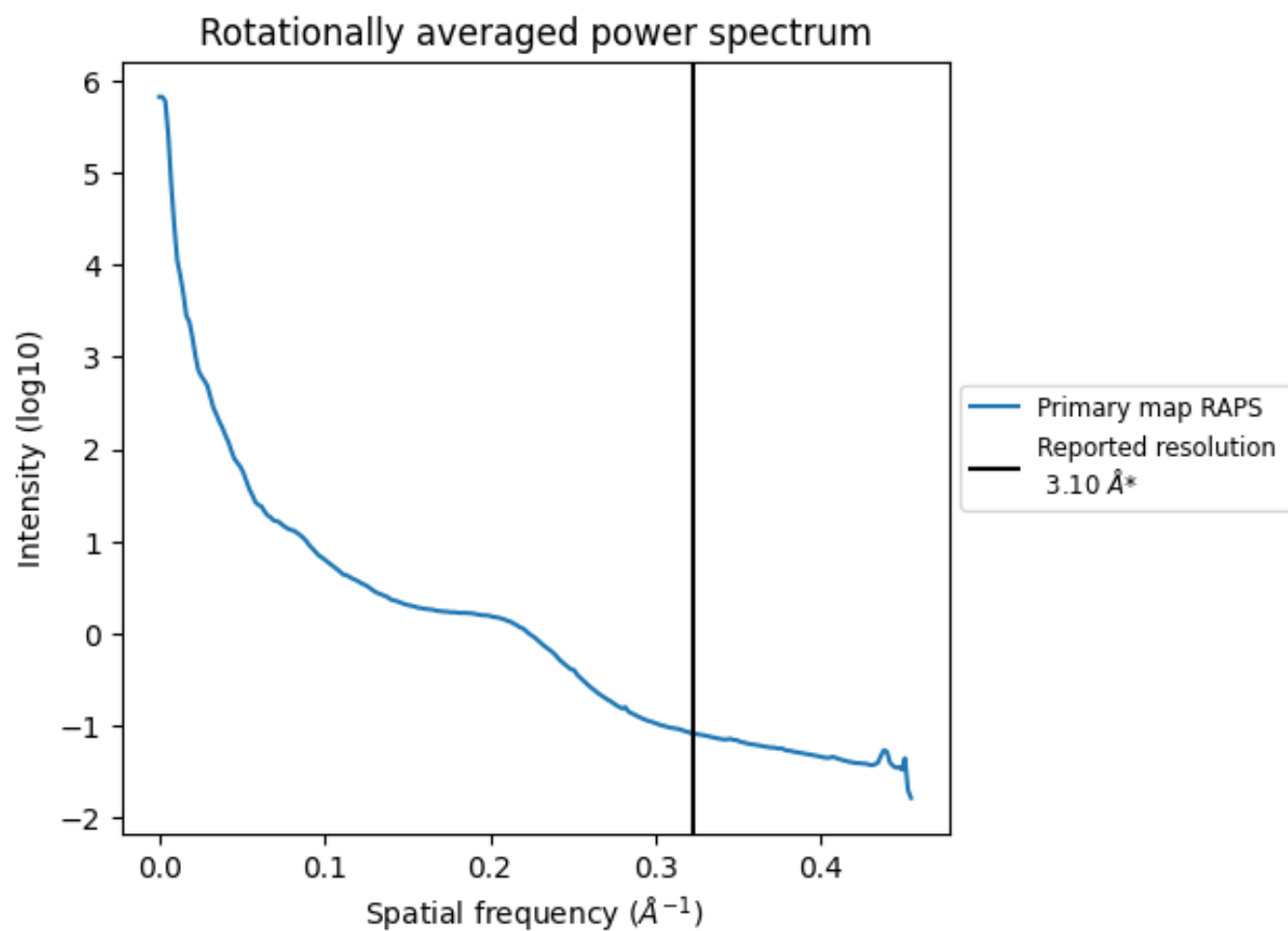
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1637 nm³; this corresponds to an approximate mass of 1479 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 0.323 $\text{\AA}^{-1}$

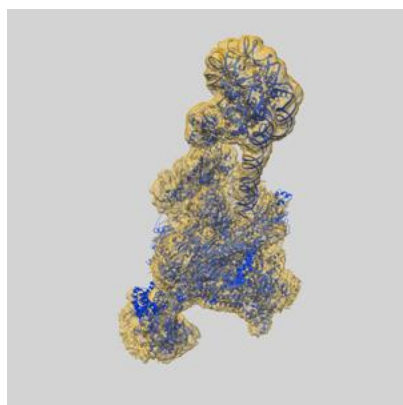
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

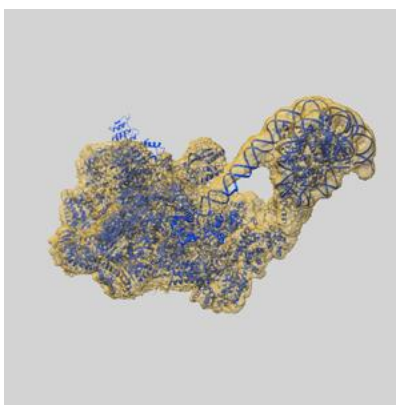
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48043 and PDB model 9EH1. Per-residue inclusion information can be found in section [3](#) on page [11](#).

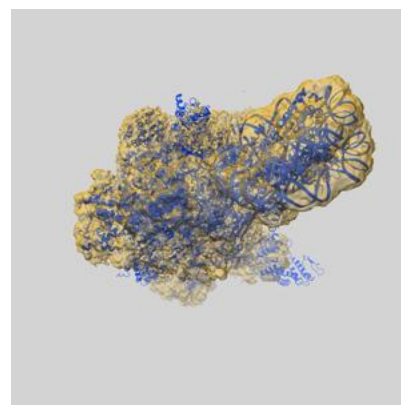
9.1 Map-model overlay [i](#)



X



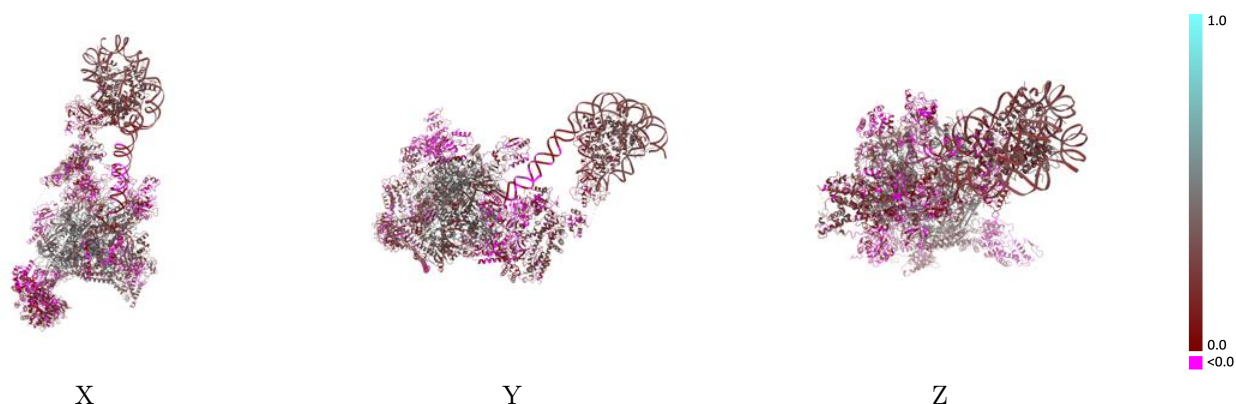
Y



Z

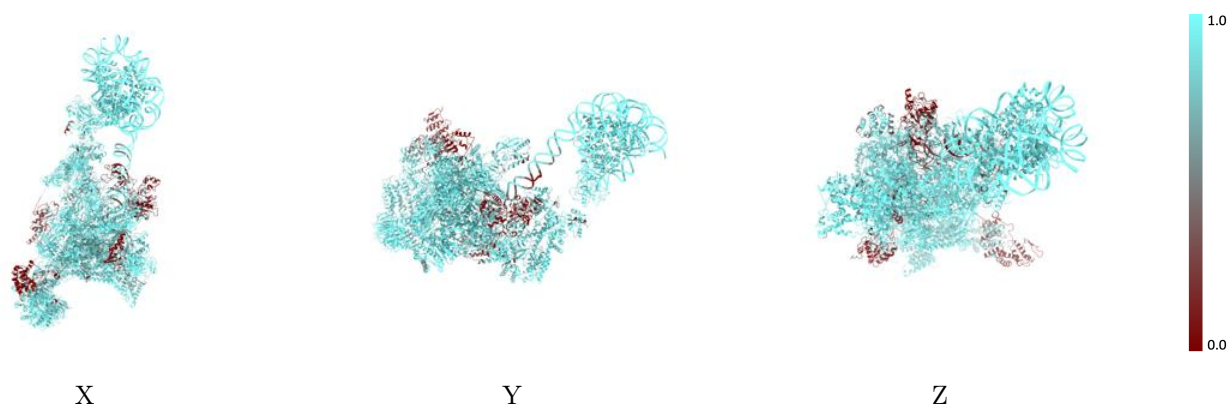
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



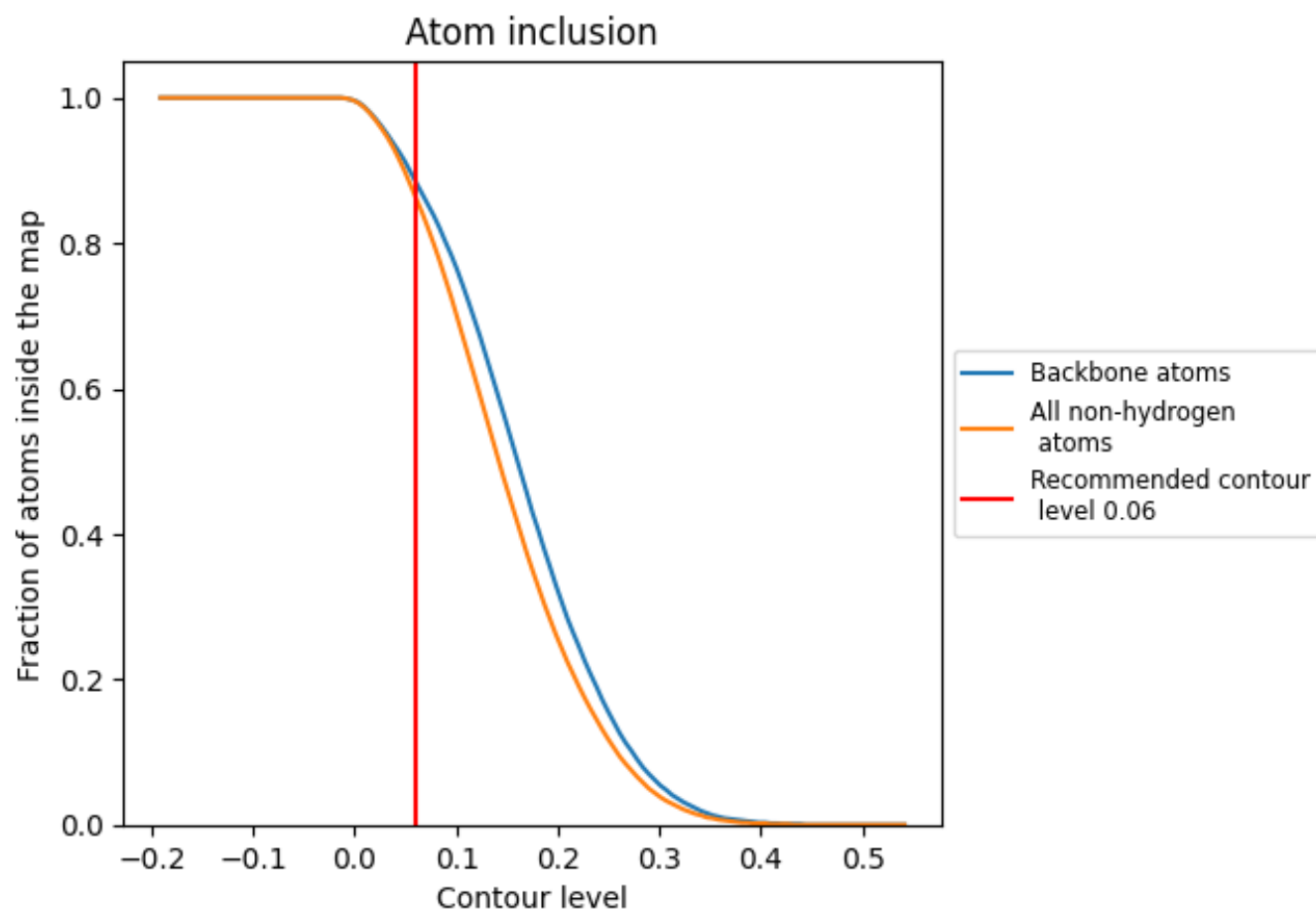
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.2370
A	 0.9620	 0.3750
B	 0.9810	 0.3880
C	 0.9810	 0.4090
D	 0.8910	 0.1570
E	 0.9820	 0.3570
F	 0.9700	 0.4160
G	 0.9310	 0.2010
H	 0.9620	 0.3890
I	 0.9750	 0.3110
J	 0.9900	 0.4130
K	 0.9890	 0.3960
L	 0.9630	 0.3620
M	 0.7290	 0.1230
N	 0.9360	 0.2050
O	 0.7340	 0.0310
P	 0.9060	 0.2330
Q	 0.7450	 0.0870
R	 0.8020	 0.1050
S	 0.9440	 0.2190
T	 0.9260	 0.2130
U	 0.2970	 0.0170
V	 0.5100	 0.0470
W	 0.9700	 0.1190
X	 0.9820	 0.1770
Y	 0.1140	 -0.0010
Z	 0.5390	 0.0810
a	 0.9700	 0.2300
b	 0.9650	 0.2710
c	 0.9810	 0.3290
d	 0.9800	 0.3090
e	 0.9830	 0.2920
f	 0.9830	 0.3410
g	 0.9490	 0.2390
h	 0.9620	 0.2450
l	 0.9160	 0.1130

