



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 4, 2017 – 03:12 PM EST

PDB ID : 6AZ1
EMDB ID: : EMD-7024
Title : Cryo-EM structure of the small subunit of Leishmania ribosome bound to paromomycin
Authors : Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Matzov, D.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : unknown
Resolution : 2.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

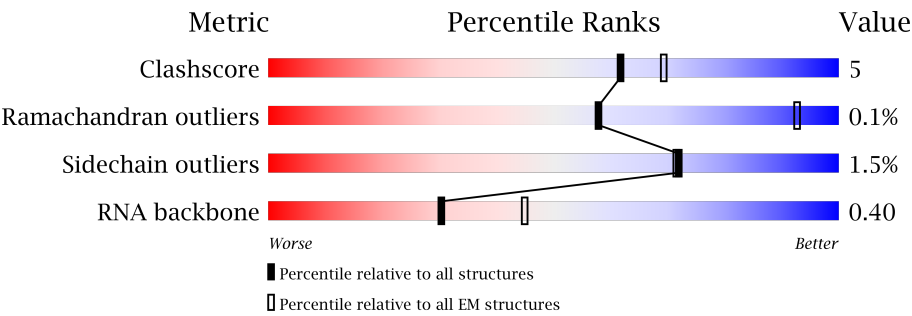
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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








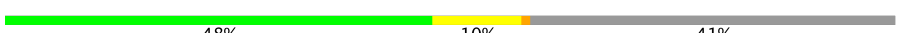











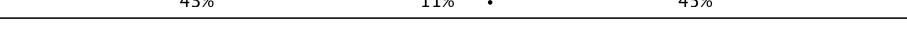







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	A	264	<div><div>68%17%15%</div><div></div></div>
2	B	246	<div><div>75%11%14%</div><div></div></div>
3	C	219	<div><div>81%16%</div><div></div></div>
4	D	190	<div><div>88%7%</div><div></div></div>
5	E	273	<div><div>80%15%5%</div><div></div></div>
6	F	265	<div><div>73%10%17%</div><div></div></div>
7	G	249	<div><div>84%11%</div><div></div></div>
8	H	190	<div><div>88%8%</div><div></div></div>

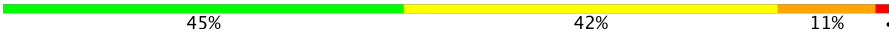


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Mol	Chain	Length	Quality of chain
9	I	200	
10	J	130	
11	K	220	
12	L	149	
13	M	116	
14	N	153	
15	O	144	
16	P	143	
17	Q	141	
18	R	153	
19	S	57	
20	T	151	
21	U	173	
22	V	143	
23	W	152	
24	X	179	
25	Y	159	
26	Z	137	
27	a	120	
28	b	112	
29	c	86	
30	d	87	
31	e	66	
32	f	152	
33	g	312	

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Mol	Chain	Length	Quality of chain
34	1	2203	
35	2	76	
36	3	77	
37	4	76	
38	5	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	OMG	1	509	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein s1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	3	0
			1829	1147	350	320	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	GLY	conflict	UNP E9BRS2

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	211	Total	C	N	O	S	2	0
			1676	1066	306	292	12		

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	212	Total	C	N	O	S	5	0
			1668	1059	307	289	13		

- Molecule 4 is a protein called ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	182	Total	C	N	O	S	1	0
			1504	948	304	244	8		

- Molecule 5 is a protein called ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	2	0
			2029	1292	395	333	9		

- Molecule 6 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	220	Total	C	N	O	S	0	0
			1656	1062	298	286	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	THR	ALA	conflict	UNP E9BNF0
F	8	GLN	-	insertion	UNP E9BNF0
F	10	ALA	ASN	conflict	UNP E9BNF0
F	12	ALA	GLY	conflict	UNP E9BNF0
F	13	ALA	VAL	conflict	UNP E9BNF0
F	14	ASP	GLU	conflict	UNP E9BNF0
F	15	VAL	ALA	conflict	UNP E9BNF0

- Molecule 7 is a protein called ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	238	Total	C	N	O	S	1	0
			1796	1123	366	304	3		

- Molecule 8 is a protein called ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	184	Total	C	N	O	S	1	0
			1438	893	283	255	7		

- Molecule 9 is a protein called ribosomal protein S7e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	200	Total	C	N	O	S	0	0
			1613	1033	303	270	7		

- Molecule 10 is a protein called ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 11 is a protein called ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	183	Total	C	N	O	S	0	0
			1403	885	294	222	2		

- Molecule 12 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1127	724	209	191	3		

- Molecule 13 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	102	Total	C	N	O	S	1	0
			809	505	149	153	2		

- Molecule 14 is a protein called ribosomal protein S10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	91	Total	C	N	O	S	1	0
			728	473	127	123	5		

- Molecule 15 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	137	Total	C	N	O	S	2	0
			1032	637	205	183	7		

- Molecule 16 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	142	Total	C	N	O	S	3	0
			1134	716	229	186	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	18	ARG	CYS	conflict	UNP E9BFB6
P	34	ALA	SER	conflict	UNP E9BFB6
P	36	LYS	ARG	conflict	UNP E9BFB6
P	127	SER	ASN	conflict	UNP E9BFB6

- Molecule 17 is a protein called ribosomal protein S12e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			746	462	130	149	5		

- Molecule 18 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1080	680	210	186	4		

- Molecule 19 is a protein called ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	54	Total	C	N	O	S	0	0
			441	272	90	73	6		

- Molecule 20 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	142	Total	C	N	O	S	0	0
			1153	727	228	190	8		

- Molecule 21 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	156	Total	C	N	O	S	0	0
			1241	786	249	201	5		

- Molecule 22 is a protein called ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	122	Total	C	N	O	S	1	0
			935	587	187	156	5		

- Molecule 23 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			822	530	158	130	4		

- Molecule 24 is a protein called ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	152	Total	C	N	O	S	1	0
			1202	765	235	198	4		

- Molecule 25 is a protein called ribosomal protein S21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	88	Total	C	N	O	S	0	0
			664	409	122	129	4		

- Molecule 26 is a protein called ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	127	Total	C	N	O	S	1	0
			1032	664	199	166	3		

- Molecule 27 is a protein called ribosomal protein S25e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	72	Total	C	N	O	S	0	0
			544	348	94	99	3		

- Molecule 28 is a protein called ribosomal protein S26e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	103	Total	C	N	O	S	0	0
			796	496	164	129	7		

- Molecule 29 is a protein called ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	84	Total	C	N	O	S	0	0
			656	407	128	113	8		

- Molecule 30 is a protein called ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 31 is a protein called ribosomal protein S30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	59	Total	C	N	O	S	0	0
			449	280	97	71	1		

- Molecule 32 is a protein called ribosomal protein S31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	60	Total	C	N	O	S	0	0
			385	242	71	69	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	5	ILE	VAL	conflict	UNP E9BTC5

- Molecule 33 is a protein called LACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	300	Total	C	N	O	S	1	0
			2240	1410	395	423	12		

- Molecule 34 is a RNA chain called ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	1760	Total	C	N	O	P	0	0
			37613	16832	6780	12242	1759		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1539	M1Y	U	conflict	GB 322500086
1	1543	C4J	U	conflict	GB 322500086

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	G	-	expression tag	GB 1229082179

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2	C	-	expression tag	GB 1229082179
2	3	G	-	expression tag	GB 1229082179
2	70	C	G	conflict	GB 1229082179

- Molecule 36 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	77	Total	C	N	O	P	0	0
			1639	732	297	534	76		

- Molecule 37 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	G	-	expression tag	GB 1229082179
4	2	C	-	expression tag	GB 1229082179
4	3	G	-	expression tag	GB 1229082179
4	70	C	G	conflict	GB 1229082179

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

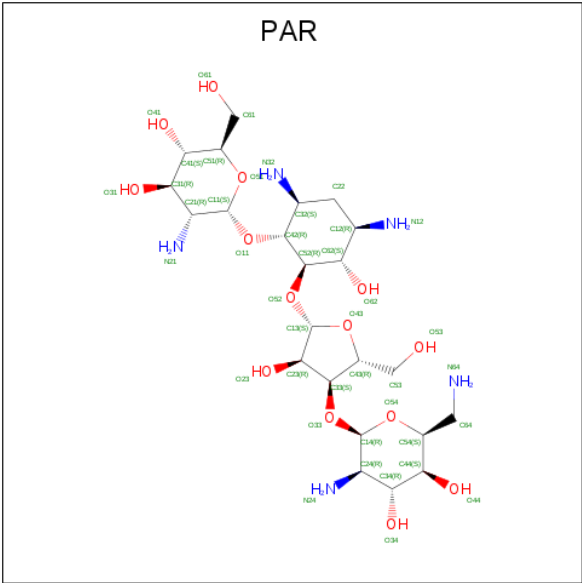
Mol	Chain	Residues	Atoms		AltConf
39	1	20	Total	Mg	0
			20	20	
39	D	1	Total	Mg	0
			1	1	
39	C	1	Total	Mg	0
			1	1	
39	5	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
39	S	1	Total	Mg	0
			1	1	

- Molecule 40 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0
40	1	1	252	138	30	84	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	D	2	Total	O	0
			2	2	
41	E	1	Total	O	0
			1	1	

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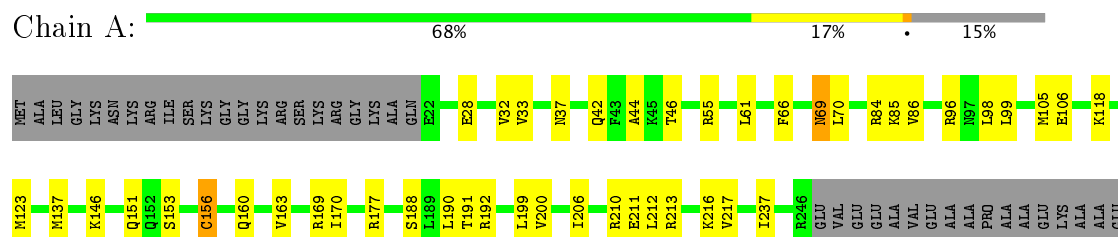
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Mol	Chain	Residues	Atoms		AltConf
41	F	3	Total 3	O 3	0
41	G	1	Total 1	O 1	0
41	H	1	Total 1	O 1	0
41	K	1	Total 1	O 1	0
41	L	1	Total 1	O 1	0
41	M	3	Total 3	O 3	0
41	O	1	Total 1	O 1	0
41	P	6	Total 6	O 6	0
41	R	2	Total 2	O 2	0
41	S	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	X	4	Total 4	O 4	0
41	Y	1	Total 1	O 1	0
41	Z	1	Total 1	O 1	0
41	b	1	Total 1	O 1	0
41	c	2	Total 2	O 2	0
41	f	1	Total 1	O 1	0
41	1	217	Total 217	O 217	0
41	2	2	Total 2	O 2	0
41	3	3	Total 3	O 3	0
41	5	3	Total 3	O 3	0

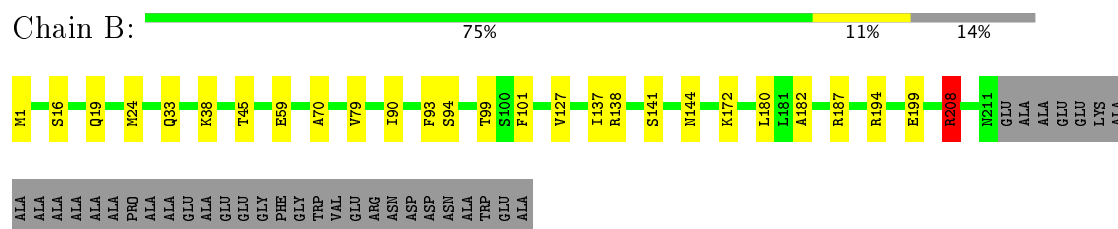
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

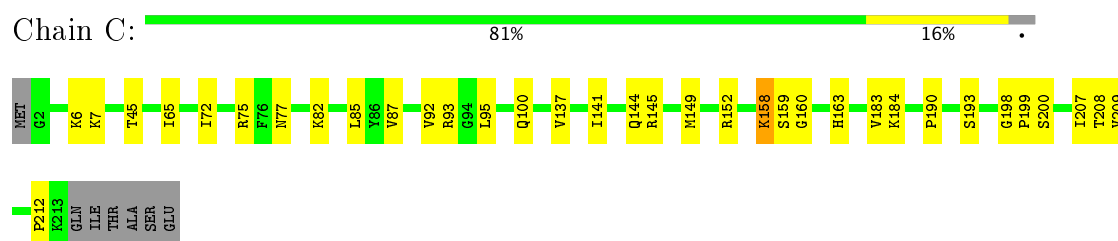
- Molecule 1: Ribosomal protein s1e



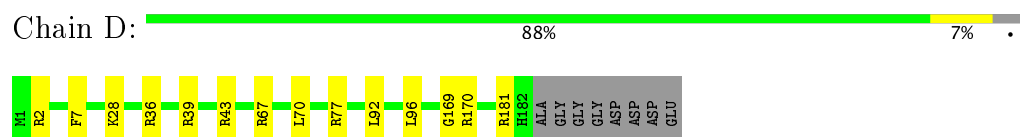
- Molecule 2: ribosomal protein S2



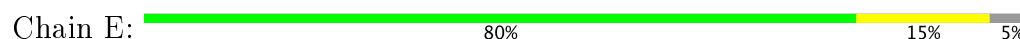
- Molecule 3: ribosomal protein S3



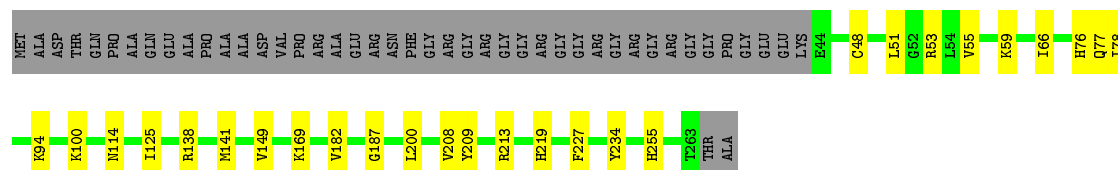
- Molecule 4: ribosomal protein S4



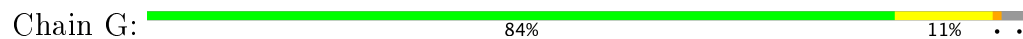
- Molecule 5: ribosomal protein S4e



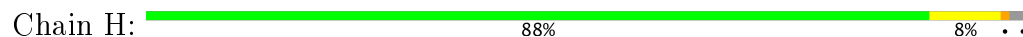
- Molecule 6: ribosomal protein S5



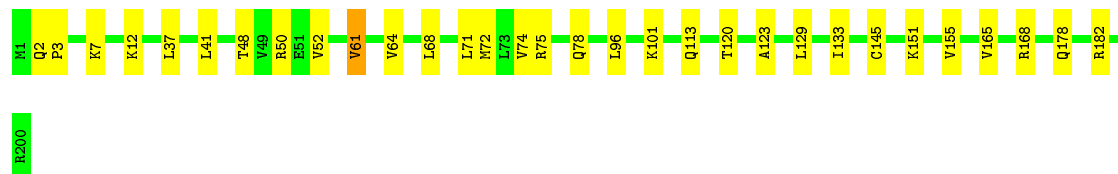
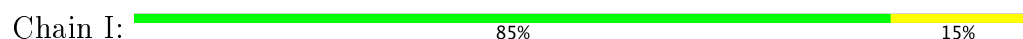
- Molecule 7: ribosomal protein S6e



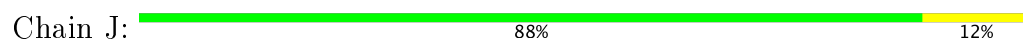
- Molecule 8: ribosomal protein S7



- Molecule 9: ribosomal protein S7e



- Molecule 10: ribosomal protein S8




- Molecule 11: ribosomal protein S8e

Chain Q: 

MET ALA GLU THR VAL ARG VAL GLU VAL PRO ALA VAL GLU ASN VAL VAL ASP VAL ALA PRO GLU SER LEU E27 R31 Q35 A40 N41 Q42 L47 S48 I63 D66 D87 L88 I89 E92 K96 T115 I123 D124 F126 G127 L137

S138 Q139 L140 H141

- Molecule 18: ribosomal protein S13

Chain R: 


MET S2 R25 K26 V27 A30 L31 L32 M33 V34 V37 F41 L44 I51 L60 I68 Q88 R89 T96 S101 H121 R125 H143 GLY LYS THR VAL GLY VAL SER ARG GLY LYS

- Molecule 19: ribosomal protein S14

Chain S: 


MET GLY HIS L4 D5 Q6 W7 R10 K17 K22 C25 S26 D27 Q28 K29 A30 L31 L37 N38 V39 C40 R41 Q42 C43 F53 L56 R57

- Molecule 20: ribosomal protein S15

Chain T: 

MET V2 R3 S14 A15 L16 S41 S48 R55 R69 R73 L80 R109 Y129 V132 K133 Q134 S143 SER THR ALA SER ALA MET VAL ALA

- Molecule 21: ribosomal protein S17

Chain U: 

MET SER ALA P5 H19 Q26 R38 K39 H40 V41 R48 K51 G54 R87 V90 Y112 Q113 R114 R118 P132 V139 K160 SER ALA ALA ASP LYS MET GLY LYS LYS PHE ALA LYS ASN

- Molecule 22: ribosomal protein S17e

Chain V: 

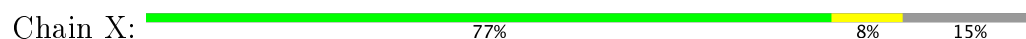
MET G2 R5 K10 V17 E18 K19 D27 M31 I35 V38 T39 I40 K45 L46 K49 M58 K59 R63 R67 G68 I69 M82 I95 D102 R118 R119 R122 A123 ASP ALA ALA VAL ALA VAL LYS LYS ALA ALA PRO ARG ARG

GLN GLN LYS SER SER LYS

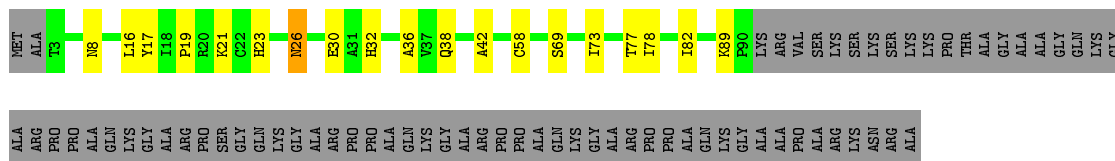
- Molecule 23: ribosomal protein S19

Chain W: 

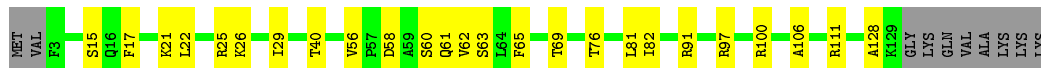
- Molecule 24: ribosomal protein S19e



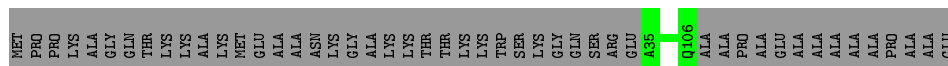
- Molecule 25: ribosomal protein S21e



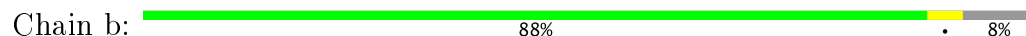
- Molecule 26: ribosomal protein S24e



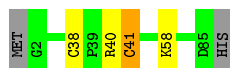
- Molecule 27: ribosomal protein S25e



- Molecule 28: ribosomal protein S26e



- Molecule 29: ribosomal protein S27e




- Molecule 30: ribosomal protein S28e

Chain d:  72% 25%

MET ALA ASP SER LYS LYS ASP ASN LYS LYS THR THR GLU VAL VAL THR GLN THR ASP GLN A21 L25 R36 L85 ARG

- Molecule 31: ribosomal protein S30e

Chain e:  88% 11%

MET G2 K47 THR VAL LYS PRO GLY GLU K54 N58 G66

- Molecule 32: ribosomal protein S31e

Chain f:  34% 5% 61%

MET GLN ILE PHE ILE LYS ASN LYS ALA GLY ARG SER VAL ALA VAL ARG VAL SER ARG VAL ILE ALA GLU ASP THR VAL ALA SER LEU LYS ALA GLN ALA ASN VAL THR CYS GLN GLY LYS LEU PHE PHE ALA MET CYS LEU ALA GLU THR LEU ALA TYR GLY LEU SER LYS GLU SER THR VAL ASP LYS P83 K99 Y100 F101 H122 H123 Y139 CYS GLY LYS CYS H144 L145 T146 TYR LYS ALA GLU SER LYS VAL ASP Y100 F101 H122 H123 Y139 CYS GLY LYS CYS H144 L145 T146 TYR LYS ALA GLU SER LYS

- Molecule 33: LACK1

Chain g:  94%

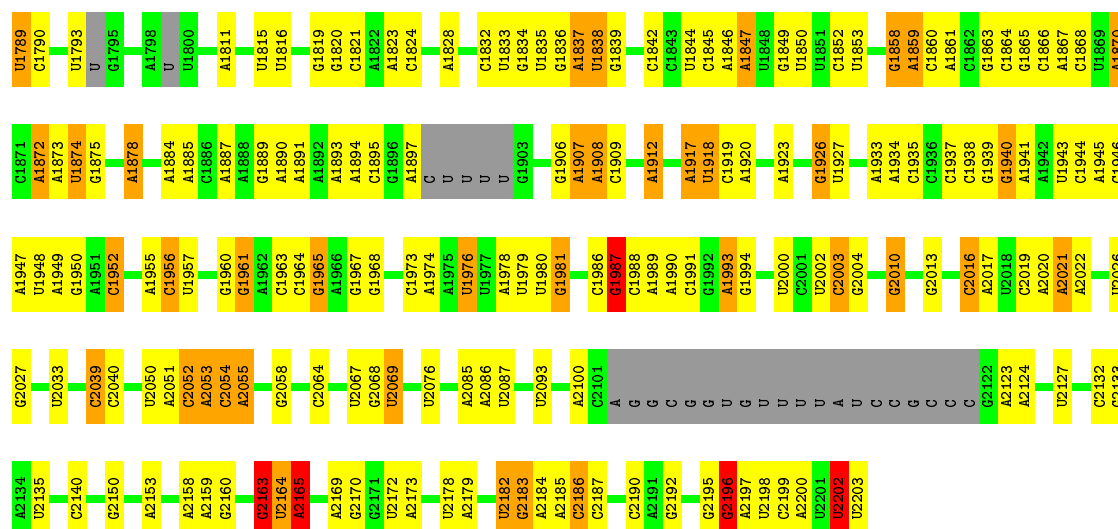
M1 M44 H48 S48 VAL ASP SER D53 L104 P160 SER LEU HIS PRO I166 L190 P274 K299 D300 N301 S309 ASP ALA GLU

- Molecule 34: ribosomal RNA 18S

Chain 1:  42% 28% 8% 20%

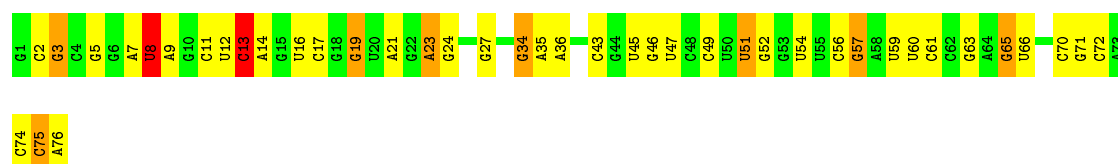
G1 A2 U3 G10 U13 C14 G16 C17 A22 C25 C31 U32 U33 G34 U35 U36 A39 G42 A43 C44 U45 U46 U47 C50 C54 A55 C58 C59 G63 A64 A65 U66 C67 A68 G71 G72 A73 U U U G77 A82 C85 U86 G87 C88 G89 C90 U95 U96 C97 A98 U99 U100 A101 C102 A103 U104 C105 A112 A113 U114 C115 U116 G117 A122 A123 A124 A125 A126 U127 G128 U129 U130 G131 G134 U135 U C138 A144 A145 U146 U147 U151 U152 G157 G158 C159 A161 C167 C171 A174 U175 A176 G180 A181 A185 G190 G191 U192 G193 U195 C196 U197 A200 C207 A215 A216 C217 A218 A219 A220 A221 A222 A223 A224 A225 A226 A227 A228 A229 A230 A231 A232 A233 A234 A235 A236 A237 A238 A239 A240 A241 A242 A243 A244 A245 A246 A247 A248 A249 A250 A251 A252 A253 A254 A255 A256 C259 A260 A261 A262 A263 A264 A265 A266 C267 A268 A269 A270 A271 A272 A273 A274 A275 A276 A277 A278 A279 A280 A281 A282 A283 A284 A285 A286 A287 A288 A289 A290 A291 A292 A293 A294 A295 A296 A297 A298 A299 A300 A301 A302 A303 A304 A305 A306 A307 A308 A309 A310 A311 A312 A313 A314 A315 A316 A317 A318 A319 A320 A321 A322 A323 A324 A325 A326 A327 A328 A329 A330 A331 A332 A333 A334 A335 A336 A337 A338 A339 A340 A341 A342 A343 A344 A345 A346 A347 A348 A349 A350 A351 A352 A353 A354 A355 A356 A357 A358 A359 A360 A361 A362 A363 A364 A365 A366 A367 A368 A369 A370 A371 A372 A373 A374 A375 A376 A377 A378 A379 A380 A381 A382 A383 A384 A385 A386 A387 A388 A389 A390 A391 A392 A393 A394 A395 A396 A397 A398 A399 A400 A401 A402 A403 A404 A405 A406 A407 A408 A409 A410 A411 A412 A413 A414 A415 A416 A417 A418 A419 A420 A421 A422 A423 A424 A425 A426 A427 A428 A429 A430 A431 A432 A433 A434 A435 A436 A437 A438 A439 A440 A441 A442 A443 A444 A445 A446 A447 A448 A449 A450 A451 A452 A453 A454 A455 A456 A457 A458 A459 A460 A461 A462 A463 A464 A465 A466 A467 A468 A469 A470 A471 A472 A473 A474 A475 A476 A477 A478 A479 A480 A481 A482 A483 A484 A485 A486 A487 A488 A489 A490 A491 A492 A493 A494 A495 A496 A497 A498 A499 A500 A501

A1723	A1485	G1551	C1634	G1653	U1566	C1408	U1409	U1408	G1241	C1141	G	U	U	G	G192	A731	C657	U569	A502
G1724	G1466	G1552	U1635	G1570	C1473	U	U	C	G1242	G1142	C	U	C	U	U	U732	U658	A570	C503
	U1636	A1554	U1637	G1571	G	A	C	G	U1243	A1145	C	G	G	U	C	U	U660	A571	U506
	U1638	U1559	U1639	G1572	G	C	C	C	G1244	A1146	U	G	U	C	U	U	U661	A572	A507
	U1640	A1560	C1561	A1576	G	C	C	C	A1248	A1147	A	U	U	U	U	U	U662	C573	A508
	U1641	A1560	C1561	A1577	G	U	U	U	G1249	A1152	C	G	U	U	U	U	U663	C574	G509
	G1642	U1566	C1561	A1578	G	C	C	C	A1250	A1153	C	U	U	U	U	U	U664	C575	G510
	G1643	U1566	C1561	A1579	G	U	U	U	A1251	C1157	C	G	U	U	U	U	U665	A576	
		U1653	U1654	A1579	G	C	C	C	U1252	A1157	C	U	U	U	U	U	U666	C577	
		U1654	U1655	A1580	G	C	C	C	U1253	A1160	C	U	U	U	U	U	U667	A578	
		U1655	U1656	A1581	G	C	C	C	U1254	G1161	C	U	U	U	U	U	U668	C579	
		U1656	U1657	A1582	G	C	C	C	U1255	A1162	C	U	U	U	U	U	U669	A580	
		U1657	U1658	A1583	G	C	C	C	U1256	A1163	C	U	U	U	U	U	U670	G588	
		U1658	U1659	A1584	G	C	C	C	U1257	A1164	C	U	U	U	U	U	U671	U589	
		U1659	U1660	A1585	G	C	C	C	U1258	A1165	C	U	U	U	U	U	U672	A590	
		U1660	U1661	A1586	G	C	C	C	U1259	A1166	C	U	U	U	U	U	U673	A591	
		U1661	U1662	A1587	G	C	C	C	U1260	A1167	C	U	U	U	U	U	U674	C592	
		U1662	U1663	A1588	G	C	C	C	U1261	A1168	C	U	U	U	U	U	U675	A593	
		U1663	U1664	A1589	G	C	C	C	U1262	A1169	C	U	U	U	U	U	U676	A594	
		U1664	U1665	A1590	G	C	C	C	U1263	A1170	C	U	U	U	U	U	U677	G600	
		U1665	U1666	A1591	G	C	C	C	U1264	A1171	C	U	U	U	U	U	U678	G601	
		U1666	U1667	A1592	G	C	C	C	U1265	A1172	C	U	U	U	U	U	U679	A602	
		U1667	U1668	A1593	G	C	C	C	U1266	A1173	C	U	U	U	U	U	U680	C603	
		U1668	U1669	A1594	G	C	C	C	U1267	A1174	C	U	U	U	U	U	U681	A604	
		U1669	U1670	A1595	G	C	C	C	U1268	A1175	C	U	U	U	U	U	U682	A605	
		U1670	U1671	A1596	G	C	C	C	U1269	A1176	C	U	U	U	U	U	U683	A606	
		U1671	U1672	A1597	G	C	C	C	U1270	A1177	C	U	U	U	U	U	U684	U607	
		U1672	U1673	A1598	G	C	C	C	U1271	A1178	C	U	U	U	U	U	U685	C608	
		U1673	U1674	A1599	G	C	C	C	U1272	A1179	C	U	U	U	U	U	U686	G609	
		U1674	U1675	A1600	G	C	C	C	U1273	A1180	C	U	U	U	U	U	U687	A610	
		U1675	U1676	A1601	G	C	C	C	U1274	A1181	C	U	U	U	U	U	U688	A611	
		U1676	U1677	A1602	G	C	C	C	U1275	A1182	C	U	U	U	U	U	U689	C612	
		U1677	U1678	A1603	G	C	C	C	U1276	A1183	C	U	U	U	U	U	U690	A613	
		U1678	U1679	A1604	G	C	C	C	U1277	A1184	C	U	U	U	U	U	U691	A614	
		U1679	U1680	A1605	G	C	C	C	U1278	A1185	C	U	U	U	U	U	U692	C615	
		U1680	U1681	A1606	G	C	C	C	U1279	A1186	C	U	U	U	U	U	U693	A616	
		U1681	U1682	A1607	G	C	C	C	U1280	A1187	C	U	U	U	U	U	U694	G617	
		U1682	U1683	A1608	G	C	C	C	U1281	A1188	C	U	U	U	U	U	U695	A618	
		U1683	U1684	A1609	G	C	C	C	U1282	A1189	C	U	U	U	U	U	U696	C619	
		U1684	U1685	A1610	G	C	C	C	U1283	A1190	C	U	U	U	U	U	U697	G620	
		U1685	U1686	A1611	G	C	C	C	U1284	A1191	C	U	U	U	U	U	U698	C621	
		U1686	U1687	A1612	G	C	C	C	U1285	A1192	C	U	U	U	U	U	U699	C622	
		U1687	U1688	A1613	G	C	C	C	U1286	A1193	C	U	U	U	U	U	U700	G623	
		U1688	U1689	A1614	G	C	C	C	U1287	A1194	C	U	U	U	U	U	U701	C624	
		U1689	U1690	A1615	G	C	C	C	U1288	A1195	C	U	U	U	U	U	U702	G625	
		U1690	U1691	A1616	G	C	C	C	U1289	A1196	C	U	U	U	U	U	U703	A619	
		U1691	U1692	A1617	G	C	C	C	U1290	A1197	C	U	U	U	U	U	U704	C620	
		U1692	U1693	A1618	G	C	C	C	U1291	A1198	C	U	U	U	U	U	U705	G621	
		U1693	U1694	A1619	G	C	C	C	U1292	A1199	C	U	U	U	U	U	U706	C622	
		U1694	U1695	A1620	G	C	C	C	U1293	A1200	C	U	U	U	U	U	U707	G623	
		U1695	U1696	A1621	G	C	C	C	U1294	A1201	C	U	U	U	U	U	U708	A619	
		U1696	U1697	A1622	G	C	C	C	U1295	A1202	C	U	U	U	U	U	U709	C620	
		U1697	U1698	A1623	G	C	C	C	U1296	A1203	C	U	U	U	U	U	U710	G621	
		U1698	U1699	A1624	G	C	C	C	U1297	A1204	C	U	U	U	U	U	U711	C622	
		U1699	U1700	A1625	G	C	C	C	U1298	A1205	C	U	U	U	U	U	U712	G623	
		U1700	U1701	A1626	G	C	C	C	U1299	A1206	C	U	U	U	U	U	U713	A619	
		U1701	U1702	A1627	G	C	C	C	U1300	A1207	C	U	U	U	U	U	U714	C620	
		U1702	U1703	A1628	G	C	C	C	U1301	A1208	C	U	U	U	U	U	U715	G621	
		U1703	U1704	A1629	G	C	C	C	U1302	A1209	C	U	U	U	U	U	U716	C622	
		U1704	U1705	A1630	G	C	C	C	U1303	A1210	C	U	U	U	U	U	U717	G623	
		U1705	U1706	A1631	G	C	C	C	U1304	A1211	C	U	U	U	U	U	U718	A619	
		U1706	U1707	A1632	G	C	C	C	U1305	A1212	C	U	U	U	U	U	U719	C620	
		U1707	U1708	A1633	G	C	C	C	U1306	A1213	C	U	U	U	U	U	U720	G621	
		U1708	U1709	A1634	G	C	C	C	U1307	A1214	C	U	U	U	U	U	U721	C622	
		U1709	U1710	A1635	G	C	C	C	U1308	A1215	C	U	U	U	U	U	U722	G623	
		U1710	U1711	A1636	G	C	C	C	U1309	A1216	C	U	U	U	U	U	U723	A619	
		U1711	U1712	A1637	G	C	C	C	U1310	A1217	C	U	U	U	U	U	U724	C620	
		U1712	U1713	A1638	G	C	C	C	U1311	A1218	C	U	U	U	U	U	U725	G621	
		U1713	U1714	A1639	G	C	C	C	U1312	A1219	C	U	U	U	U	U	U726	A619	
		U1714	U1715	A1640	G	C	C	C	U1313	A1220	C	U	U	U	U	U	U727	C622	
		U1715	U1716	A1641	G	C	C	C	U1314	A1221	C	U	U	U	U	U	U728	G623	
		U1716	U1717	A1642	G	C	C	C	U1315	A1222	C	U	U	U	U	U	U729	A619	
		U1717	U1718	A1643	G	C	C	C	U1316	A1223	C	U	U	U	U	U	U730	C620	
		U1718	U1719	A1644	G	C	C	C	U1317	A1224	C	U	U	U	U	U	U731	G621	
		U1719	U1720	A1645	G	C	C	C	U1318	A1225	C	U	U	U	U	U	U732	A619	
		U1720	U1721	A1646	G	C	C	C	U1319	A1226	C	U	U	U	U	U	U733	C622	
		U1721	U1722	A1647	G	C	C	C	U1320	A1227	C	U	U	U	U	U	U734	G623	
		U1722	U1723	A1648	G	C	C	C	U1321	A1228	C	U	U	U	U	U	U735	A619	
		U1723	U1724	A1649	G	C	C	C	U1322	A1229	C	U	U	U	U	U	U736	C620	
		U1724	U1725	A1650	G	C	C	C	U1323	A1230	C	U	U	U	U	U	U737	G621	
		U1725	U1726	A1651	G	C	C	C	U1324	A1231	C	U	U	U	U	U	U738	A619	
		U1726	U1727	A1652	G	C	C	C	U1325	A1232	C	U	U	U	U	U	U739	C622	
		U1727	U1728	A1653	G	C	C	C	U1326	A1233	C	U	U	U	U	U	U740	G623	
		U1728	U1729	A1654	G	C	C	C	U1327	A1234	C	U	U	U	U	U	U741	A619	
		U1729	U1730	A1655	G	C	C	C	U1328	A1235	C	U	U	U	U	U	U742	C620	
		U1730	U1731	A1656	G	C	C	C	U1329	A1236	C	U	U	U	U	U	U743	G621	
		U1731	U1732	A1657	G	C	C	C	U1330	A1237	C	U	U	U	U	U	U744	A619	
		U1732	U1733	A1658	G	C	C	C	U1331	A1238	C	U	U	U	U	U	U745	C622	
		U1733	U1734	A1659	G	C	C	C	U1332	A1239	C	U	U						



• Molecule 35: tRNA-Phe

Chain 2: 45% 42% 11%



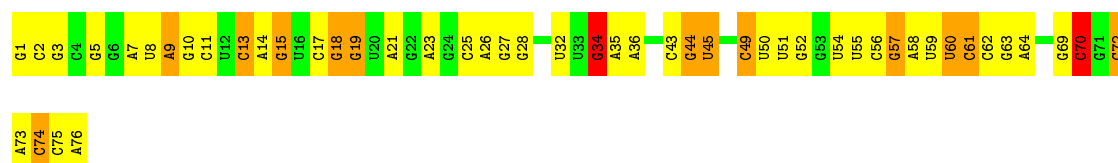
• Molecule 36: P-site tRNA

Chain 3: 62% 30% 8%



• Molecule 37: E-site tRNA

Chain 4: 34% 46% 17%



• Molecule 38: mRNA

Chain 5: 54% 38% 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141028	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	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, PAR, OMG, OMU, MA6, MIA, MG, 5MC, M1Y, 4OC, 7MG, A2M, C4J

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.52	0/1860	0.69	2/2503 (0.1%)
10	J	0.64	0/1031	0.64	0/1382
11	K	0.55	0/1425	0.68	0/1916
12	L	0.53	0/1148	0.68	1/1543 (0.1%)
13	M	0.41	0/819	0.69	0/1109
14	N	0.48	0/753	0.62	0/1024
15	O	0.57	0/1047	0.67	1/1408 (0.1%)
16	P	0.51	0/1163	0.75	4/1554 (0.3%)
17	Q	0.30	0/749	0.81	3/1028 (0.3%)
18	R	0.44	0/1099	0.65	0/1489
19	S	0.49	0/446	0.73	0/591
2	B	0.53	0/1713	0.64	1/2316 (0.0%)
20	T	0.60	0/1176	0.73	0/1577
21	U	0.60	0/1270	0.66	0/1710
22	V	0.40	0/945	0.60	0/1267
23	W	0.40	0/841	0.56	0/1144
24	X	0.51	0/1236	0.67	0/1659
25	Y	0.52	0/674	0.64	0/914
26	Z	0.47	0/1056	0.67	0/1407
27	a	0.45	0/549	0.66	0/743
28	b	0.68	1/813 (0.1%)	0.80	1/1092 (0.1%)
29	c	0.65	0/669	0.72	1/897 (0.1%)
3	C	0.46	0/1700	0.64	0/2274
30	d	0.41	0/468	0.76	1/630 (0.2%)
31	e	0.45	0/456	0.57	0/603
32	f	0.29	0/393	0.68	1/540 (0.2%)
33	g	0.44	0/2294	0.72	3/3131 (0.1%)
34	1	1.06	0/41155	1.23	426/64074 (0.7%)
35	2	0.46	0/1783	0.98	6/2776 (0.2%)
36	3	0.59	0/1831	1.04	8/2853 (0.3%)
37	4	0.43	1/1809 (0.1%)	1.16	22/2819 (0.8%)
38	5	1.00	0/279	1.29	3/431 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	D	0.48	0/1533	0.62	1/2057 (0.0%)
5	E	0.50	0/2074	0.70	1/2797 (0.0%)
6	F	0.51	0/1692	0.62	0/2295
7	G	0.41	0/1823	0.65	2/2449 (0.1%)
8	H	0.47	0/1460	0.68	1/1959 (0.1%)
9	I	0.58	0/1644	0.68	1/2217 (0.0%)
All	All	0.82	2/84876 (0.0%)	1.02	490/124178 (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
12	L	0	1
15	O	0	1
16	P	0	3
17	Q	0	1
19	S	0	2
2	B	0	2
21	U	0	2
26	Z	0	1
29	c	0	2
32	f	0	4
33	g	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	78	CYS	CB-SG	6.89	1.94	1.82
37	4	75	C	C1'-N1	5.14	1.56	1.48

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	78	CYS	CA-CB-SG	13.35	138.02	114.00
34	1	1956	C	N1-C2-O2	13.04	126.72	118.90
34	1	1973	C	N1-C2-O2	11.17	125.60	118.90
34	1	1956	C	N3-C2-O2	-10.96	114.23	121.90
34	1	1510	C	C2-N1-C1'	10.23	130.05	118.80
37	4	60	U	C2-N1-C1'	9.95	129.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	354	C	C2-N1-C1'	9.88	129.66	118.80
34	1	1510	C	N3-C2-O2	-9.84	115.02	121.90
34	1	2039	C	C6-N1-C2	-9.58	116.47	120.30
34	1	1510	C	N1-C2-O2	9.32	124.49	118.90
34	1	1838	U	N3-C2-O2	-9.27	115.71	122.20
34	1	775	C	C2-N1-C1'	9.24	128.96	118.80
34	1	1838	U	C2-N1-C1'	9.18	128.72	117.70
34	1	1222	C	C6-N1-C2	-9.16	116.64	120.30
34	1	1212	C	N1-C2-O2	9.01	124.31	118.90
34	1	354	C	N3-C2-O2	-8.91	115.66	121.90
34	1	775	C	N1-C2-O2	8.86	124.21	118.90
34	1	88	C	C6-N1-C2	-8.85	116.76	120.30
34	1	147	U	C2-N1-C1'	8.83	128.30	117.70
34	1	1179	U	N3-C2-O2	-8.78	116.05	122.20
34	1	1222	C	C5-C6-N1	8.76	125.38	121.00
34	1	1408	C	C2-N1-C1'	8.60	128.26	118.80
34	1	1973	C	N3-C2-O2	-8.48	115.96	121.90
34	1	395	U	C2-N1-C1'	8.48	127.88	117.70
17	Q	47	LEU	CA-CB-CG	8.41	134.64	115.30
34	1	1956	C	C2-N1-C1'	8.35	127.98	118.80
34	1	632	C	C5-C6-N1	8.30	125.15	121.00
37	4	49	C	N1-C2-O2	8.28	123.86	118.90
34	1	1626	C	N1-C2-O2	8.26	123.86	118.90
34	1	2039	C	C2-N1-C1'	8.24	127.87	118.80
34	1	1192	U	C5-C6-N1	8.16	126.78	122.70
34	1	1222	C	N1-C2-O2	8.16	123.80	118.90
34	1	1973	C	C2-N1-C1'	8.14	127.76	118.80
37	4	60	U	N1-C2-O2	8.12	128.49	122.80
34	1	741	C	C2-N1-C1'	8.07	127.68	118.80
34	1	1473	C	C6-N1-C2	-8.04	117.09	120.30
34	1	2040	C	C6-N1-C2	-8.02	117.09	120.30
34	1	1408	C	N1-C2-O2	8.01	123.70	118.90
34	1	589	U	N1-C2-O2	7.97	128.38	122.80
34	1	147	U	N3-C2-O2	-7.95	116.63	122.20
34	1	313	G	C4-N9-C1'	7.93	136.81	126.50
34	1	2039	C	N3-C2-O2	-7.92	116.35	121.90
34	1	624	C	C5-C6-N1	7.92	124.96	121.00
34	1	354	C	N1-C2-O2	7.89	123.64	118.90
34	1	85	C	N1-C2-O2	7.89	123.63	118.90
34	1	276	G	OP1-P-O3'	7.84	122.44	105.20
34	1	1359	C	C2-N1-C1'	7.83	127.41	118.80
34	1	2052	C	C6-N1-C2	-7.80	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1595	G	C4-N9-C1'	7.79	136.63	126.50
34	1	2	A	O5'-P-OP1	-7.77	98.71	105.70
34	1	1212	C	C2-N1-C1'	7.76	127.33	118.80
34	1	624	C	C6-N1-C2	-7.66	117.23	120.30
34	1	2040	C	N3-C2-O2	-7.65	116.54	121.90
34	1	1581	G	C4-N9-C1'	7.65	136.45	126.50
34	1	565	U	N3-C2-O2	-7.64	116.85	122.20
34	1	1	G	O4'-C1'-N9	7.62	114.30	108.20
37	4	60	U	N3-C2-O2	-7.59	116.89	122.20
34	1	1510	C	C6-N1-C1'	-7.55	111.75	120.80
29	c	38	CYS	CA-CB-SG	7.54	127.58	114.00
34	1	1489	A	P-O3'-C3'	7.52	128.72	119.70
34	1	319	C	N1-C2-O2	7.44	123.36	118.90
34	1	842	U	N1-C2-O2	7.43	128.00	122.80
34	1	632	C	C6-N1-C2	-7.34	117.36	120.30
37	4	49	C	C2-N1-C1'	7.34	126.87	118.80
34	1	1421	C	C6-N1-C2	-7.33	117.37	120.30
34	1	565	U	N1-C2-O2	7.29	127.90	122.80
37	4	32	U	N1-C2-O2	7.29	127.90	122.80
34	1	1626	C	N3-C2-O2	-7.28	116.81	121.90
34	1	1250	A	P-O3'-C3'	7.27	128.43	119.70
34	1	298	C	N1-C2-O2	7.26	123.26	118.90
34	1	1956	C	C6-N1-C2	-7.26	117.40	120.30
37	4	32	U	C2-N1-C1'	7.26	126.41	117.70
34	1	398	C	C5-C6-N1	7.22	124.61	121.00
34	1	671	G	P-O3'-C3'	7.20	128.34	119.70
34	1	32	U	N3-C2-O2	-7.17	117.18	122.20
34	1	589	U	C2-N1-C1'	7.12	126.25	117.70
34	1	1145	A	P-O3'-C3'	7.11	128.24	119.70
34	1	842	U	C2-N1-C1'	7.10	126.22	117.70
34	1	1287	U	C2-N1-C1'	7.10	126.22	117.70
36	3	28	C	C6-N1-C2	-7.09	117.46	120.30
34	1	775	C	N3-C2-O2	-7.08	116.95	121.90
34	1	592	C	N1-C2-O2	7.07	123.14	118.90
34	1	17	C	C6-N1-C2	-7.04	117.48	120.30
34	1	589	U	N3-C2-O2	-7.03	117.28	122.20
34	1	2040	C	C2-N1-C1'	7.01	126.52	118.80
34	1	689	U	N3-C2-O2	-7.01	117.30	122.20
34	1	689	U	C2-N1-C1'	7.00	126.10	117.70
34	1	741	C	N1-C2-O2	6.99	123.09	118.90
37	4	34	G	P-O3'-C3'	6.98	128.08	119.70
37	4	60	U	C5-C6-N1	6.98	126.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1788	U	C2-N1-C1'	6.98	126.07	117.70
34	1	618	C	N1-C2-O2	6.97	123.08	118.90
34	1	1287	U	N3-C2-O2	-6.96	117.33	122.20
34	1	1275	C	P-O3'-C3'	6.94	128.03	119.70
36	3	28	C	N1-C2-O2	6.93	123.06	118.90
33	g	190	LEU	CA-CB-CG	6.93	131.24	115.30
34	1	1595	G	C8-N9-C1'	-6.92	118.01	127.00
34	1	1222	C	C2-N1-C1'	6.91	126.40	118.80
34	1	1838	U	N1-C2-O2	6.91	127.64	122.80
34	1	354	C	C6-N1-C2	-6.91	117.53	120.30
34	1	147	U	N1-C2-O2	6.88	127.62	122.80
7	G	69	LEU	CA-CB-CG	6.87	131.11	115.30
34	1	1654	U	N3-C2-O2	-6.87	117.39	122.20
34	1	837	G	N3-C2-N2	-6.86	115.09	119.90
36	3	28	C	N3-C2-O2	-6.86	117.10	121.90
34	1	842	U	N3-C2-O2	-6.86	117.40	122.20
2	B	180	LEU	CA-CB-CG	6.86	131.08	115.30
34	1	514	C	N1-C2-O2	6.85	123.01	118.90
34	1	1525	C	C6-N1-C2	-6.85	117.56	120.30
36	3	28	C	C2-N1-C1'	6.84	126.33	118.80
34	1	887	U	C2-N1-C1'	6.83	125.90	117.70
34	1	1610	U	N3-C2-O2	-6.83	117.42	122.20
34	1	395	U	N3-C2-O2	-6.82	117.43	122.20
34	1	1131	C	C6-N1-C2	-6.81	117.58	120.30
34	1	1542	C	N1-C2-O2	6.80	122.98	118.90
34	1	1190	C	C6-N1-C2	-6.80	117.58	120.30
34	1	1222	C	N3-C2-O2	-6.80	117.14	121.90
34	1	354	C	C6-N1-C1'	-6.78	112.67	120.80
34	1	1	G	C4-N9-C1'	-6.77	117.69	126.50
34	1	319	C	C6-N1-C2	-6.77	117.59	120.30
34	1	2182	U	N1-C2-O2	6.76	127.53	122.80
34	1	664	U	N3-C2-O2	-6.75	117.47	122.20
34	1	1131	C	C2-N1-C1'	6.75	126.23	118.80
34	1	1419	U	C5-C6-N1	6.75	126.08	122.70
34	1	1581	G	N7-C8-N9	6.75	116.47	113.10
34	1	2165	A	N9-C1'-C2'	-6.73	104.60	112.00
34	1	1408	C	C5-C6-N1	6.73	124.36	121.00
34	1	398	C	C6-N1-C2	-6.72	117.61	120.30
34	1	485	C	C6-N1-C2	-6.71	117.62	120.30
34	1	1654	U	C2-N1-C1'	6.67	125.70	117.70
34	1	1636	U	P-O3'-C3'	6.67	127.70	119.70
16	P	16	LEU	CA-CB-CG	6.66	130.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1626	C	C2-N1-C1'	6.66	126.13	118.80
34	1	655	U	N3-C2-O2	-6.66	117.54	122.20
34	1	1559	U	P-O3'-C3'	6.66	127.69	119.70
34	1	1131	C	N1-C2-O2	6.61	122.87	118.90
34	1	1361	U	C2-N1-C1'	6.61	125.64	117.70
34	1	1108	A	P-O3'-C3'	6.60	127.62	119.70
34	1	2165	A	C4'-C3'-O3'	6.59	126.18	113.00
34	1	85	C	C6-N1-C2	-6.58	117.67	120.30
34	1	1520	U	N3-C2-O2	-6.57	117.60	122.20
34	1	1619	G	N7-C8-N9	6.56	116.38	113.10
34	1	1520	U	N1-C2-O2	6.55	127.38	122.80
34	1	1511	C	N1-C2-O2	6.55	122.83	118.90
34	1	1944	C	N1-C2-O2	6.55	122.83	118.90
34	1	104	U	N3-C2-O2	-6.54	117.62	122.20
34	1	1276	G	P-O3'-C3'	6.54	127.54	119.70
34	1	85	C	N3-C2-O2	-6.52	117.34	121.90
37	4	49	C	C5-C6-N1	6.51	124.25	121.00
34	1	2003	C	C2-N1-C1'	6.50	125.95	118.80
34	1	1421	C	C5-C6-N1	6.49	124.25	121.00
34	1	1788	U	N1-C2-O2	6.49	127.34	122.80
34	1	1	G	OP1-P-O3'	6.47	119.44	105.20
34	1	592	C	C2-N1-C1'	6.46	125.91	118.80
34	1	1	G	P-O3'-C3'	6.46	127.45	119.70
34	1	759	U	O4'-C1'-N1	6.45	113.36	108.20
34	1	503	C	C2-N1-C1'	6.44	125.89	118.80
34	1	2202	U	N3-C2-O2	-6.42	117.71	122.20
34	1	1542	C	N3-C2-O2	-6.42	117.41	121.90
30	d	25	LEU	CA-CB-CG	6.42	130.06	115.30
34	1	1610	U	N1-C2-O2	6.41	127.29	122.80
34	1	1141	C	N1-C2-O2	6.41	122.75	118.90
34	1	1188	G	N3-C4-N9	6.41	129.85	126.00
34	1	503	C	N1-C2-O2	6.40	122.74	118.90
34	1	95	C	N1-C2-O2	6.39	122.73	118.90
34	1	994	U	N3-C2-O2	-6.39	117.73	122.20
34	1	332	C	N1-C2-O2	6.39	122.73	118.90
34	1	565	U	C2-N1-C1'	6.39	125.36	117.70
17	Q	47	LEU	C-N-CA	6.38	137.64	121.70
37	4	32	U	N3-C2-O2	-6.38	117.74	122.20
34	1	775	C	C6-N1-C1'	-6.37	113.16	120.80
34	1	689	U	N1-C2-O2	6.36	127.25	122.80
34	1	1787	A	P-O3'-C3'	6.35	127.32	119.70
34	1	1533	U	N3-C2-O2	-6.33	117.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1775	C	N1-C2-O2	6.33	122.69	118.90
34	1	2052	C	C5-C6-N1	6.33	124.16	121.00
34	1	1408	C	C6-N1-C2	-6.31	117.77	120.30
34	1	313	G	N3-C4-C5	-6.31	125.44	128.60
34	1	313	G	C8-N9-C1'	-6.31	118.80	127.00
34	1	147	U	C6-N1-C1'	-6.30	112.38	121.20
34	1	1641	U	C5-C6-N1	6.29	125.85	122.70
34	1	372	C	C6-N1-C2	-6.29	117.79	120.30
34	1	297	U	N3-C2-O2	-6.28	117.80	122.20
34	1	1190	C	C5-C6-N1	6.28	124.14	121.00
34	1	1874	U	C2-N1-C1'	6.28	125.24	117.70
34	1	1473	C	C5-C6-N1	6.27	124.14	121.00
34	1	1500	C	C6-N1-C2	-6.27	117.79	120.30
34	1	1538	U	N1-C2-O2	6.27	127.19	122.80
34	1	2182	U	N3-C2-O2	-6.26	117.81	122.20
34	1	1183	G	N1-C6-O6	-6.26	116.14	119.90
34	1	1961	G	N3-C4-N9	-6.26	122.25	126.00
34	1	306	U	P-O3'-C3'	6.24	127.19	119.70
34	1	50	C	C6-N1-C2	-6.24	117.81	120.30
34	1	17	C	C5-C6-N1	6.22	124.11	121.00
34	1	887	U	N1-C2-O2	6.20	127.14	122.80
34	1	915	A	P-O3'-C3'	6.20	127.14	119.70
34	1	1610	U	C2-N1-C1'	6.20	125.14	117.70
38	5	1	C	N1-C2-O2	6.19	122.61	118.90
34	1	335	C	N1-C2-O2	6.19	122.61	118.90
9	I	68	LEU	CA-CB-CG	6.19	129.53	115.30
34	1	1212	C	N3-C2-O2	-6.18	117.57	121.90
34	1	1976	U	N3-C2-O2	-6.17	117.88	122.20
34	1	403	G	O4'-C1'-N9	6.16	113.13	108.20
34	1	403	G	P-O3'-C3'	6.16	127.09	119.70
34	1	1944	C	N3-C2-O2	-6.16	117.59	121.90
17	Q	137	LEU	CA-CB-CG	6.15	129.44	115.30
34	1	2039	C	N1-C2-O2	6.15	122.59	118.90
37	4	60	U	C6-N1-C1'	-6.13	112.61	121.20
34	1	757	C	P-O3'-C3'	6.13	127.05	119.70
34	1	319	C	N3-C2-O2	-6.12	117.62	121.90
34	1	2202	U	P-O3'-C3'	6.11	127.03	119.70
34	1	1619	G	C8-N9-C4	-6.10	103.96	106.40
34	1	454	C	C6-N1-C2	-6.09	117.86	120.30
34	1	775	C	C6-N1-C2	-6.09	117.86	120.30
34	1	1216	C	C6-N1-C2	-6.09	117.86	120.30
34	1	592	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1952	C	C5-C6-N1	6.08	124.04	121.00
34	1	2040	C	N1-C2-O2	6.08	122.55	118.90
34	1	32	U	N1-C2-O2	6.07	127.05	122.80
16	P	113	GLY	N-CA-C	6.07	128.27	113.10
34	1	13	U	C5-C6-N1	6.05	125.72	122.70
37	4	49	C	C6-N1-C2	-6.04	117.88	120.30
32	f	121	PRO	C-N-CA	6.03	136.77	121.70
34	1	789	G	P-O3'-C3'	6.02	126.93	119.70
34	1	1500	C	C5-C6-N1	6.02	124.01	121.00
34	1	1783	C	C6-N1-C2	-6.01	117.90	120.30
34	1	638	C	C6-N1-C2	-6.00	117.90	120.30
34	1	619	A	C6-N1-C2	5.99	122.20	118.60
34	1	2050	U	C5-C6-N1	5.99	125.69	122.70
34	1	381	G	C2-N3-C4	5.98	114.89	111.90
34	1	1473	C	N1-C2-O2	5.97	122.48	118.90
34	1	608	C	C6-N1-C2	-5.97	117.91	120.30
34	1	1419	U	N1-C2-O2	5.97	126.98	122.80
34	1	1538	U	N3-C2-O2	-5.97	118.02	122.20
34	1	514	C	N3-C2-O2	-5.96	117.73	121.90
34	1	372	C	N1-C2-O2	5.95	122.47	118.90
37	4	70	C	N1-C2-O2	5.95	122.47	118.90
34	1	2196	G	OP1-P-O3'	5.95	118.28	105.20
34	1	396	G	P-O3'-C3'	5.94	126.83	119.70
34	1	14	C	C5-C6-N1	5.93	123.97	121.00
34	1	335	C	C2-N1-C1'	5.93	125.32	118.80
34	1	398	C	C2-N3-C4	5.93	122.86	119.90
33	g	104	LEU	CA-CB-CG	5.92	128.91	115.30
34	1	1944	C	C6-N1-C2	-5.91	117.94	120.30
35	2	66	U	N1-C2-O2	5.91	126.94	122.80
34	1	276	G	P-O3'-C3'	5.91	126.79	119.70
34	1	14	C	C6-N1-C2	-5.90	117.94	120.30
16	P	101	LEU	CA-CB-CG	5.90	128.86	115.30
34	1	1991	C	C5-C6-N1	5.89	123.94	121.00
34	1	50	C	N3-C2-O2	-5.89	117.78	121.90
34	1	313	G	N3-C4-N9	5.89	129.53	126.00
34	1	887	U	N3-C2-O2	-5.89	118.08	122.20
34	1	1581	G	C8-N9-C1'	-5.88	119.35	127.00
37	4	49	C	N3-C2-O2	-5.87	117.79	121.90
34	1	31	C	C6-N1-C2	-5.87	117.95	120.30
34	1	1654	U	C6-N1-C2	-5.86	117.48	121.00
34	1	1120	U	C2-N1-C1'	5.86	124.73	117.70
34	1	88	C	C5-C6-N1	5.85	123.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1511	C	N3-C2-O2	-5.84	117.81	121.90
34	1	632	C	C2-N1-C1'	5.83	125.22	118.80
34	1	1642	C	C6-N1-C2	-5.83	117.97	120.30
34	1	624	C	N1-C2-O2	5.82	122.39	118.90
34	1	1987	G	O4'-C1'-N9	5.81	112.85	108.20
34	1	1554	A	C4-N9-C1'	5.81	136.76	126.30
34	1	88	C	N3-C2-O2	-5.81	117.84	121.90
34	1	1131	C	C5-C6-N1	5.80	123.90	121.00
34	1	955	A	O5'-P-OP1	5.79	117.65	110.70
34	1	395	U	N1-C2-O2	5.78	126.85	122.80
34	1	1181	C	C2-N1-C1'	5.78	125.15	118.80
34	1	1473	C	N3-C2-O2	-5.77	117.86	121.90
34	1	433	G	O4'-C1'-N9	5.76	112.81	108.20
34	1	1179	U	N1-C2-O2	5.76	126.83	122.80
34	1	1257	U	N3-C2-O2	-5.75	118.18	122.20
34	1	1257	U	C2-N1-C1'	5.74	124.59	117.70
34	1	319	C	C5-C6-N1	5.74	123.87	121.00
34	1	2187	C	N1-C2-O2	5.74	122.34	118.90
34	1	1188	G	N3-C4-C5	-5.74	125.73	128.60
34	1	1237	C	C5-C6-N1	5.74	123.87	121.00
34	1	1188	G	C6-C5-N7	-5.72	126.97	130.40
34	1	1196	U	N1-C2-O2	5.71	126.80	122.80
34	1	1408	C	C6-N1-C1'	-5.71	113.95	120.80
34	1	1864	C	C2-N1-C1'	5.69	125.05	118.80
34	1	1511	C	C6-N1-C2	-5.68	118.03	120.30
34	1	425	C	C6-N1-C2	-5.68	118.03	120.30
34	1	36	U	C5-C6-N1	5.68	125.54	122.70
34	1	1425	U	N3-C2-O2	-5.66	118.24	122.20
34	1	2053	A	P-O3'-C3'	5.66	126.49	119.70
34	1	367	A	O5'-P-OP2	-5.65	100.61	105.70
34	1	1768	U	C2-N1-C1'	5.65	124.48	117.70
34	1	90	C	C5-C6-N1	5.65	123.83	121.00
34	1	1408	C	N3-C2-O2	-5.65	117.95	121.90
38	5	10	C	N1-C2-O2	5.65	122.29	118.90
34	1	1181	C	N3-C2-O2	-5.64	117.95	121.90
34	1	1276	G	O5'-P-OP1	-5.64	100.62	105.70
34	1	1161	G	C4-N9-C1'	5.64	133.83	126.50
34	1	1131	C	N3-C2-O2	-5.63	117.96	121.90
34	1	1775	C	C6-N1-C2	-5.63	118.05	120.30
34	1	615	C	C6-N1-C2	-5.62	118.05	120.30
34	1	1838	U	C6-N1-C1'	-5.62	113.33	121.20
34	1	659	G	C4-N9-C1'	5.62	133.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1991	C	C6-N1-C2	-5.62	118.05	120.30
16	P	130	LEU	CA-CB-CG	5.60	128.19	115.30
34	1	659	G	N3-C4-N9	5.60	129.36	126.00
34	1	1973	C	C6-N1-C1'	-5.60	114.08	120.80
34	1	1533	U	N1-C2-O2	5.60	126.72	122.80
34	1	994	U	N1-C2-O2	5.59	126.71	122.80
34	1	104	U	N1-C2-O2	5.58	126.71	122.80
34	1	1858	G	P-O3'-C3'	5.57	126.38	119.70
34	1	1609	U	N3-C2-O2	-5.57	118.30	122.20
35	2	66	U	N3-C2-O2	-5.56	118.31	122.20
34	1	1196	U	N3-C2-O2	-5.56	118.31	122.20
34	1	1918	U	N1-C2-O2	5.56	126.69	122.80
34	1	1361	U	C5-C6-N1	5.54	125.47	122.70
34	1	1508	C	N1-C2-O2	5.53	122.22	118.90
34	1	741	C	C6-N1-C1'	-5.53	114.16	120.80
34	1	1874	U	C6-N1-C1'	-5.53	113.46	121.20
34	1	1120	U	N1-C2-O2	5.52	126.67	122.80
15	O	39	ASP	C-N-CA	5.52	135.50	121.70
34	1	297	U	N1-C2-O2	5.52	126.66	122.80
34	1	619	A	N1-C2-N3	-5.51	126.54	129.30
34	1	1460	G	O4'-C1'-N9	5.51	112.61	108.20
34	1	1859	A	C4-N9-C1'	5.51	136.22	126.30
34	1	862	G	O4'-C1'-N9	5.50	112.60	108.20
37	4	13	C	P-O3'-C3'	5.50	126.31	119.70
34	1	332	C	C5-C6-N1	5.50	123.75	121.00
34	1	85	C	C5-C6-N1	5.50	123.75	121.00
34	1	1486	C	C6-N1-C2	-5.50	118.10	120.30
34	1	1359	C	C6-N1-C2	-5.50	118.10	120.30
34	1	1581	G	C8-N9-C4	-5.49	104.20	106.40
34	1	1609	U	N1-C2-O2	5.49	126.64	122.80
34	1	1973	C	C6-N1-C2	-5.49	118.10	120.30
34	1	676	C	N1-C2-O2	5.49	122.19	118.90
1	A	199	LEU	CA-CB-CG	5.48	127.91	115.30
34	1	1788	U	N3-C2-O2	-5.48	118.36	122.20
34	1	659	G	C8-N9-C1'	-5.48	119.88	127.00
34	1	381	G	C4-N9-C1'	5.47	133.62	126.50
7	G	69	LEU	CB-CG-CD1	5.47	120.30	111.00
34	1	503	C	C6-N1-C1'	-5.46	114.25	120.80
34	1	1654	U	N1-C2-O2	5.46	126.62	122.80
33	g	301	ASN	N-CA-C	5.45	125.70	111.00
34	1	1679	C	N1-C2-O2	5.45	122.17	118.90
34	1	836	C	C6-N1-C2	-5.44	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1181	C	N1-C2-O2	5.44	122.17	118.90
34	1	1537	U	C2-N1-C1'	5.44	124.23	117.70
34	1	1146	G	O5'-P-OP1	-5.43	100.81	105.70
37	4	60	U	C6-N1-C2	-5.43	117.74	121.00
34	1	1525	C	N3-C2-O2	-5.43	118.10	121.90
34	1	591	A	P-O3'-C3'	5.43	126.22	119.70
34	1	298	C	C2-N1-C1'	5.43	124.77	118.80
34	1	1161	G	P-O3'-C3'	5.42	126.21	119.70
34	1	99	U	N3-C2-O2	-5.42	118.41	122.20
34	1	417	U	C5-C6-N1	5.42	125.41	122.70
34	1	1	G	C8-N9-C1'	5.42	134.04	127.00
34	1	31	C	C5-C6-N1	5.41	123.70	121.00
34	1	1421	C	C4-C5-C6	-5.41	114.70	117.40
34	1	1769	C	C5-C6-N1	5.41	123.70	121.00
34	1	1525	C	C5-C6-N1	5.41	123.70	121.00
34	1	1212	C	C6-N1-C1'	-5.41	114.31	120.80
37	4	72	C	C6-N1-C2	-5.41	118.14	120.30
34	1	1359	C	C5-C6-N1	5.40	123.70	121.00
34	1	883	G	O4'-C1'-N9	5.40	112.52	108.20
34	1	760	G	C4-N9-C1'	5.39	133.51	126.50
34	1	151	U	N1-C2-O2	5.39	126.57	122.80
34	1	1940	G	N3-C4-N9	5.39	129.23	126.00
34	1	496	A	C2-N3-C4	5.39	113.29	110.60
34	1	454	C	C5-C6-N1	5.39	123.69	121.00
34	1	1359	C	O4'-C1'-N1	5.39	112.51	108.20
34	1	335	C	C6-N1-C2	-5.38	118.15	120.30
34	1	332	C	C2-N1-C1'	5.38	124.72	118.80
34	1	319	C	C2-N1-C1'	5.38	124.72	118.80
34	1	510	G	N9-C1'-C2'	-5.37	106.09	112.00
34	1	951	U	N1-C2-O2	5.37	126.56	122.80
34	1	741	C	C6-N1-C2	-5.37	118.15	120.30
34	1	1698	U	N3-C2-O2	-5.37	118.44	122.20
34	1	2039	C	N3-C4-C5	-5.36	119.75	121.90
34	1	1419	U	C2-N1-C1'	5.35	124.11	117.70
34	1	1510	C	C6-N1-C2	-5.35	118.16	120.30
34	1	1595	G	N3-C4-N9	5.34	129.21	126.00
34	1	372	C	N3-C2-O2	-5.34	118.16	121.90
34	1	608	C	C5-C6-N1	5.34	123.67	121.00
34	1	2202	U	C2-N1-C1'	5.34	124.10	117.70
34	1	1485	A	C5-C6-N6	-5.33	119.43	123.70
34	1	95	C	N3-C2-O2	-5.33	118.17	121.90
34	1	1628	U	N1-C2-O2	5.33	126.53	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	760	G	O4'-C1'-N9	5.32	112.46	108.20
34	1	1207	U	C5-C6-N1	5.32	125.36	122.70
35	2	8	U	C2-N1-C1'	5.32	124.08	117.70
36	3	39	C	C6-N1-C2	-5.31	118.17	120.30
34	1	14	C	N1-C2-O2	5.31	122.09	118.90
34	1	2186	C	C6-N1-C2	-5.31	118.18	120.30
34	1	238	G	P-O3'-C3'	5.30	126.07	119.70
34	1	355	U	N3-C2-O2	-5.30	118.49	122.20
36	3	34	C	C2-N1-C1'	5.29	124.62	118.80
34	1	1237	C	C6-N1-C2	-5.29	118.19	120.30
34	1	403	G	C5-C6-O6	-5.28	125.43	128.60
34	1	1956	C	C5-C6-N1	5.28	123.64	121.00
34	1	1769	C	C6-N1-C2	-5.28	118.19	120.30
34	1	297	U	C2-N1-C1'	5.28	124.03	117.70
34	1	1654	U	C5-C6-N1	5.28	125.34	122.70
34	1	1371	U	N3-C2-O2	-5.28	118.51	122.20
34	1	1634	C	C6-N1-C2	-5.28	118.19	120.30
34	1	1489	A	OP2-P-O3'	5.27	116.80	105.20
34	1	1554	A	C8-N9-C1'	-5.27	118.21	127.70
34	1	335	C	C5-C6-N1	5.27	123.63	121.00
34	1	342	C	C6-N1-C2	-5.27	118.19	120.30
4	D	92	LEU	CA-CB-CG	5.26	127.41	115.30
34	1	506	U	C5-C6-N1	5.26	125.33	122.70
34	1	1359	C	C6-N1-C1'	-5.26	114.48	120.80
34	1	298	C	N3-C2-O2	-5.25	118.22	121.90
34	1	741	C	N3-C2-O2	-5.25	118.23	121.90
34	1	36	U	N3-C2-O2	-5.25	118.53	122.20
1	A	156	CYS	CA-CB-SG	5.23	123.42	114.00
34	1	1768	U	N3-C2-O2	-5.23	118.54	122.20
34	1	2064	C	C6-N1-C2	-5.22	118.21	120.30
34	1	664	U	N1-C2-O2	5.21	126.45	122.80
37	4	74	C	C2-N1-C1'	5.21	124.53	118.80
8	H	78	LEU	CA-CB-CG	5.21	127.28	115.30
34	1	355	U	N1-C2-O2	5.21	126.45	122.80
34	1	1939	G	C8-N9-C4	5.21	108.48	106.40
37	4	74	C	N1-C2-O2	5.20	122.02	118.90
34	1	1371	U	N1-C2-O2	5.20	126.44	122.80
34	1	2182	U	C5-C6-N1	5.20	125.30	122.70
34	1	664	U	C6-N1-C2	-5.19	117.89	121.00
35	2	13	C	P-O3'-C3'	5.19	125.93	119.70
34	1	1918	U	C2-N1-C1'	5.19	123.92	117.70
34	1	1522	G	N3-C4-N9	5.18	129.11	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1859	A	C8-N9-C1'	-5.18	118.37	127.70
34	1	167	C	C6-N1-C2	-5.18	118.23	120.30
34	1	675	U	C5-C6-N1	5.18	125.29	122.70
34	1	1361	U	C6-N1-C1'	-5.18	113.95	121.20
34	1	618	C	N3-C2-O2	-5.18	118.28	121.90
34	1	1212	C	C5-C6-N1	5.18	123.59	121.00
34	1	1918	U	N3-C2-O2	-5.18	118.58	122.20
34	1	1956	C	C6-N1-C1'	-5.18	114.59	120.80
34	1	90	C	C6-N1-C2	-5.16	118.23	120.30
34	1	1533	U	C2-N1-C1'	5.16	123.89	117.70
34	1	592	C	C6-N1-C1'	-5.16	114.61	120.80
34	1	1525	C	N1-C2-O2	5.16	121.99	118.90
34	1	2186	C	N3-C4-C5	-5.15	119.84	121.90
37	4	13	C	OP1-P-O3'	5.15	116.54	105.20
34	1	313	G	C8-N9-C4	-5.14	104.34	106.40
34	1	2163	G	N9-C1'-C2'	-5.14	106.34	112.00
34	1	676	C	N3-C2-O2	-5.14	118.30	121.90
34	1	2132	C	C6-N1-C2	-5.14	118.24	120.30
34	1	913	G	C2'-C3'-O3'	-5.14	98.19	109.50
34	1	1642	C	N1-C2-O2	5.14	121.98	118.90
34	1	313	G	C2-N3-C4	5.14	114.47	111.90
34	1	2190	C	C6-N1-C2	-5.14	118.24	120.30
34	1	424	C	C6-N1-C2	-5.13	118.25	120.30
34	1	395	U	C6-N1-C1'	-5.13	114.02	121.20
37	4	70	C	N3-C2-O2	-5.13	118.31	121.90
34	1	36	U	N1-C2-O2	5.12	126.38	122.80
34	1	837	G	N1-C2-N2	5.12	120.81	116.20
34	1	1939	G	N9-C4-C5	-5.12	103.35	105.40
34	1	151	U	N3-C2-O2	-5.11	118.62	122.20
12	L	111	LEU	CA-CB-CG	5.11	127.06	115.30
5	E	6	LEU	CA-CB-CG	5.11	127.05	115.30
34	1	381	G	N3-C4-C5	-5.11	126.05	128.60
34	1	787	G	O4'-C1'-N9	5.11	112.29	108.20
34	1	1864	C	N1-C2-O2	5.11	121.96	118.90
34	1	588	G	O4'-C1'-N9	5.10	112.28	108.20
34	1	1838	U	C6-N1-C2	-5.09	117.95	121.00
34	1	426	G	C2-N3-C4	5.08	114.44	111.90
34	1	2202	U	N1-C2-O2	5.08	126.36	122.80
34	1	1698	U	C2-N1-C1'	5.08	123.79	117.70
34	1	675	U	N1-C2-O2	5.07	126.35	122.80
34	1	1467	U	N3-C2-O2	-5.07	118.65	122.20
34	1	741	C	C5-C6-N1	5.06	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	1981	G	C4-N9-C1'	5.06	133.08	126.50
38	5	1	C	N3-C2-O2	-5.06	118.36	121.90
34	1	1120	U	N3-C2-O2	-5.05	118.66	122.20
34	1	1455	C	C6-N1-C2	-5.05	118.28	120.30
34	1	1157	C	C6-N1-C2	-5.05	118.28	120.30
34	1	1467	U	N1-C2-O2	5.05	126.34	122.80
34	1	655	U	N1-C2-O2	5.04	126.33	122.80
35	2	34	G	P-O3'-C3'	5.04	125.75	119.70
34	1	1419	U	N3-C2-O2	-5.04	118.67	122.20
34	1	1775	C	C5-C6-N1	5.04	123.52	121.00
34	1	952	U	N1-C2-O2	5.03	126.32	122.80
35	2	60	U	C2-N1-C1'	5.03	123.74	117.70
34	1	159	C	C6-N1-C2	-5.02	118.29	120.30
34	1	755	C	C6-N1-C2	-5.02	118.29	120.30
34	1	50	C	N1-C2-O2	5.02	121.91	118.90
36	3	28	C	C5-C6-N1	5.01	123.51	121.00
34	1	303	C	C4-C5-C6	-5.01	114.90	117.40
34	1	621	C	C6-N1-C2	-5.01	118.30	120.30
34	1	2100	A	C4-N9-C1'	5.01	135.31	126.30
34	1	1184	C	N1-C2-O2	5.00	121.90	118.90
36	3	34	C	C6-N1-C2	-5.00	118.30	120.30
34	1	1490	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208[A]	ARG	Peptide
2	B	208[B]	ARG	Peptide
12	L	109	ALA	Peptide
15	O	97	ARG	Peptide
16	P	106	GLY	Peptide
16	P	112	VAL	Peptide
16	P	86	PRO	Peptide
17	Q	48	SER	Peptide
19	S	5	ASP	Peptide
19	S	6	GLN	Peptide
21	U	19	HIS	Peptide
21	U	54	GLY	Peptide
26	Z	65	PHE	Peptide
29	c	40	ARG	Peptide
29	c	41	CYS	Peptide

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Mol	Chain	Res	Type	Group
32	f	122	HIS	Peptide
32	f	144	HIS	Peptide
32	f	145	LEU	Peptide
32	f	99	LYS	Peptide
33	g	300	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1829	0	1914	28	0
2	B	1676	0	1713	16	0
3	C	1668	0	1738	22	0
4	D	1504	0	1573	10	0
5	E	2029	0	2121	24	0
6	F	1656	0	1699	15	0
7	G	1796	0	1827	20	0
8	H	1438	0	1466	10	0
9	I	1613	0	1674	17	0
10	J	1014	0	1044	11	0
11	K	1403	0	1451	15	0
12	L	1127	0	1181	17	0
13	M	809	0	849	21	0
14	N	728	0	691	9	0
15	O	1032	0	1055	14	0
16	P	1134	0	1204	15	0
17	Q	746	0	647	10	0
18	R	1080	0	1067	12	0
19	S	441	0	451	13	0
20	T	1153	0	1219	13	0
21	U	1241	0	1255	8	0
22	V	935	0	961	21	0
23	W	822	0	801	13	0
24	X	1202	0	1230	9	0
25	Y	664	0	657	11	0
26	Z	1032	0	1101	19	0
27	a	544	0	566	0	0
28	b	796	0	810	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	656	0	661	0	0
30	d	466	0	476	0	0
31	e	449	0	476	0	0
32	f	385	0	293	0	0
33	g	2240	0	2094	0	0
34	1	37613	0	19015	314	0
35	2	1626	0	834	10	0
36	3	1639	0	837	8	0
37	4	1619	0	822	14	0
38	5	251	0	130	1	0
39	1	20	0	0	0	0
39	5	1	0	0	0	0
39	C	1	0	0	0	0
39	D	1	0	0	0	0
39	S	1	0	0	0	0
40	1	252	0	269	13	0
41	1	217	0	0	8	0
41	2	2	0	0	0	0
41	3	3	0	0	0	0
41	5	3	0	0	0	0
41	D	2	0	0	0	0
41	E	1	0	0	0	0
41	F	3	0	0	0	0
41	G	1	0	0	0	0
41	H	1	0	0	0	0
41	K	1	0	0	0	0
41	L	1	0	0	0	0
41	M	3	0	0	0	0
41	O	1	0	0	0	0
41	P	6	0	0	1	0
41	R	2	0	0	0	0
41	S	1	0	0	0	0
41	T	4	0	0	0	0
41	X	4	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	1	0
41	b	1	0	0	0	0
41	c	2	0	0	0	0
41	f	1	0	0	0	0
All	All	80594	0	59872	608	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 5.

All (608) 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)
34:1:489:A:N1	34:1:509:OMG:CM2	1.87	1.37
40:1:2305:PAR:O43	40:1:2305:PAR:C13	1.63	1.25
40:1:2302:PAR:C13	40:1:2302:PAR:O43	1.64	1.22
40:1:2304:PAR:O43	40:1:2304:PAR:C13	1.63	1.16
34:1:576:A:O2'	34:1:577:U:H5'	1.47	1.13
40:1:2307:PAR:C13	40:1:2307:PAR:O43	1.63	1.10
34:1:912:A2M:HM'2	34:1:913:G:H5'	1.12	1.10
34:1:576:A:O2'	34:1:577:U:C5'	2.00	1.09
34:1:905:A:H8	34:1:905:A:H5'	1.13	1.08
34:1:1575:G:H2'	34:1:1576:A:C8	1.89	1.08
19:S:29:LYS:HE2	34:1:1551:G:OP1	1.55	1.05
34:1:1575:G:H2'	34:1:1576:A:H8	1.22	1.02
34:1:574:C:H2'	34:1:575:C:C6	1.94	1.02
34:1:489:A:N1	34:1:509:OMG:HM21	1.79	0.97
34:1:761:A:C2	41:1:2473:HOH:O	2.17	0.96
34:1:489:A:N1	34:1:509:OMG:HM22	1.79	0.94
23:W:27:LEU:CD1	23:W:35:LEU:HD11	1.98	0.94
34:1:905:A:C8	34:1:905:A:H5'	2.03	0.93
34:1:489:A:N1	34:1:509:OMG:HM23	1.81	0.93
34:1:912:A2M:HM'2	34:1:913:G:C5'	2.00	0.91
34:1:912:A2M:CM'	34:1:913:G:H5'	1.99	0.91
34:1:489:A:C2	34:1:509:OMG:CM2	2.53	0.91
34:1:573:C:C2'	34:1:574:C:H5'	2.01	0.89
34:1:1576:A:N1	34:1:1577:U:C4	2.41	0.88
34:1:489:A:C2	34:1:509:OMG:HM21	2.07	0.88
34:1:574:C:H2'	34:1:575:C:H6	1.34	0.87
34:1:601:G:O2'	34:1:602:A:H5'	1.73	0.87
23:W:27:LEU:HD13	23:W:35:LEU:HD11	1.57	0.86
34:1:573:C:H2'	34:1:574:C:H5'	1.55	0.85
34:1:1241:G:O2'	34:1:1242:A:H5'	1.79	0.82
13:M:62:THR:HG22	34:1:1551:G:O6	1.79	0.82
20:T:109:ARG:HH12	34:1:1188:G:H1	1.24	0.82
34:1:1926:G:H5''	34:1:1926:G:H8	1.47	0.79
34:1:1963:C:C2'	34:1:1964:C:H5'	2.13	0.78
34:1:1551:G:N3	34:1:1551:G:H2'	1.96	0.78
34:1:911:A:H2'	34:1:912:A2M:H8	1.65	0.77
25:Y:23:HIS:HD2	25:Y:58:CYS:H	1.34	0.76
34:1:1114:G:H1	34:1:1207:U:H3	1.33	0.76
34:1:574:C:O2'	34:1:575:C:O4'	2.03	0.76
34:1:2165:A:OP2	41:1:2401:HOH:O	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:2163:G:O2'	34:1:2164:U:H5'	1.88	0.74
34:1:2010:G:H1	34:1:2026:U:H3	1.34	0.73
34:1:1295:G:H1	34:1:1419:U:H3	1.34	0.73
35:2:11:C:H42	35:2:24:G:H1	1.35	0.73
23:W:31:PRO:O	23:W:35:LEU:HG	1.88	0.73
10:J:2:THR:N	34:1:1281:C:HO2'	1.85	0.73
34:1:1540:G:O6	34:1:1549:C:N4	2.17	0.72
34:1:1288:G:H1	34:1:1426:U:H3	1.35	0.71
34:1:1464:OMG:HM22	34:1:1485:A:H61	1.55	0.71
34:1:575:C:O2'	34:1:576:A:H5'	1.89	0.71
34:1:958:G:H22	34:1:977:G:H1	1.38	0.71
34:1:1241:G:C2'	34:1:1242:A:H5'	2.21	0.71
34:1:354:C:H5	34:1:400:G:H1	1.38	0.70
34:1:1540:G:N1	34:1:1549:C:N3	2.35	0.70
1:A:118:LYS:HB2	34:1:2202:U:H2'	1.72	0.70
34:1:761:A:H2	41:1:2473:HOH:O	1.63	0.70
9:I:120:THR:HG22	9:I:123:ALA:H	1.56	0.69
34:1:911:A:O2'	34:1:912:A2M:O5'	2.10	0.69
34:1:1963:C:O2'	34:1:1964:C:H5'	1.94	0.68
34:1:1369:U:H3	34:1:1412:G:H1	1.41	0.68
15:O:139:ARG:NH1	34:1:2192:G:OP2	2.27	0.67
1:A:44:ALA:HB1	15:O:40:THR:HG21	1.74	0.67
9:I:101:LYS:H	34:1:989:G:H1	1.42	0.67
7:G:152:ARG:HH12	34:1:131:G:H5''	1.60	0.67
16:P:15[B]:ARG:NH2	34:1:396:G:N7	2.42	0.67
2:B:70:ALA:HB2	25:Y:42:ALA:HB2	1.77	0.66
34:1:951:U:H3	34:1:984:G:H1	1.41	0.66
22:V:35:ILE:HA	22:V:38:VAL:HG22	1.76	0.66
17:Q:31:ARG:O	17:Q:35:GLN:NE2	2.29	0.66
6:F:125:ILE:HD12	6:F:227:PHE:HB2	1.76	0.65
13:M:77:PHE:HB3	19:S:53:PHE:HB3	1.78	0.65
34:1:1576:A:C2	34:1:1577:U:C5	2.85	0.65
34:1:1961:G:N2	34:1:1987:G:O2'	2.25	0.65
4:D:2:ARG:NH2	34:1:509:OMG:OP1	2.31	0.64
34:1:87:G:N2	34:1:495:A:OP1	2.28	0.64
11:K:57:ALA:HB2	11:K:196:GLY:HA2	1.79	0.64
34:1:1963:C:H2'	34:1:1964:C:H5'	1.80	0.64
34:1:1240:A:H2'	34:1:1241:G:H5'	1.78	0.64
26:Z:63:SER:HB3	26:Z:81:LEU:HB2	1.80	0.63
34:1:568:U:O2'	34:1:574:C:N4	2.31	0.63
34:1:1619:G:HO2'	34:1:1849:G:HO2'	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:489:A:N6	34:1:509:OMG:HN22	1.96	0.62
23:W:110:ASN:HD22	23:W:127:SER:HB2	1.62	0.62
34:1:381:G:H5''	34:1:383:C:H41	1.64	0.62
34:1:1298:U:H3	34:1:1416:G:H1	1.45	0.62
34:1:847:A:N1	34:1:906:U:O4	2.33	0.62
34:1:1241:G:H2'	34:1:1242:A:C5'	2.30	0.62
34:1:905:A:H8	34:1:905:A:C5'	2.03	0.62
1:A:69:ASN:ND2	1:A:84:ARG:O	2.33	0.62
22:V:10:LYS:NZ	34:1:1668:C:O2'	2.31	0.61
7:G:180:GLN:NE2	34:1:65:A:OP1	2.33	0.61
8:H:24:LEU:HD11	8:H:132:ARG:HD2	1.81	0.61
5:E:8:ARG:NH1	34:1:490:U:O3'	2.34	0.61
20:T:109:ARG:NH1	34:1:1188:G:H1	1.98	0.61
1:A:61:LEU:HD13	1:A:98:LEU:HD21	1.82	0.61
16:P:2:THR:HG23	34:1:664:U:O4	2.00	0.60
34:1:783:A:H2	34:1:837:G:H22	1.48	0.60
12:L:41:PRO:O	34:1:1723:A:N6	2.33	0.60
18:R:25:ARG:HB2	18:R:30:ALA:HB2	1.82	0.60
34:1:286:G:N2	34:1:289:G:OP1	2.34	0.60
1:A:200:VAL:HG22	1:A:212:LEU:HB3	1.83	0.60
25:Y:30:GLU:OE1	25:Y:32:HIS:NE2	2.34	0.60
3:C:159:SER:HB3	34:1:1680:G:H5''	1.82	0.60
7:G:4:ASN:ND2	34:1:157:G:O2'	2.34	0.60
34:1:576:A:O2'	34:1:577:U:O4'	2.17	0.60
12:L:32:GLN:NE2	34:1:1724:G:O2'	2.34	0.60
11:K:191:ARG:NH2	34:1:375:G:N7	2.45	0.60
34:1:489:A:C2	34:1:509:OMG:HM22	2.30	0.60
1:A:123:MET:SD	1:A:123:MET:N	2.75	0.59
1:A:46:THR:HG21	1:A:66:PHE:HE1	1.67	0.59
34:1:1926:G:C5'	34:1:1926:G:C8	2.85	0.59
19:S:29:LYS:CE	34:1:1551:G:OP1	2.43	0.59
26:Z:40:THR:HG21	34:1:576:A:C2	2.38	0.59
37:4:15:G:N1	37:4:59:U:O2	2.35	0.59
3:C:208:THR:HG23	22:V:40:ILE:HG13	1.83	0.59
4:D:170:ARG:NH1	34:1:559:G:N7	2.48	0.59
4:D:7:PHE:O	34:1:25:C:N4	2.35	0.59
34:1:1241:G:H2'	34:1:1242:A:H5'	1.85	0.59
34:1:907:A:C2'	34:1:908:A:H5'	2.32	0.59
26:Z:40:THR:HG21	34:1:576:A:H2	1.68	0.59
35:2:3:G:N2	35:2:70:C:O2	2.36	0.59
9:I:113:GLN:HE22	34:1:910:A:H61	1.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:56:VAL:HB	26:Z:61:GLN:HE21	1.68	0.59
21:U:118:ARG:NH2	34:1:352:C:OP1	2.35	0.58
34:1:315:A:N6	34:1:333:G:O2'	2.36	0.58
3:C:144:GLN:O	34:1:1627:A:O2'	2.19	0.58
34:1:1980:U:H4'	34:1:2019:C:H4'	1.85	0.58
34:1:911:A:H2'	34:1:912:A2M:C8	2.33	0.58
34:1:431:G:OP2	34:1:466:G:O2'	2.22	0.58
34:1:1233:A:H2'	34:1:1234:G:O4'	2.04	0.58
35:2:19:G:O2'	35:2:57:G:N2	2.36	0.58
34:1:1926:G:H8	34:1:1926:G:C5'	2.16	0.58
1:A:151:GLN:HE21	1:A:153:SER:HB2	1.69	0.57
9:I:7:LYS:NZ	9:I:41:LEU:O	2.37	0.57
12:L:141:ARG:NH1	34:1:2002:U:OP1	2.37	0.57
7:G:90:GLY:HA3	7:G:94:GLU:HG2	1.86	0.57
34:1:2163:G:H2'	34:1:2164:U:C6	2.39	0.57
34:1:576:A:H2'	34:1:577:U:C6	2.38	0.57
34:1:689:U:H5'	34:1:690:G:H5'	1.87	0.57
34:1:1926:G:H5''	34:1:1926:G:C8	2.34	0.57
5:E:170:ILE:HD11	5:E:233:GLN:HG3	1.86	0.57
12:L:47:PRO:HG2	12:L:50:LEU:HB2	1.84	0.57
34:1:912:A2M:O3'	34:1:912:A2M:HM'2	2.05	0.57
5:E:250:ARG:NH1	34:1:864:G:OP1	2.37	0.57
3:C:193:SER:HA	3:C:200:SER:HA	1.87	0.57
9:I:165:VAL:HG23	9:I:168:ARG:HB2	1.87	0.57
34:1:1240:A:C2'	34:1:1241:G:H5'	2.35	0.57
26:Z:15:SER:OG	34:1:878:C:N4	2.37	0.57
34:1:1536:A:HO2'	34:1:1561:C:HO2'	1.51	0.56
24:X:89:CYS:HA	24:X:92:VAL:HB	1.86	0.56
26:Z:69:THR:HG22	26:Z:76:THR:HG22	1.87	0.56
2:B:33:GLN:HE21	2:B:38:LYS:HG3	1.71	0.56
7:G:80:ARG:NH2	7:G:87:THR:O	2.38	0.56
12:L:56:GLU:OE2	12:L:88:ARG:NH2	2.38	0.56
18:R:88:GLN:HA	18:R:96:THR:HG23	1.87	0.56
34:1:760:G:N2	41:1:2442:HOH:O	2.35	0.56
4:D:36:ARG:NH1	37:4:34:G:OP1	96.65	0.56
34:1:601:G:HO2'	34:1:602:A:H5'	1.71	0.56
13:M:45:VAL:HG11	13:M:88:LEU:HD12	1.88	0.56
10:J:31:SER:H	10:J:34:VAL:HG22	1.71	0.56
34:1:691:G:H1	34:1:754:G:H1	1.52	0.56
17:Q:63:ILE:HG22	17:Q:89:ILE:HB	1.87	0.56
23:W:49:ARG:NH2	34:1:1968:G:OP1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:52:VAL:HG21	9:I:178:GLN:HG3	1.88	0.56
11:K:75:ARG:NH1	34:1:307:C:OP1	2.39	0.55
2:B:1:MET:N	2:B:59:GLU:O	2.39	0.55
26:Z:128:ALA:O	41:Z:201:HOH:O	2.18	0.55
34:1:1576:A:C2	34:1:1577:U:C4	2.94	0.55
34:1:47:A:N7	34:1:96:U:O2'	2.40	0.55
20:T:3:ARG:HH12	34:1:1281:C:H5''	1.70	0.55
34:1:760:G:H5'	34:1:761:A:OP2	2.07	0.55
34:1:459:A:H5''	34:1:460:C:H5	1.70	0.55
8:H:8:LEU:HD21	8:H:55:VAL:HG21	1.88	0.55
14:N:53:VAL:HG12	14:N:105:THR:HG22	1.87	0.55
4:D:70:LEU:HB2	5:E:247:ILE:HG12	1.89	0.55
34:1:2150:G:N7	40:1:2306:PAR:O44	2.39	0.55
11:K:48:ALA:HB1	34:1:377:A:H5'	1.89	0.55
12:L:18:LYS:HD3	12:L:19:LYS:HG3	1.89	0.55
34:1:1868:C:N4	41:1:2449:HOH:O	2.36	0.55
34:1:576:A:O2'	34:1:577:U:O5'	2.24	0.55
1:A:169:ARG:HH22	34:1:1410:C:H5	1.55	0.55
14:N:67:THR:HG22	14:N:69:GLY:H	1.71	0.55
34:1:262:U:H1'	34:1:966:G:H22	1.71	0.55
3:C:141:ILE:HD13	3:C:149:MET:HE2	1.89	0.55
34:1:691:G:H22	34:1:754:G:H22	1.55	0.55
34:1:1530:G:H5'	34:1:1542:C:H41	1.72	0.55
34:1:1572:C:H42	34:1:1615:G:H1	1.53	0.54
34:1:1577:U:O2	34:1:1577:U:H5''	2.06	0.54
24:X:137:LYS:NZ	34:1:1917:A:O2'	2.40	0.54
34:1:508:A:N3	34:1:508:A:H2'	2.22	0.54
37:4:18:G:H5''	37:4:60:U:H2'	1.88	0.54
15:O:23:VAL:HG22	15:O:87:HIS:HB2	1.89	0.54
16:P:90:CYS:HA	16:P:93:PHE:HD2	1.73	0.54
3:C:209:VAL:HG22	22:V:39:THR:HG22	1.89	0.54
37:4:18:G:N2	37:4:61:C:O2'	2.40	0.54
3:C:93:ARG:O	3:C:100:GLN:NE2	2.39	0.54
19:S:7:TRP:NE1	34:1:1569:G:O6	2.39	0.54
34:1:1618:U:HO2'	34:1:1619:G:H8	1.56	0.54
19:S:10:ARG:NH2	34:1:1853:U:OP1	2.41	0.54
34:1:469:G:O2'	34:1:508:A:OP1	2.24	0.54
8:H:45:ARG:HH12	8:H:51:ARG:HH21	1.55	0.54
2:B:90:ILE:HG22	2:B:101:PHE:HB2	1.90	0.54
3:C:6:LYS:HD2	13:M:22:THR:HG21	1.89	0.54
34:1:1241:G:H2'	34:1:1242:A:O5'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:74:VAL:O	9:I:78:GLN:N	2.41	0.53
23:W:88:ARG:NH2	23:W:127:SER:O	2.41	0.53
5:E:63:ARG:NH2	34:1:497:A:OP2	2.35	0.53
34:1:761:A:H2	34:1:773:A:H2	1.54	0.53
5:E:95:ARG:HG2	5:E:111:LEU:HB2	1.90	0.53
34:1:785:G:O4'	34:1:787:G:N2	2.42	0.53
6:F:48:CYS:O	6:F:53:ARG:NH2	2.42	0.53
34:1:1548:A:H62	34:1:2021:A2M:HM'2	1.72	0.53
40:1:2305:PAR:N64	40:1:2305:PAR:O44	2.41	0.53
34:1:956:A:H61	34:1:979:U:H3	1.57	0.53
5:E:129:ALA:HB3	5:E:133:VAL:HG13	1.91	0.53
7:G:6:ALA:HB3	7:G:115:THR:HG22	1.90	0.53
16:P:101:LEU:HB3	16:P:124:LYS:HB3	1.91	0.53
34:1:1241:G:C2'	34:1:1242:A:C5'	2.86	0.53
22:V:17:VAL:HG13	22:V:58:MET:HE2	1.90	0.53
11:K:121:LEU:HD12	11:K:180:ARG:HE	1.74	0.53
34:1:905:A:C8	34:1:905:A:C5'	2.85	0.53
1:A:146:LYS:HB3	1:A:210:ARG:HB2	1.89	0.53
7:G:163:ARG:HH11	34:1:66:U:H6	1.56	0.53
11:K:8:LEU:HB3	11:K:20:ILE:HD12	1.89	0.53
1:A:28:GLU:HB3	1:A:96:ARG:HH12	1.74	0.53
20:T:16:LEU:HD12	34:1:1108:A:H3'	1.90	0.52
34:1:759:U:O2'	34:1:760:G:N3	2.32	0.52
34:1:862:G:H21	34:1:890:A:H62	1.58	0.52
3:C:145[A]:ARG:NH2	38:5:12:A:O3'	2.41	0.52
25:Y:38:GLN:HG2	25:Y:58:CYS:HB3	1.91	0.52
34:1:576:A:O2'	34:1:577:U:C4'	2.55	0.52
34:1:791:G:O2'	34:1:792:G:N2	2.42	0.52
36:3:1:C:H2'	36:3:2:G:H8	1.75	0.52
34:1:2067:U:O2'	34:1:2068:G:H5'	2.09	0.52
34:1:649:U:O4	40:1:2305:PAR:N24	2.42	0.52
1:A:32:VAL:HG22	1:A:98:LEU:HD12	1.91	0.52
5:E:103:LYS:NZ	34:1:889:A:OP1	2.41	0.52
17:Q:87:ASP:HB3	17:Q:139:GLN:HE22	1.74	0.52
34:1:1251:G:N2	34:1:2183:G:OP1	2.43	0.52
1:A:190:LEU:HD13	1:A:217:VAL:HG11	1.91	0.52
12:L:43:GLN:HE21	34:1:1723:A:H8	1.57	0.52
14:N:63:THR:HA	14:N:76:PRO:HA	1.92	0.52
9:I:12:LYS:HE3	9:I:48:THR:HB	1.91	0.52
15:O:88:VAL:HG13	15:O:122:ILE:HA	1.91	0.52
11:K:64:ASN:ND2	34:1:305:U:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:50:U:H3	37:4:64:A:H61	1.58	0.52
34:1:1574:G:H2'	34:1:1575:G:H8	1.75	0.51
34:1:1870:A:H4'	34:1:1960:G:H4'	1.92	0.51
34:1:574:C:O2'	34:1:575:C:H5'	2.10	0.51
3:C:160:GLY:O	3:C:163:HIS:ND1	2.36	0.51
8:H:35:VAL:HG21	12:L:49:THR:HG23	1.91	0.51
10:J:57:ARG:HG3	34:1:1109:A:H4'	1.90	0.51
34:1:1574:G:H2'	34:1:1575:G:C8	2.45	0.51
34:1:1912:A:H61	34:1:1927:U:H3	1.57	0.51
34:1:95:C:H1'	34:1:469:G:H5'	1.91	0.51
10:J:24:GLN:HE21	10:J:64:ASN:HD21	1.58	0.51
3:C:152:ARG:HH12	34:1:1824:C:H5''	1.75	0.51
3:C:65:ILE:HD12	3:C:87:VAL:HG23	1.93	0.51
6:F:55:VAL:HG21	6:F:78:ILE:HG23	1.93	0.51
18:R:121:HIS:HD2	23:W:128:MET:HG2	1.76	0.51
34:1:573:C:C3'	34:1:574:C:H5'	2.38	0.51
6:F:182:VAL:HB	6:F:209:TYR:HB2	1.93	0.51
22:V:5:ARG:HB2	22:V:10:LYS:HE3	1.91	0.51
34:1:481:A:O2'	34:1:513:G:N2	2.39	0.51
1:A:160:GLN:HA	1:A:163:VAL:HG22	1.93	0.51
5:E:92:THR:HG22	26:Z:21:LYS:HB2	1.92	0.51
15:O:33:THR:HG21	15:O:67:ALA:HB2	1.93	0.51
34:1:1136:U:O2'	34:1:1236:U:OP1	2.26	0.51
24:X:79:PRO:O	34:1:1878:A:O2'	2.29	0.51
12:L:35:ILE:HG12	12:L:71:ILE:HB	1.93	0.51
2:B:187:ARG:HD3	2:B:194:ARG:HG2	1.92	0.51
6:F:114:ASN:HD22	6:F:141:MET:HA	1.76	0.51
34:1:276:G:H21	34:1:277:U:H1'	1.75	0.50
36:3:21:A:H5''	36:3:46:A:H62	1.75	0.50
5:E:120:LEU:HD21	5:E:233:GLN:HB2	1.93	0.50
8:H:77:ARG:NH1	34:1:1945:A:OP1	2.42	0.50
34:1:525:A:H62	34:1:556:A:H61	1.59	0.50
7:G:183:ILE:HD13	34:1:146:U:H4'	1.93	0.50
2:B:16:SER:O	34:1:1184:C:N4	62.88	0.50
7:G:59:LYS:HD3	7:G:110:ALA:HB2	1.94	0.50
34:1:1963:C:O5'	34:1:1963:C:H6	1.94	0.50
34:1:343:G:N2	41:1:2465:HOH:O	2.43	0.50
3:C:137:VAL:HG22	3:C:183:VAL:HG12	1.94	0.50
17:Q:123:ILE:HG22	17:Q:125:ASP:H	1.76	0.50
26:Z:91:ARG:NH2	34:1:498:C:N3	2.60	0.50
2:B:144:ASN:ND2	25:Y:36:ALA:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:MET:SD	10:J:117:ARG:NH2	2.85	0.50
26:Z:106:ALA:O	34:1:503:C:N4	2.36	0.50
1:A:37:ASN:ND2	1:A:188:SER:OG	2.44	0.50
22:V:118:ARG:HE	34:1:727:U:H5''	1.75	0.50
36:3:58:A:O2'	36:3:61:C:N4	2.44	0.50
18:R:125:ARG:NH2	23:W:130:TYR:OH	2.42	0.50
26:Z:97:ARG:HG2	26:Z:100:ARG:HH21	1.76	0.50
26:Z:25:ARG:HD2	26:Z:81:LEU:HD22	1.94	0.50
34:1:1964:C:O2'	34:1:1965:G:OP2	2.28	0.50
16:P:1:MET:N	41:P:202:HOH:O	2.44	0.50
19:S:56:LEU:HD23	34:1:1686:C:H4'	1.93	0.50
22:V:119[B]:ARG:NH1	34:1:727:U:OP2	2.45	0.49
7:G:2[A]:LYS:HB3	7:G:15:GLN:HE21	1.77	0.49
10:J:112:ASP:OD1	10:J:112:ASP:N	2.45	0.49
35:2:7:A:H61	35:2:65:G:H22	1.60	0.49
13:M:23:SER:HB3	13:M:29:VAL:HB	1.94	0.49
20:T:14:SER:HB2	34:1:1206:C:H5''	1.94	0.49
34:1:190:G:O2'	34:1:304:A:OP1	2.26	0.49
34:1:471:A:N3	34:1:483:U:O2'	2.40	0.49
7:G:71:SER:HA	7:G:101:ARG:HH22	1.78	0.49
34:1:1621:OMU:H4'	34:1:1622:G:O5'	2.13	0.49
7:G:95:ARG:NH1	34:1:2093:U:OP1	2.40	0.49
34:1:1510:C:H5	34:1:1515:A:H61	1.61	0.49
25:Y:16:LEU:HD12	25:Y:17:TYR:HB3	1.93	0.49
15:O:24:VAL:HB	15:O:86:LEU:HD13	1.95	0.49
21:U:112:TYR:O	21:U:114:ARG:N	2.44	0.49
40:1:2307:PAR:N64	40:1:2307:PAR:O44	2.36	0.49
36:3:4:G:H2'	36:3:5:G:H8	1.78	0.48
37:4:25:C:H2'	37:4:26:A:H8	1.78	0.48
14:N:73:PHE:HB3	14:N:75:VAL:HG23	1.93	0.48
35:2:51:U:H3	35:2:63:G:H1	1.60	0.48
37:4:1:G:H22	37:4:72:C:H42	1.60	0.48
15:O:136[A]:LYS:HB3	15:O:136[A]:LYS:HE3	1.52	0.48
24:X:60:ILE:HG21	24:X:86:TYR:HE1	1.77	0.48
34:1:1574:G:C6	34:1:1575:G:C6	3.01	0.48
34:1:508:A:H2'	34:1:509:OMG:O4'	2.14	0.48
18:R:31:LEU:HD11	18:R:68:ILE:HG21	1.95	0.48
34:1:1576:A:N1	34:1:1577:U:C5	2.79	0.48
34:1:761:A:O5'	34:1:761:A:H8	1.97	0.48
26:Z:111:ARG:HH12	34:1:487:C:H5	1.61	0.48
26:Z:62:VAL:HG22	26:Z:82:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:2:GLY:HA2	34:1:1789:U:H5''	1.96	0.48
37:4:9:A:H8	37:4:11:C:H41	1.60	0.48
35:2:13:C:H42	35:2:46:G:H21	1.60	0.48
35:2:75:C:H2'	35:2:76:A:H8	1.79	0.48
5:E:121:MET:HA	5:E:139:HIS:HE1	1.78	0.48
19:S:30:ALA:HB2	34:1:1551:G:H5''	1.96	0.48
20:T:129:TYR:HA	20:T:132:VAL:HG12	1.96	0.48
34:1:467:C:O2	34:1:470:C:N4	2.39	0.48
35:2:12:U:H3	35:2:23:A:H61	1.62	0.48
24:X:164:ASP:OD2	34:1:1709:A:O2'	2.31	0.48
34:1:1844:U:H4'	34:1:1847:A:H1'	1.95	0.48
13:M:99:THR:HG21	13:M:111:ILE:HD11	1.96	0.48
18:R:89:ARG:NH2	23:W:43:LEU:O	2.47	0.48
22:V:27:ASP:O	22:V:31:ASN:ND2	2.45	0.48
34:1:54:C:O2'	34:1:507:G:N7	2.44	0.48
15:O:136[B]:LYS:HB2	15:O:136[B]:LYS:HE3	1.53	0.48
34:1:576:A:H2'	34:1:577:U:H6	1.79	0.47
2:B:127:VAL:HG21	2:B:137:ILE:HD11	1.96	0.47
36:3:47:U:O2'	36:3:50:U:OP1	2.29	0.47
15:O:128:ILE:O	34:1:1133:U:O2'	2.30	0.47
12:L:61:VAL:HG22	12:L:65:TYR:HD2	1.79	0.47
13:M:18[B]:ARG:NH1	34:1:1698:U:OP1	2.47	0.47
16:P:17:ARG:HH22	34:1:659:G:H21	1.63	0.47
21:U:26:GLN:HE22	21:U:48:ARG:HE	1.61	0.47
13:M:63:ARG:HG2	34:1:1551:G:C8	2.49	0.47
34:1:1776:U:H1'	34:1:1777:OMU:H5	1.95	0.47
34:1:870:A:N6	41:1:2469:HOH:O	2.47	0.47
37:4:1:G:N2	37:4:73:A:N7	2.62	0.47
34:1:276:G:N2	34:1:277:U:O2	2.48	0.47
2:B:79:VAL:HG22	2:B:90:ILE:HD12	1.96	0.47
18:R:89:ARG:HB2	34:1:1967:G:H4'	1.97	0.47
35:2:7:A:H5'	35:2:8:U:H5	1.79	0.47
3:C:92:VAL:HG11	3:C:95:LEU:HG	1.96	0.47
9:I:182:ARG:NH2	34:1:689:U:OP1	2.48	0.47
5:E:138:THR:HG22	5:E:140:ASP:H	1.80	0.47
14:N:49:PHE:HE1	14:N:111:ILE:HG23	1.79	0.47
26:Z:17:PHE:HZ	26:Z:26:LYS:HD3	1.79	0.47
18:R:37:VAL:HG13	18:R:41:PHE:HD2	1.79	0.47
40:1:2306:PAR:N24	40:1:2306:PAR:O44	2.48	0.47
34:1:180:G:H22	34:1:316:A:H5'	1.79	0.47
34:1:910:A:C2'	34:1:911:A:H5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:215:LEU:O	7:G:219:ASN:ND2	2.48	0.47
6:F:169:LYS:NZ	10:J:91:LYS:O	2.31	0.47
34:1:724:A:O2'	34:1:725:U:O2	2.32	0.46
6:F:94:LYS:HD2	6:F:219:HIS:HB2	1.97	0.46
34:1:847:A:C2	34:1:906:U:H5	2.33	0.46
19:S:22:CYS:SG	19:S:25:CYS:N	2.87	0.46
34:1:1907:A:N1	34:1:1908:A:N6	2.63	0.46
13:M:15:GLN:HE22	13:M:92:THR:HB	1.81	0.46
17:Q:41:ASN:H	17:Q:42:GLY:HA3	1.80	0.46
34:1:1576:A:H2	34:1:1577:U:C6	2.34	0.46
36:3:1:C:H2'	36:3:2:G:C8	2.50	0.46
34:1:1227:G:H4'	34:1:2179:A:H4'	1.97	0.46
16:P:114:ASP:HB2	34:1:619:A:N1	2.31	0.46
34:1:905:A:H2'	34:1:906:U:O5'	2.16	0.46
1:A:86:VAL:HG22	1:A:105:MET:HG3	1.98	0.46
5:E:97:ARG:HB2	5:E:111:LEU:HD11	1.98	0.46
13:M:18[B]:ARG:HB2	13:M:18[B]:ARG:HH21	1.80	0.46
34:1:912:A2M:HM'3	34:1:913:G:O4'	2.16	0.45
34:1:1224:A:OP2	34:1:1270:G:N2	2.46	0.45
17:Q:40:ALA:HA	17:Q:41:ASN:HA	1.60	0.45
15:O:127:PRO:HB3	34:1:1134:A:H5''	1.98	0.45
34:1:1579:A:OP1	34:1:1580:G:O2'	2.33	0.45
34:1:339:U:H2'	34:1:340:G:C8	2.51	0.45
11:K:68:ALA:HB1	34:1:245:A:H5'	1.98	0.45
10:J:44:HIS:O	10:J:46:TYR:N	2.49	0.45
13:M:52:ARG:NH1	34:1:1694:C:O2	2.48	0.45
14:N:68:LEU:HG	14:N:73:PHE:HZ	1.80	0.45
34:1:1578:G:H4'	34:1:1581:G:H4'	1.99	0.45
6:F:51:LEU:HD11	6:F:66:ILE:HG12	1.98	0.45
20:T:55:ARG:HD3	34:1:1207:U:H5'	1.98	0.45
16:P:68:LYS:NZ	34:1:616:A:OP1	2.50	0.45
6:F:76:HIS:NE2	6:F:77:GLN:OE1	2.49	0.45
19:S:37:LEU:HG	19:S:39:VAL:HG22	1.99	0.45
20:T:48:SER:OG	34:1:1114:G:N2	2.50	0.45
34:1:1576:A:C2	34:1:1577:U:C6	3.04	0.45
17:Q:47:LEU:N	17:Q:48:SER:OG	2.50	0.45
22:V:67:ARG:HH12	34:1:1671:U:P	2.40	0.45
23:W:54:ARG:NH1	34:1:1974:A:OP2	2.49	0.45
34:1:2054:C:H5''	34:1:2055:A:C8	2.52	0.45
35:2:27:G:N1	35:2:43:C:N3	2.61	0.45
37:4:62:C:H2'	37:4:63:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:GLU:O	5:E:165:LYS:N	2.50	0.45
6:F:234:TYR:OH	25:Y:16:LEU:O	2.30	0.45
34:1:564:A:O2'	34:1:565:U:O2	2.28	0.45
34:1:847:A:C2	34:1:906:U:C5	3.05	0.45
37:4:25:C:H2'	37:4:26:A:C8	2.52	0.45
3:C:7:LYS:HG3	13:M:58:LEU:HD21	1.98	0.45
1:A:99:LEU:HD21	1:A:237:ILE:HG12	1.99	0.44
8:H:37:HIS:HE2	12:L:85:TYR:HE1	1.66	0.44
14:N:36:VAL:HG11	14:N:83:LEU:HD21	2.00	0.44
17:Q:96:LYS:H	17:Q:115:THR:HG21	1.83	0.44
7:G:223:LEU:HD21	34:1:790:U:O2'	2.18	0.44
4:D:67:ARG:NH2	34:1:892:U:O2'	2.49	0.44
10:J:76:CYS:N	34:1:1452:A:O2'	2.44	0.44
34:1:2067:U:C2'	34:1:2068:G:H5'	2.47	0.44
3:C:158[B]:LYS:HD2	34:1:1823:A:H5''	2.00	0.44
15:O:27:TYR:HD1	15:O:91:ARG:HG3	1.83	0.44
23:W:105:ASN:HB2	23:W:129:SER:HA	1.99	0.44
34:1:1276:G:O2'	34:1:1278:U:O2	2.35	0.44
34:1:1576:A:H2	34:1:1577:U:C5	2.34	0.44
16:P:3:LYS:NZ	34:1:661:OMU:OP2	2.46	0.44
1:A:55:ARG:HH22	34:1:1141:C:H5'	1.81	0.44
1:A:70:LEU:HD23	1:A:86:VAL:HG21	2.00	0.44
17:Q:126:PHE:HA	17:Q:127:GLY:HA3	1.83	0.44
26:Z:58:ASP:OD2	26:Z:60:SER:OG	2.30	0.44
34:1:259:C:H2'	34:1:260:A:H8	1.82	0.44
9:I:52:VAL:HG13	9:I:61:VAL:HG23	2.00	0.44
34:1:2013:G:O6	34:1:2022:A:N6	2.51	0.44
13:M:32:VAL:HG21	13:M:107:VAL:HG11	1.99	0.44
1:A:191:THR:HG22	1:A:192:ARG:HD2	1.99	0.44
6:F:213:ARG:NH1	34:1:1449:U:H2'	2.33	0.44
10:J:102:VAL:HB	10:J:113:HIS:HB3	1.99	0.44
21:U:87:ARG:HG2	21:U:139:VAL:HG22	1.98	0.44
26:Z:91:ARG:O	34:1:498:C:O2'	2.27	0.44
19:S:30:ALA:HB2	34:1:1551:G:C5'	2.48	0.43
1:A:69:ASN:HD22	1:A:70:LEU:H	1.65	0.43
34:1:1872:A:H5'	34:1:1993:A:H62	1.82	0.43
3:C:184:LYS:NZ	34:1:1630:G:OP1	2.50	0.43
34:1:489:A:C6	34:1:509:OMG:HM23	2.48	0.43
34:1:36:U:H4'	34:1:575:C:H5''	1.99	0.43
5:E:210:ALA:HB3	5:E:242:LEU:HD21	1.99	0.43
5:E:203:ASN:HB2	5:E:219:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:95:ARG:O	34:1:448:C:O2'	2.33	0.43
13:M:65:THR:HG1	13:M:67:CYS:HG	1.66	0.43
25:Y:77:THR:HB	25:Y:82:ILE:HB	2.00	0.43
34:1:619:A:O2'	34:1:622:C:N4	2.44	0.43
1:A:106:GLU:HG3	1:A:216:LYS:HB3	2.00	0.43
4:D:39:ARG:NH2	34:1:643:A:OP1	2.52	0.43
5:E:8:ARG:NH2	5:E:17:LEU:HB3	2.33	0.43
8:H:41[A]:ARG:HG2	8:H:41[A]:ARG:H	1.59	0.43
20:T:132:VAL:HG13	20:T:134:GLN:HG2	2.00	0.43
23:W:84:LYS:HB2	34:1:1593:G:H5'	2.01	0.43
9:I:64:VAL:HB	9:I:96:LEU:HD23	2.01	0.43
12:L:17:LYS:HG2	12:L:22:ILE:HG12	2.00	0.43
34:1:2183:G:H3'	34:1:2184:MA6:H8	2.01	0.43
34:1:434:A:O2'	34:1:2133:G:O2'	2.34	0.43
6:F:100:LYS:HA	34:1:10:G:H21	1.83	0.43
9:I:129:LEU:HD21	9:I:155:VAL:HG21	2.01	0.43
12:L:96:ILE:HG23	12:L:108:LYS:HD2	2.01	0.43
15:O:15:LYS:HG3	15:O:17:GLY:H	1.83	0.43
2:B:45:THR:OG1	22:V:102:ASP:OD2	2.22	0.43
34:1:1173:A:H1'	34:1:1235:A:C2	2.54	0.43
34:1:1464:OMG:H2'	34:1:1465:A:C8	2.53	0.43
34:1:15:U:H2'	34:1:16:G:O4'	2.19	0.43
34:1:1664:G:N2	40:1:2304:PAR:O44	2.50	0.43
1:A:33:VAL:HG12	1:A:42:GLN:HG2	2.01	0.43
5:E:69:VAL:HG22	5:E:87:VAL:HG22	2.00	0.43
12:L:51:ARG:HD3	12:L:51:ARG:HH11	1.70	0.43
26:Z:15:SER:HB3	26:Z:29:ILE:HG13	2.01	0.43
34:1:65:A:N6	34:1:82:A:OP2	2.50	0.43
5:E:135:VAL:HG12	5:E:145:ARG:HA	2.01	0.43
18:R:34:VAL:HG23	18:R:101:SER:HB3	2.00	0.43
3:C:212:PRO:HD3	22:V:19:LYS:HB3	2.01	0.43
34:1:1548:A:H4'	34:1:1549:C:H5''	2.00	0.42
22:V:67:ARG:NH1	34:1:1671:U:OP2	2.52	0.42
34:1:2068:G:H2'	34:1:2069:U:C6	2.54	0.42
4:D:96:LEU:HD12	6:F:187:GLY:HA3	2.01	0.42
16:P:54:LYS:HD3	16:P:91:LEU:HD13	2.01	0.42
34:1:458:U:O2'	34:1:461:G:O6	2.31	0.42
7:G:139:LYS:NZ	7:G:178:LYS:O	2.41	0.42
13:M:63:ARG:HB2	19:S:41:ARG:HH21	1.84	0.42
14:N:82:GLN:HE22	14:N:85:ARG:HH21	1.67	0.42
40:1:2304:PAR:H11	40:1:2304:PAR:H531	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:PRO:HG3	34:1:310:U:H5'	2.02	0.42
16:P:67:ARG:NH2	34:1:618:C:H41	2.17	0.42
3:C:45:THR:N	3:C:82:LYS:O	2.45	0.42
4:D:28:LYS:HB3	4:D:43:ARG:HB3	18.34	0.42
8:H:134:ASN:ND2	34:1:2033:U:OP1	2.53	0.42
22:V:119[A]:ARG:HA	22:V:119[A]:ARG:HD2	1.54	0.42
24:X:96:ILE:HG22	24:X:155:LEU:HB2	2.01	0.42
7:G:49:TYR:OH	7:G:122:GLN:O	2.32	0.42
22:V:45:LYS:HG2	22:V:49:LYS:HE2	2.02	0.42
34:1:2153:A:N6	40:1:2306:PAR:O62	2.37	0.42
16:P:48:LYS:HG3	34:1:478:C:H5''	2.01	0.42
36:3:9:G:O2'	36:3:10:G:N7	2.48	0.42
34:1:1226:A:N3	34:1:2178:U:O2'	2.52	0.42
34:1:2196:G:OP1	41:1:2403:HOH:O	2.22	0.42
1:A:206:ILE:O	34:1:1413:C:O2'	2.30	0.42
16:P:105:PHE:HA	34:1:648:A:H5''	2.01	0.42
34:1:1577:U:O2	34:1:1577:U:H3'	2.19	0.42
3:C:72:ILE:HD12	3:C:85:LEU:HD21	2.01	0.42
13:M:33:THR:HG23	13:M:86:ILE:HD11	2.02	0.42
21:U:90:VAL:HG21	21:U:132:PRO:HB2	2.01	0.42
2:B:93:PHE:HD1	2:B:182:ALA:HB2	1.85	0.42
34:1:1964:C:O2'	34:1:1965:G:P	2.78	0.42
34:1:509:OMG:HM22	34:1:510:G:O4'	2.19	0.42
34:1:569:U:O2'	34:1:571:A:N7	2.38	0.42
34:1:784:C:H2'	34:1:787:G:N2	2.34	0.42
5:E:66:LEU:HD23	26:Z:22:LEU:HD22	2.02	0.42
23:W:90:VAL:HB	23:W:123:LEU:HD23	2.02	0.42
20:T:3:ARG:HB3	34:1:1112:A:H5''	2.02	0.42
34:1:1189:G:H5'	34:1:1224:A:H4'	2.02	0.42
21:U:51:LYS:HD2	34:1:296:C:H4'	2.01	0.42
34:1:601:G:H2'	34:1:602:A:C8	2.55	0.42
34:1:979:U:H2'	34:1:980:G:C8	2.55	0.42
1:A:151:GLN:HE22	1:A:156:CYS:HB3	1.85	0.42
11:K:106:ALA:HB2	11:K:184:VAL:HG23	2.02	0.42
11:K:49:ARG:HD3	34:1:377:A:C8	2.54	0.42
34:1:1621:OMU:O5'	34:1:1621:OMU:H6	2.20	0.41
13:M:24:ARG:HD2	13:M:79:LEU:HD11	2.02	0.41
16:P:46:HIS:CD2	16:P:103:SER:HB3	2.55	0.41
34:1:1664:G:H1	34:1:1682:G:H5'	1.84	0.41
2:B:19:GLN:HG2	22:V:95:ILE:HG12	2.02	0.41
11:K:23:LYS:HD3	34:1:429:G:H5''	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:59:LYS:HB3	22:V:63:ARG:HH12	1.85	0.41
34:1:1979:OMU:H1'	34:1:1979:OMU:HM23	1.63	0.41
34:1:1979:OMU:P	34:1:1979:OMU:H6	2.59	0.41
36:3:9:G:H21	36:3:46:A:H5''	1.85	0.41
6:F:59:LYS:HB3	6:F:255:HIS:CE1	2.56	0.41
34:1:2164:U:H4'	34:1:2185:MA6:C2	2.50	0.41
13:M:18[B]:ARG:NH2	13:M:114:LEU:HD11	2.35	0.41
19:S:31:LEU:HA	19:S:40:CYS:HA	2.03	0.41
34:1:44:C:OP2	34:1:480:A:N6	2.51	0.41
1:A:170:ILE:HD11	1:A:212:LEU:HD11	2.03	0.41
2:B:138:ARG:O	2:B:141:SER:OG	2.35	0.41
12:L:109:ALA:HA	12:L:112:LYS:HB3	2.02	0.41
12:L:27:VAL:HG22	12:L:71:ILE:HG12	2.01	0.41
18:R:27:VAL:HG23	18:R:60:LEU:HD11	2.02	0.41
24:X:38:LEU:HD23	24:X:38:LEU:HA	1.87	0.41
34:1:1551:G:C2'	34:1:1551:G:N3	2.73	0.41
19:S:17:LYS:NZ	34:1:2016:C:OP1	2.41	0.41
4:D:169:GLY:HA3	34:1:557:A:H5'	2.03	0.41
34:1:602:A:O2'	34:1:603:C:P	2.79	0.41
34:1:97:C:H2'	34:1:421:A:H4'	2.02	0.41
37:4:3:G:H1	37:4:70:C:H42	1.69	0.41
9:I:2:GLN:HA	9:I:3:PRO:HD3	1.86	0.41
20:T:73:ARG:NH1	34:1:914:G:H5'	2.36	0.41
22:V:69:ILE:HD12	22:V:69:ILE:HA	1.95	0.41
24:X:33:ARG:NH2	24:X:40:ASP:OD2	2.54	0.41
2:B:94:SER:OG	2:B:99:THR:O	2.27	0.41
11:K:87:SER:HB3	11:K:90:LEU:HD13	2.03	0.41
16:P:5:ASN:HA	21:U:114:ARG:HH12	1.85	0.41
21:U:38:ARG:HA	21:U:41:VAL:HG12	2.02	0.41
25:Y:17:TYR:CZ	25:Y:19:PRO:HB3	2.55	0.41
13:M:62:THR:CG2	34:1:1551:G:O6	2.62	0.41
11:K:56:ARG:HH22	34:1:376:U:P	2.43	0.41
20:T:133:LYS:HD3	34:1:913:G:N2	2.35	0.41
7:G:223:LEU:HA	7:G:223:LEU:HD13	4.32	0.41
15:O:71:ALA:HB1	15:O:112:LEU:HD12	2.01	0.41
25:Y:21:LYS:HD2	25:Y:26:ASN:ND2	2.36	0.41
34:1:321:G:H1	34:1:328:C:H42	1.69	0.41
3:C:198:GLY:HA2	3:C:199:PRO:HD3	1.91	0.41
9:I:37:LEU:HB3	9:I:41:LEU:HD12	2.02	0.41
10:J:102:VAL:O	10:J:113:HIS:N	2.54	0.41
11:K:67:TRP:NE1	11:K:204:GLU:OE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1523:A:H2'	34:1:1524:G:C8	2.56	0.41
25:Y:69:SER:O	25:Y:73:ILE:HG12	2.21	0.41
37:4:44:G:C5	37:4:45:U:H1'	2.56	0.41
5:E:249:GLU:OE2	5:E:253:ARG:NE	2.42	0.41
9:I:71:LEU:O	9:I:75:ARG:HG2	2.21	0.41
13:M:80:LYS:NZ	34:1:1687:A:OP1	2.45	0.40
7:G:193:LYS:NZ	34:1:329:C:OP2	2.44	0.40
2:B:24:MET:SD	2:B:172:LYS:HB3	2.61	0.40
8:H:135:GLU:OE2	8:H:139:GLN:NE2	2.45	0.40
8:H:6:PRO:HB3	8:H:34:TYR:CE2	2.56	0.40
34:1:1836:G:H5''	34:1:1837:A:H5'	2.03	0.40
20:T:41:SER:HB3	20:T:80:LEU:HD23	2.02	0.40
24:X:46:TRP:HZ2	24:X:163:ALA:HA	1.86	0.40
34:1:1291:U:H5	40:1:2303:PAR:H43	1.87	0.40
34:1:910:A:O2'	34:1:911:A:H5'	2.22	0.40
9:I:72:MET:HB2	34:1:991:G:N2	2.37	0.40
3:C:207:ILE:HD11	22:V:46:LEU:HD13	2.03	0.40
7:G:7:TYR:HD1	7:G:116:ILE:HB	1.86	0.40
9:I:145:CYS:SG	9:I:151:LYS:HG2	2.61	0.40
14:N:115[B]:ARG:NH1	14:N:121:ALA:O	2.55	0.40
34:1:2164:U:H4'	34:1:2185:MA6:H2	2.03	0.40
34:1:761:A:C2	34:1:773:A:H2	2.37	0.40
37:4:19:G:OP2	37:4:57:G:N1	2.53	0.40
2:B:208[A]:ARG:HH21	22:V:82:MET:HG3	1.86	0.40
6:F:200:LEU:HD13	6:F:208:VAL:HG11	2.03	0.40
12:L:48:ASP:HA	12:L:51:ARG:HG2	2.03	0.40
13:M:26:ALA:HB2	13:M:82:TYR:CZ	2.57	0.40
1:A:44:ALA:CB	15:O:40:THR:HG21	2.48	0.40
17:Q:66:ASP:HB3	17:Q:92:GLU:HA	2.03	0.40
18:R:44:LEU:HA	18:R:44:LEU:HD13	1.95	0.40
1:A:211:GLU:OE2	1:A:213:ARG:NH2	2.54	0.40
5:E:158:VAL:HB	5:E:168:ASP:HB3	2.04	0.40
5:E:178:VAL:HA	5:E:224:VAL:HA	2.03	0.40
5:E:28:PRO:HG2	5:E:35:LEU:HG	2.04	0.40
18:R:27:VAL:HG21	18:R:51:ILE:HG21	2.04	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	
1	A	226/264 (86%)	209 (92%)	17 (8%)	0	100	100
2	B	211/246 (86%)	200 (95%)	11 (5%)	0	100	100
3	C	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	32	60
4	D	181/190 (95%)	176 (97%)	5 (3%)	0	100	100
5	E	260/273 (95%)	246 (95%)	14 (5%)	0	100	100
6	F	218/265 (82%)	206 (94%)	12 (6%)	0	100	100
7	G	237/249 (95%)	222 (94%)	15 (6%)	0	100	100
8	H	181/190 (95%)	173 (96%)	8 (4%)	0	100	100
9	I	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
10	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
11	K	179/220 (81%)	170 (95%)	9 (5%)	0	100	100
12	L	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
13	M	101/116 (87%)	94 (93%)	7 (7%)	0	100	100
14	N	90/153 (59%)	85 (94%)	5 (6%)	0	100	100
15	O	137/144 (95%)	128 (93%)	9 (7%)	0	100	100
16	P	143/143 (100%)	134 (94%)	8 (6%)	1 (1%)	25	53
17	Q	113/141 (80%)	107 (95%)	6 (5%)	0	100	100
18	R	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	S	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
20	T	140/151 (93%)	132 (94%)	8 (6%)	0	100	100
21	U	154/173 (89%)	141 (92%)	13 (8%)	0	100	100
22	V	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
23	W	106/152 (70%)	100 (94%)	6 (6%)	0	100	100
24	X	151/179 (84%)	141 (93%)	10 (7%)	0	100	100
25	Y	86/159 (54%)	85 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
27	a	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
28	b	101/112 (90%)	96 (95%)	5 (5%)	0	100	100
29	c	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
30	d	63/87 (72%)	61 (97%)	2 (3%)	0	100	100
31	e	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
32	f	56/152 (37%)	40 (71%)	14 (25%)	2 (4%)	4	9
33	g	295/312 (95%)	264 (90%)	30 (10%)	1 (0%)	44	73
All	All	4756/5531 (86%)	4466 (94%)	285 (6%)	5 (0%)	58	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	87	ASN
32	f	123	PRO
32	f	122	HIS
3	C	190	PRO
33	g	274	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	
1	A	197/223 (88%)	191 (97%)	6 (3%)	46	76
2	B	180/202 (89%)	176 (98%)	4 (2%)	57	84
3	C	176/184 (96%)	172 (98%)	4 (2%)	56	84
4	D	158/164 (96%)	156 (99%)	2 (1%)	73	91
5	E	207/225 (92%)	203 (98%)	4 (2%)	62	87
6	F	170/208 (82%)	168 (99%)	2 (1%)	75	92
7	G	171/208 (82%)	166 (97%)	5 (3%)	48	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	149/159 (94%)	146 (98%)	3 (2%)	60	86
9	I	173/187 (92%)	170 (98%)	3 (2%)	66	88
10	J	108/111 (97%)	108 (100%)	0	100	100
11	K	130/176 (74%)	130 (100%)	0	100	100
12	L	113/120 (94%)	112 (99%)	1 (1%)	82	94
13	M	93/104 (89%)	93 (100%)	0	100	100
14	N	72/129 (56%)	70 (97%)	2 (3%)	49	79
15	O	103/113 (91%)	98 (95%)	5 (5%)	29	58
16	P	117/116 (101%)	113 (97%)	4 (3%)	42	73
17	Q	60/119 (50%)	60 (100%)	0	100	100
18	R	106/130 (82%)	105 (99%)	1 (1%)	82	94
19	S	47/49 (96%)	45 (96%)	2 (4%)	33	64
20	T	124/132 (94%)	123 (99%)	1 (1%)	85	95
21	U	128/150 (85%)	127 (99%)	1 (1%)	85	95
22	V	91/124 (73%)	88 (97%)	3 (3%)	43	73
23	W	78/131 (60%)	78 (100%)	0	100	100
24	X	122/147 (83%)	120 (98%)	2 (2%)	68	89
25	Y	72/117 (62%)	68 (94%)	4 (6%)	25	51
26	Z	109/118 (92%)	109 (100%)	0	100	100
27	a	58/95 (61%)	58 (100%)	0	100	100
28	b	81/93 (87%)	78 (96%)	3 (4%)	39	70
29	c	72/76 (95%)	70 (97%)	2 (3%)	49	79
30	d	46/75 (61%)	45 (98%)	1 (2%)	57	84
31	e	43/54 (80%)	42 (98%)	1 (2%)	56	84
32	f	26/126 (21%)	24 (92%)	2 (8%)	15	34
33	g	232/266 (87%)	229 (99%)	3 (1%)	73	91
All	All	3812/4631 (82%)	3741 (98%)	71 (2%)	72	87

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	85	LYS

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Mol	Chain	Res	Type
1	A	137[A]	MET
1	A	137[B]	MET
1	A	177[A]	ARG
1	A	177[B]	ARG
2	B	199[A]	GLU
2	B	199[B]	GLU
2	B	208[A]	ARG
2	B	208[B]	ARG
3	C	75	ARG
3	C	77	ASN
3	C	158[A]	LYS
3	C	158[B]	LYS
4	D	77	ARG
4	D	181	ARG
5	E	75[A]	ARG
5	E	75[B]	ARG
5	E	95	ARG
5	E	244	MET
6	F	138	ARG
6	F	149	VAL
7	G	2[A]	LYS
7	G	2[B]	LYS
7	G	32	ARG
7	G	101	ARG
7	G	163	ARG
8	H	41[A]	ARG
8	H	41[B]	ARG
8	H	151	ASN
9	I	50	ARG
9	I	61	VAL
9	I	133	ILE
12	L	133	LYS
14	N	115[A]	ARG
14	N	115[B]	ARG
15	O	59[A]	ARG
15	O	59[B]	ARG
15	O	135	ARG
15	O	136[A]	LYS
15	O	136[B]	LYS
16	P	19[A]	ARG
16	P	19[B]	ARG
16	P	71[A]	ARG

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Mol	Chain	Res	Type
16	P	71[B]	ARG
18	R	32	ARG
19	S	27	ASN
19	S	43	CYS
20	T	69	ARG
21	U	39	LYS
22	V	119[A]	ARG
22	V	119[B]	ARG
22	V	122	ARG
24	X	39[A]	LYS
24	X	39[B]	LYS
25	Y	8	ASN
25	Y	26	ASN
25	Y	78	ILE
25	Y	89	LYS
28	b	28	CYS
28	b	88	VAL
28	b	95	ASN
29	c	41	CYS
29	c	58	LYS
30	d	36	ARG
31	e	58	ASN
32	f	100	TYR
32	f	101	PHE
33	g	44	ASN
33	g	299[A]	LYS
33	g	299[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
2	B	33	GLN
2	B	96	HIS
2	B	102	HIS
3	C	77	ASN
4	D	65	HIS
4	D	122	HIS
4	D	132	HIS
4	D	138	GLN
5	E	5	HIS
5	E	72	HIS

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Mol	Chain	Res	Type
5	E	185	ASN
5	E	203	ASN
7	G	4	ASN
7	G	99	ASN
7	G	113	ASN
7	G	219	ASN
8	H	151	ASN
9	I	34	HIS
9	I	89	HIS
9	I	113	GLN
9	I	196	GLN
10	J	64	ASN
11	K	64	ASN
11	K	194	GLN
12	L	11	GLN
12	L	32	GLN
12	L	43	GLN
14	N	82	GLN
15	O	31	ASN
16	P	20	ASN
16	P	63	ASN
19	S	27	ASN
19	S	47	ASN
20	T	134	GLN
21	U	24	GLN
21	U	107	HIS
23	W	108	GLN
23	W	110	ASN
24	X	80	GLN
25	Y	8	ASN
25	Y	23	HIS
25	Y	26	ASN
25	Y	71	HIS
26	Z	61	GLN
28	b	84	HIS
28	b	95	ASN
29	c	27	GLN
29	c	50	HIS
30	d	41	GLN
31	e	17	GLN
31	e	58	ASN
31	e	60	GLN

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Mol	Chain	Res	Type
33	g	10	HIS
33	g	44	ASN
33	g	59	HIS
33	g	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	1725/2203 (78%)	551 (31%)	35 (2%)
35	2	74/76 (97%)	29 (39%)	2 (2%)
36	3	76/77 (98%)	20 (26%)	0
37	4	75/76 (98%)	34 (45%)	2 (2%)
38	5	11/13 (84%)	2 (18%)	0
All	All	1961/2445 (80%)	636 (32%)	39 (1%)

All (636) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	2	A
34	1	3	U
34	1	14	C
34	1	17	C
34	1	22	A
34	1	25	C
34	1	34	G
34	1	36	U
34	1	39	A
34	1	42	G
34	1	44	C
34	1	46	U
34	1	47	A
34	1	55	A
34	1	58	C
34	1	59	C
34	1	63	G
34	1	68	A
34	1	71	G
34	1	95	C
34	1	96	U
34	1	98	A2M
34	1	101	A

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Mol	Chain	Res	Type
34	1	102	C
34	1	103	A
34	1	105	C
34	1	112	A
34	1	114	U
34	1	115	OMC
34	1	117	G
34	1	122	A
34	1	124	A
34	1	125	A
34	1	126	A
34	1	128	C
34	1	129	U
34	1	134	G
34	1	144	A
34	1	145	A
34	1	146	U
34	1	152	A
34	1	161	A
34	1	171	C
34	1	174	A
34	1	176	A
34	1	181	A
34	1	185	A
34	1	192	U
34	1	197	U
34	1	230	G
34	1	238	G
34	1	239	C
34	1	249	A
34	1	250	C
34	1	256	A
34	1	262	U
34	1	264	C
34	1	266	U
34	1	274	C
34	1	275	A
34	1	276	G
34	1	277	U
34	1	278	A
34	1	281	A
34	1	282	C

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Mol	Chain	Res	Type
34	1	284	C
34	1	287	C
34	1	288	A
34	1	297	U
34	1	298	C
34	1	304	A
34	1	307	C
34	1	308	C
34	1	309	G
34	1	310	U
34	1	315	A
34	1	316	A
34	1	317	G
34	1	332	C
34	1	335	C
34	1	336	U
34	1	337	U
34	1	339	U
34	1	340	G
34	1	343	G
34	1	348	A
34	1	352	C
34	1	353	C
34	1	356	A
34	1	358	C
34	1	360	G
34	1	371	C
34	1	372	C
34	1	373	G
34	1	377	A
34	1	381	G
34	1	382	A
34	1	396	G
34	1	397	A
34	1	403	G
34	1	404	C
34	1	423	U
34	1	431	G
34	1	432	G
34	1	439	G
34	1	442	A
34	1	443	A

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Mol	Chain	Res	Type
34	1	444	A
34	1	445	U
34	1	447	G
34	1	459	A
34	1	460	C
34	1	462	G
34	1	465	G
34	1	466	G
34	1	467	C
34	1	469	G
34	1	472	G
34	1	473	G
34	1	477	G
34	1	481	A
34	1	482	U
34	1	483	U
34	1	487	C
34	1	488	A
34	1	491	G
34	1	494	A
34	1	495	A
34	1	501	A
34	1	502	A
34	1	503	C
34	1	507	G
34	1	508	A
34	1	516	A
34	1	520	G
34	1	521	A
34	1	523	A
34	1	525	A
34	1	554	U
34	1	557	A
34	1	558	U
34	1	559	G
34	1	562	G
34	1	563	G
34	1	565	U
34	1	566	A
34	1	568	U
34	1	570	A
34	1	572	A

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Mol	Chain	Res	Type
34	1	574	C
34	1	576	A
34	1	578	C
34	1	579	C
34	1	580	A
34	1	588	G
34	1	591	A
34	1	592	C
34	1	593	A
34	1	594	A
34	1	600	G
34	1	602	A
34	1	603	C
34	1	604	A
34	1	606	G
34	1	607	U
34	1	608	C
34	1	614	C
34	1	617	G
34	1	624	C
34	1	626	G
34	1	627	U
34	1	628	A
34	1	629	A
34	1	631	U
34	1	643	A
34	1	657	C
34	1	658	U
34	1	659	G
34	1	660	U
34	1	662	G
34	1	663	C
34	1	668	A2M
34	1	669	A
34	1	670	A
34	1	671	G
34	1	672	G
34	1	685	A
34	1	686	C
34	1	688	G
34	1	690	G
34	1	694	U

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Mol	Chain	Res	Type
34	1	721	U
34	1	722	C
34	1	723	C
34	1	724	A
34	1	728	C
34	1	729	G
34	1	731	A
34	1	740	C
34	1	741	C
34	1	742	C
34	1	751	G
34	1	756	C
34	1	757	C
34	1	758	G
34	1	759	U
34	1	762	A
34	1	771	G
34	1	776	A
34	1	785	G
34	1	787	G
34	1	788	A
34	1	789	G
34	1	790	U
34	1	791	G
34	1	792	G
34	1	834	U
34	1	842	U
34	1	844	U
34	1	845	U
34	1	855	U
34	1	856	A
34	1	862	G
34	1	863	C
34	1	866	G
34	1	867	A
34	1	872	A
34	1	875	A
34	1	876	G
34	1	883	G
34	1	884	A
34	1	890	A
34	1	893	A

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Mol	Chain	Res	Type
34	1	894	G
34	1	895	A
34	1	903	G
34	1	905	A
34	1	906	U
34	1	907	A
34	1	908	A
34	1	911	A
34	1	912	A2M
34	1	913	G
34	1	914	G
34	1	916	G
34	1	918	A
34	1	950	U
34	1	952	U
34	1	954	A
34	1	955	A
34	1	972	A
34	1	981	U
34	1	982	G
34	1	987	A
34	1	990	U
34	1	991	G
34	1	992	C
34	1	994	U
34	1	997	C
34	1	1102	G
34	1	1103	G
34	1	1105	A
34	1	1109	A
34	1	1118	G
34	1	1123	G
34	1	1129	A
34	1	1133	U
34	1	1139	G
34	1	1142	G
34	1	1145	A
34	1	1146	G
34	1	1147	A
34	1	1152	A
34	1	1153	A
34	1	1160	A

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Mol	Chain	Res	Type
34	1	1161	G
34	1	1162	A
34	1	1180	A
34	1	1182	A
34	1	1189	G
34	1	1191	A
34	1	1192	U
34	1	1199	A
34	1	1207	U
34	1	1213	A
34	1	1217	A
34	1	1218	A
34	1	1234	G
34	1	1235	A
34	1	1237	C
34	1	1239	A
34	1	1244	G
34	1	1248	A
34	1	1250	A
34	1	1251	G
34	1	1252	A
34	1	1263	C
34	1	1271	C
34	1	1272	A
34	1	1275	C
34	1	1276	G
34	1	1277	A
34	1	1278	U
34	1	1279	G
34	1	1290	A
34	1	1359	C
34	1	1360	U
34	1	1361	U
34	1	1362	A
34	1	1363	C
34	1	1364	G
34	1	1365	U
34	1	1368	C
34	1	1369	U
34	1	1371	U
34	1	1409	U
34	1	1410	C

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Mol	Chain	Res	Type
34	1	1411	A
34	1	1413	C
34	1	1419	U
34	1	1421	C
34	1	1425	U
34	1	1432	C
34	1	1443	U
34	1	1444	G
34	1	1449	U
34	1	1452	A
34	1	1461	G
34	1	1463	G
34	1	1465	A
34	1	1466	G
34	1	1477	A
34	1	1478	OMG
34	1	1484	A
34	1	1489	A
34	1	1490	A
34	1	1493	A
34	1	1498	G
34	1	1502	G
34	1	1503	A
34	1	1507	G
34	1	1510	C
34	1	1511	C
34	1	1515	A
34	1	1520	U
34	1	1523	A
34	1	1535	A
34	1	1537	U
34	1	1544	5MC
34	1	1546	A
34	1	1548	A
34	1	1549	C
34	1	1550	OMG
34	1	1551	G
34	1	1552	G
34	1	1554	A
34	1	1559	U
34	1	1560	A
34	1	1566	U

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Mol	Chain	Res	Type
34	1	1569	G
34	1	1570	G
34	1	1576	A
34	1	1579	A
34	1	1580	G
34	1	1581	G
34	1	1582	A
34	1	1588	A
34	1	1589	G
34	1	1592	U
34	1	1593	G
34	1	1595	G
34	1	1596	U
34	1	1597	G
34	1	1598	U
34	1	1601	U
34	1	1603	U
34	1	1607	G
34	1	1608	A
34	1	1616	A
34	1	1617	A
34	1	1619	G
34	1	1622	G
34	1	1636	U
34	1	1637	U
34	1	1639	G
34	1	1641	U
34	1	1643	G
34	1	1653	U
34	1	1657	U
34	1	1658	U
34	1	1659	U
34	1	1664	G
34	1	1666	U
34	1	1667	U
34	1	1673	A
34	1	1677	G
34	1	1699	A
34	1	1700	G
34	1	1702	A
34	1	1703	U
34	1	1706	A

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Mol	Chain	Res	Type
34	1	1712	G
34	1	1713	C
34	1	1714	C
34	1	1715	C
34	1	1716	A
34	1	1717	U
34	1	1718	A
34	1	1723	A
34	1	1762	A
34	1	1769	C
34	1	1770	G
34	1	1772	A
34	1	1773	U
34	1	1776	U
34	1	1777	OMU
34	1	1782	G
34	1	1788	U
34	1	1789	U
34	1	1790	C
34	1	1793	U
34	1	1811	A
34	1	1815	U
34	1	1816	U
34	1	1819	G
34	1	1820	G
34	1	1821	C
34	1	1828	A
34	1	1832	C
34	1	1833	OMU
34	1	1834	G
34	1	1835	U
34	1	1837	A
34	1	1838	U
34	1	1839	G
34	1	1842	C
34	1	1845	C
34	1	1846	A
34	1	1847	A
34	1	1850	U
34	1	1852	C
34	1	1858	G
34	1	1859	A

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Mol	Chain	Res	Type
34	1	1860	C
34	1	1861	A
34	1	1863	G
34	1	1865	OMG
34	1	1866	OMC
34	1	1867	A
34	1	1870	A
34	1	1872	A
34	1	1873	A
34	1	1874	U
34	1	1875	G
34	1	1878	A
34	1	1884	A
34	1	1885	A
34	1	1887	A
34	1	1889	G
34	1	1890	A
34	1	1891	A
34	1	1893	A
34	1	1894	A
34	1	1895	C
34	1	1897	A
34	1	1906	G
34	1	1907	A
34	1	1908	A
34	1	1909	C
34	1	1912	A
34	1	1917	A
34	1	1918	U
34	1	1919	C
34	1	1920	A
34	1	1923	A
34	1	1926	G
34	1	1933	A
34	1	1934	A
34	1	1935	C
34	1	1937	C
34	1	1938	C
34	1	1940	G
34	1	1941	A
34	1	1943	U
34	1	1946	C

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Mol	Chain	Res	Type
34	1	1947	A
34	1	1948	U
34	1	1949	A
34	1	1950	G
34	1	1952	C
34	1	1955	A
34	1	1956	C
34	1	1957	U
34	1	1965	G
34	1	1976	U
34	1	1978	A
34	1	1981	G
34	1	1986	C
34	1	1987	G
34	1	1988	C
34	1	1989	A
34	1	1990	A
34	1	1993	A
34	1	1994	G
34	1	2000	U
34	1	2003	C
34	1	2004	G
34	1	2010	G
34	1	2016	C
34	1	2017	A
34	1	2020	A
34	1	2021	A2M
34	1	2027	G
34	1	2039	C
34	1	2051	A
34	1	2052	C
34	1	2053	A
34	1	2054	C
34	1	2055	A
34	1	2058	G
34	1	2069	U
34	1	2076	U
34	1	2085	A
34	1	2086	A
34	1	2087	U
34	1	2123	A
34	1	2124	A

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Mol	Chain	Res	Type
34	1	2127	U
34	1	2135	U
34	1	2140	OMC
34	1	2158	A
34	1	2159	A
34	1	2160	G
34	1	2163	G
34	1	2164	U
34	1	2165	A
34	1	2169	A
34	1	2170	G
34	1	2172	U
34	1	2173	A
34	1	2182	U
34	1	2183	G
34	1	2186	C
34	1	2195	G
34	1	2196	G
34	1	2197	A
34	1	2198	U
34	1	2199	C
34	1	2200	A
34	1	2202	U
34	1	2203	U
35	2	2	C
35	2	3	G
35	2	5	G
35	2	8	U
35	2	9	A
35	2	14	A
35	2	16	U
35	2	17	C
35	2	19	G
35	2	21	A
35	2	23	A
35	2	34	G
35	2	35	A
35	2	36	A
35	2	45	U
35	2	47	U
35	2	49	C
35	2	51	U

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Mol	Chain	Res	Type
35	2	52	G
35	2	54	U
35	2	56	C
35	2	57	G
35	2	59	U
35	2	61	C
35	2	65	G
35	2	71	G
35	2	72	C
35	2	74	C
35	2	75	C
36	3	6	G
36	3	8	U
36	3	9	G
36	3	10	G
36	3	14	A
36	3	16	C
36	3	18	U
36	3	19	G
36	3	20	G
36	3	21	A
36	3	22	G
36	3	29	G
36	3	42	G
36	3	47	U
36	3	48	C
36	3	58	A
36	3	61	C
36	3	63	G
36	3	69	C
36	3	70	G
37	4	2	C
37	4	5	G
37	4	7	A
37	4	8	U
37	4	9	A
37	4	10	G
37	4	14	A
37	4	15	G
37	4	17	C
37	4	18	G
37	4	19	G

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Mol	Chain	Res	Type
37	4	21	A
37	4	23	A
37	4	27	G
37	4	28	G
37	4	34	G
37	4	35	A
37	4	36	A
37	4	43	C
37	4	44	G
37	4	45	U
37	4	49	C
37	4	51	U
37	4	52	G
37	4	54	U
37	4	55	U
37	4	56	C
37	4	57	G
37	4	58	A
37	4	61	C
37	4	69	G
37	4	70	C
37	4	74	C
37	4	76	A
38	5	5	A
38	5	8	U

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	1	1	G
34	1	238	G
34	1	276	G
34	1	306	U
34	1	381	G
34	1	396	G
34	1	403	G
34	1	494	A
34	1	576	A
34	1	591	A
34	1	602	A
34	1	603	C
34	1	671	G

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Mol	Chain	Res	Type
34	1	757	C
34	1	789	G
34	1	905	A
34	1	913	G
34	1	915	A
34	1	1108	A
34	1	1145	A
34	1	1161	G
34	1	1250	A
34	1	1275	C
34	1	1276	G
34	1	1489	A
34	1	1550	OMG
34	1	1551	G
34	1	1559	U
34	1	1636	U
34	1	1787	A
34	1	1858	G
34	1	1926	G
34	1	2053	A
34	1	2164	U
34	1	2202	U
35	2	13	C
35	2	34	G
37	4	13	C
37	4	34	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	OMC	1	115	34	15,22,23	1.24	2 (13%)	19,31,34	1.27	2 (10%)
34	OMG	1	1464	34	18,26,27	1.66	3 (16%)	22,38,41	2.24	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	OMG	1	1478	34	18,26,27	1.66	4 (22%)	22,38,41	2.18	4 (18%)
34	M1Y	1	1539	34	16,22,23	2.33	5 (31%)	21,32,35	2.59	5 (23%)
34	C4J	1	1543	34	16,29,30	1.82	4 (25%)	20,42,45	0.86	0
34	5MC	1	1544	34	15,22,23	1.40	3 (20%)	17,32,35	0.93	2 (11%)
34	OMG	1	1550	34	18,26,27	1.19	3 (16%)	22,38,41	2.22	6 (27%)
34	OMU	1	1621	34	14,22,23	1.18	1 (7%)	18,31,34	3.03	3 (16%)
34	OMG	1	1623	34	18,26,27	1.76	4 (22%)	22,38,41	2.07	3 (13%)
34	OMG	1	1647	34	18,26,27	1.76	4 (22%)	22,38,41	2.13	4 (18%)
34	OMU	1	1777	34	14,22,23	1.26	2 (14%)	18,31,34	2.98	3 (16%)
34	OMC	1	18	34	15,22,23	1.08	2 (13%)	19,31,34	1.30	2 (10%)
34	OMG	1	1829	34	18,26,27	1.81	5 (27%)	22,38,41	2.10	3 (13%)
34	OMU	1	1833	34	14,22,23	0.89	1 (7%)	18,31,34	3.02	3 (16%)
34	OMG	1	1865	34	18,26,27	1.76	4 (22%)	22,38,41	2.14	4 (18%)
34	OMC	1	1866	34	15,22,23	1.35	2 (13%)	19,31,34	1.41	2 (10%)
34	OMU	1	1979	34	14,22,23	0.97	1 (7%)	18,31,34	2.81	2 (11%)
34	7MG	1	1995	36,34	20,26,27	1.52	3 (15%)	22,39,42	1.81	3 (13%)
34	A2M	1	2021	34	18,25,26	2.49	2 (11%)	20,36,39	1.37	5 (25%)
34	OMU	1	2048	34	14,22,23	1.04	2 (14%)	18,31,34	2.93	3 (16%)
34	4OC	1	2059	34	16,23,24	0.68	0	19,32,35	0.89	1 (5%)
34	5MC	1	2061	34	15,22,23	1.43	3 (20%)	17,32,35	1.12	2 (11%)
34	OMC	1	2140	34	15,22,23	0.76	0	19,31,34	1.26	2 (10%)
34	OMG	1	2151	34	18,26,27	1.69	2 (11%)	22,38,41	2.15	4 (18%)
34	MA6	1	2184	34	16,26,27	1.14	2 (12%)	18,38,41	3.53	4 (22%)
34	MA6	1	2185	34	16,26,27	1.13	1 (6%)	18,38,41	4.09	5 (27%)
34	A2M	1	28	34	18,25,26	2.45	3 (16%)	20,36,39	1.15	2 (10%)
34	OMU	1	33	34	14,22,23	1.29	2 (14%)	18,31,34	2.88	3 (16%)
34	OMC	1	38	34	15,22,23	1.00	1 (6%)	19,31,34	1.29	2 (10%)
34	A2M	1	479	34	18,25,26	2.43	3 (16%)	20,36,39	1.15	2 (10%)
34	OMG	1	509	34	18,26,27	1.24	2 (11%)	22,38,41	2.17	6 (27%)
34	OMU	1	661	34	14,22,23	1.08	1 (7%)	18,31,34	2.80	3 (16%)
34	A2M	1	668	34	18,25,26	2.89	4 (22%)	20,36,39	1.11	2 (10%)
34	OMU	1	8	34	14,22,23	1.06	0	18,31,34	2.77	3 (16%)
34	A2M	1	912	34	18,25,26	0.97	1 (5%)	20,36,39	1.71	2 (10%)
34	A2M	1	98	34	18,25,26	2.42	2 (11%)	20,36,39	1.23	3 (15%)
35	MIA	2	37	35	23,31,32	1.17	3 (13%)	25,44,47	1.32	3 (12%)

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
34	OMC	1	115	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1464	34	-	0/5/27/28	0/3/3/3
34	OMG	1	1478	34	-	0/5/27/28	0/3/3/3
34	MIY	1	1539	34	-	0/7/25/26	0/2/2/2
34	C4J	1	1543	34	-	0/12/34/35	0/2/2/2
34	5MC	1	1544	34	-	0/3/25/26	0/2/2/2
34	OMG	1	1550	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1621	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1623	34	-	0/5/27/28	0/3/3/3
34	OMG	1	1647	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1777	34	-	0/5/27/28	0/2/2/2
34	OMC	1	18	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1829	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1833	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1865	34	-	0/5/27/28	0/3/3/3
34	OMC	1	1866	34	-	0/5/27/28	0/2/2/2
34	OMU	1	1979	34	-	0/5/27/28	0/2/2/2
34	7MG	1	1995	36,34	-	0/7/37/38	0/3/3/3
34	A2M	1	2021	34	-	0/5/27/28	0/3/3/3
34	OMU	1	2048	34	-	0/5/27/28	0/2/2/2
34	4OC	1	2059	34	-	0/7/29/30	0/2/2/2
34	5MC	1	2061	34	-	0/3/25/26	0/2/2/2
34	OMC	1	2140	34	-	0/5/27/28	0/2/2/2
34	OMG	1	2151	34	-	0/5/27/28	0/3/3/3
34	MA6	1	2184	34	-	0/7/29/30	0/3/3/3
34	MA6	1	2185	34	-	0/7/29/30	0/3/3/3
34	A2M	1	28	34	-	0/5/27/28	0/3/3/3
34	OMU	1	33	34	-	0/5/27/28	0/2/2/2
34	OMC	1	38	34	-	0/5/27/28	0/2/2/2
34	A2M	1	479	34	-	0/5/27/28	0/3/3/3
34	OMG	1	509	34	-	0/5/27/28	0/3/3/3
34	OMU	1	661	34	-	0/5/27/28	0/2/2/2
34	A2M	1	668	34	-	0/5/27/28	0/3/3/3
34	OMU	1	8	34	-	0/5/27/28	0/2/2/2
34	A2M	1	912	34	-	0/5/27/28	0/3/3/3
34	A2M	1	98	34	-	0/5/27/28	0/3/3/3
35	MIA	2	37	35	-	0/11/33/34	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	668	A2M	O5'-C5'	-10.58	1.30	1.44
34	1	2021	A2M	O5'-C5'	-9.40	1.31	1.44
34	1	98	A2M	O5'-C5'	-9.32	1.31	1.44
34	1	28	A2M	O5'-C5'	-9.22	1.31	1.44
34	1	479	A2M	O5'-C5'	-8.81	1.32	1.44
34	1	1543	C4J	C4-N3	-4.81	1.31	1.38
34	1	1539	M1Y	C5-C1'	-4.70	1.48	1.52
34	1	668	A2M	O4'-C4'	-3.92	1.36	1.45
34	1	115	OMC	C4-N3	-3.88	1.28	1.35
34	1	1866	OMC	C4-N3	-3.50	1.29	1.35
34	1	479	A2M	O4'-C4'	-3.47	1.37	1.45
34	1	1543	C4J	O4'-C1'	-3.39	1.39	1.44
34	1	2185	MA6	C5-C4	-3.38	1.32	1.40
34	1	2184	MA6	C5-C4	-3.08	1.33	1.40
34	1	1539	M1Y	O4'-C1'	-3.07	1.39	1.44
35	2	37	MIA	O5'-C5'	-2.86	1.40	1.44
34	1	1865	OMG	O5'-C5'	-2.74	1.40	1.44
34	1	1544	5MC	CM5-C5	-2.73	1.45	1.51
34	1	1866	OMC	O5'-C5'	-2.70	1.41	1.44
34	1	38	OMC	C4-N3	-2.69	1.30	1.35
34	1	28	A2M	O3'-C3'	-2.67	1.36	1.43
34	1	18	OMC	C4-N3	-2.66	1.30	1.35
34	1	2061	5MC	C4-N3	-2.63	1.31	1.35
34	1	1544	5MC	C4-N3	-2.61	1.31	1.35
34	1	1539	M1Y	C2'-C1'	-2.59	1.51	1.53
34	1	2061	5MC	CM5-C5	-2.53	1.46	1.51
34	1	1647	OMG	O5'-C5'	-2.50	1.41	1.44
34	1	98	A2M	O4'-C4'	-2.44	1.39	1.45
34	1	668	A2M	O4'-C1'	-2.37	1.38	1.41
34	1	1543	C4J	O4-C4	-2.34	1.18	1.24
34	1	2021	A2M	O2'-C2'	-2.32	1.36	1.42
34	1	1829	OMG	O5'-C5'	-2.32	1.41	1.44
34	1	1543	C4J	O5'-C5'	-2.31	1.41	1.44
34	1	2061	5MC	O5'-C5'	-2.30	1.41	1.44
34	1	115	OMC	O5'-C5'	-2.28	1.41	1.44
34	1	33	OMU	O5'-C5'	-2.19	1.41	1.44
34	1	2048	OMU	O5'-C5'	-2.16	1.41	1.44
34	1	1550	OMG	O5'-C5'	-2.13	1.41	1.44
34	1	18	OMC	O5'-C5'	-2.13	1.41	1.44
34	1	668	A2M	O3'-C3'	-2.12	1.38	1.43
34	1	1544	5MC	O5'-C5'	-2.07	1.41	1.44
34	1	1777	OMU	O5'-C5'	-2.07	1.41	1.44
34	1	2184	MA6	C5-N7	-2.07	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	1995	7MG	O5'-C5'	-2.06	1.41	1.44
34	1	1478	OMG	O5'-C5'	-2.02	1.41	1.44
34	1	28	A2M	O4'-C4'	-2.01	1.40	1.45
34	1	479	A2M	O3'-C3'	-2.00	1.38	1.43
34	1	1833	OMU	C4-N3	2.03	1.36	1.33
34	1	1647	OMG	C2-N2	2.04	1.38	1.34
34	1	1865	OMG	C2-N2	2.12	1.38	1.34
34	1	1829	OMG	C4-N3	2.13	1.39	1.35
34	1	1464	OMG	C2-N2	2.17	1.38	1.34
34	1	1623	OMG	C2-N2	2.20	1.38	1.34
34	1	1478	OMG	C2-N2	2.21	1.38	1.34
34	1	1995	7MG	C4-N3	2.21	1.37	1.34
34	1	1829	OMG	C2-N2	2.25	1.38	1.34
34	1	1464	OMG	C2-N1	2.26	1.39	1.35
34	1	1647	OMG	C2-N1	2.26	1.39	1.35
34	1	1623	OMG	C4-N3	2.26	1.39	1.35
34	1	2151	OMG	C2-N1	2.33	1.39	1.35
34	1	661	OMU	C4-N3	2.35	1.37	1.33
34	1	2048	OMU	C4-N3	2.37	1.37	1.33
35	2	37	MIA	C2-N1	2.38	1.37	1.34
34	1	1865	OMG	C2-N1	2.41	1.39	1.35
34	1	1478	OMG	C2-N1	2.44	1.39	1.35
34	1	509	OMG	C5-C4	2.45	1.46	1.40
34	1	1550	OMG	C5-C4	2.48	1.46	1.40
34	1	1623	OMG	C2-N1	2.53	1.40	1.35
34	1	1979	OMU	C4-N3	2.59	1.37	1.33
34	1	912	A2M	C5-C4	2.67	1.46	1.40
34	1	1829	OMG	C2-N1	2.76	1.40	1.35
34	1	1550	OMG	C6-C5	3.18	1.47	1.41
34	1	1621	OMU	C4-N3	3.18	1.38	1.33
35	2	37	MIA	C6-N1	3.22	1.37	1.33
34	1	33	OMU	C4-N3	3.39	1.39	1.33
34	1	509	OMG	C6-C5	3.43	1.47	1.41
34	1	1777	OMU	C4-N3	3.53	1.39	1.33
34	1	1539	M1Y	C6-N1	3.79	1.37	1.33
34	1	1995	7MG	C6-N1	4.71	1.41	1.33
34	1	1539	M1Y	C4-N3	5.18	1.42	1.33
34	1	1478	OMG	C6-N1	5.35	1.42	1.33
34	1	1464	OMG	C6-N1	5.40	1.42	1.33
34	1	1865	OMG	C6-N1	5.55	1.43	1.33
34	1	2151	OMG	C6-N1	5.64	1.43	1.33
34	1	1647	OMG	C6-N1	5.69	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	1623	OMG	C6-N1	5.74	1.43	1.33
34	1	1829	OMG	C6-N1	5.76	1.43	1.33

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	2185	MA6	N3-C2-N1	-11.47	118.87	128.86
34	1	2185	MA6	N1-C6-N6	-10.86	105.47	117.00
34	1	2184	MA6	N3-C2-N1	-9.86	120.27	128.86
34	1	2184	MA6	N1-C6-N6	-9.23	107.20	117.00
34	1	1539	M1Y	C5-C4-N3	-8.20	118.71	125.43
34	1	1829	OMG	C5-C6-N1	-7.87	112.28	123.48
34	1	2151	OMG	C5-C6-N1	-7.80	112.37	123.48
34	1	1478	OMG	C5-C6-N1	-7.79	112.39	123.48
34	1	1623	OMG	C5-C6-N1	-7.78	112.41	123.48
34	1	1464	OMG	C5-C6-N1	-7.63	112.62	123.48
34	1	1865	OMG	C5-C6-N1	-7.63	112.62	123.48
34	1	1647	OMG	C5-C6-N1	-7.59	112.67	123.48
34	1	1995	7MG	C5-C6-N1	-6.43	113.28	123.37
34	1	912	A2M	N3-C2-N1	-6.05	123.59	128.86
34	1	1550	OMG	C6-C5-C4	-4.32	116.55	120.84
34	1	1621	OMU	CM2-O2'-C2'	-4.14	103.21	114.54
35	2	37	MIA	C12-N6-C6	-4.04	118.05	123.26
34	1	1539	M1Y	C5-C1'-C2'	-3.91	108.81	115.55
34	1	1478	OMG	C2-N3-C4	-3.87	110.64	115.16
34	1	509	OMG	C5-C6-N1	-3.79	118.08	123.48
34	1	2151	OMG	C2-N3-C4	-3.74	110.79	115.16
34	1	1550	OMG	C5-C6-N1	-3.62	118.33	123.48
34	1	509	OMG	C6-C5-C4	-3.61	117.25	120.84
34	1	1777	OMU	C5-C4-N3	-3.50	114.77	123.12
34	1	1464	OMG	C2-N3-C4	-3.45	111.13	115.16
34	1	1539	M1Y	O4'-C1'-C5	-3.45	104.59	109.93
34	1	1550	OMG	N3-C2-N1	-3.39	122.51	127.46
34	1	1647	OMG	C2-N3-C4	-3.20	111.42	115.16
34	1	509	OMG	C4-C5-N7	-3.18	106.34	109.41
34	1	1621	OMU	C5-C4-N3	-3.12	115.66	123.12
34	1	1623	OMG	C2-N3-C4	-3.11	111.53	115.16
34	1	1833	OMU	C5-C4-N3	-2.98	116.00	123.12
34	1	509	OMG	N3-C2-N1	-2.96	123.14	127.46
34	1	1865	OMG	C2-N3-C4	-2.90	111.77	115.16
34	1	1829	OMG	C2-N3-C4	-2.88	111.80	115.16
34	1	1979	OMU	C5-C4-N3	-2.83	116.37	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	912	A2M	C4-C5-N7	-2.82	106.69	109.41
34	1	2048	OMU	C5-C4-N3	-2.82	116.40	123.12
34	1	33	OMU	C5-C4-N3	-2.72	116.63	123.12
34	1	1478	OMG	CM2-O2'-C2'	-2.69	107.18	114.54
34	1	661	OMU	C5-C4-N3	-2.68	116.71	123.12
34	1	2140	OMC	CM2-O2'-C2'	-2.68	107.21	114.54
34	1	1647	OMG	CM2-O2'-C2'	-2.65	107.28	114.54
34	1	2059	4OC	CM4-N4-C4	-2.62	120.68	122.94
34	1	1550	OMG	C4-C5-N7	-2.61	106.89	109.41
34	1	8	OMU	C5-C4-N3	-2.59	116.95	123.12
34	1	38	OMC	CM2-O2'-C2'	-2.56	107.53	114.54
34	1	115	OMC	CM2-O2'-C2'	-2.54	107.59	114.54
34	1	1777	OMU	CM2-O2'-C2'	-2.48	107.77	114.54
34	1	1865	OMG	CM2-O2'-C2'	-2.42	107.94	114.54
34	1	661	OMU	CM2-O2'-C2'	-2.39	108.01	114.54
34	1	18	OMC	CM2-O2'-C2'	-2.29	108.27	114.54
34	1	33	OMU	CM2-O2'-C2'	-2.29	108.28	114.54
34	1	8	OMU	CM2-O2'-C2'	-2.25	108.39	114.54
34	1	1866	OMC	CM2-O2'-C2'	-2.23	108.45	114.54
34	1	2048	OMU	CM2-O2'-C2'	-2.17	108.59	114.54
34	1	479	A2M	C2-N1-C6	-2.17	114.97	118.77
34	1	1539	M1Y	O2'-C2'-C1'	-2.15	107.34	112.21
34	1	1833	OMU	CM2-O2'-C2'	-2.14	108.68	114.54
34	1	98	A2M	C2-N1-C6	-2.05	115.18	118.77
34	1	2021	A2M	O5'-C5'-C4'	-2.01	101.93	109.01
34	1	2185	MA6	C4-C5-N7	-2.00	107.47	109.41
34	1	28	A2M	C4-C5-N7	2.00	111.34	109.41
34	1	1464	OMG	C4-C5-N7	2.00	111.34	109.41
34	1	2021	A2M	O4'-C4'-C3'	2.03	109.20	105.17
34	1	2061	5MC	CM5-C5-C6	2.03	122.72	118.67
34	1	2151	OMG	C4-C5-N7	2.03	111.38	109.41
34	1	1544	5MC	CM5-C5-C6	2.04	122.73	118.67
34	1	668	A2M	N3-C2-N1	2.06	130.65	128.86
34	1	2021	A2M	C4-C5-N7	2.13	111.47	109.41
34	1	2021	A2M	C4'-O4'-C1'	2.13	112.04	109.77
34	1	98	A2M	C4-C5-N7	2.16	111.50	109.41
34	1	98	A2M	N3-C2-N1	2.22	130.79	128.86
34	1	28	A2M	N3-C2-N1	2.22	130.79	128.86
34	1	668	A2M	C4-C5-N7	2.23	111.56	109.41
34	1	1464	OMG	O2'-C2'-C1'	2.24	113.33	108.75
35	2	37	MIA	N3-C2-N1	2.39	131.14	126.85
34	1	2061	5MC	C5-C4-N3	2.40	125.10	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	37	MIA	C4-C5-N7	2.52	111.85	109.41
34	1	1544	5MC	C5-C4-N3	2.63	125.48	121.22
34	1	2021	A2M	N3-C2-N1	2.74	131.24	128.86
34	1	479	A2M	N3-C2-N1	2.76	131.26	128.86
34	1	1464	OMG	CM2-O2'-C2'	2.91	122.51	114.54
34	1	1995	7MG	C5-C4-N9	3.17	110.93	106.31
34	1	1464	OMG	C6-N1-C2	3.25	120.73	116.06
34	1	2184	MA6	C2-N1-C6	3.36	120.08	111.82
34	1	1865	OMG	C6-N1-C2	3.44	121.00	116.06
34	1	2151	OMG	C6-N1-C2	3.58	121.21	116.06
34	1	1647	OMG	C6-N1-C2	3.63	121.28	116.06
34	1	2185	MA6	C2-N1-C6	3.66	120.80	111.82
34	1	1995	7MG	C6-N1-C2	3.70	121.39	116.06
34	1	1478	OMG	C6-N1-C2	3.71	121.39	116.06
34	1	1623	OMG	C6-N1-C2	3.71	121.40	116.06
34	1	115	OMC	C5-C4-N3	3.79	126.19	121.68
34	1	38	OMC	C5-C4-N3	3.84	126.24	121.68
34	1	1829	OMG	C6-N1-C2	3.93	121.71	116.06
34	1	2140	OMC	C5-C4-N3	3.97	126.40	121.68
34	1	18	OMC	C5-C4-N3	4.07	126.52	121.68
34	1	509	OMG	C6-N1-C2	4.13	122.00	116.06
34	1	1866	OMC	C5-C4-N3	4.27	126.76	121.68
34	1	1550	OMG	C6-N1-C2	4.36	122.33	116.06
34	1	2184	MA6	C5-C6-N6	4.64	132.95	122.58
34	1	1550	OMG	C2-N3-C4	5.03	121.04	115.16
34	1	509	OMG	C2-N3-C4	5.25	121.29	115.16
34	1	1539	M1Y	C4-N3-C2	5.31	119.80	115.16
34	1	2185	MA6	C5-C6-N6	5.39	134.62	122.58
34	1	8	OMU	C4-N3-C2	10.65	123.28	114.13
34	1	1621	OMU	C4-N3-C2	11.04	123.61	114.13
34	1	1979	OMU	C4-N3-C2	11.17	123.73	114.13
34	1	661	OMU	C4-N3-C2	11.19	123.74	114.13
34	1	33	OMU	C4-N3-C2	11.32	123.86	114.13
34	1	2048	OMU	C4-N3-C2	11.63	124.12	114.13
34	1	1833	OMU	C4-N3-C2	11.71	124.19	114.13
34	1	1777	OMU	C4-N3-C2	11.73	124.21	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	1	1464	OMG	2	0
34	1	1621	OMU	2	0
34	1	1777	OMU	1	0
34	1	1979	OMU	2	0
34	1	2021	A2M	1	0
34	1	2184	MA6	1	0
34	1	2185	MA6	2	0
34	1	509	OMG	12	0
34	1	661	OMU	1	0
34	1	912	A2M	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 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
40	PAR	1	2302	-	45,45,45	3.60	9 (20%)	60,67,67	1.44	12 (20%)
40	PAR	1	2303	34	45,45,45	3.51	10 (22%)	60,67,67	1.85	11 (18%)
40	PAR	1	2304	-	45,45,45	3.65	9 (20%)	60,67,67	1.50	9 (15%)
40	PAR	1	2305	-	45,45,45	3.43	8 (17%)	60,67,67	1.54	11 (18%)
40	PAR	1	2306	-	45,45,45	3.52	9 (20%)	60,67,67	1.34	7 (11%)
40	PAR	1	2307	-	45,45,45	3.56	9 (20%)	60,67,67	1.12	2 (3%)

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
40	PAR	1	2302	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2303	34	-	1/18/94/94	0/4/4/4
40	PAR	1	2304	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2305	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2306	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2307	-	-	0/18/94/94	0/4/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2304	PAR	C13-C23	-17.05	1.30	1.52
40	1	2302	PAR	C13-C23	-16.50	1.31	1.52
40	1	2307	PAR	C13-C23	-16.35	1.31	1.52
40	1	2303	PAR	C13-C23	-15.92	1.32	1.52
40	1	2306	PAR	C13-C23	-15.90	1.32	1.52
40	1	2305	PAR	C13-C23	-15.26	1.33	1.52
40	1	2303	PAR	O43-C43	-7.35	1.28	1.45
40	1	2306	PAR	O43-C43	-6.78	1.29	1.45
40	1	2305	PAR	O43-C43	-6.65	1.29	1.45
40	1	2304	PAR	O43-C43	-6.58	1.30	1.45
40	1	2307	PAR	O43-C43	-6.45	1.30	1.45
40	1	2302	PAR	O43-C43	-6.41	1.30	1.45
40	1	2302	PAR	C31-C21	-5.45	1.46	1.53
40	1	2304	PAR	C31-C21	-4.94	1.47	1.53
40	1	2306	PAR	C31-C21	-4.91	1.47	1.53
40	1	2307	PAR	C31-C21	-4.41	1.48	1.53
40	1	2306	PAR	C34-C24	-4.39	1.48	1.53
40	1	2305	PAR	C31-C21	-4.33	1.48	1.53
40	1	2305	PAR	C34-C24	-4.22	1.48	1.53
40	1	2307	PAR	C34-C24	-4.13	1.48	1.53
40	1	2303	PAR	C34-C24	-4.03	1.48	1.53
40	1	2303	PAR	C31-C21	-3.98	1.48	1.53
40	1	2304	PAR	C34-C24	-3.76	1.48	1.53
40	1	2303	PAR	O33-C33	-3.71	1.34	1.43
40	1	2304	PAR	O33-C33	-3.59	1.35	1.43
40	1	2302	PAR	O33-C33	-3.34	1.35	1.43
40	1	2302	PAR	C34-C24	-3.34	1.49	1.53
40	1	2306	PAR	O33-C33	-3.21	1.36	1.43
40	1	2307	PAR	O33-C33	-3.17	1.36	1.43
40	1	2302	PAR	C21-N21	-2.23	1.43	1.47
40	1	2304	PAR	C21-N21	-2.01	1.44	1.47
40	1	2305	PAR	O23-C23	2.01	1.47	1.43
40	1	2306	PAR	O51-C51	2.02	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2303	PAR	O51-C51	2.05	1.49	1.44
40	1	2307	PAR	O51-C51	2.07	1.49	1.44
40	1	2303	PAR	O11-C42	2.29	1.49	1.43
40	1	2302	PAR	O51-C11	2.60	1.48	1.41
40	1	2304	PAR	O51-C11	2.63	1.48	1.41
40	1	2306	PAR	O51-C11	2.91	1.49	1.41
40	1	2303	PAR	O51-C11	2.97	1.49	1.41
40	1	2307	PAR	O51-C11	2.99	1.49	1.41
40	1	2305	PAR	O51-C11	3.01	1.49	1.41
40	1	2305	PAR	O54-C14	3.77	1.51	1.41
40	1	2303	PAR	O54-C14	3.91	1.51	1.41
40	1	2304	PAR	O54-C14	3.97	1.51	1.41
40	1	2306	PAR	O54-C14	4.02	1.51	1.41
40	1	2302	PAR	O54-C14	4.18	1.52	1.41
40	1	2307	PAR	O54-C14	4.25	1.52	1.41
40	1	2303	PAR	O43-C13	11.73	1.62	1.41
40	1	2306	PAR	O43-C13	11.91	1.63	1.41
40	1	2307	PAR	O43-C13	12.26	1.63	1.41
40	1	2305	PAR	O43-C13	12.28	1.63	1.41
40	1	2304	PAR	O43-C13	12.35	1.63	1.41
40	1	2302	PAR	O43-C13	12.49	1.64	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2303	PAR	C14-O33-C33	-6.50	102.17	118.00
40	1	2303	PAR	C31-C41-C51	-4.43	102.41	110.22
40	1	2304	PAR	C14-O33-C33	-3.72	108.93	118.00
40	1	2302	PAR	O11-C11-C21	-3.38	101.78	108.20
40	1	2304	PAR	C13-O52-C52	-3.14	110.34	118.00
40	1	2302	PAR	C31-C21-N21	-2.90	105.10	111.00
40	1	2306	PAR	C14-O33-C33	-2.89	110.96	118.00
40	1	2305	PAR	O52-C13-O43	-2.73	108.48	111.43
40	1	2304	PAR	O34-C34-C24	-2.71	105.69	110.31
40	1	2305	PAR	C64-C54-C44	-2.58	108.56	113.30
40	1	2304	PAR	C61-C51-C41	-2.55	107.03	113.00
40	1	2302	PAR	C14-O33-C33	-2.54	111.81	118.00
40	1	2307	PAR	C13-O52-C52	-2.54	111.82	118.00
40	1	2305	PAR	C13-O52-C52	-2.53	111.83	118.00
40	1	2305	PAR	O33-C14-O54	-2.52	104.57	110.70
40	1	2306	PAR	C62-C12-N12	-2.38	106.25	110.92
40	1	2304	PAR	O31-C31-C21	-2.38	106.26	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2306	PAR	C31-C21-N21	-2.31	106.29	111.00
40	1	2303	PAR	C31-C21-N21	-2.30	106.33	111.00
40	1	2304	PAR	C62-C12-N12	-2.24	106.53	110.92
40	1	2302	PAR	O62-C62-C12	-2.21	105.74	109.82
40	1	2303	PAR	O34-C34-C24	-2.20	106.58	110.31
40	1	2305	PAR	C31-C41-C51	-2.19	106.36	110.22
40	1	2302	PAR	C53-C43-C33	-2.18	107.78	114.89
40	1	2304	PAR	O34-C34-C44	-2.10	105.78	110.36
40	1	2302	PAR	C11-C21-N21	-2.07	106.47	110.20
40	1	2307	PAR	C14-O33-C33	-2.06	112.97	118.00
40	1	2302	PAR	C62-C12-N12	-2.05	106.91	110.92
40	1	2306	PAR	C61-C51-C41	-2.03	108.25	113.00
40	1	2306	PAR	C34-C24-N24	-2.02	106.89	111.00
40	1	2302	PAR	O11-C42-C32	-2.00	104.32	108.96
40	1	2305	PAR	O51-C51-C61	2.08	111.38	106.41
40	1	2306	PAR	C62-C52-C42	2.08	116.46	111.65
40	1	2305	PAR	C14-O33-C33	2.09	123.09	118.00
40	1	2303	PAR	C11-C21-C31	2.13	115.88	109.96
40	1	2302	PAR	C34-C44-C54	2.17	114.04	110.22
40	1	2305	PAR	O33-C14-C24	2.21	112.40	108.20
40	1	2303	PAR	O51-C11-C21	2.28	115.19	110.06
40	1	2302	PAR	C14-C24-C34	2.28	116.31	109.96
40	1	2303	PAR	O33-C14-C24	2.57	113.09	108.20
40	1	2303	PAR	C11-O51-C51	2.59	118.59	113.72
40	1	2305	PAR	O33-C33-C23	2.67	120.26	111.47
40	1	2305	PAR	O54-C54-C44	2.84	114.89	109.66
40	1	2302	PAR	C22-C12-C62	2.85	114.38	110.14
40	1	2302	PAR	O54-C14-C24	2.85	116.48	110.06
40	1	2303	PAR	O41-C41-C51	2.97	116.76	109.28
40	1	2306	PAR	C13-C23-C33	4.06	107.02	102.07
40	1	2304	PAR	C31-C41-C51	4.12	117.48	110.22
40	1	2303	PAR	O11-C42-C52	4.18	118.24	107.50
40	1	2305	PAR	C13-C23-C33	4.35	107.37	102.07
40	1	2304	PAR	O51-C51-C41	4.36	117.69	109.66
40	1	2303	PAR	O52-C13-C23	5.61	119.59	107.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	2303	PAR	C52-O52-C13-C23

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	1	2302	PAR	1	0
40	1	2303	PAR	1	0
40	1	2304	PAR	3	0
40	1	2305	PAR	3	0
40	1	2306	PAR	3	0
40	1	2307	PAR	2	0

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
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	960:C	O3'	961:U	P	10.63