Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Oct 29, 2019 – 11:08 AM EDT

PDB ID	:	6J4W
EMDB ID:	:	EMD-0671
Title	:	RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-5) of the nucleosome
Authors	:	Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on	:	2019-01-10
Resolution	:	7.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

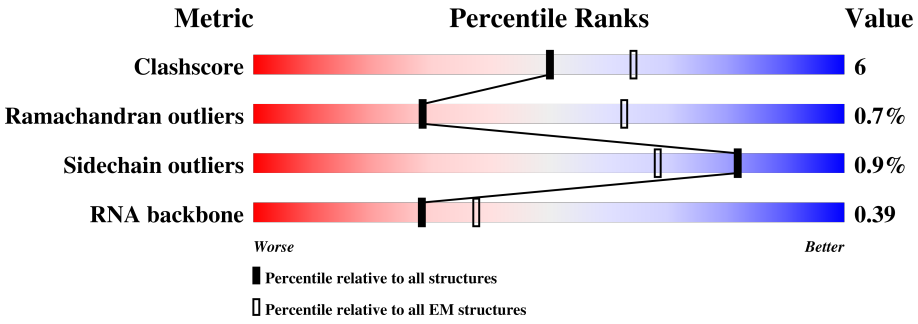
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1743	74% 6% 19%
2	B	1227	84% 9% • 6%
3	C	304	76% 11% 13%
4	D	186	80% 9% • 10%
5	E	214	90% 9%
6	F	155	50% 5% 46%
7	G	171	89% 11%
8	H	145	82% 10% 8%

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Mol	Chain	Length	Quality of chain
9	I	115	81% 16%
10	J	72	85% 7% 8%
11	K	118	95%
12	L	72	57% 6% 38%
13	P	16	19% 31% 44% 6%
14	T	198	68% 17% 14%
15	N	198	61% 20% 17%
16	M	113	44% 12% 43%
17	V	108	81% 12% 6%
18	W	911	22% 8% 70%
19	a	139	69% 30%
19	e	139	69% 30%
20	b	106	75% 25%
20	f	106	73% 26%
21	c	133	77% 23%
21	g	133	78% 21%
22	d	129	73% 26%
22	h	129	71% 28%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 48001 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1412	11123	7014	1938	2101	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1157	9228	5816	1630	1724	58	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	168	1314	812	237	263	2	0	0

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta.

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

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

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

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

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

- Molecule 13 is a RNA chain called RNA (5'-R(P*GP*UP*GP*UP*UP*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			347	153	60	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	171	Total	C	N	O	P	0	0
			3487	1652	676	989	170		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	165	Total	C	N	O	P	0	0
			3397	1616	592	1024	165		

- Molecule 16 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 18 is a protein called Spt5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Histone H3.3.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 20 is a protein called Histone H4.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

- Molecule 21 is a protein called Histone H2A type 1-B/E.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 22 is a protein called Histone H2B type 1-J.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
23	J	1	Total Zn 1 1	0
23	B	1	Total Zn 1 1	0
23	I	2	Total Zn 2 2	0
23	C	1	Total Zn 1 1	0
23	V	1	Total Zn 1 1	0
23	A	2	Total Zn 2 2	0
23	L	1	Total Zn 1 1	0
23	M	1	Total Zn 1 1	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

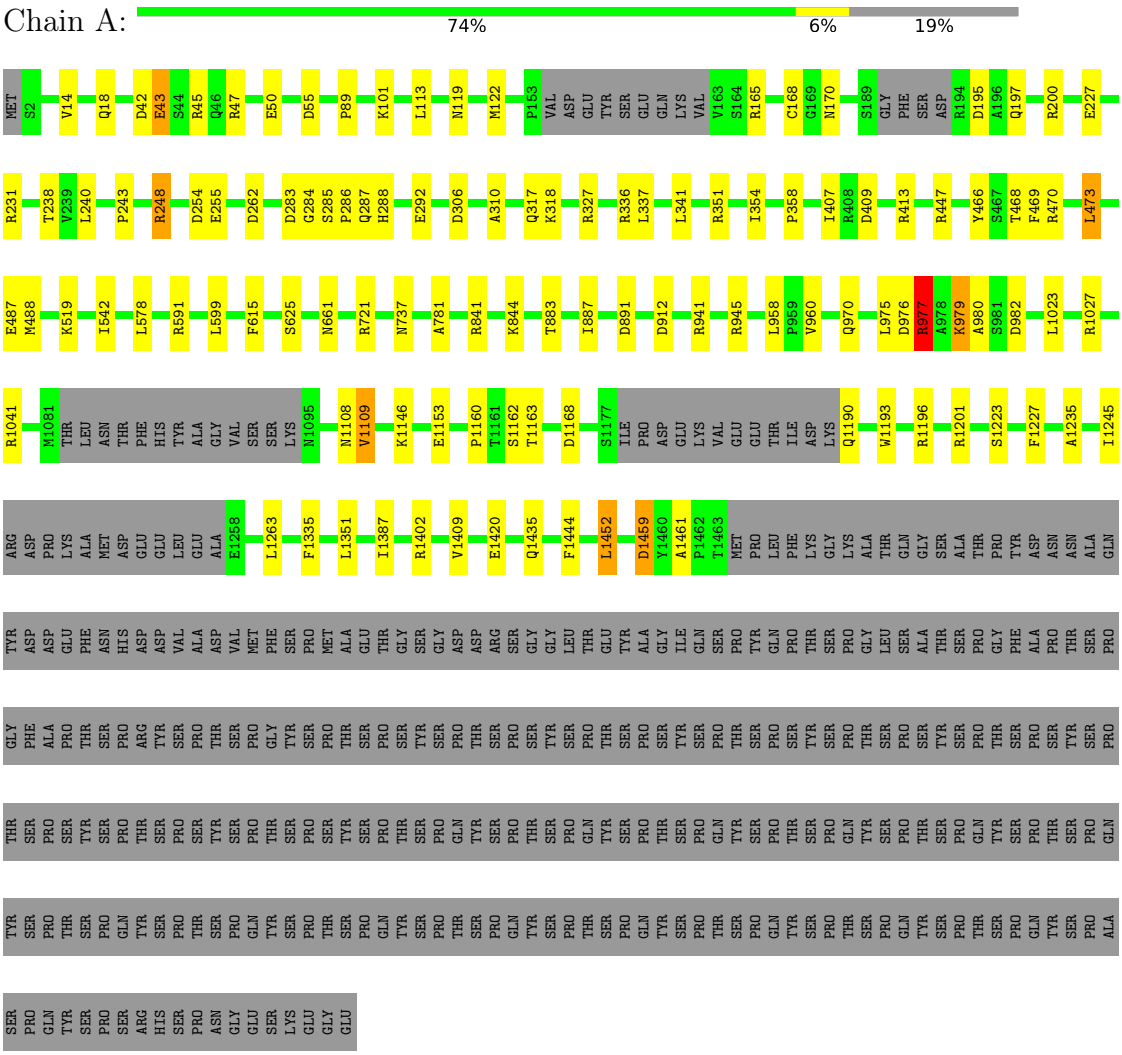
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total Mg 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

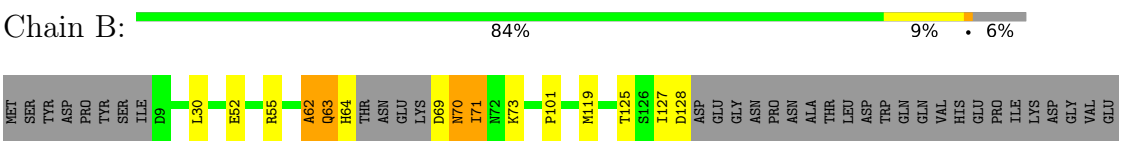
• Molecule 1: DNA-directed RNA polymerase subunit

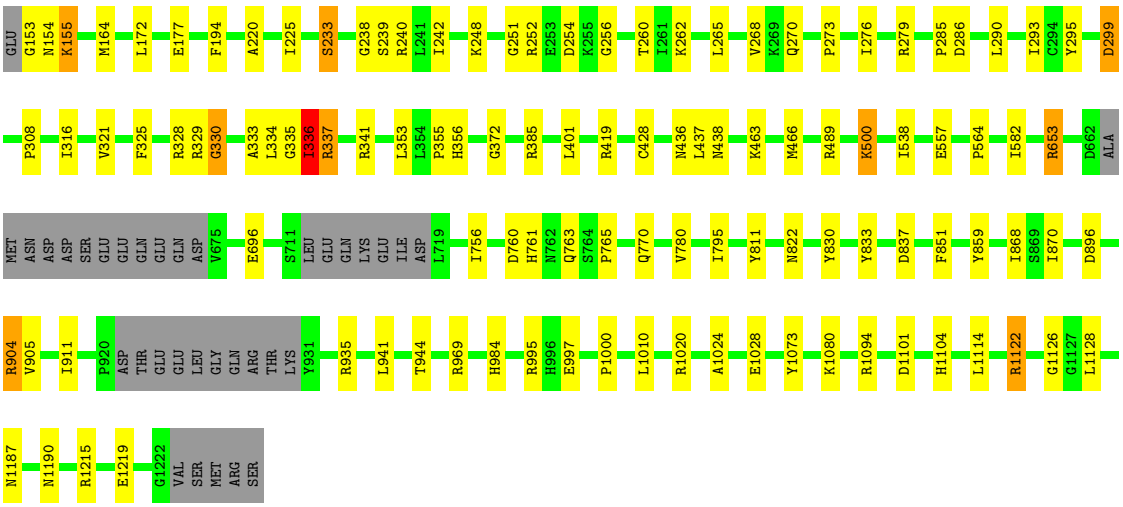
Chain A:



• Molecule 2: DNA-directed RNA polymerase subunit beta

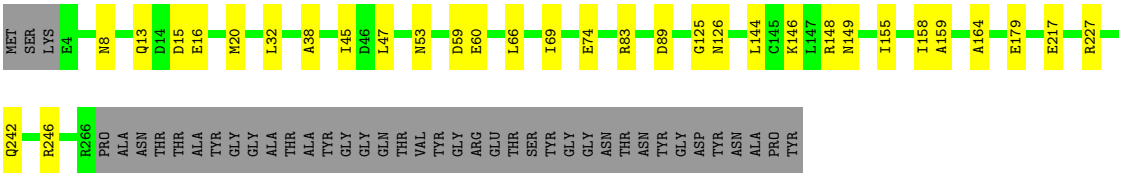
Chain B:





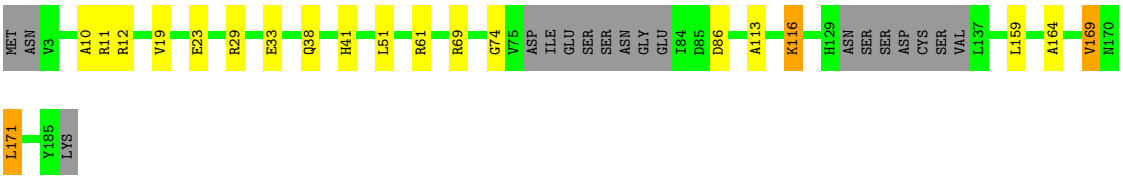
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:



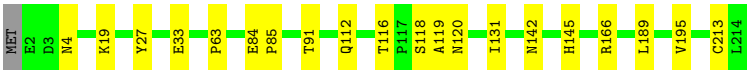
• Molecule 4: RNA polymerase II subunit B32

Chain D:



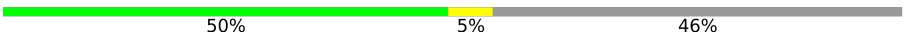
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

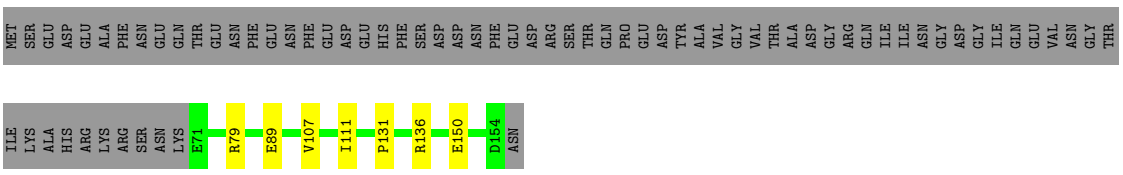
Chain E:



• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

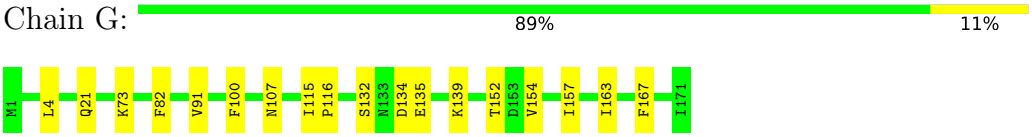
Chain F:





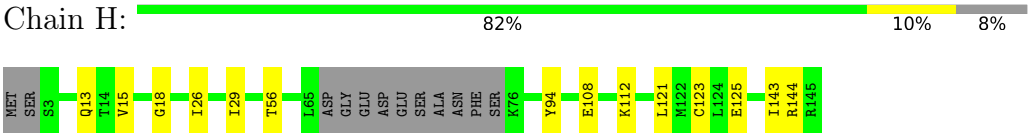
• Molecule 7: RNA polymerase II subunit

Chain G:



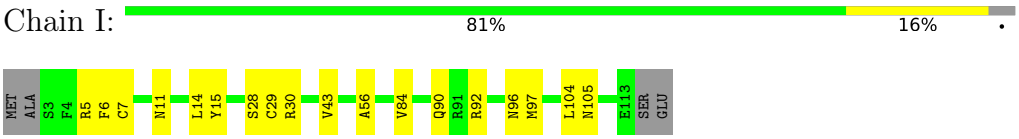
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



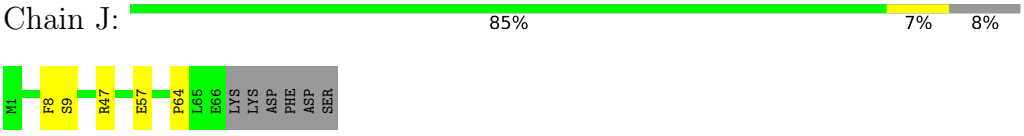
• Molecule 9: DNA-directed RNA polymerase subunit

Chain I:



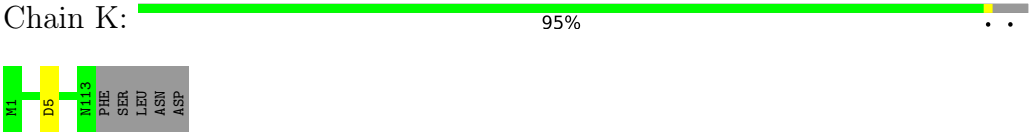
• Molecule 10: RNA polymerase subunit ABC10-beta

Chain J:



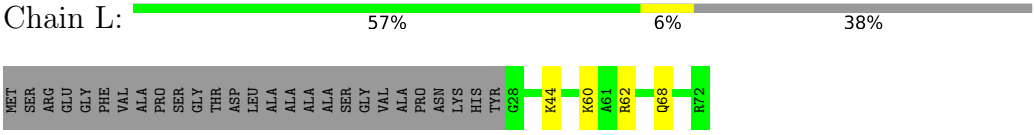
• Molecule 11: RNA polymerase II subunit B12.5

Chain K:



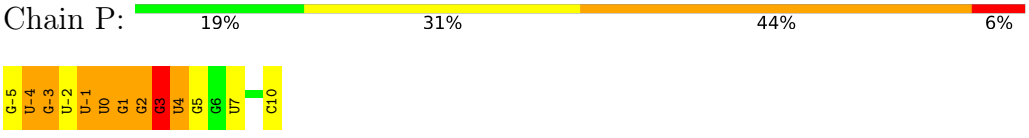
• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:



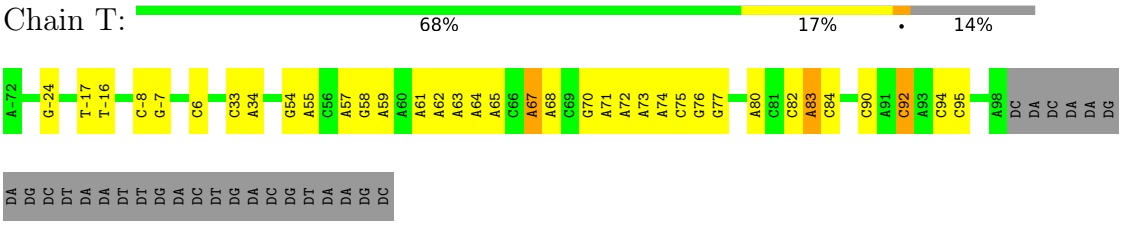
• Molecule 13: RNA (5'-R(P*GP*UP*GP*UP*UP*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3')

Chain P:



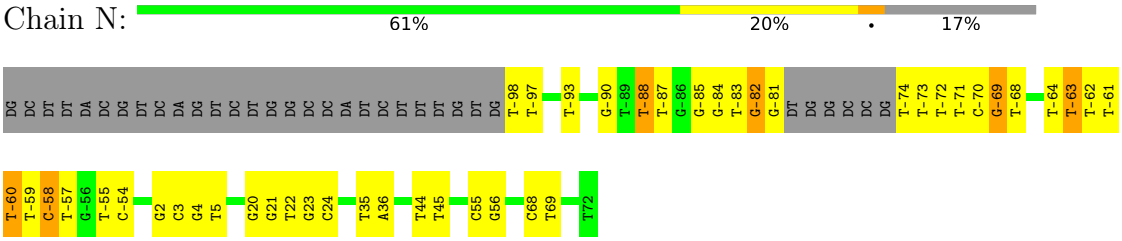
• Molecule 14: DNA (198-MER)

Chain T:



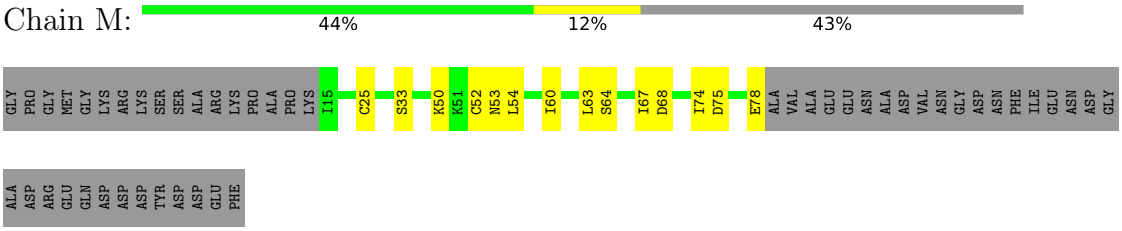
• Molecule 15: DNA (198-MER)

Chain N:



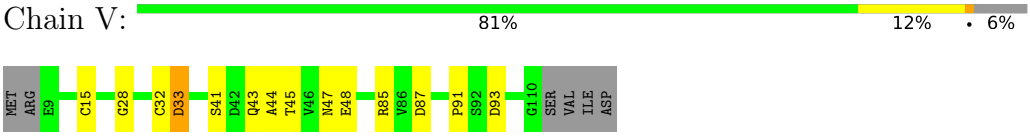
• Molecule 16: Transcription elongation factor 1 homolog

Chain M:



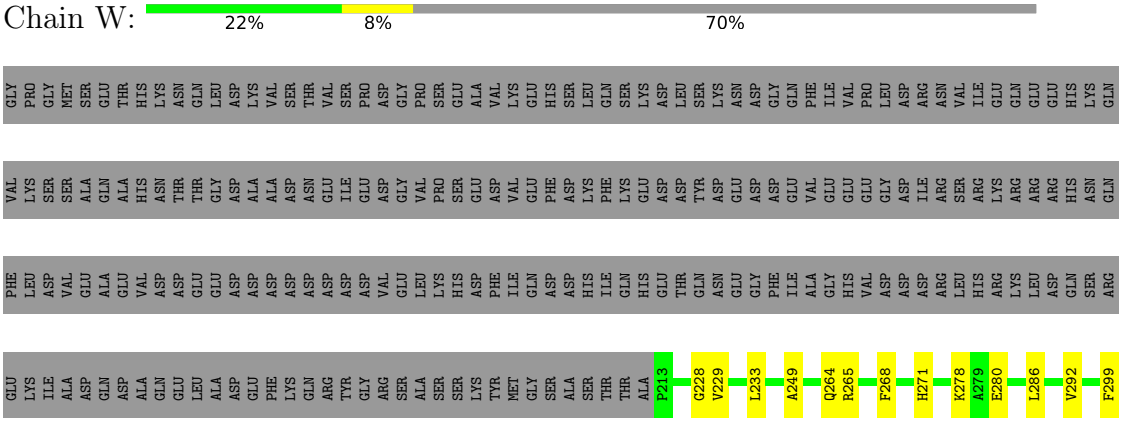
• Molecule 17: Transcription elongation factor SPT4

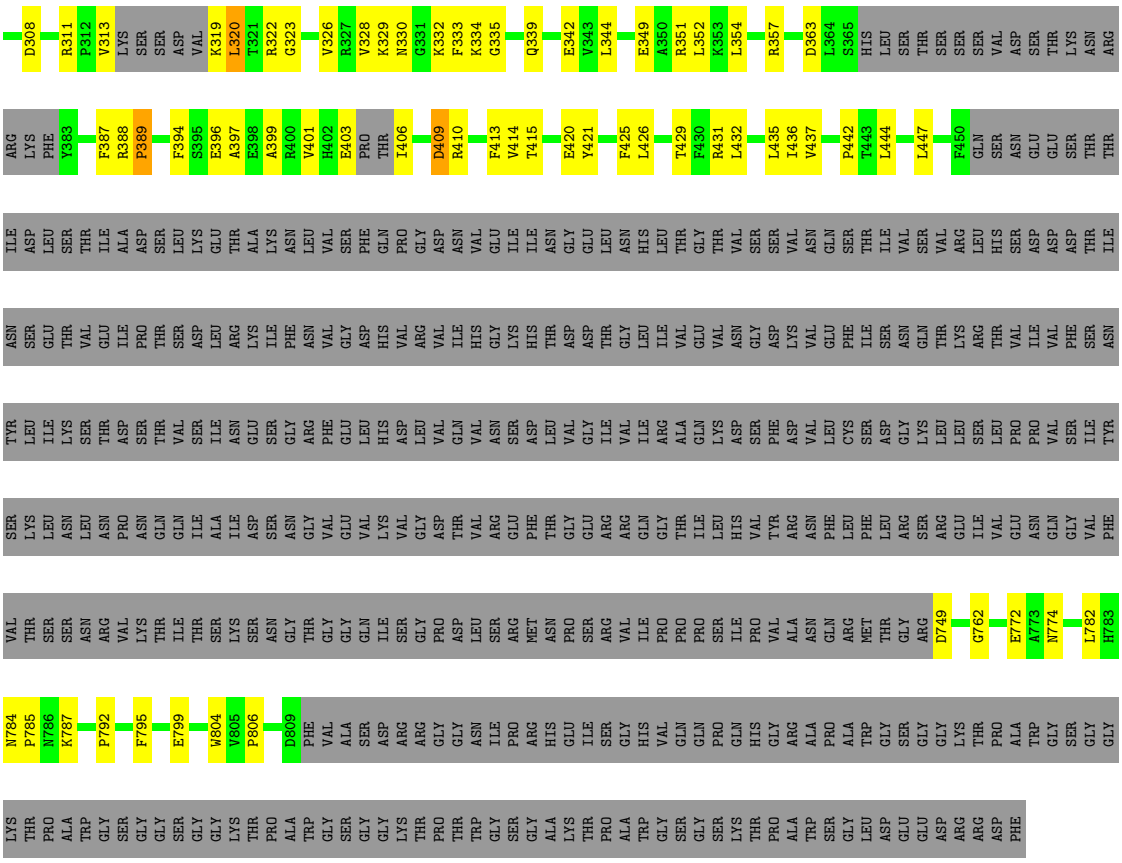
Chain V:



• Molecule 18: Spt5

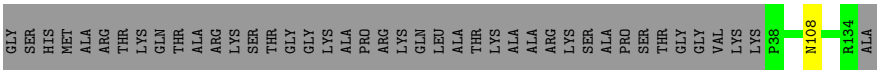
Chain W:





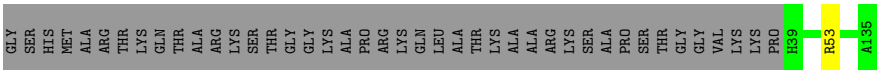
• Molecule 19: Histone H3.3

Chain a:



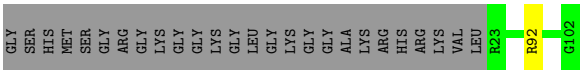
• Molecule 19: Histone H3.3

Chain e:



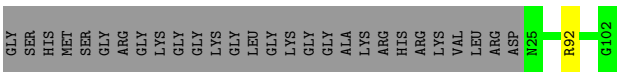
• Molecule 20: Histone H4

Chain b:



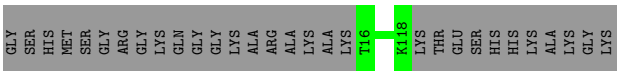
• Molecule 20: Histone H4

Chain f:



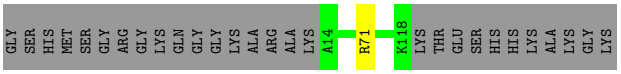
• Molecule 21: Histone H2A type 1-B/E

Chain c:



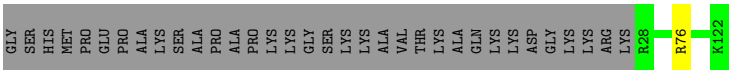
• Molecule 21: Histone H2A type 1-B/E

Chain g:



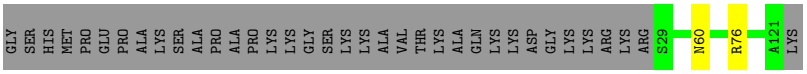
• Molecule 22: Histone H2B type 1-J

Chain d:



• Molecule 22: Histone H2B type 1-J

Chain h:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.44	0/11329	0.67	6/15310 (0.0%)
10	J	0.56	0/554	0.75	0/742
11	K	0.44	0/953	0.65	0/1291
12	L	0.45	0/365	0.76	0/484
13	P	1.21	6/387 (1.6%)	1.32	2/603 (0.3%)
14	T	0.95	6/3920 (0.2%)	1.06	4/6038 (0.1%)
15	N	0.94	12/3801 (0.3%)	1.06	0/5872
16	M	0.25	0/513	0.45	0/693
17	V	0.46	0/808	0.60	0/1097
18	W	0.40	0/2267	0.68	4/3048 (0.1%)
19	a	0.34	0/809	0.54	0/1085
19	e	0.38	0/807	0.52	0/1081
2	B	0.48	0/9407	0.71	6/12685 (0.0%)
20	b	0.38	0/645	0.57	0/862
20	f	0.40	0/626	0.56	0/837
21	c	0.35	0/806	0.52	0/1089
21	g	0.35	0/820	0.52	0/1107
22	d	0.38	0/757	0.54	0/1015
22	h	0.38	0/736	0.56	0/990
3	C	0.46	0/2139	0.72	1/2895 (0.0%)
4	D	0.32	0/1326	0.68	1/1788 (0.1%)
5	E	0.42	0/1772	0.64	0/2385
6	F	0.45	0/687	0.64	0/931
7	G	0.35	0/1353	0.71	0/1837
8	H	0.42	0/1069	0.67	0/1444
9	I	0.34	0/934	0.80	2/1257 (0.2%)
All	All	0.55	24/49590 (0.0%)	0.76	26/68466 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	-69	DG	C1'-N9	-9.52	1.33	1.47
13	P	-5	G	C1'-N9	-7.25	1.36	1.46
13	P	2	G	C1'-N9	-7.20	1.36	1.46
13	P	3	G	C1'-N9	-6.91	1.37	1.46
15	N	-81	DG	C1'-N9	-6.86	1.37	1.47
15	N	-82	DG	C1'-N9	-6.78	1.37	1.47
13	P	4	U	C1'-N1	6.77	1.58	1.48
14	T	83	DA	C1'-N9	-6.34	1.38	1.47
13	P	-3	G	C1'-N9	-6.08	1.38	1.46
15	N	-63	DT	C1'-N1	5.65	1.56	1.49
13	P	7	U	C1'-N1	5.43	1.56	1.48
15	N	-93	DT	C1'-N1	5.32	1.56	1.49
15	N	-97	DT	C1'-N1	5.31	1.56	1.49
15	N	-88	DT	C1'-N1	5.30	1.56	1.49
15	N	-87	DT	C1'-N1	5.26	1.56	1.49
14	T	95	DC	C1'-N1	5.26	1.56	1.49
15	N	-98	DT	C1'-N1	5.25	1.56	1.49
14	T	90	DC	C1'-N1	5.23	1.56	1.49
14	T	80	DA	C1'-N9	-5.20	1.40	1.47
15	N	-60	DT	C1'-N1	5.18	1.55	1.49
15	N	-58	DC	C1'-N1	5.14	1.55	1.49
15	N	-59	DT	C1'-N1	5.13	1.55	1.49
14	T	94	DC	C1'-N1	5.11	1.55	1.49
14	T	92	DC	C1'-N1	5.02	1.55	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	W	389	PRO	CA-N-CD	-8.55	99.53	111.50
1	A	473	LEU	CA-CB-CG	-8.23	96.36	115.30
2	B	63	GLN	N-CA-CB	-7.69	96.75	110.60
2	B	63	GLN	N-CA-C	-6.91	92.34	111.00
18	W	749	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	721	ARG	NE-CZ-NH1	-6.44	117.08	120.30
9	I	5	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	B	811	TYR	CB-CG-CD1	-5.93	117.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	306	ASP	CB-CG-OD1	5.89	123.61	118.30
14	T	67	DA	OP1-P-O3'	5.75	117.85	105.20
1	A	1452	LEU	CA-CB-CG	5.72	128.46	115.30
2	B	336	ILE	CA-CB-CG2	5.71	122.32	110.90
14	T	33	DC	O4'-C1'-N1	5.70	111.99	108.00
14	T	6	DC	O4'-C4'-C3'	-5.69	102.22	104.50
4	D	169	VAL	CA-CB-CG1	5.56	119.24	110.90
13	P	4	U	C2-N1-C1'	5.43	124.22	117.70
14	T	34	DA	O4'-C4'-C3'	-5.43	102.33	104.50
2	B	1010	LEU	CA-CB-CG	5.42	127.77	115.30
13	P	4	U	C6-N1-C1'	-5.41	113.63	121.20
9	I	5	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	330	GLY	N-CA-C	5.37	126.51	113.10
1	A	55	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	55	ASP	CB-CG-OD2	-5.20	113.62	118.30
18	W	409	ASP	CB-CG-OD2	5.19	122.97	118.30
18	W	363	ASP	CB-CG-OD2	5.15	122.94	118.30
3	C	15	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11147	96	0
2	B	9228	0	9232	122	0
3	C	2098	0	2059	18	0
4	D	1314	0	1314	10	0
5	E	1740	0	1754	24	0
6	F	677	0	693	5	0
7	G	1324	0	1342	11	0
8	H	1052	0	1050	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	917	0	868	9	0
10	J	545	0	561	4	0
11	K	932	0	944	1	0
12	L	359	0	358	2	0
13	P	347	0	170	22	0
14	T	3487	0	1904	77	0
15	N	3397	0	1872	95	0
16	M	505	0	496	24	0
17	V	792	0	757	7	0
18	W	2226	0	2273	144	0
19	a	797	0	835	0	0
19	e	796	0	832	0	0
20	b	638	0	676	0	0
20	f	619	0	659	0	0
21	c	796	0	848	0	0
21	g	810	0	866	0	0
22	d	746	0	771	0	0
22	h	725	0	745	0	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	V	1	0	0	0	0
24	A	1	0	0	0	0
All	All	48001	0	45026	533	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 6.

All (533) 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)
18:W:333:PHE:CD1	18:W:354:LEU:HD21	1.73	1.24
1:A:288:HIS:CD2	18:W:299:PHE:CZ	2.26	1.23
2:B:337:ARG:HD2	16:M:78:GLU:OE1	1.39	1.20
2:B:463:LYS:HD2	15:N:-84:DG:N2	1.56	1.20
18:W:409:ASP:HB2	18:W:413:PHE:CD2	1.73	1.20
18:W:333:PHE:CG	18:W:354:LEU:HD21	1.80	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:62:DA:N6	15:N:-62:DT:H3	1.45	1.15
18:W:332:LYS:HD2	18:W:389:PRO:HD3	1.24	1.12
14:T:73:DA:C2'	14:T:74:DA:H5"	1.79	1.11
2:B:419:ARG:HH11	15:N:-83:DT:H1'	1.14	1.10
5:E:118:SER:OG	15:N:-61:DT:O3'	1.70	1.09
18:W:399:ALA:HB1	18:W:406:ILE:HD11	1.27	1.09
14:T:73:DA:H2"	14:T:74:DA:C5'	1.82	1.08
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.31	1.08
18:W:409:ASP:HB2	18:W:413:PHE:HD2	1.04	1.07
1:A:976:ASP:O	1:A:977:ARG:HB2	1.51	1.07
18:W:320:LEU:HD22	18:W:432:LEU:HD13	1.37	1.05
2:B:419:ARG:NH1	15:N:-83:DT:H1'	1.71	1.05
14:T:61:DA:H1'	14:T:62:DA:OP2	1.57	1.04
14:T:74:DA:N6	15:N:-74:DT:O4	1.91	1.03
18:W:320:LEU:HD22	18:W:432:LEU:CD1	1.88	1.03
18:W:399:ALA:CB	18:W:406:ILE:HD11	1.90	1.00
1:A:288:HIS:CD2	18:W:299:PHE:CE1	2.49	1.00
14:T:62:DA:H61	15:N:-62:DT:H3	1.02	0.99
2:B:62:ALA:O	2:B:70:ASN:HA	1.62	0.98
18:W:396:GLU:OE2	18:W:414:VAL:HG23	1.64	0.98
13:P:-2:U:HO2'	13:P:-1:U:H5	1.11	0.96
18:W:399:ALA:HB1	18:W:406:ILE:CD1	1.95	0.96
14:T:92:DC:H5"	18:W:330:ASN:HD21	1.25	0.95
5:E:118:SER:OG	15:N:-60:DT:P	2.23	0.95
2:B:62:ALA:HB3	2:B:71:ILE:CG2	1.97	0.95
15:N:-58:DC:H2"	15:N:-57:DT:H71	1.49	0.94
18:W:409:ASP:CB	18:W:413:PHE:CD2	2.50	0.94
2:B:62:ALA:CB	2:B:71:ILE:CG2	2.46	0.93
1:A:286:PRO:CG	18:W:268:PHE:CZ	2.51	0.93
2:B:337:ARG:CD	16:M:78:GLU:OE1	2.16	0.93
1:A:288:HIS:NE2	18:W:299:PHE:CZ	2.36	0.92
18:W:409:ASP:CB	18:W:413:PHE:HD2	1.81	0.92
18:W:394:PHE:HE2	18:W:396:GLU:HG2	1.37	0.90
14:T:68:DA:N6	15:N:-69:DG:O6	2.03	0.90
2:B:463:LYS:HD2	15:N:-84:DG:H22	1.34	0.89
1:A:288:HIS:NE2	18:W:299:PHE:CE1	2.41	0.89
1:A:197:GLN:NE2	16:M:50:LYS:HB3	1.87	0.88
2:B:62:ALA:CB	2:B:71:ILE:HG23	2.03	0.88
14:T:58:DG:C6	14:T:59:DA:N6	2.42	0.88
17:V:85:ARG:NH1	17:V:87:ASP:OD1	2.07	0.88
2:B:463:LYS:CD	15:N:-84:DG:N2	2.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:399:ALA:C	18:W:406:ILE:CD1	2.43	0.86
5:E:118:SER:OG	15:N:-60:DT:OP1	1.93	0.86
18:W:333:PHE:CG	18:W:354:LEU:CD2	2.59	0.86
5:E:118:SER:HG	15:N:-60:DT:P	1.97	0.85
18:W:409:ASP:O	18:W:410:ARG:HG3	1.75	0.85
18:W:320:LEU:CD2	18:W:432:LEU:HD13	2.05	0.85
14:T:68:DA:N6	15:N:-69:DG:C6	2.45	0.85
18:W:329:LYS:HD2	18:W:436:ILE:HG13	1.59	0.84
18:W:332:LYS:HD2	18:W:388:ARG:HB2	1.59	0.84
18:W:399:ALA:CB	18:W:406:ILE:CD1	2.55	0.84
14:T:61:DA:C1'	14:T:62:DA:OP2	2.24	0.84
14:T:62:DA:C2	15:N:-61:DT:O2	2.31	0.84
2:B:62:ALA:HB3	2:B:71:ILE:HG22	1.59	0.83
13:P:10:C:O2	14:T:77:DG:N2	2.09	0.83
14:T:58:DG:C2	14:T:59:DA:C6	2.66	0.83
18:W:352:LEU:HD11	18:W:435:LEU:CD1	2.07	0.83
1:A:197:GLN:HE22	16:M:50:LYS:HB3	1.40	0.83
18:W:388:ARG:HB2	18:W:389:PRO:HD3	1.58	0.83
2:B:62:ALA:CB	2:B:71:ILE:HG22	2.09	0.82
14:T:62:DA:N1	15:N:-62:DT:O2	2.11	0.82
2:B:500:LYS:HD3	2:B:500:LYS:H	1.42	0.82
16:M:33:SER:HA	16:M:50:LYS:HE2	1.63	0.81
1:A:286:PRO:HG2	18:W:268:PHE:CZ	2.14	0.81
18:W:357:ARG:C	18:W:389:PRO:HG2	2.02	0.81
1:A:286:PRO:HG2	18:W:268:PHE:CE2	2.16	0.80
18:W:399:ALA:C	18:W:406:ILE:HD11	2.02	0.80
15:N:-84:DG:OP2	15:N:-84:DG:H2'	1.82	0.79
2:B:328:ARG:HD3	16:M:68:ASP:OD1	1.81	0.79
18:W:328:VAL:HA	18:W:435:LEU:HD23	1.64	0.78
18:W:357:ARG:HB3	18:W:389:PRO:HD2	1.64	0.78
18:W:394:PHE:CE2	18:W:396:GLU:HG2	2.18	0.78
2:B:328:ARG:CD	16:M:68:ASP:OD1	2.32	0.78
5:E:118:SER:HB2	15:N:-60:DT:C5'	2.14	0.78
14:T:92:DC:H5"	18:W:330:ASN:ND2	1.99	0.78
2:B:419:ARG:NH1	15:N:-83:DT:C1'	2.45	0.78
14:T:72:DA:N1	15:N:-72:DT:O2	2.17	0.77
15:N:-58:DC:H2"	15:N:-57:DT:C7	2.15	0.77
1:A:288:HIS:CE1	18:W:299:PHE:CE1	2.74	0.76
13:P:1:G:H2'	13:P:2:G:C8	2.21	0.76
5:E:116:THR:CG2	15:N:-61:DT:H5"	2.14	0.76
1:A:286:PRO:CD	18:W:268:PHE:CZ	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:319:LYS:O	18:W:320:LEU:CB	2.33	0.75
14:T:-24:DG:N2	15:N:24:DC:O2	2.18	0.75
14:T:54:DG:C4	14:T:55:DA:N7	2.54	0.75
14:T:54:DG:C2	14:T:55:DA:C4	2.75	0.75
14:T:57:DA:H1'	14:T:58:DG:H5'	1.68	0.75
1:A:288:HIS:CE1	18:W:299:PHE:HE1	2.04	0.75
2:B:463:LYS:CE	15:N:-84:DG:H21	2.00	0.74
1:A:101:LYS:NZ	15:N:-68:DT:OP1	2.20	0.74
14:T:54:DG:N3	14:T:55:DA:C8	2.55	0.74
1:A:45:ARG:HG2	1:A:45:ARG:O	1.88	0.73
2:B:868:ILE:HG12	15:N:-90:DG:OP1	1.89	0.73
5:E:116:THR:HB	15:N:-61:DT:H5"	1.71	0.73
14:T:54:DG:C4	14:T:55:DA:C8	2.77	0.73
18:W:328:VAL:HG22	18:W:435:LEU:HD21	1.70	0.73
18:W:396:GLU:OE2	18:W:414:VAL:CG2	2.36	0.72
15:N:-84:DG:H1'	15:N:-83:DT:C7	2.19	0.72
14:T:61:DA:C2'	14:T:62:DA:OP2	2.37	0.72
15:N:-85:DG:OP1	18:W:233:LEU:HD13	1.90	0.71
18:W:326:VAL:HG21	18:W:435:LEU:HD13	1.71	0.71
18:W:388:ARG:HB2	18:W:389:PRO:CD	2.19	0.71
13:P:3:G:N1	14:T:84:DC:N3	2.37	0.71
18:W:323:GLY:HA2	18:W:339:GLN:HE21	1.54	0.70
2:B:500:LYS:N	2:B:500:LYS:HD3	2.06	0.70
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.56	0.70
14:T:61:DA:C6	14:T:62:DA:N6	2.59	0.70
14:T:-24:DG:N1	15:N:24:DC:N3	2.38	0.70
15:N:-71:DT:H2"	15:N:-70:DC:C5	2.27	0.70
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.40	0.70
2:B:71:ILE:HD12	2:B:127:ILE:HG23	1.73	0.70
18:W:320:LEU:HD22	18:W:432:LEU:HD11	1.74	0.70
18:W:357:ARG:HB3	18:W:389:PRO:CD	2.22	0.70
18:W:332:LYS:HG3	18:W:388:ARG:CB	2.22	0.69
2:B:935:ARG:NH2	13:P:0:U:C4	2.61	0.68
18:W:357:ARG:O	18:W:389:PRO:HG2	1.94	0.68
15:N:-73:DT:H2"	15:N:-72:DT:H5"	1.76	0.68
2:B:935:ARG:NH2	13:P:0:U:C5	2.62	0.68
18:W:357:ARG:HB3	18:W:389:PRO:HG2	1.75	0.68
18:W:329:LYS:CD	18:W:436:ILE:HG13	2.24	0.67
2:B:463:LYS:HD2	15:N:-84:DG:H21	1.54	0.67
14:T:58:DG:N2	14:T:59:DA:C2	2.62	0.67
18:W:399:ALA:CA	18:W:406:ILE:HD11	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-58:DC:C2	15:N:-57:DT:C4	2.82	0.67
14:T:61:DA:H2"	14:T:62:DA:OP2	1.94	0.67
5:E:118:SER:HB2	15:N:-60:DT:H5"	1.75	0.67
14:T:54:DG:H2"	14:T:55:DA:OP2	1.94	0.67
2:B:63:GLN:OE1	18:W:249:ALA:HA	1.96	0.66
5:E:116:THR:CB	15:N:-61:DT:H5"	2.25	0.66
13:P:3:G:O6	14:T:84:DC:N4	2.19	0.66
1:A:243:PRO:O	1:A:248:ARG:NH1	2.28	0.66
12:L:68:GLN:HB3	18:W:784:ASN:HD21	1.61	0.66
18:W:332:LYS:CD	18:W:388:ARG:HB2	2.24	0.66
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.61	0.66
14:T:58:DG:N1	14:T:59:DA:C6	2.64	0.66
18:W:409:ASP:O	18:W:410:ARG:CG	2.43	0.66
18:W:329:LYS:HD2	18:W:436:ILE:CG1	2.25	0.66
14:T:73:DA:H2"	14:T:74:DA:H5"	0.85	0.65
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.78	0.65
18:W:351:ARG:HG2	18:W:429:THR:HG22	1.78	0.65
1:A:197:GLN:HE22	16:M:50:LYS:CB	2.09	0.65
18:W:352:LEU:CD1	18:W:435:LEU:HD11	2.19	0.65
18:W:409:ASP:CB	18:W:413:PHE:CE2	2.80	0.64
18:W:333:PHE:CD1	18:W:354:LEU:CD2	2.65	0.64
2:B:463:LYS:CD	15:N:-84:DG:H21	2.08	0.64
2:B:896:ASP:OD2	12:L:60:LYS:NZ	2.30	0.64
2:B:335:GLY:HA2	16:M:74:ILE:HD13	1.78	0.64
2:B:70:ASN:O	2:B:127:ILE:HA	1.97	0.64
13:P:5:G:C2	14:T:83:DA:C2	2.85	0.64
4:D:159:LEU:HD21	7:G:167:PHE:HB2	1.80	0.64
14:T:62:DA:N6	15:N:-62:DT:N3	2.23	0.64
1:A:286:PRO:CG	18:W:268:PHE:CE2	2.80	0.64
2:B:63:GLN:OE1	18:W:249:ALA:CA	2.46	0.63
18:W:329:LYS:CG	18:W:436:ILE:HG13	2.29	0.63
14:T:61:DA:C2	14:T:62:DA:C5	2.87	0.63
14:T:83:DA:H2"	14:T:84:DC:H5"	1.81	0.63
18:W:332:LYS:HG3	18:W:388:ARG:HB3	1.79	0.63
2:B:62:ALA:HB3	2:B:71:ILE:HG23	1.70	0.63
14:T:62:DA:N1	15:N:-62:DT:C2	2.67	0.63
18:W:437:VAL:O	18:W:437:VAL:HG22	1.98	0.63
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.63
2:B:62:ALA:HB3	2:B:71:ILE:H	1.64	0.62
1:A:286:PRO:HD3	18:W:268:PHE:CZ	2.34	0.62
16:M:25:CYS:SG	16:M:54:LEU:HD21	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:61:DA:N1	14:T:62:DA:C6	2.68	0.62
1:A:288:HIS:CG	18:W:299:PHE:CE1	2.87	0.61
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.33	0.61
2:B:220:ALA:O	2:B:252:ARG:NH2	2.33	0.61
18:W:357:ARG:HB3	18:W:389:PRO:CG	2.31	0.61
4:D:19:VAL:O	4:D:29:ARG:NH1	2.33	0.61
14:T:67:DA:N6	15:N:-68:DT:O4	2.33	0.61
2:B:328:ARG:HD3	16:M:68:ASP:HA	1.83	0.61
9:I:29:CYS:SG	9:I:30:ARG:N	2.74	0.61
1:A:288:HIS:NE2	18:W:299:PHE:HZ	1.97	0.61
4:D:41:HIS:HB3	7:G:73:LYS:HD3	1.82	0.61
5:E:118:SER:CB	15:N:-61:DT:O3'	2.49	0.60
17:V:44:ALA:O	17:V:48:GLU:HG2	2.01	0.60
18:W:328:VAL:HG22	18:W:435:LEU:CD2	2.30	0.60
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.35	0.60
8:H:56:THR:HB	8:H:144:ARG:HB3	1.83	0.60
1:A:318:LYS:HG2	15:N:-85:DG:O6	2.02	0.60
15:N:-63:DT:H2"	15:N:-62:DT:H6	1.67	0.60
13:P:1:G:N2	13:P:2:G:C2	2.69	0.60
14:T:62:DA:H2"	14:T:63:DA:C8	2.37	0.60
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.84	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.35	0.59
18:W:396:GLU:CD	18:W:414:VAL:CG2	2.70	0.59
2:B:859:TYR:HD2	2:B:911:ILE:HD11	1.67	0.59
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.59
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.85	0.59
5:E:118:SER:CB	15:N:-60:DT:OP1	2.51	0.59
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.35	0.59
18:W:399:ALA:O	18:W:406:ILE:CD1	2.50	0.59
18:W:397:ALA:O	18:W:401:VAL:HG23	2.03	0.59
1:A:976:ASP:O	1:A:977:ARG:CB	2.37	0.59
18:W:328:VAL:HA	18:W:435:LEU:CD2	2.33	0.59
18:W:394:PHE:CE2	18:W:396:GLU:CG	2.86	0.58
5:E:118:SER:OG	15:N:-61:DT:C3'	2.51	0.58
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.85	0.58
1:A:42:ASP:O	1:A:43:GLU:HG3	2.03	0.58
18:W:319:LYS:O	18:W:320:LEU:HB3	2.02	0.58
18:W:394:PHE:HE2	18:W:396:GLU:CG	2.14	0.58
2:B:233:SER:HG	2:B:356:HIS:HD1	1.50	0.58
18:W:389:PRO:HD2	18:W:389:PRO:O	2.04	0.58
2:B:328:ARG:HD2	16:M:68:ASP:OD1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:58:DG:C2	14:T:59:DA:N1	2.72	0.58
14:T:61:DA:N1	14:T:62:DA:N6	2.52	0.58
18:W:413:PHE:CE1	18:W:420:GLU:HB3	2.38	0.58
1:A:197:GLN:CD	16:M:50:LYS:HB3	2.24	0.58
14:T:54:DG:C2	14:T:55:DA:C5	2.92	0.57
2:B:295:TYR:HD1	2:B:564:PRO:HB3	1.69	0.57
2:B:337:ARG:HB2	16:M:75:ASP:OD1	2.04	0.57
16:M:54:LEU:C	16:M:54:LEU:HD12	2.24	0.57
18:W:319:LYS:O	18:W:320:LEU:HB2	2.03	0.57
2:B:30:LEU:O	2:B:489:ARG:NH1	2.38	0.57
3:C:20:MET:SD	3:C:227:ARG:NH2	2.75	0.57
5:E:116:THR:HG21	15:N:-61:DT:H5”	1.87	0.57
5:E:118:SER:CB	15:N:-60:DT:P	2.91	0.57
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.34	0.57
15:N:-83:DT:H6	15:N:-83:DT:O5’	1.88	0.57
1:A:1459:ASP:N	1:A:1459:ASP:OD1	2.34	0.56
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.56
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.87	0.56
8:H:13:GLN:HE22	8:H:29:ILE:HD12	1.70	0.56
18:W:332:LYS:CG	18:W:388:ARG:HB2	2.35	0.56
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.39	0.56
14:T:62:DA:N1	15:N:-61:DT:O2	2.38	0.56
13:P:-1:U:H2’	13:P:-1:U:O2	2.05	0.56
18:W:409:ASP:OD2	18:W:415:THR:OG1	2.21	0.56
2:B:268:VAL:HA	2:B:330:GLY:HA2	1.88	0.56
15:N:22:DT:H2”	15:N:23:DG:H5”	1.88	0.56
14:T:58:DG:N1	14:T:59:DA:N6	2.53	0.56
2:B:935:ARG:NH2	13:P:0:U:O4	2.39	0.56
17:V:43:GLN:NE2	17:V:47:ASN:OD1	2.39	0.56
2:B:334:LEU:HD22	16:M:67:ILE:CD1	2.37	0.55
18:W:344:LEU:CD1	18:W:349:GLU:HB2	2.35	0.55
2:B:822:ASN:O	10:J:47:ARG:NH1	2.39	0.55
15:N:-63:DT:H2’	15:N:-62:DT:C7	2.36	0.55
14:T:61:DA:C2	14:T:62:DA:C6	2.94	0.55
2:B:62:ALA:HB1	2:B:71:ILE:HG22	1.90	0.54
3:C:83:ARG:HG2	18:W:762:GLY:HA2	1.88	0.54
2:B:52:GLU:OE2	2:B:55:ARG:NH1	16.93	0.54
18:W:396:GLU:CD	18:W:414:VAL:HG21	2.27	0.54
1:A:409:ASP:N	1:A:409:ASP:OD1	2.40	0.54
2:B:270:GLN:HB3	2:B:329:ARG:HD3	1.89	0.54
15:N:-85:DG:OP1	18:W:233:LEU:CD1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-63:DT:H2'	15:N:-62:DT:H72	1.90	0.54
2:B:904:ARG:NH1	18:W:782:LEU:O	2.41	0.54
13:P:1:G:O2'	13:P:2:G:O4'	2.23	0.54
18:W:352:LEU:HD11	18:W:435:LEU:HD21	1.90	0.53
15:N:-85:DG:H4'	15:N:-84:DG:O5'	2.08	0.53
14:T:92:DC:C5'	18:W:330:ASN:HD21	2.11	0.53
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.73	0.53
1:A:288:HIS:CD2	18:W:299:PHE:HZ	2.18	0.53
1:A:50:GLU:OE1	18:W:444:LEU:HD11	2.09	0.53
1:A:286:PRO:CD	18:W:268:PHE:CE1	2.92	0.53
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.74	0.53
18:W:772:GLU:OE2	18:W:774:ASN:ND2	2.42	0.53
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.90	0.53
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.91	0.52
17:V:41:SER:HB2	17:V:45:THR:HB	1.91	0.52
14:T:61:DA:H1'	14:T:62:DA:P	2.49	0.52
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.74	0.52
2:B:944:THR:HG21	2:B:1122:ARG:HE	1.75	0.52
15:N:-58:DC:C4	15:N:-57:DT:O4	2.63	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
4:D:113:ALA:O	4:D:116:LYS:NZ	2.43	0.51
1:A:1402:ARG:NH2	1:A:1420:GLU:OE1	2.43	0.51
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.93	0.51
1:A:50:GLU:CD	18:W:444:LEU:HD11	2.31	0.51
2:B:333:ALA:HB3	2:B:336:ILE:HD11	1.92	0.51
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.93	0.51
2:B:62:ALA:HB2	2:B:71:ILE:HG23	1.89	0.51
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.44	0.51
2:B:760:ASP:OD1	2:B:760:ASP:N	2.38	0.51
2:B:62:ALA:HB3	2:B:71:ILE:N	2.26	0.51
15:N:-63:DT:H2"	15:N:-62:DT:C6	2.43	0.51
18:W:409:ASP:HB2	18:W:413:PHE:CE2	2.35	0.51
18:W:286:LEU:HD22	18:W:292:VAL:HG21	1.93	0.50
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.75	0.50
2:B:63:GLN:OE1	18:W:249:ALA:HB1	2.11	0.50
18:W:349:GLU:HG2	18:W:431:ARG:HA	1.92	0.50
3:C:74:GLU:O	3:C:246:ARG:NH2	2.33	0.50
2:B:463:LYS:CD	15:N:-84:DG:H22	2.14	0.50
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.44	0.50
15:N:-61:DT:H2"	15:N:-60:DT:C6	2.46	0.50
4:D:33:GLU:O	4:D:38:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.50
18:W:403:GLU:O	18:W:403:GLU:HG3	2.12	0.50
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.50
1:A:310:ALA:HB2	14:T:72:DA:OP1	2.12	0.50
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.77	0.50
14:T:62:DA:C2	15:N:-62:DT:O2	2.64	0.50
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.93	0.49
2:B:260:THR:HG22	2:B:308:PRO:HB2	1.93	0.49
15:N:68:DC:H2"	15:N:69:DT:H5'	1.95	0.49
1:A:1146:LYS:NZ	2:B:254:ASP:OD2	2.38	0.49
2:B:419:ARG:NH1	15:N:-83:DT:C2	2.74	0.49
18:W:413:PHE:HE1	18:W:420:GLU:HB3	1.78	0.49
2:B:859:TYR:HE2	2:B:941:LEU:HD12	1.77	0.49
15:N:-88:DT:OP1	18:W:334:LYS:HE3	2.12	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.95	0.49
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.46	0.49
5:E:27:TYR:HA	5:E:63:PRO:HA	1.95	0.49
14:T:64:DA:H2'	14:T:65:DA:C8	2.47	0.49
1:A:841:ARG:NH2	1:A:1108:ASN:OD1	2.46	0.49
1:A:1153:GLU:OE1	1:A:1196:ARG:NH1	2.45	0.49
18:W:357:ARG:CB	18:W:389:PRO:HG2	2.42	0.49
18:W:399:ALA:O	18:W:406:ILE:HD12	2.13	0.49
2:B:1101:ASP:O	2:B:1122:ARG:NH1	2.45	0.48
14:T:74:DA:H2"	14:T:75:DC:H5'	1.94	0.48
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.36	0.48
1:A:43:GLU:OE2	18:W:335:GLY:O	2.31	0.48
1:A:14:VAL:H	1:A:1435:GLN:NE2	2.10	0.48
13:P:-4:U:OP1	13:P:-4:U:H4'	2.14	0.48
14:T:63:DA:H2'	14:T:64:DA:C8	2.49	0.48
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.96	0.48
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.96	0.48
15:N:68:DC:H2'	15:N:69:DT:C6	2.48	0.48
18:W:409:ASP:OD2	18:W:413:PHE:CE2	2.66	0.48
3:C:74:GLU:HG3	3:C:242:GLN:HE22	1.77	0.48
14:T:68:DA:N1	15:N:-69:DG:N1	2.62	0.48
18:W:308:ASP:HA	18:W:311:ARG:HG3	1.96	0.48
18:W:396:GLU:CD	18:W:414:VAL:HG23	2.30	0.48
1:A:113:LEU:O	1:A:165:ARG:NH2	2.47	0.47
1:A:1193:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.47
14:T:62:DA:N1	15:N:-61:DT:C2	2.83	0.47
15:N:-71:DT:C2	15:N:-70:DC:C4	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:91:PRO:HB2	17:V:93:ASP:OD1	2.14	0.47
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.97	0.47
10:J:9:SER:OG	10:J:47:ARG:NH2	2.47	0.47
18:W:388:ARG:CB	18:W:389:PRO:CD	2.88	0.47
1:A:283:ASP:N	1:A:283:ASP:OD1	2.46	0.47
2:B:401:LEU:HD13	2:B:538:ILE:HG21	1.96	0.47
1:A:254:ASP:OD1	1:A:254:ASP:N	2.48	0.47
5:E:19:LYS:NZ	5:E:33:GLU:O	2.38	0.47
16:M:52:CYS:O	16:M:53:ASN:HB2	2.15	0.47
18:W:437:VAL:CG2	18:W:437:VAL:O	2.61	0.47
2:B:63:GLN:OE1	18:W:249:ALA:CB	2.62	0.47
15:N:4:DG:H4'	15:N:5:DT:H5'	1.97	0.47
18:W:413:PHE:HZ	18:W:420:GLU:CD	2.17	0.47
5:E:189:LEU:HD13	5:E:213:CYS:HB2	1.96	0.46
18:W:399:ALA:CB	18:W:406:ILE:HD13	2.44	0.46
5:E:142:ASN:HB3	5:E:145:HIS:HD2	1.80	0.46
14:T:70:DG:H2'	14:T:71:DA:C8	2.50	0.46
1:A:286:PRO:HG3	18:W:268:PHE:CZ	2.46	0.46
1:A:542:ILE:HD12	1:A:578:LEU:HD13	1.98	0.46
1:A:912:ASP:OD1	1:A:912:ASP:N	2.42	0.46
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.47	0.46
13:P:-2:U:O5'	13:P:-2:U:H6	1.98	0.46
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.46
2:B:969:ARG:HH22	3:C:59:ASP:HB2	1.80	0.46
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.79	0.46
15:N:-72:DT:H6	15:N:-72:DT:H5"	1.79	0.46
1:A:1109:VAL:HG13	1:A:1335:PHE:HE2	1.80	0.46
11:K:5:ASP:OD1	18:W:787:LYS:NZ	2.48	0.46
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.97	0.46
1:A:887:ILE:O	1:A:945:ARG:NH2	2.41	0.46
2:B:557:GLU:HB2	2:B:582:ILE:HD12	1.97	0.46
15:N:-83:DT:O4	15:N:-82:DG:C2	2.68	0.46
13:P:-1:U:H2'	13:P:0:U:H5"	1.97	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.46
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.81	0.46
6:F:79:ARG:NH1	6:F:150:GLU:OE2	2.49	0.45
13:P:2:G:O5'	13:P:2:G:H8	1.99	0.45
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.80	0.45
3:C:45:ILE:HA	3:C:159:ALA:HA	1.99	0.45
15:N:2:DG:H1'	15:N:3:DC:H5'	1.98	0.45
15:N:-63:DT:C6	15:N:-62:DT:H72	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:-2:U:O5'	13:P:-2:U:C6	2.69	0.45
2:B:436:ASN:O	2:B:438:ASN:N	2.48	0.45
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.98	0.45
15:N:-58:DC:C2	15:N:-57:DT:N3	2.85	0.45
2:B:419:ARG:NH1	15:N:-83:DT:N1	2.59	0.45
13:P:5:G:H1	14:T:82:DC:H42	1.64	0.45
18:W:352:LEU:CD1	18:W:435:LEU:HD21	2.46	0.45
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.37	0.45
9:I:96:ASN:OD1	9:I:97:MET:N	2.48	0.45
15:N:-71:DT:H2"	15:N:-70:DC:H5	1.79	0.45
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.98	0.45
2:B:1219:GLU:O	4:D:12:ARG:NH2	2.49	0.45
13:P:1:G:N2	13:P:2:G:N3	2.64	0.45
15:N:20:DG:H2"	15:N:21:DG:H5"	1.98	0.45
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.40	0.45
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.99	0.45
2:B:64:HIS:O	2:B:64:HIS:CG	2.70	0.45
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.99	0.45
14:T:68:DA:C6	15:N:-69:DG:N1	2.85	0.45
1:A:1162:SER:OG	1:A:1163:THR:N	2.49	0.44
7:G:116:PRO:HD2	7:G:163:ILE:HG13	1.99	0.44
18:W:322:ARG:HD3	18:W:342:GLU:HA	1.99	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.44
2:B:276:ILE:HD11	16:M:63:LEU:HD21	2.00	0.44
2:B:62:ALA:HB1	2:B:71:ILE:CG2	2.42	0.44
13:P:3:G:N2	14:T:84:DC:O2	2.49	0.44
18:W:409:ASP:OD2	18:W:413:PHE:HE2	2.00	0.44
2:B:325:PHE:CE1	16:M:63:LEU:HB3	2.52	0.44
1:A:286:PRO:O	1:A:288:HIS:N	2.50	0.44
15:N:-71:DT:H2"	15:N:-70:DC:C6	2.52	0.44
14:T:54:DG:N3	14:T:55:DA:N9	2.65	0.44
14:T:62:DA:H2"	14:T:63:DA:O4'	2.17	0.44
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.99	0.44
5:E:119:ALA:N	15:N:-60:DT:OP1	2.51	0.44
4:D:23:GLU:HB3	7:G:82:PHE:HD1	1.83	0.44
2:B:870:ILE:HG13	18:W:387:PHE:CZ	2.52	0.44
15:N:-58:DC:C5	15:N:-57:DT:O4	2.71	0.44
17:V:28:GLY:HA3	17:V:33:ASP:CG	2.38	0.44
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.49	0.44
2:B:334:LEU:HD22	16:M:67:ILE:HD11	2.00	0.44
2:B:70:ASN:HB2	2:B:128:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:935:ARG:CZ	13:P:0:U:O4	2.66	0.44
18:W:399:ALA:O	18:W:406:ILE:HD11	2.14	0.43
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.88	0.43
18:W:333:PHE:CD2	18:W:354:LEU:CD2	3.00	0.43
18:W:344:LEU:HD11	18:W:349:GLU:HB2	2.00	0.43
1:A:1461:ALA:HB1	7:G:21:GLN:HB2	1.99	0.43
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.99	0.43
15:N:-64:DT:C6	15:N:-63:DT:H72	2.53	0.43
18:W:442:PRO:HB2	18:W:447:LEU:CD1	2.48	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.43
7:G:91:VAL:HG23	7:G:139:LYS:HA	2.01	0.43
15:N:-73:DT:H2”	15:N:-72:DT:C5’	2.45	0.43
14:T:58:DG:C2	14:T:59:DA:C5	3.07	0.43
18:W:421:TYR:HA	18:W:425:PHE:O	2.19	0.43
1:A:891:ASP:HA	1:A:941:ARG:HH12	1.83	0.43
3:C:148:ARG:HG2	3:C:149:ASN:H	1.83	0.43
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.43
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.77	0.43
18:W:332:LYS:HE3	18:W:357:ARG:HB2	2.01	0.43
1:A:1263:LEU:HA	1:A:1263:LEU:HD12	1.93	0.43
2:B:71:ILE:HG12	2:B:73:LYS:HE3	2.00	0.43
15:N:-85:DG:H2”	15:N:-84:DG:C8	2.53	0.43
14:T:75:DC:H6	14:T:75:DC:H3’	1.83	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.00	0.43
18:W:792:PRO:HG2	18:W:795:PHE:CD2	2.54	0.43
1:A:407:ILE:HG12	1:A:413:ARG:HG2	2.00	0.43
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.52	0.43
14:T:76:DG:N1	14:T:77:DG:C6	2.87	0.43
2:B:336:ILE:H	2:B:341:ARG:HH21	1.67	0.42
2:B:334:LEU:HD22	16:M:67:ILE:HD13	2.00	0.42
14:T:58:DG:N3	14:T:59:DA:C5	2.87	0.42
6:F:107:VAL:HG11	6:F:111:ILE:HD11	2.00	0.42
15:N:44:DT:H2”	15:N:45:DT:C5	2.54	0.42
15:N:-84:DG:O3’	15:N:-83:DT:H71	2.19	0.42
2:B:463:LYS:HE3	15:N:-84:DG:H21	1.82	0.42
14:T:-8:DC:H2”	14:T:-7:DG:C8	2.54	0.42
18:W:352:LEU:HD11	18:W:435:LEU:CD2	2.49	0.42
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.42
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.42
1:A:468:THR:OG1	1:A:470:ARG:NH1	2.52	0.42
2:B:154:ASN:OD1	2:B:155:LYS:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:TYR:N	9:I:28:SER:O	2.37	0.42
14:T:58:DG:N2	14:T:59:DA:N1	2.67	0.42
2:B:119:MET:O	2:B:153:GLY:N	2.53	0.42
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.51	0.42
14:T:-17:DT:H2"	14:T:-16:DT:C6	2.54	0.42
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.93	0.42
15:N:55:DC:H2"	15:N:56:DG:C8	2.55	0.42
2:B:101:PRO:HG2	2:B:172:LEU:HD11	2.01	0.42
1:A:615:PHE:HB3	8:H:121:LEU:HD21	2.01	0.42
1:A:286:PRO:O	1:A:288:HIS:ND1	2.52	0.42
7:G:152:THR:HA	7:G:157:ILE:HG22	2.02	0.42
9:I:84:VAL:HG22	9:I:104:LEU:HD21	2.01	0.42
15:N:-55:DT:H2"	15:N:-54:DC:C5	2.54	0.42
14:T:58:DG:C6	14:T:59:DA:C6	3.07	0.42
16:M:60:ILE:HB	16:M:64:SER:OG	2.20	0.42
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.59	0.42
1:A:292:GLU:OE1	18:W:271:HIS:HE1	2.02	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.41
1:A:883:THR:O	1:A:1027:ARG:NH2	2.52	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
14:T:76:DG:C6	14:T:77:DG:C6	3.08	0.41
18:W:278:LYS:HD2	18:W:280:GLU:OE2	2.20	0.41
2:B:251:GLY:HA2	2:B:256:GLY:HA3	2.02	0.41
5:E:189:LEU:HD11	5:E:195:VAL:HG13	2.01	0.41
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.55	0.41
13:P:3:G:H2'	13:P:4:U:O4'	2.19	0.41
18:W:352:LEU:HD21	18:W:435:LEU:CD1	2.50	0.41
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.85	0.41
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.78	0.41
2:B:233:SER:OG	2:B:356:HIS:ND1	2.43	0.41
2:B:63:GLN:OE1	18:W:249:ALA:O	2.38	0.41
5:E:118:SER:HB2	15:N:-60:DT:P	2.59	0.41
14:T:74:DA:C6	15:N:-74:DT:O4	2.66	0.41
18:W:784:ASN:HB2	18:W:785:PRO:HD3	2.02	0.41
2:B:325:PHE:CZ	16:M:63:LEU:HD23	2.55	0.41
1:A:781:ALA:N	2:B:696:GLU:OE2	2.45	0.41
14:T:54:DG:N2	14:T:55:DA:C4	2.88	0.41
18:W:228:GLY:HA3	18:W:299:PHE:CZ	2.55	0.41
18:W:322:ARG:CD	18:W:342:GLU:HG3	2.51	0.41
4:D:69:ARG:HG2	4:D:74:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:35:DT:H4'	15:N:36:DA:H5'	2.02	0.41
14:T:71:DA:H2'	14:T:72:DA:C8	2.55	0.41
18:W:322:ARG:CD	18:W:342:GLU:HA	2.51	0.41
18:W:409:ASP:C	18:W:410:ARG:HG3	2.37	0.41
1:A:591:ARG:HH11	1:A:591:ARG:HD3	1.74	0.41
15:N:-85:DG:H2"	15:N:-84:DG:O5'	2.21	0.41
2:B:262:LYS:HA	2:B:273:PRO:HA	2.03	0.41
2:B:71:ILE:O	2:B:73:LYS:HG3	2.20	0.41
3:C:125:GLY:HA2	3:C:126:ASN:HA	1.75	0.41
14:T:70:DG:C6	14:T:71:DA:C6	3.08	0.41
1:A:447:ARG:HB2	1:A:488:MET:HG2	2.03	0.40
1:A:519:LYS:NZ	1:A:625:SER:O	2.46	0.40
1:A:979:LYS:O	1:A:980:ALA:C	2.58	0.40
2:B:653:ARG:HE	2:B:653:ARG:HB3	1.70	0.40
3:C:32:LEU:HA	3:C:32:LEU:HD12	1.83	0.40
1:A:1351:LEU:HD12	1:A:1351:LEU:HA	1.83	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HB3	2.04	0.40
2:B:463:LYS:CE	15:N:-84:DG:N2	2.71	0.40
18:W:229:VAL:HG21	18:W:286:LEU:HD11	2.03	0.40
1:A:285:SER:O	1:A:285:SER:OG	2.30	0.40
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.93	0.40
2:B:904:ARG:HG2	2:B:905:VAL:N	2.36	0.40
3:C:66:LEU:HD11	3:C:155:ILE:HD12	2.02	0.40
18:W:265:ARG:HD2	18:W:265:ARG:HA	1.71	0.40
1:A:195:ASP:N	1:A:195:ASP:OD1	2.53	0.40
1:A:970:GLN:HA	1:A:975:LEU:HB2	2.03	0.40
2:B:293:ILE:HG12	2:B:372:GLY:HA2	2.04	0.40
18:W:354:LEU:HD23	18:W:426:LEU:HD23	2.03	0.40
18:W:799:GLU:HB3	18:W:804:TRP:CZ3	2.56	0.40
1:A:841:ARG:NE	1:A:1387:ILE:O	2.44	0.40
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.54	0.40
1:A:197:GLN:OE1	16:M:50:LYS:HB3	2.21	0.40
14:T:55:DA:C2	15:N:-54:DC:C2	3.10	0.40
15:N:-85:DG:H4'	15:N:-84:DG:OP1	2.21	0.40
14:T:54:DG:C4	14:T:55:DA:C5	3.08	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	1400/1743 (80%)	1343 (96%)	47 (3%)	10 (1%)	24	67
2	B	1145/1227 (93%)	1082 (94%)	55 (5%)	8 (1%)	24	67
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	21	65
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	6	39
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	14	56
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	11	50
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	19	61
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	11	50
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	7	41
16	M	62/113 (55%)	58 (94%)	4 (6%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	21	65
19	a	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
19	e	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
20	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
20	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
21	c	101/133 (76%)	95 (94%)	6 (6%)	0	100	100
21	g	103/133 (77%)	97 (94%)	6 (6%)	0	100	100
22	d	93/129 (72%)	90 (97%)	3 (3%)	0	100	100
22	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	5045/6668 (76%)	4814 (95%)	198 (4%)	33 (1%)	28	67

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL
1	A	1109	VAL
2	B	155	LYS
2	B	239	SER
2	B	337	ARG
3	C	89	ASP
7	G	134	ASP
8	H	108	GLU
12	L	44	LYS
18	W	320	LEU
1	A	284	GLY
1	A	977	ARG
1	A	1223	SER
2	B	62	ALA
2	B	177	GLU
2	B	299	ASP
4	D	169	VAL
4	D	171	LEU
7	G	154	VAL
8	H	18	GLY
1	A	979	LYS
4	D	10	ALA
4	D	164	ALA
9	I	56	ALA
1	A	47	ARG
2	B	437	LEU
3	C	217	GLU
1	A	43	GLU
2	B	238	GLY
10	J	64	PRO
18	W	806	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1225/1528 (80%)	1218 (99%)	7 (1%)	87 93
2	B	1012/1077 (94%)	1001 (99%)	11 (1%)	76 88
3	C	236/264 (89%)	235 (100%)	1 (0%)	92 95
4	D	143/160 (89%)	140 (98%)	3 (2%)	56 78
5	E	196/197 (100%)	193 (98%)	3 (2%)	67 85
6	F	75/137 (55%)	75 (100%)	0	100 100
7	G	148/148 (100%)	148 (100%)	0	100 100
8	H	120/130 (92%)	120 (100%)	0	100 100
9	I	106/109 (97%)	105 (99%)	1 (1%)	81 90
10	J	60/66 (91%)	60 (100%)	0	100 100
11	K	104/109 (95%)	104 (100%)	0	100 100
12	L	38/56 (68%)	37 (97%)	1 (3%)	49 73
16	M	61/99 (62%)	61 (100%)	0	100 100
17	V	86/92 (94%)	85 (99%)	1 (1%)	74 87
18	W	241/796 (30%)	239 (99%)	2 (1%)	83 92
19	a	83/112 (74%)	82 (99%)	1 (1%)	74 87
19	e	82/112 (73%)	81 (99%)	1 (1%)	74 87
20	b	65/81 (80%)	64 (98%)	1 (2%)	67 85
20	f	63/81 (78%)	62 (98%)	1 (2%)	65 84
21	c	82/102 (80%)	82 (100%)	0	100 100
21	g	83/102 (81%)	82 (99%)	1 (1%)	74 87
22	d	81/107 (76%)	80 (99%)	1 (1%)	74 87
22	h	79/107 (74%)	77 (98%)	2 (2%)	50 74
All	All	4469/5772 (77%)	4431 (99%)	38 (1%)	82 90

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	248	ARG
1	A	473	LEU
1	A	661	ASN
1	A	737	ASN
1	A	977	ARG
1	A	1459	ASP

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Mol	Chain	Res	Type
2	B	69	ASP
2	B	70	ASN
2	B	71	ILE
2	B	233	SER
2	B	240	ARG
2	B	428	CYS
2	B	466	MET
2	B	500	LYS
2	B	653	ARG
2	B	904	ARG
2	B	1122	ARG
3	C	8	ASN
4	D	11	ARG
4	D	116	LYS
4	D	171	LEU
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
9	I	105	ASN
12	L	62	ARG
17	V	33	ASP
18	W	264	GLN
18	W	313	VAL
19	a	108	ASN
20	b	92	ARG
22	d	76	ARG
19	e	53	ARG
20	f	92	ARG
21	g	71	ARG
22	h	60	ASN
22	h	76	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	GLN
1	A	651	GLN
1	A	661	ASN
1	A	787	HIS
1	A	1190	GLN
1	A	1435	GLN

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Mol	Chain	Res	Type
2	B	887	HIS
2	B	996	HIS
3	C	8	ASN
3	C	13	GLN
3	C	242	GLN
5	E	4	ASN
5	E	145	HIS
5	E	193	GLN
8	H	13	GLN
9	I	12	ASN
9	I	90	GLN
9	I	105	ASN
16	M	65	GLN
18	W	330	ASN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
18	W	784	ASN
19	a	68	GLN
22	d	81	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	U
13	P	-3	G
13	P	-1	U
13	P	0	U
13	P	1	G
13	P	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.