



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:49 am GMT

PDB ID : 3JAM
EMDB ID: : EMD-3047
Title : CryoEM structure of 40S-eIF1A-eIF1 complex from yeast
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-17
Resolution : 3.46 Å(reported)
Based on PDB ID : 3J80

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

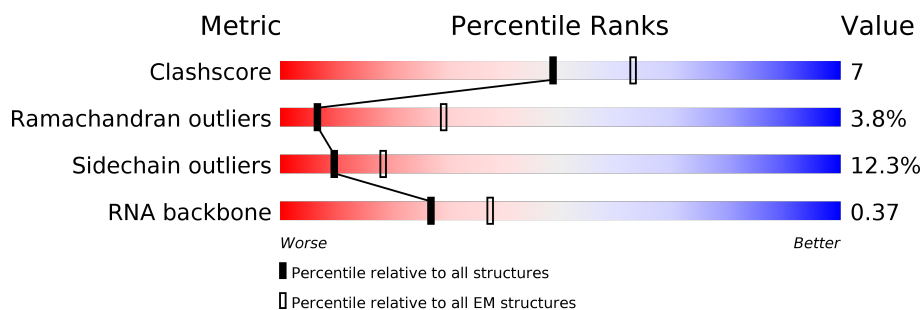
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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 3.46 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	1799	41% 44% 13% .
2	A	254	57% 20% 5% 18%
3	B	255	64% 20% . 13%
4	C	259	66% 15% . 16%
5	D	237	69% 21% . 6%
6	E	261	74% 22% .
7	F	227	69% 20% . 9%
8	G	236	75% 19% . .

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Mol	Chain	Length	Quality of chain
9	H	190	
10	I	201	
11	J	188	
12	K	106	
13	L	156	
14	M	134	
15	N	151	
16	O	137	
17	P	142	
18	Q	143	
19	R	136	
20	S	146	
21	T	144	
22	U	117	
23	V	87	
24	W	130	
25	X	145	
26	Y	135	
27	Z	108	
28	a	119	
29	b	82	
30	c	67	
31	d	56	
32	e	63	
33	f	150	

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Mol	Chain	Length	Quality of chain
34	g	326	<div><div></div><div>86%</div><div>11%</div><div>••</div></div>
35	h	25	<div><div></div><div>92%</div><div>8%</div></div>
36	i	153	<div><div></div><div>57%</div><div>6%</div><div>37%</div></div>
37	j	108	<div><div></div><div>69%</div><div>10%</div><div>20%</div></div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77850 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	223	Total	C	N	O	S	0	0
			1774	1120	325	326	3		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 8 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 9 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	184	Total	C	N	O		0	0
			1483	950	270	263			

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 11 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 14 is a protein called eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	122	Total	C	N	O	0	0
			922	575	167	180		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 18 is a protein called uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	125	Total	C	N	O	S	0	0
			991	619	182	187	3		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 24 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	98	Total	C	N	O	S	0	0
			779	480	165	129	5		

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 30 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 32 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	53	Total	C	N	O	S	0	0
			428	268	87	72	1		

- Molecule 33 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	96	Total	C	N	O	S	0	0
			778	482	144	147	5		

- Molecule 37 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	78	Total	Mg	0
			78	78	
38	J	1	Total	Mg	0
			1	1	
38	f	1	Total	Mg	0
			1	1	

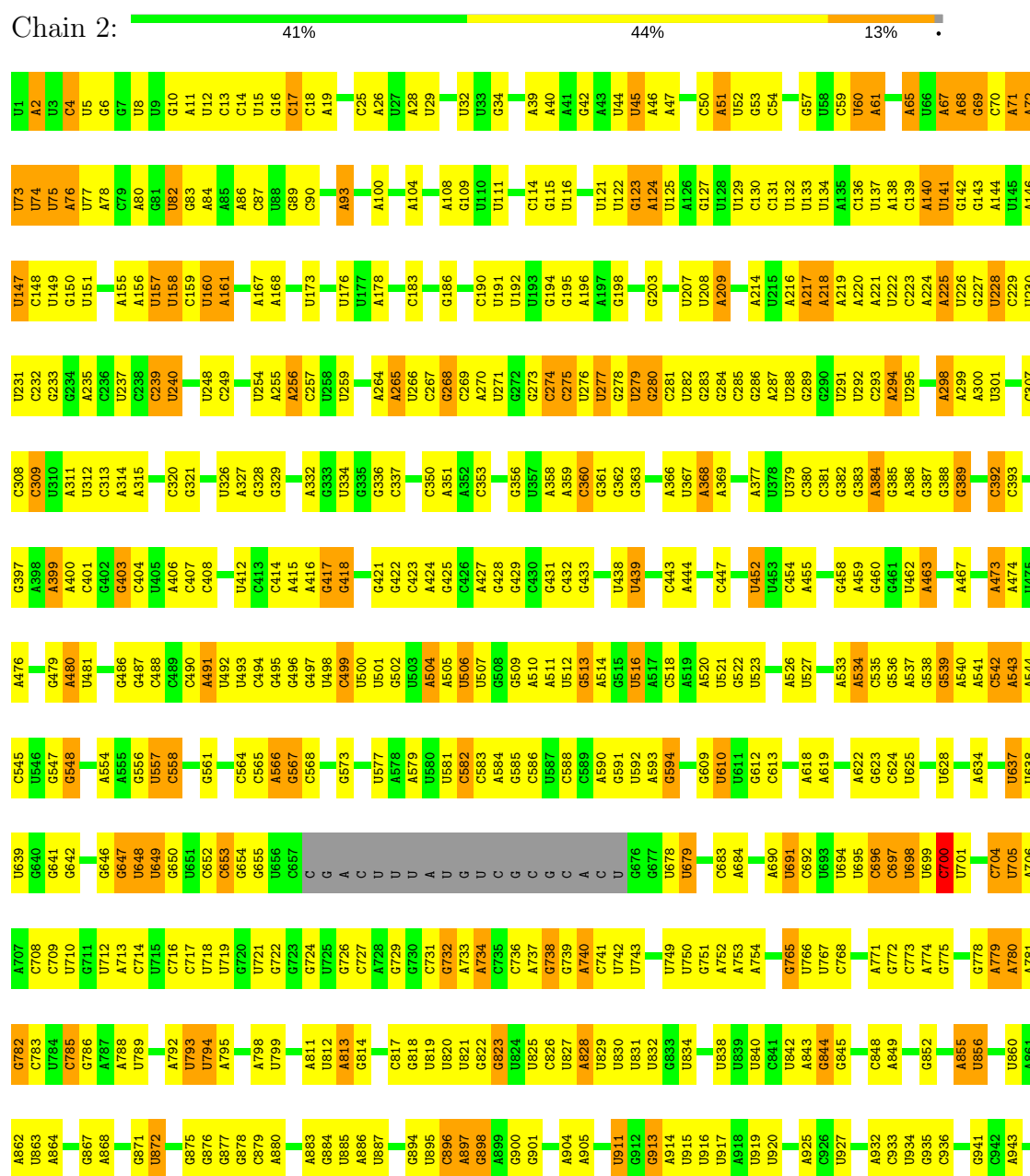
- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

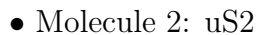
Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

3 Residue-property plots

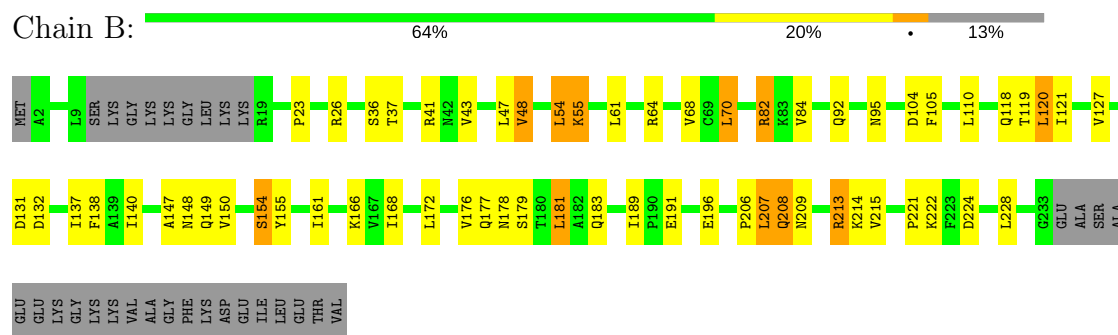
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 18S rRNA

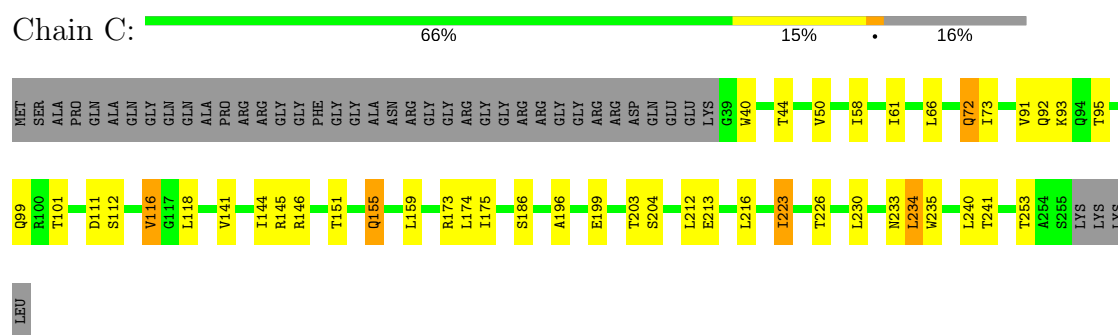




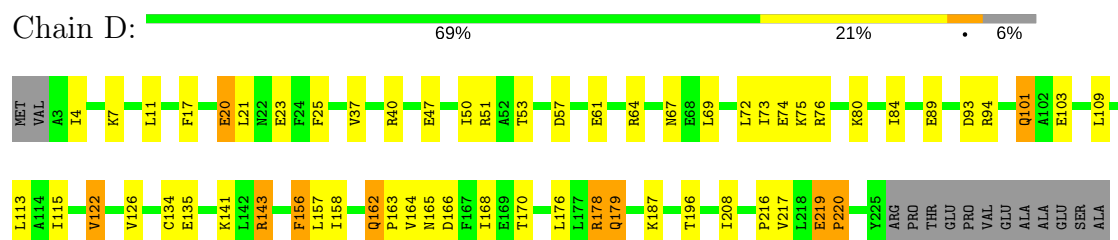
- Molecule 3: eS1



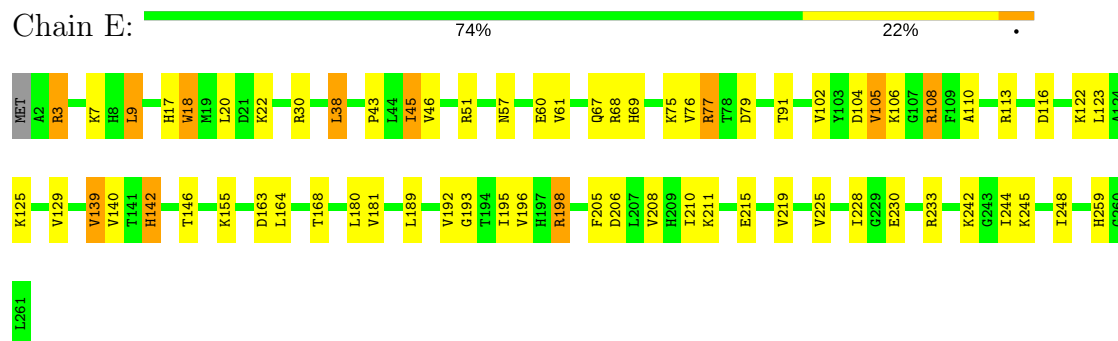
- Molecule 4: uS5



- Molecule 5: uS3

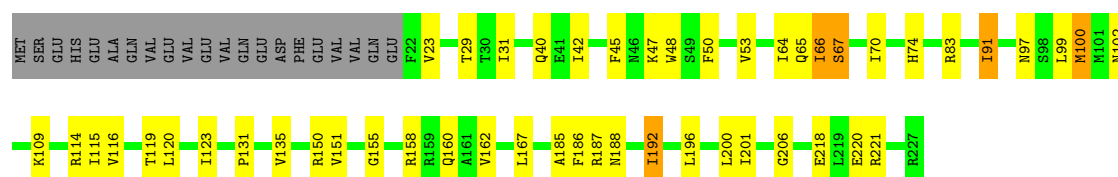


- Molecule 6: eS4



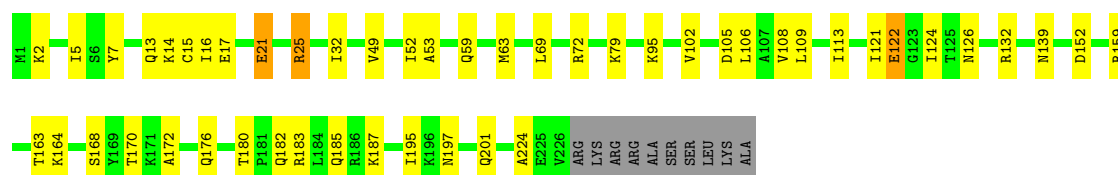
- Molecule 7: uS7





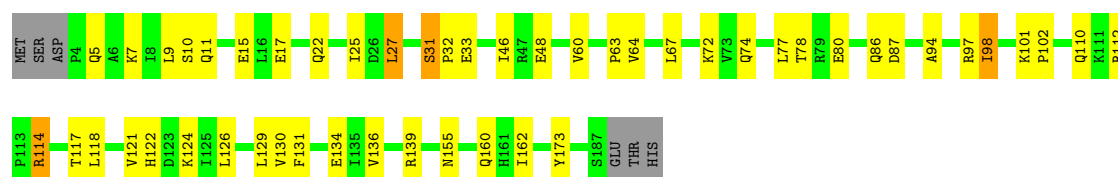
• Molecule 8: eS6

Chain G: 75% 19%



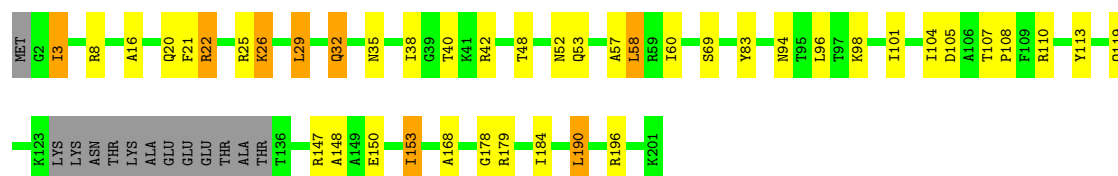
• Molecule 9: eS7

Chain H: 71% 24%



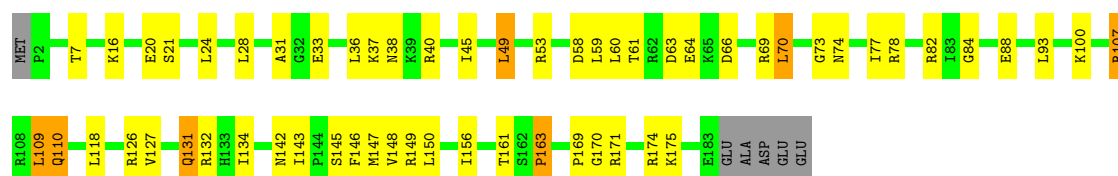
• Molecule 10: eS8

Chain I: 72% 17% 6%



• Molecule 11: uS4

Chain J: 66% 27%




• Molecule 12: eS10

Chain K: 59% 27% 9%



PRO
GLN
GLY
LYS
TYR

• Molecule 13: uS17

Chain L:  83% 15% ...


MET S2 T3 Q8 S9 E10 Q14 T21 K32 K36 K37 V38 I54 D55 I66 I78 R79 M80 R81 R82 T83 I84 R99 K105 V111 I122 V125 R129 R136 F137 M138 V139 L140 A143 F156

• Molecule 14: eS12

Chain M:  67% 18% 6% 9%

MET SER ASP VAL GLU VAL GLN VAL PRO VAL A13 E14 I17 I18 D19 A20 L21 K22 L25 L29 D32 L38 R39 A44 L45 G50 L55 V59 T60 E61 L67 L71 V77 L79 T80 K81 R82 A92 G93 I97 D98 R104 K105 S110 N116 Q134

• Molecule 15: uS15

Chain N:  81% 18% .

MET G2 R3 K9 K27 E35 T38 K39 Y40 A41 R42 I50 L53 L54 R55 V60 K64 R73 L88 V96 R99 K100 H101 L102 F103 R104 R105 R106 K107 K112 F113 R114 I118 R121 N138 N151

• Molecule 16: uS11

Chain O:  73% 18% . 7%

MET ALA ASN VAL GLN ALA LYS ASP ASN S11 R18 R24 D25 H29 E37 A40 R41 V42 K49 S55 A64 Q65 I81 T86 G87 S91 Q99 L102 R103 A104 L110 R111 I112 G113 R114 I115 E116 P120 V121 P122 S123 D124 L137

• Molecule 17: uS19

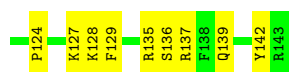
Chain P:  61% 23% . 13%

MET SER GLU ALA ALA PRO R6 K9 Y17 K18 G19 V20 D21 L22 E23 K24 L25 R28 P29 T30 F33 V34 K35 R40 R47 Q48 P53 M57 A62 L65 E69 H79 L80 R81 I84 G89 K100 V101 P109 V112 I121 T122 Y123 T124 P125 V126 R127 H128 G129 R130 ALA GLY THR SER ARG PHE ILE PRO LEU ARG

• Molecule 18: uS9

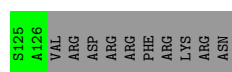
Chain Q:  68% 26% . 5%

MET SER T3 S6 V7 K14 A18 V19 V22 L28 I29 L38 V39 Q40 I43 L44 R45 V48 P51 L52 L53 L54 V55 G56 F60 D64 V69 Q77 V78 I81 Q94 V97 K102 L105 F109 Y112 D113 R114 S121



• Molecule 19: eS17

Chain R: 66% 19% 8%



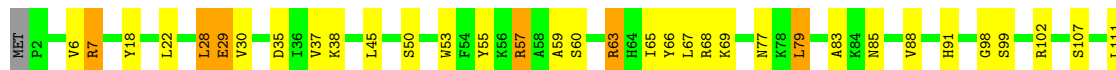
• Molecule 20: uS13

Chain S: 66% 29% 5%



• Molecule 21: eS19

Chain T: 73% 22% 5%



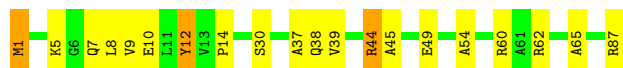
• Molecule 22: uS10

Chain U: 70% 19% 9%



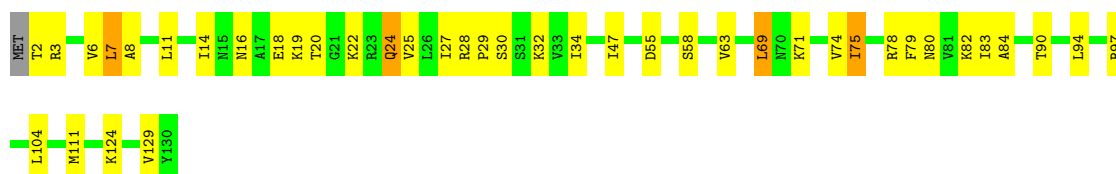
• Molecule 23: eS21

Chain V: 77% 20% 3%



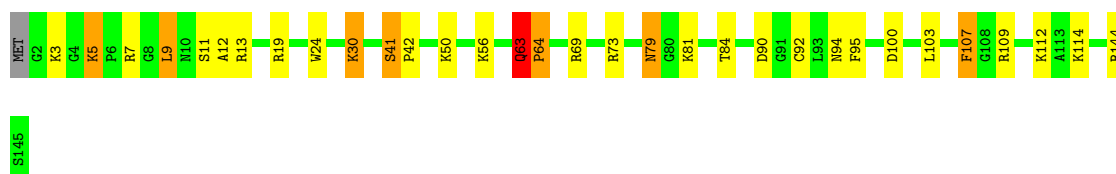
• Molecule 24: uS8

Chain W: 68% 28% 4%



• Molecule 25: uS12

Chain X: 77% 17% 5% ..



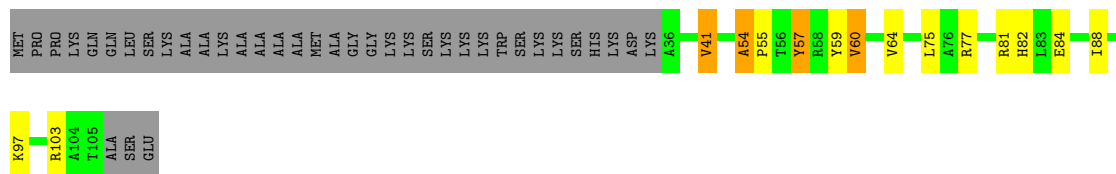
• Molecule 26: eS24

Chain Y: 76% 20% . .



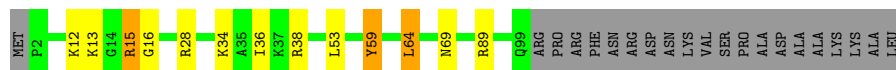
• Molecule 27: eS25

Chain Z: 51% 10% . 35%



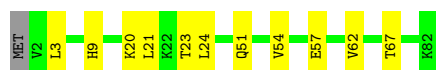
• Molecule 28: eS26

Chain a: 71% 8% . 18%



• Molecule 29: eS27

Chain b: 85% 13% .



• Molecule 30: eS28

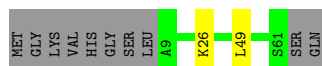
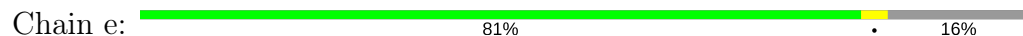
Chain c: 84% 10% 6%



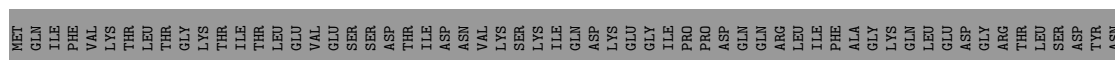
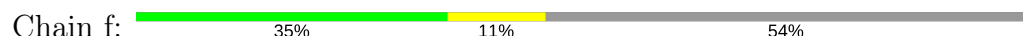
- Molecule 31: uS14



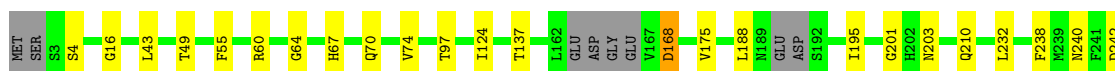
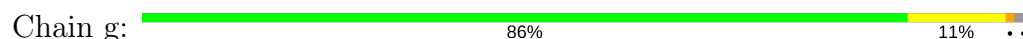
- Molecule 32: eS30



- Molecule 33: eS31



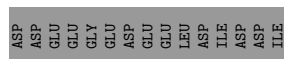
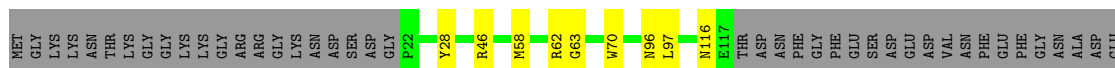
- Molecule 34: RACK1



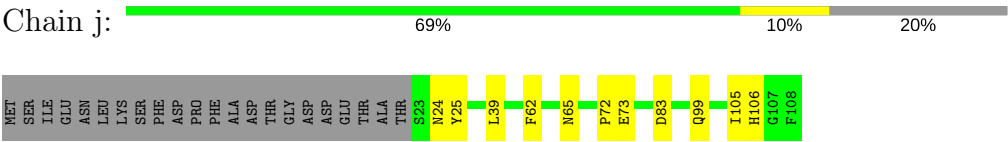
- Molecule 35: eL41



- Molecule 36: eIF1A



● Molecule 37: eIF1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	86055	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (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	2	0.27	0/42269	0.69	8/65862 (0.0%)
10	I	0.42	0/1515	0.74	2/2029 (0.1%)
11	J	0.43	0/1495	0.82	1/2001 (0.0%)
12	K	0.49	0/831	0.74	0/1123
13	L	0.41	0/1276	0.64	0/1718
14	M	0.46	0/929	0.77	0/1255
15	N	0.44	0/1210	0.77	0/1628
16	O	0.41	0/953	0.73	0/1279
17	P	0.46	0/1000	0.72	0/1343
18	Q	0.44	0/1125	0.74	1/1510 (0.1%)
19	R	0.43	0/1002	0.82	2/1346 (0.1%)
2	A	0.44	0/1666	0.78	1/2279 (0.0%)
20	S	0.42	0/1212	0.75	1/1629 (0.1%)
21	T	0.45	0/1129	0.79	1/1520 (0.1%)
22	U	0.40	0/857	0.69	0/1158
23	V	0.40	0/696	0.72	0/938
24	W	0.39	0/1039	0.77	2/1399 (0.1%)
25	X	0.41	0/1137	0.74	0/1516
26	Y	0.41	0/1075	0.72	0/1433
27	Z	0.48	0/567	0.70	0/762
28	a	0.38	0/791	0.69	0/1059
29	b	0.39	0/619	0.65	0/837
3	B	0.41	0/1798	0.73	2/2421 (0.1%)
30	c	0.42	0/496	0.73	0/666
31	d	0.44	0/457	0.67	0/607
32	e	0.40	0/435	0.72	0/579
33	f	0.50	0/562	0.70	0/751
34	g	0.44	0/2521	0.63	0/3431
35	h	0.43	0/234	0.88	0/300
36	i	0.40	0/788	0.67	0/1051
37	j	0.43	0/703	0.69	0/938
4	C	0.42	0/1659	0.71	0/2252

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	D	0.44	0/1769	0.72	0/2378
6	E	0.39	0/2122	0.70	1/2861 (0.0%)
7	F	0.44	0/1628	0.78	0/2198
8	G	0.41	0/1835	0.71	0/2451
9	H	0.44	0/1507	0.76	2/2028 (0.1%)
All	All	0.36	0/82907	0.71	24/120536 (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
12	K	0	1
17	P	0	1
18	Q	0	1
25	X	0	1
26	Y	0	1
All	All	0	5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1315	G	C2'-C3'-O3'	7.09	125.10	109.50
20	S	105	LEU	CA-CB-CG	7.01	131.42	115.30
10	I	29	LEU	CA-CB-CG	6.92	131.22	115.30
3	B	181	LEU	CA-CB-CG	6.79	130.92	115.30
1	2	1534	G	C2'-C3'-O3'	6.15	123.53	113.70
9	H	118	LEU	CA-CB-CG	6.12	129.37	115.30
10	I	190	LEU	CA-CB-CG	6.10	129.34	115.30
1	2	1491	A	C2'-C3'-O3'	5.79	122.96	113.70
21	T	79	LEU	CA-CB-CG	5.71	128.44	115.30
2	A	201	LEU	CA-CB-CG	5.59	128.15	115.30
6	E	38	LEU	CA-CB-CG	5.58	128.14	115.30
19	R	100	LEU	CA-CB-CG	5.57	128.11	115.30
19	R	16	LEU	CA-CB-CG	5.55	128.07	115.30
1	2	828	A	C2'-C3'-O3'	5.52	122.53	113.70
11	J	150	LEU	CA-CB-CG	5.44	127.80	115.30
1	2	1501	A	C2'-C3'-O3'	5.38	122.31	113.70
24	W	69	LEU	CA-CB-CG	5.34	127.59	115.30
9	H	77	LEU	CA-CB-CG	5.30	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1320	A	N9-C1'-C2'	5.22	120.78	114.00
1	2	277	U	C2'-C3'-O3'	5.16	121.96	113.70
3	B	120	LEU	CA-CB-CG	5.12	127.08	115.30
1	2	700	C	C2'-C3'-O3'	5.11	121.88	113.70
18	Q	52	LEU	CA-CB-CG	5.08	126.98	115.30
24	W	7	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	K	87	PHE	Peptide
17	P	28	MET	Peptide
18	Q	40	GLN	Peptide
25	X	63	GLN	Peptide
26	Y	29	HIS	Peptide

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	2	37797	0	19016	570	0
2	A	1626	0	1633	28	0
3	B	1774	0	1834	18	0
4	C	1629	0	1710	20	0
5	D	1744	0	1826	18	0
6	E	2078	0	2157	20	0
7	F	1609	0	1679	22	0
8	G	1812	0	1911	21	0
9	H	1483	0	1579	16	0
10	I	1489	0	1504	17	0
11	J	1471	0	1554	22	0
12	K	809	0	810	12	0
13	L	1248	0	1311	15	0
14	M	922	0	953	9	0
15	N	1187	0	1251	6	0
16	O	942	0	979	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	980	0	1026	15	0
18	Q	1105	0	1170	23	0
19	R	991	0	1039	15	0
20	S	1193	0	1217	20	0
21	T	1110	0	1124	18	0
22	U	845	0	913	9	0
23	V	687	0	682	12	0
24	W	1021	0	1056	19	0
25	X	1119	0	1198	14	0
26	Y	1061	0	1111	11	0
27	Z	558	0	585	6	0
28	a	779	0	828	0	0
29	b	609	0	631	0	0
30	c	494	0	534	0	0
31	d	446	0	436	0	0
32	e	428	0	468	0	0
33	f	549	0	564	0	0
34	g	2466	0	2406	0	0
35	h	233	0	284	0	0
36	i	778	0	779	0	0
37	j	695	0	729	0	0
38	2	78	0	0	0	0
38	J	1	0	0	0	0
38	f	1	0	0	0	0
39	a	1	0	0	0	0
39	b	1	0	0	0	0
39	f	1	0	0	0	0
All	All	77850	0	60487	893	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 7.

All (893) 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)
1:2:51:A:N6	1:2:439:U:H3	1.05	1.41
1:2:1593:U:H3	1:2:1598:A:N6	1.13	1.40
1:2:480:A:N1	1:2:506:U:O4	1.62	1.33
1:2:628:U:N3	1:2:969:A:N6	1.77	1.32
1:2:1079:U:O4	1:2:1090:A:N1	1.66	1.25
1:2:480:A:N1	1:2:506:U:C4	2.13	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:864:A:N1	1:2:964:U:O4	1.83	1.11
1:2:1292:U:C4	1:2:1321:A:N1	2.22	1.08
1:2:51:A:N1	1:2:439:U:O4	1.87	1.08
1:2:1292:U:O4	1:2:1321:A:N1	1.86	1.07
1:2:299:A:H2'	1:2:300:A:C8	1.91	1.06
1:2:1037:U:H3	1:2:1091:A:N6	1.54	1.05
1:2:1593:U:O4	1:2:1598:A:N1	1.90	1.04
1:2:864:A:N1	1:2:964:U:C4	2.28	1.01
1:2:628:U:N3	1:2:969:A:C6	2.26	1.01
1:2:628:U:C2	1:2:969:A:N6	2.28	1.00
1:2:480:A:C2	1:2:506:U:O4	2.16	0.98
1:2:1037:U:O4	1:2:1091:A:N1	1.98	0.97
1:2:51:A:N6	1:2:439:U:N3	1.83	0.95
1:2:989:C:H5	1:2:1013:G:H1	1.08	0.95
1:2:1590:A:H2'	1:2:1591:A:C8	2.02	0.94
1:2:548:G:H1	1:2:588:C:H5	1.15	0.94
1:2:1238:U:H1'	1:2:1247:C:H42	1.32	0.94
1:2:1037:U:H3	1:2:1091:A:H61	0.98	0.93
1:2:239:C:H4'	1:2:240:U:OP2	1.69	0.92
1:2:628:U:C4	1:2:969:A:N6	2.37	0.91
1:2:8:U:N3	1:2:1138:A:N6	2.18	0.91
1:2:1079:U:H3	1:2:1090:A:N6	1.70	0.90
24:W:8:ALA:HA	24:W:74:VAL:HG21	1.54	0.89
24:W:6:VAL:HG12	24:W:34:ILE:HD11	1.57	0.87
1:2:894:G:H1	1:2:916:U:H3	1.22	0.86
1:2:1540:G:H22	1:2:1566:C:H2'	1.39	0.86
1:2:1290:G:N2	1:2:1323:G:H22	1.73	0.86
1:2:1601:U:H2'	1:2:1602:U:C6	2.12	0.84
2:A:62:ARG:HH11	2:A:62:ARG:HG2	1.44	0.82
1:2:1292:U:C4	1:2:1321:A:C2	2.67	0.82
1:2:1450:U:H2'	1:2:1451:G:C8	2.16	0.81
1:2:480:A:C6	1:2:506:U:O4	2.34	0.81
1:2:991:A:N6	1:2:1011:U:H3	1.76	0.81
1:2:1170:A:H2'	1:2:1171:G:C8	2.17	0.80
1:2:867:G:H1	1:2:959:U:H3	1.29	0.80
1:2:1292:U:O4	1:2:1321:A:C6	2.35	0.79
1:2:1450:U:H2'	1:2:1451:G:H8	1.48	0.78
1:2:864:A:C2	1:2:964:U:C4	2.71	0.78
1:2:1593:U:N3	1:2:1598:A:N6	1.90	0.78
1:2:1137:A:H2'	1:2:1138:A:C8	2.19	0.77
1:2:168:A:H5'	8:G:176:GLN:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1319:U:O2'	1:2:1321:A:OP1	2.04	0.76
1:2:157:U:H4'	1:2:158:U:OP1	1.85	0.76
2:A:70:PRO:HB3	2:A:94:GLY:HA3	1.66	0.74
1:2:291:U:H2'	1:2:292:U:C6	2.23	0.74
1:2:1079:U:N3	1:2:1090:A:N6	2.33	0.74
1:2:1173:C:N3	1:2:1464:G:C2	2.56	0.74
1:2:793:U:H3'	1:2:794:U:C5'	2.18	0.73
2:A:124:THR:HG22	2:A:174:TRP:HE1	1.52	0.73
11:J:109:LEU:HB2	11:J:146:PHE:HB3	1.69	0.73
1:2:749:U:H2'	1:2:750:U:C6	2.23	0.73
1:2:1033:C:HO2'	24:W:2:THR:N	1.87	0.73
1:2:1378:U:H2'	1:2:1379:U:C6	2.23	0.73
26:Y:129:ALA:O	26:Y:133:ASN:HB2	1.89	0.73
1:2:864:A:C6	1:2:964:U:O4	2.40	0.73
4:C:144:ILE:HD13	4:C:196:ALA:HB1	1.70	0.72
1:2:1079:U:C4	1:2:1090:A:N1	2.57	0.72
1:2:150:G:H21	8:G:13:GLN:HE22	1.37	0.72
1:2:255:A:H2'	1:2:256:A:O4'	1.90	0.72
1:2:590:A:H2'	1:2:591:G:C8	2.25	0.71
1:2:298:A:H2'	1:2:299:A:H5'	1.71	0.70
1:2:991:A:H61	1:2:1011:U:H3	1.34	0.70
1:2:65:A:H2	1:2:84:A:H62	1.39	0.70
1:2:1670:G:H2'	1:2:1671:G:H8	1.56	0.70
7:F:48:TRP:HZ2	7:F:120:LEU:HB3	1.57	0.70
1:2:1670:G:H2'	1:2:1671:G:C8	2.26	0.70
1:2:121:U:H2'	1:2:122:U:C6	2.27	0.70
5:D:25:PHE:HE2	5:D:50:ILE:HG12	1.57	0.70
26:Y:41:ARG:HG2	26:Y:57:VAL:HG23	1.74	0.69
1:2:140:A:H2	1:2:265:A:H4'	1.57	0.69
21:T:7:ARG:HH11	21:T:7:ARG:HG2	1.57	0.69
1:2:1143:U:H2'	1:2:1144:U:C6	2.27	0.69
2:A:50:VAL:HA	2:A:53:THR:HG23	1.73	0.69
1:2:1477:A:OP1	21:T:57:ARG:HG2	1.91	0.69
1:2:793:U:H3'	1:2:794:U:H5''	1.75	0.69
1:2:1292:U:O4	1:2:1321:A:C2	2.46	0.69
1:2:1343:A:H2'	1:2:1344:A:C8	2.27	0.69
19:R:34:LEU:O	19:R:38:ILE:HG12	1.93	0.67
1:2:1290:G:N2	1:2:1323:G:N2	2.42	0.67
1:2:1455:C:O2'	1:2:1456:G:H5'	1.95	0.67
11:J:49:LEU:HD13	11:J:53:ARG:HH12	1.58	0.67
11:J:77:ILE:HD11	11:J:93:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:71:A:H3'	1:2:72:A:H5''	1.76	0.67
1:2:984:G:H1	1:2:1015:C:H5	1.43	0.67
1:2:8:U:C4	1:2:1138:A:N6	2.63	0.66
1:2:51:A:N1	1:2:439:U:C4	2.64	0.66
16:O:81:ILE:HB	16:O:115:ILE:HG22	1.77	0.66
1:2:991:A:N6	1:2:1011:U:N3	2.37	0.66
1:2:1289:U:H2'	1:2:1290:G:C8	2.30	0.66
24:W:11:LEU:HD12	24:W:74:VAL:HG22	1.77	0.66
1:2:1316:C:H2'	1:2:1317:G:O4'	1.94	0.66
1:2:1778:G:O2'	1:2:1779:A:C8	2.48	0.66
1:2:1292:U:C5	1:2:1321:A:C2	2.84	0.66
1:2:1290:G:H22	1:2:1323:G:H22	1.45	0.65
1:2:1290:G:H22	1:2:1323:G:N2	1.95	0.65
1:2:45:U:O2'	1:2:46:A:H2'	1.97	0.65
1:2:868:A:H61	1:2:957:U:H5	1.42	0.65
1:2:1679:A:H2	1:2:1718:G:H21	1.44	0.65
1:2:1570:G:N3	1:2:1570:G:H5''	2.12	0.65
1:2:61:A:H8	1:2:268:G:HO2'	1.41	0.65
1:2:979:G:H4'	1:2:1774:A:H4'	1.78	0.65
1:2:61:A:H8	1:2:268:G:O2'	1.78	0.64
1:2:512:U:H2'	1:2:513:G:C8	2.33	0.64
1:2:1174:U:H2'	1:2:1175:G:H8	1.62	0.64
7:F:115:ILE:O	7:F:119:THR:HG23	1.97	0.64
18:Q:55:VAL:HG21	18:Q:105:LEU:HG	1.80	0.64
9:H:98:ILE:HD11	9:H:121:VAL:HG11	1.79	0.64
1:2:1320:A:H4'	1:2:1321:A:OP1	1.98	0.64
1:2:537:A:C8	1:2:542:C:N4	2.66	0.63
1:2:700:C:H42	1:2:738:G:H1	1.45	0.63
21:T:60:SER:O	21:T:63:ARG:HG3	1.99	0.63
7:F:123:ILE:HB	7:F:131:PRO:HB3	1.80	0.63
1:2:1363:G:N2	1:2:1364:C:C2	2.66	0.63
7:F:115:ILE:HG12	7:F:192:ILE:HD13	1.81	0.63
20:S:57:ARG:HH22	27:Z:75:LEU:HD11	1.62	0.63
1:2:8:U:H3	1:2:1138:A:N6	1.95	0.63
1:2:991:A:H5'	1:2:991:A:N3	2.14	0.62
1:2:1417:G:C6	1:2:1418:C:N3	2.67	0.62
1:2:1279:C:H2'	1:2:1280:G:H8	1.64	0.62
1:2:221:A:H61	1:2:838:U:H3	1.48	0.62
17:P:30:THR:O	17:P:34:VAL:HG23	1.99	0.62
24:W:8:ALA:HA	24:W:74:VAL:CG2	2.27	0.62
1:2:68:A:H2	8:G:132:ARG:NH2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1583:U:H3	1:2:1609:A:H2	1.47	0.62
1:2:17:C:O2'	1:2:1136:A:N1	2.28	0.62
1:2:1462:G:N1	1:2:1463:C:C4	2.68	0.62
5:D:219:GLU:HG2	5:D:220:PRO:HD2	1.80	0.62
18:Q:77:GLN:O	18:Q:81:ILE:HG13	2.00	0.62
1:2:1452:G:H4'	17:P:122:THR:HG21	1.82	0.61
1:2:539:G:N2	1:2:541:A:N7	2.46	0.61
3:B:54:LEU:O	3:B:55:LYS:HB2	2.00	0.61
13:L:54:ILE:HG23	13:L:55:ASP:H	1.66	0.61
20:S:37:GLY:HA2	20:S:105:LEU:HD21	1.82	0.61
24:W:90:THR:HG23	24:W:94:LEU:HD12	1.82	0.61
3:B:176:VAL:HG12	3:B:177:GLN:H	1.66	0.61
1:2:1462:G:N2	1:2:1463:C:C2	2.69	0.61
13:L:66:ILE:HG13	13:L:140:LEU:HD21	1.83	0.61
1:2:1349:G:N1	1:2:1374:C:C2	2.69	0.61
1:2:1240:G:H1'	17:P:79:HIS:HB2	1.82	0.60
1:2:1217:G:H5''	1:2:1442:A:N6	2.16	0.60
1:2:61:A:C8	1:2:268:G:O2'	2.52	0.60
1:2:516:U:H3	1:2:534:A:H61	1.48	0.60
9:H:31:SER:HB2	9:H:32:PRO:HD3	1.84	0.60
6:E:9:LEU:HB2	6:E:30:ARG:HB2	1.83	0.60
10:I:57:ALA:HB2	10:I:178:GLY:HA2	1.83	0.60
1:2:512:U:H4'	11:J:131:GLN:HG3	1.84	0.60
4:C:116:VAL:HG22	4:C:144:ILE:HD11	1.83	0.60
1:2:1277:G:C6	1:2:1278:C:N3	2.70	0.59
11:J:38:ASN:HB3	11:J:40:ARG:H	1.65	0.59
1:2:1079:U:O4	1:2:1090:A:C2	2.52	0.59
7:F:66:ILE:HD12	7:F:67:SER:H	1.67	0.59
7:F:114:ARG:HH22	18:Q:43:ILE:HB	1.68	0.59
5:D:69:LEU:HA	5:D:72:LEU:HD12	1.85	0.59
1:2:124:A:H2'	1:2:125:U:O4'	2.03	0.59
1:2:732:G:H1'	1:2:734:A:N6	2.18	0.58
4:C:233:ASN:HB2	23:V:1:MET:HG3	1.84	0.58
25:X:79:ASN:HD22	25:X:81:LYS:H	1.52	0.58
1:2:1349:G:C6	1:2:1374:C:N3	2.72	0.58
1:2:406:A:H2'	1:2:407:C:C6	2.39	0.58
1:2:911:U:C2	1:2:913:G:N2	2.72	0.58
1:2:1349:G:C2	1:2:1374:C:O2	2.56	0.58
1:2:1085:A:H2'	1:2:1086:A:C8	2.38	0.58
4:C:50:VAL:HG21	4:C:73:ILE:HG23	1.85	0.58
1:2:1562:U:H2'	1:2:1563:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1265:U:H2'	1:2:1266:G:C8	2.39	0.58
1:2:1602:U:H5'	18:Q:129:PHE:HB3	1.86	0.58
1:2:1177:G:H3'	1:2:1178:G:H8	1.68	0.57
1:2:1598:A:H2'	1:2:1598:A:N3	2.19	0.57
10:I:107:THR:N	10:I:108:PRO:HD2	2.18	0.57
1:2:1581:A:H5''	18:Q:135:ARG:HH21	1.69	0.57
21:T:22:LEU:HB3	21:T:55:TYR:HD2	1.68	0.57
1:2:1754:A:H5'	1:2:1754:A:H8	1.69	0.57
1:2:299:A:H2'	1:2:300:A:H8	1.63	0.57
5:D:40:ARG:HB2	5:D:47:GLU:HB2	1.85	0.57
1:2:1061:A:H2'	1:2:1062:U:O4'	2.04	0.57
1:2:1584:A:H5''	18:Q:136:SER:HB3	1.87	0.57
1:2:704:C:H4'	1:2:705:U:OP1	2.04	0.57
8:G:7:TYR:HD1	8:G:113:ILE:HG23	1.68	0.57
9:H:46:ILE:HG12	9:H:60:VAL:HG12	1.86	0.57
1:2:1442:A:H4'	1:2:1443:G:H5'	1.85	0.57
5:D:170:THR:HG22	5:D:187:LYS:HG2	1.86	0.57
9:H:101:LYS:HA	9:H:112:ARG:NH2	2.18	0.57
1:2:1387:C:O2'	19:R:52:GLY:HA3	2.04	0.57
1:2:1781:C:H2'	1:2:1782:C:C6	2.39	0.57
1:2:813:A:N1	1:2:856:U:O4	2.38	0.56
7:F:120:LEU:HD23	7:F:131:PRO:HB2	1.86	0.56
14:M:98:ASP:HB2	14:M:104:ARG:HG3	1.86	0.56
1:2:1584:A:H1'	1:2:1609:A:N6	2.20	0.56
1:2:363:G:N2	1:2:380:C:C2	2.72	0.56
2:A:205:ARG:HH22	19:R:84:TYR:HB3	1.71	0.56
5:D:162:GLN:N	5:D:163:PRO:HD2	2.21	0.56
1:2:1593:U:C4	1:2:1598:A:N1	2.71	0.56
15:N:114:ARG:HH11	15:N:114:ARG:HG2	1.70	0.56
1:2:1237:A:N6	1:2:1247:C:H41	2.04	0.56
1:2:1267:G:H1	1:2:1439:C:H42	1.51	0.56
1:2:1653:A:N6	1:2:1743:G:H1'	2.21	0.56
1:2:10:G:C6	1:2:1631:A:C2	2.94	0.56
1:2:207:U:H2'	1:2:208:U:C6	2.40	0.56
1:2:5:U:H2'	1:2:6:G:H8	1.71	0.56
1:2:813:A:N6	1:2:856:U:N3	2.52	0.56
1:2:925:A:H8	1:2:925:A:H5''	1.71	0.56
4:C:144:ILE:HG12	4:C:223:ILE:HG23	1.87	0.56
1:2:140:A:H61	8:G:187:LYS:HB2	1.71	0.56
8:G:32:ILE:HG23	8:G:53:ALA:HA	1.88	0.56
1:2:1531:C:H2'	1:2:1532:G:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:353:C:H5''	10:I:16:ALA:HB2	1.87	0.55
19:R:28:PHE:HA	19:R:55:THR:HG21	1.88	0.55
1:2:1778:G:O2'	1:2:1779:A:H8	1.86	0.55
23:V:5:LYS:HB2	23:V:7:GLN:HE21	1.70	0.55
1:2:1619:U:H2'	1:2:1620:G:C8	2.42	0.55
1:2:798:A:C2	1:2:799:U:C2	2.94	0.55
18:Q:78:VAL:HA	18:Q:81:ILE:HD12	1.87	0.55
1:2:1671:G:C2	1:2:1672:C:C2	2.95	0.55
1:2:1710:A:H2'	1:2:1711:G:H4'	1.87	0.55
27:Z:59:TYR:HB3	27:Z:64:VAL:HG11	1.87	0.55
14:M:21:LEU:HD21	14:M:80:ILE:HG21	1.89	0.55
1:2:69:G:H1	1:2:82:U:H3	1.54	0.55
22:U:57:ARG:HG2	22:U:89:ARG:HD2	1.88	0.55
1:2:1086:A:H2'	1:2:1087:A:C8	2.41	0.55
1:2:1559:U:H2'	1:2:1560:G:H8	1.71	0.55
19:R:93:LEU:HD12	19:R:100:LEU:HB3	1.89	0.54
11:J:132:ARG:HH22	26:Y:65:GLY:HA2	1.72	0.54
1:2:216:A:H2'	1:2:217:A:C8	2.42	0.54
15:N:114:ARG:O	15:N:118:ILE:HG12	2.07	0.54
24:W:18:GLU:HG2	24:W:69:LEU:O	2.06	0.54
1:2:1772:G:H2'	1:2:1773:U:O4'	2.07	0.54
1:2:864:A:C2	1:2:964:U:O4	2.55	0.54
4:C:66:LEU:HD22	7:F:160:GLN:HG2	73.64	0.54
1:2:1173:C:C2	1:2:1464:G:N2	2.75	0.54
1:2:240:U:C6	1:2:240:U:H5''	2.42	0.54
1:2:561:G:C2	1:2:583:C:C2	2.95	0.54
1:2:1037:U:C4	1:2:1091:A:N1	2.74	0.54
1:2:1654:U:H3	1:2:1742:A:H61	1.55	0.54
1:2:360:C:C2	1:2:383:G:N2	2.76	0.54
1:2:428:G:H1'	1:2:439:U:O2	2.08	0.54
4:C:61:ILE:HA	4:C:66:LEU:HD12	1.88	0.54
1:2:1333:U:H2'	1:2:1334:U:O4'	2.07	0.54
1:2:1771:C:H2'	1:2:1772:G:C8	2.42	0.54
4:C:234:LEU:HD11	23:V:14:PRO:HD2	1.89	0.54
6:E:211:LYS:HD3	6:E:215:GLU:HG2	1.90	0.54
1:2:1137:A:H2'	1:2:1138:A:N7	2.22	0.54
1:2:123:G:H3'	1:2:124:A:H5''	1.90	0.54
1:2:363:G:C2	1:2:380:C:C2	2.96	0.54
11:J:82:ARG:HH21	11:J:149:ARG:HD3	1.71	0.54
1:2:1279:C:H2'	1:2:1280:G:C8	2.41	0.54
1:2:1343:A:H4'	1:2:1344:A:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:126:LEU:HG	9:H:173:TYR:CE1	2.43	0.54
1:2:542:C:O2	1:2:542:C:O4'	2.24	0.54
1:2:1085:A:C2	1:2:1086:A:C2	2.95	0.54
1:2:628:U:C4	1:2:969:A:C6	2.93	0.53
4:C:240:LEU:HD21	23:V:54:ALA:HB2	1.89	0.53
1:2:1096:U:H1'	4:C:173:ARG:HD2	1.89	0.53
1:2:989:C:H5	1:2:1013:G:N1	1.91	0.53
1:2:283:G:O6	8:G:185:GLN:HG3	2.08	0.53
14:M:22:LYS:HA	14:M:25:LEU:HD12	1.91	0.53
21:T:65:ILE:HG22	21:T:124:ILE:HG13	1.88	0.53
1:2:273:G:C6	1:2:274:C:N4	2.77	0.53
6:E:193:GLY:HA3	6:E:210:ILE:CG2	2.37	0.53
1:2:328:G:H5''	10:I:98:LYS:HB3	1.90	0.53
12:K:8:ARG:O	12:K:12:TYR:HD1	1.92	0.53
1:2:1185:U:O4	1:2:1199:G:N2	2.39	0.53
1:2:294:A:H2'	1:2:295:U:O4'	2.08	0.53
1:2:647:G:N3	1:2:647:G:H2'	2.23	0.53
1:2:1239:U:H2'	1:2:1240:G:H5''	1.90	0.53
1:2:698:U:H2'	1:2:699:U:C6	2.44	0.53
1:2:1474:C:H2'	1:2:1475:G:H8	1.74	0.53
1:2:1589:C:H2'	1:2:1590:A:H8	1.72	0.53
1:2:1770:C:H5''	1:2:1770:C:C6	2.44	0.53
1:2:256:A:C2	1:2:257:C:C2	2.96	0.53
12:K:16:PHE:HE2	12:K:86:ILE:HD13	1.73	0.53
1:2:883:A:H2'	1:2:884:G:C8	2.44	0.53
2:A:155:TYR:HB3	23:V:60:ARG:HH21	1.74	0.53
18:Q:39:VAL:HG21	18:Q:48:VAL:HG21	1.91	0.53
1:2:1272:G:N7	1:2:1428:U:H3'	2.23	0.53
1:2:14:C:O2	1:2:1140:G:C2	2.62	0.53
1:2:1771:C:C2	1:2:1787:G:C2	2.97	0.53
4:C:118:LEU:HD11	4:C:216:LEU:HB3	1.91	0.53
2:A:179:ARG:HD3	2:A:183:ARG:CZ	2.39	0.53
3:B:138:PHE:HB2	3:B:213:ARG:O	2.08	0.53
8:G:2:LYS:HG3	8:G:17:GLU:HG3	1.91	0.53
1:2:1583:U:OP1	18:Q:124:PRO:HA	2.08	0.53
1:2:1449:C:O2'	1:2:1450:U:H5'	2.08	0.52
1:2:486:G:H1	1:2:499:C:H42	1.57	0.52
1:2:490:C:H2'	1:2:491:A:H4'	1.91	0.52
1:2:700:C:C2	1:2:739:G:N1	2.77	0.52
1:2:1455:C:O3'	20:S:137:HIS:HB2	2.10	0.52
1:2:1053:U:H2'	1:2:1054:U:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1173:C:N4	1:2:1464:G:C6	2.77	0.52
1:2:50:C:O2	1:2:429:G:C2	2.62	0.52
8:G:159:ARG:HE	8:G:172:ALA:HB2	1.75	0.52
27:Z:81:ARG:HA	27:Z:84:GLU:HB3	1.91	0.52
1:2:294:A:C2	1:2:295:U:C2	2.97	0.52
26:Y:43:LYS:O	26:Y:46:GLU:HG2	2.10	0.52
1:2:1015:C:O4'	1:2:1015:C:O2	2.26	0.52
1:2:1214:C:H2'	1:2:1215:C:C6	2.45	0.52
1:2:12:U:H2'	1:2:13:C:C6	2.45	0.52
1:2:239:C:C4'	1:2:240:U:OP2	2.49	0.52
1:2:1097:U:H1'	24:W:71:LYS:HD2	1.91	0.52
1:2:142:G:H2'	1:2:143:G:C8	2.44	0.52
12:K:15:LEU:O	12:K:19:GLY:N	2.42	0.52
13:L:3:THR:HA	13:L:82:ARG:HH21	1.74	0.52
1:2:1223:A:H61	1:2:1258:U:H3	1.56	0.52
12:K:13:GLN:HA	12:K:80:LEU:HD11	1.91	0.52
2:A:35:PRO:HG3	23:V:87:ARG:HH21	1.75	0.52
1:2:1566:C:OP1	20:S:36:ARG:HG3	2.10	0.52
1:2:487:G:H1	1:2:498:U:H5	1.58	0.52
1:2:653:C:N4	1:2:679:U:H3	2.08	0.52
1:2:916:U:O2'	16:O:29:HIS:HD2	1.92	0.52
23:V:60:ARG:HA	23:V:65:ALA:HB2	1.91	0.52
1:2:1604:C:H2'	1:2:1605:G:C8	2.44	0.51
9:H:98:ILE:HG13	9:H:121:VAL:HG21	1.93	0.51
7:F:29:THR:HG23	18:Q:28:LEU:HD23	1.92	0.51
19:R:57:LEU:O	19:R:60:ARG:HG2	2.10	0.51
24:W:20:THR:HG23	24:W:22:LYS:HG2	1.92	0.51
1:2:813:A:H2'	1:2:813:A:N3	2.25	0.51
1:2:511:A:H5''	11:J:163:PRO:HG2	1.91	0.51
1:2:1210:A:H1'	17:P:99:GLY:O	2.10	0.51
1:2:1217:G:H5''	1:2:1442:A:H61	1.74	0.51
1:2:1771:C:H2'	1:2:1772:G:H8	1.73	0.51
1:2:958:U:H2'	1:2:958:U:O2	2.09	0.51
7:F:48:TRP:CZ2	7:F:120:LEU:HB3	2.42	0.51
13:L:122:ILE:HG13	13:L:143:ALA:HB3	1.92	0.51
1:2:813:A:N6	1:2:856:U:H3	2.08	0.51
1:2:864:A:C2	1:2:964:U:C5	2.97	0.51
1:2:487:G:C2	1:2:499:C:C2	2.99	0.51
1:2:1121:G:H5''	1:2:1121:G:H8	1.76	0.51
5:D:126:VAL:HG11	5:D:134:CYS:HB2	1.93	0.51
2:A:45:VAL:HA	16:O:99:GLN:HE22	52.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:82:LYS:O	24:W:84:ALA:N	2.44	0.51
1:2:1611:U:O2	1:2:1611:U:O4'	2.29	0.51
1:2:538:G:O5'	1:2:538:G:H8	1.94	0.51
1:2:5:U:H2'	1:2:6:G:C8	2.45	0.51
13:L:21:THR:HG22	13:L:32:LYS:H	1.75	0.51
1:2:1137:A:C5	1:2:1138:A:N6	2.79	0.50
1:2:452:U:O2	1:2:452:U:H3'	2.11	0.50
1:2:868:A:N6	1:2:957:U:H5	2.08	0.50
15:N:54:LEU:HB3	15:N:60:VAL:HB	1.92	0.50
17:P:17:TYR:HB2	17:P:25:LEU:HD21	1.93	0.50
1:2:1398:A:H5'	19:R:60:ARG:HH12	1.77	0.50
1:2:1540:G:N2	1:2:1566:C:H2'	2.19	0.50
1:2:653:C:H42	1:2:679:U:H3	1.60	0.50
12:K:82:LEU:HD22	12:K:86:ILE:HG21	1.93	0.50
13:L:125:VAL:HG22	13:L:137:PHE:HB3	1.93	0.50
19:R:23:LYS:HG2	19:R:23:LYS:O	2.10	0.50
25:X:63:GLN:HB3	25:X:64:PRO:CD	2.42	0.50
1:2:1542:U:H3'	1:2:1543:A:H5''	1.94	0.50
1:2:1586:G:N1	1:2:1587:C:C2	2.79	0.50
18:Q:7:VAL:HG23	18:Q:22:VAL:HG23	1.92	0.50
1:2:1671:G:C6	1:2:1672:C:C4	3.00	0.50
1:2:228:U:H3	1:2:235:A:H61	1.58	0.50
1:2:385:G:H2'	1:2:386:A:C8	2.46	0.50
2:A:50:VAL:HA	2:A:53:THR:CG2	2.40	0.50
20:S:37:GLY:CA	20:S:105:LEU:HD21	2.42	0.50
1:2:1038:A:H4'	23:V:62:ARG:HH12	1.76	0.50
1:2:51:A:N6	1:2:439:U:C2	2.64	0.50
1:2:1783:U:H2'	1:2:1784:G:H8	1.76	0.50
19:R:20:TYR:O	19:R:24:LEU:HB2	2.12	0.50
3:B:43:VAL:HG11	3:B:68:VAL:HG11	1.93	0.50
5:D:178:ARG:HH21	5:D:179:GLN:HE22	1.60	0.50
1:2:1588:G:OP1	21:T:91:HIS:HB2	2.11	0.50
1:2:141:U:H2'	1:2:142:G:H8	1.77	0.49
4:C:173:ARG:HB3	4:C:204:SER:HB2	1.94	0.49
5:D:20:GLU:HG2	12:K:61:TRP:CE3	2.47	0.49
17:P:100:LYS:HG2	17:P:101:VAL:HG23	1.93	0.49
19:R:41:ILE:HD13	19:R:47:ARG:HG3	1.93	0.49
1:2:1389:A:H2'	1:2:1390:U:C6	2.48	0.49
1:2:388:G:C2	1:2:408:C:C2	3.01	0.49
1:2:454:C:H3'	1:2:455:A:H8	1.77	0.49
1:2:900:G:H2'	1:2:901:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:969:A:N6	1:2:970:A:C4	2.80	0.49
1:2:768:C:H1'	11:J:143:ILE:HG21	1.94	0.49
17:P:62:ALA:HA	17:P:65:LEU:HD12	1.94	0.49
21:T:18:TYR:HB3	21:T:59:ALA:HB1	1.94	0.49
1:2:567:G:H4'	25:X:90:ASP:HA	1.93	0.49
1:2:71:A:H3'	1:2:72:A:C5'	2.41	0.49
6:E:198:ARG:HG2	6:E:208:VAL:HG12	1.95	0.49
13:L:8:GLN:NE2	13:L:14:GLN:H	2.10	0.49
1:2:1330:A:OP1	19:R:45:ARG:NH2	2.42	0.49
24:W:8:ALA:CA	24:W:74:VAL:HG21	2.34	0.49
1:2:1170:A:H2'	1:2:1171:G:H8	1.74	0.49
1:2:1671:G:H2'	1:2:1672:C:C6	2.48	0.49
1:2:1651:C:C2	1:2:1746:G:C2	3.01	0.49
1:2:883:A:H2'	1:2:884:G:H8	1.77	0.49
2:A:120:LEU:HD11	2:A:144:ILE:HD12	1.94	0.49
1:2:1066:C:H5''	3:B:150:VAL:HG23	1.94	0.49
9:H:134:GLU:HB2	9:H:155:ASN:HD21	1.77	0.49
1:2:1538:G:H1	1:2:1569:C:H42	1.60	0.49
22:U:51:VAL:HB	22:U:94:GLU:HB2	1.94	0.49
26:Y:53:ASP:HB3	26:Y:96:LEU:HD21	1.94	0.49
1:2:698:U:H3	1:2:740:A:H61	1.60	0.49
6:E:106:LYS:HB3	6:E:108:ARG:HE	1.78	0.49
5:D:72:LEU:HD22	12:K:65:TYR:HB3	1.94	0.49
26:Y:29:HIS:HB3	26:Y:32:ARG:O	2.12	0.49
1:2:1355:U:H2'	1:2:1356:G:H8	1.77	0.49
1:2:1464:G:N2	1:2:1465:C:C2	2.81	0.49
1:2:590:A:H2'	1:2:591:G:H8	1.75	0.49
1:2:1471:U:H5'	7:F:192:ILE:HD11	1.93	0.49
1:2:782:G:N2	1:2:783:C:C2	2.81	0.49
1:2:1292:U:O4	1:2:1293:G:C5	2.66	0.48
1:2:1472:G:H2'	1:2:1473:A:C8	2.48	0.48
1:2:473:A:H8	1:2:473:A:H5''	1.78	0.48
3:B:121:ILE:HG12	3:B:161:ILE:HG23	1.95	0.48
1:2:1499:C:C2	1:2:1505:G:C2	3.01	0.48
1:2:1586:G:H1	1:2:1606:U:H3	1.60	0.48
1:2:1653:A:H61	1:2:1743:G:H1'	1.75	0.48
1:2:871:G:H2'	1:2:872:U:O4'	2.13	0.48
1:2:999:C:O2	1:2:999:C:O4'	2.29	0.48
1:2:293:C:H2'	1:2:294:A:H5''	1.95	0.48
1:2:228:U:H2'	1:2:229:C:C6	2.48	0.48
1:2:298:A:C2'	1:2:299:A:H5'	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:609:G:N3	1:2:609:G:H2'	2.27	0.48
1:2:60:U:H5'	1:2:454:C:N4	2.28	0.48
8:G:32:ILE:HD11	8:G:63:MET:HB3	1.95	0.48
17:P:22:LEU:HD23	17:P:109:PRO:HG2	1.96	0.48
26:Y:27:VAL:HG11	26:Y:35:VAL:HG21	1.95	0.48
1:2:281:C:H2'	1:2:282:U:O4'	2.14	0.48
3:B:168:ILE:O	3:B:172:LEU:HG	2.12	0.48
10:I:104:ILE:HD13	10:I:168:ALA:HB3	1.94	0.48
1:2:1164:G:H2'	1:2:1165:A:C8	2.48	0.48
6:E:140:VAL:HG22	6:E:146:THR:HG22	1.96	0.48
19:R:26:MET:HG2	19:R:62:GLN:HE22	1.78	0.48
22:U:34:LEU:HD11	22:U:89:ARG:HG3	1.96	0.48
25:X:11:SER:O	25:X:13:ARG:N	2.47	0.48
1:2:1267:G:H1	1:2:1439:C:N4	2.11	0.48
1:2:823:G:N2	1:2:848:C:C2	2.82	0.48
1:2:1174:U:H2'	1:2:1175:G:C8	2.47	0.48
1:2:1266:G:HO2'	1:2:1446:G:HO2'	1.61	0.48
1:2:879:C:H2'	1:2:880:A:O4'	2.14	0.48
1:2:977:A:H2'	1:2:978:A:O4'	2.13	0.48
1:2:1502:G:OP2	21:T:99:SER:HB3	2.12	0.48
1:2:1577:U:O2'	18:Q:139:GLN:HA	2.13	0.48
1:2:1225:A:H5''	1:2:1226:A:O5'	2.14	0.48
1:2:1173:C:C2	1:2:1464:G:C2	3.02	0.48
6:E:76:VAL:O	6:E:77:ARG:HB2	2.13	0.48
21:T:83:ALA:HB1	21:T:91:HIS:HB3	1.94	0.48
1:2:1252:U:H5''	14:M:39:ARG:HH22	1.79	0.47
1:2:542:C:H4'	1:2:543:A:OP2	2.13	0.47
21:T:6:VAL:HB	21:T:66:TYR:CE1	2.49	0.47
2:A:3:LEU:HD13	23:V:39:VAL:HG11	1.95	0.47
1:2:1073:G:N2	1:2:1074:C:C2	2.82	0.47
1:2:1593:U:C2	1:2:1598:A:N6	2.73	0.47
1:2:480:A:C6	1:2:506:U:C4	2.95	0.47
1:2:732:G:H1'	1:2:734:A:H61	1.78	0.47
1:2:700:C:N3	1:2:739:G:C6	2.83	0.47
1:2:989:C:H2'	1:2:990:G:O4'	2.14	0.47
2:A:189:PRO:HA	23:V:44:ARG:HH22	1.78	0.47
13:L:99:ARG:NH1	25:X:7:ARG:O	2.45	0.47
1:2:896:C:N4	1:2:913:G:C6	2.82	0.47
20:S:91:ASP:HB3	20:S:95:GLY:H	1.79	0.47
1:2:1044:C:C2	1:2:1073:G:C2	3.01	0.47
5:D:61:GLU:H	5:D:64:ARG:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:116:U:H3	1:2:299:A:H2	1.56	0.47
19:R:28:PHE:HZ	19:R:48:ASN:ND2	2.12	0.47
20:S:48:LYS:HD3	21:T:35:ASP:HB3	1.95	0.47
4:C:144:ILE:CD1	4:C:196:ALA:HB1	2.40	0.47
11:J:170:GLY:HA2	11:J:174:ARG:HD3	1.96	0.47
26:Y:42:GLU:HG3	26:Y:52:LYS:HD2	1.97	0.47
1:2:588:C:O4'	1:2:588:C:O2	2.32	0.47
5:D:164:VAL:HA	5:D:168:ILE:HD12	1.96	0.47
1:2:1558:U:H2'	1:2:1559:U:O4'	2.15	0.47
1:2:1782:C:H2'	1:2:1783:U:C6	2.49	0.47
1:2:18:C:H2'	1:2:19:A:H8	1.78	0.47
5:D:53:THR:HA	5:D:94:ARG:HH21	1.80	0.47
6:E:105:VAL:HG12	6:E:244:ILE:H	1.80	0.47
7:F:74:HIS:CD2	7:F:109:LYS:HD2	2.49	0.47
1:2:1794:C:H5'	1:2:1795:A:C2	2.50	0.47
1:2:218:A:H2'	1:2:219:A:H8	1.79	0.47
1:2:690:A:H2'	1:2:691:U:O4'	2.15	0.47
1:2:1262:G:C2	1:2:1263:G:H1'	2.50	0.47
1:2:1363:G:N1	1:2:1364:C:C4	2.83	0.47
3:B:119:THR:HG23	3:B:155:TYR:HD1	1.79	0.47
1:2:147:U:H5''	1:2:148:C:H5	1.78	0.47
11:J:148:VAL:HG11	11:J:156:ILE:HD11	1.96	0.47
1:2:1450:U:O2'	17:P:79:HIS:HD2	1.97	0.46
1:2:767:U:O2	1:2:767:U:O4'	2.32	0.46
1:2:89:G:C6	1:2:90:C:C4	3.02	0.46
21:T:37:VAL:HG22	21:T:38:LYS:H	1.79	0.46
2:A:66:ALA:HB2	23:V:37:ALA:HB2	1.96	0.46
1:2:209:A:H8	1:2:209:A:H5''	1.80	0.46
1:2:140:A:C2	1:2:265:A:H4'	2.45	0.46
1:2:384:A:H5'	10:I:25:ARG:HH22	1.79	0.46
1:2:557:U:H5'	1:2:558:C:OP1	2.14	0.46
1:2:798:A:H2'	1:2:799:U:C6	2.50	0.46
4:C:92:GLN:HG2	4:C:101:THR:HG22	1.97	0.46
7:F:40:GLN:HE22	18:Q:56:GLY:HA2	1.80	0.46
11:J:84:GLY:HA3	11:J:107:ARG:HH11	1.80	0.46
13:L:54:ILE:HG23	13:L:55:ASP:N	2.30	0.46
2:A:45:VAL:HA	16:O:99:GLN:NE2	52.91	0.46
22:U:17:VAL:HG13	22:U:96:PRO:HG3	1.98	0.46
1:2:10:G:C5	1:2:1631:A:C2	3.03	0.46
1:2:1179:C:H1'	1:2:1458:A:H61	1.81	0.46
1:2:1437:C:N4	1:2:1438:C:N4	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:274:C:N4	1:2:275:C:N4	2.64	0.46
1:2:360:C:C2	1:2:383:G:C2	3.03	0.46
1:2:843:A:H2'	1:2:844:G:C8	2.50	0.46
5:D:101:GLN:HG3	5:D:122:VAL:HG22	1.97	0.46
14:M:77:VAL:HG12	14:M:79:LEU:HB2	1.97	0.46
20:S:38:VAL:HG22	20:S:101:LEU:HD22	1.97	0.46
1:2:1353:G:C2	1:2:1354:C:C2	3.03	0.46
1:2:1466:U:H2'	1:2:1467:A:O4'	2.16	0.46
1:2:254:U:H2'	1:2:255:A:H5'	1.98	0.46
1:2:700:C:N4	1:2:738:G:H1	2.12	0.46
11:J:63:ASP:O	11:J:66:ASP:HB3	2.15	0.46
15:N:35:GLU:HA	15:N:38:ILE:HG12	1.98	0.46
18:Q:69:VAL:HG21	18:Q:81:ILE:HG12	1.96	0.46
20:S:112:ASP:HA	20:S:115:ARG:HD2	1.98	0.46
20:S:88:ARG:HH22	20:S:108:LYS:HB3	1.81	0.46
1:2:1120:C:O2	1:2:1126:G:C2	2.69	0.46
1:2:1655:U:H4'	1:2:1656:G:O5'	2.15	0.46
1:2:52:U:H2'	1:2:53:G:C8	2.50	0.46
1:2:75:U:H4'	1:2:76:A:OP1	2.15	0.46
22:U:22:ILE:HG21	22:U:100:VAL:HG11	1.97	0.46
1:2:1590:A:C2	1:2:1591:A:C6	3.04	0.46
1:2:160:U:O2'	1:2:161:A:OP2	2.29	0.46
1:2:521:U:H5'	1:2:522:G:OP2	2.16	0.46
11:J:61:THR:HA	24:W:97:ARG:HH12	1.80	0.46
1:2:1082:G:H3'	1:2:1083:A:H5''	1.98	0.46
1:2:1754:A:C5'	1:2:1754:A:H8	2.29	0.46
1:2:642:G:C2	1:2:692:C:C2	3.04	0.46
1:2:89:G:N1	1:2:90:C:C2	2.84	0.46
1:2:1367:G:H5''	21:T:69:LYS:HG2	1.97	0.46
1:2:1038:A:O2'	1:2:1039:G:O5'	2.30	0.45
1:2:1177:G:H3'	1:2:1178:G:C8	2.50	0.45
6:E:45:ILE:HA	6:E:61:VAL:HG11	1.98	0.45
6:E:68:ARG:HH12	6:E:76:VAL:HG21	1.81	0.45
11:J:59:LEU:HD13	11:J:73:GLY:HA2	1.98	0.45
20:S:63:GLN:HA	20:S:66:LEU:HD12	1.98	0.45
1:2:981:U:H6	1:2:981:U:H5''	1.82	0.45
13:L:78:THR:HG22	13:L:84:ILE:HD11	1.97	0.45
22:U:34:LEU:CD1	22:U:89:ARG:HG3	2.46	0.45
24:W:6:VAL:HG12	24:W:34:ILE:CD1	2.38	0.45
1:2:1349:G:C2	1:2:1374:C:C2	3.04	0.45
8:G:2:LYS:HB3	8:G:108:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:113:TYR:CE1	10:I:153:ILE:HD11	2.51	0.45
1:2:1671:G:C5	1:2:1672:C:C4	3.04	0.45
1:2:326:U:H2'	1:2:327:A:C8	2.51	0.45
15:N:40:TYR:HB3	15:N:50:ILE:HG12	1.98	0.45
7:F:114:ARG:NH2	18:Q:43:ILE:HB	2.29	0.45
1:2:1238:U:C1'	1:2:1247:C:H42	2.16	0.45
1:2:1472:G:H2'	1:2:1473:A:H8	1.81	0.45
1:2:637:U:O4'	1:2:637:U:O2	2.34	0.45
3:B:48:VAL:HG21	3:B:61:LEU:HD11	1.98	0.45
22:U:96:PRO:HG2	22:U:99:ILE:HD13	1.97	0.45
1:2:1091:A:O2'	1:2:1092:A:H3'	2.17	0.45
1:2:1180:U:H2'	1:2:1181:U:O4'	2.17	0.45
1:2:1687:A:H2	1:2:1709:C:H42	1.64	0.45
1:2:28:A:H2'	1:2:29:U:O4'	2.17	0.45
17:P:17:TYR:HB3	17:P:18:LYS:H	1.66	0.45
1:2:1240:G:C1'	17:P:79:HIS:HB2	2.45	0.45
21:T:77:ASN:OD1	21:T:98:GLY:HA2	2.17	0.45
1:2:1588:G:C2	1:2:1589:C:C2	3.04	0.45
1:2:17:C:H2'	1:2:18:C:C6	2.52	0.45
1:2:648:U:O2'	1:2:649:U:C6	2.68	0.45
5:D:74:GLU:HG3	5:D:84:ILE:HD12	1.99	0.45
7:F:97:ASN:O	7:F:100:MET:HB2	2.16	0.45
11:J:21:SER:HA	11:J:24:LEU:HD12	1.98	0.45
1:2:1323:G:H4'	2:A:113:ARG:HH21	1.81	0.45
1:2:1332:C:H2'	1:2:1333:U:C6	2.51	0.45
1:2:414:C:O2	1:2:418:G:C2	2.70	0.45
1:2:556:G:C6	1:2:558:C:N4	2.84	0.45
1:2:969:A:H3'	1:2:969:A:C8	2.52	0.45
1:2:637:U:OP2	24:W:32:LYS:HD2	2.17	0.45
1:2:1171:G:C2	1:2:1172:C:C2	3.05	0.45
1:2:1277:G:C6	1:2:1278:C:C4	3.05	0.45
1:2:1338:C:O2'	1:2:1340:A:N7	2.44	0.45
1:2:1171:G:C6	1:2:1172:C:C4	3.05	0.45
1:2:1537:G:O6	20:S:27:ASN:HB2	2.16	0.45
1:2:1637:C:H2'	1:2:1638:C:O4'	2.17	0.45
13:L:66:ILE:HG21	13:L:140:LEU:HD11	1.99	0.45
24:W:75:ILE:HD11	24:W:79:PHE:HD2	1.82	0.45
1:2:1073:G:N1	1:2:1074:C:C4	2.85	0.44
1:2:1402:C:H2'	1:2:1403:G:H8	1.82	0.44
1:2:222:U:H2'	1:2:223:C:C6	2.52	0.44
1:2:1353:G:C6	1:2:1354:C:C4	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:159:LEU:HD22	4:C:226:THR:HG21	2.00	0.44
12:K:25:LYS:HD2	12:K:59:PHE:HZ	1.82	0.44
1:2:334:U:H4'	13:L:129:ARG:HD3	1.98	0.44
17:P:124:THR:HA	17:P:125:PRO:HD3	1.87	0.44
19:R:24:LEU:HA	19:R:34:LEU:HD13	1.99	0.44
1:2:1494:U:O2	1:2:1509:G:O6	2.35	0.44
1:2:280:G:C2	1:2:281:C:C2	3.06	0.44
1:2:462:U:H2'	1:2:463:A:C8	2.53	0.44
1:2:504:A:H8	1:2:504:A:H5''	1.82	0.44
1:2:947:G:C2	1:2:948:C:C2	3.05	0.44
6:E:104:ASP:HB3	6:E:110:ALA:HB2	1.98	0.44
1:2:1064:A:H2'	1:2:1065:C:O4'	2.17	0.44
1:2:1268:U:H5'	1:2:1268:U:O2	2.17	0.44
1:2:1290:G:H2'	1:2:1291:G:H8	1.81	0.44
1:2:1291:G:C4	1:2:1292:U:O2	2.71	0.44
1:2:1441:U:H4'	1:2:1444:A:N3	2.32	0.44
1:2:561:G:N2	1:2:583:C:C2	2.85	0.44
4:C:40:TRP:CE2	4:C:72:GLN:HG3	2.53	0.44
11:J:127:VAL:O	11:J:131:GLN:HB2	2.18	0.44
11:J:31:ALA:HA	11:J:36:LEU:HD12	1.98	0.44
12:K:60:SER:HB2	12:K:65:TYR:HE2	1.83	0.44
25:X:41:SER:HA	25:X:42:PRO:HD3	1.87	0.44
1:2:1175:G:C2	1:2:1176:C:C2	3.05	0.44
1:2:186:G:H22	1:2:196:A:H2'	1.82	0.44
1:2:775:G:C6	1:2:785:C:N4	2.86	0.44
1:2:1279:C:O2'	22:U:70:THR:HG22	2.17	0.44
1:2:1396:U:H3'	1:2:1397:C:H5'	2.00	0.44
1:2:1613:C:C5	7:F:83:ARG:HA	2.52	0.44
1:2:1673:C:C2	1:2:1725:G:C2	3.06	0.44
3:B:176:VAL:C	3:B:178:ASN:H	2.21	0.44
5:D:109:LEU:HD21	5:D:115:ILE:HG23	1.99	0.44
1:2:93:A:H1'	6:E:3:ARG:HB3	1.99	0.44
10:I:42:ARG:HB3	10:I:58:LEU:O	2.18	0.44
25:X:50:LYS:HG3	25:X:103:LEU:HD23	2.00	0.44
26:Y:128:LYS:O	26:Y:132:ARG:HB2	2.17	0.44
1:2:14:C:C2	1:2:1140:G:C2	3.05	0.44
1:2:480:A:H61	1:2:506:U:H3	1.66	0.44
1:2:72:A:H4'	1:2:73:U:OP1	2.16	0.44
1:2:772:G:C6	1:2:773:C:N3	2.86	0.44
1:2:897:A:N3	1:2:898:G:H1'	2.32	0.44
1:2:1402:C:H2'	1:2:1403:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:279:U:H4'	1:2:280:G:O5'	2.18	0.44
1:2:389:G:H5''	1:2:389:G:N3	2.33	0.44
1:2:566:A:N1	1:2:582:C:H1'	2.33	0.44
1:2:221:A:N6	1:2:838:U:H3	2.12	0.44
1:2:89:G:C2	1:2:90:C:C2	3.06	0.44
1:2:417:G:C8	8:G:59:GLN:HG2	2.53	0.44
16:O:24:ASN:HA	16:O:55:SER:HB3	1.99	0.44
18:Q:48:VAL:HG22	18:Q:78:VAL:HG13	2.00	0.44
20:S:25:ASN:HD21	27:Z:41:VAL:HG13	1.82	0.44
1:2:1137:A:H2'	1:2:1138:A:H8	1.80	0.44
1:2:1178:G:C6	1:2:1179:C:N3	2.86	0.44
1:2:1290:G:H8	1:2:1290:G:O5'	2.01	0.44
1:2:1603:G:C6	1:2:1604:C:C4	3.05	0.44
1:2:51:A:C6	1:2:439:U:N3	2.68	0.44
1:2:592:U:H4'	1:2:594:G:H4'	1.98	0.44
1:2:765:G:C6	11:J:149:ARG:HB2	2.52	0.44
1:2:842:U:H2'	1:2:843:A:C8	2.52	0.44
12:K:46:LEU:HD13	12:K:66:TYR:CD2	2.53	0.44
13:L:14:GLN:HB3	13:L:54:ILE:HG21	1.98	0.44
17:P:21:ASP:H	17:P:24:LYS:HD2	1.82	0.44
25:X:109:ARG:HB3	25:X:112:LYS:HB2	2.00	0.44
25:X:5:LYS:HG3	25:X:5:LYS:H	1.62	0.44
1:2:1178:G:C2	1:2:1179:C:C2	3.06	0.43
1:2:1277:G:C2	1:2:1278:C:C2	3.06	0.43
1:2:151:U:H3	1:2:161:A:H61	1.66	0.43
1:2:309:C:C2	1:2:356:G:C2	3.06	0.43
1:2:885:U:H2'	1:2:886:A:O4'	2.18	0.43
8:G:14:LYS:HZ1	8:G:122:GLU:HB2	1.83	0.43
10:I:148:ALA:C	10:I:150:GLU:H	2.21	0.43
18:Q:51:PRO:HA	18:Q:109:PHE:HE1	1.83	0.43
26:Y:37:LYS:HA	26:Y:40:LEU:HD12	2.00	0.43
1:2:1270:G:H2'	1:2:1271:U:C6	2.53	0.43
1:2:1481:A:H2'	1:2:1482:G:C8	2.52	0.43
1:2:1486:G:H3'	1:2:1513:A:H61	1.82	0.43
1:2:1589:C:C2	1:2:1590:A:C8	3.07	0.43
21:T:28:LEU:O	21:T:29:GLU:HB2	2.17	0.43
1:2:1059:U:H2'	1:2:1060:U:H4'	2.00	0.43
1:2:1178:G:C6	1:2:1179:C:C4	3.05	0.43
1:2:10:G:C6	1:2:11:A:C5	3.06	0.43
1:2:1315:G:C2	1:2:1316:C:C2	3.07	0.43
1:2:1774:A:H2'	1:2:1775:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:102:PRO:HD2	9:H:112:ARG:HH21	1.84	0.43
9:H:22:GLN:HA	9:H:25:ILE:HD12	2.00	0.43
24:W:16:ASN:O	24:W:20:THR:HG22	2.18	0.43
1:2:1736:U:H2'	1:2:1737:C:C6	2.53	0.43
1:2:1754:A:H5'	1:2:1754:A:C8	2.52	0.43
1:2:516:U:H3	1:2:534:A:N6	2.13	0.43
1:2:585:G:C2	1:2:586:C:C2	3.07	0.43
3:B:137:ILE:HG22	3:B:215:VAL:HG13	2.01	0.43
7:F:135:VAL:HA	7:F:200:LEU:HD22	2.01	0.43
23:V:38:GLN:HG3	23:V:49:GLU:HG2	1.99	0.43
1:2:1603:G:C2	1:2:1604:C:C2	3.07	0.43
3:B:110:LEU:HD13	3:B:213:ARG:HD2	2.00	0.43
1:2:1118:G:H8	1:2:1118:G:H5''	1.83	0.43
2:A:68:PRO:HD2	2:A:119:ARG:HH12	1.84	0.43
14:M:44:ALA:HB1	14:M:50:GLY:HA3	2.00	0.43
16:O:64:ALA:HB3	16:O:104:ALA:HB3	2.00	0.43
20:S:116:LEU:HA	20:S:119:ILE:HG12	2.01	0.43
1:2:1154:G:C2	1:2:1622:C:C2	3.07	0.43
1:2:1156:A:H2'	1:2:1159:A:N7	2.33	0.43
1:2:1457:C:H5'	20:S:131:LEU:HD22	2.01	0.43
1:2:1675:C:H2'	1:2:1676:A:O4'	2.19	0.43
1:2:392:C:H2'	1:2:393:C:C6	2.53	0.43
3:B:208:GLN:HG2	3:B:209:ASN:N	2.34	0.43
9:H:31:SER:CB	9:H:32:PRO:HD3	2.49	0.43
18:Q:6:SER:HA	18:Q:22:VAL:O	2.18	0.43
27:Z:54:ALA:H	27:Z:55:PRO:HD2	1.82	0.43
1:2:1454:C:O2	1:2:1454:C:O4'	2.34	0.43
1:2:537:A:H2	1:2:539:G:H22	1.60	0.43
2:A:193:GLN:HA	2:A:194:PRO:HD3	1.81	0.43
1:2:1497:G:C2	1:2:1498:C:C2	3.07	0.43
1:2:155:A:H2'	1:2:156:A:O4'	2.19	0.43
10:I:83:TYR:HD2	10:I:101:ILE:HD13	1.82	0.43
1:2:1408:A:H2'	1:2:1409:A:C8	2.54	0.43
1:2:1590:A:C2	1:2:1602:U:N3	2.84	0.43
1:2:612:G:H4'	1:2:613:C:OP1	2.19	0.43
8:G:163:THR:HG22	8:G:168:SER:HA	2.01	0.43
24:W:24:GLN:HA	24:W:63:VAL:O	2.19	0.43
1:2:1216:A:H4'	12:K:44:LYS:HD3	2.01	0.42
1:2:452:U:O2	1:2:452:U:C2'	2.66	0.42
6:E:17:HIS:HB3	6:E:108:ARG:HA	2.00	0.42
1:2:1203:A:H2'	1:2:1203:A:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1620:G:C2	1:2:1621:C:C2	3.07	0.42
1:2:1661:G:C6	1:2:1662:C:C4	3.07	0.42
1:2:1671:G:C6	1:2:1672:C:N4	2.87	0.42
6:E:18:TRP:CZ2	6:E:43:PRO:HD3	2.54	0.42
14:M:25:LEU:HD13	14:M:92:ALA:HB2	2.02	0.42
15:N:55:ARG:HA	15:N:60:VAL:O	2.19	0.42
1:2:1542:U:H4'	20:S:132:ARG:HH11	1.84	0.42
1:2:779:A:H3'	1:2:780:A:H4'	2.01	0.42
10:I:107:THR:N	10:I:108:PRO:CD	2.83	0.42
16:O:121:VAL:HA	16:O:122:PRO:HD3	1.93	0.42
1:2:1175:G:C6	1:2:1176:C:C4	3.08	0.42
1:2:1343:A:C2	1:2:1344:A:C6	3.07	0.42
1:2:1391:C:H2'	1:2:1392:G:H8	1.84	0.42
1:2:1496:G:O6	1:2:1507:C:N4	2.52	0.42
1:2:1542:U:H5'	20:S:136:GLN:HE22	1.85	0.42
1:2:50:C:N3	1:2:429:G:C6	2.88	0.42
1:2:696:C:H4'	1:2:697:C:OP1	2.19	0.42
3:B:70:LEU:HD13	3:B:82:ARG:HG2	2.01	0.42
4:C:66:LEU:HB3	7:F:151:VAL:HG11	69.23	0.42
9:H:67:LEU:HD13	9:H:94:ALA:HB2	2.01	0.42
2:A:50:VAL:HG22	19:R:109:LEU:HD21	2.01	0.42
21:T:28:LEU:HD21	21:T:30:VAL:HG23	2.01	0.42
25:X:24:TRP:HE3	25:X:30:LYS:HG2	1.85	0.42
1:2:1073:G:C6	1:2:1074:C:N4	2.88	0.42
1:2:240:U:H5''	1:2:240:U:H6	1.84	0.42
1:2:699:U:H2'	1:2:700:C:C6	2.54	0.42
3:B:92:GLN:HB2	3:B:95:ASN:HB2	2.00	0.42
1:2:1377:C:H1'	18:Q:19:VAL:HG11	2.00	0.42
1:2:121:U:O2	1:2:122:U:C2	2.73	0.42
1:2:1500:G:N7	21:T:102:ARG:NH2	2.66	0.42
1:2:15:U:H2'	1:2:16:G:O4'	2.19	0.42
1:2:520:A:H2'	1:2:521:U:O4'	2.19	0.42
1:2:52:U:H2'	1:2:53:G:H8	1.84	0.42
1:2:878:G:C2	1:2:879:C:C2	3.07	0.42
8:G:14:LYS:NZ	8:G:122:GLU:HB2	2.35	0.42
1:2:1292:U:O4	1:2:1293:G:C4	2.72	0.42
1:2:1497:G:C6	1:2:1498:C:C4	3.08	0.42
1:2:1770:C:H5''	1:2:1770:C:H6	1.83	0.42
1:2:53:G:C2	1:2:54:C:C2	3.07	0.42
1:2:737:A:O2'	1:2:738:G:H8	2.02	0.42
1:2:782:G:C2	1:2:783:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:55:LEU:HB3	14:M:81:LYS:HG2	2.01	0.42
1:2:917:U:H4'	16:O:18:ARG:HD3	2.02	0.42
1:2:1527:C:O5'	1:2:1527:C:H6	2.03	0.42
1:2:1533:U:H4'	1:2:1534:G:C2	2.54	0.42
1:2:1560:G:C2	1:2:1561:C:C2	3.08	0.42
1:2:1586:G:C6	1:2:1587:C:C4	3.07	0.42
1:2:454:C:H3'	1:2:455:A:C8	2.52	0.42
2:A:131:GLN:HE21	2:A:135:GLU:HG3	1.84	0.42
2:A:21:ARG:HD2	2:A:24:LEU:HD13	2.01	0.42
10:I:107:THR:HG22	10:I:110:ARG:HH21	1.85	0.42
1:2:1132:A:H2'	1:2:1133:C:O4'	2.19	0.42
1:2:1307:G:C2	1:2:1308:C:C2	3.08	0.42
1:2:1654:U:H3	1:2:1742:A:N6	2.18	0.42
1:2:1661:G:C2	1:2:1662:C:C2	3.08	0.42
1:2:1679:A:H2	1:2:1718:G:N2	2.16	0.42
1:2:473:A:C8	1:2:473:A:H5''	2.55	0.42
2:A:176:LEU:O	2:A:180:GLU:HG2	2.20	0.42
3:B:36:SER:HA	3:B:41:ARG:HD2	2.02	0.42
9:H:9:LEU:HD21	9:H:17:GLU:HB3	2.00	0.42
11:J:110:GLN:HE22	11:J:126:ARG:HD3	1.84	0.42
1:2:1544:G:H2'	1:2:1545:A:O4'	2.19	0.42
1:2:1564:U:H5''	20:S:39:GLY:H	1.84	0.42
1:2:1598:A:H1'	1:2:1599:G:H5'	2.02	0.42
1:2:896:C:C4	1:2:913:G:C6	3.07	0.42
1:2:935:G:C2	1:2:936:C:C2	3.08	0.42
2:A:37:VAL:HG13	2:A:149:LEU:HD23	2.01	0.42
2:A:90:ALA:HA	2:A:95:ALA:HB3	2.02	0.42
10:I:58:LEU:H	10:I:58:LEU:HG	1.69	0.42
22:U:39:ALA:HA	22:U:42:ILE:HG12	2.02	0.42
1:2:147:U:H3'	1:2:148:C:H6	1.83	0.41
1:2:53:G:C6	1:2:54:C:C4	3.07	0.41
1:2:623:G:C2	1:2:624:C:C2	3.08	0.41
6:E:18:TRP:HB3	6:E:20:LEU:HG	2.02	0.41
8:G:102:VAL:HG13	8:G:106:LEU:HD22	2.01	0.41
8:G:21:GLU:HB2	8:G:25:ARG:HH12	1.84	0.41
9:H:46:ILE:CG1	9:H:60:VAL:HG12	2.49	0.41
11:J:163:PRO:HG3	11:J:169:PRO:O	2.20	0.41
13:L:84:ILE:HD13	13:L:111:VAL:HG21	2.02	0.41
1:2:1094:U:H4'	24:W:19:LYS:NZ	2.34	0.41
1:2:1213:U:H2'	1:2:1214:C:C6	2.55	0.41
1:2:1673:C:C2	1:2:1725:G:N2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:886:A:C6	1:2:887:U:C4	3.08	0.41
10:I:38:ILE:HA	10:I:60:ILE:O	2.20	0.41
18:Q:18:ALA:HB2	18:Q:69:VAL:HG13	2.01	0.41
25:X:107:PHE:CE1	25:X:114:LYS:HD2	2.55	0.41
1:2:1397:C:H4'	1:2:1398:A:O5'	2.20	0.41
1:2:431:G:C6	1:2:432:C:N3	2.88	0.41
1:2:44:U:H3'	1:2:45:U:H5'	2.02	0.41
1:2:751:G:H2'	1:2:752:A:C8	2.56	0.41
3:B:149:GLN:HE22	3:B:154:SER:HB3	1.86	0.41
5:D:75:LYS:HB3	12:K:22:VAL:HB	2.02	0.41
18:Q:54:LEU:HD11	18:Q:112:TYR:HB3	2.02	0.41
1:2:568:C:H41	25:X:69:ARG:HH12	1.68	0.41
1:2:1278:C:H2'	1:2:1279:C:O4'	2.20	0.41
1:2:1332:C:H2'	1:2:1333:U:H6	1.86	0.41
1:2:1726:U:H2'	1:2:1727:C:C6	2.55	0.41
1:2:16:G:C6	1:2:17:C:N4	2.89	0.41
1:2:624:C:H2'	1:2:625:U:C6	2.55	0.41
1:2:69:G:C2	1:2:70:C:C2	3.08	0.41
1:2:73:U:H4'	1:2:74:U:OP1	2.21	0.41
1:2:86:A:H2'	1:2:87:C:H6	1.85	0.41
17:P:17:TYR:HA	17:P:112:VAL:HG11	2.02	0.41
21:T:7:ARG:HE	21:T:67:LEU:HD22	1.85	0.41
25:X:92:CYS:HA	25:X:95:PHE:HD2	1.85	0.41
1:2:1460:G:C6	1:2:1461:C:C4	3.09	0.41
1:2:268:G:C2	1:2:269:C:C2	3.08	0.41
1:2:4:C:H4'	4:C:186:SER:HB3	2.03	0.41
1:2:556:G:N2	1:2:558:C:C2	2.88	0.41
1:2:628:U:O4	1:2:969:A:N7	2.54	0.41
1:2:884:G:H2'	1:2:885:U:O4'	2.20	0.41
2:A:170:ILE:HG12	2:A:170:ILE:H	1.57	0.41
4:C:174:LEU:HD23	4:C:203:THR:HG22	2.01	0.41
1:2:886:A:H5''	16:O:120:PRO:HB3	2.03	0.41
1:2:1080:A:O2'	1:2:1081:C:H2'	2.20	0.41
1:2:1202:A:H3'	1:2:1203:A:H8	1.85	0.41
1:2:1474:C:H2'	1:2:1475:G:C8	2.54	0.41
1:2:1480:C:H5	1:2:1523:A:H62	1.66	0.41
1:2:1560:G:C6	1:2:1561:C:C4	3.09	0.41
1:2:280:G:C6	1:2:281:C:C4	3.09	0.41
1:2:328:G:H2'	1:2:329:G:H8	1.85	0.41
1:2:504:A:H8	1:2:504:A:C5'	2.33	0.41
1:2:609:G:H5''	1:2:610:U:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:93:A:C6	1:2:397:G:C6	3.09	0.41
2:A:157:ASP:O	2:A:158:VAL:HB	2.20	0.41
9:H:27:LEU:HD11	9:H:80:GLU:HB3	2.02	0.41
24:W:14:ILE:HD11	24:W:27:ILE:HD11	2.03	0.41
1:2:1218:A:N6	1:2:1263:G:O2'	2.53	0.41
1:2:1632:C:O2	1:2:1632:C:H2'	2.21	0.41
1:2:69:G:C6	1:2:70:C:C4	3.09	0.41
1:2:886:A:C2	1:2:925:A:C2	3.08	0.41
1:2:952:G:H2'	1:2:953:G:C8	2.56	0.41
20:S:86:LEU:HA	20:S:99:HIS:HD2	1.85	0.41
1:2:10:G:C6	1:2:1631:A:H2	2.37	0.41
1:2:1679:A:H5'	1:2:1680:U:C6	2.55	0.41
5:D:73:ILE:HG22	5:D:84:ILE:HD13	2.03	0.41
1:2:399:A:C2	10:I:26:LYS:HG3	2.55	0.41
14:M:45:LEU:HD13	14:M:71:LEU:HB3	2.02	0.41
20:S:88:ARG:HG3	20:S:91:ASP:HA	2.02	0.41
1:2:1144:U:C4	1:2:1145:G:N7	2.89	0.41
1:2:1746:G:H2'	1:2:1747:A:C8	2.55	0.41
1:2:360:C:N3	1:2:383:G:C2	2.88	0.41
3:B:23:PRO:HB3	3:B:26:ARG:NH2	2.36	0.41
6:E:45:ILE:HG22	6:E:46:VAL:N	2.36	0.41
9:H:114:ARG:HA	9:H:117:THR:HG23	2.02	0.41
10:I:3:ILE:HD11	10:I:32:GLN:HE21	1.86	0.41
16:O:87:GLY:HA3	16:O:120:PRO:HD2	2.01	0.41
18:Q:38:LEU:O	18:Q:40:GLN:N	2.53	0.41
13:L:99:ARG:HG2	25:X:9:LEU:HA	2.02	0.41
1:2:1012:A:H2'	1:2:1013:G:O4'	2.21	0.41
1:2:1796:U:H4'	1:2:1797:U:O5'	2.21	0.41
1:2:362:G:C2	1:2:381:C:C2	3.09	0.41
1:2:367:U:C2'	1:2:368:A:H5'	2.51	0.41
1:2:67:A:N6	1:2:83:G:O2'	2.54	0.41
17:P:30:THR:HA	17:P:33:PHE:CD2	2.55	0.41
1:2:1031:G:C6	1:2:1032:C:C4	3.09	0.41
1:2:1067:C:H2'	1:2:1068:A:H8	1.86	0.41
1:2:1118:G:C8	1:2:1118:G:H5''	2.56	0.41
6:E:125:LYS:HB3	6:E:142:HIS:HB2	2.03	0.41
6:E:57:ASN:O	6:E:61:VAL:HG23	2.21	0.41
8:G:5:ILE:HD13	8:G:16:ILE:HD12	2.02	0.41
1:2:158:U:H6	26:Y:117:LYS:HA	1.85	0.41
1:2:1143:U:O2	1:2:1144:U:C2	2.74	0.40
8:G:14:LYS:HD3	8:G:16:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:70:LEU:O	11:J:74:ASN:HB2	2.20	0.40
1:2:1588:G:C6	1:2:1589:C:C4	3.09	0.40
1:2:284:G:C2	1:2:285:C:C2	3.09	0.40
2:A:62:ARG:NH1	2:A:62:ARG:HG2	2.19	0.40
6:E:129:VAL:HG22	6:E:139:VAL:HG23	2.03	0.40
7:F:218:GLU:O	7:F:221:ARG:HG2	2.21	0.40
7:F:64:ILE:HG23	7:F:91:ILE:HG21	2.03	0.40
7:F:91:ILE:HG13	7:F:91:ILE:H	1.58	0.40
18:Q:52:LEU:HA	18:Q:60:PHE:CE1	2.56	0.40
1:2:403:G:C2	1:2:404:C:C2	3.09	0.40
6:E:122:LYS:HB2	6:E:164:LEU:HD12	2.03	0.40
7:F:185:ALA:HB2	7:F:192:ILE:HG23	2.01	0.40
27:Z:57:TYR:H	27:Z:103:ARG:HG2	1.86	0.40
1:2:108:A:H2'	1:2:109:G:C8	2.56	0.40
1:2:1424:C:HO2'	1:2:1426:G:H8	1.69	0.40
2:A:122:ILE:HA	2:A:144:ILE:O	2.22	0.40
8:G:121:ILE:HB	8:G:124:ILE:HG22	2.03	0.40
8:G:197:ASN:O	8:G:201:GLN:HG2	2.22	0.40
1:2:855:A:H62	9:H:97:ARG:H	1.69	0.40
1:2:332:A:H5'	10:I:48:THR:HB	2.04	0.40
1:2:1185:U:H2'	1:2:1186:U:O4'	2.22	0.40
1:2:1711:G:N3	1:2:1711:G:H2'	2.36	0.40
1:2:225:A:N3	1:2:225:A:H2'	2.36	0.40
1:2:366:A:H2'	1:2:367:U:O4'	2.21	0.40
1:2:585:G:C6	1:2:586:C:C4	3.09	0.40
1:2:2:A:C2	4:C:175:ILE:HD13	2.56	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	
2	A	206/254 (81%)	171 (83%)	27 (13%)	8 (4%)	3	30
3	B	219/255 (86%)	187 (85%)	20 (9%)	12 (6%)	2	20
4	C	215/259 (83%)	192 (89%)	17 (8%)	6 (3%)	6	38
5	D	221/237 (93%)	195 (88%)	17 (8%)	9 (4%)	3	29
6	E	258/261 (99%)	226 (88%)	25 (10%)	7 (3%)	6	39
7	F	204/227 (90%)	167 (82%)	28 (14%)	9 (4%)	3	27
8	G	224/236 (95%)	205 (92%)	15 (7%)	4 (2%)	10	47
9	H	182/190 (96%)	157 (86%)	16 (9%)	9 (5%)	2	23
10	I	184/201 (92%)	168 (91%)	9 (5%)	7 (4%)	4	30
11	J	180/188 (96%)	154 (86%)	20 (11%)	6 (3%)	4	34
12	K	94/106 (89%)	79 (84%)	9 (10%)	6 (6%)	1	17
13	L	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	9	45
14	M	120/134 (90%)	95 (79%)	18 (15%)	7 (6%)	2	19
15	N	148/151 (98%)	138 (93%)	9 (6%)	1 (1%)	25	67
16	O	125/137 (91%)	108 (86%)	11 (9%)	6 (5%)	2	24
17	P	121/142 (85%)	100 (83%)	12 (10%)	9 (7%)	1	13
18	Q	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8	43
19	R	123/136 (90%)	104 (85%)	14 (11%)	5 (4%)	3	29
20	S	143/146 (98%)	116 (81%)	17 (12%)	10 (7%)	1	14
21	T	141/144 (98%)	125 (89%)	12 (8%)	4 (3%)	6	38
22	U	104/117 (89%)	93 (89%)	9 (9%)	2 (2%)	9	46
23	V	85/87 (98%)	70 (82%)	10 (12%)	5 (6%)	2	19
24	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	3	30
25	X	142/145 (98%)	121 (85%)	15 (11%)	6 (4%)	3	28
26	Y	132/135 (98%)	119 (90%)	7 (5%)	6 (4%)	3	26
27	Z	68/108 (63%)	51 (75%)	13 (19%)	4 (6%)	2	19
28	a	96/119 (81%)	82 (85%)	8 (8%)	6 (6%)	1	17
29	b	79/82 (96%)	68 (86%)	8 (10%)	3 (4%)	4	30
30	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
31	d	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
32	e	51/63 (81%)	45 (88%)	5 (10%)	1 (2%)	9	45
33	f	67/150 (45%)	40 (60%)	20 (30%)	7 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	g	312/326 (96%)	253 (81%)	51 (16%)	8 (3%)	6	39
35	h	23/25 (92%)	23 (100%)	0	0	100	100
36	i	94/153 (61%)	83 (88%)	9 (10%)	2 (2%)	8	44
37	j	84/108 (78%)	70 (83%)	11 (13%)	3 (4%)	4	32
All	All	4976/5574 (89%)	4281 (86%)	506 (10%)	189 (4%)	7	30

All (189) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	95	ALA
3	B	55	LYS
3	B	148	ASN
4	C	141	VAL
5	D	217	VAL
5	D	220	PRO
7	F	67	SER
8	G	69	LEU
8	G	122	GLU
9	H	31	SER
9	H	64	VAL
9	H	74	GLN
9	H	136	VAL
10	I	22	ARG
10	I	147	ARG
10	I	153	ILE
12	K	60	SER
12	K	83	PRO
12	K	88	PRO
13	L	55	ASP
14	M	97	ILE
15	N	138	ASN
16	O	124	ASP
17	P	29	PRO
18	Q	39	VAL
19	R	71	PHE
24	W	78	ARG
24	W	83	ILE
25	X	12	ALA
25	X	64	PRO
26	Y	30	PRO
28	a	13	LYS

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Mol	Chain	Res	Type
36	i	63	GLY
37	j	72	PRO
2	A	166	GLY
3	B	147	ALA
3	B	179	SER
3	B	221	PRO
6	E	3	ARG
6	E	242	LYS
6	E	245	LYS
7	F	45	PHE
7	F	66	ILE
7	F	206	GLY
8	G	224	ALA
9	H	110	GLN
12	K	54	PHE
12	K	87	PHE
16	O	40	ALA
17	P	101	VAL
19	R	24	LEU
20	S	7	GLU
20	S	141	THR
22	U	49	LYS
22	U	118	ILE
23	V	9	VAL
23	V	30	SER
23	V	45	ALA
24	W	30	SER
25	X	3	LYS
26	Y	31	ASN
26	Y	34	ASN
27	Z	88	ILE
29	b	21	LEU
34	g	4	SER
36	i	96	ASN
2	A	202	TYR
3	B	54	LEU
3	B	154	SER
3	B	222	LYS
4	C	151	THR
4	C	155	GLN
4	C	253	THR
5	D	143	ARG

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Mol	Chain	Res	Type
5	D	156	PHE
5	D	216	PRO
7	F	100	MET
7	F	102	ASN
10	I	35	ASN
10	I	40	THR
10	I	52	ASN
11	J	118	LEU
14	M	93	GLY
14	M	98	ASP
14	M	110	SER
16	O	91	SER
18	Q	14	LYS
19	R	26	MET
19	R	124	VAL
20	S	6	GLN
20	S	9	GLY
20	S	60	GLU
20	S	61	LEU
21	T	28	LEU
21	T	50	SER
23	V	10	GLU
23	V	12	TYR
25	X	41	SER
25	X	63	GLN
26	Y	4	ALA
27	Z	54	ALA
28	a	59	TYR
29	b	51	GLN
33	f	87	THR
33	f	111	GLU
33	f	143	HIS
34	g	16	GLY
34	g	201	GLY
34	g	275	GLU
34	g	293	ASP
2	A	103	THR
2	A	158	VAL
2	A	195	TRP
3	B	214	LYS
4	C	44	THR
5	D	93	ASP

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Mol	Chain	Res	Type
5	D	219	GLU
6	E	67	GLN
6	E	205	PHE
7	F	53	VAL
7	F	155	GLY
9	H	63	PRO
9	H	98	ILE
11	J	134	ILE
11	J	171	ARG
12	K	92	LEU
13	L	105	LYS
14	M	78	PRO
14	M	82	VAL
16	O	25	ASP
16	O	114	ARG
17	P	28	MET
17	P	129	GLY
20	S	51	ASP
20	S	120	ARG
24	W	29	PRO
24	W	58	SER
25	X	144	ARG
26	Y	36	SER
28	a	36	ILE
37	j	24	ASN
37	j	106	HIS
3	B	207	LEU
3	B	224	ASP
4	C	112	SER
5	D	157	LEU
5	D	196	THR
6	E	195	ILE
7	F	23	VAL
8	G	152	ASP
9	H	10	SER
10	I	94	ASN
11	J	147	MET
14	M	32	ASP
16	O	42	VAL
17	P	17	TYR
17	P	69	GLU
17	P	121	ILE

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Mol	Chain	Res	Type
18	Q	97	VAL
19	R	99	VAL
21	T	29	GLU
21	T	88	VAL
27	Z	41	VAL
28	a	15	ARG
28	a	64	LEU
29	b	62	VAL
32	e	49	LEU
33	f	118	ARG
34	g	168	ASP
2	A	5	SER
2	A	21	ARG
3	B	206	PRO
6	E	105	VAL
9	H	131	PHE
11	J	110	GLN
11	J	163	PRO
13	L	3	THR
20	S	25	ASN
26	Y	64	TYR
33	f	98	VAL
34	g	64	GLY
17	P	48	GLY
17	P	53	PRO
20	S	14	ILE
33	f	126	PRO
27	Z	60	VAL
33	f	102	VAL
34	g	278	ILE
28	a	16	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	174/211 (82%)	145 (83%)	29 (17%)	2	14
3	B	198/228 (87%)	173 (87%)	25 (13%)	5	26
4	C	176/203 (87%)	157 (89%)	19 (11%)	7	33
5	D	185/196 (94%)	155 (84%)	30 (16%)	3	15
6	E	223/224 (100%)	186 (83%)	37 (17%)	2	14
7	F	174/194 (90%)	154 (88%)	20 (12%)	6	29
8	G	192/200 (96%)	174 (91%)	18 (9%)	10	39
9	H	164/170 (96%)	145 (88%)	19 (12%)	6	29
10	I	147/159 (92%)	129 (88%)	18 (12%)	6	27
11	J	153/158 (97%)	130 (85%)	23 (15%)	3	19
12	K	88/96 (92%)	75 (85%)	13 (15%)	3	19
13	L	136/137 (99%)	128 (94%)	8 (6%)	23	60
14	M	97/109 (89%)	80 (82%)	17 (18%)	2	12
15	N	127/128 (99%)	110 (87%)	17 (13%)	4	23
16	O	96/104 (92%)	85 (88%)	11 (12%)	6	29
17	P	105/119 (88%)	93 (89%)	12 (11%)	7	29
18	Q	117/119 (98%)	100 (86%)	17 (14%)	4	20
19	R	112/124 (90%)	92 (82%)	20 (18%)	2	11
20	S	128/129 (99%)	109 (85%)	19 (15%)	3	19
21	T	117/118 (99%)	103 (88%)	14 (12%)	6	27
22	U	96/107 (90%)	85 (88%)	11 (12%)	6	29
23	V	73/73 (100%)	69 (94%)	4 (6%)	25	62
24	W	110/111 (99%)	97 (88%)	13 (12%)	6	28
25	X	119/120 (99%)	108 (91%)	11 (9%)	11	40
26	Y	108/109 (99%)	98 (91%)	10 (9%)	10	40
27	Z	60/88 (68%)	55 (92%)	5 (8%)	13	45
28	a	83/100 (83%)	73 (88%)	10 (12%)	6	27
29	b	71/72 (99%)	63 (89%)	8 (11%)	7	30
30	c	55/59 (93%)	48 (87%)	7 (13%)	5	25
31	d	46/48 (96%)	45 (98%)	1 (2%)	57	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	e	47/55 (86%)	46 (98%)	1 (2%)	59	84
33	f	58/133 (44%)	48 (83%)	10 (17%)	2	13
34	g	265/272 (97%)	231 (87%)	34 (13%)	5	25
35	h	23/23 (100%)	21 (91%)	2 (9%)	12	43
36	i	83/130 (64%)	76 (92%)	7 (8%)	13	45
37	j	77/96 (80%)	69 (90%)	8 (10%)	8	35
All	All	4283/4722 (91%)	3755 (88%)	528 (12%)	10	27

All (528) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	9	LEU
2	A	15	GLN
2	A	28	ASN
2	A	32	HIS
2	A	33	GLN
2	A	37	VAL
2	A	50	VAL
2	A	53	THR
2	A	58	VAL
2	A	59	LEU
2	A	62	ARG
2	A	88	LYS
2	A	93	THR
2	A	108	THR
2	A	109	ASN
2	A	111	ILE
2	A	112	THR
2	A	123	VAL
2	A	133	ILE
2	A	134	LYS
2	A	157	ASP
2	A	165	ARG
2	A	167	LYS
2	A	170	ILE
2	A	177	LEU
2	A	193	GLN
2	A	198	MET
2	A	201	LEU
2	A	205	ARG

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Mol	Chain	Res	Type
3	B	37	THR
3	B	47	LEU
3	B	48	VAL
3	B	64	ARG
3	B	70	LEU
3	B	82	ARG
3	B	84	VAL
3	B	104	ASP
3	B	105	PHE
3	B	118	GLN
3	B	120	LEU
3	B	127	VAL
3	B	131	ASP
3	B	132	ASP
3	B	140	ILE
3	B	166	LYS
3	B	181	LEU
3	B	183	GLN
3	B	189	ILE
3	B	191	GLU
3	B	196	GLU
3	B	207	LEU
3	B	208	GLN
3	B	213	ARG
3	B	228	LEU
4	C	58	ILE
4	C	72	GLN
4	C	91	VAL
4	C	93	LYS
4	C	95	THR
4	C	99	GLN
4	C	111	ASP
4	C	116	VAL
4	C	145	ARG
4	C	146	ARG
4	C	155	GLN
4	C	199	GLU
4	C	212	LEU
4	C	213	GLU
4	C	223	ILE
4	C	230	LEU
4	C	234	LEU

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Mol	Chain	Res	Type
4	C	235	TRP
4	C	241	THR
5	D	4	ILE
5	D	7	LYS
5	D	11	LEU
5	D	17	PHE
5	D	20	GLU
5	D	21	LEU
5	D	23	GLU
5	D	37	VAL
5	D	51	ARG
5	D	57	ASP
5	D	67	ASN
5	D	76	ARG
5	D	80	LYS
5	D	89	GLU
5	D	101	GLN
5	D	103	GLU
5	D	113	LEU
5	D	122	VAL
5	D	135	GLU
5	D	141	LYS
5	D	143	ARG
5	D	156	PHE
5	D	158	ILE
5	D	162	GLN
5	D	165	ASN
5	D	166	ASP
5	D	176	LEU
5	D	178	ARG
5	D	179	GLN
5	D	208	ILE
6	E	7	LYS
6	E	9	LEU
6	E	18	TRP
6	E	22	LYS
6	E	38	LEU
6	E	45	ILE
6	E	51	ARG
6	E	60	GLU
6	E	69	HIS
6	E	75	LYS

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Mol	Chain	Res	Type
6	E	77	ARG
6	E	79	ASP
6	E	91	THR
6	E	102	VAL
6	E	108	ARG
6	E	113	ARG
6	E	116	ASP
6	E	123	LEU
6	E	139	VAL
6	E	142	HIS
6	E	155	LYS
6	E	163	ASP
6	E	168	THR
6	E	180	LEU
6	E	181	VAL
6	E	189	LEU
6	E	192	VAL
6	E	196	VAL
6	E	198	ARG
6	E	206	ASP
6	E	219	VAL
6	E	225	VAL
6	E	228	ILE
6	E	230	GLU
6	E	233	ARG
6	E	248	ILE
6	E	259	HIS
7	F	31	ILE
7	F	42	ILE
7	F	47	LYS
7	F	50	PHE
7	F	65	GLN
7	F	70	ILE
7	F	91	ILE
7	F	99	LEU
7	F	116	VAL
7	F	150	ARG
7	F	158	ARG
7	F	162	VAL
7	F	167	LEU
7	F	186	PHE
7	F	187	ARG

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Mol	Chain	Res	Type
7	F	188	ASN
7	F	192	ILE
7	F	196	LEU
7	F	201	ILE
7	F	220	GLU
8	G	15	CYS
8	G	21	GLU
8	G	25	ARG
8	G	49	VAL
8	G	52	ILE
8	G	72	ARG
8	G	79	LYS
8	G	95	LYS
8	G	105	ASP
8	G	109	LEU
8	G	126	ASN
8	G	139	ASN
8	G	164	LYS
8	G	170	THR
8	G	180	THR
8	G	182	GLN
8	G	183	ARG
8	G	195	ILE
9	H	5	GLN
9	H	7	LYS
9	H	11	GLN
9	H	15	GLU
9	H	27	LEU
9	H	33	GLU
9	H	48	GLU
9	H	72	LYS
9	H	78	THR
9	H	86	GLN
9	H	87	ASP
9	H	114	ARG
9	H	122	HIS
9	H	124	LYS
9	H	129	LEU
9	H	130	VAL
9	H	139	ARG
9	H	160	GLN
9	H	162	ILE

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Mol	Chain	Res	Type
10	I	3	ILE
10	I	8	ARG
10	I	20	GLN
10	I	21	PHE
10	I	22	ARG
10	I	26	LYS
10	I	29	LEU
10	I	32	GLN
10	I	53	GLN
10	I	58	LEU
10	I	69	SER
10	I	96	LEU
10	I	105	ASP
10	I	119	GLN
10	I	179	ARG
10	I	184	ILE
10	I	190	LEU
10	I	196	ARG
11	J	7	THR
11	J	16	LYS
11	J	20	GLU
11	J	28	LEU
11	J	33	GLU
11	J	37	LYS
11	J	45	ILE
11	J	49	LEU
11	J	58	ASP
11	J	60	LEU
11	J	64	GLU
11	J	69	ARG
11	J	70	LEU
11	J	78	ARG
11	J	88	GLU
11	J	100	LYS
11	J	107	ARG
11	J	109	LEU
11	J	131	GLN
11	J	142	ASN
11	J	145	SER
11	J	161	THR
11	J	175	LYS
12	K	14	HIS

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Mol	Chain	Res	Type
12	K	16	PHE
12	K	17	GLN
12	K	21	LEU
12	K	27	PHE
12	K	35	ILE
12	K	36	ASP
12	K	40	LEU
12	K	48	SER
12	K	63	TYR
12	K	76	LEU
12	K	86	ILE
12	K	87	PHE
13	L	10	GLU
13	L	36	LYS
13	L	38	VAL
13	L	55	ASP
13	L	80	MET
13	L	84	ILE
13	L	136	ARG
13	L	138	ASN
14	M	14	GLU
14	M	17	ILE
14	M	19	ASP
14	M	21	LEU
14	M	22	LYS
14	M	29	LEU
14	M	38	LEU
14	M	55	LEU
14	M	59	VAL
14	M	61	GLU
14	M	67	LEU
14	M	77	VAL
14	M	79	LEU
14	M	80	ILE
14	M	82	VAL
14	M	105	LYS
14	M	116	ASN
15	N	3	ARG
15	N	9	LYS
15	N	27	LYS
15	N	42	ARG
15	N	53	LEU

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Mol	Chain	Res	Type
15	N	64	LYS
15	N	73	ARG
15	N	88	LEU
15	N	96	VAL
15	N	99	ARG
15	N	100	LYS
15	N	102	LEU
15	N	104	ARG
15	N	106	ARG
15	N	107	LYS
15	N	112	LYS
15	N	121	ARG
16	O	24	ASN
16	O	37	GLU
16	O	49	LYS
16	O	65	GLN
16	O	86	THR
16	O	102	LEU
16	O	110	LEU
16	O	112	ILE
16	O	114	ARG
16	O	116	GLU
16	O	124	ASP
17	P	9	LYS
17	P	17	TYR
17	P	20	VAL
17	P	35	LYS
17	P	40	ARG
17	P	47	ARG
17	P	57	MET
17	P	79	HIS
17	P	81	ARG
17	P	84	ILE
17	P	126	VAL
17	P	127	ARG
18	Q	7	VAL
18	Q	19	VAL
18	Q	29	ILE
18	Q	45	ARG
18	Q	48	VAL
18	Q	53	LEU
18	Q	54	LEU

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Mol	Chain	Res	Type
18	Q	64	ASP
18	Q	94	GLN
18	Q	102	LYS
18	Q	113	ASP
18	Q	114	ARG
18	Q	121	SER
18	Q	127	LYS
18	Q	128	LYS
18	Q	137	ARG
18	Q	142	TYR
19	R	5	ARG
19	R	6	THR
19	R	16	LEU
19	R	17	ILE
19	R	24	LEU
19	R	26	MET
19	R	27	ASP
19	R	32	LYS
19	R	38	ILE
19	R	41	ILE
19	R	46	LEU
19	R	48	ASN
19	R	60	ARG
19	R	61	ILE
19	R	67	ARG
19	R	72	LYS
19	R	81	LYS
19	R	93	LEU
19	R	100	LEU
19	R	120	SER
20	S	16	ARG
20	S	18	LEU
20	S	20	THR
20	S	38	VAL
20	S	45	LEU
20	S	47	CYS
20	S	49	LYS
20	S	53	ASP
20	S	88	ARG
20	S	90	LYS
20	S	91	ASP
20	S	94	ASP

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Mol	Chain	Res	Type
20	S	105	LEU
20	S	109	LEU
20	S	111	ASP
20	S	112	ASP
20	S	126	ARG
20	S	140	THR
20	S	145	ARG
21	T	7	ARG
21	T	45	LEU
21	T	53	TRP
21	T	57	ARG
21	T	63	ARG
21	T	68	ARG
21	T	79	LEU
21	T	85	ASN
21	T	107	SER
21	T	111	LEU
21	T	116	ILE
21	T	124	ILE
21	T	129	LEU
21	T	140	LEU
22	U	21	LYS
22	U	34	LEU
22	U	36	ASN
22	U	40	ASN
22	U	41	ILE
22	U	43	LYS
22	U	62	VAL
22	U	64	LYS
22	U	65	ILE
22	U	92	ASP
22	U	118	ILE
23	V	1	MET
23	V	8	LEU
23	V	12	TYR
23	V	44	ARG
24	W	3	ARG
24	W	7	LEU
24	W	24	GLN
24	W	25	VAL
24	W	28	ARG
24	W	47	ILE

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Mol	Chain	Res	Type
24	W	55	ASP
24	W	75	ILE
24	W	80	ASN
24	W	104	LEU
24	W	111	MET
24	W	124	LYS
24	W	129	VAL
25	X	5	LYS
25	X	9	LEU
25	X	19	ARG
25	X	30	LYS
25	X	56	LYS
25	X	73	ARG
25	X	79	ASN
25	X	84	THR
25	X	94	ASN
25	X	100	ASP
25	X	107	PHE
26	Y	8	ARG
26	Y	10	ARG
26	Y	20	ARG
26	Y	31	ASN
26	Y	34	ASN
26	Y	35	VAL
26	Y	57	VAL
26	Y	70	THR
26	Y	84	LYS
26	Y	99	LYS
27	Z	57	TYR
27	Z	60	VAL
27	Z	77	ARG
27	Z	82	HIS
27	Z	97	LYS
28	a	12	LYS
28	a	15	ARG
28	a	28	ARG
28	a	34	LYS
28	a	38	ARG
28	a	53	LEU
28	a	59	TYR
28	a	64	LEU
28	a	69	ASN

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Mol	Chain	Res	Type
28	a	89	ARG
29	b	3	LEU
29	b	9	HIS
29	b	20	LYS
29	b	23	THR
29	b	24	LEU
29	b	54	VAL
29	b	57	GLU
29	b	67	THR
30	c	8	THR
30	c	11	LYS
30	c	16	LEU
30	c	30	VAL
30	c	32	PHE
30	c	38	ARG
30	c	48	VAL
31	d	32	ARG
32	e	26	LYS
33	f	82	LYS
33	f	85	TYR
33	f	90	LYS
33	f	93	HIS
33	f	94	LYS
33	f	96	LYS
33	f	105	TYR
33	f	109	ASP
33	f	116	LYS
33	f	129	PHE
34	g	43	LEU
34	g	49	THR
34	g	55	PHE
34	g	60	ARG
34	g	67	HIS
34	g	70	GLN
34	g	74	VAL
34	g	97	THR
34	g	124	ILE
34	g	137	THR
34	g	168	ASP
34	g	175	VAL
34	g	188	LEU
34	g	195	ILE

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Mol	Chain	Res	Type
34	g	203	ASN
34	g	210	GLN
34	g	232	LEU
34	g	238	PHE
34	g	240	ASN
34	g	242	ASP
34	g	244	LYS
34	g	271	ASP
34	g	273	GLU
34	g	275	GLU
34	g	276	VAL
34	g	284	GLU
34	g	292	GLN
34	g	293	ASP
34	g	299	LEU
34	g	304	ASP
34	g	308	LEU
34	g	314	ASP
34	g	316	VAL
34	g	321	GLN
35	h	12	ARG
35	h	16	LYS
36	i	28	TYR
36	i	46	ARG
36	i	58	MET
36	i	62	ARG
36	i	70	TRP
36	i	97	LEU
36	i	116	ASN
37	j	25	TYR
37	j	39	LEU
37	j	62	PHE
37	j	65	ASN
37	j	73	GLU
37	j	83	ASP
37	j	99	GLN
37	j	105	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	109	ASN

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Mol	Chain	Res	Type
2	A	131	GLN
3	B	101	HIS
3	B	220	GLN
4	C	99	GLN
5	D	67	ASN
5	D	159	HIS
5	D	162	GLN
5	D	165	ASN
5	D	179	GLN
6	E	50	ASN
6	E	112	HIS
6	E	130	GLN
6	E	224	ASN
7	F	36	GLN
7	F	39	GLN
7	F	40	GLN
7	F	46	ASN
7	F	188	ASN
7	F	226	ASN
8	G	10	ASN
8	G	13	GLN
8	G	139	ASN
9	H	42	GLN
9	H	155	ASN
10	I	116	HIS
12	K	17	GLN
12	K	58	GLN
13	L	8	GLN
13	L	22	ASN
15	N	62	GLN
16	O	12	GLN
16	O	29	HIS
16	O	80	HIS
16	O	99	GLN
17	P	79	HIS
18	Q	83	GLN
19	R	48	ASN
19	R	62	GLN
19	R	83	GLN
19	R	105	GLN
20	S	25	ASN
20	S	78	HIS

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Mol	Chain	Res	Type
20	S	99	HIS
20	S	122	HIS
21	T	25	GLN
21	T	64	HIS
21	T	85	ASN
21	T	91	HIS
21	T	93	HIS
21	T	101	ASN
21	T	106	GLN
22	U	40	ASN
22	U	44	ASN
22	U	105	GLN
23	V	7	GLN
24	W	24	GLN
25	X	18	HIS
25	X	22	ASN
25	X	79	ASN
27	Z	44	GLN
27	Z	82	HIS
28	a	17	HIS
29	b	42	ASN
31	d	10	HIS
36	i	44	ASN
36	i	55	ASN
36	i	85	GLN
37	j	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1799 (98%)	675 (37%)	0

All (675) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	32	U

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Mol	Chain	Res	Type
1	2	34	G
1	2	39	A
1	2	40	A
1	2	42	G
1	2	45	U
1	2	47	A
1	2	51	A
1	2	57	G
1	2	59	C
1	2	60	U
1	2	61	A
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	78	A
1	2	80	A
1	2	82	U
1	2	93	A
1	2	100	A
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	123	G
1	2	124	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	136	C
1	2	137	U

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Mol	Chain	Res	Type
1	2	138	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	144	A
1	2	146	A
1	2	147	U
1	2	149	U
1	2	157	U
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	167	A
1	2	173	U
1	2	176	U
1	2	178	A
1	2	183	C
1	2	190	C
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	203	G
1	2	209	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	224	A
1	2	225	A
1	2	226	U
1	2	227	G
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	233	G
1	2	237	U
1	2	239	C
1	2	240	U

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Mol	Chain	Res	Type
1	2	248	U
1	2	249	C
1	2	256	A
1	2	259	U
1	2	264	A
1	2	265	A
1	2	266	U
1	2	267	C
1	2	268	G
1	2	270	A
1	2	271	U
1	2	274	C
1	2	275	C
1	2	276	U
1	2	277	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	286	G
1	2	287	A
1	2	288	U
1	2	289	G
1	2	294	A
1	2	298	A
1	2	301	U
1	2	307	C
1	2	308	C
1	2	309	C
1	2	311	A
1	2	312	U
1	2	313	C
1	2	314	A
1	2	315	A
1	2	320	C
1	2	321	G
1	2	336	G
1	2	337	C
1	2	350	C
1	2	351	A
1	2	358	A
1	2	359	A
1	2	360	C

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Mol	Chain	Res	Type
1	2	361	G
1	2	368	A
1	2	369	A
1	2	377	A
1	2	379	U
1	2	382	G
1	2	384	A
1	2	387	G
1	2	389	G
1	2	392	C
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	412	U
1	2	415	A
1	2	416	A
1	2	417	G
1	2	418	G
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A
1	2	433	G
1	2	438	U
1	2	439	U
1	2	443	C
1	2	444	A
1	2	447	C
1	2	452	U
1	2	458	G
1	2	459	A
1	2	460	G
1	2	463	A
1	2	467	A
1	2	473	A
1	2	474	A
1	2	476	A
1	2	479	G
1	2	480	A

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Mol	Chain	Res	Type
1	2	481	U
1	2	488	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	494	C
1	2	495	G
1	2	496	G
1	2	497	G
1	2	499	C
1	2	500	U
1	2	501	U
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	510	A
1	2	513	G
1	2	514	A
1	2	516	U
1	2	518	C
1	2	523	U
1	2	526	A
1	2	527	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	536	G
1	2	539	G
1	2	540	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	547	G
1	2	548	G
1	2	554	A
1	2	557	U
1	2	558	C
1	2	564	C

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Mol	Chain	Res	Type
1	2	565	C
1	2	566	A
1	2	567	G
1	2	573	G
1	2	577	U
1	2	579	A
1	2	581	U
1	2	582	C
1	2	584	A
1	2	593	A
1	2	594	G
1	2	610	U
1	2	618	A
1	2	619	A
1	2	622	A
1	2	634	A
1	2	637	U
1	2	638	U
1	2	639	U
1	2	641	G
1	2	646	G
1	2	647	G
1	2	648	U
1	2	649	U
1	2	650	G
1	2	652	C
1	2	653	C
1	2	654	G
1	2	655	G
1	2	678	U
1	2	679	U
1	2	683	C
1	2	684	A
1	2	691	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	701	U
1	2	704	C

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Mol	Chain	Res	Type
1	2	705	U
1	2	706	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	712	U
1	2	713	A
1	2	714	C
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	724	G
1	2	726	G
1	2	727	C
1	2	729	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	740	A
1	2	741	C
1	2	742	U
1	2	743	U
1	2	753	A
1	2	754	A
1	2	765	G
1	2	766	U
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	785	C
1	2	786	G
1	2	788	A

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Mol	Chain	Res	Type
1	2	789	U
1	2	792	A
1	2	793	U
1	2	794	U
1	2	795	A
1	2	811	A
1	2	812	U
1	2	813	A
1	2	814	G
1	2	817	C
1	2	818	G
1	2	819	U
1	2	820	U
1	2	821	U
1	2	822	G
1	2	823	G
1	2	825	U
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	831	U
1	2	832	U
1	2	834	U
1	2	840	U
1	2	844	G
1	2	845	G
1	2	849	A
1	2	852	G
1	2	855	A
1	2	856	U
1	2	860	U
1	2	862	A
1	2	863	U
1	2	872	U
1	2	875	G
1	2	876	G
1	2	877	G
1	2	895	U
1	2	896	C
1	2	897	A

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Mol	Chain	Res	Type
1	2	898	G
1	2	904	A
1	2	905	A
1	2	911	U
1	2	913	G
1	2	914	A
1	2	915	U
1	2	919	U
1	2	920	U
1	2	927	U
1	2	932	A
1	2	933	C
1	2	934	U
1	2	941	G
1	2	943	A
1	2	950	A
1	2	958	U
1	2	959	U
1	2	965	A
1	2	969	A
1	2	972	A
1	2	978	A
1	2	981	U
1	2	983	G
1	2	987	A
1	2	991	A
1	2	993	G
1	2	994	A
1	2	1003	U
1	2	1011	U
1	2	1020	C
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A

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Mol	Chain	Res	Type
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1062	U
1	2	1065	C
1	2	1071	C
1	2	1075	A
1	2	1080	A
1	2	1081	C
1	2	1082	G
1	2	1083	A
1	2	1091	A
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1098	U
1	2	1099	G
1	2	1107	G
1	2	1108	G
1	2	1110	G
1	2	1113	G
1	2	1118	G
1	2	1121	G
1	2	1130	A
1	2	1137	A
1	2	1142	A
1	2	1149	G
1	2	1150	A
1	2	1157	C
1	2	1158	C
1	2	1166	G
1	2	1167	U
1	2	1173	C
1	2	1175	G
1	2	1184	U
1	2	1189	C
1	2	1190	U
1	2	1193	A

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Mol	Chain	Res	Type
1	2	1194	C
1	2	1195	A
1	2	1196	C
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1203	A
1	2	1204	C
1	2	1211	G
1	2	1212	G
1	2	1215	C
1	2	1216	A
1	2	1217	G
1	2	1218	A
1	2	1222	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1234	C
1	2	1236	G
1	2	1238	U
1	2	1240	G
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1244	G
1	2	1246	U
1	2	1247	C
1	2	1250	U
1	2	1254	G
1	2	1258	U
1	2	1259	U
1	2	1265	U
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1274	A
1	2	1282	U
1	2	1283	C

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Mol	Chain	Res	Type
1	2	1284	U
1	2	1296	G
1	2	1298	G
1	2	1305	C
1	2	1306	U
1	2	1307	G
1	2	1313	U
1	2	1314	U
1	2	1316	C
1	2	1317	G
1	2	1320	A
1	2	1321	A
1	2	1323	G
1	2	1324	A
1	2	1336	A
1	2	1339	U
1	2	1340	A
1	2	1343	A
1	2	1344	A
1	2	1347	A
1	2	1349	G
1	2	1350	G
1	2	1351	U
1	2	1353	G
1	2	1356	G
1	2	1358	C
1	2	1359	A
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1368	U
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1380	A
1	2	1384	G
1	2	1388	U
1	2	1389	A
1	2	1396	U

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Mol	Chain	Res	Type
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1404	A
1	2	1410	G
1	2	1411	U
1	2	1412	U
1	2	1413	U
1	2	1416	G
1	2	1425	A
1	2	1426	G
1	2	1429	C
1	2	1430	U
1	2	1433	G
1	2	1434	A
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1445	C
1	2	1446	G
1	2	1449	C
1	2	1450	U
1	2	1454	C
1	2	1456	G
1	2	1457	C
1	2	1458	A
1	2	1460	G
1	2	1461	C
1	2	1463	C
1	2	1464	G
1	2	1467	A
1	2	1468	C
1	2	1469	A
1	2	1471	U
1	2	1475	G
1	2	1476	G
1	2	1481	A
1	2	1484	G
1	2	1485	A
1	2	1487	U
1	2	1488	A
1	2	1489	C

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Mol	Chain	Res	Type
1	2	1490	A
1	2	1491	A
1	2	1492	C
1	2	1494	U
1	2	1495	U
1	2	1498	C
1	2	1501	A
1	2	1502	G
1	2	1504	G
1	2	1505	G
1	2	1506	U
1	2	1507	C
1	2	1508	U
1	2	1509	G
1	2	1512	U
1	2	1514	A
1	2	1519	G
1	2	1520	U
1	2	1521	G
1	2	1522	A
1	2	1531	C
1	2	1532	G
1	2	1533	U
1	2	1534	G
1	2	1535	C
1	2	1536	U
1	2	1537	G
1	2	1539	G
1	2	1543	A
1	2	1546	G
1	2	1552	U
1	2	1553	A
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1563	C
1	2	1566	C
1	2	1569	C
1	2	1570	G
1	2	1571	A
1	2	1573	G
1	2	1580	U

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Mol	Chain	Res	Type
1	2	1581	A
1	2	1583	U
1	2	1588	G
1	2	1591	A
1	2	1593	U
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1598	A
1	2	1599	G
1	2	1603	G
1	2	1605	G
1	2	1606	U
1	2	1613	C
1	2	1614	G
1	2	1616	C
1	2	1617	C
1	2	1632	C
1	2	1633	A
1	2	1634	C
1	2	1643	G
1	2	1647	G
1	2	1655	U
1	2	1656	G
1	2	1678	G
1	2	1679	A
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1696	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U

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Mol	Chain	Res	Type
1	2	1703	C
1	2	1705	A
1	2	1706	U
1	2	1707	C
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1725	G
1	2	1729	A
1	2	1730	A
1	2	1742	A
1	2	1743	G
1	2	1748	A
1	2	1750	U
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1760	A
1	2	1763	A
1	2	1764	A
1	2	1766	G
1	2	1767	U
1	2	1770	C
1	2	1777	U
1	2	1778	G
1	2	1779	A
1	2	1780	A
1	2	1781	C
1	2	1784	G
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1794	C
1	2	1795	A
1	2	1796	U
1	2	1797	U
1	2	1798	A

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 83 ligands modelled in this entry, 83 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.