



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

PDB ID : 4CE4
EMDB ID: : EMD-2490
Title : 39S large subunit of the porcine mitochondrial ribosome
Authors : Greber, B.J.; Boehringer, D.; Leitner, A.; Bieri, P.; Voigts-Hoffmann, F.;
Erzberger, J.P.; Leibundgut, M.; Aebersold, R.; Ban, N.
Deposited on : 2013-11-08
Resolution : 4.90 Å(reported)
Based on PDB ID : 3V2D 1R73 2QYQ 1QF6 1O0W 2CW9 2XZN 1J26 1S3A

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

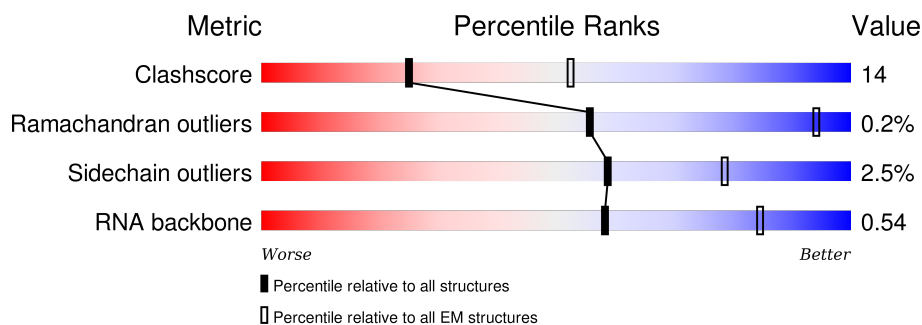
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	0	148	<div> <div>42%</div> <div>9%</div> <div>.</div> <div>49%</div> </div>
2	1	256	<div> <div>17%</div> <div>5%</div> <div>77%</div> </div>
3	2	252	<div> <div>24%</div> <div>6%</div> <div>70%</div> </div>
4	3	161	<div> <div>25%</div> <div>11%</div> <div>63%</div> </div>
5	5	146	<div> <div>25%</div> <div>21%</div> <div>53%</div> </div>
6	6	65	<div> <div>52%</div> <div>22%</div> <div>26%</div> </div>
7	7	95	<div> <div>31%</div> <div>15%</div> <div>55%</div> </div>
8	8	188	<div> <div>20%</div> <div>12%</div> <div>68%</div> </div>


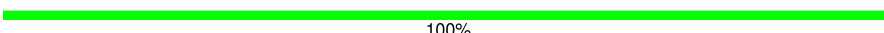

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Mol	Chain	Length	Quality of chain
9	9	100	
10	A	1570	
11	B	29	
12	D	306	
13	E	399	
14	F	224	
15	I	268	
16	N	178	
17	O	145	
18	P	288	
19	Q	208	
20	R	169	
21	S	180	
22	T	292	
23	U	132	
24	V	207	
25	W	134	
26	X	87	
27	Y	216	
28	b	380	
29	c	301	
30	h	298	
31	i	312	
32	l	166	
33	o	56	

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Mol	Chain	Length	Quality of chain
34	u	205	 42% 56%
35	v	91	 100%
35	w	91	 100%
36	x	85	 100%
37	z	426	 100%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 65473 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 MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	76	Total	C	N	O	S	0	0
			607	392	114	99	2		

- Molecule 2 is a protein called MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	58	Total	C	N	O	S	0	0
			489	312	90	85	2		

- Molecule 3 is a protein called MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	76	Total	C	N	O	S	0	0
			633	394	116	119	4		

- Molecule 4 is a protein called MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	59	Total	C	N	O	S	0	0
			491	321	95	74	1		

- Molecule 5 is a protein called MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	68	Total	C	N	O	S	0	0
			508	317	103	83	5		

- Molecule 6 is a protein called MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 7 is a protein called MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			362	224	82	55	1		

- Molecule 8 is a protein called MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	60	Total	C	N	O	S	0	0
			520	338	106	74	2		

- Molecule 9 is a protein called MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	36	Total	C	N	O	S	0	0
			316	200	68	45	3		

- Molecule 10 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1444	Total	C	N	O	P	0	0
			30656	13760	5548	9904	1444		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	INSERTION	GB AJ002189

- Molecule 11 is a RNA chain called UNASSIGNED RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	B	29	Total	C	O	P	0	0
			348	145	174	29		

- Molecule 12 is a protein called MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	200	Total	C	N	O	S	0	0
			1531	944	309	269	9		

- Molecule 13 is a protein called MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	208	Total	C	N	O	S	0	0
			1621	1040	300	274	7		

- Molecule 14 is a protein called MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	224	Total	C	N	O	S	0	0
			1713	1101	310	298	4		

- Molecule 15 is a protein called MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	57	Total	C	N	O	0	0
			447	282	79	86		

- Molecule 16 is a protein called MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	147	Total	C	N	O	S	0	0
			1178	756	210	204	8		

- Molecule 17 is a protein called MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	114	Total	C	N	O	S	0	0
			891	559	175	153	4		

- Molecule 18 is a protein called MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	169	Total	C	N	O	S	0	0
			1309	816	258	233	2		

- Molecule 19 is a protein called MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	154	Total	C	N	O	S	0	0
			1179	758	218	195	8		

- Molecule 20 is a protein called MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	120	Total	C	N	O	S	0	0
			982	619	187	172	4		

- Molecule 21 is a protein called MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	94	Total	C	N	O	S	0	0
			748	467	146	131	4		

- Molecule 22 is a protein called MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	119	Total	C	N	O	S	0	0
			962	615	166	177	4		

- Molecule 23 is a protein called MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	123	Total	C	N	O	S	0	0
			1018	647	212	156	3		

- Molecule 24 is a protein called MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	109	Total	C	N	O	S	0	0
			877	565	156	154	2		

- Molecule 25 is a protein called MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	134	Total	C	N	O	S	0	0
			1058	679	191	182	6		

- Molecule 26 is a protein called MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	87	Total	C	N	O	S	0	0
			689	436	133	118	2		

- Molecule 27 is a protein called MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	103	Total	C	N	O	S	0	0
			835	526	156	151	2		

- Molecule 28 is a protein called MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	192	Total	C	N	O	S	0	0
			1562	1006	266	284	6		

- Molecule 29 is a protein called MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	292	Total	C	N	O	S	0	0
			2310	1489	391	415	15		

- Molecule 30 is a protein called MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	272	Total	C	N	O	S	0	0
			2075	1333	344	391	7		

- Molecule 31 is a protein called MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	161	Total	C	N	O	S	0	0
			1335	845	243	239	8		

- Molecule 32 is a protein called MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	76	Total	C	N	O	S	0	0
			619	398	108	111	2		

- Molecule 33 is a protein called MRPL52.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	o	56	Total	C	N	O	0	0
			336	224	56	56		

- Molecule 34 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	90	Total	C	N	O	S	0	0
			717	444	137	132	4		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	v	91	Total	C	N	O	0	0
			546	364	91	91		
35	w	91	Total	C	N	O	0	0
			546	364	91	91		

- Molecule 36 is a protein called THIOREDOXIN FOLD.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	x	85	Total	C	N	O	0	0
			510	340	85	85		

- Molecule 37 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	z	426	Total	C	N	O	0	0
			2556	1704	426	426		

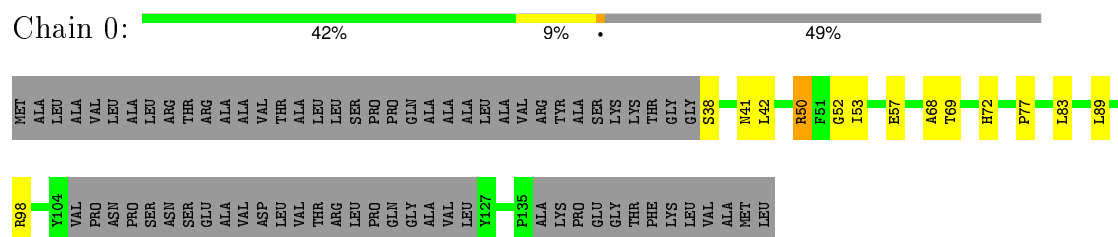
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	9	1	Total	Zn	0
			1	1	
38	5	1	Total	Zn	0
			1	1	

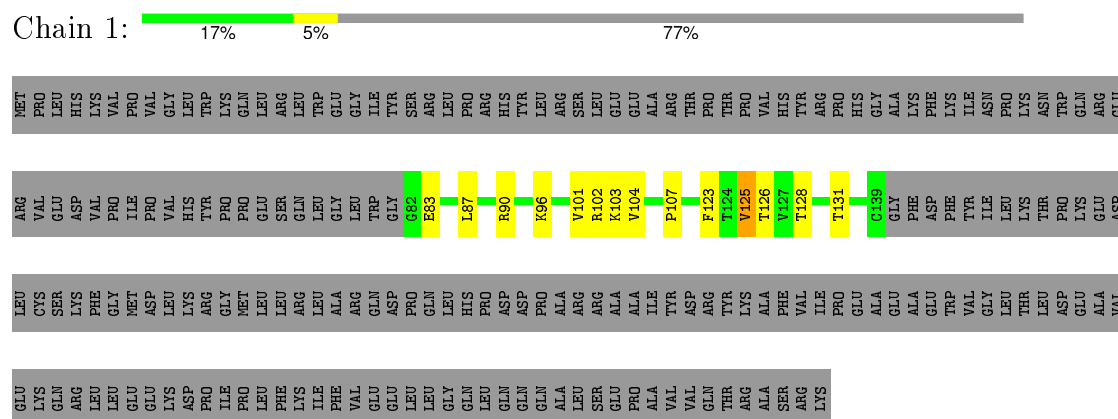
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

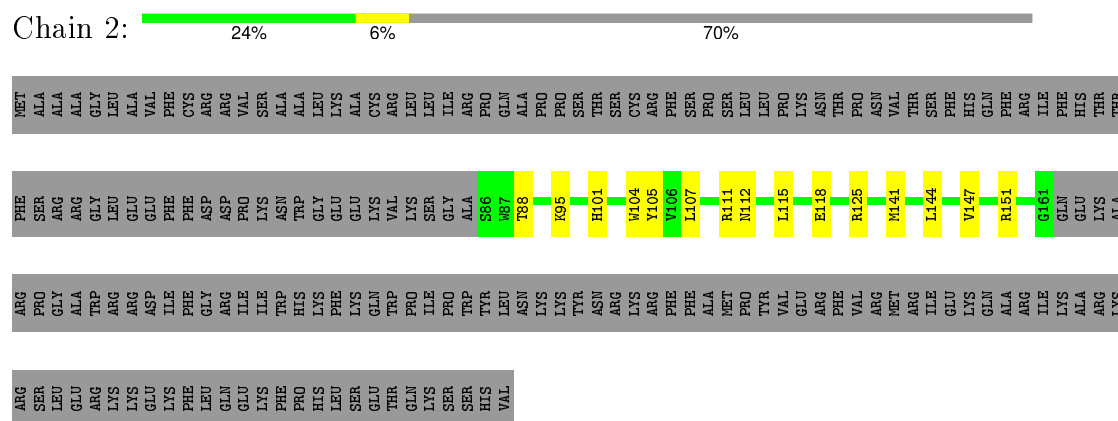
- Molecule 1: MRPL27



- Molecule 2: MRPL28



- Molecule 3: MRPL47



- Molecule 4: MRPL30

ARG	TRP	LEU	LEU	ASN	PRO	ALA	ASN	GLN	GLU	ALA	ARG	LYS	SER	GLN	THR	ASP	TRP	ILE	ARG	HIS	LYS	PHE	THR	ARG	SER	ARG	ILE	PRO	ASP	LYS	VAL	GLN	PRO	SER	THR	CYS	LEU	SER	GLU	HIS	GLU	LYS	TYR	GLY	LEU	VAL	ASP	PRO
MET	ALA	GLY	ILE	LEU	ARG	VAL	SER	VAL	GLN	ARG	PRO	GLY	ARG	LEU	THR	VAL	THR	LYS	GLY	MET	GLU	SER	LEU	ILE	CYS	GLU	LEU	THR	ASP	TRP	ILE	ARG	HIS	LYS	PHE	THR	ARG	SER	ARG	ILE	THR	ASP	TRP	ILE	ARG	ALA		

X146	ASP	THR	ASN	GLY	LYS	ALA	ILE	SER	SER	LEU	ASP	SER	PHE	TRP	MET	A79	R84	R85	R91	C92	R93	R94	R95	D108	H115	L116	K117	Q118	K119	H120	I121	G124	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	X137	X138	X139	X140	X141	X142	X143	X144	X145
	ALA	SER	ALA	MET	LEU	VAL	LEU	VAL	PRO	PRO	TRP	PRO	ALA	ALA	ARG	GLY	LEU	LEU	ASN	TRP	GLU	GLN	LEU	GLN	ARG	ASN	ARG	LEU	GLY	LEU	PRO	LEU	HIS	PRO	TRP	GLY	PRO	ALA	LEU	ALA	VAL	GLN	GLY	PRO	ALA	ILE	CYS	THR	PRO	ALA	ASN

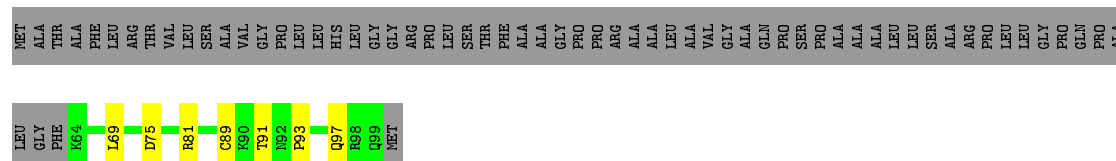
MET	PHE	LEU	SER	ALA	VAL	THR	PHE	ALA	LYS	SER	LVS	S13	K14	M20	M21	S22	G27	F28	S29	F30	R34	S35	R36	K40	H45	F56	V57	E58	Q59	K60	LVS	I1E	ARG	SER	I1U
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[illegible]

K131	K132	K133	K134	K135	A139	K141	K142	K143	M151	Q154	S155	K156	T162	THR	SER	PHE	LEU	TRP	LYS	ARG	ASN	ASP	PRO	THR	GLN	LYS	TYR	GLY	LEU	ASN	LEU	VAL																	
ILE	THR	SER	VAL	ARG	ASN	CYS	GLY	PRO	THR	PRO	VAL	ASN	ARG	VAL	PRO	HIS	LEU	LEU	PRO	ALA	SER	VAL	LYS	PRO	GLN	ASN	CYS	LEU	SER	SER	VAL	SER	GLY	R103	R104	K105	T106	V107	K108	A109	V110	T111	Y112	R113	F114	R124	R125	Y129	K120
ALA	ALA	SER	ALA	PHE	ALA	GLY	VAL	ALA	ALA	THR	VAL	ALA	ALA	VAL	PRO	HIS	LEU	LEU	PRO	ALA	SER	SER	THR	PRO	GLN	ASN	CYS	LEU	SER	SER	VAL	SER	SER	ARG	PHE	HIS	SER	HIS	ILE	GLN	THR	SER	ALA	LEU	SER	ALA	PRO	ARG	LEU

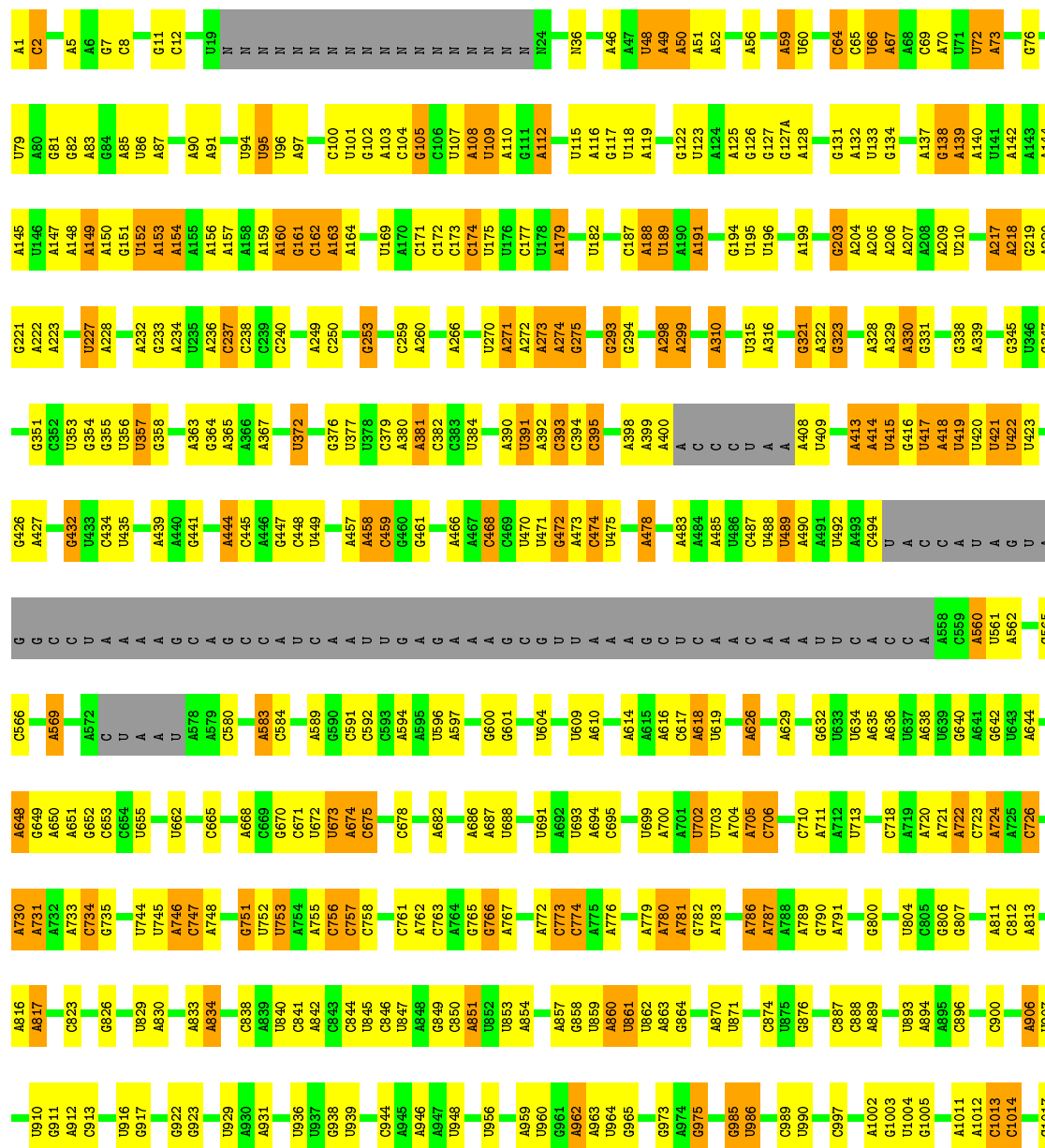
- Molecule 9: MRPL36

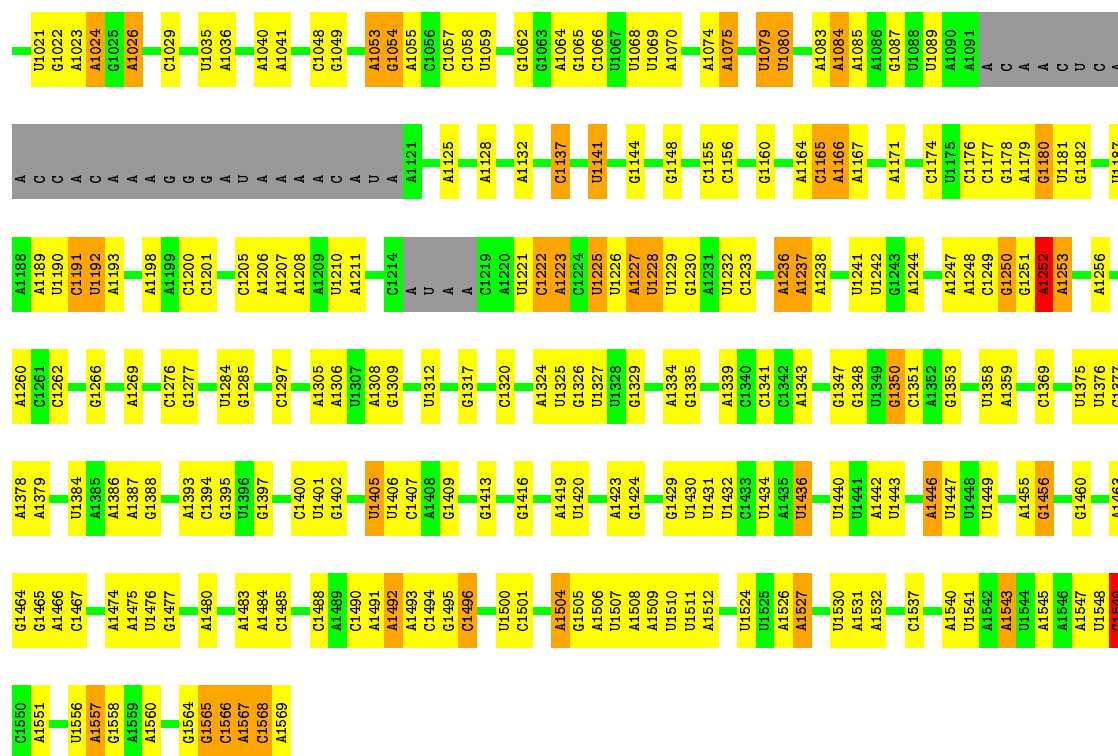
Chain 9:  29% 7% 64%



- Molecule 10: 16S rRNA

Chain A:  50% 32% 10% 8%



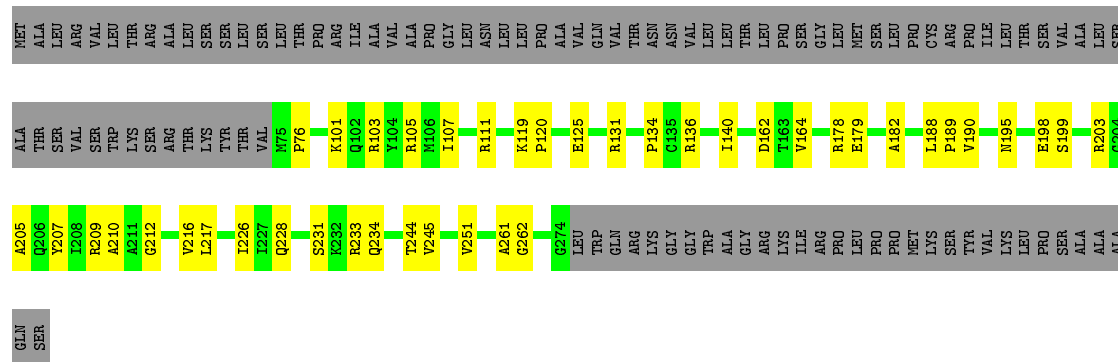


Chain B: 93% 7%



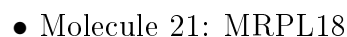
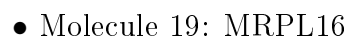
• Molecule 12: MRPL2

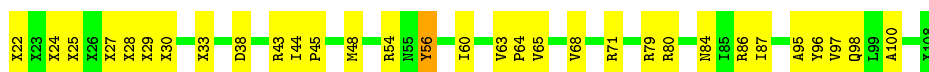
Chain D: 52% 14% 35%



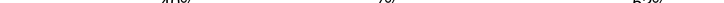
Chain E: 36% 16% 48%

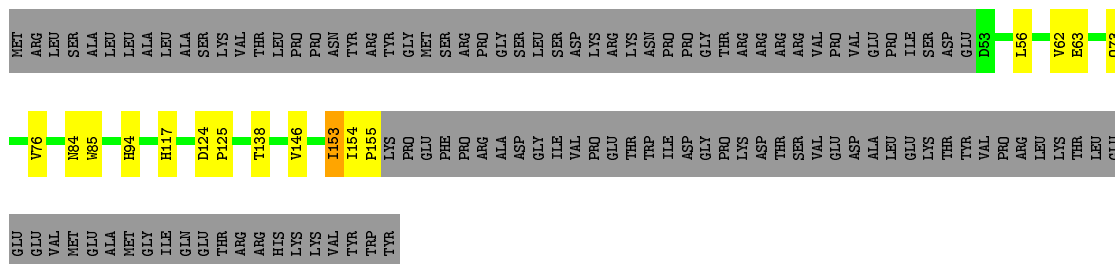






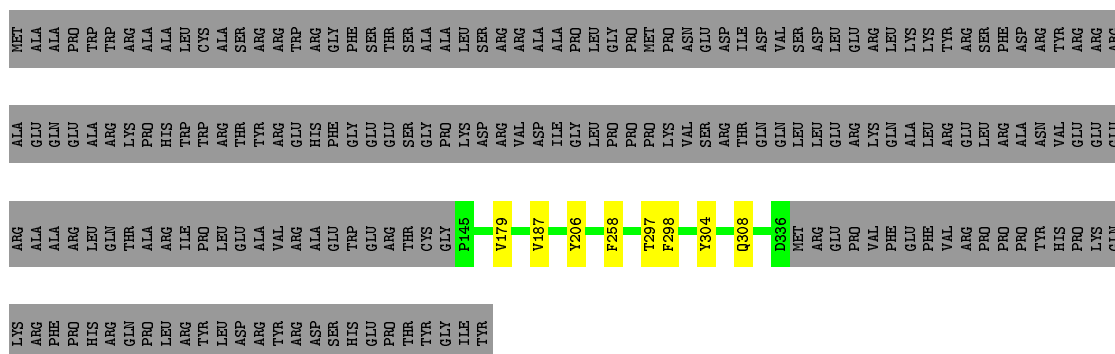
- Molecule 27: MRPL24

Chain Y:  40% 7% 52%



- Molecule 28: MRPL38

Chain b:  48% . 49%



- Molecule 29: MRPL39

Chain c:  93% 7%



- Molecule 30: MRPL44

Chain h: 90% 9%



- Molecule 31: MRPL45

Chain i:  50% 1% 48%



ARG LYS ALA PRO GLY LEU VAL ILE PRO HIS GLU ARG VAL LEU GLU ARG CYS THR ALA TYR VAL PRO PRO GLU VAL ILE Y104 Y116 Y149 E249 Y253 Y256 Y264 ILE ILE PRO

TRP ALA PRO THR LYS GLN PRO ILE LEU THR MET ILE GLY PRO GLN LEU LYS TRP GLU PHE GLU GLU GLU TYR GLN GLY VAL HIS LYS PRO GLN PRO ILE SER PHE VAL ARG ASN ASP SER

- Molecule 32: MRPL49

Chain l:  42% 54%

MET ALA ALA THR VAL LEU CYS GLY VAL LEU ARG TRP ARG THR GLY VAL PRO GLY LEU CYS GLY LEU GLY THR ARG ARG LEU SER GLN GLY THR ARG GLY THR PRO GLU VAL HIS LYS PRO GLN PRO ILE SER PHE VAL ARG ASN ASP SER

PRO LYS HIS GLU THR PRO THR TRP GLY LEU PHE VAL ARG ARG M91 I100 S129 T135 V143 F153 L157 F166

- Molecule 33: MRPL52

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: ICT1

Chain u:  42% 56%

MET ALA ALA ALA CYS ARG LEU ARG TRP GLY LEU ASN ARG ALA ALA TRP LEU LEU PRO PRO THR THR TYR PRO ARG ARG ALA HIS LYS VAL GLU GLY ARG GLU PHE GLN SER ILE TYR SER LEU LYS ASP THR ALA TRP ARG

LEU PRO ASP ASP ALA LYS Q67 G85 PRO GLY GLN ASN VAL ASN R93 R140 Y141 R144 F163 ALA LYS GLU PRO SER ARG GLU ASP ALA LEU GLU ARG ARG SER ARG ARG ILE GLU MET ASN ARG GLU ARG LEU TYR PRO LYS ARG ARG LYS ARG GLY SER ASP THR ALA TRP ARG

ARG ARG VAL ASP VAL ASP

- Molecule 35: UNASSIGNED HELICES

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: UNASSIGNED HELICES

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: THIOREDOXIN FOLD

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: UNASSIGNED HELICES

Chain z:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON I AND FEI FALCON II	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0	0.20	0/624	0.34	0/836
10	A	0.16	0/34230	0.72	8/53284 (0.0%)
12	D	0.19	0/1557	0.36	0/2093
13	E	0.21	0/1662	0.37	0/2246
14	F	0.20	0/1582	0.38	0/2148
15	I	0.20	0/450	0.37	0/603
16	N	0.21	0/1211	0.40	0/1639
17	O	0.21	0/907	0.40	0/1224
18	P	0.21	0/1254	0.40	0/1686
19	Q	0.21	0/1104	0.36	0/1483
2	1	0.20	0/498	0.41	0/670
20	R	0.21	0/1000	0.38	0/1342
21	S	0.18	0/763	0.36	0/1033
22	T	0.22	0/978	0.39	0/1318
23	U	0.21	0/986	0.36	0/1319
24	V	0.21	0/866	0.41	0/1168
25	W	0.20	0/931	0.33	0/1241
26	X	0.20	0/585	0.37	0/788
27	Y	0.20	0/853	0.40	0/1155
28	b	0.21	0/1616	0.39	0/2205
29	c	0.29	1/2171 (0.0%)	0.43	1/2937 (0.0%)
3	2	0.19	0/641	0.32	0/862
30	h	0.23	0/1918	0.38	0/2597
31	i	0.21	0/1366	0.41	0/1844
32	l	0.22	0/632	0.42	0/855
34	u	0.20	0/726	0.38	0/975
4	3	0.19	0/501	0.40	0/671
5	5	0.19	0/393	0.37	0/524
6	6	0.21	0/396	0.36	0/526
7	7	0.19	0/370	0.35	0/492
8	8	0.21	0/529	0.33	0/698
9	9	0.20	0/322	0.32	0/424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.19	1/63622 (0.0%)	0.60	9/92886 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
29	c	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	141	ARG	C-N	6.05	1.48	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	753	U	C2-N1-C1'	7.69	126.93	117.70
10	A	1549	C	N3-C2-O2	-7.49	116.66	121.90
10	A	753	U	N1-C2-O2	7.31	127.92	122.80
10	A	753	U	N3-C2-O2	-6.98	117.31	122.20
10	A	1549	C	C6-N1-C2	-6.66	117.64	120.30
10	A	1549	C	N1-C2-O2	5.79	122.37	118.90
29	c	100	SER	O-C-N	5.52	131.54	122.70
10	A	1252	A	C2-N3-C4	5.46	113.33	110.60
10	A	64	C	N1-C2-O2	5.29	122.08	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	c	70	THR	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	0	607	0	611	9	0
2	1	489	0	501	8	0
3	2	633	0	649	13	0
4	3	491	0	559	16	0
5	5	508	0	527	33	0
6	6	391	0	429	8	0
7	7	362	0	382	15	0
8	8	520	0	585	31	0
9	9	316	0	341	5	0
10	A	30656	0	15523	415	0
11	B	348	0	234	2	0
12	D	1531	0	1569	29	0
13	E	1621	0	1680	48	0
14	F	1713	0	1762	49	0
15	I	447	0	472	10	0
16	N	1178	0	1185	31	0
17	O	891	0	941	19	0
18	P	1309	0	1335	51	0
19	Q	1179	0	1211	34	0
20	R	982	0	995	15	0
21	S	748	0	752	12	0
22	T	962	0	987	29	0
23	U	1018	0	1099	29	0
24	V	877	0	925	25	0
25	W	1058	0	1069	38	0
26	X	689	0	708	22	0
27	Y	835	0	838	8	0
28	b	1562	0	1469	0	0
29	c	2310	0	2310	0	0
30	h	2075	0	2091	0	0
31	i	1335	0	1323	0	0
32	l	619	0	628	0	0
33	o	336	0	338	0	0
34	u	717	0	730	0	0
35	v	546	0	556	0	0
35	w	546	0	556	0	0
36	x	510	0	514	0	0
37	z	2556	0	2598	0	0
38	5	1	0	0	0	0
38	9	1	0	0	0	0
All	All	65473	0	50982	814	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 14.

All (814) 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)
13:E:258:THR:OG1	13:E:351:LYS:NZ	2.02	0.92
10:A:1543:A:OP1	13:E:351:LYS:NZ	2.05	0.89
10:A:444:A:OP2	19:Q:67:LYS:NZ	2.03	0.89
8:8:108:LYS:NZ	10:A:79:U:O4	2.06	0.89
10:A:83:A:OP2	10:A:1233:C:O2'	1.94	0.86
10:A:122:G:N2	10:A:125:A:OP2	2.09	0.85
10:A:1402:G:OP2	10:A:1402:G:N2	2.09	0.85
10:A:758:C:N4	10:A:765:G:O6	2.10	0.84
10:A:240:C:OP1	14:F:117:ARG:NH1	2.11	0.84
19:Q:134:LYS:NZ	19:Q:143:GLY:O	2.11	0.83
4:3:78:ARG:O	4:3:83:LYS:NZ	2.11	0.83
10:A:1022:G:N1	10:A:1026:A:OP2	2.11	0.82
17:O:143:ASN:ND2	22:T:156:GLU:OE2	2.11	0.82
1:0:50:ARG:NH1	10:A:1198:A:OP1	2.13	0.81
10:A:1180:G:H21	10:A:1229:U:H3	1.23	0.81
8:8:156:LYS:NZ	10:A:426:G:OP2	2.13	0.81
10:A:134:G:N1	10:A:137:A:OP2	2.14	0.80
22:T:182:ARG:HH12	22:T:190:LEU:HD11	1.46	0.79
5:5:94:ARG:NE	10:A:642:G:OP2	2.15	0.79
10:A:1558:G:O2'	10:A:1560:A:OP2	1.98	0.79
10:A:259:C:H42	10:A:316:A:H61	1.26	0.79
10:A:203:G:OP2	10:A:203:G:N2	2.14	0.78
8:8:141:LYS:NZ	10:A:1241:U:OP1	2.16	0.78
3:2:125:ARG:HH12	10:A:678:C:H1'	1.49	0.77
10:A:1526:A:H3'	10:A:1527:A:H5''	1.66	0.77
10:A:182:U:OP1	18:P:47:ARG:NH1	2.17	0.77
12:D:162:ASP:OD1	12:D:178:ARG:NH1	2.18	0.77
8:8:142:ARG:NH2	10:A:1190:U:OP2	2.17	0.77
10:A:829:U:OP2	10:A:834:A:N6	2.17	0.77
8:8:130:LYS:NZ	10:A:1232:U:H5'	2.00	0.77
22:T:165:GLU:HB2	22:T:168:ASN:HB2	1.66	0.77
10:A:478:A:O2'	23:U:100:LYS:NZ	2.17	0.77
16:N:14:PHE:HE2	16:N:44:LYS:HZ2	1.30	0.76
10:A:1416:G:N2	10:A:1419:A:OP2	2.18	0.76
14:F:70:UNK:HG3	14:F:75:UNK:HG1	1.68	0.76
24:V:123:GLU:HG2	24:V:125:ASP:H	1.51	0.75
19:Q:64:ARG:HD2	19:Q:144:LYS:HD3	1.67	0.75
10:A:702:U:H5	26:X:33:UNK:HG1	1.53	0.74
10:A:1566:C:OP2	13:E:203:VAL:HG13	1.88	0.73
10:A:600:G:OP2	18:P:45:ARG:NH2	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1369:C:O2'	17:O:34:LYS:NZ	2.21	0.73
10:A:112:A:OP1	14:F:115:LYS:NZ	2.18	0.73
3:2:111:ARG:HH11	3:2:141:MET:HB3	1.53	0.73
7:7:91:LYS:HD2	10:A:118:U:H5''	1.69	0.72
10:A:347:G:OP2	14:F:142:ARG:NH2	2.21	0.72
16:N:115:ASN:O	16:N:119:ARG:NH1	2.23	0.72
10:A:626:A:N7	18:P:39:ARG:NH2	2.37	0.72
13:E:199:GLY:HA2	13:E:225:GLN:H	1.54	0.72
10:A:589:A:O2'	24:V:122:ASN:ND2	2.22	0.72
10:A:800:G:N2	10:A:985:G:OP2	2.19	0.72
10:A:601:G:OP1	18:P:35:LYS:NZ	2.22	0.71
10:A:163:A:N1	10:A:1013:C:O2'	2.24	0.71
10:A:1164:A:N6	10:A:1171:A:OP2	2.23	0.71
10:A:441:G:H5''	19:Q:144:LYS:NZ	2.06	0.71
10:A:418:A:HO2'	10:A:419:U:C4'	2.03	0.70
24:V:133:ARG:HG2	24:V:161:GLU:HG2	1.74	0.70
10:A:1012:A:H5''	23:U:34:ARG:NH1	2.07	0.70
10:A:1066:C:O2	10:A:1419:A:O2'	2.10	0.70
2:1:90:ARG:NH1	10:A:1074:A:O3'	2.24	0.70
7:7:84:ARG:NH1	10:A:126:G:OP1	2.25	0.70
16:N:22:ASP:O	16:N:26:GLN:NE2	2.25	0.69
5:5:95:ARG:NH1	10:A:154:A:OP2	2.23	0.69
14:F:70:UNK:HG2	14:F:72:UNK:HG3	1.74	0.69
25:W:119:LEU:HD22	25:W:123:GLN:HE21	1.56	0.69
8:8:130:LYS:HZ3	10:A:1232:U:H5'	1.55	0.69
17:O:85:LEU:HD21	17:O:130:ARG:HH12	1.57	0.69
1:0:41:ASN:ND2	10:A:1176:C:OP2	2.25	0.69
10:A:1084:A:OP2	15:I:116:LYS:NZ	2.20	0.68
10:A:199:A:N3	14:F:147:ARG:NH2	2.41	0.68
10:A:419:U:H2'	10:A:420:U:C6	2.28	0.68
14:F:221:LEU:HG	14:F:223:HIS:H	1.55	0.68
8:8:142:ARG:HH21	10:A:1190:U:H5''	1.57	0.68
9:9:93:PRO:HB2	10:A:1348:G:H5''	1.75	0.68
10:A:1017:C:H5''	13:E:301:ARG:HG2	1.75	0.68
10:A:59:A:O2'	10:A:60:U:O2	2.10	0.68
13:E:225:GLN:HG3	13:E:226:LYS:HG2	1.76	0.68
11:B:1:N:H5'	21:S:108:ARG:HD3	1.74	0.67
10:A:1241:U:H2'	10:A:1242:U:C6	2.30	0.67
10:A:973:G:O2'	10:A:975:G:OP2	2.08	0.67
10:A:761:C:OP2	10:A:763:C:N4	2.26	0.67
8:8:105:LYS:HG2	10:A:76:G:N7	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1035:U:O4	16:N:119:ARG:NH2	2.28	0.67
17:O:46:LEU:HD11	17:O:77:ILE:HG21	1.77	0.67
10:A:1068:U:H2'	10:A:1070:A:OP2	1.96	0.66
4:3:74:SER:HB2	10:A:471:U:H5''	1.77	0.66
10:A:395:C:HO2'	10:A:413:A:H2	1.42	0.66
10:A:826:G:O6	10:A:838:C:N4	2.19	0.66
10:A:189:U:OP2	24:V:181:ARG:NH2	2.30	0.65
13:E:154:LYS:NZ	13:E:342:GLY:O	2.22	0.65
6:6:40:LYS:HB3	6:6:58:GLU:HB3	1.77	0.65
13:E:180:VAL:HB	13:E:242:THR:H	1.61	0.65
10:A:11:G:O2'	10:A:112:A:N6	2.30	0.65
20:R:34:THR:HG23	20:R:85:LEU:HD11	1.79	0.64
10:A:294:G:OP2	25:W:158:GLY:N	2.28	0.64
10:A:85:A:O2'	18:P:64:ARG:NH1	2.30	0.64
10:A:149:A:H2'	25:W:147:ARG:HH22	1.62	0.64
13:E:204:SER:HB2	13:E:223:PRO:HB3	1.78	0.64
27:Y:56:LEU:HD21	27:Y:76:VAL:HG21	1.79	0.64
10:A:1053:A:N7	14:F:137:ARG:NH2	2.42	0.64
12:D:212:GLY:HA2	12:D:251:VAL:HG12	1.79	0.64
10:A:137:A:HO2'	10:A:139:A:H8	1.46	0.64
7:7:88:LYS:NZ	10:A:127:G:OP2	2.31	0.63
10:A:179:A:O2'	23:U:48:ARG:NH2	2.31	0.63
10:A:441:G:H5''	19:Q:144:LYS:HZ3	1.64	0.62
10:A:1087:G:OP2	15:I:122:ARG:NH2	2.31	0.62
18:P:98:LEU:HD23	18:P:101:LEU:HD12	1.81	0.62
8:8:143:ARG:NH2	10:A:1206:A:N1	2.40	0.62
10:A:109:U:O2	14:F:147:ARG:NH1	2.32	0.62
15:I:108:ARG:O	15:I:147:ARG:NH1	2.28	0.62
8:8:124:ARG:HH12	10:A:1201:C:H5''	1.65	0.62
10:A:786:A:H3'	20:R:10:SER:HB3	1.80	0.62
27:Y:146:VAL:HG12	27:Y:153:ILE:HA	1.82	0.62
10:A:1353:G:N2	10:A:1464:G:O2'	2.32	0.62
10:A:675:C:N3	10:A:700:A:N6	2.48	0.62
23:U:29:ARG:O	23:U:30:HIS:ND1	2.32	0.62
10:A:911:G:O2'	10:A:913:C:N4	2.33	0.62
16:N:39:LEU:HD23	16:N:112:LEU:HD11	1.83	0.61
8:8:104:ARG:NH1	10:A:207:A:H1'	2.15	0.61
10:A:1504:A:H2'	10:A:1505:G:H8	1.64	0.61
10:A:50:A:N6	10:A:345:G:O2'	2.32	0.61
10:A:1506:A:H2'	10:A:1507:U:C6	2.35	0.61
13:E:264:LYS:HD2	13:E:312:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1182:G:H1	10:A:1222:C:H42	1.49	0.61
2:1:90:ARG:HD2	2:1:103:LYS:HD2	1.82	0.61
10:A:153:A:H8	10:A:153:A:OP1	1.83	0.61
10:A:104:C:N4	14:F:104:LYS:O	2.34	0.61
10:A:569:A:H4'	16:N:29:GLY:HA3	1.83	0.61
10:A:906:A:H62	10:A:910:U:H3	1.47	0.61
4:3:85:ILE:HG23	4:3:109:LYS:HB3	1.81	0.61
3:2:88:THR:HG23	3:2:147:VAL:HG22	1.81	0.61
10:A:162:C:H42	10:A:1011:A:H61	1.48	0.61
16:N:67:PHE:O	16:N:72:TRP:NE1	2.33	0.60
21:S:160:ARG:HA	21:S:163:HIS:HB3	1.83	0.60
10:A:1250:G:N2	18:P:77:ARG:NH1	2.49	0.60
12:D:125:GLU:HB2	12:D:164:VAL:HB	1.83	0.60
10:A:1227:A:O2'	10:A:1228:U:O4'	2.18	0.60
10:A:339:A:OP2	10:A:1064:A:O2'	2.19	0.60
13:E:272:ARG:NH2	13:E:308:MET:O	2.34	0.60
23:U:33:GLY:O	23:U:36:ASN:ND2	2.34	0.60
10:A:160:A:OP2	10:A:1035:U:N3	2.32	0.60
16:N:21:LEU:HD13	16:N:31:LEU:HD11	1.83	0.60
10:A:985:G:N2	10:A:989:C:O2'	2.35	0.60
3:2:112:ASN:OD1	26:X:22:UNK:N	2.35	0.60
14:F:143:SER:HB3	14:F:146:TRP:HD1	1.67	0.60
14:F:120:VAL:HG12	14:F:122:GLY:H	1.66	0.60
10:A:418:A:O2'	10:A:419:U:O4'	2.12	0.59
10:A:1564:G:H2'	10:A:1565:G:C8	2.38	0.59
14:F:273:LEU:HA	14:F:276:UNK:HG3	1.84	0.59
10:A:858:G:H3'	12:D:209:ARG:HH21	1.68	0.59
10:A:1252:A:N3	10:A:1252:A:H2'	2.18	0.59
24:V:136:LYS:HD3	24:V:158:VAL:HB	1.84	0.59
6:6:14:LYS:H	6:6:35:SER:HB3	1.67	0.59
8:8:139:ALA:HA	8:8:142:ARG:NH1	2.18	0.59
14:F:219:VAL:HG21	14:F:248:LEU:HD13	1.85	0.59
10:A:1013:C:O2'	10:A:1014:C:OP1	2.19	0.59
3:2:111:ARG:HE	3:2:115:LEU:HD11	1.68	0.58
10:A:1353:G:H21	10:A:1465:G:H5'	1.68	0.58
12:D:111:ARG:NH2	12:D:125:GLU:OE1	2.37	0.58
16:N:62:THR:HG21	16:N:127:LEU:HB3	1.86	0.58
10:A:840:U:H4'	12:D:261:ALA:HB2	1.85	0.58
17:O:53:ARG:HD3	17:O:54:PRO:HD2	1.85	0.58
15:I:123:LEU:HA	15:I:128:LEU:HB2	1.85	0.58
10:A:1557:A:OP2	20:R:11:HIS:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:789:A:H61	10:A:997:C:H42	1.52	0.58
10:A:237:C:O2'	18:P:51:ARG:NH2	2.36	0.57
10:A:137:A:H4'	10:A:138:G:H5'	1.85	0.57
24:V:123:GLU:OE2	24:V:167:LYS:NZ	2.37	0.57
10:A:159:A:H5''	16:N:119:ARG:NH1	2.20	0.57
10:A:1504:A:H2'	10:A:1505:G:C8	2.39	0.57
26:X:24:UNK:HG1	26:X:56:TYR:OH	2.04	0.57
1:0:42:LEU:HD22	10:A:1155:C:H5''	1.86	0.57
25:W:81:SER:H	25:W:110:LYS:NZ	2.03	0.57
25:W:90:LYS:HA	25:W:93:ARG:NH1	2.20	0.57
3:2:111:ARG:NH1	3:2:141:MET:HB3	2.19	0.57
10:A:191:A:OP2	10:A:1320:C:O2'	2.21	0.57
17:O:99:ARG:NH2	22:T:161:GLU:OE1	2.34	0.57
15:I:98:LEU:HD21	15:I:105:LEU:HD12	1.86	0.57
4:3:110:LEU:HD11	4:3:119:ILE:HG12	1.86	0.57
5:5:93:ARG:NH2	10:A:640:G:OP1	2.38	0.56
10:A:859:U:OP2	12:D:209:ARG:NE	2.38	0.56
6:6:21:MET:HA	6:6:27:GLY:HA2	1.87	0.56
4:3:106:VAL:HA	4:3:109:LYS:NZ	2.19	0.56
13:E:344:LYS:NZ	22:T:91:LYS:NZ	2.53	0.56
25:W:81:SER:CB	25:W:110:LYS:HZ1	2.18	0.56
10:A:485:A:N6	10:A:580:C:H42	2.04	0.56
10:A:470:U:O2'	10:A:483:A:N3	2.39	0.56
13:E:150:LEU:HD21	13:E:244:LEU:HD23	1.87	0.56
1:0:57:GLU:HG3	1:0:98:ARG:HA	1.87	0.56
16:N:6:LYS:HG2	24:V:110:TRP:HH2	1.71	0.56
10:A:1305:A:H2'	10:A:1306:A:H8	1.70	0.56
10:A:458:A:H2'	10:A:459:C:H2'	1.88	0.56
10:A:600:G:N7	18:P:44:ARG:NH2	2.54	0.56
10:A:634:U:H1'	14:F:147:ARG:NH1	2.21	0.56
4:3:68:ILE:HD12	4:3:122:LEU:HD12	1.88	0.56
10:A:1003:G:H5''	25:W:110:LYS:HB3	1.87	0.56
19:Q:71:ASP:HA	19:Q:155:LYS:HE2	1.88	0.56
10:A:391:U:H2'	10:A:392:A:N3	2.21	0.56
5:5:95:ARG:NH2	10:A:151:G:OP1	2.39	0.56
13:E:257:VAL:HG11	13:E:340:VAL:HG22	1.87	0.56
10:A:1004:U:OP2	25:W:110:LYS:NZ	2.30	0.55
14:F:103:GLN:HA	14:F:106:PHE:CE2	2.41	0.55
13:E:303:TRP:O	13:E:306:THR:OG1	2.19	0.55
4:3:71:ARG:HH21	4:3:74:SER:HA	1.71	0.55
10:A:911:G:H21	10:A:912:A:N6	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:87:LEU:HD23	2:1:104:VAL:HG12	1.87	0.55
10:A:1460:G:N2	10:A:1463:A:OP2	2.39	0.55
10:A:560:A:N6	10:A:1312:U:OP1	2.39	0.55
17:O:44:SER:HB2	17:O:117:THR:H	1.71	0.55
24:V:179:GLN:HB2	24:V:184:TYR:HB3	1.89	0.55
19:Q:64:ARG:NH1	19:Q:132:THR:HB	2.22	0.55
12:D:198:GLU:HA	12:D:205:ALA:HA	1.88	0.55
10:A:1058:C:H2'	10:A:1059:U:H6	1.71	0.55
25:W:123:GLN:OE1	25:W:135:ARG:NH2	2.36	0.55
8:8:124:ARG:NH2	10:A:1201:C:OP1	2.39	0.55
17:O:98:PRO:HB3	22:T:162:ILE:HG12	1.88	0.55
14:F:66:UNK:HB1	14:F:80:THR:HB	1.88	0.55
20:R:17:ARG:HA	20:R:25:ARG:HH21	1.72	0.55
23:U:34:ARG:O	23:U:38:CYS:N	2.40	0.55
10:A:1500:U:H2'	10:A:1501:C:C6	2.42	0.54
16:N:61:ASN:ND2	16:N:131:GLU:OE2	2.32	0.54
20:R:82:GLU:HG3	20:R:84:ASP:H	1.73	0.54
22:T:152:ARG:HG3	22:T:161:GLU:HG2	1.90	0.54
18:P:35:LYS:HD2	18:P:36:PRO:HD2	1.87	0.54
10:A:648:A:H2'	10:A:780:A:H2'	1.88	0.54
10:A:618:A:H8	10:A:618:A:OP2	1.91	0.54
10:A:187:C:H2'	24:V:181:ARG:HH12	1.71	0.54
10:A:367:A:N6	10:A:432:G:H5''	2.23	0.54
10:A:1494:C:H4'	13:E:271:ARG:NH1	2.23	0.54
10:A:249:A:H2'	10:A:250:C:C6	2.43	0.54
19:Q:83:THR:OG1	19:Q:123:ARG:NH2	2.41	0.54
10:A:1397:G:O2'	10:A:1400:C:OP2	2.22	0.54
10:A:395:C:O2'	10:A:413:A:H2	1.91	0.54
10:A:1384:U:H2'	10:A:1386:A:OP2	2.08	0.54
19:Q:98:HIS:HA	19:Q:151:VAL:HG12	1.88	0.54
10:A:420:U:H2'	10:A:421:U:O4'	2.08	0.54
10:A:108:A:O2'	10:A:109:U:OP2	2.18	0.54
10:A:260:A:OP2	12:D:101:LYS:NZ	2.41	0.54
16:N:16:ARG:HH11	16:N:124:ARG:HH11	1.55	0.54
10:A:119:A:H62	10:A:127(A):G:H21	1.56	0.54
10:A:160:A:H2	10:A:173:C:H5'	1.72	0.54
10:A:626:A:H62	18:P:39:ARG:HH21	1.54	0.54
5:5:132:UNK:O	5:5:135:UNK:HG3	2.08	0.54
5:5:108:ASP:OD1	5:5:119:LYS:HB3	2.08	0.54
10:A:137:A:O2'	10:A:139:A:H8	1.91	0.53
3:2:101:HIS:HA	3:2:104:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:786:A:OP1	10:A:1558:G:N1	2.42	0.53
10:A:734:C:OP2	12:D:103:ARG:NH2	2.41	0.53
14:F:90:ALA:HB2	18:P:10:UNK:HG1	1.91	0.53
22:T:120:THR:HG23	22:T:130:THR:HG23	1.90	0.53
10:A:604:U:H3	10:A:626:A:H61	1.56	0.53
18:P:99:ASN:HB2	18:P:144:GLY:HA3	1.90	0.53
10:A:1024:A:N3	10:A:1276:C:O2'	2.35	0.53
10:A:1053:A:H62	14:F:137:ARG:HH12	1.56	0.53
10:A:217:A:H61	10:A:227:U:H4'	1.73	0.53
4:3:120:LYS:HD2	4:3:121:PRO:HD2	1.89	0.53
16:N:16:ARG:HD3	16:N:124:ARG:NH1	2.24	0.53
13:E:203:VAL:HG21	13:E:225:GLN:OE1	2.08	0.53
10:A:780:A:H5''	10:A:781:A:OP2	2.08	0.53
18:P:102:GLN:NE2	18:P:144:GLY:O	2.41	0.53
10:A:1075:A:N6	10:A:1137:C:N3	2.57	0.53
22:T:116:ILE:HD12	22:T:178:LYS:HD2	1.91	0.53
20:R:14:VAL:HG22	20:R:15:PHE:H	1.74	0.53
10:A:182:U:O2'	10:A:355:G:OP2	2.20	0.53
10:A:644:A:N1	25:W:155:ARG:NH1	2.56	0.53
15:I:116:LYS:HB2	15:I:120:ARG:NH1	2.24	0.53
10:A:1079:U:O2'	10:A:1080:U:OP1	2.22	0.53
9:9:89:CYS:SG	9:9:91:THR:OG1	2.66	0.53
10:A:163:A:H2'	23:U:35:LYS:NZ	2.24	0.53
10:A:1070:A:H61	10:A:1141:U:H3	1.56	0.52
18:P:73:PRO:HD2	18:P:76:LEU:HD12	1.91	0.52
10:A:310:A:H5'	12:D:262:GLY:HA2	1.91	0.52
23:U:35:LYS:HD3	23:U:45:ALA:HB2	1.90	0.52
15:I:123:LEU:HB3	15:I:129:ALA:HB3	1.91	0.52
21:S:82:ARG:HG3	21:S:93:LEU:HB2	1.90	0.52
10:A:911:G:H21	10:A:912:A:H62	1.55	0.52
13:E:239:LYS:NZ	13:E:244:LEU:HD13	2.24	0.52
18:P:122:VAL:HG22	18:P:127:VAL:HG11	1.91	0.52
10:A:177:C:H4'	23:U:55:ARG:NH1	2.24	0.52
22:T:148:THR:HG22	22:T:165:GLU:HG3	1.90	0.52
19:Q:121:LEU:HB2	19:Q:162:GLU:HG3	1.91	0.52
6:6:34:ARG:HG2	6:6:36:ARG:H	1.75	0.52
8:8:125:ARG:HB3	18:P:79:PRO:HG2	1.92	0.52
19:Q:64:ARG:NH1	19:Q:144:LYS:HB3	2.25	0.52
26:X:71:ARG:NH2	26:X:96:TYR:OH	2.42	0.52
10:A:1329:G:H1	10:A:1401:U:H3	1.58	0.52
10:A:271:A:H3'	10:A:271:A:N3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:187:C:H5'	10:A:1023:A:H62	1.75	0.52
1:0:53:ILE:HG23	1:0:68:ALA:HB2	1.92	0.52
27:Y:154:ILE:N	27:Y:155:PRO:HD2	2.25	0.52
10:A:372:U:C4	10:A:1248:A:H2	2.28	0.52
16:N:113:PRO:O	16:N:118:ARG:HB2	2.10	0.52
18:P:12:UNK:HA	18:P:15:UNK:HG3	1.92	0.52
23:U:86:PHE:HE2	23:U:102:LEU:HD21	1.74	0.52
10:A:1557:A:OP1	13:E:343:HIS:NE2	2.41	0.52
14:F:89:THR:HG22	18:P:10:UNK:HG2	1.92	0.52
7:7:71:ARG:HD3	7:7:74:ARG:HH21	1.74	0.52
10:A:936:U:H1'	10:A:938:G:OP2	2.10	0.52
8:8:124:ARG:HH11	18:P:78:ILE:HD11	1.75	0.52
5:5:128:UNK:O	5:5:131:UNK:HG3	2.10	0.52
14:F:72:UNK:HG2	14:F:73:UNK:H	1.76	0.51
10:A:724:A:O2'	10:A:726:C:N4	2.44	0.51
10:A:731:A:H5'	12:D:134:PRO:HB3	1.92	0.51
17:O:60:VAL:HG12	17:O:62:ASN:H	1.75	0.51
16:N:16:ARG:NH1	16:N:124:ARG:HG2	2.26	0.51
10:A:1164:A:H4'	10:A:1165:C:OP2	2.10	0.51
10:A:1250:G:C2	18:P:77:ARG:NH1	2.78	0.51
5:5:85:ARG:NH2	10:A:1436:U:O3'	2.43	0.51
10:A:1492:A:H8	10:A:1492:A:OP2	1.93	0.51
17:O:74:LEU:HD23	17:O:83:LYS:HG2	1.93	0.51
10:A:702:U:O4'	26:X:71:ARG:NH1	2.43	0.51
10:A:1248:A:H4'	10:A:1249:C:OP2	2.10	0.51
2:1:83:GLU:HB3	2:1:107:PRO:HB3	1.93	0.51
10:A:762:A:H4'	10:A:763:C:OP2	2.09	0.51
23:U:72:ILE:HD13	23:U:102:LEU:HD23	1.93	0.51
17:O:92:PRO:HG3	17:O:99:ARG:HB2	1.91	0.51
10:A:159:A:H2'	10:A:160:A:C8	2.46	0.51
10:A:163:A:P	23:U:52:LYS:HZ1	2.34	0.51
10:A:1506:A:H2'	10:A:1507:U:H6	1.75	0.51
10:A:959:A:N3	10:A:1413:G:O2'	2.43	0.51
10:A:422:U:H2'	10:A:423:U:C6	2.47	0.50
4:3:76:LYS:HE3	10:A:472:G:H21	1.76	0.50
13:E:344:LYS:HZ2	22:T:91:LYS:NZ	2.10	0.50
13:E:150:LEU:HA	13:E:196:LEU:HD13	1.92	0.50
10:A:1128:A:OP2	10:A:1128:A:H2	1.93	0.50
27:Y:63:GLU:OE2	27:Y:73:GLN:HB2	2.10	0.50
4:3:88:MET:SD	10:A:416:G:N2	2.72	0.50
10:A:196:U:OP1	23:U:40:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:HIS:CE1	10:A:1225:U:H1'	2.46	0.50
16:N:37:VAL:HG13	16:N:42:LEU:HB2	1.93	0.50
10:A:86:U:H2'	10:A:87:A:H8	1.77	0.50
8:8:130:LYS:HZ2	10:A:1232:U:H5'	1.77	0.50
13:E:301:ARG:NH1	13:E:304:PRO:HD3	2.26	0.50
10:A:1227:A:H2'	10:A:1228:U:C6	2.47	0.50
10:A:859:U:H5''	12:D:210:ALA:HB2	1.94	0.50
23:U:127:UNK:HA	23:U:130:UNK:HG3	1.94	0.50
10:A:1526:A:C3'	10:A:1527:A:H5''	2.38	0.50
5:5:91:ARG:NH2	10:A:151:G:OP2	2.45	0.50
21:S:122:VAL:HG13	21:S:157:SER:HA	1.93	0.50
22:T:116:ILE:HG12	22:T:136:ILE:HG12	1.94	0.50
7:7:88:LYS:HZ2	7:7:90:ARG:NH2	2.10	0.50
10:A:929:U:H5	10:A:936:U:H3	1.58	0.50
13:E:183:TYR:OH	13:E:192:ARG:NH1	2.45	0.50
14:F:274:UNK:HA	14:F:277:UNK:HG3	1.93	0.50
16:N:12:ALA:O	16:N:13:THR:OG1	2.28	0.50
13:E:173:LEU:HD22	13:E:348:VAL:HG21	1.94	0.50
10:A:119:A:O2'	26:X:84:ASN:ND2	2.45	0.49
10:A:249:A:H2'	10:A:250:C:H6	1.77	0.49
18:P:10:UNK:HA	18:P:13:UNK:HG3	1.94	0.49
15:I:110:ASP:OD1	15:I:111:LEU:N	2.45	0.49
5:5:117:LYS:HE3	5:5:124:GLY:H	1.77	0.49
10:A:1058:C:H2'	10:A:1059:U:C6	2.47	0.49
10:A:488:U:H2'	10:A:489:U:C6	2.47	0.49
16:N:21:LEU:HD21	16:N:38:LYS:NZ	2.28	0.49
24:V:102:VAL:HB	24:V:138:LEU:HB3	1.93	0.49
10:A:874:C:O2'	10:A:962:A:N1	2.39	0.49
19:Q:191:SER:H	19:Q:194:UNK:HG3	1.78	0.49
8:8:109:ALA:HB1	8:8:113:ARG:HH21	1.78	0.49
3:2:95:LYS:HD3	3:2:151:ARG:HH21	1.76	0.49
7:7:85:ARG:HG2	7:7:90:ARG:HG3	1.93	0.49
10:A:1057:C:H2'	10:A:1058:C:C6	2.48	0.49
13:E:281:THR:OG1	13:E:282:HIS:N	2.44	0.49
25:W:88:LEU:HD11	25:W:109:LYS:HD3	1.95	0.49
4:3:71:ARG:HA	4:3:117:ILE:HG22	1.95	0.49
4:3:88:MET:O	10:A:416:G:O2'	2.31	0.49
26:X:44:ILE:HD13	26:X:95:ALA:HB2	1.95	0.49
10:A:1511:U:H2'	10:A:1512:A:N3	2.28	0.49
10:A:846:C:H2'	10:A:847:U:H6	1.78	0.49
10:A:1549:C:O2	10:A:1549:C:H2'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:731:A:H3'	12:D:134:PRO:HB3	1.95	0.48
10:A:1192:U:H3	10:A:1207:A:H62	1.61	0.48
10:A:209:A:H2'	10:A:210:U:C6	2.48	0.48
22:T:121:THR:HG22	22:T:123:ASP:H	1.78	0.48
7:7:66:LYS:HZ3	10:A:253:G:H22	1.60	0.48
10:A:1350:G:OP2	10:A:1351:C:H5''	2.13	0.48
10:A:1449:U:H1'	17:O:63:LYS:NZ	2.29	0.48
1:0:77:PRO:HB3	1:0:89:LEU:HD22	1.96	0.48
20:R:53:ARG:HA	20:R:105:THR:HG21	1.95	0.48
7:7:70:VAL:HG12	10:A:36:N:OP2	2.13	0.48
25:W:144:THR:HG23	25:W:173:PHE:HB2	1.94	0.48
10:A:152:U:H3'	10:A:153:A:H5''	1.94	0.48
5:5:141:UNK:HA	5:5:144:UNK:HG3	1.95	0.48
23:U:125:UNK:HA	23:U:128:UNK:HG3	1.95	0.48
5:5:130:UNK:HA	5:5:133:UNK:HG3	1.94	0.48
10:A:293:G:O2'	25:W:161:ARG:NH2	2.35	0.48
10:A:1393:A:OP1	10:A:1395:G:O2'	2.26	0.48
3:2:115:LEU:HD22	3:2:118:GLU:OE1	2.14	0.48
12:D:216:VAL:HG13	12:D:228:GLN:HB3	1.95	0.48
22:T:182:ARG:NH1	22:T:190:LEU:HD11	2.22	0.48
10:A:81:G:N2	10:A:85:A:OP2	2.41	0.48
25:W:71:ILE:HD11	25:W:130:HIS:HB2	1.96	0.48
5:5:127:UNK:HA	5:5:130:UNK:HG3	1.96	0.48
10:A:746:A:OP2	10:A:747:C:OP2	2.32	0.48
10:A:773:C:O2'	10:A:774:C:O2	2.31	0.48
10:A:1495:G:H1'	10:A:1496:C:H2'	1.96	0.48
19:Q:64:ARG:NH2	19:Q:145:GLY:O	2.47	0.48
5:5:137:UNK:HA	5:5:140:UNK:HG3	1.96	0.48
19:Q:197:UNK:HA	19:Q:200:UNK:HG3	1.95	0.48
10:A:1358:U:H2'	10:A:1359:A:C8	2.49	0.48
24:V:178:PHE:HD1	24:V:185:GLN:HG2	1.77	0.48
18:P:38:ARG:NH1	18:P:45:ARG:NH1	2.62	0.48
5:5:138:UNK:HA	5:5:141:UNK:HG3	1.95	0.48
2:1:123:PHE:HE2	2:1:125:VAL:HG13	1.79	0.48
26:X:45:PRO:HG2	26:X:48:MET:HB2	1.96	0.47
10:A:1276:C:H2'	10:A:1277:G:H8	1.79	0.47
10:A:187:C:C2'	24:V:181:ARG:HH12	2.26	0.47
10:A:86:U:H2'	10:A:87:A:C8	2.48	0.47
12:D:107:ILE:HG13	12:D:136:ARG:NH1	2.28	0.47
26:X:79:ARG:HG2	26:X:86:ARG:HG2	1.96	0.47
10:A:861:U:H4'	10:A:862:U:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:29:UNK:HG2	26:X:33:UNK:CG	12.91	0.47
10:A:271:A:N6	10:A:273:A:N7	2.62	0.47
10:A:1475:A:H2'	10:A:1476:U:C6	2.50	0.47
25:W:151:LEU:HB3	25:W:153:ARG:NH1	2.29	0.47
16:N:16:ARG:HH11	16:N:124:ARG:NH1	2.12	0.47
10:A:417:U:H5'	10:A:418:A:OP2	2.14	0.47
8:8:104:ARG:O	10:A:76:G:H8	1.97	0.47
22:T:89:PRO:HA	22:T:92:PHE:HD2	1.79	0.47
12:D:226:ILE:HG21	12:D:234:GLN:HE21	1.80	0.47
22:T:138:ILE:HA	22:T:187:LEU:HD12	1.96	0.47
23:U:25:LEU:HA	23:U:28:ALA:HB3	1.97	0.47
7:7:85:ARG:NH1	7:7:92:SER:O	2.48	0.47
10:A:1564:G:H2'	10:A:1565:G:H8	1.78	0.47
7:7:82:ILE:HG23	7:7:93:LEU:HD13	1.96	0.47
10:A:1005:G:H4'	25:W:165:MET:HG3	1.96	0.47
10:A:299:A:OP2	10:A:299:A:H8	1.96	0.47
10:A:66:U:H2'	10:A:67:A:C8	2.49	0.47
10:A:1250:G:N2	18:P:77:ARG:HH11	2.12	0.47
15:I:95:GLU:HB3	15:I:111:LEU:HD11	1.97	0.47
8:8:154:GLN:NE2	10:A:1200:C:O2'	2.37	0.47
10:A:408:A:N1	10:A:1166:A:H2'	2.29	0.47
14:F:186:ASP:HB3	14:F:258:THR:HA	1.96	0.47
10:A:597:A:H4'	18:P:53:HIS:CD2	2.50	0.47
10:A:448:C:H4'	10:A:1317:G:O2'	2.15	0.47
5:5:93:ARG:NH1	10:A:642:G:OP2	2.48	0.47
5:5:131:UNK:O	5:5:134:UNK:HG3	2.14	0.47
5:5:134:UNK:HA	5:5:137:UNK:HG3	1.97	0.47
8:8:105:LYS:HE2	10:A:76:G:C6	2.49	0.47
13:E:325:TRP:CD1	13:E:337:ASN:HB2	2.50	0.47
10:A:786:A:C5	20:R:17:ARG:HD2	2.49	0.47
10:A:315:U:H2'	10:A:316:A:H8	1.78	0.47
3:2:111:ARG:HH11	3:2:141:MET:CB	2.24	0.47
10:A:1222:C:H3'	10:A:1223:A:H5''	1.96	0.47
21:S:126:GLU:HB3	21:S:130:ARG:NH1	2.29	0.47
25:W:130:HIS:HD2	25:W:132:VAL:HG22	1.80	0.47
19:Q:89:ILE:HD12	19:Q:161:VAL:HB	1.97	0.47
14:F:199:ASP:N	14:F:199:ASP:OD1	2.47	0.47
19:Q:200:UNK:HA	19:Q:203:UNK:HG3	1.97	0.46
25:W:196:UNK:HA	25:W:199:UNK:HG3	1.96	0.46
23:U:126:UNK:HA	23:U:129:UNK:HG3	1.97	0.46
10:A:363:A:O2'	10:A:384:U:OP1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:161:G:N2	10:A:173:C:OP1	2.48	0.46
10:A:474:C:H2'	10:A:475:U:C6	2.50	0.46
10:A:163:A:H2'	23:U:35:LYS:HZ1	1.80	0.46
4:3:106:VAL:HA	4:3:109:LYS:HZ1	1.79	0.46
23:U:59:LEU:HG	23:U:62:ARG:HD2	1.97	0.46
10:A:787:A:O2'	13:E:266:PHE:O	2.33	0.46
10:A:356:U:O4	18:P:58:GLN:NE2	2.48	0.46
12:D:131:ARG:O	12:D:140:ILE:N	2.46	0.46
10:A:478:A:HO2'	23:U:100:LYS:HZ2	1.56	0.46
10:A:419:U:H2'	10:A:420:U:C5	2.51	0.46
26:X:56:TYR:HD1	26:X:60:ILE:HD12	1.81	0.46
19:Q:194:UNK:HA	19:Q:197:UNK:HG3	1.96	0.46
10:A:376:G:O2'	18:P:56:GLU:OE1	2.33	0.46
3:2:125:ARG:HH21	10:A:699:U:H1'	1.81	0.46
18:P:38:ARG:HH11	18:P:45:ARG:NH2	2.14	0.46
19:Q:195:UNK:HA	19:Q:198:UNK:HG3	1.98	0.46
19:Q:201:UNK:HA	19:Q:204:UNK:HG3	1.96	0.46
10:A:421:U:HO2'	10:A:422:U:P	2.38	0.46
5:5:134:UNK:HG1	20:R:41:ARG:NH2	2.31	0.46
23:U:123:ARG:HA	23:U:126:UNK:HG3	1.98	0.46
12:D:119:LYS:HA	12:D:120:PRO:HD3	1.82	0.46
24:V:136:LYS:NZ	24:V:139:LEU:HD23	2.31	0.46
13:E:344:LYS:NZ	22:T:91:LYS:HZ1	2.13	0.46
5:5:133:UNK:HA	5:5:136:UNK:HG3	1.98	0.46
10:A:72:U:O2'	10:A:73:A:OP1	2.31	0.46
13:E:165:GLY:O	22:T:170:ARG:NH2	2.48	0.46
23:U:35:LYS:HG2	23:U:41:LEU:HB3	1.97	0.46
25:W:104:LEU:HD12	25:W:119:LEU:HD12	1.98	0.46
12:D:190:VAL:HA	12:D:217:LEU:HD23	1.97	0.46
10:A:377:U:O2	18:P:69:GLY:HA3	2.15	0.46
14:F:278:UNK:HA	14:F:281:UNK:HG3	1.97	0.46
10:A:816:A:H3'	10:A:817:A:H5''	1.98	0.46
10:A:1053:A:H2'	14:F:131:LYS:HZ3	1.81	0.46
10:A:103:A:C2	10:A:105:G:C8	3.04	0.46
20:R:9:ILE:HG23	20:R:11:HIS:H	1.81	0.46
10:A:944:C:OP1	17:O:52:HIS:NE2	2.41	0.46
16:N:21:LEU:HD21	16:N:38:LYS:HZ2	1.81	0.46
10:A:1476:U:H2'	10:A:1477:G:O4'	2.16	0.46
10:A:321:G:OP1	10:A:323:G:O2'	2.27	0.46
9:9:69:LEU:HD22	9:9:97:GLN:HB3	1.98	0.46
19:Q:66:ARG:O	19:Q:129:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:68:VAL:HG22	26:X:97:VAL:HG12	1.98	0.45
10:A:294:G:O6	25:W:159:ARG:NH1	2.48	0.45
14:F:86:VAL:HG11	14:F:273:LEU:HD13	1.97	0.45
10:A:219:G:OP1	14:F:168:LYS:NZ	2.49	0.45
10:A:367:A:H61	10:A:432:G:H5''	1.80	0.45
10:A:1079:U:HO2'	10:A:1080:U:P	2.38	0.45
25:W:142:GLU:HB3	25:W:175:LYS:HB2	1.98	0.45
8:8:151:ASN:HD22	10:A:1200:C:H5''	1.81	0.45
12:D:199:SER:HB3	12:D:207:TYR:HE1	1.82	0.45
10:A:916:U:H2'	10:A:917:G:H8	1.81	0.45
10:A:1284:U:H2'	10:A:1285:G:H8	1.81	0.45
18:P:23:SER:H	18:P:26:ASN:HD22	1.64	0.45
10:A:473:A:H4'	10:A:583:A:H2'	1.99	0.45
18:P:68:GLU:OE2	18:P:74:PHE:N	2.49	0.45
10:A:1484:A:H2'	10:A:1485:C:H6	1.81	0.45
10:A:1002:A:H2'	10:A:1003:G:H8	1.81	0.45
26:X:38:ASP:O	26:X:98:GLN:NE2	2.49	0.45
10:A:1566:C:H2'	13:E:206:PHE:CZ	2.51	0.45
10:A:188:A:OP2	24:V:181:ARG:NH2	2.49	0.45
25:W:90:LYS:HG3	25:W:93:ARG:NH1	2.31	0.45
10:A:893:U:H3	10:A:896:C:H41	1.63	0.45
10:A:851:A:N6	12:D:203:ARG:O	2.50	0.45
13:E:269:VAL:HG21	13:E:291:PRO:HB3	1.97	0.45
13:E:193:MET:HG2	13:E:231:ASN:HD22	1.81	0.45
10:A:195:U:O2'	10:A:1012:A:OP1	2.34	0.45
10:A:1484:A:H2'	10:A:1485:C:C6	2.51	0.45
10:A:609:U:H2'	10:A:610:A:H8	1.82	0.45
10:A:756:C:O2'	10:A:757:C:O4'	2.35	0.45
10:A:790:G:H2'	10:A:791:A:H8	1.81	0.45
24:V:159:ARG:HB2	24:V:203:GLU:HB2	1.99	0.45
10:A:107:U:H1'	10:A:110:A:C2	2.52	0.45
10:A:234:A:O2'	18:P:35:LYS:N	2.37	0.45
10:A:2:C:H42	10:A:149:A:N6	2.15	0.45
10:A:938:G:H2'	10:A:939:U:C6	2.51	0.45
20:R:37:VAL:HG13	20:R:85:LEU:HD22	1.99	0.45
10:A:1506:A:H2	10:A:1506:A:OP2	2.00	0.45
10:A:66:U:O2'	10:A:67:A:OP1	2.33	0.45
23:U:123:ARG:HH22	24:V:150:LYS:NZ	2.14	0.45
22:T:161:GLU:OE1	22:T:191:ARG:NH2	2.50	0.45
14:F:73:UNK:HG2	14:F:74:UNK:HG3	1.98	0.45
5:5:84:ARG:NH2	10:A:638:A:O2'	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:298:A:H4'	10:A:299:A:H5'	1.98	0.45
9:9:81:ARG:NH1	10:A:1524:U:C4	2.85	0.45
26:X:64:PRO:HB2	26:X:100:ALA:HB2	1.98	0.45
10:A:705:A:OP2	10:A:706:C:H5	2.00	0.45
11:B:21:N:OP2	21:S:119:THR:HG21	2.17	0.45
10:A:1343:A:OP2	10:A:1343:A:H2	1.99	0.45
10:A:753:U:O2	10:A:753:U:H2'	2.16	0.45
10:A:944:C:OP2	17:O:78:ARG:NH2	2.50	0.45
10:A:1241:U:H2'	10:A:1242:U:H6	1.78	0.45
10:A:860:A:C6	12:D:233:ARG:NH1	2.82	0.45
1:O:38:SER:OG	19:Q:142:GLY:O	2.34	0.45
13:E:351:LYS:HB2	13:E:351:LYS:HE3	1.71	0.44
20:R:22:PRO:HA	20:R:25:ARG:NH1	2.32	0.44
4:3:71:ARG:HB2	4:3:91:LEU:HD13	1.99	0.44
3:2:101:HIS:O	3:2:105:TYR:HB2	2.18	0.44
10:A:1156:C:O2'	10:A:1249:C:OP2	2.33	0.44
10:A:1557:A:OP2	10:A:1558:G:OP2	2.34	0.44
10:A:1182:G:H1	10:A:1222:C:N4	2.15	0.44
10:A:448:C:H2'	10:A:449:U:C6	2.52	0.44
10:A:380:A:H3'	10:A:381:A:C2	2.52	0.44
6:6:30:PHE:CZ	10:A:1241:U:H4'	2.53	0.44
13:E:200:GLY:H	13:E:225:GLN:HB3	1.82	0.44
10:A:609:U:O2	14:F:104:LYS:NZ	2.39	0.44
10:A:174:C:H2'	10:A:175:U:H6	1.82	0.44
17:O:32:ILE:N	17:O:67:GLY:O	2.51	0.44
10:A:1566:C:H4'	10:A:1567:A:OP2	2.16	0.44
18:P:56:GLU:HG2	18:P:62:ARG:HA	1.99	0.44
12:D:195:ASN:OD1	12:D:244:THR:OG1	2.24	0.44
26:X:27:UNK:HB2	26:X:30:UNK:CG	2.47	0.44
14:F:263:LEU:HB3	14:F:264:PRO:HD3	1.99	0.44
10:A:434:C:H2'	10:A:435:U:C6	2.52	0.44
2:1:128:THR:HG22	2:1:131:THR:H	1.83	0.44
10:A:415:U:H3'	10:A:416:G:C8	2.51	0.44
10:A:367:A:H61	10:A:432:G:C5'	2.30	0.44
10:A:357:U:H5'	18:P:43:ARG:HH12	1.83	0.44
10:A:804:U:H2'	10:A:806:G:OP2	2.17	0.44
16:N:16:ARG:HH12	16:N:124:ARG:HG2	1.83	0.44
13:E:344:LYS:CD	22:T:91:LYS:HZ1	2.31	0.44
14:F:66:UNK:HG2	14:F:189:ILE:O	2.18	0.44
7:7:66:LYS:HZ3	10:A:253:G:N2	2.15	0.44
5:5:139:UNK:HA	5:5:142:UNK:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:54:ARG:HG3	26:X:65:VAL:HB	1.99	0.44
21:S:126:GLU:HB3	21:S:130:ARG:HH12	1.82	0.44
10:A:849:G:N7	12:D:231:SER:OG	2.43	0.44
25:W:75:ARG:HG3	25:W:118:VAL:HG22	1.99	0.44
5:5:115:HIS:ND1	5:5:117:LYS:HE2	2.33	0.44
10:A:861:U:H5''	10:A:862:U:H5	1.82	0.44
10:A:706:C:H42	10:A:751:G:H1	1.66	0.44
21:S:158:ILE:HA	21:S:161:LEU:HD12	1.99	0.44
12:D:76:PRO:HB3	12:D:105:ARG:HH11	1.83	0.44
10:A:315:U:H2'	10:A:316:A:C8	2.52	0.44
2:1:101:VAL:HG11	10:A:1074:A:H1'	2.00	0.44
9:9:75:ASP:OD2	9:9:91:THR:HG21	2.17	0.44
14:F:277:UNK:HA	14:F:280:UNK:HG3	1.99	0.44
25:W:77:GLN:H	25:W:171:HIS:CE1	2.36	0.44
10:A:842:A:O2'	10:A:871:U:OP1	2.30	0.44
13:E:273:TRP:HB3	13:E:307:LYS:HD3	1.98	0.44
14:F:109:ILE:H	14:F:109:ILE:HG13	1.52	0.44
14:F:276:UNK:HA	14:F:279:UNK:HG3	1.99	0.43
5:5:140:UNK:HA	5:5:143:UNK:HG3	2.00	0.43
25:W:73:HIS:HD2	25:W:118:VAL:HG13	1.83	0.43
10:A:1347:G:H1	10:A:1358:U:H3	1.66	0.43
10:A:1476:U:C4	10:A:1477:G:C5	3.06	0.43
14:F:262:THR:HG23	14:F:264:PRO:HD2	2.00	0.43
10:A:392:A:H2'	10:A:393:C:O4'	2.18	0.43
8:8:124:ARG:NH1	18:P:78:ILE:HD11	2.33	0.43
10:A:609:U:H2'	10:A:610:A:C8	2.53	0.43
13:E:340:VAL:HA	13:E:341:PRO:HD3	1.91	0.43
12:D:179:GLU:HA	12:D:245:VAL:HG23	2.00	0.43
24:V:116:ASP:OD1	24:V:117:LEU:N	2.51	0.43
4:3:76:LYS:HD3	10:A:471:U:C4	2.53	0.43
14:F:276:UNK:O	14:F:279:UNK:HG3	2.17	0.43
5:5:136:UNK:HA	5:5:139:UNK:HG3	1.99	0.43
10:A:94:U:H2'	10:A:95:U:O4'	2.18	0.43
10:A:1308:A:H2'	10:A:1309:G:C8	2.52	0.43
16:N:14:PHE:CZ	16:N:53:CYS:HB2	2.53	0.43
10:A:1053:A:H3'	14:F:131:LYS:HZ3	1.82	0.43
25:W:80:TYR:HD1	25:W:110:LYS:HD2	1.83	0.43
16:N:6:LYS:HG2	24:V:110:TRP:CH2	2.52	0.43
8:8:151:ASN:ND2	10:A:1200:C:H5''	2.34	0.43
10:A:1284:U:H2'	10:A:1285:G:C8	2.53	0.43
10:A:1210:U:H2'	10:A:1211:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1003:G:H5''	25:W:110:LYS:HD3	2.00	0.43
10:A:461:G:H1	10:A:468:C:N4	2.17	0.43
14:F:275:UNK:HA	14:F:278:UNK:HG3	2.00	0.43
14:F:97:HIS:CE1	18:P:29:PRO:HG3	2.53	0.43
2:1:102:ARG:HD2	10:A:48:U:C5	2.53	0.43
19:Q:202:UNK:HA	19:Q:205:UNK:HG3	1.99	0.43
7:7:63:ARG:HH12	10:A:123:U:H4'	1.83	0.43
10:A:1455:A:H4'	10:A:1456:G:H4'	2.01	0.43
10:A:220:A:H2	10:A:223:A:N7	2.17	0.43
10:A:138:G:H1'	27:Y:94:HIS:CE1	2.54	0.43
10:A:372:U:N3	10:A:1248:A:H2	2.17	0.43
19:Q:203:UNK:O	19:Q:206:UNK:HG3	2.18	0.43
21:S:126:GLU:OE2	21:S:160:ARG:HD3	2.19	0.43
10:A:730:A:H4'	10:A:731:A:OP2	2.15	0.43
25:W:197:UNK:HA	25:W:200:UNK:HG3	2.00	0.43
6:6:20:MET:HB2	6:6:29:SER:HB3	2.01	0.43
10:A:1568:C:H5'	13:E:205:HIS:CD2	2.54	0.43
16:N:112:LEU:HD13	16:N:121:MET:HE3	2.00	0.43
10:A:49:A:H5'	10:A:50:A:OP2	2.19	0.43
19:Q:198:UNK:HA	19:Q:201:UNK:HG3	1.99	0.43
3:2:107:LEU:HD12	3:2:144:LEU:HD22	2.00	0.43
24:V:168:THR:OG1	24:V:169:GLU:N	2.52	0.43
16:N:26:GLN:HA	16:N:27:PRO:HD3	1.90	0.43
8:8:105:LYS:HG2	10:A:76:G:C8	2.53	0.43
13:E:273:TRP:CD1	13:E:307:LYS:HB3	2.53	0.43
18:P:81:TYR:HD1	18:P:81:TYR:HA	1.73	0.43
18:P:46:GLY:O	18:P:48:LYS:N	2.50	0.43
10:A:413:A:C6	10:A:414:A:C8	3.07	0.43
10:A:357:U:H5'	18:P:43:ARG:NH1	2.34	0.43
19:Q:199:UNK:O	19:Q:202:UNK:HG3	2.19	0.43
18:P:129:ILE:HG22	18:P:131:PRO:HD3	2.01	0.43
10:A:1378:A:H2'	10:A:1379:A:C8	2.53	0.43
10:A:163:A:OP2	23:U:48:ARG:HD3	2.18	0.42
18:P:101:LEU:O	18:P:105:ILE:HG13	2.18	0.42
10:A:217:A:H4'	10:A:218:A:H5'	2.00	0.42
5:5:139:UNK:HB1	10:A:653:C:H5''	2.01	0.42
13:E:222:PRO:O	13:E:224:LYS:HG2	2.18	0.42
10:A:1334:A:H2'	10:A:1335:G:C8	2.54	0.42
22:T:153:ASN:HD21	22:T:155:ILE:HD11	1.84	0.42
12:D:188:LEU:HD12	12:D:189:PRO:HD2	2.00	0.42
10:A:1205:C:H2'	10:A:1206:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:72:TYR:HD1	25:W:175:LYS:HG2	1.84	0.42
10:A:1040:A:H2'	10:A:1041:A:C8	2.54	0.42
25:W:190:UNK:HA	25:W:193:UNK:HG3	2.00	0.42
14:F:207:ALA:HA	14:F:212:TRP:HD1	1.83	0.42
10:A:1405:U:OP2	10:A:1405:U:H6	2.02	0.42
17:O:99:ARG:N	22:T:161:GLU:O	2.45	0.42
10:A:217:A:N6	10:A:227:U:H4'	2.34	0.42
5:5:129:UNK:O	5:5:132:UNK:HG3	2.19	0.42
12:D:182:ALA:HB2	12:D:244:THR:HG22	2.01	0.42
25:W:138:LEU:HD21	25:W:176:LEU:HD23	2.01	0.42
24:V:171:TRP:HA	24:V:172:PRO:HD3	1.89	0.42
5:5:84:ARG:HH11	23:U:34:ARG:CZ	2.32	0.42
24:V:139:LEU:HG	24:V:158:VAL:HG11	2.01	0.42
22:T:98:ASP:OD2	22:T:145:LEU:HB2	2.19	0.42
21:S:89:HIS:HB3	21:S:107:THR:HB	2.00	0.42
8:8:135:LYS:NZ	10:A:1229:U:OP1	2.44	0.42
19:Q:203:UNK:HA	19:Q:206:UNK:HG3	2.01	0.42
25:W:140:VAL:HG22	25:W:176:LEU:HD11	2.01	0.42
10:A:1191:C:H42	10:A:1208:A:H61	1.68	0.42
10:A:173:C:N3	16:N:50:LEU:HD11	2.35	0.42
16:N:26:GLN:NE2	16:N:31:LEU:HD22	2.35	0.42
10:A:1023:A:H4'	10:A:1024:A:C8	2.55	0.42
10:A:1252:A:H4'	10:A:1253:A:OP2	2.16	0.42
25:W:81:SER:HB3	25:W:110:LYS:HZ1	1.83	0.42
25:W:200:UNK:HA	25:W:203:UNK:HG3	2.02	0.42
13:E:263:GLY:HA2	13:E:313:GLY:HA3	2.02	0.42
6:6:22:SER:HB3	6:6:56:PHE:CZ	2.54	0.42
21:S:131:VAL:O	21:S:135:ARG:HG2	2.19	0.42
10:A:944:C:H2'	10:A:946:A:OP2	2.20	0.42
16:N:44:LYS:HE3	16:N:55:ASP:OD2	2.20	0.42
22:T:114:GLY:HA2	22:T:187:LEU:HD11	2.00	0.42
18:P:100:ARG:O	18:P:104:LEU:HG	2.20	0.42
10:A:329:A:H2'	10:A:330:A:H4'	2.01	0.42
10:A:833:A:H5'	10:A:1429:G:H4'	2.01	0.42
8:8:114:PHE:CZ	18:P:78:ILE:HG13	2.55	0.42
25:W:70:GLU:HG3	25:W:177:VAL:HG22	2.01	0.42
10:A:448:C:O2'	10:A:1317:G:H4'	2.20	0.42
10:A:916:U:H2'	10:A:917:G:C8	2.54	0.42
18:P:104:LEU:HD22	18:P:109:ARG:CZ	2.49	0.42
10:A:720:A:H2'	10:A:721:A:C8	2.54	0.42
14:F:253:MET:HB2	14:F:253:MET:HE3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:118:GLN:HB2	25:W:106:PHE:CE1	2.55	0.42
18:P:47:ARG:HE	18:P:48:LYS:HE2	1.84	0.42
27:Y:56:LEU:HD11	27:Y:62:VAL:HG11	2.02	0.42
26:X:80:ARG:HE	26:X:87:ILE:HD11	1.84	0.42
10:A:364:G:N1	10:A:596:U:OP2	2.36	0.42
17:O:32:ILE:HG13	17:O:86:ILE:HD13	2.02	0.42
24:V:122:ASN:O	24:V:195:THR:OG1	2.26	0.42
21:S:122:VAL:HG11	21:S:160:ARG:HD2	2.02	0.42
24:V:200:ASN:OD1	24:V:201:SER:N	2.53	0.42
17:O:131:GLU:HB2	17:O:134:PHE:HD2	1.85	0.42
16:N:16:ARG:HB2	16:N:55:ASP:HA	2.02	0.41
10:A:236:A:H2'	10:A:237:C:H5''	2.02	0.41
5:5:135:UNK:O	5:5:138:UNK:HG3	2.20	0.41
5:5:127:UNK:O	5:5:130:UNK:HG3	2.19	0.41
19:Q:204:UNK:O	19:Q:207:UNK:HG3	2.20	0.41
10:A:220:A:H5''	14:F:166:PRO:HB3	2.02	0.41
10:A:194:G:H21	23:U:44:ARG:HH22	1.68	0.41
14:F:125:ARG:HB3	14:F:125:ARG:NH1	2.35	0.41
10:A:353:U:O2'	10:A:1053:A:N1	2.53	0.41
24:V:136:LYS:HZ1	24:V:139:LEU:HD23	1.86	0.41
19:Q:191:SER:H	19:Q:194:UNK:CG	2.33	0.41
19:Q:199:UNK:HA	19:Q:202:UNK:HG3	2.02	0.41
13:E:295:SER:OG	13:E:296:THR:N	2.54	0.41
22:T:102:ARG:HG3	22:T:167:TYR:CG	2.55	0.41
10:A:844:C:H2'	10:A:845:U:C6	2.55	0.41
10:A:786:A:N6	20:R:19:GLY:H	2.19	0.41
10:A:766:G:H2'	10:A:767:A:C8	2.55	0.41
10:A:1306:A:H5''	19:Q:184:PRO:HB3	2.01	0.41
19:Q:196:UNK:HA	19:Q:199:UNK:HG3	2.01	0.41
1:0:52:GLY:N	1:0:69:THR:O	2.50	0.41
15:I:134:PRO:HA	15:I:137:LYS:HB3	2.02	0.41
10:A:863:A:H2'	10:A:864:G:C8	2.55	0.41
10:A:51:A:H2'	10:A:52:A:C8	2.55	0.41
8:8:130:LYS:NZ	10:A:1233:C:P	2.94	0.41
10:A:188:A:OP2	10:A:189:U:OP2	2.38	0.41
10:A:353:U:H2'	10:A:354:G:C8	2.55	0.41
19:Q:106:ARG:HG3	19:Q:122:TRP:CZ2	2.55	0.41
8:8:132:LYS:NZ	10:A:1230:G:H2'	2.35	0.41
26:X:56:TYR:CD1	26:X:60:ILE:HD12	2.56	0.41
10:A:461:G:H1	10:A:468:C:H42	1.67	0.41
10:A:298:A:C4'	10:A:299:A:OP2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:28:UNK:HB2	26:X:30:UNK:HG3	5.82	0.41
22:T:119:VAL:HG22	22:T:174:ILE:HG12	2.02	0.41
18:P:20:UNK:HG2	18:P:22:VAL:H	1.85	0.41
10:A:416:G:P	10:A:416:G:H8	2.44	0.41
5:5:84:ARG:HH11	23:U:34:ARG:NH2	2.18	0.41
10:A:1440:U:H5''	13:E:304:PRO:HA	2.02	0.41
10:A:1070:A:N6	10:A:1141:U:H3	2.18	0.41
7:7:88:LYS:HZ2	7:7:90:ARG:HH21	1.66	0.41
10:A:218:A:H2'	10:A:219:G:C8	2.55	0.41
10:A:271:A:C6	10:A:273:A:N7	2.88	0.41
22:T:117:LEU:HD22	22:T:176:VAL:HG22	2.02	0.41
18:P:155:GLU:HA	18:P:175:THR:HB	2.02	0.41
10:A:1160:G:H1	10:A:1176:C:H42	1.69	0.41
10:A:1023:A:H4'	10:A:1024:A:H8	1.86	0.41
14:F:216:VAL:HG22	14:F:258:THR:HB	2.03	0.41
10:A:90:A:H2'	10:A:91:A:C8	2.56	0.41
20:R:33:LEU:HD21	20:R:56:ALA:HA	2.02	0.41
7:7:53:GLY:HA2	10:A:765:G:H21	1.86	0.41
22:T:182:ARG:HA	22:T:204:MET:SD	2.61	0.41
10:A:1002:A:H2'	10:A:1003:G:C8	2.56	0.41
5:5:135:UNK:HA	5:5:138:UNK:HG3	2.03	0.41
10:A:271:A:N6	10:A:275:G:N1	2.69	0.41
6:6:45:HIS:HB3	6:6:56:PHE:CD1	2.55	0.41
14:F:217:LEU:HD23	14:F:259:LEU:HD21	2.03	0.41
10:A:1446:A:C6	10:A:1447:U:C4	3.08	0.41
23:U:109:GLU:HG3	24:V:100:PHE:CZ	2.56	0.41
10:A:1021:U:H2'	10:A:1022:G:C8	2.56	0.41
10:A:11:G:H5''	10:A:12:C:OP2	2.20	0.41
7:7:91:LYS:HE3	7:7:91:LYS:HB2	1.90	0.41
10:A:422:U:C4	10:A:423:U:C4	3.09	0.41
10:A:562:A:N6	10:A:1017:C:O2'	2.53	0.41
14:F:90:ALA:HA	14:F:91:PRO:HD3	1.93	0.41
26:X:27:UNK:HB2	26:X:30:UNK:HG1	2.03	0.41
10:A:1148:G:N2	19:Q:141:GLY:HA3	2.35	0.41
14:F:113:LYS:NZ	14:F:158:PRO:HB3	2.36	0.41
27:Y:84:ASN:HB3	27:Y:117:HIS:CE1	2.56	0.41
13:E:251:PRO:HG3	13:E:326:ARG:HA	2.03	0.41
10:A:1236:A:O2'	10:A:1237:A:OP1	2.28	0.41
18:P:68:GLU:HB3	18:P:71:GLN:HE21	1.86	0.41
26:X:63:VAL:HA	26:X:64:PRO:HD3	1.94	0.41
19:Q:205:UNK:O	19:Q:208:UNK:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:274:A:N6	10:A:722:A:O2'	2.55	0.41
8:8:130:LYS:HE3	18:P:79:PRO:HB3	2.03	0.40
10:A:137:A:O2'	10:A:139:A:C8	2.72	0.40
10:A:985:G:H4'	10:A:986:U:O5'	2.22	0.40
10:A:472:G:H2'	10:A:473:A:C2	2.56	0.40
8:8:124:ARG:HD2	18:P:78:ILE:HD12	2.03	0.40
10:A:461:G:O2'	10:A:485:A:O2'	2.22	0.40
25:W:199:UNK:HA	25:W:202:UNK:HG3	2.03	0.40
10:A:790:G:H2'	10:A:791:A:C8	2.56	0.40
10:A:650:A:H2'	10:A:651:A:C8	2.55	0.40
10:A:1053:A:C2'	14:F:131:LYS:HZ3	2.33	0.40
13:E:256:ASP:OD2	13:E:353:SER:HA	2.21	0.40
17:O:120:LYS:O	17:O:121:THR:OG1	2.31	0.40
22:T:194:LEU:HB2	22:T:197:TYR:HD2	1.85	0.40
10:A:673:U:OP2	10:A:674:A:N6	2.52	0.40
10:A:485:A:H61	10:A:580:C:N4	2.18	0.40
26:X:25:UNK:CG	26:X:43:ARG:HB2	2.51	0.40
10:A:648:A:H4'	10:A:783:A:OP2	2.21	0.40
18:P:113:THR:HG23	18:P:153:ASN:HD22	1.87	0.40
8:8:107:VAL:O	8:8:111:ILE:HG12	2.21	0.40
10:A:1182:G:N2	10:A:1222:C:N3	2.59	0.40
10:A:339:A:OP2	10:A:1065:G:H5'	2.21	0.40
13:E:171:THR:HG21	13:E:340:VAL:HG23	2.04	0.40
13:E:259:ALA:HB3	13:E:341:PRO:HB2	2.04	0.40
10:A:177:C:H4'	23:U:55:ARG:HH12	1.86	0.40
10:A:72:U:HO2'	10:A:73:A:P	2.43	0.40
10:A:1378:A:H2'	10:A:1379:A:H8	1.87	0.40
10:A:232:A:H2'	10:A:233:G:C8	2.57	0.40
25:W:192:UNK:HA	25:W:195:UNK:HG3	2.03	0.40
20:R:48:ARG:O	20:R:52:LEU:HB2	2.21	0.40
10:A:635:A:H2'	10:A:636:A:C8	2.56	0.40
16:N:18:TRP:CD1	16:N:56:HIS:HB3	2.56	0.40
4:3:77:ARG:NH2	10:A:470:U:O4	2.54	0.40
10:A:1054:G:H5''	10:A:1324:A:C2	2.57	0.40
13:E:280:ALA:HA	13:E:288:HIS:ND1	2.36	0.40
27:Y:124:ASP:HA	27:Y:125:PRO:HD3	1.93	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	0	72/148 (49%)	69 (96%)	3 (4%)	0	100	100
2	1	56/256 (22%)	51 (91%)	5 (9%)	0	100	100
3	2	74/252 (29%)	73 (99%)	1 (1%)	0	100	100
4	3	57/161 (35%)	56 (98%)	1 (2%)	0	100	100
5	5	47/146 (32%)	44 (94%)	3 (6%)	0	100	100
6	6	46/65 (71%)	43 (94%)	3 (6%)	0	100	100
7	7	41/95 (43%)	41 (100%)	0	0	100	100
8	8	58/188 (31%)	58 (100%)	0	0	100	100
9	9	34/100 (34%)	34 (100%)	0	0	100	100
12	D	198/306 (65%)	188 (95%)	10 (5%)	0	100	100
13	E	206/399 (52%)	194 (94%)	12 (6%)	0	100	100
14	F	196/224 (88%)	188 (96%)	8 (4%)	0	100	100
15	I	55/268 (20%)	47 (86%)	8 (14%)	0	100	100
16	N	145/178 (82%)	132 (91%)	13 (9%)	0	100	100
17	O	112/145 (77%)	109 (97%)	3 (3%)	0	100	100
18	P	155/288 (54%)	144 (93%)	10 (6%)	1 (1%)	30	74
19	Q	136/208 (65%)	131 (96%)	5 (4%)	0	100	100
20	R	118/169 (70%)	107 (91%)	11 (9%)	0	100	100
21	S	92/180 (51%)	87 (95%)	5 (5%)	0	100	100
22	T	117/292 (40%)	113 (97%)	4 (3%)	0	100	100
23	U	114/132 (86%)	110 (96%)	3 (3%)	1 (1%)	21	67
24	V	104/207 (50%)	97 (93%)	7 (7%)	0	100	100
25	W	109/134 (81%)	106 (97%)	3 (3%)	0	100	100
26	X	68/87 (78%)	68 (100%)	0	0	100	100
27	Y	101/216 (47%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	190/380 (50%)	179 (94%)	10 (5%)	1 (0%)	34	77
29	c	259/301 (86%)	246 (95%)	12 (5%)	1 (0%)	39	80
30	h	239/298 (80%)	220 (92%)	18 (8%)	1 (0%)	39	80
31	i	159/312 (51%)	148 (93%)	11 (7%)	0	100	100
32	l	74/166 (45%)	70 (95%)	3 (4%)	1 (1%)	14	58
34	u	86/205 (42%)	77 (90%)	9 (10%)	0	100	100
All	All	3518/6506 (54%)	3325 (94%)	187 (5%)	6 (0%)	56	86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	l	143	VAL
23	U	14	VAL
28	b	187	VAL
18	P	47	ARG
30	h	223	MET
29	c	71	ASP

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	0	62/115 (54%)	60 (97%)	2 (3%)	46	77
2	1	54/229 (24%)	51 (94%)	3 (6%)	26	65
3	2	72/228 (32%)	72 (100%)	0	100	100
4	3	56/147 (38%)	56 (100%)	0	100	100
5	5	44/108 (41%)	43 (98%)	1 (2%)	58	83
6	6	45/60 (75%)	45 (100%)	0	100	100
7	7	39/78 (50%)	39 (100%)	0	100	100
8	8	54/162 (33%)	52 (96%)	2 (4%)	41	74
9	9	34/77 (44%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	158/248 (64%)	158 (100%)	0	100	100
13	E	173/320 (54%)	171 (99%)	2 (1%)	78	90
14	F	166/166 (100%)	161 (97%)	5 (3%)	48	78
15	I	50/228 (22%)	48 (96%)	2 (4%)	38	72
16	N	127/157 (81%)	126 (99%)	1 (1%)	86	93
17	O	99/123 (80%)	97 (98%)	2 (2%)	63	86
18	P	129/235 (55%)	125 (97%)	4 (3%)	47	78
19	Q	111/155 (72%)	106 (96%)	5 (4%)	34	70
20	R	101/143 (71%)	96 (95%)	5 (5%)	30	67
21	S	80/153 (52%)	78 (98%)	2 (2%)	55	82
22	T	107/258 (42%)	105 (98%)	2 (2%)	65	86
23	U	100/109 (92%)	98 (98%)	2 (2%)	63	86
24	V	94/173 (54%)	92 (98%)	2 (2%)	61	85
25	W	95/95 (100%)	94 (99%)	1 (1%)	80	91
26	X	62/62 (100%)	61 (98%)	1 (2%)	70	88
27	Y	91/192 (47%)	88 (97%)	3 (3%)	45	77
28	b	165/328 (50%)	158 (96%)	7 (4%)	36	71
29	c	236/244 (97%)	228 (97%)	8 (3%)	44	76
30	h	206/230 (90%)	203 (98%)	3 (2%)	72	89
31	i	148/281 (53%)	143 (97%)	5 (3%)	44	76
32	l	68/147 (46%)	63 (93%)	5 (7%)	17	56
34	u	79/177 (45%)	76 (96%)	3 (4%)	40	74
All	All	3105/5428 (57%)	3027 (98%)	78 (2%)	59	82

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	50	ARG
1	0	83	LEU
2	1	96	LYS
2	1	125	VAL
2	1	126	THR
5	5	121	ILE
8	8	129	TYR

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Mol	Chain	Res	Type
8	8	134	TRP
13	E	287	THR
13	E	317	ARG
14	F	92	ARG
14	F	114	THR
14	F	159	THR
14	F	203	LEU
14	F	234	THR
15	I	130	VAL
15	I	136	ASN
16	N	11	TRP
17	O	75	LEU
17	O	77	ILE
18	P	61	THR
18	P	81	TYR
18	P	130	GLN
18	P	147	THR
19	Q	77	THR
19	Q	82	PHE
19	Q	83	THR
19	Q	90	LEU
19	Q	149	HIS
20	R	36	LEU
20	R	52	LEU
20	R	74	ARG
20	R	104	TYR
20	R	124	ILE
21	S	117	TYR
21	S	163	HIS
22	T	166	LEU
22	T	177	VAL
23	U	30	HIS
23	U	81	LEU
24	V	148	LEU
24	V	158	VAL
25	W	119	LEU
26	X	56	TYR
27	Y	85	TRP
27	Y	138	THR
27	Y	153	ILE
28	b	179	VAL
28	b	206	TYR

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Mol	Chain	Res	Type
28	b	258	PHE
28	b	297	THR
28	b	298	PHE
28	b	304	TYR
28	b	308	GLN
29	c	69	LYS
29	c	70	THR
29	c	126	THR
29	c	165	ARG
29	c	180	VAL
29	c	207	ILE
29	c	280	VAL
29	c	305	HIS
30	h	184	PHE
30	h	230	GLU
30	h	233	THR
31	i	116	VAL
31	i	149	HIS
31	i	249	GLU
31	i	253	VAL
31	i	256	TYR
32	l	100	ILE
32	l	129	SER
32	l	135	THR
32	l	153	PHE
32	l	157	LEU
34	u	140	ARG
34	u	141	TYR
34	u	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	ASN
1	0	72	HIS
3	2	119	GLN
5	5	83	ASN
8	8	151	ASN
8	8	154	GLN
9	9	99	GLN
12	D	234	GLN
13	E	231	ASN

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Mol	Chain	Res	Type
16	N	26	GLN
16	N	48	HIS
17	O	33	GLN
18	P	26	ASN
18	P	53	HIS
18	P	71	GLN
20	R	31	ASN
23	U	36	ASN
23	U	79	HIS
23	U	89	ASN
24	V	122	ASN
25	W	73	HIS
25	W	130	HIS
25	W	157	HIS
25	W	171	HIS
26	X	73	GLN
26	X	84	ASN
26	X	98	GLN
27	Y	118	ASN
28	b	147	HIS
28	b	191	ASN
28	b	307	HIS
28	b	320	GLN
32	l	92	HIS
32	l	141	ASN
34	u	103	HIS
34	u	122	HIS
34	u	124	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1431/1570 (91%)	368 (25%)	25 (1%)
11	B	0/29	-	-
All	All	1431/1599 (89%)	368 (25%)	25 (1%)

All (368) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	2	C
10	A	5	A

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Mol	Chain	Res	Type
10	A	7	G
10	A	8	C
10	A	46	A
10	A	48	U
10	A	49	A
10	A	50	A
10	A	56	A
10	A	59	A
10	A	64	C
10	A	65	C
10	A	66	U
10	A	67	A
10	A	69	C
10	A	70	A
10	A	73	A
10	A	82	G
10	A	95	U
10	A	96	U
10	A	97	A
10	A	100	C
10	A	101	U
10	A	102	G
10	A	105	G
10	A	108	A
10	A	109	U
10	A	112	A
10	A	116	A
10	A	117	G
10	A	128	A
10	A	131	G
10	A	132	A
10	A	133	U
10	A	138	G
10	A	139	A
10	A	140	A
10	A	142	A
10	A	144	A
10	A	145	A
10	A	147	A
10	A	148	A
10	A	149	A
10	A	150	A

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Mol	Chain	Res	Type
10	A	152	U
10	A	153	A
10	A	154	A
10	A	156	A
10	A	157	A
10	A	160	A
10	A	161	G
10	A	162	C
10	A	163	A
10	A	164	A
10	A	169	U
10	A	171	C
10	A	172	C
10	A	174	C
10	A	179	A
10	A	188	A
10	A	189	U
10	A	191	A
10	A	203	G
10	A	204	A
10	A	205	A
10	A	206	A
10	A	217	A
10	A	218	A
10	A	221	G
10	A	222	A
10	A	227	U
10	A	228	A
10	A	237	C
10	A	238	C
10	A	253	G
10	A	266	A
10	A	270	U
10	A	271	A
10	A	272	A
10	A	273	A
10	A	274	A
10	A	275	G
10	A	293	G
10	A	299	A
10	A	310	A
10	A	321	G

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Mol	Chain	Res	Type
10	A	322	A
10	A	323	G
10	A	328	A
10	A	330	A
10	A	331	G
10	A	338	G
10	A	351	G
10	A	357	U
10	A	358	G
10	A	365	A
10	A	372	U
10	A	379	C
10	A	381	A
10	A	382	C
10	A	390	A
10	A	391	U
10	A	393	C
10	A	394	C
10	A	395	C
10	A	398	A
10	A	399	A
10	A	400	A
10	A	409	U
10	A	413	A
10	A	414	A
10	A	415	U
10	A	417	U
10	A	418	A
10	A	419	U
10	A	421	U
10	A	422	U
10	A	427	A
10	A	432	G
10	A	439	A
10	A	444	A
10	A	445	C
10	A	447	G
10	A	457	A
10	A	458	A
10	A	459	C
10	A	466	A
10	A	468	C

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Mol	Chain	Res	Type
10	A	472	G
10	A	474	C
10	A	478	A
10	A	487	C
10	A	489	U
10	A	490	A
10	A	492	U
10	A	494	C
10	A	560	A
10	A	561	U
10	A	565	C
10	A	566	C
10	A	569	A
10	A	583	A
10	A	584	C
10	A	591	C
10	A	592	C
10	A	594	A
10	A	614	A
10	A	616	A
10	A	617	C
10	A	618	A
10	A	619	U
10	A	626	A
10	A	629	A
10	A	632	G
10	A	648	A
10	A	649	G
10	A	652	G
10	A	655	U
10	A	662	U
10	A	665	C
10	A	668	A
10	A	670	G
10	A	671	C
10	A	673	U
10	A	674	A
10	A	675	C
10	A	682	A
10	A	686	A
10	A	687	A
10	A	688	U

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Mol	Chain	Res	Type
10	A	691	U
10	A	693	U
10	A	694	A
10	A	695	C
10	A	702	U
10	A	703	U
10	A	704	A
10	A	705	A
10	A	706	C
10	A	710	C
10	A	711	A
10	A	713	U
10	A	718	C
10	A	722	A
10	A	723	C
10	A	724	A
10	A	726	C
10	A	731	A
10	A	733	A
10	A	734	C
10	A	735	G
10	A	744	U
10	A	745	U
10	A	746	A
10	A	747	C
10	A	748	A
10	A	752	U
10	A	755	A
10	A	757	C
10	A	766	G
10	A	772	A
10	A	773	C
10	A	774	C
10	A	776	A
10	A	779	A
10	A	780	A
10	A	781	A
10	A	782	G
10	A	787	A
10	A	807	G
10	A	811	A
10	A	812	C

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Mol	Chain	Res	Type
10	A	813	A
10	A	817	A
10	A	823	C
10	A	830	A
10	A	834	A
10	A	841	C
10	A	850	C
10	A	851	A
10	A	853	U
10	A	854	A
10	A	857	A
10	A	861	U
10	A	870	A
10	A	876	G
10	A	887	C
10	A	888	C
10	A	889	A
10	A	894	A
10	A	900	C
10	A	906	A
10	A	907	U
10	A	922	G
10	A	923	G
10	A	931	A
10	A	948	U
10	A	956	U
10	A	960	U
10	A	962	A
10	A	963	A
10	A	964	U
10	A	965	G
10	A	975	G
10	A	985	G
10	A	986	U
10	A	990	U
10	A	1013	C
10	A	1014	C
10	A	1024	A
10	A	1026	A
10	A	1029	C
10	A	1036	A
10	A	1048	C

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Mol	Chain	Res	Type
10	A	1049	G
10	A	1053	A
10	A	1054	G
10	A	1055	A
10	A	1062	G
10	A	1069	U
10	A	1075	A
10	A	1080	U
10	A	1083	A
10	A	1084	A
10	A	1085	A
10	A	1089	U
10	A	1125	A
10	A	1132	A
10	A	1137	C
10	A	1141	U
10	A	1144	G
10	A	1165	C
10	A	1166	A
10	A	1167	A
10	A	1174	C
10	A	1177	C
10	A	1178	G
10	A	1179	A
10	A	1180	G
10	A	1181	U
10	A	1187	U
10	A	1189	A
10	A	1191	C
10	A	1192	U
10	A	1193	A
10	A	1221	U
10	A	1222	C
10	A	1223	A
10	A	1225	U
10	A	1226	U
10	A	1227	A
10	A	1228	U
10	A	1236	A
10	A	1237	A
10	A	1238	A
10	A	1244	A

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Mol	Chain	Res	Type
10	A	1247	A
10	A	1250	G
10	A	1251	G
10	A	1252	A
10	A	1253	A
10	A	1256	A
10	A	1260	A
10	A	1262	C
10	A	1266	G
10	A	1269	A
10	A	1297	C
10	A	1325	U
10	A	1326	G
10	A	1327	U
10	A	1339	A
10	A	1341	C
10	A	1350	G
10	A	1376	U
10	A	1377	C
10	A	1387	A
10	A	1388	G
10	A	1394	C
10	A	1405	U
10	A	1406	U
10	A	1407	C
10	A	1409	G
10	A	1420	U
10	A	1423	A
10	A	1424	G
10	A	1430	U
10	A	1431	U
10	A	1432	U
10	A	1434	U
10	A	1436	U
10	A	1442	A
10	A	1443	U
10	A	1446	A
10	A	1456	G
10	A	1466	A
10	A	1467	C
10	A	1474	A
10	A	1480	A

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Mol	Chain	Res	Type
10	A	1483	A
10	A	1488	C
10	A	1490	C
10	A	1491	A
10	A	1492	A
10	A	1493	A
10	A	1496	C
10	A	1504	A
10	A	1508	A
10	A	1509	A
10	A	1510	U
10	A	1527	A
10	A	1530	U
10	A	1531	A
10	A	1532	A
10	A	1537	C
10	A	1540	A
10	A	1541	U
10	A	1543	A
10	A	1545	A
10	A	1547	A
10	A	1548	U
10	A	1549	C
10	A	1551	A
10	A	1556	U
10	A	1557	A
10	A	1565	G
10	A	1567	A
10	A	1568	C
10	A	1569	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1	A
10	A	66	U
10	A	72	U
10	A	115	U
10	A	273	A
10	A	298	A
10	A	418	A
10	A	618	A

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Mol	Chain	Res	Type
10	A	672	U
10	A	702	U
10	A	730	A
10	A	746	A
10	A	751	G
10	A	756	C
10	A	786	A
10	A	860	A
10	A	985	G
10	A	1013	C
10	A	1079	U
10	A	1166	A
10	A	1236	A
10	A	1252	A
10	A	1375	U
10	A	1566	C
10	A	1568	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.