



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 21, 2018 – 08:37 PM EST

PDB ID : 5OOM  
EMDB ID: : EMD-3843  
Title : Structure of a native assembly intermediate of the human mitochondrial ribosome with unfolded interfacial rRNA  
Authors : Brown, A.; Rathore, S.; Kimanius, D.; Aibara, S.; Bai, X.C.; Rorbach, J.; Amunts, A.; Ramakrishnan, V.  
Deposited on : 2017-08-08  
Resolution : 3.03 Å(reported)  
Based on PDB ID : 3J9M

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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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) : rb-20030736

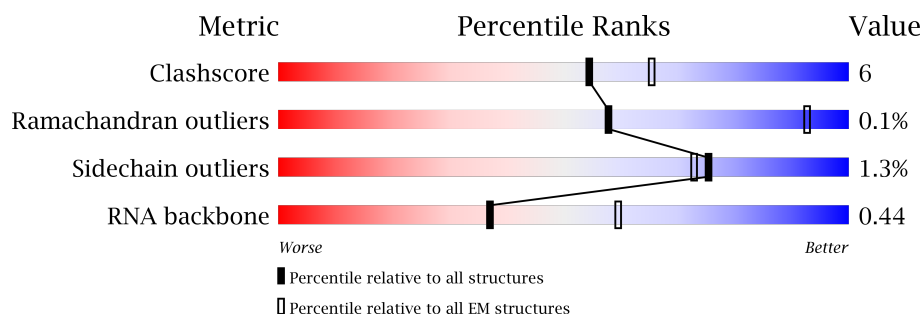
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.03 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.



















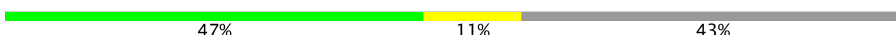








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	A	1559	30% 29% 10% . 30%
2	B	69	43% 32% . . 19%
3	D	305	58% 14% 28%
4	E	348	68% 14% 18%
5	F	311	66% 14% . 20%
6	H	267	30% 6% 64%
7	I	261	48% 12% 39%
8	J	192	50% 22% . 27%











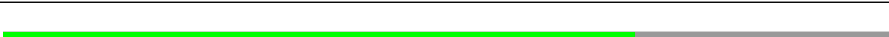


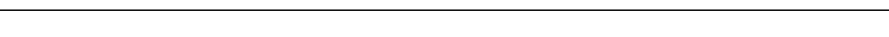
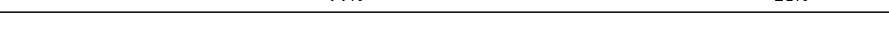
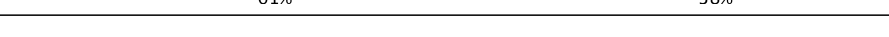



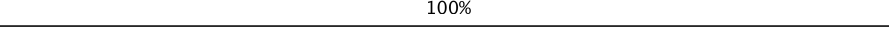

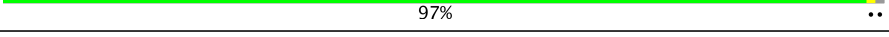
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Mol	Chain	Length	Quality of chain
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	
29	5	423	
30	6	380	
31	7	338	
32	8	206	
33	9	137	

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Mol	Chain	Length	Quality of chain
34	a	142	
35	b	215	
36	c	332	
37	d	306	
38	e	279	
39	f	212	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	k	112	
45	l	138	
46	m	128	
47	o	102	
48	p	206	
49	q	222	
50	r	196	
51	s	439	
52	t	28	
53	u	234	
54	v	70	
55	w	156	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 90739 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1092	Total	C	N	O	P	0	0
			23184	10409	4202	7481	1092		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	220	Total	C	N	O	S	0	0
			1706	1059	339	299	9		

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	285	Total	C	N	O	S	0	0
			2258	1457	384	406	11		

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total	C	N	O	0	0
			784	498	152	134		

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	159	Total	C	N	O	S	0	0
			1305	835	239	224	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	139	Total	C	N	O	S	0	0
			1154	734	220	197	3		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 31 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 32 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 33 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 34 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 36 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 39 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 44 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	79	Total	C	N	O	S	0	0
			665	420	130	112	3		

- Molecule 48 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 51 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 52 is a protein called Unknown protein or protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 53 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 54 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 55 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

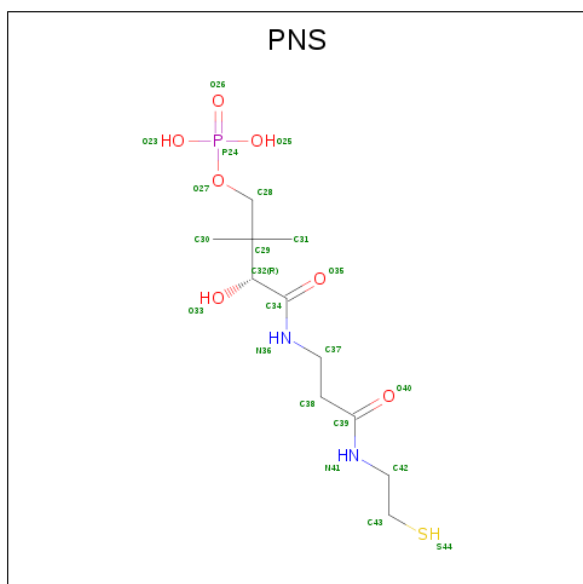
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	W	1	Total	Mg	0
			1	1	
56	A	47	Total	Mg	0
			47	47	
56	g	1	Total	Mg	0
			1	1	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	0	1	Total	Zn	0
			1	1	
57	I	1	Total	Zn	0
			1	1	

- Molecule 58 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).

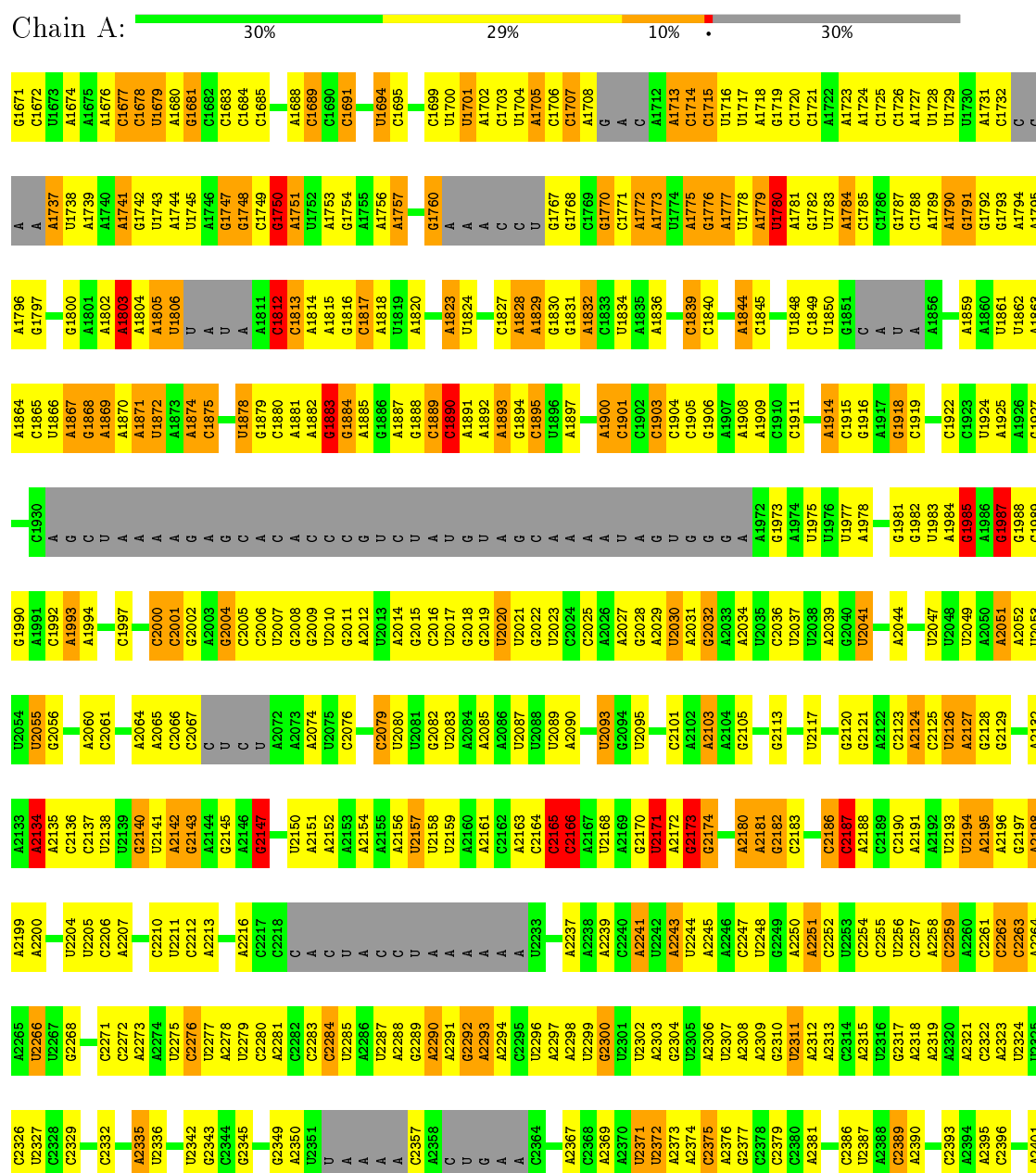


Mol	Chain	Residues	Atoms						AltConf
58	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

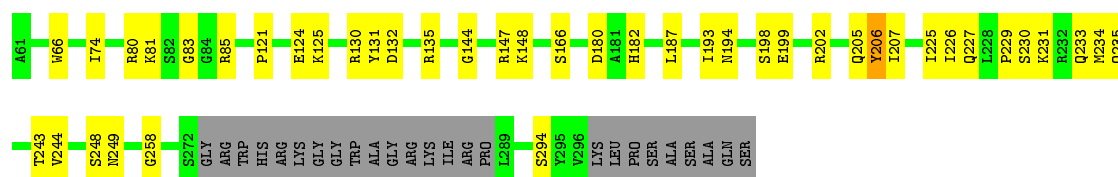
### 3 Residue-property plots

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: 16S ribosomal RNA

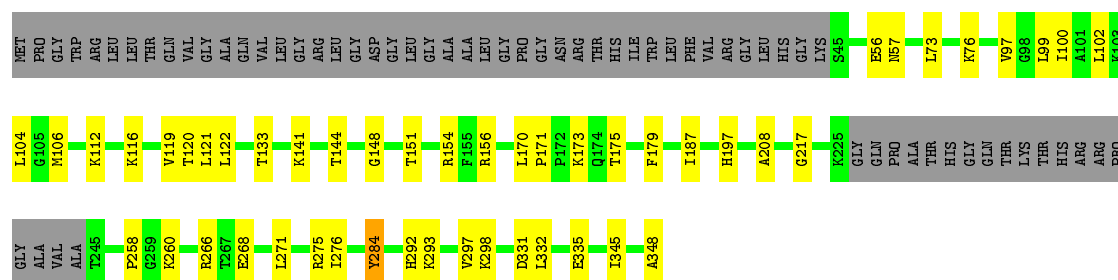






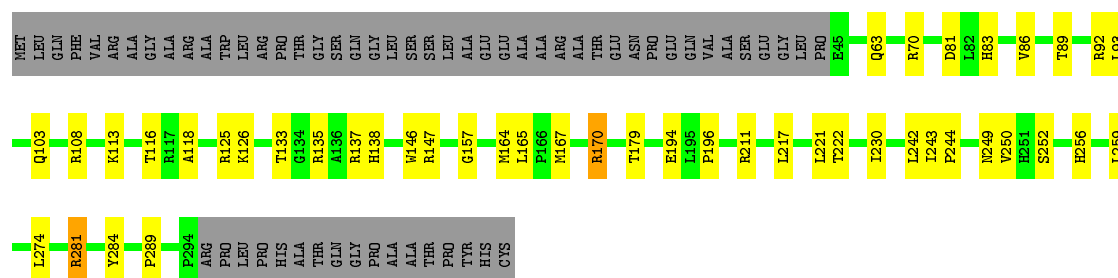
- Molecule 4: 39S ribosomal protein L3, mitochondrial

Chain E: 68% 14% 18%



- Molecule 5: 39S ribosomal protein L4, mitochondrial

Chain F: 66% 14% 20%



- Molecule 6: 39S ribosomal protein L9, mitochondrial

Chain H: 30% 6% 64%



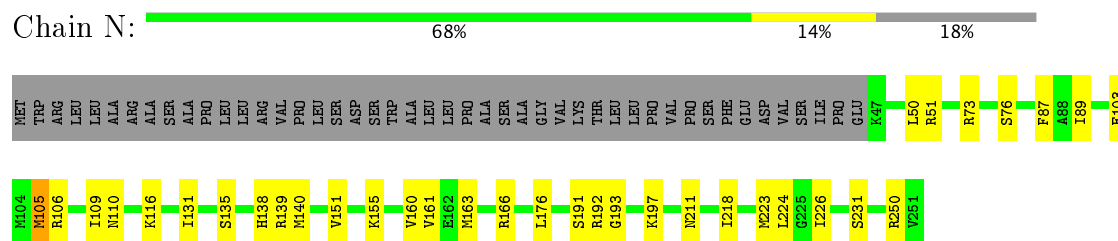
- Molecule 7: 39S ribosomal protein L10, mitochondrial

Chain I: 48% 12% 39%

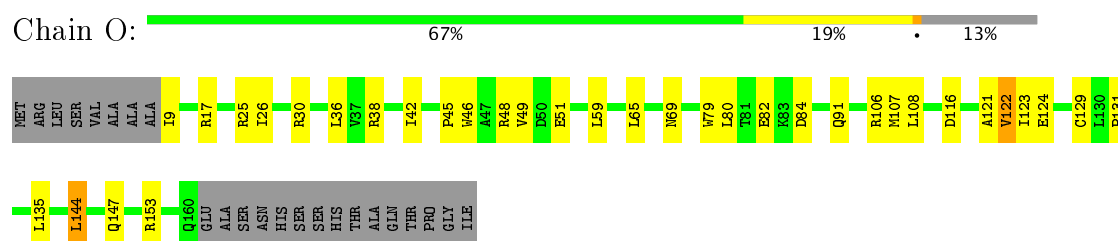




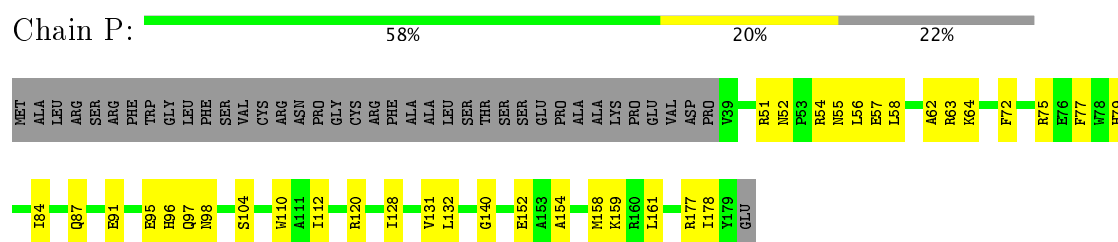
- Molecule 12: 39S ribosomal protein L16, mitochondrial



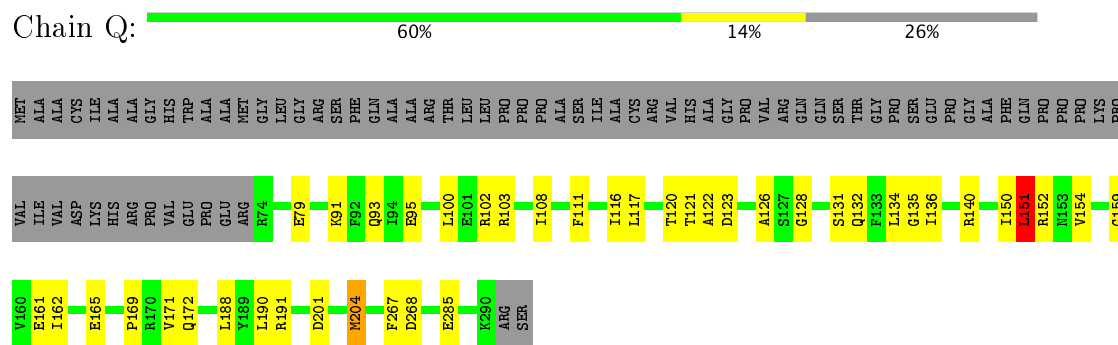
- Molecule 13: 39S ribosomal protein L17, mitochondrial



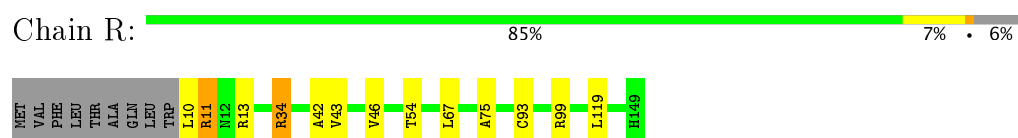
- Molecule 14: 39S ribosomal protein L18, mitochondrial



- Molecule 15: 39S ribosomal protein L19, mitochondrial

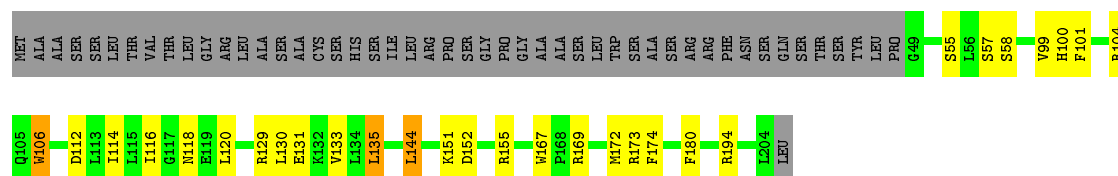


- Molecule 16: 39S ribosomal protein L20, mitochondrial



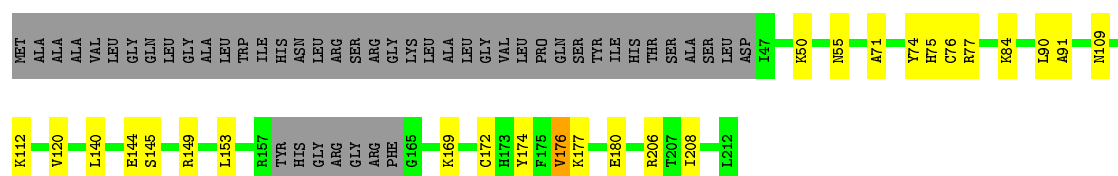
- Molecule 17: 39S ribosomal protein L21, mitochondrial

Chain S: 



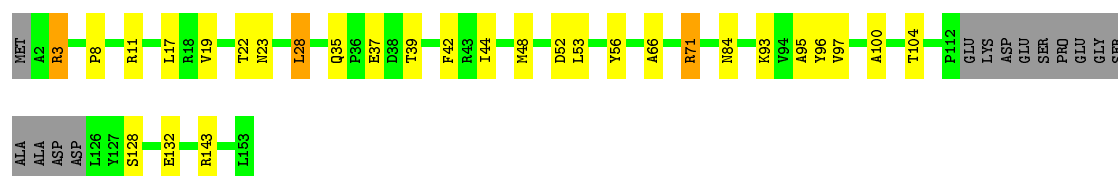
- Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T: 



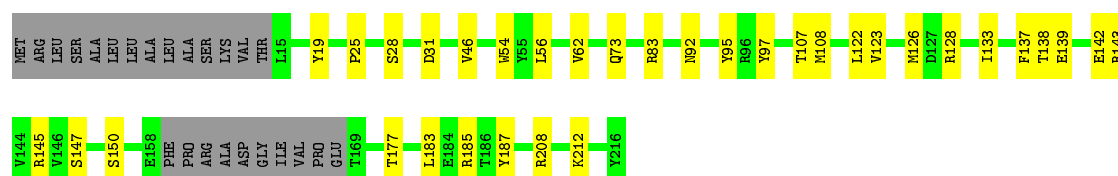
- Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U: 



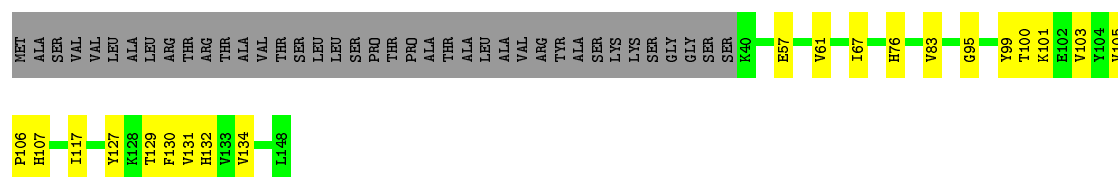
- Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V: 




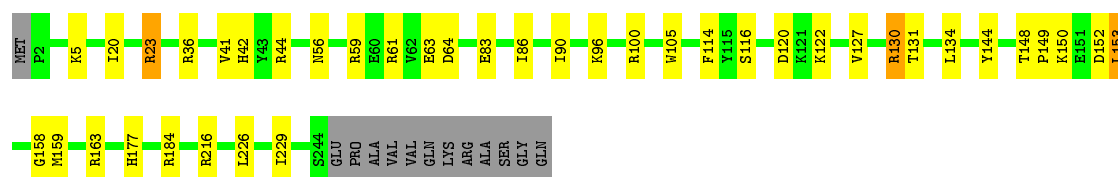
- Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W: 



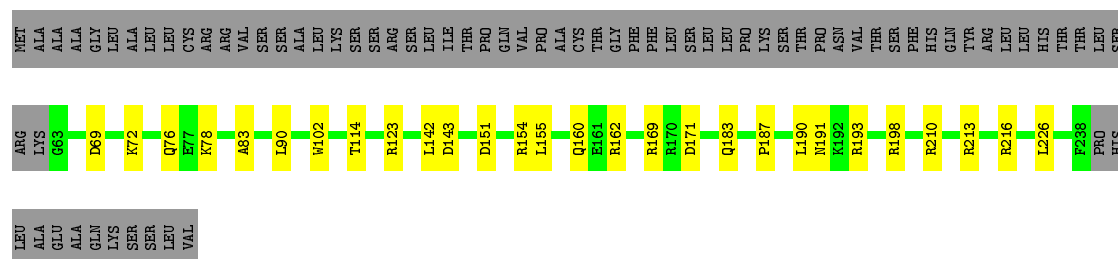
- Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X: 



- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 59% 11% 30%



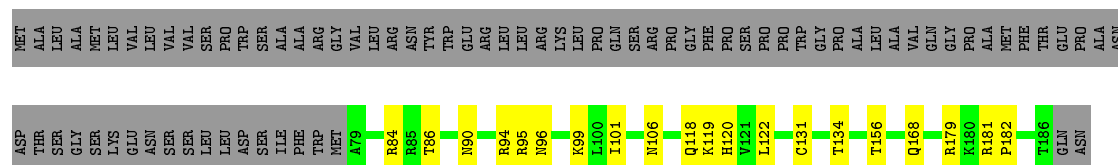
- Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 65% 10% 25%



- Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0: 47% 11% 43%



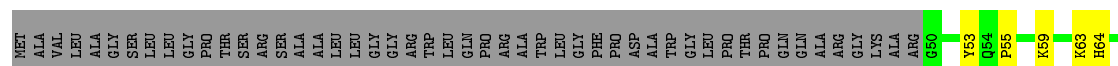
- Molecule 26: 39S ribosomal protein L33, mitochondrial

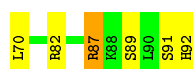
Chain 1: 58% 22% 20%



- Molecule 27: 39S ribosomal protein L34, mitochondrial

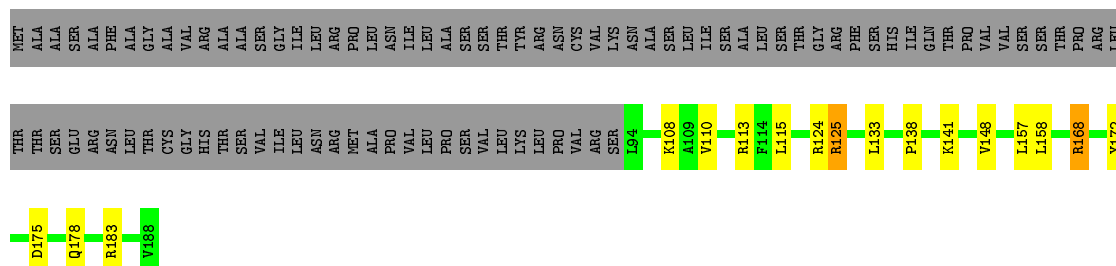
Chain 2: 35% 11% 53%





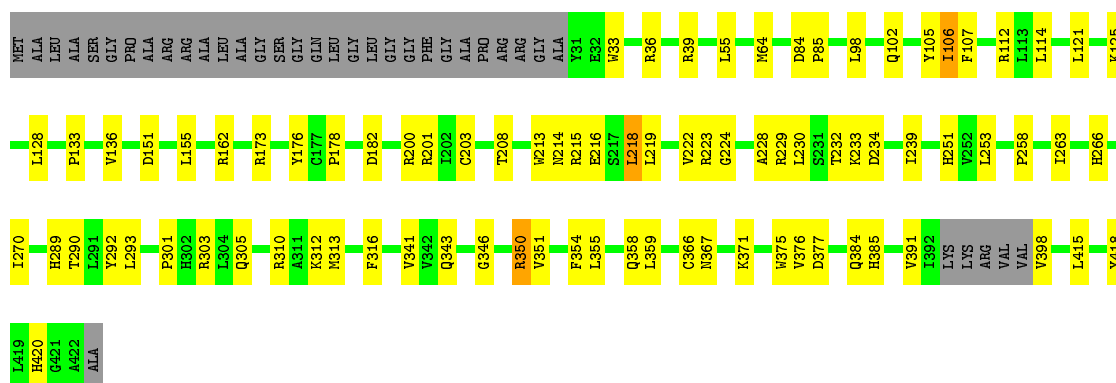
- Molecule 28: 39S ribosomal protein L35, mitochondrial

Chain 3: 41% 8% 49%



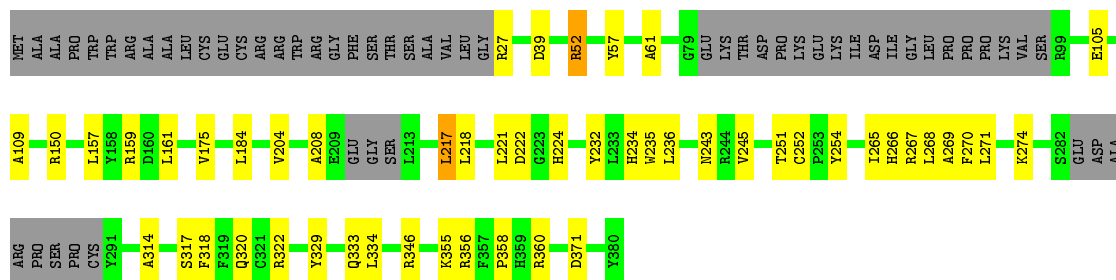
- Molecule 29: 39S ribosomal protein L37, mitochondrial

Chain 5: 71% 19% 9%



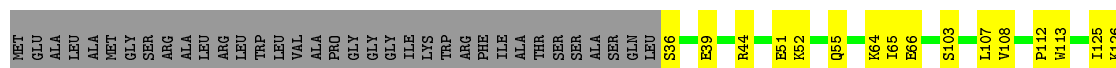
- Molecule 30: 39S ribosomal protein L38, mitochondrial

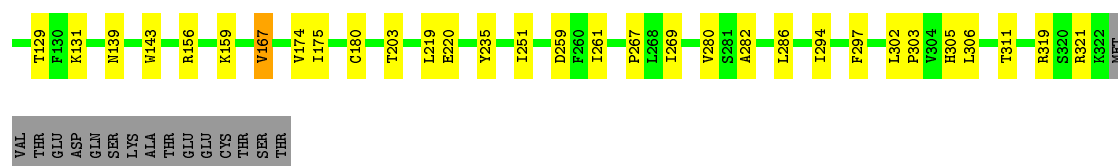
Chain 6: 72% 13% 15%



- Molecule 31: 39S ribosomal protein L39, mitochondrial

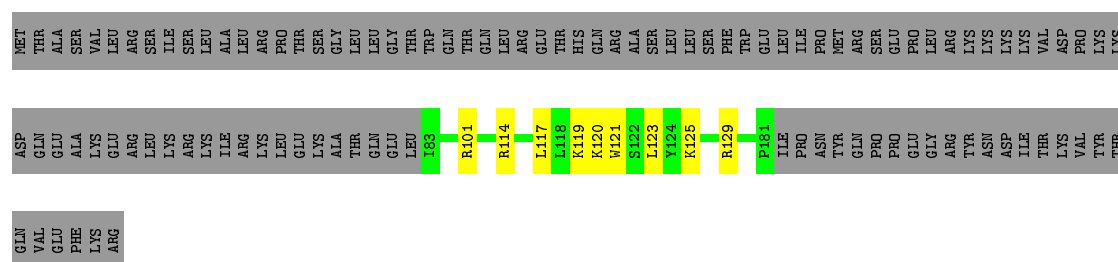
Chain 7: 71% 14% 15%





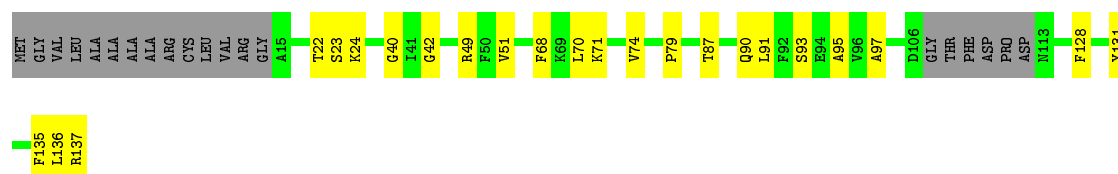
- Molecule 32: 39S ribosomal protein L40, mitochondrial

Chain 8: 44% 52%



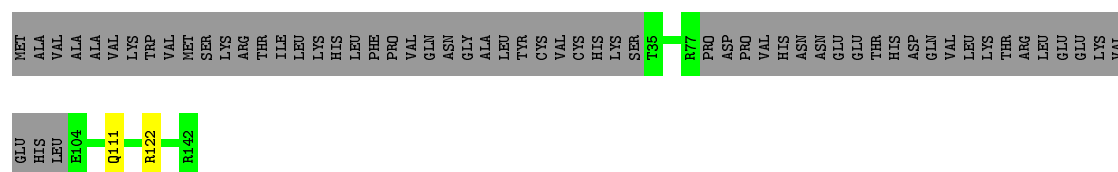
- Molecule 33: 39S ribosomal protein L41, mitochondrial

Chain 9: 69% 17% 15%



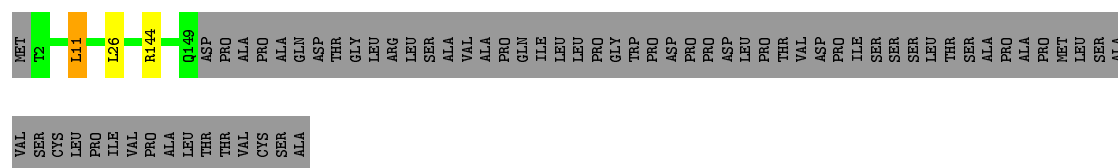
- Molecule 34: 39S ribosomal protein L42, mitochondrial

Chain a: 56% 42%



- Molecule 35: 39S ribosomal protein L43, mitochondrial

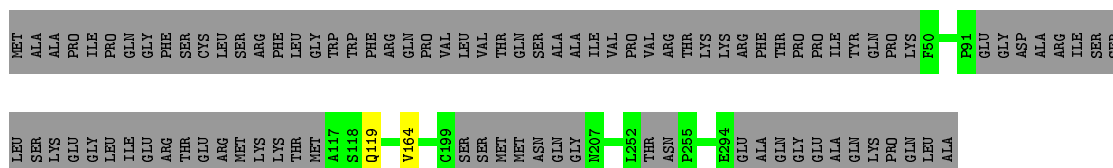
Chain b: 67% 31%



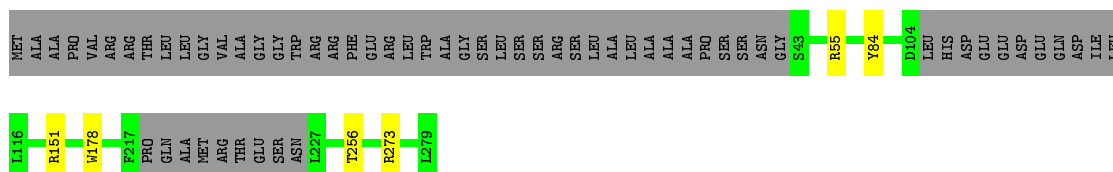
- Molecule 36: 39S ribosomal protein L44, mitochondrial

Chain c: 82% 17%

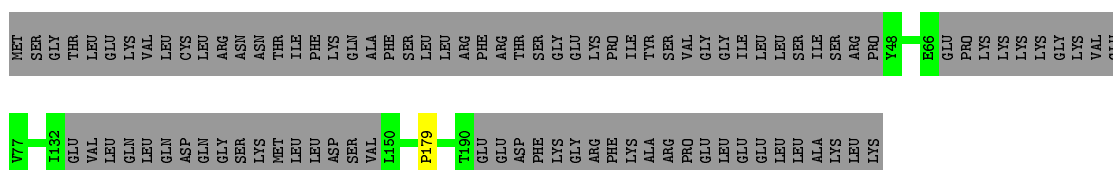
- Molecule 37: 39S ribosomal protein L45, mitochondrial



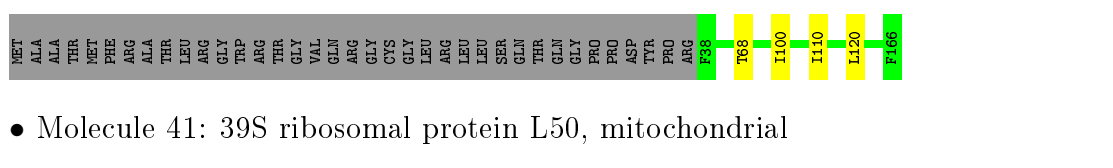
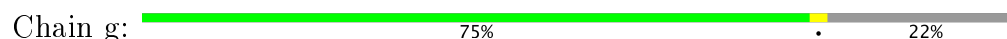
- Molecule 38: 39S ribosomal protein L46, mitochondrial



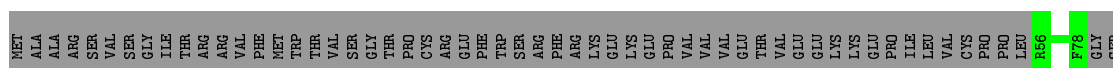
- Molecule 39: 39S ribosomal protein L48, mitochondrial



- Molecule 40: 39S ribosomal protein L49, mitochondrial



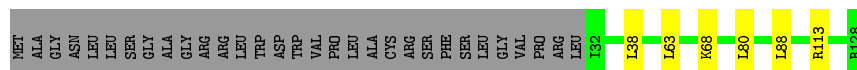
- Molecule 41: 39S ribosomal protein L50, mitochondrial





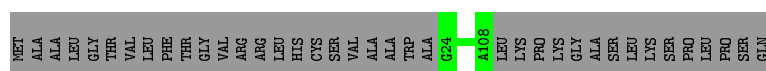
- Molecule 42: 39S ribosomal protein L51, mitochondrial

Chain i: 71% 5% 24%



- Molecule 43: 39S ribosomal protein L52, mitochondrial

Chain j: 69% 31%



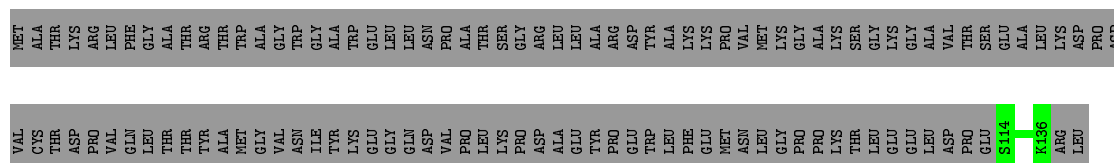
- Molecule 44: 39S ribosomal protein L53, mitochondrial

Chain k: 71% 29%



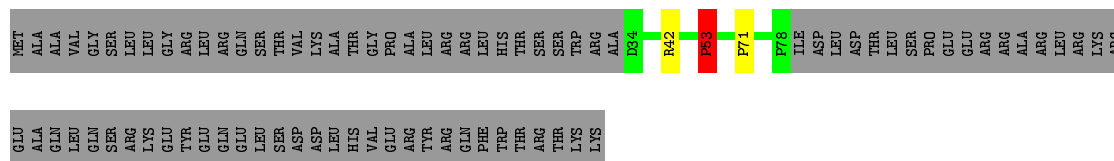
- Molecule 45: 39S ribosomal protein L54, mitochondrial

Chain l: 17% 83%



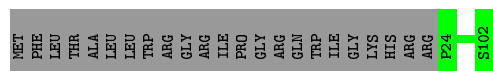
- Molecule 46: 39S ribosomal protein L55, mitochondrial

Chain m: 33% 65%



- Molecule 47: Ribosomal protein 63, mitochondrial

Chain o: 77% 23%



- Molecule 48: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1

- Molecule 50: 39S ribosomal protein S18a, mitochondrial

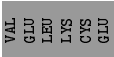
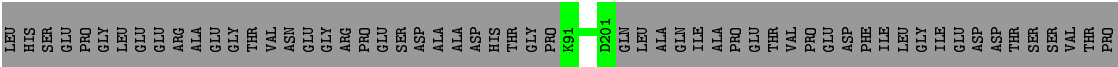
- Molecule 51: 39S ribosomal protein S30, mitochondrial

- Molecule 52: Unknown protein or protein extension

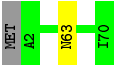
There are no outlier residues recorded for this chain.

- Molecule 53: Mitochondrial assembly of ribosomal large subunit protein 1

MET	GLY	PRO	GLY	GLY	ARG	VAL	ARG	ALA	ALA	ALA	LEU	LEU	ALA	PRO	PRO	MET	LEU	TRP	ARG	ARG	ALA	ALA	VAL	VAL	SER	SER	SER	VAL	VAL	ALA	ALA	GLY	GLY	GLU	GLY	GLY	LEU	LEU	ARG	ARG	LEU	LEU	LEU	VAL	VAL	VAL	GLN	ARG	ARG	LEU	PRO	PRO	VAL	VAL	GLY	GLY	ARG	ALA	ALA	ALA	CYS	PHE	CYS	GLN	THR	PRO	ASN	PHE	VAL	VAL	ARG	ARG	GLY
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- Molecule 54: MIEF1 upstream open reading frame protein



- Molecule 55: Acyl carrier protein, mitochondrial



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.56	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	130841	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, PNS

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	1.77	301/25926 (1.2%)	1.45	433/40305 (1.1%)
10	L	0.51	0/904	0.63	1/1218 (0.1%)
11	M	0.88	1/2359 (0.0%)	0.80	4/3185 (0.1%)
12	N	0.56	0/1697	0.63	0/2281
13	O	0.84	1/1269 (0.1%)	0.83	2/1708 (0.1%)
14	P	0.68	0/1173	0.71	1/1588 (0.1%)
15	Q	0.60	1/1846 (0.1%)	0.69	2/2487 (0.1%)
16	R	1.04	3/1174 (0.3%)	0.89	5/1572 (0.3%)
17	S	0.91	1/1276 (0.1%)	0.82	2/1729 (0.1%)
18	T	1.00	1/1335 (0.1%)	0.76	2/1796 (0.1%)
19	U	0.87	0/1183	0.78	1/1600 (0.1%)
2	B	0.71	0/1328	1.26	10/2056 (0.5%)
20	V	0.73	0/1616	0.64	0/2189
21	W	0.92	2/881 (0.2%)	0.72	0/1188
22	X	0.68	0/2090	0.69	1/2825 (0.0%)
23	Y	0.83	0/1552	0.71	1/2079 (0.0%)
24	Z	0.82	1/1003 (0.1%)	0.74	0/1354
25	0	0.85	1/895 (0.1%)	0.74	0/1201
26	1	0.63	0/438	0.81	0/583
27	2	1.05	1/357 (0.3%)	0.84	0/475
28	3	1.03	0/852	0.79	1/1136 (0.1%)
29	5	0.65	0/3250	0.70	2/4429 (0.0%)
3	D	0.58	0/1736	0.65	0/2335
30	6	0.66	0/2726	0.65	2/3715 (0.1%)
31	7	0.67	1/2391 (0.0%)	0.67	0/3234
32	8	0.39	0/855	0.55	0/1152
33	9	0.75	0/972	0.68	0/1306
34	a	0.84	0/709	0.65	0/963
35	b	0.92	0/1202	0.78	2/1626 (0.1%)
36	c	0.78	0/2264	0.71	1/3059 (0.0%)
37	d	0.64	0/1790	0.66	0/2423
38	e	0.30	0/1797	0.59	2/2422 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	f	0.47	0/931	0.58	0/1259
4	E	0.74	0/2322	0.71	1/3148 (0.0%)
40	g	0.91	0/1102	0.77	1/1503 (0.1%)
41	h	0.63	0/847	0.71	1/1150 (0.1%)
42	i	1.05	1/849 (0.1%)	0.87	5/1135 (0.4%)
43	j	0.75	0/698	0.64	0/940
44	k	0.32	0/635	0.60	0/855
45	l	0.29	0/226	0.43	0/299
46	m	0.29	0/379	0.75	1/510 (0.2%)
47	o	0.74	0/682	0.66	0/916
48	p	0.53	0/1071	0.62	0/1433
49	q	0.58	0/1107	0.59	0/1498
5	F	0.94	1/2071 (0.0%)	0.81	0/2817
50	r	0.69	0/1238	0.67	0/1676
51	s	0.80	0/3114	0.77	5/4225 (0.1%)
53	u	0.40	0/949	0.59	0/1281
54	v	0.35	0/597	0.58	0/796
55	w	0.31	0/647	0.61	0/871
6	H	0.65	0/798	0.71	0/1073
7	I	0.41	0/1308	0.68	2/1761 (0.1%)
8	J	0.30	0/1077	0.58	0/1452
9	K	0.84	0/1495	0.76	2/2029 (0.1%)
All	All	1.11	317/94989 (0.3%)	1.00	493/133846 (0.4%)

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
26	1	0	1
31	7	0	1
40	g	0	1
46	m	0	1
51	s	0	1
8	J	0	1
All	All	0	6

All (317) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1789	A	N9-C4	-9.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2308	A	N9-C4	-8.74	1.32	1.37
1	A	1751	A	N9-C8	-7.99	1.31	1.37
1	A	1864	A	C5-C4	-7.96	1.33	1.38
42	i	68	LYS	C-N	-7.79	1.16	1.34
1	A	2152	A	N9-C4	-7.70	1.33	1.37
1	A	1818	A	N9-C4	-7.56	1.33	1.37
1	A	2004	G	N7-C5	-7.40	1.34	1.39
1	A	1785	C	C4-C5	-7.31	1.37	1.43
24	Z	151	LEU	C-N	-7.25	1.17	1.34
1	A	2051	A	N9-C4	-7.18	1.33	1.37
1	A	1772	A	C5-C4	-7.14	1.33	1.38
1	A	2307	U	C2-N3	-7.07	1.32	1.37
1	A	1787	G	C5-C4	-6.95	1.33	1.38
1	A	1864	A	N9-C4	-6.84	1.33	1.37
1	A	1680	A	N7-C5	-6.82	1.35	1.39
1	A	1866	U	C2-N3	-6.80	1.32	1.37
1	A	1828	A	N7-C5	-6.79	1.35	1.39
1	A	1916	G	C5-C4	-6.74	1.33	1.38
1	A	1773	A	N9-C4	-6.69	1.33	1.37
1	A	1790	A	N9-C4	-6.69	1.33	1.37
1	A	2292	G	N9-C8	-6.68	1.33	1.37
1	A	2673	G	C5-C4	-6.68	1.33	1.38
1	A	1983	U	C2-N3	-6.66	1.33	1.37
1	A	1683	C	N3-C4	-6.65	1.29	1.33
1	A	2675	G	C5-C4	-6.64	1.33	1.38
1	A	2373	A	N9-C4	-6.61	1.33	1.37
1	A	1984	A	N9-C4	-6.58	1.33	1.37
1	A	2138	U	C2-N3	-6.55	1.33	1.37
1	A	1900	A	N9-C4	-6.54	1.33	1.37
1	A	1770	G	C2-N3	-6.54	1.27	1.32
1	A	1831	G	C5-C4	-6.54	1.33	1.38
1	A	1793	G	C6-N1	-6.53	1.34	1.39
1	A	1744	A	N7-C5	-6.51	1.35	1.39
1	A	1771	C	N3-C4	-6.51	1.29	1.33
1	A	2302	U	C2-N3	-6.48	1.33	1.37
1	A	2294	A	N9-C4	-6.47	1.33	1.37
1	A	2289	G	C5-C4	-6.46	1.33	1.38
1	A	1904	C	N1-C6	-6.44	1.33	1.37
13	O	122	VAL	CB-CG2	-6.42	1.39	1.52
1	A	2292	G	N7-C5	-6.42	1.35	1.39
1	A	1747	G	C5-C4	-6.41	1.33	1.38
1	A	2276	C	N1-C6	-6.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1678	C	N1-C6	-6.39	1.33	1.37
1	A	2276	C	N3-C4	-6.38	1.29	1.33
1	A	1984	A	C5-C4	-6.37	1.34	1.38
1	A	2298	A	N7-C5	-6.36	1.35	1.39
1	A	1754	G	N1-C2	-6.33	1.32	1.37
1	A	1897	A	N9-C4	-6.33	1.34	1.37
1	A	2009	G	N7-C5	-6.32	1.35	1.39
1	A	1867	A	N7-C5	-6.31	1.35	1.39
1	A	1793	G	C5-C4	-6.30	1.33	1.38
1	A	1793	G	N1-C2	-6.29	1.32	1.37
1	A	1803	A	N9-C4	-6.28	1.34	1.37
1	A	1884	G	N9-C4	-6.24	1.32	1.38
1	A	2288	A	N7-C5	-6.23	1.35	1.39
1	A	1879	G	C8-N7	-6.22	1.27	1.30
1	A	1916	G	N7-C5	-6.21	1.35	1.39
1	A	2150	U	C2-N3	-6.20	1.33	1.37
1	A	1789	A	C5-C4	-6.19	1.34	1.38
1	A	1828	A	C5-C4	-6.19	1.34	1.38
1	A	1914	A	N7-C5	-6.16	1.35	1.39
1	A	2292	G	C8-N7	-6.14	1.27	1.30
1	A	2312	A	C5-C4	-6.14	1.34	1.38
1	A	2276	C	C4-C5	-6.12	1.38	1.43
1	A	1792	G	C5-C4	-6.10	1.34	1.38
1	A	1787	G	N7-C5	-6.08	1.35	1.39
1	A	1879	G	N7-C5	-6.08	1.35	1.39
1	A	2019	G	N9-C8	-6.06	1.33	1.37
1	A	1880	C	N3-C4	-6.03	1.29	1.33
1	A	1884	G	C5-C4	-6.02	1.34	1.38
1	A	1867	A	N9-C4	-6.00	1.34	1.37
1	A	1792	G	N1-C2	-5.99	1.32	1.37
16	R	43	VAL	CB-CG2	-5.98	1.40	1.52
1	A	2020	U	C2-N3	-5.98	1.33	1.37
1	A	1775	A	C5-C4	-5.98	1.34	1.38
1	A	1796	A	N9-C4	-5.98	1.34	1.37
31	7	143	TRP	CB-CG	-5.97	1.39	1.50
1	A	1908	A	N9-C4	-5.96	1.34	1.37
1	A	2681	G	N9-C8	-5.96	1.33	1.37
1	A	2421	G	C5-C4	-5.94	1.34	1.38
1	A	1683	C	N1-C6	-5.92	1.33	1.37
18	T	172	CYS	CB-SG	-5.92	1.72	1.81
1	A	1844	A	N9-C4	-5.91	1.34	1.37
1	A	1739	A	N9-C4	-5.89	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1879	G	C5-C4	-5.88	1.34	1.38
1	A	2304	G	N9-C4	-5.88	1.33	1.38
1	A	2308	A	C6-N1	-5.88	1.31	1.35
1	A	2145	G	C6-N1	-5.87	1.35	1.39
1	A	1914	A	N9-C4	-5.86	1.34	1.37
1	A	2343	G	C2-N3	-5.86	1.28	1.32
1	A	2714	A	N9-C4	-5.86	1.34	1.37
1	A	1903	C	N3-C4	-5.85	1.29	1.33
1	A	1775	A	C6-N1	-5.83	1.31	1.35
1	A	2678	A	N7-C5	-5.82	1.35	1.39
1	A	1770	G	N9-C4	-5.81	1.33	1.38
1	A	1679	U	C2-N3	-5.80	1.33	1.37
1	A	1742	G	C5-C4	-5.80	1.34	1.38
1	A	2128	G	C5-C4	-5.77	1.34	1.38
1	A	2454	G	C5-C4	-5.77	1.34	1.38
1	A	2676	A	N7-C5	-5.76	1.35	1.39
1	A	2673	G	N9-C8	-5.76	1.33	1.37
1	A	1830	G	C5-C4	-5.75	1.34	1.38
1	A	2376	A	C5-C4	-5.75	1.34	1.38
1	A	2291	A	N9-C4	-5.74	1.34	1.37
1	A	2372	U	C2-N3	-5.72	1.33	1.37
1	A	2147	G	C6-N1	-5.72	1.35	1.39
1	A	1748	G	N7-C5	-5.71	1.35	1.39
1	A	1680	A	C5-C4	-5.70	1.34	1.38
1	A	1865	C	N3-C4	-5.70	1.29	1.33
1	A	2298	A	N9-C4	-5.70	1.34	1.37
1	A	2684	C	N1-C6	-5.69	1.33	1.37
1	A	2004	G	C5-C4	-5.69	1.34	1.38
1	A	2007	U	C4-C5	-5.69	1.38	1.43
1	A	1988	G	C5-C4	-5.67	1.34	1.38
1	A	1750	G	N7-C5	-5.66	1.35	1.39
1	A	1753	A	C5-C4	-5.66	1.34	1.38
1	A	2655	G	C5-C4	-5.66	1.34	1.38
1	A	1915	C	C4-C5	-5.66	1.38	1.43
1	A	1789	A	N7-C5	-5.66	1.35	1.39
1	A	1751	A	C8-N7	-5.65	1.27	1.31
1	A	2014	A	N9-C4	-5.65	1.34	1.37
1	A	1797	G	C5-C4	-5.65	1.34	1.38
1	A	1741	A	C5-C4	-5.63	1.34	1.38
1	A	2250	A	N9-C4	-5.63	1.34	1.37
25	0	131	CYS	CB-SG	-5.62	1.72	1.81
1	A	1897	A	N7-C5	-5.62	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2151	A	N7-C5	-5.61	1.35	1.39
1	A	2699	C	N3-C4	-5.61	1.30	1.33
1	A	2700	G	C5-C4	-5.61	1.34	1.38
1	A	1790	A	N7-C5	-5.61	1.35	1.39
1	A	2308	A	N7-C5	-5.61	1.35	1.39
1	A	2676	A	C5-C6	-5.61	1.36	1.41
1	A	1869	A	N9-C4	-5.60	1.34	1.37
1	A	2675	G	N1-C2	-5.59	1.33	1.37
1	A	2129	G	C5-C4	-5.59	1.34	1.38
1	A	2012	A	N7-C5	-5.58	1.35	1.39
1	A	2152	A	C5-C4	-5.58	1.34	1.38
1	A	2290	A	C5-C6	-5.57	1.36	1.41
1	A	2369	A	N9-C4	-5.57	1.34	1.37
1	A	1739	A	C2-N3	-5.55	1.28	1.33
1	A	1867	A	N3-C4	-5.54	1.31	1.34
1	A	1879	G	N9-C8	-5.54	1.33	1.37
1	A	2682	A	N7-C5	-5.53	1.35	1.39
1	A	1981	G	C6-N1	-5.53	1.35	1.39
1	A	1787	G	N9-C8	-5.51	1.33	1.37
1	A	1791	G	C5-C4	-5.51	1.34	1.38
1	A	1788	C	N1-C6	-5.51	1.33	1.37
1	A	1813	C	N3-C4	-5.51	1.30	1.33
1	A	2375	C	C4-C5	-5.51	1.38	1.43
1	A	2308	A	C5-C4	-5.49	1.34	1.38
1	A	1883	G	C5-C4	-5.47	1.34	1.38
1	A	1702	A	N9-C4	-5.47	1.34	1.37
1	A	2152	A	N3-C4	-5.47	1.31	1.34
1	A	2018	G	C5-C4	-5.46	1.34	1.38
1	A	1906	G	C5-C4	-5.45	1.34	1.38
1	A	2011	G	C5-C4	-5.45	1.34	1.38
1	A	3218	A	N7-C5	-5.43	1.35	1.39
1	A	2044	A	N9-C4	-5.43	1.34	1.37
1	A	1767	G	C6-N1	-5.43	1.35	1.39
1	A	2143	G	C5-C4	-5.43	1.34	1.38
1	A	2009	G	C8-N7	-5.43	1.27	1.30
1	A	2051	A	C5-C4	-5.43	1.34	1.38
1	A	1757	A	N7-C5	-5.42	1.35	1.39
1	A	3213	A	N7-C5	-5.42	1.35	1.39
1	A	1790	A	N9-C8	-5.42	1.33	1.37
1	A	1863	A	C5-C4	-5.41	1.34	1.38
1	A	2290	A	N9-C4	-5.41	1.34	1.37
15	Q	204	MET	C-N	-5.41	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1864	A	C5-C6	-5.40	1.36	1.41
1	A	1865	C	N1-C6	-5.40	1.33	1.37
1	A	2672	A	N9-C4	-5.39	1.34	1.37
1	A	1803	A	N3-C4	-5.39	1.31	1.34
1	A	2278	A	C5-C4	-5.39	1.34	1.38
1	A	1881	A	C6-N1	-5.38	1.31	1.35
1	A	1816	G	C5-C4	-5.37	1.34	1.38
1	A	1894	G	C6-N1	-5.37	1.35	1.39
1	A	2006	C	N1-C6	-5.37	1.33	1.37
1	A	1767	G	N7-C5	-5.36	1.36	1.39
1	A	1859	A	N9-C4	-5.35	1.34	1.37
1	A	1753	A	N9-C4	-5.35	1.34	1.37
1	A	1748	G	C8-N7	-5.35	1.27	1.30
17	S	106	TRP	CB-CG	-5.34	1.40	1.50
1	A	2683	C	N1-C6	-5.34	1.33	1.37
1	A	1751	A	N7-C5	-5.34	1.36	1.39
1	A	1903	C	C4-C5	-5.33	1.38	1.43
1	A	2004	G	N9-C8	-5.33	1.34	1.37
1	A	2152	A	C6-N1	-5.33	1.31	1.35
1	A	2254	C	C4-C5	-5.33	1.38	1.43
21	W	83	VAL	CB-CG2	-5.32	1.41	1.52
1	A	2684	C	N3-C4	-5.32	1.30	1.33
1	A	1795	A	C5-C4	-5.32	1.35	1.38
1	A	2250	A	C5-C4	-5.32	1.35	1.38
1	A	1678	C	N3-C4	-5.31	1.30	1.33
1	A	2103	A	C5-C4	-5.31	1.35	1.38
1	A	1785	C	N1-C6	-5.31	1.33	1.37
1	A	1791	G	N7-C5	-5.30	1.36	1.39
1	A	1891	A	N9-C4	-5.30	1.34	1.37
1	A	2681	G	C8-N7	-5.30	1.27	1.30
1	A	1771	C	C4-C5	-5.30	1.38	1.43
1	A	2147	G	C5-C4	-5.29	1.34	1.38
1	A	2293	A	C5-C4	-5.29	1.35	1.38
1	A	1792	G	N9-C8	-5.29	1.34	1.37
1	A	1844	A	N7-C5	-5.29	1.36	1.39
5	F	284	TYR	CD1-CE1	-5.29	1.31	1.39
1	A	1768	G	N1-C2	-5.29	1.33	1.37
1	A	2289	G	N3-C4	-5.28	1.31	1.35
1	A	2289	G	C2-N3	-5.28	1.28	1.32
1	A	2680	U	C2-N3	-5.28	1.34	1.37
1	A	1787	G	C6-N1	-5.28	1.35	1.39
1	A	2121	G	C6-N1	-5.28	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1768	G	C5-C4	-5.26	1.34	1.38
1	A	2293	A	N7-C5	-5.26	1.36	1.39
1	A	1879	G	C6-N1	-5.26	1.35	1.39
1	A	2289	G	N9-C4	-5.25	1.33	1.38
1	A	1784	A	C6-N1	-5.25	1.31	1.35
1	A	2300	G	C6-N1	-5.24	1.35	1.39
1	A	1885	A	N9-C4	-5.24	1.34	1.37
16	R	93	CYS	CB-SG	-5.24	1.73	1.81
1	A	1674	A	N7-C5	-5.24	1.36	1.39
1	A	1868	G	C6-N1	-5.24	1.35	1.39
1	A	2312	A	N7-C5	-5.24	1.36	1.39
1	A	2689	C	N3-C4	-5.23	1.30	1.33
1	A	2304	G	C2-N3	-5.23	1.28	1.32
1	A	1982	G	C5-C4	-5.23	1.34	1.38
1	A	2309	A	N7-C5	-5.23	1.36	1.39
1	A	1889	C	C4-C5	-5.22	1.38	1.43
1	A	1906	G	N1-C2	-5.22	1.33	1.37
1	A	2134	A	C5-C4	-5.22	1.35	1.38
1	A	1684	C	N3-C4	-5.22	1.30	1.33
1	A	2145	G	C5-C4	-5.22	1.34	1.38
1	A	2683	C	C4-C5	-5.22	1.38	1.43
1	A	1867	A	C5-C4	-5.21	1.35	1.38
1	A	2304	G	C5-C4	-5.21	1.34	1.38
1	A	1779	A	N7-C5	-5.21	1.36	1.39
1	A	2317	G	C5-C4	-5.20	1.34	1.38
1	A	1679	U	C5-C6	-5.20	1.29	1.34
1	A	1818	A	N7-C5	-5.20	1.36	1.39
1	A	2343	G	N1-C2	-5.20	1.33	1.37
1	A	1772	A	N3-C4	-5.19	1.31	1.34
1	A	2278	A	N9-C4	-5.19	1.34	1.37
1	A	2103	A	N9-C4	-5.19	1.34	1.37
1	A	1862	U	C2-N3	-5.19	1.34	1.37
1	A	1894	G	N1-C2	-5.18	1.33	1.37
1	A	1881	A	N3-C4	-5.17	1.31	1.34
1	A	1705	A	N9-C4	-5.17	1.34	1.37
1	A	1791	G	N9-C8	-5.17	1.34	1.37
1	A	2291	A	C8-N7	-5.17	1.27	1.31
1	A	1772	A	N9-C8	-5.17	1.33	1.37
1	A	2089	U	C2-N3	-5.17	1.34	1.37
1	A	1829	A	C5-C4	-5.16	1.35	1.38
1	A	1918	G	C2-N3	-5.16	1.28	1.32
1	A	2019	G	C5-C4	-5.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1773	A	C5-C4	-5.16	1.35	1.38
27	2	87	ARG	CG-CD	-5.16	1.39	1.51
1	A	2303	A	C5-C6	-5.15	1.36	1.41
1	A	2309	A	C6-N1	-5.15	1.31	1.35
1	A	2454	G	N9-C8	-5.15	1.34	1.37
1	A	2279	U	C2-N3	-5.14	1.34	1.37
1	A	2673	G	C6-N1	-5.14	1.35	1.39
1	A	1884	G	N9-C8	-5.14	1.34	1.37
1	A	2422	U	C2-N3	-5.14	1.34	1.37
1	A	2304	G	C8-N7	-5.14	1.27	1.30
1	A	1985	G	C5-C4	-5.14	1.34	1.38
1	A	1880	C	C4-C5	-5.13	1.38	1.43
1	A	1893	A	N3-C4	-5.13	1.31	1.34
1	A	1778	U	C2-N3	-5.13	1.34	1.37
1	A	2137	C	C4-C5	-5.13	1.38	1.43
1	A	2007	U	C2-N3	-5.12	1.34	1.37
1	A	1683	C	C2-N3	-5.12	1.31	1.35
1	A	1894	G	C5-C4	-5.12	1.34	1.38
1	A	2120	G	C5-C4	-5.11	1.34	1.38
1	A	2292	G	N9-C4	-5.11	1.33	1.38
1	A	2008	G	N9-C8	-5.11	1.34	1.37
1	A	2136	C	C4-C5	-5.11	1.38	1.43
1	A	2137	C	N3-C4	-5.11	1.30	1.33
1	A	1741	A	N9-C4	-5.10	1.34	1.37
1	A	2303	A	C5-C4	-5.10	1.35	1.38
1	A	1884	G	C2-N3	-5.09	1.28	1.32
1	A	1753	A	N7-C5	-5.09	1.36	1.39
1	A	2298	A	C5-C6	-5.09	1.36	1.41
1	A	2273	A	N7-C5	-5.09	1.36	1.39
16	R	11	ARG	CB-CG	-5.09	1.38	1.52
1	A	2683	C	C5-C6	-5.08	1.30	1.34
1	A	2335	A	C5-C4	-5.08	1.35	1.38
1	A	1893	A	C5-C4	-5.08	1.35	1.38
1	A	1987	G	C6-N1	-5.08	1.35	1.39
1	A	2128	G	C2-N3	-5.08	1.28	1.32
1	A	2672	A	N7-C5	-5.08	1.36	1.39
1	A	1790	A	C5-C4	-5.07	1.35	1.38
1	A	1830	G	N9-C8	-5.07	1.34	1.37
1	A	2343	G	C5-C4	-5.07	1.34	1.38
1	A	2004	G	C8-N7	-5.06	1.27	1.30
1	A	2304	G	N1-C2	-5.06	1.33	1.37
1	A	1828	A	C5-C6	-5.06	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	61	VAL	CB-CG1	-5.05	1.42	1.52
1	A	1868	G	C5-C4	-5.05	1.34	1.38
1	A	2677	A	N9-C4	-5.05	1.34	1.37
1	A	1815	A	N7-C5	-5.05	1.36	1.39
1	A	1770	G	N3-C4	-5.04	1.31	1.35
1	A	2302	U	C4-C5	-5.04	1.39	1.43
1	A	2275	U	C2-N3	-5.03	1.34	1.37
1	A	2453	G	C8-N7	-5.03	1.27	1.30
1	A	2004	G	N3-C4	-5.03	1.31	1.35
11	M	188	CYS	CB-SG	-5.03	1.73	1.81
1	A	1840	C	N3-C4	-5.02	1.30	1.33
1	A	2290	A	N7-C5	-5.02	1.36	1.39
1	A	2304	G	N9-C8	-5.02	1.34	1.37
1	A	2707	A	N9-C4	-5.02	1.34	1.37
1	A	2681	G	C6-N1	-5.02	1.36	1.39
1	A	1830	G	N1-C2	-5.01	1.33	1.37
1	A	1863	A	N7-C5	-5.01	1.36	1.39
1	A	2124	A	N7-C5	-5.01	1.36	1.39
1	A	2696	A	C5-C4	-5.01	1.35	1.38
1	A	1915	C	N1-C6	-5.01	1.34	1.37
1	A	2277	U	C2-N3	-5.00	1.34	1.37
1	A	1889	C	N1-C6	-5.00	1.34	1.37

All (493) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2066	C	N1-C2-O2	10.36	125.12	118.90
1	A	2322	C	N1-C2-O2	10.29	125.08	118.90
1	A	2252	C	C5-C6-N1	10.02	126.01	121.00
38	e	178	TRP	C-N-CA	10.01	146.71	121.70
1	A	2372	U	N3-C2-O2	-9.99	115.21	122.20
1	A	1729	U	N3-C2-O2	-9.96	115.23	122.20
1	A	1840	C	C6-N1-C2	-9.73	116.41	120.30
1	A	1715	C	C2-N1-C1'	9.69	129.46	118.80
1	A	2275	U	N3-C2-O2	-9.64	115.45	122.20
1	A	2322	C	C2-N1-C1'	9.56	129.32	118.80
1	A	2898	U	N3-C2-O2	-9.48	115.56	122.20
1	A	2066	C	N3-C2-O2	-9.33	115.37	121.90
1	A	1701	U	N1-C2-O2	9.29	129.30	122.80
1	A	3212	C	C2-N1-C1'	9.24	128.97	118.80
1	A	2252	C	C6-N1-C2	-9.21	116.62	120.30
1	A	1701	U	N3-C2-O2	-9.19	115.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2386	C	N1-C2-O2	9.15	124.39	118.90
1	A	2684	C	N1-C2-O2	9.02	124.31	118.90
1	A	1782	G	O4'-C1'-N9	9.02	115.41	108.20
1	A	1823	A	P-O3'-C3'	8.97	130.47	119.70
1	A	2379	C	N1-C2-O2	8.93	124.26	118.90
1	A	1813	C	C2-N1-C1'	8.85	128.54	118.80
1	A	1850	U	N3-C2-O2	-8.78	116.05	122.20
1	A	1791	G	O5'-P-OP2	-8.71	97.86	105.70
1	A	2187	C	N3-C2-O2	-8.62	115.87	121.90
1	A	1715	C	N1-C2-O2	8.59	124.05	118.90
1	A	3134	C	N1-C2-O2	8.51	124.00	118.90
1	A	1813	C	N3-C2-O2	-8.50	115.95	121.90
1	A	2375	C	C5-C6-N1	8.49	125.25	121.00
1	A	2372	U	N1-C2-O2	8.46	128.72	122.80
1	A	2898	U	C2-N1-C1'	8.39	127.77	117.70
1	A	2750	U	N3-C2-O2	-8.34	116.36	122.20
1	A	2322	C	N3-C2-O2	-8.30	116.09	121.90
1	A	2066	C	C2-N1-C1'	8.21	127.83	118.80
1	A	2135	A	C2-N3-C4	8.19	114.69	110.60
17	S	135	LEU	CA-CB-CG	8.15	134.05	115.30
1	A	2684	C	C2-N1-C1'	8.07	127.67	118.80
1	A	1780	U	P-O3'-C3'	8.04	129.35	119.70
1	A	1792	G	C4-C5-N7	8.03	114.01	110.80
1	A	1725	C	N1-C2-O2	8.03	123.72	118.90
1	A	2165	C	P-O3'-C3'	7.92	129.20	119.70
1	A	2379	C	C2-N1-C1'	7.92	127.51	118.80
1	A	2852	C	N1-C2-O2	7.81	123.59	118.90
1	A	2150	U	N1-C2-O2	7.81	128.26	122.80
1	A	1806	U	N3-C2-O2	-7.78	116.75	122.20
15	Q	151	LEU	CB-CG-CD2	-7.75	97.83	111.00
1	A	1743	U	C5-C6-N1	7.73	126.56	122.70
1	A	2186	C	N1-C2-O2	7.73	123.54	118.90
1	A	1890	C	C6-N1-C2	-7.70	117.22	120.30
1	A	1916	G	C5-C6-O6	-7.66	124.00	128.60
1	A	2005	C	C6-N1-C2	-7.64	117.25	120.30
1	A	1776	G	C8-N9-C4	-7.63	103.35	106.40
1	A	1689	C	N1-C2-O2	7.63	123.48	118.90
1	A	2900	C	C5-C6-N1	7.62	124.81	121.00
1	A	3134	C	N3-C2-O2	-7.60	116.58	121.90
16	R	34	ARG	CB-CG-CD	-7.57	91.91	111.60
1	A	2329	C	C6-N1-C2	-7.57	117.27	120.30
1	A	2416	U	N1-C2-O2	7.56	128.09	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1715	C	C6-N1-C1'	-7.54	111.75	120.80
1	A	1984	A	C8-N9-C4	7.54	108.82	105.80
1	A	1783	U	C5-C6-N1	7.53	126.46	122.70
19	U	28	LEU	CA-CB-CG	7.52	132.59	115.30
1	A	1813	C	N1-C2-O2	7.51	123.41	118.90
1	A	1993	A	C2-N3-C4	7.46	114.33	110.60
1	A	3192	C	N1-C2-O2	7.44	123.36	118.90
1	A	2687	C	C6-N1-C2	-7.42	117.33	120.30
1	A	2423	C	C6-N1-C2	-7.41	117.33	120.30
1	A	1817	C	C6-N1-C2	-7.37	117.35	120.30
1	A	2150	U	N3-C2-O2	-7.36	117.05	122.20
1	A	1868	G	N1-C6-O6	-7.36	115.48	119.90
51	s	229	LEU	CA-CB-CG	7.35	132.21	115.30
1	A	2357	C	N3-C2-O2	-7.35	116.76	121.90
1	A	2343	G	C2-N3-C4	7.34	115.57	111.90
1	A	1805	A	N1-C6-N6	-7.34	114.19	118.60
1	A	2093	U	N1-C2-O2	7.33	127.93	122.80
1	A	2681	G	O5'-P-OP2	-7.32	99.11	105.70
1	A	1814	A	C8-N9-C4	-7.31	102.88	105.80
1	A	2750	U	N1-C2-O2	7.30	127.91	122.80
1	A	2080	U	N3-C2-O2	-7.29	117.09	122.20
1	A	2259	C	N1-C2-O2	7.29	123.28	118.90
51	s	374	LEU	CA-CB-CG	7.26	132.01	115.30
1	A	2087	U	C5-C6-N1	7.24	126.32	122.70
1	A	1701	U	C2-N1-C1'	7.21	126.35	117.70
1	A	2000	C	N1-C2-O2	7.21	123.22	118.90
1	A	2138	U	N3-C2-O2	-7.19	117.17	122.20
1	A	1748	G	C4-C5-N7	7.18	113.67	110.80
1	A	3212	C	N1-C2-O2	7.18	123.21	118.90
1	A	1806	U	N1-C2-O2	7.17	127.82	122.80
1	A	2211	U	N1-C2-O2	7.13	127.79	122.80
41	h	96	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	1725	C	O5'-P-OP2	-7.12	99.30	105.70
1	A	1685	C	N1-C2-O2	7.09	123.15	118.90
1	A	2852	C	C2-N1-C1'	7.07	126.58	118.80
1	A	1840	C	C5-C6-N1	7.05	124.53	121.00
1	A	2030	U	P-O3'-C3'	7.05	128.16	119.70
1	A	1689	C	C2-N1-C1'	7.04	126.54	118.80
1	A	3201	A	P-O3'-C3'	7.04	128.14	119.70
1	A	2457	A	P-O3'-C3'	7.03	128.13	119.70
1	A	1729	U	N1-C2-O2	7.02	127.72	122.80
1	A	2322	C	C6-N1-C2	-6.99	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2277	U	C5-C6-N1	6.98	126.19	122.70
1	A	2379	C	N3-C2-O2	-6.97	117.02	121.90
1	A	2135	A	C8-N9-C4	-6.96	103.02	105.80
1	A	2372	U	C2-N1-C1'	6.96	126.05	117.70
1	A	1732	C	C6-N1-C2	-6.96	117.52	120.30
1	A	2186	C	C6-N1-C2	-6.93	117.53	120.30
1	A	2292	G	N7-C8-N9	6.93	116.57	113.10
1	A	1793	G	N1-C6-O6	-6.92	115.75	119.90
1	A	2684	C	N3-C2-O2	-6.90	117.07	121.90
2	B	1658	U	N1-C2-O2	6.87	127.61	122.80
1	A	2093	U	N3-C2-O2	-6.86	117.39	122.20
1	A	2280	C	N1-C2-O2	6.86	123.02	118.90
42	i	63	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	2211	U	N3-C2-O2	-6.84	117.41	122.20
1	A	3212	C	C5-C6-N1	6.84	124.42	121.00
1	A	1879	G	C6-C5-N7	-6.81	126.31	130.40
1	A	2076	C	C6-N1-C2	-6.81	117.58	120.30
1	A	2357	C	N1-C2-O2	6.80	122.98	118.90
7	I	183	ASP	CB-CG-OD1	6.78	124.41	118.30
1	A	2020	U	N1-C2-O2	6.77	127.54	122.80
1	A	2416	U	N3-C2-O2	-6.76	117.47	122.20
1	A	2898	U	C6-N1-C2	-6.75	116.95	121.00
1	A	2127	A	N1-C2-N3	-6.75	125.92	129.30
1	A	2263	C	C6-N1-C2	-6.74	117.61	120.30
1	A	2243	A	P-O3'-C3'	6.73	127.78	119.70
1	A	2852	C	N3-C2-O2	-6.72	117.19	121.90
1	A	2871	U	N3-C2-O2	-6.72	117.50	122.20
1	A	2140	G	C8-N9-C4	-6.70	103.72	106.40
1	A	1989	C	C5-C6-N1	6.69	124.35	121.00
1	A	2186	C	C5-C6-N1	6.69	124.35	121.00
1	A	1784	A	C5-C6-N1	6.69	121.05	117.70
1	A	1813	C	C6-N1-C1'	-6.68	112.79	120.80
22	X	153	LEU	CA-CB-CG	6.67	130.64	115.30
1	A	2386	C	C2-N1-C1'	6.65	126.11	118.80
1	A	1695	C	C6-N1-C2	-6.64	117.64	120.30
1	A	2379	C	C6-N1-C1'	-6.64	112.83	120.80
16	R	34	ARG	CG-CD-NE	6.63	125.73	111.80
1	A	2843	C	C6-N1-C2	-6.63	117.65	120.30
36	c	203	LEU	CB-CG-CD1	-6.62	99.75	111.00
1	A	1695	C	N3-C2-O2	-6.61	117.27	121.90
1	A	2671	C	C6-N1-C2	-6.60	117.66	120.30
1	A	2187	C	C6-N1-C2	-6.58	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2136	C	C2-N1-C1'	6.57	126.03	118.80
1	A	2656	U	N3-C2-O2	-6.57	117.60	122.20
1	A	1778	U	N3-C2-O2	-6.56	117.61	122.20
1	A	2271	C	C6-N1-C2	-6.55	117.68	120.30
1	A	1792	G	C5-N7-C8	-6.54	101.03	104.30
1	A	1751	A	N7-C8-N9	6.52	117.06	113.80
1	A	1823	A	C8-N9-C4	-6.52	103.19	105.80
1	A	2747	U	N1-C2-O2	6.51	127.36	122.80
1	A	1776	G	N7-C8-N9	6.51	116.36	113.10
1	A	2687	C	C5-C6-N1	6.50	124.25	121.00
1	A	2284	C	C2-N1-C1'	6.49	125.94	118.80
1	A	3104	U	N3-C2-O2	-6.49	117.66	122.20
18	T	176	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	A	1714	C	N1-C2-O2	6.46	122.78	118.90
1	A	2157	U	C5-C6-N1	6.46	125.93	122.70
1	A	2846	G	O4'-C1'-N9	6.46	113.37	108.20
1	A	2408	U	C5-C6-N1	6.45	125.93	122.70
1	A	2386	C	N3-C2-O2	-6.45	117.39	121.90
1	A	1750	G	C4-C5-N7	6.43	113.37	110.80
1	A	2164	C	N1-C2-O2	6.43	122.76	118.90
1	A	1881	A	N1-C6-N6	-6.42	114.75	118.60
1	A	1875	C	C6-N1-C2	-6.42	117.73	120.30
1	A	2292	G	C5-N7-C8	-6.42	101.09	104.30
1	A	3212	C	C6-N1-C1'	-6.41	113.11	120.80
1	A	2747	U	C2-N1-C1'	6.39	125.37	117.70
2	B	1658	U	N3-C2-O2	-6.38	117.73	122.20
1	A	1725	C	N3-C2-O2	-6.38	117.44	121.90
1	A	2135	A	N7-C8-N9	6.37	116.99	113.80
1	A	2322	C	C6-N1-C1'	-6.37	113.16	120.80
1	A	1715	C	N3-C2-O2	-6.36	117.45	121.90
1	A	3212	C	O4'-C1'-N1	6.36	113.29	108.20
1	A	1983	U	N3-C4-C5	6.35	118.41	114.60
1	A	1747	G	C6-N1-C2	-6.35	121.29	125.10
1	A	1684	C	C6-N1-C2	-6.34	117.76	120.30
1	A	2300	G	C4-C5-N7	6.34	113.33	110.80
1	A	3192	C	N3-C2-O2	-6.31	117.48	121.90
1	A	3192	C	C2-N1-C1'	6.29	125.72	118.80
1	A	1834	U	C5-C6-N1	6.28	125.84	122.70
9	K	125	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	A	1721	C	N1-C2-O2	6.27	122.66	118.90
1	A	2747	U	C5-C6-N1	6.27	125.83	122.70
1	A	2322	C	C5-C6-N1	6.27	124.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1785	C	C4-C5-C6	-6.24	114.28	117.40
1	A	2117	U	N1-C2-O2	6.23	127.16	122.80
1	A	1783	U	O5'-P-OP2	-6.22	100.10	105.70
1	A	2871	U	N1-C2-O2	6.22	127.15	122.80
1	A	2272	C	C6-N1-C2	-6.21	117.82	120.30
11	M	184	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	1806	U	C2-N1-C1'	6.20	125.14	117.70
1	A	2865	C	N3-C2-O2	-6.20	117.56	121.90
1	A	1768	G	N9-C4-C5	-6.20	102.92	105.40
1	A	1732	C	C5-C6-N1	6.18	124.09	121.00
1	A	1784	A	C4-C5-N7	6.16	113.78	110.70
1	A	2275	U	N1-C2-O2	6.16	127.11	122.80
1	A	3125	A	C5-C6-N6	-6.16	118.77	123.70
40	g	120	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	2311	U	N3-C2-O2	-6.14	117.90	122.20
1	A	1785	C	C5-C6-N1	6.14	124.07	121.00
1	A	3222	C	C6-N1-C2	-6.13	117.85	120.30
1	A	2061	C	C6-N1-C2	-6.13	117.85	120.30
1	A	1772	A	C2-N3-C4	6.12	113.66	110.60
1	A	1772	A	C5-C6-N1	6.12	120.76	117.70
1	A	1783	U	C2-N1-C1'	6.12	125.04	117.70
1	A	2928	C	C6-N1-C2	-6.11	117.86	120.30
1	A	1725	C	C6-N1-C2	-6.10	117.86	120.30
1	A	1695	C	N1-C2-O2	6.10	122.56	118.90
1	A	2750	U	C2-N1-C1'	6.10	125.02	117.70
1	A	2082	G	N3-C2-N2	-6.10	115.63	119.90
1	A	1743	U	C6-N1-C2	-6.09	117.34	121.00
46	m	53	PRO	O-C-N	-6.09	112.96	122.70
7	I	182	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	1845	C	C5-C6-N1	6.09	124.04	121.00
1	A	1839	C	C5-C6-N1	6.08	124.04	121.00
1	A	2266	U	N3-C2-O2	-6.08	117.95	122.20
1	A	2928	C	C2-N1-C1'	6.07	125.48	118.80
1	A	1714	C	C2-N1-C1'	6.06	125.47	118.80
1	A	1783	U	N1-C2-O2	6.05	127.04	122.80
1	A	2793	C	N1-C2-O2	6.05	122.53	118.90
1	A	2303	A	C4-C5-N7	6.04	113.72	110.70
1	A	2865	C	N1-C2-O2	6.04	122.52	118.90
1	A	3212	C	C6-N1-C2	-6.03	117.89	120.30
1	A	1747	G	N3-C2-N2	-6.02	115.69	119.90
1	A	2684	C	C6-N1-C1'	-6.02	113.58	120.80
1	A	1919	C	N1-C2-O2	6.01	122.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	161	LEU	CA-CB-CG	6.01	129.12	115.30
18	T	90	LEU	CB-CG-CD2	-6.01	100.79	111.00
16	R	119	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	2205	U	N3-C2-O2	-5.99	118.01	122.20
1	A	2912	C	N1-C2-O2	5.99	122.49	118.90
1	A	2507	A	P-O3'-C3'	5.99	126.88	119.70
2	B	1607	U	P-O3'-C3'	5.98	126.88	119.70
1	A	2266	U	N1-C2-O2	5.97	126.98	122.80
1	A	3124	U	N3-C4-O4	5.97	123.58	119.40
1	A	2900	C	C2-N1-C1'	5.96	125.36	118.80
1	A	2336	U	N3-C2-O2	-5.96	118.03	122.20
1	A	1778	U	C5-C6-N1	5.95	125.68	122.70
1	A	1725	C	C5-C6-N1	5.94	123.97	121.00
1	A	2375	C	C6-N1-C2	-5.93	117.93	120.30
1	A	2255	C	C6-N1-C2	-5.93	117.93	120.30
1	A	2186	C	C2-N1-C1'	5.92	125.32	118.80
1	A	1750	G	O4'-C1'-N9	5.92	112.93	108.20
1	A	2076	C	C2-N1-C1'	5.92	125.31	118.80
1	A	3157	C	C2-N1-C1'	5.90	125.29	118.80
1	A	1783	U	N3-C2-O2	-5.90	118.07	122.20
1	A	1738	U	N3-C2-O2	-5.90	118.07	122.20
1	A	2304	G	C5-N7-C8	-5.89	101.35	104.30
1	A	2912	C	N3-C2-O2	-5.89	117.78	121.90
1	A	2080	U	N1-C2-O2	5.88	126.92	122.80
1	A	1748	G	C6-C5-N7	-5.88	126.87	130.40
1	A	1720	C	C6-N1-C2	-5.88	117.95	120.30
1	A	2186	C	N3-C2-O2	-5.87	117.79	121.90
1	A	2079	C	N1-C2-O2	5.85	122.41	118.90
42	i	63	LEU	CB-CG-CD1	-5.84	101.06	111.00
1	A	2416	U	C2-N1-C1'	5.84	124.71	117.70
1	A	2067	C	N1-C2-O2	5.83	122.40	118.90
1	A	1671	G	O4'-C1'-N9	5.83	112.86	108.20
1	A	1984	A	N9-C4-C5	-5.83	103.47	105.80
1	A	1832	A	C8-N9-C4	5.81	108.13	105.80
1	A	2247	C	N1-C2-O2	5.79	122.38	118.90
1	A	1880	C	C6-N1-C2	-5.79	117.98	120.30
1	A	2284	C	N3-C2-O2	-5.79	117.84	121.90
1	A	1689	C	N3-C2-O2	-5.79	117.85	121.90
1	A	2329	C	C2-N1-C1'	5.79	125.17	118.80
1	A	2252	C	C2-N1-C1'	5.79	125.16	118.80
1	A	2136	C	C5-C6-N1	5.78	123.89	121.00
1	A	2263	C	C2-N1-C1'	5.77	125.15	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1691	C	C5-C6-N1	5.77	123.89	121.00
1	A	1875	C	C5-C6-N1	5.77	123.88	121.00
2	B	1633	U	N1-C2-O2	5.76	126.83	122.80
1	A	2067	C	C6-N1-C2	-5.75	118.00	120.30
1	A	1785	C	C5-C4-N4	-5.75	116.17	120.20
1	A	2000	C	N3-C2-O2	-5.74	117.88	121.90
1	A	2101	C	C6-N1-C2	-5.72	118.01	120.30
1	A	2868	C	C5-C6-N1	5.72	123.86	121.00
1	A	2654	U	N3-C2-O2	-5.72	118.20	122.20
42	i	88	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	2303	A	C4-C5-C6	-5.70	114.15	117.00
13	O	144	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	3134	C	C6-N1-C2	-5.70	118.02	120.30
1	A	1707	C	N3-C2-O2	-5.70	117.91	121.90
1	A	1890	C	C5-C6-N1	5.70	123.85	121.00
29	5	415	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	2254	C	N1-C2-O2	5.69	122.31	118.90
1	A	3106	C	C6-N1-C2	-5.69	118.03	120.30
17	S	144	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	2697	G	N9-C4-C5	-5.67	103.13	105.40
1	A	2900	C	C6-N1-C2	-5.67	118.03	120.30
1	A	3192	C	C6-N1-C2	-5.67	118.03	120.30
1	A	2276	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2005	C	C5-C6-N1	5.65	123.82	121.00
10	L	90	CYS	C-N-CA	-5.65	107.58	121.70
1	A	2303	A	C5-N7-C8	-5.64	101.08	103.90
1	A	3134	C	C2-N1-C1'	5.63	125.00	118.80
1	A	1915	C	C5-C6-N1	5.63	123.81	121.00
1	A	2834	C	C6-N1-C2	-5.63	118.05	120.30
1	A	2135	A	N3-C4-C5	-5.63	122.86	126.80
2	B	1635	C	N1-C2-O2	5.62	122.28	118.90
1	A	1694	U	N1-C2-O2	5.61	126.73	122.80
1	A	2049	U	C5-C6-N1	5.61	125.51	122.70
1	A	2066	C	C6-N1-C2	-5.61	118.06	120.30
1	A	1768	G	C4-C5-N7	5.61	113.04	110.80
1	A	2066	C	C6-N1-C1'	-5.60	114.08	120.80
1	A	1784	A	C5-N7-C8	-5.60	101.10	103.90
29	5	359	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	2441	C	C6-N1-C2	-5.60	118.06	120.30
1	A	1701	U	C6-N1-C1'	-5.59	113.37	121.20
1	A	1859	A	C4-C5-N7	5.59	113.50	110.70
1	A	1714	C	N3-C2-O2	-5.59	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1715	C	O4'-C1'-N1	5.59	112.67	108.20
1	A	2671	C	C5-C6-N1	5.59	123.80	121.00
1	A	2000	C	C6-N1-C2	-5.59	118.06	120.30
1	A	2343	G	N3-C4-C5	-5.58	125.81	128.60
1	A	2300	G	C5-N7-C8	-5.57	101.52	104.30
1	A	2124	A	C8-N9-C4	-5.57	103.57	105.80
1	A	1850	U	N1-C2-O2	5.56	126.69	122.80
1	A	1778	U	C6-N1-C2	-5.56	117.66	121.00
1	A	1905	C	C6-N1-C2	-5.56	118.08	120.30
9	K	65	ILE	CG1-CB-CG2	-5.53	99.23	111.40
42	i	80	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	1823	A	N7-C8-N9	5.53	116.56	113.80
1	A	1671	G	C4-C5-N7	5.51	113.00	110.80
1	A	2004	G	C8-N9-C4	-5.51	104.20	106.40
1	A	2871	U	C5-C6-N1	5.51	125.45	122.70
1	A	1725	C	C2-N1-C1'	5.50	124.86	118.80
11	M	154	ILE	CG1-CB-CG2	-5.50	99.31	111.40
1	A	1823	A	C2-N3-C4	5.49	113.34	110.60
2	B	1607	U	C2-N1-C1'	5.48	124.28	117.70
1	A	1770	G	N3-C4-C5	5.48	131.34	128.60
1	A	1743	U	N3-C2-O2	-5.47	118.37	122.20
1	A	1863	A	N1-C2-N3	-5.47	126.56	129.30
1	A	2117	U	N3-C2-O2	-5.47	118.37	122.20
1	A	3125	A	C4-C5-N7	5.47	113.43	110.70
1	A	1685	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2138	U	N1-C2-O2	5.46	126.62	122.80
1	A	2252	C	C4-C5-C6	-5.46	114.67	117.40
30	6	184	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	1895	C	N3-C4-C5	5.45	124.08	121.90
1	A	1689	C	C6-N1-C1'	-5.45	114.26	120.80
16	R	11	ARG	CG-CD-NE	-5.45	100.36	111.80
1	A	2437	C	C6-N1-C2	-5.44	118.12	120.30
11	M	96	LEU	CB-CG-CD2	-5.44	101.75	111.00
13	O	59	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	2205	U	N1-C2-O2	5.44	126.61	122.80
1	A	2443	C	C2-N1-C1'	5.44	124.78	118.80
1	A	1685	C	C2-N1-C1'	5.43	124.78	118.80
1	A	1817	C	C5-C6-N1	5.43	123.72	121.00
1	A	1770	G	N3-C4-N9	-5.43	122.74	126.00
1	A	1922	C	C5-C6-N1	5.43	123.72	121.00
1	A	1973	G	N3-C4-N9	-5.42	122.75	126.00
1	A	3125	A	N9-C4-C5	-5.42	103.63	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	67	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	2865	C	C6-N1-C2	-5.42	118.13	120.30
1	A	2445	U	C2-N1-C1'	5.41	124.19	117.70
1	A	2001	C	N3-C4-C5	5.41	124.06	121.90
1	A	2020	U	N3-C2-O2	-5.41	118.42	122.20
1	A	2129	G	C4-C5-N7	5.40	112.96	110.80
1	A	1997	C	N3-C4-C5	5.40	124.06	121.90
1	A	1915	C	C6-N1-C2	-5.40	118.14	120.30
1	A	2375	C	C2-N1-C1'	5.40	124.74	118.80
1	A	2017	U	N3-C2-O2	-5.39	118.43	122.20
1	A	1879	G	N3-C4-N9	5.38	129.23	126.00
1	A	2929	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1869	A	O5'-P-OP1	-5.38	100.86	105.70
1	A	2854	U	N1-C2-O2	5.38	126.56	122.80
1	A	1792	G	N9-C4-C5	-5.37	103.25	105.40
1	A	2141	U	O5'-P-OP1	-5.37	100.86	105.70
1	A	2377	G	N1-C6-O6	-5.36	116.68	119.90
1	A	2660	U	N3-C2-O2	-5.36	118.45	122.20
1	A	2729	U	N3-C2-O2	-5.36	118.45	122.20
1	A	2473	A	C4-N9-C1'	5.35	135.94	126.30
51	s	301	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	2898	U	N1-C2-N3	5.35	118.11	114.90
1	A	2258	A	C4-C5-N7	5.35	113.37	110.70
1	A	2417	C	N3-C2-O2	-5.34	118.16	121.90
1	A	2287	U	C5-C6-N1	5.34	125.37	122.70
1	A	2441	C	C5-C6-N1	5.34	123.67	121.00
1	A	2793	C	C6-N1-C2	-5.34	118.16	120.30
1	A	1987	G	C4-N9-C1'	5.34	133.44	126.50
1	A	3157	C	N3-C2-O2	-5.33	118.17	121.90
1	A	3222	C	C5-C6-N1	5.33	123.66	121.00
1	A	1903	C	C6-N1-C2	-5.32	118.17	120.30
1	A	1699	C	N1-C2-O2	5.32	122.09	118.90
1	A	1884	G	C8-N9-C4	5.32	108.53	106.40
1	A	2329	C	N3-C2-O2	-5.32	118.17	121.90
1	A	2688	C	C5-C6-N1	5.32	123.66	121.00
1	A	2857	U	C5-C6-N1	5.32	125.36	122.70
1	A	2129	G	N9-C4-C5	-5.31	103.28	105.40
1	A	2445	U	C6-N1-C1'	-5.31	113.77	121.20
51	s	299	PHE	CB-CG-CD1	5.31	124.51	120.80
1	A	2667	U	N3-C2-O2	-5.30	118.49	122.20
1	A	2252	C	N1-C2-O2	5.29	122.07	118.90
1	A	1916	G	C6-N1-C2	-5.28	121.93	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1751	A	C4-N9-C1'	5.28	135.80	126.30
1	A	2047	U	N1-C2-O2	5.27	126.49	122.80
35	b	26	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	1879	G	C8-N9-C1'	-5.26	120.16	127.00
35	b	11	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	2259	C	N3-C2-O2	-5.26	118.22	121.90
23	Y	226	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	1754	G	N3-C2-N2	5.26	123.58	119.90
28	3	157	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	2375	C	C4-C5-C6	-5.25	114.77	117.40
1	A	1777	A	O4'-C1'-N9	5.25	112.40	108.20
1	A	2809	C	C6-N1-C2	-5.24	118.20	120.30
1	A	1984	A	N1-C2-N3	-5.24	126.68	129.30
1	A	2898	U	O4'-C1'-N1	5.23	112.39	108.20
1	A	1884	G	N3-C4-C5	5.23	131.22	128.60
1	A	2135	A	O4'-C1'-N9	5.23	112.38	108.20
1	A	2164	C	N3-C2-O2	-5.23	118.24	121.90
1	A	2258	A	C5-N7-C8	-5.23	101.28	103.90
42	i	38	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	2276	C	C5-C6-N1	5.21	123.60	121.00
1	A	2650	C	N1-C2-O2	5.21	122.02	118.90
1	A	2871	U	C2-N1-C1'	5.20	123.94	117.70
1	A	2173	G	N3-C4-N9	5.19	129.11	126.00
1	A	3214	C	C6-N1-C2	-5.18	118.23	120.30
1	A	1672	C	N3-C4-C5	5.18	123.97	121.90
1	A	2302	U	C5-C4-O4	-5.18	122.79	125.90
1	A	2930	U	N3-C2-O2	-5.18	118.58	122.20
1	A	2823	U	N3-C2-O2	-5.17	118.58	122.20
1	A	2473	A	C2-N3-C4	5.17	113.19	110.60
1	A	2311	U	N1-C2-O2	5.16	126.41	122.80
1	A	2656	U	N1-C2-O2	5.16	126.41	122.80
1	A	2171	U	C5-C6-N1	5.15	125.28	122.70
1	A	1828	A	N1-C2-N3	-5.15	126.72	129.30
1	A	1783	U	C6-N1-C2	-5.15	117.91	121.00
1	A	2300	G	C4-N9-C1'	5.15	133.19	126.50
1	A	1778	U	C2-N1-C1'	5.15	123.88	117.70
1	A	1789	A	C4-C5-C6	-5.15	114.43	117.00
1	A	1726	C	C5-C6-N1	5.14	123.57	121.00
1	A	2093	U	C2-N1-C1'	5.14	123.87	117.70
1	A	2868	C	C4-C5-C6	-5.14	114.83	117.40
1	A	1805	A	P-O3'-C3'	5.14	125.87	119.70
1	A	1839	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2445	U	N1-C2-O2	5.13	126.39	122.80
1	A	2667	U	N1-C2-O2	5.13	126.39	122.80
1	A	2688	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1872	U	N1-C2-O2	5.12	126.39	122.80
1	A	2241	A	C4-C5-N7	5.12	113.26	110.70
1	A	1681	G	N1-C6-O6	-5.12	116.83	119.90
1	A	1780	U	OP1-P-O3'	5.12	116.47	105.20
1	A	1694	U	N3-C2-O2	-5.12	118.62	122.20
2	B	1659	U	N1-C2-O2	5.12	126.38	122.80
30	6	217	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	1845	C	C4-C5-C6	-5.11	114.84	117.40
1	A	2166	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2080	U	C2-N1-C1'	5.10	123.82	117.70
1	A	1741	A	C5-C6-N6	-5.10	119.62	123.70
1	A	2076	C	C5-C6-N1	5.10	123.55	121.00
1	A	1879	G	N9-C4-C5	-5.09	103.36	105.40
1	A	2727	C	N3-C2-O2	-5.09	118.34	121.90
1	A	2905	A	P-O3'-C3'	5.09	125.81	119.70
1	A	2697	G	C4-C5-N7	5.08	112.83	110.80
51	s	299	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	A	1713	A	P-O3'-C3'	5.08	125.80	119.70
1	A	1784	A	N9-C4-C5	-5.08	103.77	105.80
15	Q	151	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	2025	C	C5-C6-N1	5.08	123.54	121.00
1	A	1844	A	C5-N7-C8	-5.08	101.36	103.90
1	A	2750	U	C5-C6-N1	5.08	125.24	122.70
1	A	1723	A	N1-C6-N6	-5.08	115.56	118.60
1	A	2280	C	N3-C2-O2	-5.08	118.35	121.90
1	A	2136	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1844	A	C4-C5-N7	5.07	113.24	110.70
2	B	1659	U	N3-C2-O2	-5.07	118.65	122.20
1	A	2251	A	C2-N3-C4	5.07	113.13	110.60
1	A	2854	U	N3-C2-O2	-5.07	118.65	122.20
38	e	84	TYR	CA-CB-CG	5.07	123.03	113.40
1	A	1812	C	C5-C6-N1	5.06	123.53	121.00
11	M	39	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	B	1633	U	N3-C2-O2	-5.05	118.67	122.20
1	A	1775	A	C5-C6-N1	5.04	120.22	117.70
1	A	1900	A	N3-C4-N9	-5.04	123.37	127.40
1	A	2187	C	N1-C2-O2	5.04	121.92	118.90
1	A	2898	U	N1-C2-O2	5.03	126.32	122.80
1	A	2277	U	C4-C5-C6	-5.03	116.68	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2744	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	3150	U	C5-C6-N1	5.03	125.21	122.70
1	A	1812	C	C6-N1-C2	-5.02	118.29	120.30
1	A	2186	C	P-O3'-C3'	5.02	125.72	119.70
1	A	2416	U	C5-C6-N1	5.02	125.21	122.70
1	A	1677	C	C6-N1-C1'	5.01	126.82	120.80
1	A	2834	C	C5-C6-N1	5.01	123.51	121.00
1	A	2243	A	OP2-P-O3'	5.01	116.23	105.20
1	A	2205	U	C2-N1-C1'	5.01	123.71	117.70
1	A	1737	A	C5-C6-N1	5.01	120.20	117.70
1	A	2906	C	C6-N1-C2	-5.01	118.30	120.30
1	A	3192	C	C5-C6-N1	5.01	123.50	121.00
1	A	2041	U	N3-C2-O2	-5.00	118.70	122.20
2	B	1637	C	C6-N1-C2	-5.00	118.30	120.30
4	E	187	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	25	GLY	Peptide
31	7	159	LYS	Peptide
8	J	69	LYS	Peptide
40	g	110	ILE	Peptide
46	m	53	PRO	Mainchain
51	s	270	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23184	0	11795	143	0
2	B	1191	0	607	9	0
3	D	1706	0	1754	36	0
4	E	2258	0	2264	35	0
5	F	2013	0	2044	31	0
6	H	784	0	832	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1283	0	1369	24	0
8	J	1061	0	1141	30	0
9	K	1451	0	1448	23	0
10	L	889	0	941	16	0
11	M	2305	0	2378	31	0
12	N	1654	0	1681	21	0
13	O	1245	0	1283	28	0
14	P	1148	0	1148	21	0
15	Q	1805	0	1841	31	0
16	R	1153	0	1213	10	0
17	S	1251	0	1322	26	0
18	T	1305	0	1352	17	0
19	U	1154	0	1154	24	0
20	V	1575	0	1583	21	0
21	W	859	0	888	10	0
22	X	2035	0	2054	29	0
23	Y	1517	0	1561	20	0
24	Z	978	0	1029	11	0
25	0	880	0	902	13	0
26	1	433	0	475	6	0
27	2	351	0	375	8	0
28	3	831	0	883	14	0
29	5	3156	0	3138	56	0
30	6	2640	0	2464	36	0
31	7	2334	0	2343	29	0
32	8	836	0	844	8	0
33	9	947	0	949	19	0
34	a	686	0	658	0	0
35	b	1178	0	1180	0	0
36	c	2217	0	2220	0	0
37	d	1741	0	1727	0	0
38	e	1762	0	1766	0	0
39	f	915	0	917	0	0
40	g	1067	0	1056	0	0
41	h	827	0	806	0	0
42	i	827	0	856	0	0
43	j	684	0	673	0	0
44	k	627	0	636	0	0
45	l	221	0	227	0	0
46	m	372	0	387	0	0
47	o	665	0	664	0	0
48	p	1058	0	1083	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	q	1076	0	1049	0	0
50	r	1203	0	1220	0	0
51	s	3036	0	3022	0	0
52	t	140	0	30	0	0
53	u	927	0	921	0	0
54	v	588	0	604	0	0
55	w	638	0	636	0	0
56	A	47	0	0	0	0
56	W	1	0	0	0	0
56	g	1	0	0	0	0
57	0	1	0	0	0	0
57	I	1	0	0	0	0
58	v	21	0	21	0	0
All	All	90739	0	79414	697	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 (697) 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)
29:5:105:TYR:CE2	29:5:218:LEU:HD22	1.60	1.34
1:A:3116:C:N4	1:A:3140:A:H61	1.57	1.03
1:A:3116:C:H42	1:A:3140:A:N6	1.57	1.01
22:X:144:TYR:O	22:X:148:THR:HG23	1.63	0.98
29:5:105:TYR:CE2	29:5:218:LEU:CD2	2.46	0.97
29:5:105:TYR:HE2	29:5:218:LEU:CD2	1.80	0.93
17:S:101:PHE:HD1	17:S:130:LEU:HD22	1.33	0.90
17:S:101:PHE:CE2	17:S:116:ILE:HD13	2.08	0.88
2:B:1607:U:H3	2:B:1664:G:H1	0.89	0.88
29:5:105:TYR:HE2	29:5:218:LEU:HD22	0.99	0.83
20:V:137:PHE:HD2	20:V:142:GLU:O	1.61	0.83
7:I:123:MET:HA	7:I:153:LEU:O	1.79	0.82
29:5:290:THR:HA	29:5:343:GLN:O	1.79	0.82
29:5:105:TYR:CD2	29:5:218:LEU:HD22	2.17	0.80
29:5:293:LEU:O	29:5:346:GLY:HA2	1.83	0.79
17:S:101:PHE:CD1	17:S:130:LEU:HD22	2.17	0.77
30:6:270:PHE:HB2	30:6:317:SER:O	1.84	0.77
25:0:179:ARG:HH12	25:0:182:PRO:HG3	1.50	0.76
30:6:157:LEU:O	30:6:161:LEU:HB3	1.86	0.76
1:A:1747:G:N2	1:A:1750:G:O2'	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:139:GLU:N	20:V:139:GLU:OE1	2.19	0.75
15:Q:123:ASP:OD2	15:Q:126:ALA:N	2.18	0.75
30:6:266:HIS:O	30:6:320:GLN:HA	1.86	0.75
15:Q:152:ARG:NH1	15:Q:190:LEU:O	2.20	0.74
1:A:2140:G:N3	24:Z:76:ARG:NH2	2.36	0.72
29:5:218:LEU:HD12	29:5:218:LEU:O	1.90	0.72
29:5:106:ILE:HD11	29:5:223:ARG:HE	1.56	0.71
8:J:76:ARG:NH2	24:Z:99:VAL:O	115.50	0.71
5:F:63:GLN:HG2	5:F:81:ASP:HB3	1.72	0.71
33:9:93:SER:O	33:9:97:ALA:HB3	1.92	0.70
1:A:3116:C:H42	1:A:3140:A:H61	0.78	0.69
25:0:106:ASN:HD22	25:0:118:GLN:HE21	1.38	0.69
7:I:140:TYR:HB3	7:I:143:LEU:HB2	1.73	0.69
15:Q:201:ASP:HB3	15:Q:204:MET:HB3	1.75	0.68
15:Q:120:THR:HG22	15:Q:132:GLN:HG2	1.77	0.67
22:X:150:LYS:HB2	22:X:159:MET:HE1	1.76	0.67
17:S:129:ARG:HE	17:S:155:ARG:HG3	1.60	0.67
23:Y:198:ARG:NH2	27:2:70:LEU:O	2.27	0.67
20:V:139:GLU:H	20:V:139:GLU:CD	1.97	0.66
20:V:137:PHE:CD2	20:V:142:GLU:O	2.45	0.66
2:B:1625:A:H62	14:P:87:GLN:HE22	1.40	0.66
8:J:89:TYR:O	8:J:93:ALA:HB3	1.96	0.66
30:6:329:TYR:O	30:6:333:GLN:HB2	1.95	0.66
7:I:51:THR:OG1	12:N:250:ARG:NH2	2.30	0.65
27:2:59:LYS:O	27:2:63:LYS:HB2	1.97	0.65
8:J:110:GLY:O	8:J:153:ILE:HA	1.97	0.65
1:A:2064:A:OP1	21:W:101:LYS:NZ	2.29	0.65
22:X:114:PHE:O	22:X:122:LYS:HA	1.97	0.65
29:5:106:ILE:HG22	29:5:266:HIS:HB3	1.78	0.64
5:F:211:ARG:HH11	6:H:58:ARG:HG3	87.71	0.64
29:5:208:THR:HA	29:5:224:GLY:O	1.96	0.64
1:A:2702:G:H5'	9:K:114:LYS:HE2	1.77	0.64
5:F:217:LEU:HD11	5:F:243:ILE:HD12	1.80	0.64
31:7:203:THR:HG22	31:7:280:VAL:H	1.62	0.64
15:Q:120:THR:HA	15:Q:131:SER:O	1.97	0.64
31:7:107:LEU:HB2	31:7:126:LYS:HB2	1.79	0.64
7:I:119:HIS:NE2	7:I:158:GLU:O	2.30	0.64
1:A:2673:G:H5''	18:T:112:LYS:HB2	1.80	0.63
12:N:87:PHE:HB2	12:N:163:MET:HB2	1.80	0.63
3:D:132:ASP:OD2	3:D:135:ARG:NH1	2.28	0.63
1:A:2292:G:C8	16:R:11:ARG:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:230:LEU:O	29:5:289:HIS:HB3	1.99	0.63
14:P:77:PHE:O	14:P:97:GLN:NE2	2.31	0.63
5:F:103:GLN:HE22	5:F:250:VAL:H	1.47	0.62
1:A:1790:A:OP1	27:2:82:ARG:NH1	2.31	0.62
22:X:163:ARG:HE	29:5:55:LEU:HD22	1.64	0.62
14:P:52:ASN:HB3	14:P:55:ASN:HB2	1.80	0.62
2:B:1643:A:H61	14:P:87:GLN:HE21	1.47	0.62
1:A:2143:G:OP1	17:S:173:ARG:NH2	2.31	0.62
7:I:124:LYS:HB2	7:I:153:LEU:HB2	1.82	0.62
7:I:32:ALA:HB1	12:N:73:ARG:HH21	1.64	0.62
19:U:71:ARG:NH2	19:U:96:TYR:OH	2.33	0.62
5:F:133:THR:HG21	5:F:135:ARG:HE	1.64	0.62
13:O:25:ARG:NH2	13:O:51:GLU:OE2	2.33	0.62
19:U:128:SER:O	19:U:132:GLU:HB2	2.00	0.61
1:A:2389:C:H5''	29:5:301:PRO:HB3	1.82	0.61
28:3:183:ARG:NH1	30:6:355:LYS:O	2.34	0.61
19:U:143:ARG:NH1	31:7:66:GLU:OE1	2.33	0.61
3:D:235:GLN:HB3	3:D:294:SER:HA	1.81	0.61
3:D:194:ASN:HA	3:D:207:ILE:CG2	2.30	0.61
1:A:1777:A:N6	1:A:1780:U:OP2	2.34	0.61
3:D:227:GLN:HE21	3:D:231:LYS:HG2	1.65	0.61
18:T:55:ASN:ND2	18:T:74:TYR:O	2.33	0.61
1:A:2511:C:H3'	1:A:2512:A:H8	1.65	0.60
14:P:58:LEU:HD23	14:P:177:ARG:HH21	14.72	0.60
3:D:194:ASN:HA	3:D:207:ILE:HG21	1.82	0.60
32:8:117:LEU:O	32:8:121:TRP:HB2	2.02	0.59
22:X:20:ILE:HA	22:X:23:ARG:HH11	1.67	0.59
1:A:1706:C:OP1	23:Y:193:ARG:NH2	2.33	0.59
1:A:2174:G:N2	8:J:102:ARG:O	2.33	0.59
18:T:84:LYS:HD3	18:T:149:ARG:HB3	1.84	0.59
14:P:64:LYS:HA	14:P:97:GLN:HE22	1.67	0.59
30:6:217:LEU:HD22	30:6:271:LEU:HD12	1.85	0.59
1:A:1691:C:O2	23:Y:216:ARG:NH1	2.31	0.59
22:X:144:TYR:O	22:X:148:THR:CG2	2.45	0.59
1:A:2147:G:OP1	17:S:104:ARG:NH1	2.36	0.59
9:K:63:ARG:NH1	9:K:130:ASP:OD1	2.36	0.59
1:A:2927:C:H2'	1:A:2928:C:H4'	1.84	0.59
1:A:2032:G:O2'	1:A:2865:C:O2	2.19	0.58
3:D:194:ASN:OD1	3:D:243:THR:OG1	2.21	0.58
15:Q:152:ARG:HG3	15:Q:161:GLU:HG2	1.85	0.58
17:S:101:PHE:CD1	17:S:130:LEU:CD2	2.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:177:HIS:O	22:X:184:ARG:NH2	2.37	0.58
1:A:2458:A:OP1	13:O:9:ILE:N	2.37	0.58
2:B:1607:U:O4	2:B:1664:G:O6	2.21	0.58
1:A:3146:G:O3'	4:E:266:ARG:NH1	2.36	0.58
10:L:58:ILE:HD11	10:L:76:ALA:HB2	1.84	0.58
14:P:63:ARG:HG2	14:P:177:ARG:HH11	1.69	0.58
16:R:10:LEU:HG	16:R:13:ARG:HD3	1.84	0.58
2:B:1627:C:OP1	32:8:129:ARG:NH1	2.35	0.58
18:T:153:LEU:HB2	18:T:169:LYS:HB2	1.85	0.58
26:1:43:LEU:O	26:1:55:LEU:HA	2.03	0.58
30:6:157:LEU:O	30:6:161:LEU:CB	2.52	0.58
5:F:281:ARG:HD3	11:M:125:ARG:HD3	1.84	0.58
8:J:111:LEU:HG	8:J:154:ARG:HB3	1.86	0.58
14:P:75:ARG:HG2	14:P:110:TRP:HE1	37.63	0.58
17:S:101:PHE:HE2	17:S:116:ILE:HD13	1.65	0.58
20:V:97:TYR:HA	20:V:107:THR:O	2.02	0.58
2:B:1642:G:H4'	32:8:119:LYS:HG3	1.85	0.57
3:D:207:ILE:O	3:D:207:ILE:HG22	2.03	0.57
9:K:10:GLN:NE2	18:T:206:ARG:O	2.30	0.57
8:J:138:SER:HA	8:J:141:VAL:HG12	1.85	0.57
13:O:45:PRO:HG2	13:O:48:ARG:HD2	1.86	0.57
1:A:3183:U:O2	9:K:177:ARG:NH1	2.36	0.57
29:5:112:ARG:NH2	29:5:303:ARG:O	2.38	0.57
4:E:73:LEU:HD11	32:8:114:ARG:HE	181.88	0.57
11:M:177:ALA:HB1	11:M:203:ARG:HH12	1.70	0.57
25:0:119:LYS:O	25:0:120:HIS:ND1	2.37	0.57
28:3:175:ASP:HB3	28:3:178:GLN:HB2	1.86	0.57
31:7:107:LEU:HD12	31:7:126:LYS:HD2	1.87	0.57
1:A:1812:C:OP1	18:T:50:LYS:NZ	2.37	0.57
10:L:55:PRO:HB3	10:L:77:ILE:HG12	1.87	0.57
19:U:3:ARG:O	19:U:23:ASN:ND2	2.38	0.57
22:X:61:ARG:NH2	22:X:63:GLU:OE2	2.38	0.57
29:5:216:GLU:HA	29:5:216:GLU:OE1	2.05	0.56
30:6:218:LEU:HD22	30:6:234:HIS:HB2	1.87	0.56
1:A:2276:C:H1'	16:R:11:ARG:HH22	1.69	0.56
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.38	0.56
19:U:11:ARG:NH1	20:V:212:LYS:O	2.38	0.56
19:U:8:PRO:HA	23:Y:183:GLN:HE22	1.70	0.56
31:7:51:GLU:O	31:7:55:GLN:HB2	2.06	0.56
1:A:2191:A:N6	1:A:2198:A:OP2	2.39	0.56
3:D:199:GLU:HB2	3:D:202:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:99:ARG:NH1	15:Q:161:GLU:OE1	2.39	0.56
22:X:226:LEU:HD12	23:Y:155:LEU:HB3	1.88	0.56
29:5:350:ARG:NH2	29:5:384:GLN:O	2.38	0.56
10:L:108:ILE:HA	10:L:114:PRO:HA	1.87	0.56
1:A:2372:U:O4	19:U:35:GLN:NE2	2.39	0.56
7:I:162:LYS:HD2	7:I:196:LYS:HA	1.88	0.56
20:V:142:GLU:OE1	20:V:142:GLU:HA	2.04	0.56
23:Y:72:LYS:O	23:Y:76:GLN:NE2	2.39	0.56
12:N:193:GLY:O	12:N:197:LYS:HB2	2.05	0.56
13:O:38:ARG:NH2	13:O:82:GLU:OE1	2.39	0.56
8:J:32:GLY:O	8:J:36:GLY:N	2.33	0.56
15:Q:136:ILE:O	15:Q:151:LEU:HA	2.06	0.56
17:S:99:VAL:HG22	17:S:133:VAL:HG12	1.88	0.56
24:Z:71:ARG:NH2	24:Z:92:GLU:O	2.39	0.56
3:D:130:ARG:NH1	3:D:131:TYR:O	2.39	0.55
22:X:41:VAL:HG11	22:X:83:GLU:HB3	1.87	0.55
28:3:172:TYR:HB2	28:3:175:ASP:HB2	1.88	0.55
8:J:29:ALA:HB1	8:J:50:CYS:HB2	1.87	0.55
33:9:128:PHE:HD1	33:9:135:PHE:HB3	1.71	0.55
15:Q:79:GLU:OE2	15:Q:103:ARG:NH2	2.39	0.55
30:6:204:VAL:HB	30:6:245:VAL:HG21	1.88	0.55
3:D:206:TYR:N	3:D:206:TYR:CD2	2.73	0.55
7:I:87:ALA:HA	7:I:90:PHE:HD2	1.72	0.55
9:K:52:ASP:O	18:T:206:ARG:NH1	2.37	0.55
30:6:175:VAL:HG22	30:6:204:VAL:HG22	1.88	0.55
1:A:2459:A:N6	1:A:2668:A:O2'	2.39	0.55
1:A:3202:U:OP2	4:E:141:LYS:NZ	2.39	0.55
1:A:2521:A:OP2	3:D:202:ARG:NH2	2.37	0.55
11:M:225:ASP:HB3	11:M:227:ALA:H	1.72	0.55
13:O:26:ILE:HD11	15:Q:268:ASP:HB3	1.88	0.55
19:U:19:VAL:HG22	33:9:136:LEU:HD22	1.89	0.55
1:A:1874:A:O2'	1:A:2090:A:O2'	2.23	0.55
33:9:91:LEU:O	33:9:95:ALA:HB3	2.07	0.55
13:O:42:ILE:O	13:O:122:VAL:HA	2.07	0.55
4:E:171:PRO:O	4:E:173:LYS:NZ	2.40	0.54
13:O:131:PRO:HD2	25:0:134:THR:HG22	1.89	0.54
14:P:72:PHE:HB2	21:W:107:HIS:HA	1.88	0.54
29:5:341:VAL:HG22	29:5:358:GLN:HG2	1.89	0.54
3:D:207:ILE:HG12	3:D:229:PRO:HD3	1.90	0.54
10:L:123:ILE:HD12	10:L:141:ALA:HB2	1.89	0.54
26:1:20:MET:O	26:1:29:CYS:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:201:ARG:NH1	29:5:418:TYR:O	2.41	0.54
31:7:156:ARG:NH2	31:7:259:ASP:O	2.39	0.54
4:E:268:GLU:HB3	4:E:271:LEU:HD11	1.90	0.54
1:A:2212:C:H2'	1:A:2213:A:H8	1.72	0.54
1:A:2528:G:OP1	3:D:135:ARG:NH2	2.41	0.54
6:H:58:ARG:NH1	6:H:77:HIS:O	2.41	0.54
11:M:146:ASP:OD1	11:M:146:ASP:N	2.41	0.54
7:I:191:PHE:O	7:I:195:SER:HB2	2.07	0.54
17:S:174:PHE:HA	17:S:180:PHE:O	2.08	0.54
27:2:82:ARG:HE	27:2:87:ARG:HD2	1.72	0.54
29:5:151:ASP:O	29:5:155:LEU:HB2	2.08	0.54
30:6:218:LEU:HA	30:6:269:ALA:O	2.08	0.54
7:I:191:PHE:O	7:I:195:SER:CB	2.56	0.54
14:P:79:HIS:HA	14:P:95:GLU:O	2.08	0.54
15:Q:121:THR:HG22	15:Q:171:VAL:HG12	1.90	0.54
1:A:1745:U:O4	28:3:108:LYS:NZ	2.41	0.54
15:Q:117:LEU:O	15:Q:134:LEU:HA	2.08	0.54
1:A:1884:G:O6	5:F:281:ARG:NH2	2.41	0.53
3:D:198:SER:HB2	3:D:206:TYR:OH	2.08	0.53
3:D:248:SER:OG	3:D:249:ASN:N	2.40	0.53
1:A:1985:G:OP1	1:A:1987:G:O2'	2.25	0.53
3:D:124:GLU:HG2	3:D:144:GLY:HA3	1.90	0.53
28:3:148:VAL:HG13	30:6:360:ARG:HA	1.91	0.53
1:A:1705:A:N6	33:9:40:GLY:O	2.41	0.53
3:D:166:SER:OG	3:D:182:HIS:ND1	2.39	0.53
6:H:98:LEU:HD22	6:H:102:VAL:HG21	1.90	0.53
6:H:75:ARG:HH21	22:X:100:ARG:HH22	1.55	0.53
30:6:371:ASP:OD1	30:6:371:ASP:N	2.41	0.53
4:E:56:GLU:OE2	13:O:153:ARG:NH2	2.42	0.53
8:J:128:GLU:HA	8:J:133:GLN:HE21	1.74	0.53
15:Q:111:PHE:O	15:Q:140:ARG:NH1	2.41	0.53
1:A:2529:U:O2'	3:D:206:TYR:HA	2.07	0.53
1:A:3123:G:N2	1:A:3133:A:OP2	2.42	0.53
3:D:226:ILE:O	3:D:233:GLN:HA	2.08	0.53
4:E:292:HIS:ND1	4:E:293:LYS:O	2.37	0.53
5:F:167:MET:HA	5:F:170:ARG:HE	1.74	0.53
24:Z:78:ARG:HD2	24:Z:116:LEU:HD21	1.90	0.53
30:6:105:GLU:O	30:6:109:ALA:HB2	2.08	0.53
1:A:2126:U:O4	24:Z:76:ARG:NH1	2.42	0.53
1:A:2519:G:N7	3:D:230:SER:OG	2.38	0.53
1:A:2293:A:N6	11:M:37:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:100:HIS:O	17:S:100:HIS:ND1	2.42	0.53
22:X:153:LEU:HD11	22:X:158:GLY:HA3	1.89	0.53
29:5:178:PRO:O	29:5:182:ASP:HB2	2.09	0.53
1:A:2194:U:O2'	1:A:2195:A:O4'	2.27	0.53
1:A:2191:A:OP1	8:J:142:ARG:NH2	2.42	0.53
8:J:89:TYR:O	8:J:93:ALA:CB	2.56	0.53
9:K:16:ARG:HH22	9:K:124:ARG:HH21	1.55	0.53
2:B:1637:C:H5'	30:6:52:ARG:HB3	1.90	0.53
1:A:2123:C:HO2'	1:A:2134:A:HO2'	1.56	0.53
5:F:70:ARG:NH1	5:F:194:GLU:OE1	2.41	0.53
9:K:154:ARG:NH1	9:K:157:GLU:OE2	2.41	0.53
32:8:117:LEU:O	32:8:121:TRP:CB	2.57	0.52
1:A:2180:A:H1'	1:A:2206:C:H4'	1.91	0.52
1:A:2520:C:HO2'	1:A:2529:U:H3	1.57	0.52
4:E:133:THR:OG1	4:E:144:THR:OG1	2.27	0.52
7:I:83:ARG:HG2	7:I:134:PHE:HE1	1.73	0.52
10:L:72:GLN:HA	10:L:84:ALA:O	2.09	0.52
19:U:44:ILE:HG22	19:U:93:LYS:HB3	1.90	0.52
29:5:213:TRP:O	29:5:219:LEU:HD12	2.09	0.52
16:R:54:THR:HG21	17:S:172:MET:H	1.73	0.52
17:S:152:ASP:OD1	17:S:152:ASP:N	2.42	0.52
1:A:3127:G:H2'	1:A:3128:A:H2'	1.92	0.52
1:A:2511:C:O2'	3:D:258:GLY:N	2.42	0.52
8:J:66:LEU:HB3	8:J:82:ILE:HD11	1.91	0.52
10:L:42:ASP:HB3	10:L:44:SER:H	1.74	0.52
11:M:276:ASN:ND2	11:M:279:ASP:OD1	2.43	0.52
15:Q:103:ARG:NH1	15:Q:108:ILE:HB	2.24	0.52
17:S:101:PHE:HZ	17:S:120:LEU:HD11	1.74	0.52
3:D:187:LEU:HD21	3:D:244:VAL:HG12	1.91	0.52
5:F:89:THR:H	5:F:179:THR:HG21	1.75	0.52
7:I:83:ARG:O	7:I:87:ALA:CB	2.57	0.52
11:M:168:GLU:OE1	11:M:220:ARG:NH2	2.38	0.52
10:L:95:ARG:HG3	15:Q:165:GLU:OE2	2.10	0.52
11:M:264:GLN:NE2	11:M:269:LEU:O	2.42	0.52
1:A:1889:C:OP1	11:M:133:LYS:NZ	2.39	0.52
12:N:224:LEU:HD11	13:O:38:ARG:HB3	113.83	0.52
31:7:52:LYS:HG3	31:7:219:LEU:HD11	1.92	0.52
4:E:97:VAL:O	4:E:197:HIS:NE2	2.37	0.52
23:Y:83:ALA:N	33:9:74:VAL:O	2.38	0.51
1:A:2395:A:H4'	29:5:350:ARG:HH12	1.75	0.51
1:A:2310:G:O2'	1:A:2675:G:O6	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2932:G:OP1	5:F:137:ARG:NH1	2.42	0.51
1:A:3220:A:OP1	4:E:260:LYS:NZ	2.43	0.51
5:F:221:LEU:HD23	5:F:222:THR:HG23	1.91	0.51
17:S:101:PHE:CE2	17:S:116:ILE:CD1	2.90	0.51
19:U:44:ILE:HG23	19:U:48:MET:HB3	1.92	0.51
29:5:107:PHE:HB3	29:5:222:VAL:HG12	1.92	0.51
30:6:265:ILE:HG12	30:6:322:ARG:HG2	1.91	0.51
31:7:131:LYS:HE3	31:7:305:HIS:HB3	1.92	0.51
14:P:104:SER:OG	30:6:150:ARG:NH1	2.39	0.51
9:K:21:LEU:HD12	9:K:145:LEU:HD12	1.91	0.51
22:X:64:ASP:N	22:X:64:ASP:OD1	2.37	0.51
1:A:1747:G:OP2	1:A:1749:C:N4	2.43	0.51
8:J:39:LEU:HB3	8:J:44:VAL:HG11	1.91	0.51
19:U:44:ILE:HD11	19:U:53:LEU:HG	1.92	0.51
23:Y:143:ASP:OD1	33:9:137:ARG:NH2	2.44	0.51
14:P:152:GLU:HG3	14:P:158:MET:HG3	1.92	0.51
7:I:128:ASN:HA	7:I:131:LEU:HB3	1.92	0.51
4:E:104:LEU:HB2	4:E:121:LEU:HB2	1.92	0.51
9:K:59:ILE:HB	9:K:127:LEU:HD23	1.93	0.51
4:E:102:LEU:O	4:E:122:LEU:HA	2.11	0.51
4:E:348:ALA:HB2	15:Q:128:GLY:HA3	1.93	0.51
5:F:249:ASN:N	5:F:249:ASN:OD1	2.43	0.51
13:O:147:GLN:HE21	31:7:175:ILE:HG12	1.77	0.50
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.39	0.50
21:W:106:PRO:HD2	21:W:117:ILE:HD11	1.93	0.50
1:A:2709:A:H1'	25:0:96:ASN:HD21	1.76	0.50
5:F:81:ASP:OD1	5:F:81:ASP:N	2.42	0.50
20:V:122:LEU:HD12	20:V:133:ILE:HG13	1.93	0.50
31:7:282:ALA:HB2	31:7:321:ARG:HG2	1.94	0.50
1:A:2055:U:H2'	1:A:2056:G:H8	1.76	0.50
4:E:73:LEU:HD21	32:8:114:ARG:HG3	179.40	0.50
1:A:1718:A:N3	1:A:1911:C:O2'	2.39	0.50
23:Y:102:TRP:HE3	23:Y:142:LEU:HD22	1.76	0.50
12:N:191:SER:OG	12:N:192:ARG:N	2.43	0.50
23:Y:213:ARG:HA	23:Y:216:ARG:HH21	1.75	0.50
4:E:331:ASP:OD1	4:E:331:ASP:N	2.41	0.50
17:S:135:LEU:HD23	17:S:144:LEU:HB3	1.93	0.50
22:X:130:ARG:HE	22:X:134:LEU:HD11	1.77	0.50
1:A:2409:A:O2'	29:5:270:ILE:O	2.30	0.50
5:F:165:LEU:HB2	5:F:170:ARG:HD3	1.94	0.50
8:J:49:PHE:O	8:J:53:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:249:ASN:OD1	5:F:252:SER:OG	2.29	0.49
13:O:144:LEU:HD12	31:7:302:LEU:HD23	1.93	0.49
1:A:2471:G:OP1	10:L:37:ARG:N	2.38	0.49
19:U:66:ALA:HB2	19:U:100:ALA:HB2	1.94	0.49
29:5:228:ALA:HB3	29:5:292:TYR:HB2	1.93	0.49
31:7:108:VAL:HG22	31:7:125:ILE:HG12	1.94	0.49
1:A:2051:A:H2'	1:A:2052:A:C8	2.47	0.49
1:A:2293:A:H2'	11:M:39:ARG:HH12	1.78	0.49
19:U:52:ASP:O	19:U:56:TYR:HB2	2.12	0.49
1:A:1977:U:H2'	1:A:1978:A:H8	1.77	0.49
5:F:116:THR:HG23	5:F:118:ALA:H	1.76	0.49
1:A:2182:G:H1'	1:A:2199:A:H2'	1.93	0.49
30:6:57:TYR:O	30:6:61:ALA:CB	2.60	0.49
33:9:22:THR:HG23	33:9:24:LYS:H	1.77	0.49
14:P:128:ILE:O	14:P:132:LEU:HB2	2.12	0.49
14:P:56:LEU:HB3	14:P:62:ALA:HB2	1.93	0.49
23:Y:151:ASP:OD1	23:Y:154:ARG:NH1	2.42	0.49
30:6:268:LEU:O	30:6:318:PHE:HA	2.12	0.49
1:A:2318:A:H2'	1:A:2319:A:C8	2.48	0.49
5:F:230:ILE:HG23	5:F:242:LEU:HD11	1.93	0.49
20:V:25:PRO:HG2	20:V:28:SER:HB3	1.95	0.49
29:5:136:VAL:HG22	29:5:420:HIS:CD2	2.47	0.49
1:A:2349:G:H2'	1:A:2350:A:C8	2.48	0.49
1:A:3179:G:O2'	1:A:3190:A:N6	2.42	0.49
15:Q:93:GLN:NE2	15:Q:285:GLU:OE1	2.41	0.49
1:A:1871:A:H61	1:A:1901:C:H5'	1.78	0.48
7:I:83:ARG:O	7:I:87:ALA:HB3	2.13	0.48
8:J:43:GLY:HA3	8:J:76:ARG:HH12	1.78	0.48
14:P:178:ILE:O	30:6:346:ARG:NH2	2.44	0.48
25:0:181:ARG:HD3	25:0:182:PRO:HD2	1.95	0.48
1:A:2395:A:OP1	29:5:173:ARG:NH2	2.46	0.48
30:6:222:ASP:N	30:6:222:ASP:OD1	2.44	0.48
23:Y:160:GLN:HG3	33:9:131:TYR:CG	2.48	0.48
3:D:74:ILE:HD13	3:D:148:LYS:HE3	1.94	0.48
19:U:37:GLU:HB3	19:U:104:THR:HG23	1.95	0.48
1:A:2173:G:H2'	1:A:2174:G:C8	2.48	0.48
8:J:113:THR:HA	8:J:156:VAL:HB	1.94	0.48
31:7:44:ARG:HB3	31:7:261:ILE:HD12	1.95	0.48
6:H:103:GLU:HG2	6:H:104:ASN:H	1.78	0.48
29:5:354:PHE:HB2	29:5:377:ASP:HB2	1.95	0.48
18:T:75:HIS:HD2	18:T:120:VAL:HG13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:94:LYS:HG3	11:M:129:ILE:HG22	1.95	0.48
13:O:46:TRP:HD1	13:O:121:ALA:HB2	1.79	0.48
20:V:177:THR:HG22	33:9:71:LYS:H	1.79	0.48
1:A:2815:G:N7	12:N:139:ARG:NH1	2.61	0.48
31:7:112:PRO:HB2	31:7:267:PRO:HG2	1.94	0.48
1:A:2248:U:OP1	16:R:99:ARG:NH2	2.35	0.48
1:A:2367:A:N3	23:Y:123:ARG:NH2	2.61	0.48
1:A:2740:A:N3	1:A:2921:A:O2'	2.46	0.48
9:K:21:LEU:HD11	9:K:34:MET:HE3	1.96	0.48
29:5:293:LEU:HD13	29:5:312:LYS:HE3	1.94	0.48
1:A:2191:A:H4'	8:J:142:ARG:HG3	1.94	0.48
14:P:96:HIS:ND1	14:P:98:ASN:OD1	2.46	0.48
19:U:42:PHE:HB2	19:U:95:ALA:HB3	1.96	0.48
1:A:2093:U:O2	1:A:2266:U:O2'	2.31	0.48
1:A:1909:A:H61	1:A:2010:U:H3	1.60	0.47
2:B:1609:U:O2	2:B:1616:A:N6	2.47	0.47
4:E:106:MET:HG2	4:E:120:THR:HG22	1.95	0.47
3:D:202:ARG:HE	3:D:205:GLN:NE2	2.11	0.47
29:5:200:ARG:NH2	29:5:234:ASP:OD1	2.47	0.47
1:A:1756:A:H2'	1:A:1757:A:H8	1.79	0.47
22:X:149:PRO:HD2	22:X:152:ASP:HB3	1.97	0.47
1:A:1990:G:N2	1:A:1993:A:C2	2.79	0.47
4:E:100:ILE:HA	4:E:297:VAL:O	2.15	0.47
8:J:22:ALA:H	8:J:68:THR:HG22	1.79	0.47
9:K:39:LEU:HD11	9:K:125:LEU:HB2	1.97	0.47
17:S:112:ASP:O	17:S:194:ARG:HA	2.14	0.47
30:6:355:LYS:HE3	30:6:358:PRO:HA	1.97	0.47
1:A:1883:G:N7	5:F:281:ARG:NH1	2.63	0.47
6:H:98:LEU:HD23	6:H:129:ALA:HB2	1.95	0.47
9:K:21:LEU:HD21	9:K:31:LEU:HD22	1.96	0.47
13:O:49:VAL:HG13	13:O:123:ILE:HG12	1.95	0.47
21:W:76:HIS:HB2	21:W:130:PHE:CD1	2.49	0.47
30:6:221:LEU:HD12	30:6:267:ARG:HG3	1.96	0.47
24:Z:100:HIS:HB3	24:Z:106:VAL:HG11	1.95	0.47
29:5:33:TRP:O	29:5:39:ARG:NH2	2.47	0.47
1:A:1848:U:OP1	11:M:48:LYS:NZ	2.47	0.47
1:A:2684:C:OP1	25:0:86:THR:OG1	2.22	0.47
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.34	0.47
1:A:2262:C:OP1	17:S:173:ARG:NH1	2.48	0.47
18:T:71:ALA:H	18:T:180:GLU:HB3	1.80	0.47
26:1:19:ARG:HB3	26:1:62:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:133:PRO:HG3	29:5:239:ILE:HD13	1.96	0.47
3:D:66:TRP:HA	3:D:80:ARG:HH11	1.80	0.47
9:K:21:LEU:HD22	9:K:59:ILE:HG12	1.96	0.47
13:O:79:TRP:NE1	15:Q:267:PHE:O	2.46	0.47
1:A:2854:U:H4'	28:3:138:PRO:HG2	1.97	0.47
1:A:2389:C:O2'	29:5:305:GLN:NE2	2.48	0.47
30:6:57:TYR:O	30:6:61:ALA:HB2	2.15	0.47
13:O:116:ASP:OD1	13:O:116:ASP:N	2.47	0.47
20:V:123:VAL:HG13	20:V:128:ARG:HA	1.97	0.47
1:A:2906:C:O2	26:1:19:ARG:NH2	2.47	0.47
23:Y:69:ASP:OD1	23:Y:69:ASP:N	2.47	0.47
2:B:1628:C:H5'	32:8:125:LYS:HG2	1.95	0.47
33:9:42:GLY:HA3	33:9:51:VAL:O	2.15	0.47
1:A:1800:G:N1	1:A:1803:A:OP2	2.48	0.47
15:Q:102:ARG:NH1	15:Q:169:PRO:HA	2.30	0.46
18:T:91:ALA:O	18:T:145:SER:OG	2.32	0.46
4:E:148:GLY:HA2	4:E:175:THR:O	2.15	0.46
5:F:83:HIS:HB3	5:F:86:VAL:HG12	1.97	0.46
10:L:111:ASN:OD1	10:L:111:ASN:N	2.46	0.46
1:A:1749:C:OP2	1:A:2899:C:O2'	2.29	0.46
3:D:74:ILE:HD13	3:D:148:LYS:HB2	1.98	0.46
6:H:116:LYS:HD3	6:H:120:ARG:HH22	1.81	0.46
11:M:260:LYS:NZ	11:M:265:ILE:O	2.39	0.46
12:N:160:VAL:HG12	12:N:161:VAL:HG23	1.97	0.46
19:U:28:LEU:H	23:Y:114:THR:HG22	1.80	0.46
1:A:2422:U:OP2	33:9:24:LYS:NZ	2.48	0.46
1:A:2457:A:O2'	13:O:17:ARG:NH2	2.49	0.46
7:I:52:GLU:O	12:N:211:ASN:ND2	2.43	0.46
11:M:264:GLN:NE2	11:M:267:PHE:O	2.48	0.46
29:5:162:ARG:NH2	29:5:176:TYR:OH	2.48	0.46
12:N:135:SER:HG	12:N:138:HIS:CG	2.34	0.46
29:5:310:ARG:HA	29:5:313:MET:HE2	1.98	0.46
10:L:119:ILE:HG21	10:L:123:ILE:HD11	1.96	0.46
10:L:98:PRO:HA	15:Q:162:ILE:HG13	1.98	0.46
13:O:46:TRP:CD1	13:O:121:ALA:HB2	2.50	0.46
15:Q:154:VAL:HG12	15:Q:159:GLY:HA2	1.98	0.46
13:O:108:LEU:HD13	25:0:122:LEU:HD21	1.96	0.46
1:A:1924:U:H5''	3:D:81:LYS:HB2	1.97	0.46
1:A:2268:G:N7	11:M:44:ARG:NH1	2.55	0.46
8:J:90:PHE:HE2	8:J:120:ILE:HD13	1.81	0.46
10:L:87:VAL:HG11	10:L:123:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:46:VAL:HG11	20:V:83:ARG:HA	1.97	0.46
7:I:119:HIS:HB3	7:I:121:ILE:HG22	1.97	0.46
14:P:154:ALA:HA	14:P:159:LYS:HE3	1.98	0.46
20:V:62:VAL:O	20:V:73:GLN:HA	2.15	0.46
29:5:355:LEU:HD23	29:5:376:VAL:HG12	1.97	0.46
19:U:3:ARG:H	19:U:23:ASN:HB3	1.81	0.46
19:U:17:LEU:HD21	33:9:136:LEU:HD12	1.96	0.46
1:A:1737:A:H61	1:A:1760:G:H1'	1.81	0.46
3:D:125:LYS:HB2	29:5:258:PRO:HD2	1.98	0.46
11:M:83:PHE:HB3	28:3:115:LEU:HD13	1.98	0.46
20:V:147:SER:OG	20:V:150:SER:O	2.29	0.46
20:V:54:TRP:NE1	20:V:56:LEU:O	2.49	0.46
1:A:1890:C:OP2	28:3:168:ARG:NH2	2.50	0.45
32:8:120:LYS:HA	32:8:123:LEU:HD12	1.98	0.45
1:A:2016:C:OP2	11:M:59:ARG:NH1	2.41	0.45
1:A:2103:A:HO2'	24:Z:35:LYS:N	2.14	0.45
1:A:2170:G:H4'	8:J:132:LEU:HD11	1.98	0.45
3:D:205:GLN:HB2	3:D:206:TYR:CE2	2.51	0.45
14:P:84:ILE:HB	14:P:91:GLU:HB3	1.98	0.45
1:A:2181:A:N6	1:A:2206:C:O2'	2.48	0.45
9:K:27:PRO:HG2	9:K:30:LYS:HB3	1.98	0.45
12:N:131:ILE:HD12	12:N:151:VAL:HG21	1.99	0.45
14:P:112:ILE:HD13	14:P:131:VAL:HG21	1.98	0.45
7:I:160:LYS:HG2	7:I:163:GLU:HB3	1.99	0.45
26:1:45:HIS:CD2	26:1:46:TYR:H	2.34	0.45
30:6:208:ALA:H	30:6:243:ASN:HD21	1.64	0.45
4:E:154:ARG:HB3	31:7:311:THR:HG21	1.99	0.45
1:A:2814:G:H2'	12:N:140:MET:HB2	1.99	0.45
11:M:230:PRO:O	11:M:234:LEU:HB2	2.16	0.45
14:P:54:ARG:NH1	14:P:140:GLY:O	2.50	0.45
21:W:103:VAL:HG22	21:W:127:TYR:HE1	1.81	0.45
30:6:235:TRP:HB3	30:6:254:TYR:HA	1.99	0.45
1:A:2165:C:O2'	1:A:2166:C:O4'	2.33	0.45
11:M:78:ILE:O	28:3:113:ARG:NH1	2.49	0.45
18:T:144:GLU:O	18:T:176:VAL:HA	2.17	0.45
27:2:64:HIS:HB2	27:2:92:HIS:HD2	1.82	0.45
27:2:91:SER:OG	27:2:92:HIS:N	2.50	0.45
1:A:1776:G:O6	1:A:1779:A:OP1	2.34	0.45
12:N:89:ILE:HD11	12:N:176:LEU:HD22	1.99	0.45
29:5:251:HIS:O	29:5:371:LYS:NZ	2.38	0.45
29:5:121:LEU:HD21	29:5:128:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:139:ASN:HB3	31:7:174:VAL:HG21	1.99	0.45
1:A:1688:A:OP2	22:X:5:LYS:NZ	2.47	0.45
1:A:2395:A:H1'	29:5:385:HIS:HB2	1.98	0.45
20:V:126:MET:SD	20:V:126:MET:N	2.89	0.45
22:X:150:LYS:HG3	22:X:159:MET:HE2	1.99	0.45
31:7:36:SER:HB2	31:7:39:GLU:HB2	1.98	0.45
3:D:121:PRO:HB3	3:D:166:SER:HA	1.98	0.45
19:U:28:LEU:HA	19:U:42:PHE:HA	1.99	0.45
22:X:86:ILE:HB	22:X:105:TRP:HB2	1.98	0.45
20:V:19:TYR:OH	20:V:31:ASP:OD2	2.31	0.44
1:A:2127:A:H4'	1:A:2251:A:C5	2.52	0.44
3:D:83:GLY:O	3:D:85:ARG:NH1	2.45	0.44
4:E:217:GLY:HA2	4:E:258:PRO:HB3	1.98	0.44
13:O:84:ASP:N	13:O:84:ASP:OD1	2.50	0.44
29:5:350:ARG:HE	29:5:351:VAL:HG23	1.82	0.44
22:X:127:VAL:HG22	22:X:131:THR:HB	1.99	0.44
24:Z:66:LEU:HB2	24:Z:122:LEU:HB3	1.99	0.44
29:5:200:ARG:HE	29:5:233:LYS:HD2	1.82	0.44
21:W:57:GLU:HB2	21:W:99:TYR:HD1	1.83	0.44
29:5:391:VAL:HG13	29:5:398:VAL:HB	2.00	0.44
1:A:1756:A:H2'	1:A:1757:A:C8	2.52	0.44
1:A:2420:U:O2'	33:9:23:SER:OG	2.34	0.44
4:E:119:VAL:HG11	4:E:284:TYR:HB3	1.98	0.44
4:E:56:GLU:OE1	4:E:57:ASN:ND2	2.51	0.44
12:N:116:LYS:O	12:N:166:ARG:NH1	2.51	0.44
13:O:107:MET:HA	13:O:122:VAL:O	2.18	0.44
6:H:59:TRP:HE1	22:X:96:LYS:HE2	1.83	0.44
31:7:303:PRO:HG2	31:7:306:LEU:H	1.83	0.44
1:A:2815:G:O6	12:N:139:ARG:NH2	2.42	0.44
1:A:1878:U:O3'	5:F:92:ARG:NH2	2.51	0.44
1:A:2034:A:O2'	11:M:71:GLN:OE1	2.29	0.44
13:O:108:LEU:HD11	13:O:135:LEU:HD23	1.99	0.44
17:S:100:HIS:O	17:S:100:HIS:CG	2.70	0.44
20:V:95:TYR:HB3	20:V:108:MET:SD	2.58	0.44
11:M:28:LYS:HG2	11:M:29:PRO:HD2	2.00	0.44
21:W:95:GLY:HA3	21:W:134:VAL:O	2.18	0.44
14:P:57:GLU:OE2	14:P:96:HIS:NE2	2.51	0.44
30:6:161:LEU:HD13	30:6:221:LEU:HD21	2.01	0.43
6:H:84:GLU:OE1	22:X:44:ARG:NH2	2.50	0.43
5:F:289:PRO:HD2	11:M:195:LEU:HD11	1.99	0.43
15:Q:152:ARG:NH1	15:Q:191:ARG:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3131:G:H3'	1:A:3132:G:H8	1.83	0.43
3:D:202:ARG:HH21	3:D:205:GLN:HE22	1.66	0.43
8:J:69:LYS:HD3	8:J:129:ALA:HB1	1.99	0.43
8:J:25:ARG:HA	8:J:65:PRO:HA	2.01	0.43
18:T:76:CYS:HA	18:T:174:TYR:O	2.18	0.43
22:X:56:ASN:OD1	22:X:56:ASN:N	2.48	0.43
30:6:39:ASP:OD1	30:6:39:ASP:N	2.51	0.43
4:E:76:LYS:HG3	4:E:170:LEU:HD21	2.00	0.43
1:A:1839:C:H5'	9:K:117:HIS:ND1	2.33	0.43
11:M:292:LYS:O	11:M:296:SER:OG	2.31	0.43
22:X:42:HIS:CG	22:X:86:ILE:HD11	2.54	0.43
23:Y:171:ASP:N	23:Y:171:ASP:OD1	2.51	0.43
1:A:1924:U:H2'	1:A:1925:A:C8	2.53	0.43
15:Q:91:LYS:NZ	15:Q:95:GLU:OE2	2.27	0.43
17:S:57:SER:OG	17:S:58:SER:N	2.51	0.43
1:A:2327:U:H4'	13:O:30:ARG:HH21	1.84	0.43
5:F:138:HIS:CD2	5:F:146:TRP:HE1	2.36	0.43
17:S:131:GLU:HG2	17:S:151:LYS:HE2	2.00	0.43
1:A:1868:G:N7	11:M:51:ARG:NH2	2.67	0.43
9:K:45:PRO:HB3	16:R:75:ALA:HB2	2.01	0.43
17:S:101:PHE:HB3	17:S:106:TRP:CD1	2.53	0.43
29:5:114:LEU:HD13	29:5:263:ILE:HG12	2.00	0.43
31:7:286:LEU:HD12	31:7:294:ILE:HB	2.00	0.43
33:9:128:PHE:CD1	33:9:135:PHE:HB3	2.53	0.43
1:A:2415:C:N4	33:9:49:ARG:HH12	2.17	0.43
1:A:2740:A:H2'	1:A:2741:A:C8	2.53	0.43
31:7:220:GLU:HB3	31:7:251:ILE:HD11	2.00	0.43
6:H:117:SER:O	6:H:121:ASN:HB2	2.18	0.43
12:N:76:SER:HB3	12:N:155:LYS:HB2	2.00	0.43
31:7:103:SER:HA	31:7:129:THR:HG22	2.01	0.43
31:7:180:CYS:HA	31:7:297:PHE:O	2.19	0.43
1:A:2055:U:H2'	1:A:2056:G:C8	2.52	0.43
1:A:2682:A:H5''	16:R:34:ARG:HH12	1.83	0.43
25:0:95:ARG:HD3	25:0:95:ARG:HH11	1.71	0.43
3:D:180:ASP:N	3:D:180:ASP:OD1	2.39	0.43
17:S:167:TRP:HE1	17:S:169:ARG:HH21	1.67	0.43
1:A:2371:U:H2'	19:U:71:ARG:HD3	2.01	0.43
27:2:89:SER:O	27:2:89:SER:OG	2.36	0.42
29:5:214:ASN:OD1	29:5:219:LEU:HD13	2.17	0.42
29:5:366:CYS:SG	29:5:367:ASN:N	2.92	0.42
1:A:2171:U:C2	1:A:2173:G:H4'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:125:ALA:HB2	8:J:140:VAL:HG21	2.00	0.42
12:N:50:LEU:HB2	12:N:110:ASN:HD21	1.84	0.42
16:R:42:ALA:O	16:R:46:VAL:HB	2.19	0.42
23:Y:169:ARG:HH22	29:5:64:MET:HB2	1.84	0.42
1:A:1750:G:OP2	28:3:113:ARG:NH2	2.46	0.42
1:A:2187:C:H2'	1:A:2188:A:C8	2.54	0.42
3:D:66:TRP:HB3	3:D:80:ARG:HE	1.84	0.42
8:J:49:PHE:O	8:J:53:PHE:CB	2.68	0.42
19:U:22:THR:HG21	19:U:56:TYR:HE1	1.83	0.42
30:6:236:LEU:O	30:6:251:THR:OG1	2.36	0.42
30:6:235:TRP:HA	30:6:252:CYS:O	2.19	0.42
20:V:183:LEU:HD11	33:9:79:PRO:HD2	2.02	0.42
1:A:2395:A:O2'	29:5:384:GLN:NE2	2.43	0.42
4:E:208:ALA:HB2	4:E:297:VAL:HG12	2.00	0.42
5:F:113:LYS:HG3	5:F:157:GLY:H	1.83	0.42
12:N:103:GLU:OE1	12:N:106:ARG:NH2	2.42	0.42
15:Q:122:ALA:HB2	15:Q:172:GLN:HE22	1.84	0.42
29:5:125:LYS:HA	29:5:253:LEU:HD21	2.00	0.42
31:7:108:VAL:HB	31:7:113:TRP:CD1	2.54	0.42
31:7:175:ILE:HG13	31:7:175:ILE:H	1.58	0.42
4:E:144:THR:HA	4:E:179:PHE:O	2.20	0.42
23:Y:187:PRO:HD2	23:Y:190:LEU:HD11	2.02	0.42
1:A:1977:U:H2'	1:A:1978:A:C8	2.55	0.42
1:A:2103:A:H4'	12:N:231:SER:HA	2.01	0.42
1:A:2326:C:OP2	17:S:55:SER:OG	117.33	0.42
3:D:225:ILE:HA	3:D:234:MET:O	2.20	0.42
9:K:67:PHE:HB3	9:K:71:LYS:HB2	2.01	0.42
18:T:144:GLU:HB2	18:T:177:LYS:HB3	2.01	0.42
1:A:2682:A:H5''	16:R:34:ARG:NH1	2.34	0.42
8:J:50:CYS:HA	8:J:53:PHE:HB3	2.01	0.42
11:M:118:LEU:HD21	11:M:129:ILE:HD11	2.02	0.42
18:T:109:ASN:HD21	25:0:101:ILE:HD13	1.85	0.42
31:7:219:LEU:HA	31:7:219:LEU:HD23	1.91	0.42
1:A:2913:A:H4'	1:A:2914:A:H5''	2.02	0.42
5:F:243:ILE:HG22	5:F:244:PRO:O	2.20	0.42
7:I:121:ILE:HG13	7:I:156:SER:HB2	2.01	0.42
7:I:96:ILE:HD11	7:I:153:LEU:HD22	2.01	0.42
15:Q:150:ILE:HA	15:Q:162:ILE:O	2.20	0.42
22:X:226:LEU:HD23	22:X:229:ILE:HD12	2.02	0.42
27:2:53:TYR:CZ	27:2:55:PRO:HB3	2.55	0.42
30:6:161:LEU:HD21	30:6:271:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:303:PRO:HG2	31:7:306:LEU:HB2	2.02	0.42
1:A:3146:G:N2	4:E:268:GLU:OE2	2.46	0.42
13:O:123:ILE:HD13	13:O:123:ILE:HG21	1.76	0.42
29:5:215:ARG:NH2	29:5:366:CYS:O	2.53	0.42
29:5:293:LEU:HD22	29:5:316:PHE:HD2	1.85	0.42
4:E:116:LYS:HD2	15:Q:165:GLU:OE2	2.19	0.42
4:E:276:ILE:HG13	4:E:332:LEU:HB2	2.02	0.42
5:F:83:HIS:CG	5:F:274:LEU:HD11	2.55	0.42
16:R:10:LEU:HD13	16:R:10:LEU:HA	1.87	0.42
25:0:94:ARG:HA	25:0:99:LYS:HD2	2.02	0.41
6:H:64:LEU:HB2	22:X:63:GLU:OE1	2.20	0.41
9:K:46:VAL:HG13	18:T:208:ILE:HG12	2.01	0.41
10:L:52:HIS:CE1	10:L:53:ARG:HG3	2.55	0.41
30:6:105:GLU:O	30:6:109:ALA:CB	2.68	0.41
4:E:266:ARG:HA	4:E:266:ARG:HD3	1.78	0.41
4:E:112:LYS:NZ	4:E:335:GLU:O	2.42	0.41
10:L:75:LEU:O	10:L:81:LYS:HA	2.21	0.41
11:M:129:ILE:HD13	11:M:129:ILE:HG21	1.87	0.41
13:O:106:ARG:HG2	13:O:124:GLU:HG2	2.01	0.41
33:9:68:PHE:CE2	33:9:70:LEU:HB2	2.55	0.41
1:A:2194:U:C4	7:I:125:VAL:HB	2.55	0.41
1:A:2142:A:O2'	1:A:2262:C:OP1	2.37	0.41
15:Q:100:LEU:HD23	15:Q:100:LEU:HA	1.88	0.41
25:0:90:ASN:O	25:0:94:ARG:HG2	2.20	0.41
13:O:80:LEU:HD23	13:O:80:LEU:HA	1.94	0.41
28:3:110:VAL:HG13	28:3:158:LEU:HD22	2.02	0.41
1:A:3116:C:N3	1:A:3140:A:N1	2.68	0.41
3:D:193:ILE:HD11	3:D:226:ILE:HD12	2.03	0.41
4:E:73:LEU:HD11	4:E:151:THR:HG21	2.03	0.41
6:H:55:ILE:HG21	22:X:44:ARG:HD2	2.02	0.41
4:E:99:LEU:HA	4:E:99:LEU:HD23	1.92	0.41
8:J:124:LYS:HE2	8:J:144:ILE:HG21	2.03	0.41
8:J:32:GLY:HA3	8:J:33:PRO:HD3	1.92	0.41
9:K:20:LEU:HD22	9:K:21:LEU:H	1.86	0.41
11:M:62:ARG:HA	11:M:63:PRO:HD3	1.95	0.41
12:N:218:ILE:HA	12:N:223:MET:HG3	2.03	0.41
21:W:67:ILE:HG21	21:W:131:VAL:HG11	2.02	0.41
11:M:78:ILE:HD13	28:3:124:ARG:HD2	2.03	0.41
28:3:133:LEU:HD22	28:3:141:LYS:HG2	2.02	0.41
1:A:1802:A:OP1	20:V:83:ARG:NH2	2.54	0.41
1:A:2837:A:H2'	1:A:2838:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:142:GLU:HB2	11:M:162:LEU:HD22	2.03	0.41
17:S:114:ILE:HD13	17:S:114:ILE:HG21	1.79	0.41
18:T:140:LEU:HD23	18:T:180:GLU:HA	2.02	0.41
29:5:133:PRO:HD3	29:5:375:TRP:CG	2.56	0.41
31:7:65:ILE:HG13	31:7:65:ILE:H	1.63	0.41
1:A:2677:A:H2'	1:A:2678:A:C8	2.55	0.41
5:F:70:ARG:HA	5:F:196:PRO:HD3	2.03	0.41
5:F:252:SER:O	5:F:256:HIS:ND1	2.54	0.41
7:I:188:ARG:HA	7:I:191:PHE:HD2	1.85	0.41
7:I:178:GLY:HA2	7:I:191:PHE:HE2	1.86	0.41
8:J:18:GLY:N	8:J:72:VAL:O	2.53	0.41
24:Z:50:PRO:HA	24:Z:53:HIS:HD2	1.85	0.41
4:E:179:PHE:CE1	4:E:298:LYS:HE3	2.56	0.41
5:F:164:MET:SD	5:F:170:ARG:NH1	2.93	0.41
7:I:119:HIS:HD2	7:I:121:ILE:HB	1.85	0.41
9:K:110:GLY:O	9:K:114:LYS:NZ	2.51	0.41
20:V:185:ARG:NH2	20:V:187:TYR:O	2.54	0.41
26:1:33:LYS:HE3	26:1:65:LEU:HD11	2.03	0.41
30:6:356:ARG:HD2	30:6:356:ARG:HA	1.87	0.41
9:K:36:SER:O	9:K:40:GLN:HG3	2.21	0.41
11:M:129:ILE:HD12	11:M:184:LEU:HD11	2.03	0.41
15:Q:188:LEU:HD22	15:Q:191:ARG:HH12	1.86	0.41
30:6:274:LYS:HG3	30:6:314:ALA:HB2	2.02	0.41
4:E:345:ILE:HG13	4:E:345:ILE:H	1.68	0.41
13:O:65:LEU:HB3	13:O:69:ASN:HD22	1.85	0.41
21:W:100:THR:O	21:W:129:THR:HA	2.21	0.41
31:7:269:ILE:HD13	31:7:269:ILE:HA	1.92	0.40
1:A:1871:A:O2'	1:A:1900:A:N6	2.54	0.40
1:A:2310:G:N2	1:A:2311:U:O4	2.36	0.40
1:A:3228:U:OP2	4:E:156:ARG:NH2	2.54	0.40
5:F:93:LEU:H	13:O:91:GLN:HE21	133.45	0.40
13:O:129:CYS:HG	25:O:156:THR:HG1	1.66	0.40
23:Y:90:LEU:HA	23:Y:90:LEU:HD23	1.88	0.40
29:5:203:CYS:HA	29:5:230:LEU:HA	2.03	0.40
29:5:84:ASP:HA	29:5:85:PRO:HD3	1.93	0.40
30:6:224:HIS:HA	30:6:232:TYR:CE2	2.56	0.40
33:9:87:THR:HG23	33:9:90:GLN:H	1.86	0.40
9:K:25:MET:O	9:K:149:ARG:NH1	2.55	0.40
1:A:1784:A:O2'	19:U:84:ASN:ND2	2.55	0.40
22:X:150:LYS:HB2	22:X:159:MET:CE	2.47	0.40
24:Z:40:ARG:NH2	30:6:27:ARG:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:232:THR:HG23	29:5:289:HIS:HB2	2.03	0.40
5:F:126:LYS:NZ	5:F:138:HIS:O	2.42	0.40
7:I:117:ARG:NH1	8:J:133:GLN:OE1	2.54	0.40
15:Q:116:ILE:HA	15:Q:135:GLY:O	2.22	0.40
19:U:39:THR:HA	19:U:97:VAL:O	2.21	0.40
24:Z:78:ARG:O	24:Z:83:LYS:NZ	2.55	0.40
1:A:2180:A:H4'	1:A:2181:A:C8	2.56	0.40
8:J:24:VAL:HG21	8:J:35:LEU:HD21	2.03	0.40
9:K:65:ILE:HD13	9:K:65:ILE:HG21	1.93	0.40
11:M:95:PRO:HB3	11:M:141:VAL:HG21	2.03	0.40
15:Q:102:ARG:HA	15:Q:102:ARG:HD2	1.96	0.40
28:3:125:ARG:HD2	28:3:125:ARG:HH21	1.66	0.40
31:7:167:VAL:HG23	31:7:235:TYR:HB3	2.03	0.40
1:A:1884:G:N3	1:A:1895:C:O2'	2.55	0.40
1:A:2196:A:O2'	1:A:2213:A:N1	2.50	0.40
12:N:105:MET:O	12:N:109:ILE:HB	2.22	0.40
18:T:77:ARG:HD3	18:T:120:VAL:HG22	2.03	0.40
19:U:44:ILE:HG21	19:U:44:ILE:HD13	1.80	0.40
22:X:116:SER:O	22:X:120:ASP:N	2.55	0.40
22:X:90:ILE:HG21	22:X:90:ILE:HD13	1.91	0.40
23:Y:78:LYS:HE2	23:Y:78:LYS:HB2	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
3	D	216/305 (71%)	203 (94%)	13 (6%)	0	100	100
4	E	281/348 (81%)	273 (97%)	8 (3%)	0	100	100
5	F	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
6	H	93/267 (35%)	85 (91%)	7 (8%)	1 (1%)	17	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
8	J	138/192 (72%)	120 (87%)	18 (13%)	0	100	100
9	K	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
10	L	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
11	M	285/296 (96%)	275 (96%)	10 (4%)	0	100	100
12	N	203/251 (81%)	192 (95%)	11 (5%)	0	100	100
13	O	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
14	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100
15	Q	215/292 (74%)	200 (93%)	15 (7%)	0	100	100
16	R	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
17	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100
18	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
19	U	135/153 (88%)	126 (93%)	9 (7%)	0	100	100
20	V	188/216 (87%)	183 (97%)	5 (3%)	0	100	100
21	W	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
22	X	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
24	Z	118/161 (73%)	110 (93%)	8 (7%)	0	100	100
25	0	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	87 (94%)	6 (6%)	0	100	100
29	5	383/423 (90%)	363 (95%)	20 (5%)	0	100	100
30	6	316/380 (83%)	300 (95%)	16 (5%)	0	100	100
31	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
32	8	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
33	9	113/137 (82%)	109 (96%)	4 (4%)	0	100	100
34	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
35	b	146/215 (68%)	130 (89%)	16 (11%)	0	100	100
36	c	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
37	d	203/306 (66%)	191 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	e	211/279 (76%)	179 (85%)	31 (15%)	1 (0%)	32	71
39	f	110/212 (52%)	98 (89%)	11 (10%)	1 (1%)	20	58
40	g	127/166 (76%)	115 (91%)	12 (9%)	0	100	100
41	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
42	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
43	j	83/123 (68%)	81 (98%)	2 (2%)	0	100	100
44	k	76/112 (68%)	71 (93%)	5 (7%)	0	100	100
45	l	21/138 (15%)	21 (100%)	0	0	100	100
46	m	43/128 (34%)	37 (86%)	4 (9%)	2 (5%)	3	15
47	o	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
48	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
49	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
50	r	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
51	s	366/439 (83%)	354 (97%)	12 (3%)	0	100	100
53	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
54	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
55	w	77/156 (49%)	69 (90%)	8 (10%)	0	100	100
All	All	7945/11026 (72%)	7507 (94%)	433 (5%)	5 (0%)	58	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	m	71	PRO
6	H	104	ASN
38	e	256	THR
39	f	179	PRO
46	m	53	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	179/245 (73%)	177 (99%)	2 (1%)	78	93
4	E	246/290 (85%)	244 (99%)	2 (1%)	85	95
5	F	217/262 (83%)	211 (97%)	6 (3%)	49	81
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	145/232 (62%)	144 (99%)	1 (1%)	87	95
8	J	113/150 (75%)	113 (100%)	0	100	100
9	K	155/156 (99%)	153 (99%)	2 (1%)	73	91
10	L	98/124 (79%)	97 (99%)	1 (1%)	80	93
11	M	245/249 (98%)	240 (98%)	5 (2%)	60	86
12	N	172/211 (82%)	169 (98%)	3 (2%)	66	89
13	O	133/150 (89%)	132 (99%)	1 (1%)	85	95
14	P	123/155 (79%)	121 (98%)	2 (2%)	68	89
15	Q	199/256 (78%)	198 (100%)	1 (0%)	91	97
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	141/180 (78%)	141 (100%)	0	100	100
18	T	141/176 (80%)	141 (100%)	0	100	100
19	U	124/135 (92%)	122 (98%)	2 (2%)	68	89
20	V	172/191 (90%)	167 (97%)	5 (3%)	48	80
21	W	89/119 (75%)	88 (99%)	1 (1%)	78	93
22	X	219/229 (96%)	214 (98%)	5 (2%)	56	84
23	Y	159/223 (71%)	156 (98%)	3 (2%)	62	87
24	Z	111/147 (76%)	111 (100%)	0	100	100
25	0	97/164 (59%)	95 (98%)	2 (2%)	59	86
26	1	49/60 (82%)	46 (94%)	3 (6%)	22	57
27	2	38/72 (53%)	38 (100%)	0	100	100
28	3	88/166 (53%)	86 (98%)	2 (2%)	56	84
29	5	348/368 (95%)	341 (98%)	7 (2%)	60	86
30	6	265/332 (80%)	262 (99%)	3 (1%)	78	93
31	7	263/303 (87%)	260 (99%)	3 (1%)	78	93
32	8	91/190 (48%)	90 (99%)	1 (1%)	78	93
33	9	99/112 (88%)	99 (100%)	0	100	100
34	a	78/133 (59%)	76 (97%)	2 (3%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	b	130/186 (70%)	128 (98%)	2 (2%)	70	90
36	c	241/288 (84%)	239 (99%)	2 (1%)	85	95
37	d	193/274 (70%)	191 (99%)	2 (1%)	80	93
38	e	188/236 (80%)	185 (98%)	3 (2%)	68	89
39	f	101/188 (54%)	101 (100%)	0	100	100
40	g	119/148 (80%)	117 (98%)	2 (2%)	66	89
41	h	95/148 (64%)	93 (98%)	2 (2%)	59	86
42	i	86/110 (78%)	85 (99%)	1 (1%)	75	92
43	j	68/97 (70%)	68 (100%)	0	100	100
44	k	71/90 (79%)	71 (100%)	0	100	100
45	l	23/116 (20%)	23 (100%)	0	100	100
46	m	40/113 (35%)	39 (98%)	1 (2%)	53	83
47	o	68/87 (78%)	68 (100%)	0	100	100
48	p	117/181 (65%)	116 (99%)	1 (1%)	82	94
49	q	110/178 (62%)	106 (96%)	4 (4%)	40	75
50	r	133/169 (79%)	131 (98%)	2 (2%)	70	90
51	s	326/381 (86%)	320 (98%)	6 (2%)	64	88
53	u	105/200 (52%)	105 (100%)	0	100	100
54	v	59/60 (98%)	58 (98%)	1 (2%)	66	89
55	w	73/136 (54%)	72 (99%)	1 (1%)	71	91
All	All	7147/9520 (75%)	7052 (99%)	95 (1%)	75	91

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	147	ARG
3	D	206	TYR
4	E	275	ARG
4	E	284	TYR
5	F	108	ARG
5	F	125	ARG
5	F	147	ARG
5	F	170	ARG
5	F	259	LEU
5	F	281	ARG

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Mol	Chain	Res	Type
7	I	146	LEU
9	K	16	ARG
9	K	125	LEU
10	L	39	ARG
11	M	44	ARG
11	M	47	ARG
11	M	57	ARG
11	M	96	LEU
11	M	134	ARG
12	N	51	ARG
12	N	105	MET
12	N	226	ILE
13	O	36	LEU
14	P	51	ARG
14	P	120	ARG
15	Q	151	LEU
19	U	3	ARG
19	U	71	ARG
20	V	92	ASN
20	V	138	THR
20	V	143	ARG
20	V	145	ARG
20	V	208	ARG
21	W	105	VAL
22	X	23	ARG
22	X	36	ARG
22	X	59	ARG
22	X	130	ARG
22	X	216	ARG
23	Y	162	ARG
23	Y	191	ASN
23	Y	210	ARG
25	0	84	ARG
25	0	168	GLN
26	1	34	ARG
26	1	38	ARG
26	1	61	LYS
28	3	125	ARG
28	3	168	ARG
29	5	36	ARG
29	5	98	LEU
29	5	102	GLN

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Mol	Chain	Res	Type
29	5	106	ILE
29	5	218	LEU
29	5	229	ARG
29	5	350	ARG
30	6	52	ARG
30	6	159	ARG
30	6	334	LEU
31	7	64	LYS
31	7	167	VAL
31	7	319	ARG
32	8	101	ARG
34	a	111	GLN
34	a	122	ARG
35	b	11	LEU
35	b	144	ARG
36	c	87	LEU
36	c	202	LEU
37	d	119	GLN
37	d	164	VAL
38	e	55	ARG
38	e	151	ARG
38	e	273	ARG
40	g	68	THR
40	g	100	ILE
41	h	96	LEU
41	h	120	MET
42	i	113	ARG
46	m	42	ARG
48	p	129	ARG
49	q	28	ARG
49	q	46	LEU
49	q	82	LEU
49	q	114	ARG
50	r	36	ARG
50	r	74	ARG
51	s	81	ARG
51	s	230	ARG
51	s	238	ASN
51	s	299	PHE
51	s	360	VAL
51	s	361	ILE
54	v	63	ASN

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Mol	Chain	Res	Type
55	w	106	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	205	GLN
3	D	227	GLN
4	E	184	ASN
6	H	121	ASN
10	L	142	GLN
11	M	170	ASN
13	O	147	GLN
14	P	87	GLN
16	R	89	ASN
16	R	125	HIS
17	S	118	ASN
17	S	140	ASN
18	T	210	HIS
19	U	4	ASN
19	U	82	HIS
20	V	92	ASN
21	W	62	HIS
22	X	46	HIS
23	Y	195	ASN
25	0	106	ASN
29	5	305	GLN
30	6	320	GLN
30	6	332	HIS
30	6	359	HIS
32	8	143	GLN
35	b	27	GLN
37	d	167	HIS
37	d	251	GLN
38	e	212	HIS
39	f	112	ASN
41	h	87	GLN
42	i	120	HIS
42	i	124	HIS
44	k	26	ASN
50	r	112	HIS
51	s	238	ASN
51	s	298	GLN

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Mol	Chain	Res	Type
54	v	63	ASN
55	w	103	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1071/1559 (68%)	302 (28%)	17 (1%)
2	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1122/1628 (68%)	317 (28%)	18 (1%)

All (317) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1681	G
1	A	1689	C
1	A	1694	U
1	A	1700	U
1	A	1701	U
1	A	1703	C
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1716	U
1	A	1717	U
1	A	1719	G
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1731	A
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1760	G

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Mol	Chain	Res	Type
1	A	1770	G
1	A	1773	A
1	A	1775	A
1	A	1781	A
1	A	1791	G
1	A	1794	A
1	A	1803	A
1	A	1804	A
1	A	1805	A
1	A	1806	U
1	A	1812	C
1	A	1813	C
1	A	1817	C
1	A	1820	A
1	A	1823	A
1	A	1824	U
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1849	C
1	A	1861	U
1	A	1867	A
1	A	1869	A
1	A	1870	A
1	A	1871	A
1	A	1872	U
1	A	1874	A
1	A	1875	C
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1887	A
1	A	1888	G
1	A	1890	C
1	A	1892	A
1	A	1893	A
1	A	1901	C
1	A	1903	C
1	A	1914	A

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Mol	Chain	Res	Type
1	A	1918	G
1	A	1927	G
1	A	1975	U
1	A	1985	G
1	A	1987	G
1	A	1992	C
1	A	1994	A
1	A	2000	C
1	A	2001	C
1	A	2002	G
1	A	2004	G
1	A	2015	G
1	A	2020	U
1	A	2021	U
1	A	2022	G
1	A	2023	U
1	A	2027	A
1	A	2028	G
1	A	2029	A
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2041	U
1	A	2053	U
1	A	2055	U
1	A	2060	A
1	A	2065	A
1	A	2074	A
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2095	U
1	A	2105	G
1	A	2113	G
1	A	2124	A
1	A	2125	C
1	A	2126	U
1	A	2132	A
1	A	2134	A

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Mol	Chain	Res	Type
1	A	2142	A
1	A	2147	G
1	A	2154	A
1	A	2156	A
1	A	2157	U
1	A	2158	U
1	A	2159	U
1	A	2161	A
1	A	2163	A
1	A	2166	C
1	A	2168	U
1	A	2171	U
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2180	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2190	C
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2197	G
1	A	2198	A
1	A	2200	A
1	A	2204	U
1	A	2207	A
1	A	2210	C
1	A	2216	A
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2243	A
1	A	2244	U
1	A	2245	A
1	A	2257	C
1	A	2259	C
1	A	2261	C
1	A	2262	C
1	A	2263	C

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Mol	Chain	Res	Type
1	A	2264	A
1	A	2281	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2290	A
1	A	2296	U
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2306	A
1	A	2313	A
1	A	2315	A
1	A	2321	A
1	A	2323	A
1	A	2324	U
1	A	2332	C
1	A	2335	A
1	A	2342	U
1	A	2345	G
1	A	2371	U
1	A	2374	A
1	A	2375	C
1	A	2381	A
1	A	2387	U
1	A	2389	C
1	A	2390	A
1	A	2393	C
1	A	2396	C
1	A	2401	A
1	A	2405	C
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2417	C
1	A	2418	A
1	A	2426	C
1	A	2427	C
1	A	2431	C
1	A	2435	G
1	A	2443	C

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Mol	Chain	Res	Type
1	A	2444	A
1	A	2445	U
1	A	2446	A
1	A	2449	G
1	A	2457	A
1	A	2458	A
1	A	2468	A
1	A	2508	C
1	A	2511	C
1	A	2512	A
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2526	C
1	A	2527	A
1	A	2655	G
1	A	2656	U
1	A	2659	C
1	A	2660	U
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2698	G
1	A	2699	C
1	A	2706	A
1	A	2707	A
1	A	2708	C
1	A	2709	A
1	A	2725	A
1	A	2732	G
1	A	2734	A
1	A	2739	U
1	A	2740	A
1	A	2744	U
1	A	2750	U
1	A	2752	C
1	A	2803	A
1	A	2804	A
1	A	2810	G
1	A	2813	U

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Mol	Chain	Res	Type
1	A	2814	G
1	A	2815	G
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2844	G
1	A	2846	G
1	A	2847	C
1	A	2852	C
1	A	2854	U
1	A	2859	A
1	A	2861	A
1	A	2864	U
1	A	2865	C
1	A	2870	G
1	A	2871	U
1	A	2879	A
1	A	2893	A
1	A	2895	U
1	A	2896	G
1	A	2901	A
1	A	2906	C
1	A	2910	A
1	A	2912	C
1	A	2913	A
1	A	2914	A
1	A	2915	C
1	A	2917	G
1	A	2922	A
1	A	2926	A
1	A	2928	C
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3114	U
1	A	3123	G
1	A	3124	U
1	A	3128	A
1	A	3129	A
1	A	3131	G
1	A	3134	C
1	A	3137	G

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Mol	Chain	Res	Type
1	A	3138	A
1	A	3139	G
1	A	3141	A
1	A	3150	U
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3177	A
1	A	3180	A
1	A	3183	U
1	A	3184	C
1	A	3185	A
1	A	3189	C
1	A	3190	A
1	A	3202	U
1	A	3204	C
1	A	3207	A
1	A	3217	A
1	A	3218	A
2	B	1607	U
2	B	1608	G
2	B	1609	U
2	B	1611	G
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1631	C
2	B	1632	U
2	B	1640	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1649	C
2	B	1651	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1703	C

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Mol	Chain	Res	Type
1	A	1713	A
1	A	1772	A
1	A	1780	U
1	A	1805	A
1	A	1823	A
1	A	2030	U
1	A	2125	C
1	A	2165	C
1	A	2172	A
1	A	2186	C
1	A	2243	A
1	A	2444	A
1	A	2457	A
1	A	2507	A
1	A	2905	A
1	A	3201	A
2	B	1607	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 51 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	PNS	v	101	55,54	15,20,21	2.38	5 (33%)	17,26,29	1.13	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PNS	v	101	55,54	-	0/24/26/27	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	v	101	PNS	O27-C28	-3.50	1.39	1.44
58	v	101	PNS	O35-C34	-2.17	1.19	1.23
58	v	101	PNS	O40-C39	-2.12	1.18	1.23
58	v	101	PNS	C39-N41	5.13	1.45	1.33
58	v	101	PNS	C34-N36	5.94	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	v	101	PNS	C31-C29-C32	2.55	113.25	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	Z	1
42	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	151:LEU	C	152:LYS	N	1.17
1	i	68:LYS	C	69:HIS	N	1.16