



Full wwPDB EM Model Validation Report ⓘ

Apr 15, 2020 – 01:08 PM EDT

PDB ID : 6W2S
EMDB ID : EMD-21529
Title : Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES)
bound to the small ribosomal subunit in the open state (Class 1)
Authors : Neupane, R.; Pisareva, V.; Rodriguez, C.F.; Pisarev, A.; Fernandez, I.S.
Deposited on : 2020-03-08
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

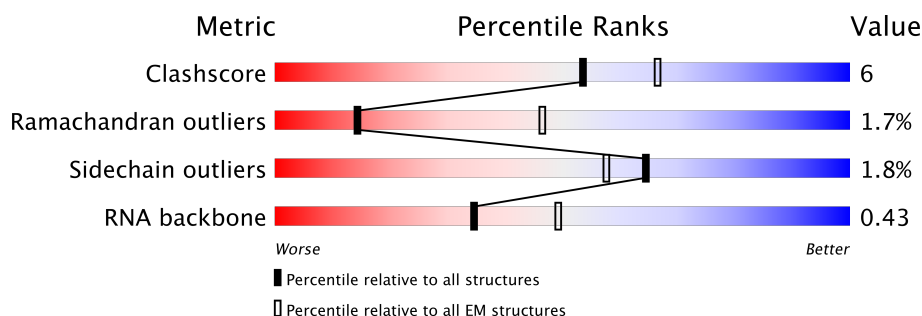
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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













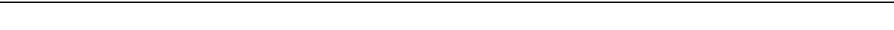

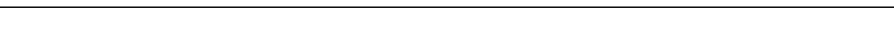
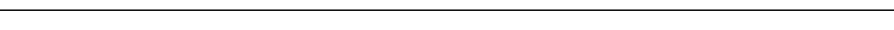











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 respectively. 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	1697	69% 27% .
2	O	377	33% 44% 13% . 10%
3	B	295	65% 7% . 26%
4	C	264	76% 5% 19%
5	D	255	82% 5% 13%
6	F	263	94% 5%
7	H	249	87% 7% . 5%

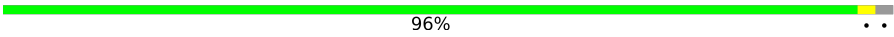

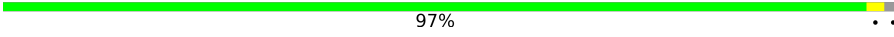

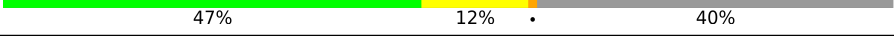


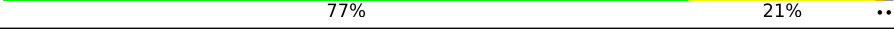
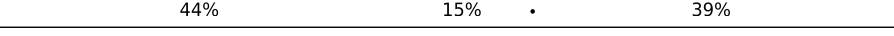

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Mol	Chain	Length	Quality of chain
8	I	194	 87% 8% 5%
9	J	208	 90% 9% .
10	K	194	 92% . 5%
11	M	158	 81% 9% 9%
12	O	151	 91% 8% .
13	P	151	 84% 6% 10%
14	W	83	 92% 8%
15	X	130	 93% . .
16	Y	143	 88% 10% ..
17	Z	134	 87% 6% 7%
18	b	115	 83% . 12%
19	c	84	 98% ..
20	f	133	 43% 57%
21	E	281	 75% 6% 19%
22	G	204	 82% 11% 6%
23	L	149	 56% 9% 36%
24	N	132	 68% 20% . 11%
25	Q	145	 61% 17% . 21%
26	R	172	 76% 6% . 17%
27	S	135	 79% 19% ..
28	T	152	 78% 16% 5%
29	U	145	 90% 7% .
30	V	119	 81% . 16%
31	a	125	 60% 40%
32	d	69	 90% 10%

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Mol	Chain	Length	Quality of chain
33	e	56	 96% ..
34	g	156	 40% . 56%
35	h	317	 97% ..
36	1	1362	 28% 10% . 61%
37	2	913	 47% 12% . 40%
38	3	462	 65% 22% . 9%
39	4	364	 46% 26% . 25%
40	5	363	 55% 30% 5% 11%
41	6	218	 77% 21% ..
42	7	607	 44% 15% . 39%
43	8	374	 68% 26% . .

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 106911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 2 is a RNA chain called CrPV 5'-UTR IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	339	Total	C	N	O	P	0	0
			7205	3222	1255	2389	339		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	569	U	C	conflict	GB 8895506
0	570	U	C	conflict	GB 8895506
0	571	U	A	conflict	GB 8895506
0	572	U	C	conflict	GB 8895506
0	574	U	C	conflict	GB 8895506
0	575	U	G	conflict	GB 8895506
0	729	G	-	expression tag	GB 8895506
0	730	G	-	expression tag	GB 8895506
0	731	A	-	expression tag	GB 8895506
0	732	U	-	expression tag	GB 8895506
0	733	C	-	expression tag	GB 8895506

- Molecule 3 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1706	1084	296	318	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TWL4
B	135	THR	MET	conflict	UNP G1TWL4
B	155	ARG	HIS	conflict	UNP G1TWL4
B	162	PRO	LEU	conflict	UNP G1TWL4

- Molecule 4 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	221	Total	C	N	O	S	0	0
			1717	1113	296	299	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	57	ASN	ASP	conflict	UNP G1SWM1
D	97	PHE	CYS	conflict	UNP G1SWM1
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	262	Total	C	N	O	S	0	0
			2072	1323	384	357	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 8 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 9 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 10 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 11 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 12 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 13 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 14 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	83	Total	C	N	O	S	0	0
			634	390	116	123	5		

- Molecule 15 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 16 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 17 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 18 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	101	Total	C	N	O	S	0	0
			816	509	170	132	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8

- Molecule 19 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 20 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 21 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 22 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	191	Total	C	N	O	S	0	0
			1499	937	283	272	7		

- Molecule 23 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 24 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 25 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	115	Total	C	N	O	S	0	0
			956	610	176	163	7		

- Molecule 26 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 27 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 28 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 29 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 30 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 31 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 33 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 34 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 35 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	534	Total	C	N	O	S	0	0
			4377	2770	778	808	21		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	547	Total	C	N	O	S	0	0
			4446	2791	785	837	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	671	GLU	VAL	conflict	UNP G1U971

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	7	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

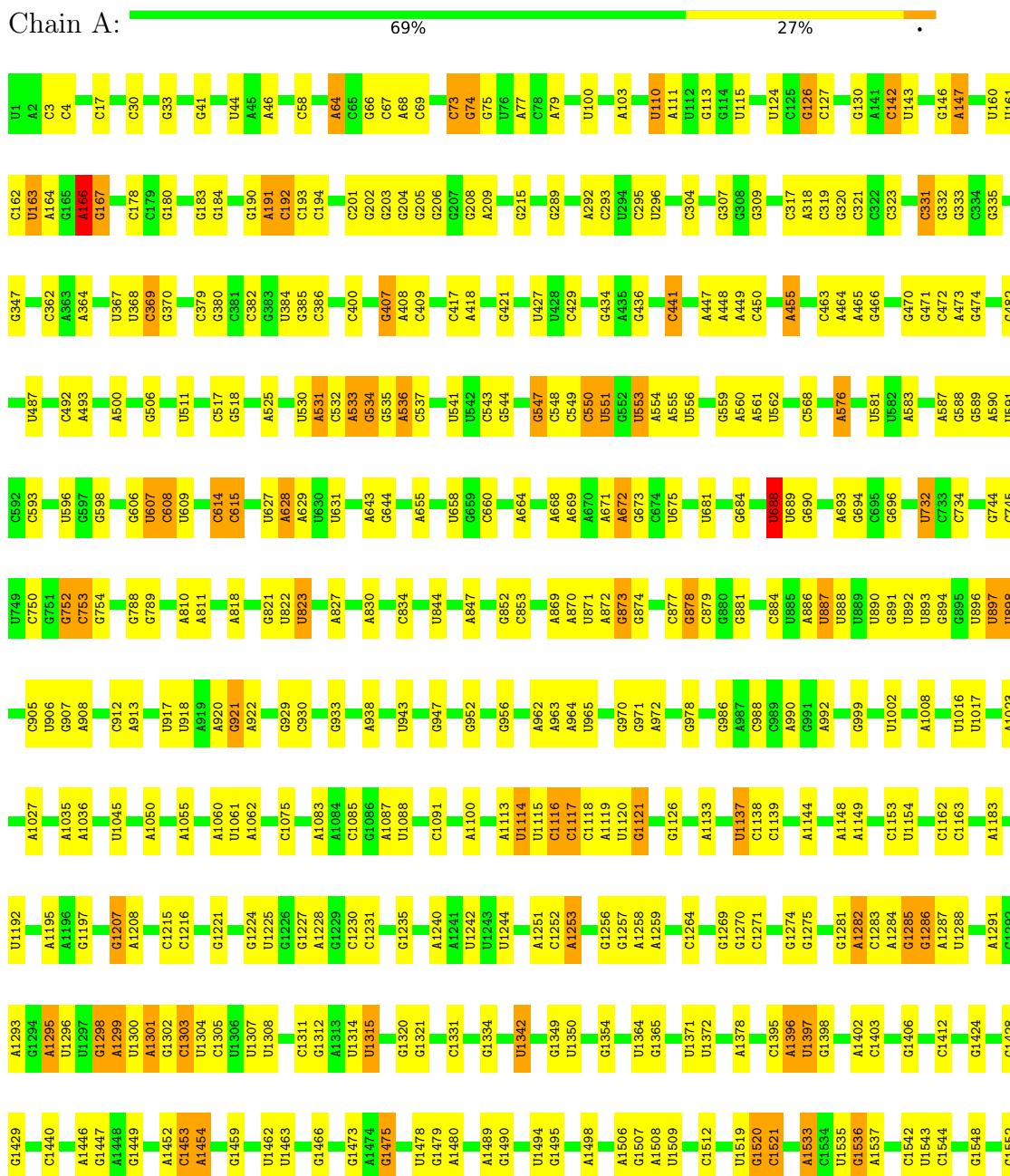
- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

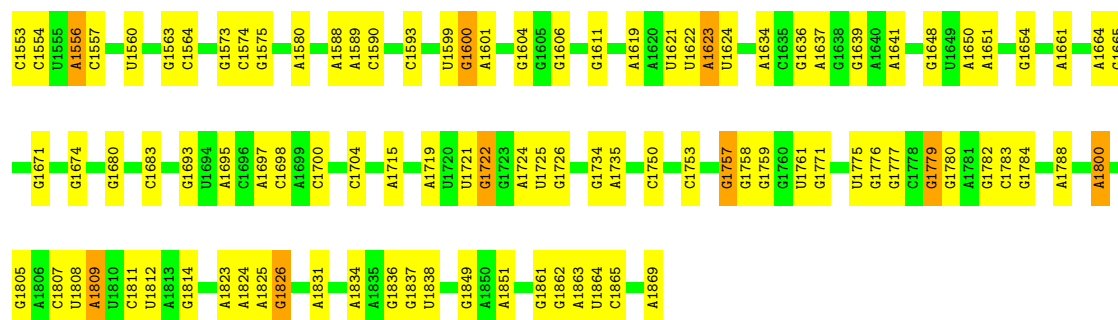
Mol	Chain	Residues	Atoms		AltConf
45	b	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

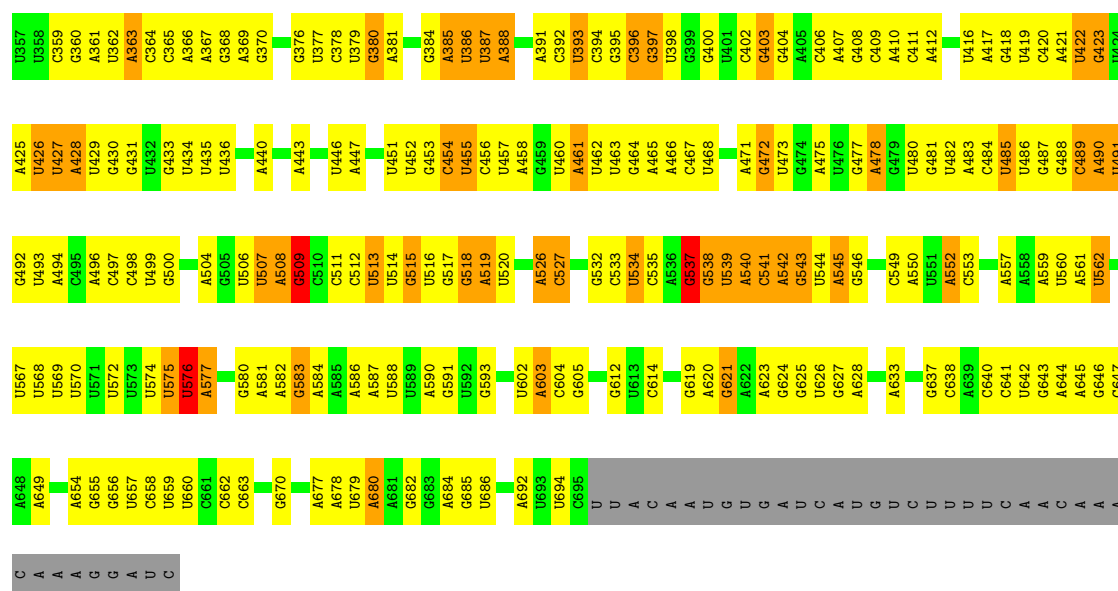
- Molecule 1: 18S rRNA





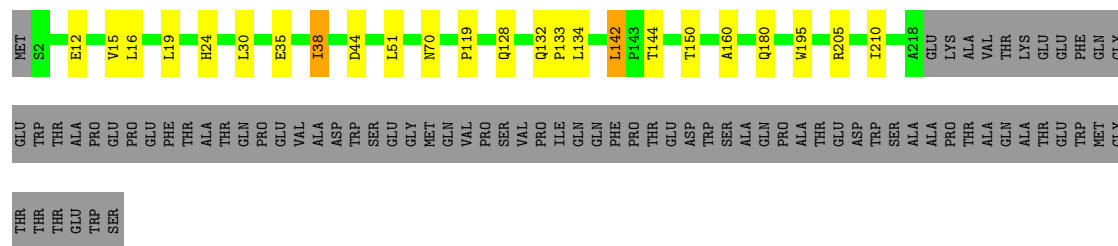
• Molecule 2: CrPV 5'-UTR IRES

Chain 0: 33% 44% 13% 10%



• Molecule 3: uS2

Chain B: 65% 7% 26%




• Molecule 4: eS1

Chain C: 76% 5% 19%



ALA
LYS
VAL
GLU
ARG
ALA
ASP
GLY
TYR
GLU
PRO
PRO
VAL
GLN
GLU
SER
SER
VAL

• Molecule 5: uS5

Chain D:  82% 5% 13%

MET
ALA
ASP
ASP
ALA
GLY
ALA
ALA
ALA
GLY
GLY
PRO
GLY
GLY
PRO
GLY
GLY
PRO
ASN
K69
L66
I81
R117
F127
L141
K211
K212
L213
L214
L215
A237
K238
Y248
K274
K278
ARG
VAL
SER
VAL
GLN
ARG
THR
GLN
ALA
PRO
ALA
VAL
ALA
THR

• Molecule 6: eS4

Chain F:  94% 5%


MET
A2
H17
L44
K51
I72
R108
V111
I129
F130
H138
L139
R191
R245
L256
K259
G263

• Molecule 7: eS6

Chain H:  87% 7% 5%


M1
P8
V49
Y84
R98
V102
L106
L109
V114
K115
K116
T125
R159
N163
K164
P169
R170
T171
K172
A173
Q186
T199
K200
K201
L237
ARG
ALA
SER
THR
SER
LYS
SER
GLU
SER
SER
GLN
LYS

• Molecule 8: eS7

Chain I:  87% 8% 5%


MET
PHE
SER
SER
A6
F19
A38
R41
E50
I60
L69
E82
S88
V92
A96
I100
S108
ARG
THR
LYS
ASN
K113
L122
R143
H157
E188
L194

• Molecule 9: eS8

Chain J:  90% 9%


MET
G2
R5
I33
R56
A57
T76
V81
K94
I101
V102
P108
R123
T130
P131
R141
I145
R178
G183
L190
G207
LYS

• Molecule 10: uS4

Chain K:  92% 5%


MET
P2
V46
L50
R80
F105
L106
P170
R175
G186
ALA
GLY
ASP
ASP
GLU
GLU
GLU
ASP

• Molecule 11: uS17

Chain M:  81% 9% 9%


MET
ALA
D3
Y10
Q18
V23
LEU
GLY
GLY
THR
GLY
LYS
GLU
K32
L33
P34
L42
P47
R69
I72
N80
R101
C116
V120
V126
T127
V128
V145
K153
GLN
PHE
GLN
LYS
PHE

- Molecule 12: uS15

Chain O:  91% 8%



- Molecule 13: uS11

Chain P:  84% 6% 10%



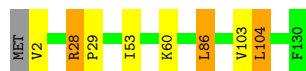
- Molecule 14: eS21

Chain W:  92% 8%




- Molecule 15: uS8

Chain X:  93%




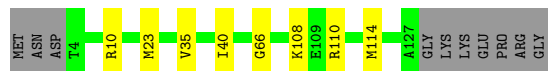
- Molecule 16: uS12

Chain Y:  88% 10%




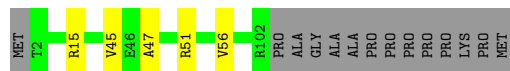
- Molecule 17: eS24

Chain Z:  87% 6% 7%



- Molecule 18: eS26

Chain b:  83% 12%



- Molecule 19: eS27

MET P2 A50 H84

- | | |
|------|-----|
| ALA | MET |
| LEU | GLN |
| SER | LEU |
| THR | PHE |
| LEU | VAL |
| GLU | ARG |
| VAL | GLN |
| ALA | ALA |
| GLY | GLU |
| ARG | LEU |
| MET | HIS |
| LEU | THR |
| GLY | LEU |
| GLY | GLU |
| LYS | VAL |
| VAL | THR |
| H76 | GLY |
| S132 | ARG |
| | GLU |
| | THR |
| | VAL |
| | ALA |
| | GLN |
| | LYS |
| | ILE |
| | ALA |
| | HIS |
| | VAL |
| | SER |
| | ALA |
| | LEU |
| | GLU |
| | GLY |
| | ILE |
| | ALA |
| | PRO |
| | GLU |
| | ASP |
| | GLN |
| | VAL |
| | VAL |
| | LEU |
| | LEU |
| | ALA |
| | GLY |
| | THR |
| | THR |
| | PRO |
| | LEU |
| | GLU |
| | ASP |
| | GLU |
| | ALA |
| | THR |
| | LEU |
| | GLY |
| | GLN |
| | CYS |
| | GLY |
| | VAL |
| | GLU |

- | | | |
|------|------|------|
| V175 | G228 | MET |
| R178 | GLY | SER |
| L182 | LYS | ALA |
| G183 | PRO | ARG |
| P191 | GLU | ARG |
| G199 | PRO | ARG |
| | PRO | ALA |
| | ALA | ALA |
| | MET | PHE |
| | THR | ARG |
| | ALA | ARG |
| | VAL | ALA |
| | THR | GLY |
| | ALA | LYS |
| | | M1 |
| | | I5 |
| | | K10 |
| | | K62 |
| | | R67 |
| | | V72 |
| | | R76 |
| | | I126 |
| | | C134 |
| | | D162 |
| | | P163 |

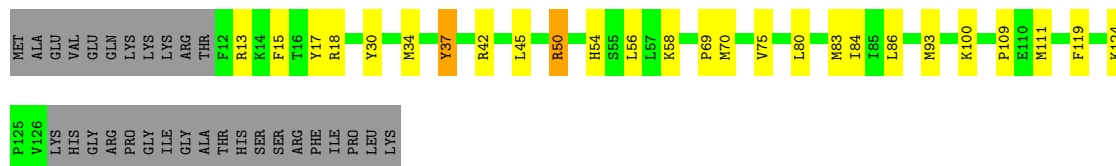
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| NET | THR | GLU | TRP | GLU | THR | ALA | ALA | ALA | PRO | ALA | VAL | ALA | GLU | GLU | T14 | F20 | I30 | L35 | I39 | A40 | Y45 | P50 | H51 | I68 | V69 | T73 | T89 | V90 | T104 | I117 | G129 | V134 | V141 | S142 | R146 | V147 | K167 | S187 | I190 | F204 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|

- | Position | Residue | Conservation |
|----------|---------|--------------|
| 1 | ALA | MI |
| 2 | VAL | Y12 |
| 3 | PRO | E13 |
| 4 | PRO | L14 |
| 5 | GLY | |
| 6 | ALA | |
| 7 | ASP | G19 |
| 8 | LYS | V20 |
| 9 | LYS | H32 |
| 10 | ALA | |
| 11 | GLU | V45 |
| 12 | ALA | |
| 13 | GLY | S51 |
| 14 | ALA | L52 |
| 15 | GLY | |
| 16 | SER | R55 |
| 17 | ALA | |
| 18 | ALA | |
| 19 | THR | K59 |
| 20 | GLU | |
| 21 | | Y70 |
| 22 | | L71 |
| 23 | | |
| 24 | | I76 |
| 25 | | |
| 26 | | R96 |
| 27 | SER | |
| 28 | ARG | |
| 29 | PRO | |
| 30 | GLU | |
| 31 | THR | |
| 32 | GLY | |
| 33 | GLY | |
| 34 | ARG | |
| 35 | PRO | |
| 36 | PRO | |
| 37 | ARG | |
| 38 | PRO | |
| 39 | LYS | |
| 40 | GLY | |
| 41 | LEU | |
| 42 | GLU | |
| 43 | GLY | |
| 44 | GLU | |
| 45 | SER | |
| 46 | ARG | |
| 47 | PRO | |
| 48 | ALA | |
| 49 | ALA | |
| 50 | ARG | |
| 51 | LEU | |
| 52 | THR | |
| 53 | ARG | |
| 54 | GLY | |
| 55 | GLU | |
| 56 | ALA | |
| 57 | ASP | |
| 58 | ARG | |
| 59 | ASP | |
| 60 | THR | |
| 61 | THR | |
| 62 | ARG | |
| 63 | ARG | |
| 64 | ARG | |
| 65 | SER | |


- [illegible]

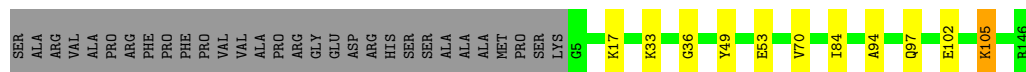
- Molecule 25: uS19

Chain Q:  61% 17% 21%




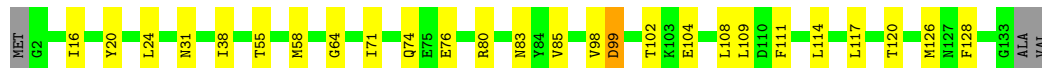
- Molecule 26: uS9

Chain R:  76% 6% 17%




- Molecule 27: eS17

Chain S:  79% 19% 2%




- Molecule 28: uS13

Chain T:  78% 16% 5%




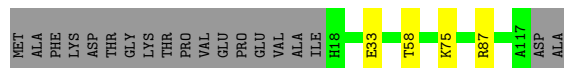
- Molecule 29: eS19

Chain U:  90% 7% 3%



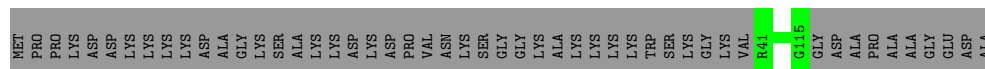
- Molecule 30: uS10

Chain V:  81% 16% 3%

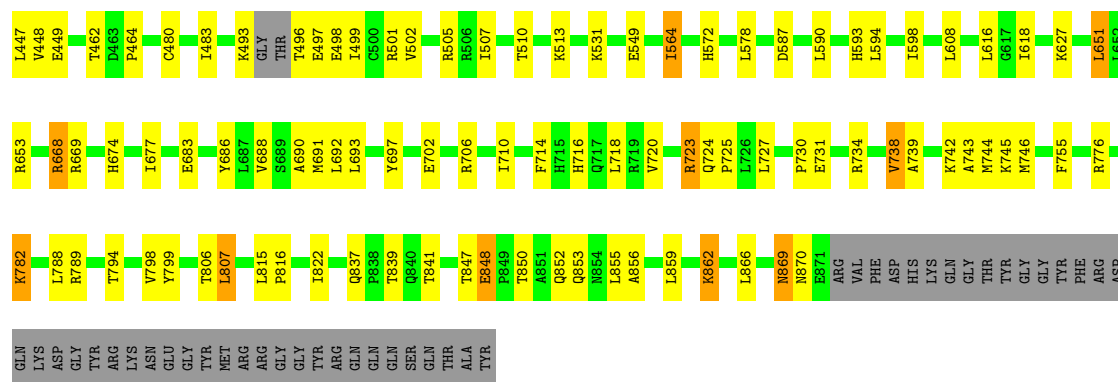


- Molecule 31: eS25

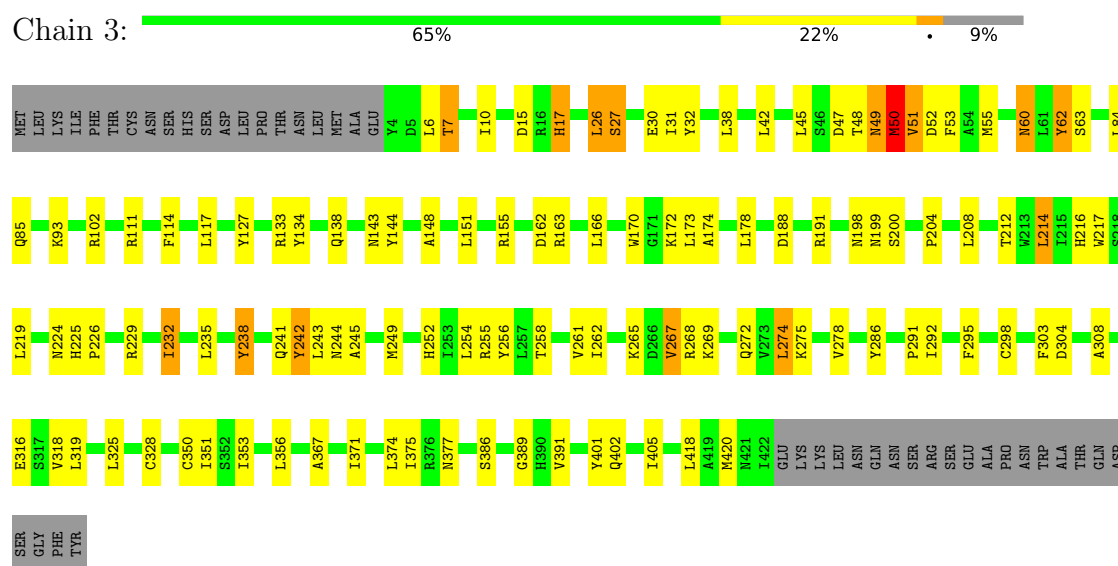
Chain a:  60% 40%



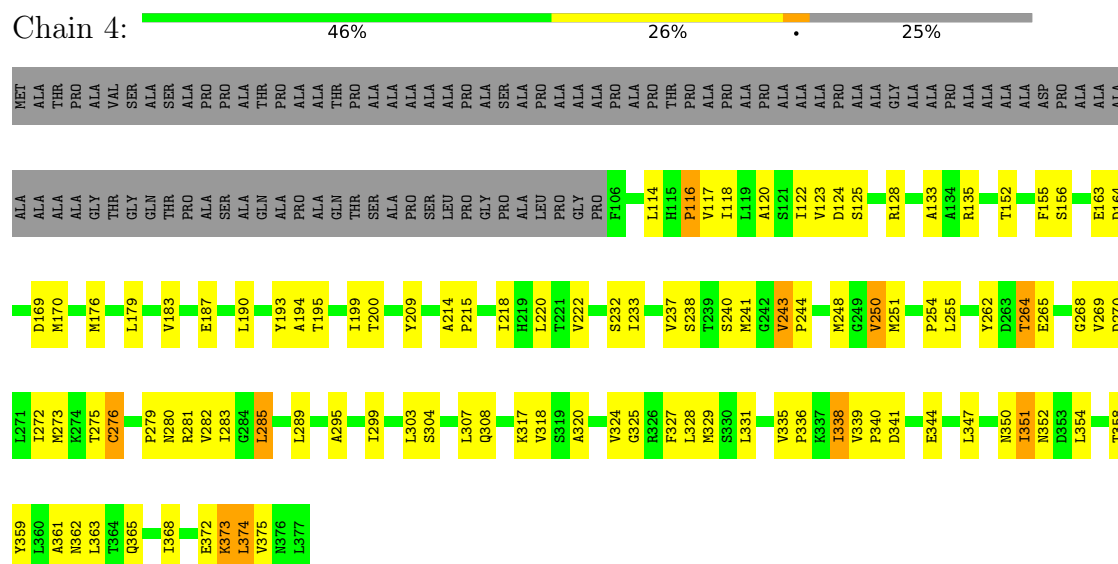




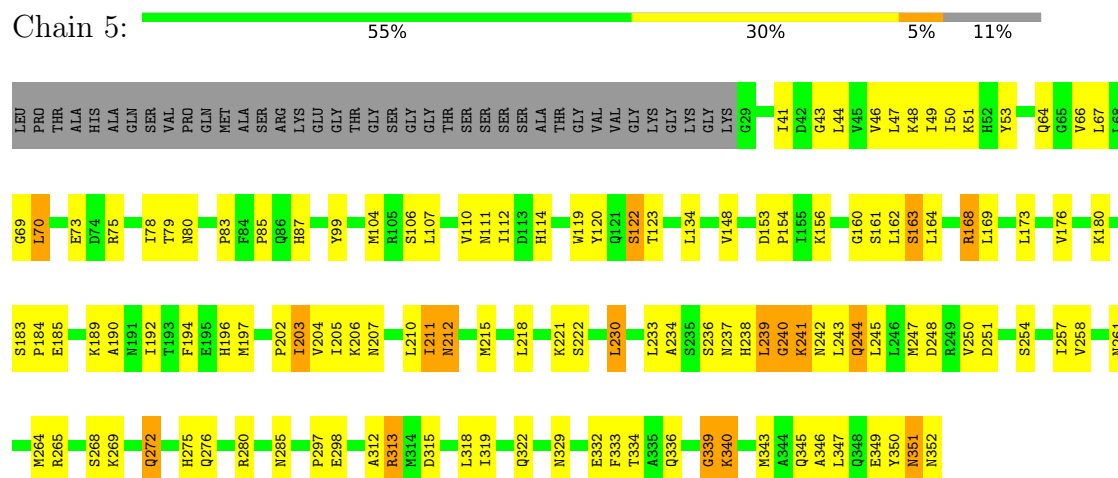
• Molecule 38: Eukaryotic translation initiation factor 3 subunit E



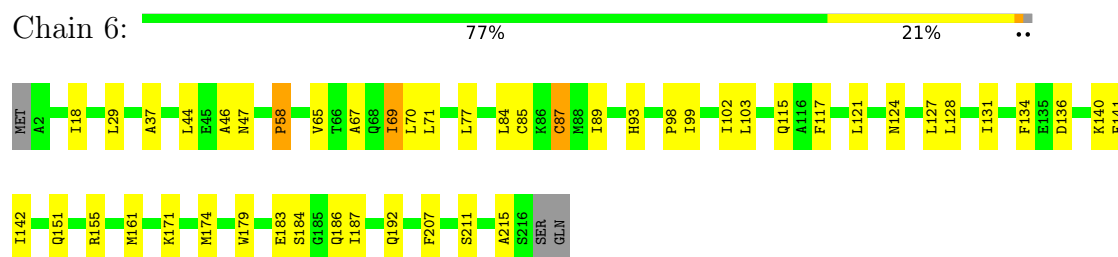
• Molecule 39: Eukaryotic translation initiation factor 3 subunit F



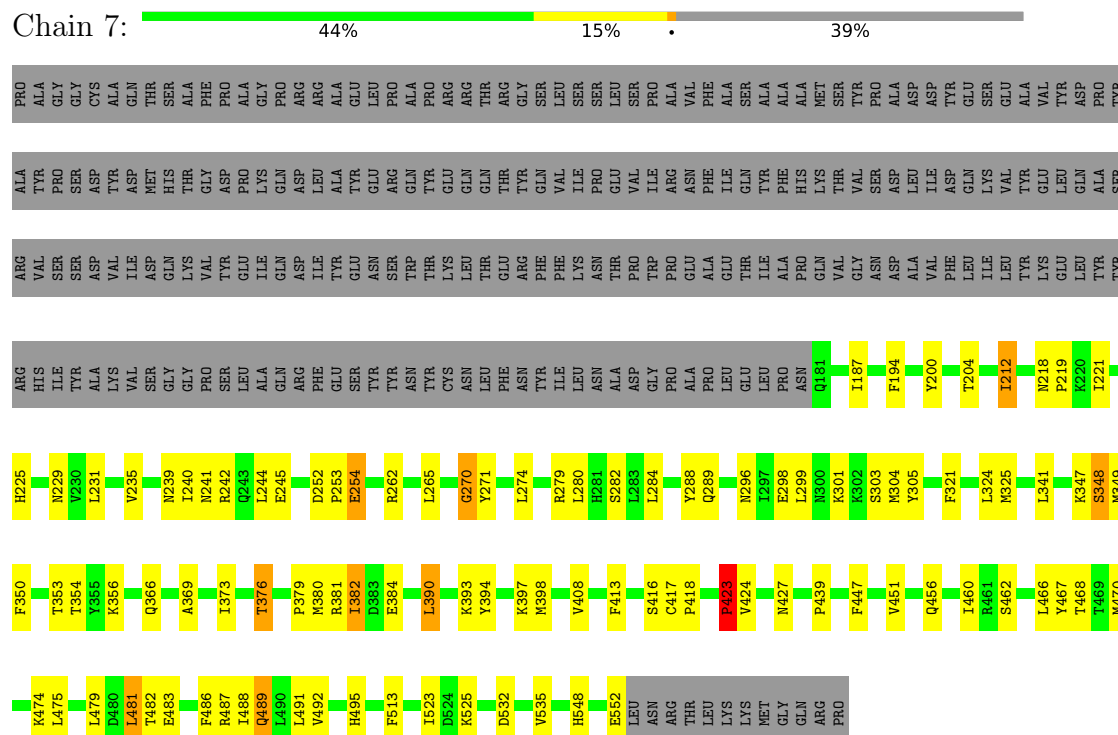
- Molecule 40: Eukaryotic translation initiation factor 3 subunit H



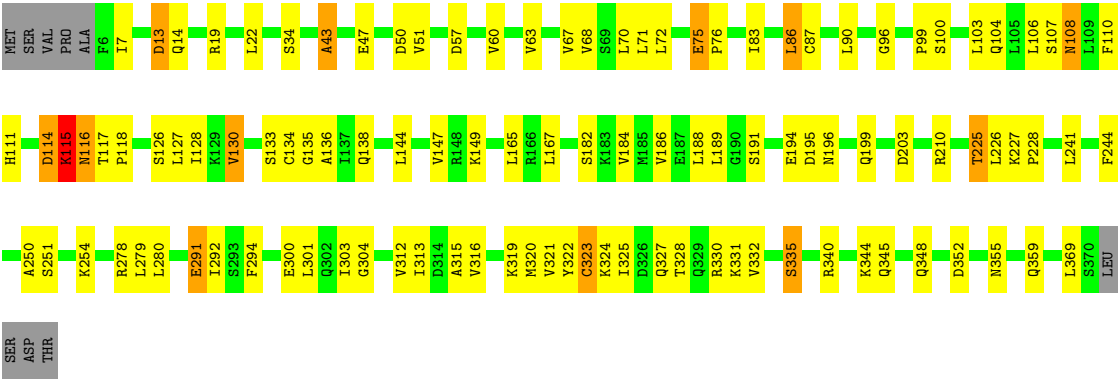
- Molecule 41: Eukaryotic translation initiation factor 3 subunit K



- Molecule 42: Eukaryotic translation initiation factor 3 subunit L



● Molecule 43: Eukaryotic translation initiation factor 3 subunit M



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36100	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 ($e^-/\text{\AA}^2$)	56.90	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/40505	0.69	5/63112 (0.0%)
2	O	0.30	2/8053 (0.0%)	0.77	2/12543 (0.0%)
3	B	0.67	0/1743	0.78	0/2370
4	C	0.67	0/1756	0.78	0/2350
5	D	0.67	0/1754	0.78	0/2370
6	F	0.67	0/2114	0.79	0/2843
7	H	0.68	0/1946	0.83	0/2590
8	I	0.68	0/1510	0.79	0/2022
9	J	0.67	0/1715	0.82	0/2287
10	K	0.67	0/1550	0.80	0/2069
11	M	0.66	0/1195	0.80	0/1597
12	O	0.67	0/1226	0.79	0/1649
13	P	0.69	0/1029	0.82	0/1380
14	W	0.70	0/641	0.82	0/858
15	X	0.67	0/1051	0.79	0/1406
16	Y	0.68	0/1116	0.81	0/1490
17	Z	0.67	0/1028	0.80	0/1366
18	b	0.66	0/830	0.82	0/1112
19	c	0.67	0/665	0.81	0/891
20	f	0.68	0/462	0.86	0/607
21	E	0.69	0/1796	0.81	0/2417
22	G	0.70	0/1521	0.81	0/2046
23	L	0.65	0/834	0.77	0/1125
24	N	0.70	0/918	0.81	0/1233
25	Q	0.67	0/974	0.85	0/1301
26	R	0.69	0/1146	0.81	0/1534
27	S	0.69	0/1082	0.83	0/1452
28	T	0.68	0/1208	0.82	0/1618
29	U	0.69	0/1115	0.79	0/1493
30	V	0.69	0/805	0.81	0/1081
31	a	0.69	0/604	0.81	0/810
32	d	0.70	0/490	0.85	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.67	0/470	0.79	0/623
34	g	0.68	0/567	0.84	0/753
35	h	0.69	0/2486	0.80	0/3384
36	1	0.68	0/4460	0.81	0/6034
37	2	0.69	0/4522	0.82	1/6102 (0.0%)
38	3	0.69	0/3538	0.83	0/4786
39	4	0.71	1/2149 (0.0%)	0.89	0/2920
40	5	0.67	0/2674	0.88	1/3606 (0.0%)
41	6	0.73	1/1772 (0.1%)	0.79	1/2396 (0.0%)
42	7	0.71	2/3185 (0.1%)	0.86	3/4296 (0.1%)
43	8	0.71	0/2963	0.85	1/3998 (0.0%)
All	All	0.54	6/113168 (0.0%)	0.77	14/162576 (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
16	Y	0	1
18	b	0	1
22	G	0	1
25	Q	0	1
27	S	0	1
36	1	0	4
37	2	0	4
38	3	0	6
39	4	0	3
40	5	0	6
42	7	0	3
43	8	0	4
All	All	0	35

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	69	ILE	CG1-CD1	-7.53	0.98	1.50
42	7	187	ILE	CG1-CD1	-6.45	1.05	1.50
39	4	351	ILE	CG1-CD1	6.23	1.93	1.50
2	0	509	G	C1'-N9	-5.98	1.38	1.46
2	0	576	U	C1'-N1	5.62	1.57	1.48
42	7	382	ILE	CG1-CD1	-5.04	1.15	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	7	382	ILE	CB-CG1-CD1	9.61	140.82	113.90
42	7	240	ILE	CB-CG1-CD1	8.06	136.47	113.90
42	7	187	ILE	CB-CG1-CD1	7.27	134.25	113.90
1	A	688	U	C2'-C3'-O3'	6.76	124.51	113.70
1	A	166	A	C2'-C3'-O3'	6.62	124.30	113.70
2	0	485	U	C2'-C3'-O3'	6.46	124.04	113.70
43	8	115	LYS	CB-CA-C	5.90	122.19	110.40
1	A	1137	U	C2'-C3'-O3'	5.88	123.10	113.70
40	5	238	HIS	CB-CA-C	5.75	121.89	110.40
41	6	69	ILE	CB-CG1-CD1	5.69	129.82	113.90
2	0	537	G	N9-C1'-C2'	5.57	121.23	114.00
37	2	587	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	1295	A	C2'-C3'-O3'	5.20	122.03	113.70
1	A	110	U	C2'-C3'-O3'	5.01	121.72	113.70

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	1	165	ARG	Peptide
36	1	483	ARG	Peptide
36	1	498	ASN	Peptide
36	1	514	MET	Peptide
37	2	564	ILE	Peptide
37	2	651	LEU	Peptide
37	2	716	HIS	Peptide
37	2	782	LYS	Peptide
38	3	27	SER	Peptide
38	3	278	VAL	Peptide
38	3	47	ASP	Peptide
38	3	49	ASN	Peptide
38	3	50	MET	Peptide
38	3	60	ASN	Peptide
39	4	243	VAL	Peptide
39	4	373	LYS	Peptide
39	4	374	LEU	Peptide
40	5	122	SER	Peptide
40	5	180	LYS	Peptide
40	5	210	LEU	Peptide
40	5	221	LYS	Peptide
40	5	272	GLN	Peptide

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Mol	Chain	Res	Type	Group
40	5	312	ALA	Peptide
42	7	225	HIS	Peptide
42	7	376	THR	Peptide
42	7	423	PRO	Peptide
43	8	115	LYS	Peptide
43	8	117	THR	Peptide
43	8	13	ASP	Peptide
43	8	332	VAL	Peptide
22	G	129	GLY	Peptide
25	Q	54	HIS	Peptide
27	S	64	GLY	Peptide
16	Y	61	GLN	Peptide
18	b	45	VAL	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	36229	0	18304	152	0
2	0	7205	0	3626	54	0
3	B	1706	0	1698	18	0
4	C	1729	0	1803	5	0
5	D	1717	0	1812	17	0
6	F	2072	0	2175	9	0
7	H	1923	0	2089	13	0
8	I	1488	0	1582	7	0
9	J	1686	0	1772	12	0
10	K	1525	0	1640	4	0
11	M	1175	0	1249	7	0
12	O	1202	0	1289	5	0
13	P	1016	0	1039	5	0
14	W	634	0	629	4	0
15	X	1034	0	1080	5	0
16	Y	1098	0	1167	7	0
17	Z	1011	0	1083	5	0
18	b	816	0	867	0	0
19	c	651	0	672	0	0
20	f	457	0	502	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	1768	0	1866	11	0
22	G	1499	0	1540	10	0
23	L	810	0	836	6	0
24	N	908	0	939	13	0
25	Q	956	0	1002	13	0
26	R	1128	0	1195	6	0
27	S	1068	0	1121	17	0
28	T	1190	0	1249	16	0
29	U	1097	0	1130	5	0
30	V	795	0	862	3	0
31	a	598	0	656	0	0
32	d	488	0	514	0	0
33	e	459	0	452	0	0
34	g	555	0	567	0	0
35	h	2429	0	2386	0	0
36	1	4377	0	4433	151	0
37	2	4446	0	4444	118	0
38	3	3465	0	3446	69	0
39	4	2111	0	2105	169	0
40	5	2624	0	2591	249	0
41	6	1737	0	1706	33	0
42	7	3109	0	3084	65	0
43	8	2918	0	2950	66	0
44	A	1	0	0	0	0
45	b	1	0	0	0	0
All	All	106911	0	87152	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1080) 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)
5:D:127:PHE:CD1	5:D:141:LEU:HD21	1.26	1.61
5:D:127:PHE:CD1	5:D:141:LEU:CD2	1.95	1.50
36:1:523:LEU:HA	36:1:526:MET:SD	1.71	1.30
37:2:710:ILE:O	37:2:714:PHE:HD2	1.09	1.29
36:1:526:MET:HG2	40:5:236:SER:O	1.26	1.28
36:1:526:MET:CB	40:5:237:ASN:HA	1.64	1.28
37:2:710:ILE:O	37:2:714:PHE:CD2	1.88	1.27
39:4:351:ILE:HA	40:5:343:MET:SD	1.82	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:710:ILE:HB	37:2:714:PHE:CE2	1.81	1.15
39:4:354:LEU:HD12	40:5:343:MET:SD	1.86	1.15
36:1:526:MET:HB3	40:5:237:ASN:HA	1.18	1.14
36:1:526:MET:CG	40:5:237:ASN:HA	1.77	1.13
36:1:526:MET:HB3	40:5:237:ASN:CA	1.81	1.11
37:2:493:LYS:HG2	37:2:498:GLU:OE2	1.60	1.02
36:1:534:LEU:HB2	40:5:230:LEU:HD13	1.40	1.01
39:4:365:GLN:HG3	40:5:329:ASN:HB3	1.44	1.00
39:4:124:ASP:C	40:5:111:ASN:HD21	1.65	0.99
36:1:530:LEU:HD21	40:5:234:ALA:HB2	1.45	0.98
39:4:358:THR:HG22	40:5:336:GLN:HA	1.49	0.94
5:D:127:PHE:CE1	5:D:141:LEU:HD21	2.03	0.93
39:4:279:PRO:HA	39:4:280:ASN:HB3	1.51	0.93
37:2:493:LYS:CG	37:2:498:GLU:OE2	2.17	0.92
5:D:127:PHE:CE1	5:D:141:LEU:CD2	2.53	0.92
5:D:127:PHE:CD1	5:D:141:LEU:HD22	2.04	0.91
3:B:70:ASN:ND2	5:D:274:MET:SD	2.43	0.91
36:1:526:MET:HG2	40:5:236:SER:C	1.92	0.90
36:1:526:MET:HB3	40:5:237:ASN:CB	2.00	0.90
37:2:710:ILE:CB	37:2:714:PHE:CE2	2.57	0.88
2:0:534:U:O2	2:0:543:G:N2	2.08	0.85
36:1:523:LEU:HD12	36:1:526:MET:SD	2.17	0.85
37:2:855:LEU:HB3	40:5:258:VAL:HB	1.58	0.85
39:4:358:THR:HA	40:5:336:GLN:HG2	1.59	0.84
36:1:534:LEU:CB	40:5:230:LEU:HD13	2.07	0.83
37:2:855:LEU:HB3	40:5:258:VAL:CB	2.07	0.83
36:1:523:LEU:HD13	40:5:241:LYS:HB2	1.60	0.83
39:4:116:PRO:HB2	40:5:47:LEU:HD13	1.60	0.82
39:4:351:ILE:CA	40:5:343:MET:SD	2.68	0.82
38:3:371:ILE:HG21	38:3:391:VAL:HG21	1.61	0.81
37:2:710:ILE:CG1	37:2:714:PHE:HE2	1.94	0.81
39:4:125:SER:N	40:5:111:ASN:HD21	1.79	0.81
28:T:124:ARG:NH1	28:T:130:ARG:O	2.14	0.80
39:4:124:ASP:C	40:5:111:ASN:ND2	2.35	0.80
40:5:261:ASN:HB3	40:5:265:ARG:HH12	1.45	0.80
36:1:526:MET:CB	40:5:237:ASN:CA	2.48	0.78
40:5:67:LEU:HD22	40:5:78:ILE:HD13	1.65	0.78
37:2:710:ILE:HD12	37:2:714:PHE:CZ	2.18	0.78
1:A:1192:U:OP2	16:Y:119:ARG:NH2	2.17	0.77
36:1:277:ASN:O	36:1:281:THR:HG23	1.85	0.77
36:1:520:ARG:NH2	36:1:521:ASN:OD1	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:794:THR:O	37:2:839:THR:OG1	2.03	0.76
2:0:537:G:O2'	2:0:540:A:N1	2.18	0.76
37:2:855:LEU:HB3	40:5:258:VAL:CA	2.16	0.76
39:4:373:LYS:HA	39:4:375:VAL:HG12	1.68	0.75
36:1:526:MET:CG	40:5:236:SER:O	2.22	0.75
36:1:446:ILE:HG23	43:8:313:ILE:HG13	1.67	0.75
39:4:354:LEU:HD13	40:5:339:GLY:C	2.06	0.75
40:5:329:ASN:HA	40:5:332:GLU:HB2	1.68	0.74
37:2:483:ILE:HD11	37:2:505:ARG:HB3	1.70	0.74
36:1:520:ARG:NH2	40:5:243:LEU:O	2.21	0.73
38:3:49:ASN:HA	38:3:50:MET:HB2	1.68	0.73
42:7:241:ASN:HD22	42:7:423:PRO:HA	1.52	0.73
36:1:526:MET:SD	40:5:237:ASN:HA	2.28	0.73
36:1:526:MET:HE3	40:5:240:GLY:N	2.04	0.73
36:1:530:LEU:O	36:1:532:LYS:N	2.22	0.73
39:4:375:VAL:O	40:5:313:ARG:HD2	1.88	0.73
1:A:1473:G:O2'	1:A:1475:G:N2	2.22	0.73
5:D:127:PHE:CE1	5:D:141:LEU:HD22	2.22	0.73
39:4:354:LEU:O	39:4:358:THR:HG23	1.89	0.72
36:1:441:GLN:HE21	36:1:479:ASP:HB3	1.54	0.72
36:1:523:LEU:HA	36:1:526:MET:CG	2.21	0.71
39:4:123:VAL:HG21	40:5:44:LEU:HD22	1.72	0.71
37:2:710:ILE:C	37:2:714:PHE:CD2	2.63	0.70
40:5:41:ILE:HG12	40:5:78:ILE:HD12	1.72	0.70
38:3:111:ARG:HA	38:3:114:PHE:HB2	1.73	0.70
36:1:101:THR:HG22	36:1:149:TRP:HB3	1.74	0.70
37:2:869:ASN:CG	40:5:272:GLN:HB2	2.12	0.70
28:T:16:LEU:HD11	28:T:72:GLN:HE21	1.56	0.69
37:2:870:ASN:HD22	40:5:272:GLN:NE2	1.91	0.69
42:7:486:PHE:H	42:7:487:ARG:C	1.95	0.69
39:4:354:LEU:CD1	40:5:343:MET:SD	2.76	0.69
36:1:229:HIS:HB3	36:1:259:LEU:HD11	1.74	0.69
36:1:523:LEU:CD1	36:1:526:MET:SD	2.81	0.69
41:6:115:GLN:HE22	42:7:491:LEU:HB3	1.57	0.69
1:A:1693:G:H21	1:A:1834:A:H8	1.40	0.69
39:4:361:ALA:HB1	40:5:332:GLU:HB3	1.73	0.68
37:2:855:LEU:CB	40:5:258:VAL:HA	2.24	0.68
39:4:156:SER:HB2	40:5:110:VAL:HG11	1.76	0.68
39:4:361:ALA:CB	40:5:332:GLU:HB3	2.24	0.68
39:4:281:ARG:CZ	39:4:283:ILE:HB	2.24	0.68
37:2:852:GLN:HE22	40:5:257:ILE:HD12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:51:SER:OG	23:L:55:ARG:NH2	2.26	0.68
37:2:855:LEU:HB3	40:5:258:VAL:HA	1.76	0.68
38:3:7:THR:HA	38:3:10:ILE:HG22	1.76	0.68
37:2:855:LEU:HD13	40:5:257:ILE:CG2	2.24	0.68
40:5:122:SER:HB2	40:5:123:THR:HA	1.76	0.67
3:B:70:ASN:CG	5:D:274:MET:SD	2.73	0.67
37:2:725:PRO:HB3	37:2:734:ARG:HG3	1.76	0.67
38:3:351:ILE:HG23	38:3:356:LEU:HD11	1.77	0.67
1:A:379:C:O2	9:J:5:ARG:NH1	2.29	0.66
36:1:529:VAL:HG23	40:5:233:LEU:HB3	1.77	0.66
37:2:710:ILE:CG1	37:2:714:PHE:CE2	2.78	0.66
37:2:710:ILE:HD12	37:2:714:PHE:CE2	2.31	0.66
39:4:276:CYS:HA	40:5:211:ILE:HG23	1.77	0.66
36:1:278:LYS:O	36:1:281:THR:OG1	2.09	0.66
37:2:372:VAL:HG11	37:2:419:PHE:HB3	1.78	0.66
1:A:818:A:OP1	10:K:80:ARG:NH2	2.29	0.66
39:4:354:LEU:HD22	40:5:339:GLY:HA3	1.78	0.65
27:S:98:VAL:HG21	27:S:117:LEU:HD22	1.78	0.65
36:1:289:ALA:HA	36:1:292:HIS:HB3	1.79	0.65
37:2:862:LYS:HB2	40:5:265:ARG:HD2	1.78	0.65
39:4:373:LYS:HD2	40:5:322:GLN:CD	2.17	0.65
40:5:297:PRO:HA	40:5:298:GLU:HB2	1.79	0.65
5:D:127:PHE:CG	5:D:141:LEU:CD2	2.77	0.65
39:4:276:CYS:SG	40:5:215:MET:N	2.70	0.65
39:4:124:ASP:O	40:5:111:ASN:ND2	2.30	0.65
36:1:522:GLN:O	36:1:526:MET:HG3	1.97	0.64
36:1:523:LEU:CA	36:1:526:MET:SD	2.67	0.64
38:3:84:LEU:HD12	38:3:85:GLN:HG2	1.78	0.64
5:D:127:PHE:HD1	5:D:141:LEU:HD21	0.78	0.64
2:0:549:C:O2'	2:0:552:A:N3	2.31	0.64
39:4:362:ASN:CG	40:5:336:GLN:HE22	2.00	0.64
41:6:142:ILE:HG23	41:6:161:MET:SD	2.37	0.64
37:2:855:LEU:HD13	40:5:257:ILE:HB	1.80	0.64
38:3:30:GLU:N	38:3:62:TYR:OH	2.31	0.63
3:B:16:LEU:HD21	27:S:117:LEU:HD11	1.79	0.63
39:4:116:PRO:CB	40:5:47:LEU:HD13	2.27	0.63
37:2:710:ILE:C	37:2:714:PHE:HD2	1.97	0.63
36:1:289:ALA:HB3	36:1:331:ILE:HG21	1.80	0.63
39:4:176:MET:SD	40:5:106:SER:OG	2.57	0.62
1:A:1117:C:O2'	1:A:1119:A:N6	2.32	0.62
36:1:530:LEU:HD21	40:5:234:ALA:CB	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:8:43:ALA:HB1	43:8:47:GLU:HB2	1.80	0.62
37:2:855:LEU:HD13	40:5:257:ILE:HG22	1.82	0.62
41:6:71:LEU:HD11	41:6:134:PHE:CD1	2.35	0.61
36:1:526:MET:HB3	40:5:237:ASN:CG	2.20	0.61
1:A:1300:U:O2	1:A:1300:U:H2'	2.00	0.61
2:0:397:G:H2'	2:0:398:U:O4'	1.99	0.61
4:C:146:ARG:HB2	4:C:149:GLN:HB2	1.82	0.61
39:4:354:LEU:HB2	40:5:343:MET:SD	2.40	0.61
41:6:215:ALA:HB2	43:8:369:LEU:HD12	1.82	0.61
36:1:525:ALA:O	36:1:529:VAL:HG22	2.00	0.61
36:1:530:LEU:HG	40:5:234:ALA:HA	1.81	0.61
39:4:155:PHE:CD2	39:4:176:MET:HG2	2.36	0.61
40:5:79:THR:HG21	40:5:112:ILE:HD11	1.83	0.61
36:1:526:MET:HB3	40:5:237:ASN:OD1	2.01	0.61
39:4:365:GLN:HG3	40:5:329:ASN:CB	2.27	0.61
39:4:279:PRO:HD2	40:5:207:ASN:N	2.15	0.61
40:5:257:ILE:HG23	40:5:261:ASN:ND2	2.16	0.61
1:A:1693:G:N2	1:A:1834:A:H8	1.99	0.61
14:W:16:LYS:HG2	14:W:23:ILE:HG22	1.81	0.60
40:5:340:LYS:HB3	41:6:207:PHE:CE1	2.35	0.60
43:8:115:LYS:CB	43:8:116:ASN:HB3	2.32	0.60
38:3:42:LEU:HD22	38:3:219:LEU:HD22	1.83	0.60
37:2:710:ILE:HG13	37:2:714:PHE:HE2	1.66	0.60
39:4:341:ASP:N	40:5:350:TYR:OH	2.34	0.60
41:6:37:ALA:HB1	41:6:131:ILE:HG12	1.84	0.60
36:1:440:LEU:HD21	36:1:471:ILE:HG23	1.82	0.60
39:4:361:ALA:HB3	40:5:336:GLN:HE21	1.67	0.60
42:7:356:LYS:HD2	42:7:424:VAL:HG13	1.82	0.60
42:7:488:ILE:HG23	42:7:492:VAL:HG23	1.84	0.60
1:A:1075:C:OP1	12:O:107:LYS:NZ	2.34	0.59
41:6:44:LEU:HD21	41:6:84:LEU:HD12	1.82	0.59
1:A:1636:G:N3	1:A:1636:G:H2'	2.16	0.59
16:Y:93:PHE:O	16:Y:140:ARG:NH2	2.35	0.59
2:0:475:A:O2'	2:0:509:G:O6	2.20	0.59
37:2:710:ILE:HD12	37:2:714:PHE:HZ	1.63	0.59
38:3:38:LEU:HA	38:3:249:MET:HG3	1.84	0.59
39:4:243:VAL:HG11	39:4:248:MET:HA	1.83	0.59
38:3:198:ASN:N	38:3:199:ASN:HA	2.17	0.59
39:4:307:LEU:HD22	39:4:324:VAL:HG11	1.83	0.59
36:1:523:LEU:O	36:1:526:MET:HB2	2.02	0.59
37:2:855:LEU:HD12	37:2:856:ALA:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:4:195:THR:HA	39:4:222:VAL:HB	1.85	0.59
1:A:1331:C:H2'	1:A:1331:C:O2	2.03	0.59
36:1:385:PRO:HA	36:1:388:LYS:HB2	1.84	0.59
39:4:152:THR:HG21	40:5:51:LYS:HE3	1.85	0.59
1:A:293:C:O2	1:A:293:C:H2'	2.03	0.59
1:A:694:G:H1	1:A:732:U:H3	1.51	0.59
16:Y:61:GLN:O	16:Y:63:ASN:N	2.36	0.59
37:2:375:LYS:O	37:2:378:ILE:HG22	2.01	0.59
1:A:963:A:H2'	1:A:964:A:O4'	2.03	0.59
36:1:530:LEU:O	40:5:230:LEU:HD12	2.03	0.58
39:4:269:VAL:HG22	40:5:47:LEU:CD2	2.33	0.58
43:8:195:ASP:N	43:8:196:ASN:HB2	2.18	0.58
40:5:346:ALA:O	40:5:350:TYR:HB3	2.02	0.58
1:A:126:G:H2'	7:H:199:THR:HG21	1.85	0.58
42:7:245:GLU:HA	42:7:439:PRO:HG2	1.85	0.58
36:1:526:MET:HE3	40:5:240:GLY:CA	2.34	0.58
36:1:530:LEU:O	40:5:230:LEU:CD1	2.52	0.58
40:5:333:PHE:HA	40:5:336:GLN:HG3	1.84	0.58
39:4:303:LEU:HD21	39:4:324:VAL:HG21	1.86	0.58
1:A:1734:G:O2'	1:A:1800:A:N6	2.36	0.58
39:4:375:VAL:HG22	40:5:313:ARG:HD2	1.84	0.58
36:1:534:LEU:HB2	40:5:230:LEU:CD1	2.25	0.58
40:5:211:ILE:HG22	40:5:212:ASN:N	2.19	0.57
1:A:986:G:C8	13:P:137:SER:O	2.57	0.57
25:Q:37:TYR:OH	25:Q:45:LEU:HD12	2.04	0.57
39:4:269:VAL:HG22	40:5:47:LEU:HD21	1.86	0.57
38:3:258:THR:O	38:3:262:ILE:HG13	2.04	0.57
39:4:265:GLU:HG2	40:5:50:ILE:HG22	1.86	0.57
43:8:108:ASN:HB2	43:8:114:ASP:HB2	1.86	0.57
8:I:100:ILE:HD11	8:I:122:LEU:HD12	1.85	0.57
39:4:338:ILE:HG13	39:4:340:PRO:HD3	1.87	0.57
1:A:672:A:N6	1:A:1027:A:OP1	2.38	0.57
40:5:80:ASN:HB3	40:5:107:LEU:HD11	1.87	0.57
40:5:69:GLY:HA2	40:5:78:ILE:HA	1.87	0.57
43:8:292:ILE:HG12	43:8:331:LYS:HB2	1.85	0.57
1:A:1396:A:O2'	1:A:1398:G:N7	2.36	0.57
40:5:104:MET:HB2	40:5:114:HIS:HB2	1.85	0.57
43:8:312:VAL:HG11	43:8:325:ILE:HG21	1.87	0.57
5:D:127:PHE:HA	5:D:141:LEU:HD23	1.86	0.57
9:J:57:ALA:HB2	9:J:183:GLY:HA2	1.87	0.57
42:7:244:LEU:HD11	42:7:254:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:348:SER:HA	42:7:349:MET:HB3	1.86	0.57
3:B:15:VAL:HG21	27:S:109:LEU:HG	1.87	0.57
25:Q:75:VAL:HG12	25:Q:93:MET:HB3	1.87	0.57
42:7:379:PRO:HA	42:7:380:MET:HB3	1.87	0.56
39:4:272:ILE:CG1	40:5:43:GLY:HA3	2.35	0.56
37:2:594:LEU:O	37:2:598:ILE:HG22	2.06	0.56
38:3:229:ARG:HA	38:3:232:ILE:HG22	1.87	0.56
39:4:336:PRO:HB3	40:5:349:GLU:C	2.24	0.56
43:8:7:ILE:HB	43:8:22:LEU:HA	1.86	0.56
36:1:455:LEU:HA	36:1:458:LEU:HB3	1.86	0.56
39:4:285:LEU:HD21	40:5:163:SER:CB	2.36	0.56
36:1:530:LEU:C	40:5:230:LEU:HD11	2.26	0.56
39:4:375:VAL:O	40:5:313:ARG:CD	2.52	0.56
39:4:340:PRO:N	40:5:350:TYR:HE1	2.04	0.56
1:A:1216:C:N4	1:A:1342:U:OP1	2.36	0.56
1:A:897:U:H3'	1:A:898:U:H5''	1.87	0.56
1:A:1016:U:O2	1:A:1016:U:H2'	2.05	0.56
15:X:86:LEU:HD11	15:X:104:LEU:HD21	1.88	0.56
39:4:304:SER:O	43:8:348:GLN:NE2	2.38	0.56
40:5:244:GLN:HB3	40:5:247:MET:HB3	1.88	0.56
40:5:257:ILE:O	40:5:261:ASN:HB2	2.06	0.56
43:8:60:VAL:HG11	43:8:99:PRO:HD3	1.88	0.56
37:2:855:LEU:HD13	40:5:257:ILE:CB	2.36	0.56
39:4:324:VAL:O	39:4:328:LEU:N	2.37	0.56
40:5:350:TYR:C	40:5:350:TYR:CD2	2.79	0.56
37:2:618:ILE:HD11	37:2:677:ILE:HG22	1.88	0.56
2:0:402:C:H3'	2:0:403:G:C5'	2.35	0.56
37:2:627:LYS:HB3	37:2:688:VAL:HG21	1.87	0.56
1:A:1091:C:HO2'	15:X:2:VAL:N	2.04	0.56
42:7:353:THR:HG23	42:7:354:THR:HA	1.88	0.55
38:3:254:LEU:HD21	38:3:286:TYR:HD2	1.71	0.55
38:3:60:ASN:HB3	38:3:62:TYR:CE2	2.41	0.55
36:1:372:ASN:HA	36:1:375:VAL:HG12	1.88	0.55
1:A:146:G:O2'	1:A:147:A:O5'	2.19	0.55
1:A:1228:A:O2'	1:A:1634:A:N3	2.23	0.55
1:A:688:U:O2	8:I:122:LEU:HD13	2.06	0.55
2:0:621:G:OP1	2:0:623:A:N6	2.40	0.55
36:1:208:ILE:HG22	36:1:218:ILE:HG21	1.88	0.55
37:2:852:GLN:HE22	40:5:257:ILE:CD1	2.19	0.55
37:2:848:GLU:OE2	40:5:251:ASP:HB2	2.06	0.55
42:7:262:ARG:NH1	42:7:282:SER:OG	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:475:LEU:HD12	42:7:513:PHE:HB2	1.88	0.55
36:1:526:MET:HG2	40:5:237:ASN:HA	1.80	0.55
43:8:60:VAL:HG12	43:8:63:VAL:HG13	1.88	0.55
39:4:281:ARG:HA	40:5:204:VAL:HG13	1.89	0.55
39:4:328:LEU:HA	39:4:331:LEU:HD12	1.88	0.55
1:A:1139:C:O4'	1:A:1139:C:O2	2.25	0.55
1:A:1298:G:H2'	1:A:1298:G:N3	2.21	0.55
1:A:190:G:HO2'	1:A:191:A:H8	1.53	0.55
1:A:384:U:O4	9:J:5:ARG:NH2	2.39	0.55
1:A:853:C:O4'	1:A:853:C:O2	2.23	0.55
1:A:896:U:H2'	1:A:897:U:O4'	2.07	0.55
37:2:727:LEU:HB2	37:2:730:PRO:HD2	1.89	0.55
39:4:251:MET:CB	43:8:67:VAL:HG11	2.37	0.55
39:4:372:GLU:OE1	39:4:373:LYS:HG3	2.06	0.55
43:8:128:ILE:HG12	43:8:167:LEU:HD22	1.89	0.55
37:2:727:LEU:O	37:2:731:GLU:HB2	2.06	0.55
38:3:229:ARG:HG2	38:3:256:TYR:HB3	1.88	0.55
39:4:128:ARG:NH2	40:5:70:LEU:HD21	2.22	0.54
2:0:507:U:H3'	2:0:508:A:C5'	2.37	0.54
36:1:519:ILE:HA	36:1:523:LEU:CD2	2.36	0.54
38:3:17:HIS:CE1	38:3:45:LEU:HD21	2.42	0.54
39:4:220:LEU:HD11	39:4:233:ILE:HG12	1.88	0.54
39:4:375:VAL:O	40:5:313:ARG:NE	2.39	0.54
37:2:859:LEU:HA	40:5:265:ARG:CZ	2.37	0.54
1:A:1252:C:OP1	30:V:75:LYS:NZ	2.38	0.54
43:8:291:GLU:HA	43:8:330:ARG:HA	1.89	0.54
1:A:533:A:O2'	1:A:534:G:O5'	2.25	0.54
21:E:175:VAL:HG22	21:E:182:LEU:HB2	1.90	0.54
2:0:526:A:H2'	2:0:527:C:H5''	1.88	0.54
2:0:583:G:HO2'	36:1:3:ALA:N	2.06	0.54
38:3:405:ILE:HG12	39:4:359:TYR:CE2	2.41	0.54
12:O:60:VAL:HG13	12:O:66:VAL:HG21	1.89	0.54
1:A:1521:C:OP2	28:T:136:THR:OG1	2.26	0.54
43:8:115:LYS:HB3	43:8:116:ASN:HB3	1.90	0.54
40:5:75:ARG:HH22	40:5:205:ILE:HD12	1.73	0.54
1:A:1533:A:H2	1:A:1536:G:N3	2.06	0.54
37:2:852:GLN:O	37:2:855:LEU:HD11	2.08	0.54
40:5:192:ILE:O	42:7:548:HIS:CE1	2.61	0.54
39:4:347:LEU:CD1	40:5:346:ALA:C	2.76	0.54
40:5:240:GLY:O	40:5:242:ASN:N	2.41	0.54
1:A:1207:G:O2'	1:A:1837:G:N2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:A:H3'	1:A:192:C:O4'	2.08	0.54
1:A:407:G:H2'	1:A:407:G:N3	2.23	0.54
36:1:207:GLN:HE22	36:1:216:THR:HB	1.73	0.53
36:1:531:ALA:HB1	39:4:327:PHE:HB3	1.89	0.53
38:3:208:LEU:HD23	38:3:243:LEU:HD23	1.90	0.53
39:4:351:ILE:HA	40:5:343:MET:CE	2.37	0.53
39:4:275:THR:HB	39:4:279:PRO:HG3	1.90	0.53
40:5:79:THR:HG21	40:5:112:ILE:CD1	2.37	0.53
21:E:62:LYS:O	21:E:67:ARG:NH1	2.40	0.53
25:Q:56:LEU:HD22	25:Q:80:LEU:HD13	1.90	0.53
36:1:526:MET:SD	40:5:237:ASN:CA	2.94	0.53
37:2:856:ALA:HA	37:2:859:LEU:HD12	1.90	0.53
10:K:46:VAL:HG21	10:K:106:LEU:HD13	1.90	0.53
2:0:426:U:O2'	2:0:427:U:O2	2.18	0.53
38:3:261:VAL:HA	38:3:265:LYS:HB3	1.90	0.53
40:5:202:PRO:HB2	40:5:205:ILE:HD11	1.91	0.53
37:2:855:LEU:CB	40:5:258:VAL:CA	2.84	0.53
3:B:24:HIS:HB3	3:B:51:LEU:HD21	1.90	0.53
25:Q:45:LEU:HD11	25:Q:86:LEU:HD21	1.91	0.53
37:2:464:PRO:HB3	37:2:668:ARG:HG3	1.90	0.53
39:4:152:THR:N	39:4:187:GLU:OE2	2.41	0.53
40:5:190:ALA:HB2	40:5:315:ASP:OD2	2.09	0.53
37:2:507:ILE:HA	37:2:510:THR:HG22	1.91	0.53
37:2:690:ALA:O	37:2:789:ARG:NH2	2.42	0.53
40:5:350:TYR:CD2	40:5:351:ASN:N	2.77	0.53
43:8:71:LEU:CD2	43:8:111:HIS:HB3	2.39	0.53
1:A:1807:C:H2'	1:A:1808:U:O4'	2.09	0.53
37:2:714:PHE:O	37:2:718:LEU:HB2	2.09	0.53
39:4:237:VAL:HB	39:4:255:LEU:HD11	1.91	0.53
39:4:123:VAL:HG21	40:5:44:LEU:CD2	2.37	0.53
1:A:1116:C:O2	1:A:1116:C:C2'	2.55	0.53
2:0:387:U:H4'	2:0:388:A:OP1	2.09	0.52
2:0:518:G:H4'	2:0:519:A:OP1	2.09	0.52
2:0:539:U:O2	2:0:539:U:H2'	2.09	0.52
37:2:738:VAL:HG11	37:2:746:MET:HG2	1.90	0.52
38:3:111:ARG:HG2	38:3:133:ARG:HG2	1.91	0.52
39:4:240:SER:N	39:4:241:MET:HB2	2.24	0.52
39:4:365:GLN:CG	40:5:329:ASN:HB3	2.29	0.52
39:4:354:LEU:HD13	40:5:339:GLY:CA	2.39	0.52
41:6:174:MET:HA	41:6:179:TRP:CE3	2.44	0.52
1:A:897:U:H3'	1:A:898:U:C5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:180:GLN:HB2	3:B:195:TRP:CE3	2.45	0.52
39:4:358:THR:CA	40:5:336:GLN:HG2	2.37	0.52
40:5:67:LEU:HD22	40:5:78:ILE:CD1	2.38	0.52
39:4:318:VAL:HG13	43:8:226:LEU:HB2	1.91	0.52
1:A:167:G:OP1	7:H:8:PRO:HB3	2.09	0.52
37:2:727:LEU:HB2	37:2:730:PRO:CD	2.39	0.52
38:3:127:TYR:OH	38:3:155:ARG:O	2.26	0.52
38:3:375:ILE:HG21	42:7:466:LEU:HD11	1.90	0.52
43:8:13:ASP:HA	43:8:14:GLN:C	2.30	0.52
1:A:533:A:N1	1:A:551:U:C4	2.78	0.52
38:3:304:ASP:HB2	38:3:308:ALA:HB2	1.92	0.52
43:8:250:ALA:HB2	43:8:279:LEU:HD11	1.92	0.52
17:Z:110:ARG:NH2	17:Z:114:MET:SD	2.83	0.52
36:1:528:SER:HA	39:4:331:LEU:HD23	1.91	0.52
40:5:194:PHE:HZ	40:5:319:ILE:HD13	1.74	0.52
42:7:321:PHE:O	42:7:324:LEU:HG	2.10	0.52
42:7:548:HIS:CE1	42:7:552:GLU:HG3	2.44	0.52
43:8:313:ILE:HA	43:8:316:VAL:HG22	1.91	0.52
36:1:526:MET:CG	40:5:237:ASN:CA	2.71	0.52
37:2:856:ALA:HA	37:2:859:LEU:HB2	1.90	0.52
40:5:265:ARG:O	40:5:269:LYS:N	2.43	0.52
43:8:280:LEU:HD22	43:8:301:LEU:HG	1.92	0.52
42:7:274:LEU:O	42:7:274:LEU:HD12	2.10	0.52
37:2:379:ILE:HD11	37:2:447:LEU:HB3	1.92	0.51
39:4:155:PHE:CE1	40:5:106:SER:HB3	2.45	0.51
40:5:134:LEU:HD11	40:5:169:LEU:HD13	1.93	0.51
41:6:155:ARG:HG2	41:6:186:GLN:HA	1.92	0.51
2:0:541:C:H2'	2:0:542:A:H8	1.73	0.51
39:4:156:SER:OG	40:5:110:VAL:HG21	2.10	0.51
37:2:683:GLU:HA	37:2:686:TYR:HB3	1.92	0.51
38:3:214:LEU:O	38:3:232:ILE:HG13	2.10	0.51
42:7:366:GLN:NE2	42:7:416:SER:OG	2.43	0.51
1:A:1834:A:H2	1:A:1837:G:H1	1.56	0.51
36:1:355:LEU:HD11	37:2:720:VAL:HB	1.91	0.51
36:1:390:LEU:HD22	36:1:410:VAL:HB	1.92	0.51
39:4:358:THR:HG22	40:5:336:GLN:CA	2.32	0.51
37:2:493:LYS:CE	37:2:498:GLU:OE2	2.59	0.51
38:3:114:PHE:HA	38:3:117:LEU:HB2	1.93	0.51
40:5:234:ALA:O	40:5:237:ASN:N	2.44	0.51
42:7:390:LEU:HA	42:7:393:LYS:HB3	1.93	0.51
43:8:147:VAL:HG13	43:8:188:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:8:196:ASN:HB3	43:8:199:GLN:HB2	1.92	0.51
1:A:1207:G:N2	2:0:694:U:OP1	2.43	0.51
36:1:452:PHE:HB2	36:1:489:ARG:HG2	1.92	0.51
37:2:731:GLU:HB3	37:2:755:PHE:CE2	2.45	0.51
37:2:852:GLN:NE2	40:5:257:ILE:HD12	2.24	0.51
43:8:340:ARG:HB3	43:8:344:LYS:HD3	1.93	0.51
3:B:205:ARG:HB3	3:B:210:ILE:HG22	1.93	0.51
1:A:581:U:H4'	17:Z:66:GLY:HA3	1.92	0.51
36:1:527:SER:HA	36:1:530:LEU:HB2	1.92	0.51
37:2:848:GLU:OE2	40:5:247:MET:HG2	2.11	0.51
42:7:229:ASN:OD1	42:7:279:ARG:NH2	2.44	0.51
36:1:113:LEU:HA	36:1:116:GLU:HB2	1.92	0.51
36:1:452:PHE:CE1	36:1:471:ILE:HD13	2.46	0.51
39:4:128:ARG:HH21	40:5:70:LEU:HD21	1.76	0.51
39:4:135:ARG:HE	39:4:194:ALA:HB1	1.75	0.51
22:G:73:THR:O	22:G:89:THR:HG21	2.11	0.51
27:S:114:LEU:HB3	27:S:117:LEU:HG	1.94	0.51
37:2:693:LEU:HD23	37:2:697:TYR:CE2	2.46	0.50
36:1:533:ALA:HB2	40:5:233:LEU:HD12	1.93	0.50
39:4:179:LEU:CD1	40:5:99:TYR:HA	2.41	0.50
1:A:547:G:H2'	1:A:549:C:H41	1.76	0.50
1:A:873:G:N3	1:A:873:G:H2'	2.25	0.50
36:1:410:VAL:HA	36:1:413:TRP:HB3	1.92	0.50
40:5:79:THR:OG1	40:5:112:ILE:HD12	2.10	0.50
43:8:294:PHE:HB2	43:8:328:THR:HA	1.93	0.50
5:D:127:PHE:HD1	5:D:141:LEU:CD2	1.70	0.50
29:U:22:LEU:HD13	29:U:28:LEU:HD21	1.93	0.50
36:1:116:GLU:O	36:1:121:ILE:HD11	2.12	0.50
36:1:384:VAL:HG13	36:1:386:GLU:HB3	1.92	0.50
38:3:295:PHE:HA	38:3:298:CYS:HB2	1.93	0.50
38:3:405:ILE:HG23	39:4:359:TYR:OH	2.11	0.50
39:4:361:ALA:CA	40:5:332:GLU:HB3	2.42	0.50
42:7:394:TYR:HA	42:7:397:LYS:HB3	1.93	0.50
43:8:100:SER:HA	43:8:103:LEU:HD12	1.93	0.50
36:1:520:ARG:HB2	40:5:241:LYS:O	2.11	0.50
38:3:238:TYR:HE1	38:3:272:GLN:HE22	1.59	0.50
38:3:316:GLU:HA	38:3:319:LEU:HB3	1.92	0.50
39:4:262:TYR:CE2	39:4:264:THR:HG22	2.46	0.50
40:5:196:HIS:CE1	40:5:322:GLN:NE2	2.79	0.50
41:6:207:PHE:CE1	41:6:211:SER:HB3	2.47	0.50
42:7:270:GLY:HA3	42:7:305:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:490:A:HI'	36:1:212:HIS:HB3	1.93	0.50
40:5:276:GLN:O	40:5:280:ARG:N	2.39	0.50
42:7:280:LEU:HD21	42:7:303:SER:HB2	1.93	0.50
1:A:1535:U:O2	1:A:1535:U:C2'	2.59	0.50
37:2:598:ILE:O	37:2:598:ILE:HG23	2.11	0.50
11:M:47:PRO:HG2	11:M:116:CYS:SG	2.52	0.50
12:O:55:ARG:NH1	12:O:56:ASP:OD1	2.44	0.50
37:2:710:ILE:HB	37:2:714:PHE:CZ	2.41	0.50
1:A:1521:C:OP1	28:T:129:LEU:HD13	2.12	0.50
37:2:870:ASN:CG	39:4:374:LEU:HD22	2.32	0.50
39:4:317:LYS:HA	39:4:320:ALA:HB3	1.94	0.50
39:4:340:PRO:C	40:5:350:TYR:CE1	2.85	0.50
1:A:534:G:N2	1:A:551:U:O2	2.34	0.50
1:A:907:G:H2'	1:A:908:A:C8	2.47	0.50
22:G:20:PHE:CZ	22:G:69:VAL:HG21	2.47	0.50
22:G:40:ALA:HB1	22:G:45:TYR:CG	2.46	0.50
37:2:445:LEU:HA	37:2:448:VAL:HG22	1.93	0.50
39:4:279:PRO:HA	39:4:280:ASN:CB	2.23	0.50
40:5:332:GLU:O	40:5:336:GLN:HG3	2.12	0.50
1:A:369:C:O4'	1:A:369:C:O2	2.27	0.50
40:5:173:LEU:HD13	40:5:194:PHE:CZ	2.47	0.49
1:A:1779:G:H3'	1:A:1780:G:H8	1.77	0.49
39:4:347:LEU:HD22	40:5:347:LEU:HB2	1.94	0.49
40:5:160:GLY:HA2	40:5:334:THR:HG23	1.94	0.49
40:5:64:GLN:O	40:5:83:PRO:HA	2.12	0.49
42:7:194:PHE:CZ	42:7:235:VAL:HG23	2.46	0.49
2:0:489:C:O4'	2:0:489:C:O2	2.28	0.49
37:2:593:HIS:NE2	38:3:7:THR:HB	2.27	0.49
43:8:278:ARG:HA	43:8:320:MET:HE1	1.94	0.49
36:1:530:LEU:HD23	40:5:230:LEU:HG	1.94	0.49
37:2:379:ILE:HG22	37:2:404:CYS:SG	2.52	0.49
39:4:118:ILE:O	39:4:122:ILE:HG13	2.12	0.49
39:4:170:MET:HG3	39:4:209:TYR:HB3	1.93	0.49
39:4:279:PRO:HB2	40:5:206:LYS:N	2.27	0.49
40:5:243:LEU:O	40:5:245:LEU:HB2	2.12	0.49
24:N:106:CYS:SG	24:N:107:SER:N	2.85	0.49
2:0:539:U:O2	2:0:539:U:C2'	2.61	0.49
40:5:153:ASP:HB2	40:5:163:SER:HA	1.95	0.49
40:5:204:VAL:HG22	40:5:204:VAL:O	2.13	0.49
40:5:41:ILE:CG1	40:5:78:ILE:HD12	2.40	0.49
36:1:533:ALA:CB	40:5:233:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:710:ILE:CD1	37:2:714:PHE:CE2	2.96	0.49
37:2:847:THR:HA	37:2:850:THR:HG22	1.95	0.49
43:8:87:CYS:HA	43:8:90:LEU:HD23	1.95	0.49
1:A:126:G:N2	1:A:180:G:O2'	2.45	0.49
1:A:531:A:H61	1:A:553:U:H3	1.61	0.49
1:A:534:G:H2'	1:A:535:G:H8	1.77	0.49
7:H:106:LEU:HD23	7:H:106:LEU:N	2.28	0.49
7:H:49:VAL:HG22	7:H:115:LYS:HB3	1.94	0.49
9:J:81:VAL:HG22	9:J:102:VAL:HG12	1.93	0.49
28:T:40:TYR:OH	28:T:71:MET:O	2.31	0.49
38:3:15:ASP:HA	38:3:208:LEU:HD13	1.93	0.49
43:8:104:GLN:HA	43:8:107:SER:HB2	1.94	0.49
43:8:70:LEU:HG	43:8:86:LEU:HD21	1.95	0.49
22:G:30:ILE:HG23	22:G:117:ILE:HD11	1.93	0.49
27:S:99:ASP:O	27:S:102:THR:HB	2.12	0.49
16:Y:128:VAL:HG21	16:Y:141:PRO:HD3	1.95	0.49
39:4:285:LEU:HB2	40:5:161:SER:HA	1.95	0.49
43:8:227:LYS:N	43:8:228:PRO:HD3	2.27	0.49
1:A:1722:G:O6	1:A:1812:U:O2	2.31	0.49
6:F:51:LYS:N	6:F:51:LYS:CD	2.75	0.49
13:P:85:CYS:SG	13:P:90:ILE:HB	2.52	0.49
38:3:7:THR:OG1	38:3:244:ASN:ND2	2.46	0.49
39:4:339:VAL:N	39:4:340:PRO:HD3	2.27	0.49
1:A:64:A:O2'	1:A:66:G:OP2	2.30	0.49
2:0:543:G:C2	2:0:544:U:C4	3.01	0.49
38:3:254:LEU:HD21	38:3:286:TYR:CD2	2.48	0.49
39:4:275:THR:O	39:4:279:PRO:HD3	2.13	0.49
26:R:70:VAL:HG11	26:R:84:ILE:HG22	1.94	0.49
40:5:244:GLN:HB2	40:5:248:ASP:HB2	1.94	0.48
4:C:175:GLU:O	4:C:187:LYS:NZ	2.46	0.48
2:0:472:G:H2'	2:0:472:G:N3	2.27	0.48
36:1:375:VAL:HG23	36:1:380:LEU:HB2	1.94	0.48
38:3:241:GLN:O	38:3:242:TYR:HB2	2.13	0.48
38:3:262:ILE:HG12	38:3:267:VAL:HG11	1.94	0.48
1:A:788:G:N3	1:A:788:G:H2'	2.27	0.48
22:G:35:LEU:HD12	22:G:147:VAL:HG23	1.95	0.48
13:P:39:ASP:N	13:P:69:SER:HB3	2.28	0.48
2:0:604:C:N4	2:0:677:A:O2'	2.46	0.48
22:G:39:ILE:HG23	22:G:68:ILE:HG21	1.94	0.48
15:X:28:ARG:CB	15:X:29:PRO:HD3	2.43	0.48
2:0:537:G:OP2	40:5:269:LYS:NZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:148:ALA:HB1	38:3:172:LYS:HD3	1.95	0.48
36:1:526:MET:SD	40:5:237:ASN:C	2.92	0.48
29:U:63:HIS:CE1	29:U:78:ILE:HD11	2.47	0.48
36:1:390:LEU:HD11	36:1:407:VAL:HA	1.95	0.48
37:2:496:THR:HA	37:2:499:ILE:HG22	1.94	0.48
39:4:183:VAL:HA	40:5:85:PRO:CB	2.43	0.48
39:4:308:GLN:NE2	43:8:345:GLN:O	2.47	0.48
39:4:341:ASP:CA	40:5:350:TYR:OH	2.61	0.48
42:7:486:PHE:N	42:7:487:ARG:C	2.66	0.48
38:3:6:LEU:HD11	38:3:204:PRO:HB3	1.95	0.48
2:0:491:U:O2'	2:0:517:G:O6	2.20	0.48
36:1:448:GLN:HE22	36:1:495:SER:HB2	1.78	0.48
36:1:526:MET:HE2	40:5:239:LEU:N	2.29	0.48
22:G:50:PRO:HG2	22:G:90:VAL:HG23	1.96	0.48
38:3:225:HIS:N	38:3:226:PRO:CD	2.77	0.48
39:4:238:SER:OG	39:4:250:VAL:HG12	2.13	0.48
42:7:298:GLU:HA	42:7:301:LYS:HB3	1.96	0.48
7:H:159:ARG:HG2	7:H:173:ALA:HB2	1.96	0.48
9:J:101:ILE:HD12	9:J:190:LEU:HD11	1.96	0.48
2:0:562:U:O2	2:0:562:U:O4'	2.31	0.48
36:1:307:ARG:HH12	36:1:318:MET:HA	1.79	0.48
37:2:855:LEU:HD22	40:5:258:VAL:N	2.28	0.48
38:3:51:VAL:O	38:3:55:MET:HG3	2.14	0.48
39:4:265:GLU:HG2	40:5:50:ILE:O	2.14	0.48
39:4:262:TYR:CE2	40:5:53:TYR:CD2	3.02	0.48
1:A:550:C:O2'	1:A:551:U:C5	2.65	0.48
1:A:877:C:H2'	1:A:878:G:O4'	2.14	0.48
7:H:102:VAL:HG21	7:H:109:LEU:HD11	1.95	0.48
39:4:152:THR:CG2	40:5:51:LYS:HE3	2.44	0.47
39:4:270:ASP:HA	39:4:273:MET:HG2	1.96	0.47
39:4:340:PRO:N	40:5:350:TYR:CE1	2.81	0.47
41:6:171:LYS:HA	41:6:174:MET:HB3	1.97	0.47
1:A:1397:U:C2'	1:A:1397:U:O2	2.61	0.47
1:A:1520:G:N3	1:A:1520:G:H2'	2.28	0.47
1:A:1761:U:H2'	1:A:1771:G:H1	1.79	0.47
37:2:480:CYS:HA	37:2:483:ILE:HG22	1.95	0.47
39:4:190:LEU:HB3	39:4:218:ILE:HB	1.96	0.47
39:4:347:LEU:HD23	39:4:351:ILE:HG12	1.95	0.47
42:7:486:PHE:HB3	42:7:487:ARG:HB3	1.96	0.47
1:A:163:U:OP1	7:H:84:TYR:HA	2.15	0.47
10:K:170:PRO:O	10:K:175:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:80:LEU:HD21	25:Q:83:MET:HB2	1.96	0.47
2:0:602:U:O2'	2:0:680:A:N7	2.43	0.47
36:1:530:LEU:CG	40:5:234:ALA:HA	2.44	0.47
41:6:71:LEU:HD22	41:6:127:LEU:HD23	1.96	0.47
42:7:470:MET:HB3	42:7:474:LYS:HB3	1.96	0.47
1:A:752:G:H4'	1:A:753:C:OP1	2.13	0.47
25:Q:18:ARG:NH1	28:T:88:LYS:O	2.47	0.47
36:1:276:TYR:HA	36:1:279:VAL:HG12	1.96	0.47
38:3:170:TRP:CZ3	38:3:173:LEU:HD22	2.50	0.47
39:4:354:LEU:HD12	40:5:343:MET:CG	2.44	0.47
1:A:1446:A:H5''	30:V:58:THR:HG23	1.96	0.47
1:A:607:U:H3'	1:A:608:C:C5'	2.44	0.47
11:M:120:VAL:HG12	11:M:145:VAL:HG11	1.96	0.47
27:S:24:LEU:HB2	27:S:58:MET:SD	2.54	0.47
37:2:493:LYS:HE2	37:2:498:GLU:OE2	2.15	0.47
37:2:862:LYS:HB2	40:5:265:ARG:CD	2.45	0.47
39:4:344:GLU:HG3	40:5:350:TYR:CD2	2.50	0.47
43:8:303:ILE:HG22	43:8:304:GLY:H	1.77	0.47
14:W:1:MET:N	14:W:1:MET:SD	2.87	0.47
38:3:174:ALA:O	38:3:178:LEU:HG	2.14	0.47
39:4:365:GLN:HA	40:5:329:ASN:OD1	2.14	0.47
36:1:478:CYS:HB3	36:1:502:ARG:HB3	1.97	0.47
38:3:367:ALA:O	38:3:371:ILE:HG12	2.15	0.47
40:5:176:VAL:HB	40:5:189:LYS:HE2	1.96	0.47
41:6:70:LEU:HD21	41:6:103:LEU:HD12	1.97	0.47
1:A:1298:G:O2'	1:A:1299:A:C8	2.66	0.47
11:M:42:LEU:HD13	11:M:72:ILE:HD11	1.97	0.47
37:2:493:LYS:HG3	37:2:498:GLU:OE2	2.09	0.47
37:2:855:LEU:CD1	40:5:257:ILE:HB	2.44	0.47
38:3:212:THR:HG22	38:3:216:HIS:CE1	2.49	0.47
39:4:183:VAL:HA	40:5:85:PRO:HG3	1.96	0.47
39:4:361:ALA:HA	40:5:332:GLU:HB3	1.95	0.47
39:4:128:ARG:HB2	40:5:111:ASN:HA	1.97	0.47
1:A:1282:A:H2'	1:A:1283:C:O4'	2.15	0.47
16:Y:63:ASN:HD22	16:Y:114:ASP:HB3	1.79	0.47
36:1:11:ALA:CB	36:1:34:VAL:HG21	2.44	0.47
40:5:154:PRO:HD2	40:5:156:LYS:HE3	1.97	0.47
1:A:1624:U:O4'	1:A:1624:U:O2	2.30	0.47
7:H:159:ARG:HB3	7:H:171:THR:HG22	1.96	0.47
28:T:26:ILE:HG22	28:T:45:LEU:HD11	1.95	0.47
36:1:218:ILE:HG23	36:1:218:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:6:70:LEU:HD13	41:6:102:ILE:HB	1.97	0.47
7:H:49:VAL:HG23	7:H:114:VAL:HB	1.97	0.47
36:1:110:GLN:O	36:1:114:ASP:N	2.48	0.47
43:8:50:ASP:OD1	43:8:51:VAL:N	2.47	0.47
1:A:1298:G:C2'	1:A:1298:G:N3	2.77	0.47
1:A:1719:A:H62	1:A:1814:G:H21	1.63	0.47
1:A:693:A:H2'	1:A:694:G:H8	1.80	0.47
5:D:212:LYS:HA	5:D:215:LEU:HD12	1.97	0.47
25:Q:15:PHE:CZ	25:Q:109:PRO:HB2	2.50	0.47
39:4:352:ASN:HD21	42:7:523:ILE:HG21	1.80	0.46
37:2:356:LEU:HB3	37:2:360:ILE:HD12	1.96	0.46
36:1:487:THR:HA	37:2:798:VAL:HG22	1.95	0.46
43:8:182:SER:O	43:8:186:VAL:HG23	2.16	0.46
38:3:254:LEU:HD12	38:3:255:ARG:N	2.30	0.46
36:1:526:MET:CE	40:5:240:GLY:N	2.75	0.46
42:7:417:CYS:HB3	42:7:418:PRO:HD3	1.97	0.46
12:O:99:ARG:NH2	12:O:119:GLU:OE2	2.48	0.46
36:1:147:THR:HA	36:1:150:VAL:HG22	1.96	0.46
36:1:383:VAL:HG13	36:1:388:LYS:HA	1.98	0.46
37:2:464:PRO:CB	37:2:668:ARG:HG3	2.45	0.46
40:5:49:ILE:HG12	40:5:120:TYR:CE2	2.51	0.46
39:4:325:GLY:HA2	39:4:328:LEU:HD12	1.98	0.46
39:4:281:ARG:CZ	40:5:202:PRO:HB3	2.46	0.46
1:A:1116:C:O2'	1:A:1117:C:C2	2.69	0.46
1:A:1118:C:O2	1:A:1118:C:O4'	2.28	0.46
4:C:149:GLN:HE21	4:C:151:ARG:HB3	1.81	0.46
7:H:116:LYS:HD2	7:H:125:THR:HG21	1.97	0.46
24:N:38:ALA:HB1	24:N:110:VAL:HG21	1.98	0.46
27:S:71:ILE:HB	27:S:74:GLN:HB2	1.96	0.46
36:1:525:ALA:O	36:1:529:VAL:HG13	2.16	0.46
38:3:134:TYR:O	38:3:138:GLN:HG2	2.15	0.46
36:1:530:LEU:HD22	40:5:230:LEU:CD2	2.46	0.46
41:6:47:ASN:HB3	41:6:69:ILE:HG23	1.98	0.46
43:8:315:ALA:HB1	43:8:320:MET:CE	2.46	0.46
1:A:1286:G:O6	24:N:36:ARG:HB3	2.16	0.46
37:2:850:THR:HA	37:2:853:GLN:HB3	1.97	0.46
40:5:257:ILE:HA	40:5:261:ASN:HD22	1.80	0.46
37:2:870:ASN:HA	40:5:272:GLN:CD	2.36	0.46
41:6:124:ASN:HA	41:6:128:LEU:HD22	1.97	0.46
43:8:319:LYS:HG3	43:8:322:TYR:HB2	1.96	0.46
1:A:1542:C:OP1	29:U:62:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:211:LYS:O	5:D:215:LEU:HG	2.16	0.46
8:I:157:HIS:HD1	8:I:188:GLU:HB2	1.79	0.46
2:0:576:U:H3'	2:0:577:A:H5''	1.98	0.46
37:2:744:MET:HA	37:2:782:LYS:HD2	1.97	0.46
1:A:1231:C:O2'	1:A:1253:A:N6	2.48	0.46
1:A:293:C:C2'	1:A:293:C:O2	2.64	0.46
6:F:44:LEU:HD13	6:F:72:ILE:HD11	1.97	0.46
22:G:141:VAL:HG23	22:G:146:ARG:HG2	1.97	0.46
1:A:380:G:P	9:J:56:ARG:HH22	2.38	0.46
24:N:58:GLU:HB3	24:N:61:TYR:HB3	1.97	0.46
24:N:62:VAL:HA	24:N:65:VAL:HG12	1.98	0.46
36:1:322:VAL:HB	36:1:379:VAL:HG13	1.98	0.46
37:2:443:CYS:HA	37:2:446:THR:HG22	1.98	0.46
38:3:386:SER:HB2	42:7:467:TYR:CZ	2.50	0.46
42:7:532:ASP:HA	42:7:535:VAL:HG22	1.97	0.46
1:A:536:A:N1	1:A:548:C:N4	2.61	0.46
7:H:98:ARG:HE	7:H:106:LEU:HD22	1.80	0.46
36:1:78:CYS:SG	36:1:82:ASN:O	2.72	0.46
36:1:534:LEU:N	40:5:230:LEU:HD13	2.31	0.46
40:5:46:VAL:O	40:5:50:ILE:HG13	2.15	0.46
21:E:5:ILE:HD12	21:E:10:LYS:HA	1.97	0.46
24:N:69:CYS:O	24:N:74:ILE:HB	2.16	0.46
37:2:493:LYS:HG3	37:2:497:GLU:OE2	2.16	0.45
36:1:246:TRP:CD2	37:2:723:ARG:HD2	2.51	0.45
38:3:26:LEU:HD22	38:3:53:PHE:CE1	2.51	0.45
39:4:375:VAL:HG22	40:5:313:ARG:CD	2.46	0.45
1:A:628:A:H61	21:E:178:ARG:HB3	1.81	0.45
1:A:823:U:O4'	1:A:823:U:O2	2.34	0.45
1:A:289:G:H5'	6:F:129:ILE:HD11	1.97	0.45
2:0:574:U:H2'	2:0:575:U:C6	2.51	0.45
38:3:268:ARG:H	38:3:269:LYS:HB3	1.80	0.45
42:7:376:THR:HA	42:7:379:PRO:HD2	1.98	0.45
27:S:31:ASN:HD21	27:S:55:THR:HB	1.81	0.45
38:3:353:ILE:HG12	38:3:389:GLY:HA3	1.97	0.45
39:4:183:VAL:HA	40:5:85:PRO:HB3	1.97	0.45
1:A:533:A:H2'	1:A:534:G:C8	2.52	0.45
21:E:1:MET:O	21:E:4:GLN:N	2.50	0.45
11:M:80:MET:SD	11:M:120:VAL:HG23	2.56	0.45
38:3:138:GLN:HG3	38:3:151:LEU:HD22	1.98	0.45
37:2:855:LEU:HB2	40:5:258:VAL:HA	1.96	0.45
39:4:375:VAL:HB	40:5:318:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:8:189:LEU:CD1	43:8:194:GLU:HB3	2.47	0.45
1:A:1331:C:C2'	1:A:1331:C:O2	2.64	0.45
37:2:815:LEU:N	37:2:816:PRO:HD2	2.31	0.45
39:4:340:PRO:CD	40:5:350:TYR:CE1	3.00	0.45
42:7:373:ILE:HG12	42:7:398:MET:HB2	1.98	0.45
43:8:241:LEU:HA	43:8:244:PHE:HB3	1.98	0.45
23:L:59:LYS:HB3	23:L:70:TYR:HB2	1.98	0.45
38:3:31:ILE:HG22	38:3:32:TYR:H	1.81	0.45
39:4:193:TYR:HB2	39:4:220:LEU:HB3	1.98	0.45
39:4:276:CYS:HA	40:5:211:ILE:CG2	2.45	0.45
39:4:373:LYS:HD2	40:5:322:GLN:NE2	2.32	0.45
41:6:65:VAL:O	41:6:69:ILE:HG12	2.16	0.45
1:A:1285:G:OP2	24:N:35:ILE:HG22	2.17	0.45
8:I:19:PHE:CZ	8:I:50:GLU:HB2	2.52	0.45
28:T:68:ILE:HG23	28:T:72:GLN:HE22	1.81	0.45
37:2:692:LEU:HD22	37:2:693:LEU:HD12	1.99	0.45
37:2:862:LYS:O	37:2:866:LEU:HG	2.17	0.45
37:2:869:ASN:ND2	40:5:268:SER:O	2.50	0.45
38:3:49:ASN:HB3	38:3:52:ASP:HB2	1.99	0.45
40:5:239:LEU:HD12	40:5:243:LEU:HD12	1.99	0.45
40:5:318:LEU:O	40:5:322:GLN:N	2.47	0.45
41:6:37:ALA:HA	41:6:131:ILE:HG23	1.99	0.45
43:8:352:ASP:HA	43:8:355:ASN:HD22	1.82	0.45
1:A:550:C:O2'	1:A:551:U:C6	2.69	0.45
2:0:541:C:H2'	2:0:542:A:C8	2.51	0.45
38:3:374:LEU:HA	38:3:377:ASN:HD22	1.82	0.45
24:N:26:LEU:HG	24:N:31:LEU:HD13	1.98	0.45
29:U:28:LEU:HD22	29:U:54:TYR:CD1	2.52	0.45
2:0:537:G:H1'	2:0:538:G:C2	2.52	0.45
39:4:375:VAL:HG21	40:5:318:LEU:HD23	1.98	0.45
37:2:859:LEU:HD23	40:5:265:ARG:NH1	2.32	0.45
1:A:1300:U:O2	1:A:1300:U:C2'	2.65	0.45
1:A:1779:G:H2'	1:A:1780:G:O4'	2.17	0.45
1:A:320:G:N2	1:A:331:C:O2'	2.46	0.45
3:B:134:LEU:CD2	3:B:144:THR:HG21	2.47	0.45
13:P:21:VAL:HG13	13:P:23:GLU:HG2	1.99	0.45
2:0:378:C:H2'	2:0:379:U:C6	2.52	0.45
36:1:119:ASP:O	36:1:121:ILE:HD12	2.16	0.45
36:1:225:SER:O	36:1:229:HIS:HB2	2.17	0.45
39:4:347:LEU:CD1	40:5:346:ALA:HB3	2.47	0.45
42:7:296:ASN:HA	42:7:299:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:402:GLN:HE22	42:7:525:LYS:HB3	1.82	0.45
36:1:449:SER:O	43:8:327:GLN:HB2	2.16	0.45
36:1:525:ALA:C	36:1:529:VAL:HG22	2.38	0.44
38:3:420:MET:HB3	42:7:347:LYS:HE2	1.99	0.44
39:4:375:VAL:HG11	40:5:318:LEU:HD23	1.98	0.44
42:7:456:GLN:O	42:7:460:ILE:HG12	2.17	0.44
1:A:1535:U:O2	1:A:1535:U:H2'	2.17	0.44
37:2:445:LEU:HD12	37:2:502:VAL:HG13	1.98	0.44
38:3:38:LEU:HD13	38:3:252:HIS:CE1	2.53	0.44
39:4:281:ARG:HA	40:5:204:VAL:O	2.17	0.44
41:6:117:PHE:O	41:6:121:LEU:HB2	2.17	0.44
5:D:66:LEU:HD11	5:D:81:ILE:HG12	2.00	0.44
6:F:129:ILE:HG22	6:F:139:LEU:HD23	1.99	0.44
37:2:440:VAL:HA	37:2:443:CYS:HB2	1.99	0.44
37:2:862:LYS:CB	40:5:265:ARG:HD2	2.47	0.44
1:A:1035:A:H2'	1:A:1036:A:O4'	2.17	0.44
1:A:455:A:O2'	1:A:1735:A:N3	2.41	0.44
2:0:427:U:H1'	2:0:428:A:C5	2.52	0.44
2:0:517:G:HO2'	2:0:518:G:C5'	2.29	0.44
36:1:43:TRP:CE3	36:1:43:TRP:O	2.70	0.44
38:3:143:ASN:N	38:3:144:TYR:HB2	2.33	0.44
1:A:1674:G:OP1	22:G:51:HIS:NE2	2.43	0.44
1:A:321:C:N3	1:A:331:C:O2	2.51	0.44
24:N:21:VAL:HA	24:N:24:THR:HG22	2.00	0.44
26:R:97:GLN:HB3	26:R:105:LYS:HG3	1.98	0.44
36:1:285:LYS:HG2	37:2:724:GLN:HE22	1.83	0.44
37:2:822:ILE:HG21	38:3:303:PHE:CE1	2.53	0.44
38:3:262:ILE:HG12	38:3:267:VAL:CG1	2.46	0.44
39:4:374:LEU:HD23	39:4:374:LEU:O	2.18	0.44
43:8:355:ASN:C	43:8:359:GLN:HE21	2.20	0.44
2:0:544:U:C4	2:0:545:A:C6	3.06	0.44
36:1:512:GLN:O	36:1:514:MET:N	2.42	0.44
39:4:358:THR:O	39:4:361:ALA:HB3	2.18	0.44
40:5:173:LEU:HD13	40:5:194:PHE:CE2	2.53	0.44
41:6:67:ALA:HB1	41:6:127:LEU:HD22	1.99	0.44
41:6:71:LEU:HD23	41:6:131:ILE:HB	2.00	0.44
1:A:1113:A:C6	1:A:1121:G:C6	3.05	0.44
1:A:1589:A:H2'	1:A:1590:C:O4'	2.17	0.44
1:A:1826:G:OP2	1:A:1826:G:H8	2.01	0.44
24:N:24:THR:HA	24:N:27:ILE:HG12	1.99	0.44
37:2:445:LEU:HD11	37:2:501:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:590:LEU:O	37:2:593:HIS:CD2	2.71	0.44
40:5:66:VAL:HA	40:5:119:TRP:HA	1.99	0.44
43:8:103:LEU:HD11	43:8:130:VAL:HG11	2.00	0.44
6:F:17:HIS:HB2	6:F:108:ARG:HA	2.00	0.44
36:1:323:LEU:HB3	36:1:383:VAL:HG23	1.99	0.44
36:1:495:SER:HA	36:1:496:ASP:HA	1.80	0.44
38:3:214:LEU:HD13	38:3:235:LEU:HD23	2.00	0.44
9:J:76:THR:HG22	9:J:108:PRO:HG2	1.99	0.44
36:1:161:LEU:HD21	36:1:177:ILE:HB	2.00	0.44
37:2:731:GLU:HB3	37:2:755:PHE:CZ	2.53	0.44
3:B:38:ILE:HD11	3:B:150:THR:CG2	2.48	0.44
26:R:102:GLU:OE1	26:R:102:GLU:N	2.51	0.44
2:O:380:G:H2'	2:O:440:A:N1	2.33	0.43
43:8:96:GLY:O	43:8:134:CYS:SG	2.76	0.43
1:A:614:C:H4'	1:A:615:C:H5''	1.99	0.43
9:J:130:THR:N	9:J:131:PRO:CD	2.81	0.43
36:1:109:GLN:HG2	36:1:113:LEU:HD12	1.99	0.43
36:1:281:THR:O	37:2:723:ARG:NH1	2.51	0.43
36:1:467:LEU:HD22	36:1:471:ILE:HD11	1.99	0.43
37:2:799:TYR:OH	37:2:837:GLN:HB2	2.18	0.43
38:3:50:MET:HG2	38:3:178:LEU:HD13	2.00	0.43
39:4:220:LEU:HD11	39:4:233:ILE:CG1	2.48	0.43
39:4:340:PRO:CD	40:5:350:TYR:HE1	2.30	0.43
39:4:372:GLU:HB2	40:5:264:MET:HE1	2.00	0.43
40:5:333:PHE:HA	40:5:336:GLN:CG	2.48	0.43
1:A:962:A:N1	1:A:1055:A:O2'	2.51	0.43
1:A:1453:C:H2'	1:A:1454:A:H4'	2.01	0.43
23:L:32:HIS:HB2	23:L:45:VAL:HG21	2.00	0.43
23:L:12:TYR:CE1	23:L:52:LEU:HD11	2.53	0.43
27:S:104:GLU:O	27:S:108:LEU:HG	2.18	0.43
36:1:452:PHE:HB2	36:1:489:ARG:CG	2.49	0.43
41:6:29:LEU:HD12	41:6:46:ALA:HA	1.99	0.43
42:7:479:LEU:HD23	42:7:482:THR:HB	2.01	0.43
43:8:133:SER:HA	43:8:136:ALA:HB3	1.99	0.43
1:A:142:C:O2	1:A:142:C:O4'	2.36	0.43
1:A:1808:U:H2'	1:A:1809:A:C8	2.53	0.43
1:A:73:C:H2'	1:A:74:G:H4'	2.00	0.43
11:M:33:LEU:HD23	11:M:34:PRO:HD2	2.01	0.43
36:1:524:THR:O	36:1:525:ALA:C	2.56	0.43
36:1:5:PHE:CZ	36:1:30:VAL:HG13	2.54	0.43
37:2:363:GLU:HB2	37:2:366:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:4:120:ALA:HB3	40:5:48:LYS:HE3	1.99	0.43
42:7:239:ASN:HA	42:7:242:ARG:HD2	2.00	0.43
42:7:397:LYS:HG3	42:7:408:VAL:CG1	2.48	0.43
1:A:1757:G:H2'	1:A:1758:G:H8	1.82	0.43
9:J:141:ARG:HB3	9:J:145:ILE:HG23	1.99	0.43
3:B:160:ALA:N	14:W:66:ASP:OD2	2.48	0.43
36:1:484:ILE:O	36:1:491:LEU:HD21	2.18	0.43
39:4:163:GLU:HA	39:4:164:ASP:HA	1.80	0.43
39:4:268:GLY:O	39:4:272:ILE:HG13	2.19	0.43
39:4:339:VAL:N	39:4:340:PRO:CD	2.81	0.43
37:2:862:LYS:HE2	40:5:265:ARG:HB3	2.01	0.43
42:7:413:PHE:HB2	42:7:451:VAL:HG21	1.99	0.43
43:8:315:ALA:HB1	43:8:320:MET:HE2	2.00	0.43
43:8:19:ARG:HD3	43:8:68:VAL:HG12	2.01	0.43
1:A:1599:U:O2	1:A:1600:G:N1	2.52	0.43
27:S:83:ASN:HB3	27:S:85:VAL:HG23	2.00	0.43
2:0:491:U:O3'	2:0:517:G:C6	2.72	0.43
36:1:523:LEU:HD22	40:5:241:LYS:HG3	1.99	0.43
38:3:188:ASP:HA	38:3:191:ARG:HB2	1.99	0.43
39:4:214:ALA:N	39:4:215:PRO:HD3	2.33	0.43
39:4:265:GLU:O	39:4:269:VAL:N	2.44	0.43
39:4:281:ARG:NE	40:5:202:PRO:HA	2.33	0.43
42:7:241:ASN:HA	42:7:244:LEU:HD12	2.01	0.43
43:8:60:VAL:O	43:8:63:VAL:HG13	2.18	0.43
8:I:69:LEU:HD22	8:I:96:ALA:HB2	2.01	0.43
17:Z:35:VAL:HG23	17:Z:40:ILE:HD11	2.00	0.43
40:5:345:GLN:HE21	40:5:349:GLU:CG	2.31	0.43
42:7:252:ASP:N	42:7:253:PRO:CD	2.82	0.43
42:7:379:PRO:HA	42:7:380:MET:CB	2.47	0.43
43:8:323:CYS:SG	43:8:324:LYS:N	2.91	0.43
3:B:70:ASN:OD1	5:D:274:MET:SD	2.77	0.43
6:F:130:PHE:O	6:F:138:HIS:N	2.45	0.43
1:A:441:C:OP2	9:J:2:GLY:N	2.52	0.43
2:0:396:C:O2	2:0:397:G:N2	2.52	0.43
36:1:159:GLN:O	36:1:163:LEU:HD23	2.18	0.43
39:4:341:ASP:HA	40:5:350:TYR:OH	2.18	0.43
42:7:475:LEU:C	42:7:475:LEU:HD23	2.39	0.43
14:W:30:ALA:O	14:W:60:ARG:HD3	2.18	0.43
2:0:517:G:O2'	2:0:518:G:O5'	2.30	0.43
2:0:534:U:C4	2:0:535:C:N4	2.86	0.43
37:2:510:THR:HA	37:2:513:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:710:ILE:CD1	37:2:714:PHE:HE2	2.31	0.43
40:5:183:SER:HB3	40:5:184:PRO:HD3	2.01	0.43
41:6:77:LEU:HD23	41:6:141:PHE:CD2	2.54	0.43
41:6:151:GLN:HE21	41:6:192:GLN:HA	1.84	0.43
42:7:479:LEU:CB	42:7:489:GLN:HE21	2.32	0.43
43:8:103:LEU:HD13	43:8:127:LEU:HA	2.01	0.43
1:A:1611:G:H4'	28:T:86:ARG:NH1	2.33	0.43
38:3:26:LEU:O	38:3:26:LEU:HG	2.19	0.43
43:8:186:VAL:HG22	43:8:203:ASP:OD1	2.18	0.43
24:N:31:LEU:HD12	24:N:33:ARG:HG3	2.01	0.43
26:R:49:TYR:O	26:R:53:GLU:HG2	2.19	0.43
28:T:124:ARG:HD3	28:T:129:LEU:HD12	2.01	0.43
2:0:393:U:H2'	2:0:394:C:O4'	2.18	0.42
36:1:446:ILE:HG13	36:1:514:MET:HG2	2.01	0.42
36:1:530:LEU:O	40:5:230:LEU:HD11	2.19	0.42
37:2:418:ILE:HG23	37:2:441:ARG:HD3	2.00	0.42
37:2:706:ARG:HA	37:2:710:ILE:HD11	2.01	0.42
39:4:285:LEU:HD21	40:5:163:SER:OG	2.18	0.42
36:1:529:VAL:O	40:5:233:LEU:HD13	2.18	0.42
42:7:244:LEU:HD21	42:7:254:GLU:HG2	2.01	0.42
43:8:135:GLY:O	43:8:138:GLN:HG2	2.19	0.42
1:A:1315:U:O4'	1:A:1315:U:O2	2.37	0.42
1:A:427:U:O4'	1:A:427:U:O2	2.37	0.42
1:A:887:U:O2	1:A:887:U:C2'	2.67	0.42
12:O:84:LEU:HD22	12:O:149:LEU:HD23	2.00	0.42
26:R:94:ALA:HA	26:R:97:GLN:HE21	1.83	0.42
1:A:1563:G:OP1	29:U:121:ARG:NH2	2.52	0.42
36:1:147:THR:N	36:1:148:PRO:CD	2.82	0.42
36:1:285:LYS:HB3	37:2:723:ARG:NE	2.34	0.42
39:4:262:TYR:HB3	39:4:265:GLU:HG3	2.01	0.42
39:4:340:PRO:C	40:5:350:TYR:HE1	2.22	0.42
39:4:156:SER:CB	40:5:110:VAL:HG11	2.47	0.42
39:4:276:CYS:HB3	40:5:215:MET:HB2	2.02	0.42
40:5:250:VAL:O	40:5:254:SER:N	2.43	0.42
42:7:265:LEU:HB3	42:7:279:ARG:HD3	2.01	0.42
43:8:126:SER:O	43:8:130:VAL:HG23	2.19	0.42
43:8:316:VAL:HA	43:8:321:VAL:O	2.19	0.42
39:4:329:MET:HG3	43:8:335:SER:O	2.19	0.42
21:E:191:PRO:O	21:E:199:GLY:HA3	2.19	0.42
36:1:410:VAL:HA	36:1:413:TRP:CB	2.49	0.42
36:1:63:LYS:HD2	36:1:66:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:725:PRO:HB2	37:2:731:GLU:HG2	2.00	0.42
39:4:128:ARG:CZ	40:5:112:ILE:HD11	2.49	0.42
43:8:70:LEU:HD23	43:8:106:LEU:HB2	2.00	0.42
1:A:191:A:N6	1:A:208:G:O2'	2.51	0.42
28:T:24:ARG:HD3	28:T:29:ALA:HA	2.01	0.42
36:1:30:VAL:O	36:1:34:VAL:HG23	2.20	0.42
36:1:428:VAL:N	36:1:429:PRO:CD	2.82	0.42
36:1:526:MET:HE2	40:5:239:LEU:H	1.85	0.42
39:4:375:VAL:O	40:5:313:ARG:CZ	2.68	0.42
39:4:282:VAL:HB	40:5:164:LEU:HD12	2.00	0.42
40:5:194:PHE:CZ	40:5:319:ILE:HD13	2.54	0.42
42:7:212:ILE:HG23	42:7:271:TYR:HE1	1.84	0.42
1:A:1113:A:H2'	1:A:1114:U:C6	2.53	0.42
25:Q:45:LEU:HG	25:Q:84:ILE:HD11	2.01	0.42
27:S:16:ILE:HG23	27:S:38:ILE:HD11	2.02	0.42
2:0:385:A:C6	2:0:386:U:C4	3.07	0.42
38:3:214:LEU:HA	38:3:217:TRP:NE1	2.34	0.42
39:4:340:PRO:CA	40:5:350:TYR:HE1	2.32	0.42
36:1:527:SER:N	40:5:237:ASN:OD1	2.52	0.42
3:B:19:LEU:HD13	27:S:102:THR:HG23	2.01	0.42
25:Q:50:ARG:O	25:Q:58:LYS:HG2	2.19	0.42
30:V:33:GLU:OE2	30:V:87:ARG:NE	2.53	0.42
36:1:48:GLU:CB	36:1:49:PRO:HD3	2.49	0.42
38:3:274:LEU:HG	38:3:275:LYS:N	2.33	0.42
39:4:372:GLU:OE2	40:5:318:LEU:HG	2.20	0.42
40:5:148:VAL:HG12	40:5:168:ARG:HB3	2.02	0.42
41:6:136:ASP:O	41:6:140:LYS:N	2.52	0.42
1:A:1536:G:H2'	1:A:1537:A:H8	1.85	0.42
1:A:549:C:C5	1:A:550:C:C2	3.08	0.42
36:1:329:ILE:HB	36:1:330:PRO:HD3	2.02	0.42
36:1:452:PHE:CE1	36:1:471:ILE:HG21	2.55	0.42
37:2:739:ALA:O	37:2:789:ARG:NH1	2.51	0.42
37:2:839:THR:HB	37:2:841:THR:HG23	2.01	0.42
37:2:869:ASN:OD1	40:5:269:LYS:O	2.37	0.42
40:5:164:LEU:HB3	40:5:203:ILE:CD1	2.49	0.42
41:6:18:ILE:O	41:6:18:ILE:HG22	2.19	0.42
42:7:475:LEU:CD2	42:7:479:LEU:HD12	2.49	0.42
4:C:79:VAL:HG13	4:C:81:PHE:CD2	2.54	0.42
3:B:12:GLU:HA	27:S:111:PHE:CZ	2.54	0.42
27:S:80:ARG:HD2	27:S:83:ASN:HD21	1.84	0.42
2:0:514:U:H2'	2:0:515:G:H1'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:6:179:TRP:CE3	41:6:187:ILE:HG21	2.55	0.42
41:6:67:ALA:HB2	41:6:98:PRO:HG2	2.01	0.42
42:7:369:ALA:O	42:7:373:ILE:HG13	2.19	0.42
39:4:254:PRO:HG3	43:8:110:PHE:CG	2.54	0.42
43:8:90:LEU:HD12	43:8:130:VAL:HG21	2.02	0.42
43:8:75:GLU:HG3	43:8:76:PRO:HD3	2.02	0.42
1:A:533:A:N6	1:A:551:U:O4	2.53	0.42
1:A:536:A:H2'	1:A:536:A:N3	2.35	0.42
22:G:187:SER:HB3	22:G:190:ILE:HG12	2.02	0.42
8:I:38:ALA:HA	8:I:41:ARG:HD3	2.02	0.42
36:1:526:MET:HA	40:5:236:SER:C	2.40	0.42
41:6:77:LEU:HD23	41:6:141:PHE:CE2	2.54	0.42
42:7:288:TYR:CE1	42:7:321:PHE:HB3	2.55	0.42
25:Q:111:MET:SD	25:Q:119:PHE:CZ	3.13	0.42
25:Q:34:MET:O	25:Q:42:ARG:HG2	2.20	0.42
2:0:394:C:H2'	2:0:396:C:C4	2.54	0.42
36:1:300:TYR:CE1	36:1:322:VAL:HG12	2.55	0.42
36:1:436:ILE:O	36:1:440:LEU:HB2	2.20	0.42
39:4:176:MET:O	39:4:176:MET:HG3	2.19	0.42
39:4:279:PRO:HD2	40:5:207:ASN:CA	2.50	0.42
1:A:1270:G:O2'	1:A:1301:A:N7	2.50	0.42
1:A:1320:G:H2'	1:A:1321:G:O4'	2.20	0.42
1:A:511:U:O2'	1:A:576:A:N6	2.53	0.42
8:I:60:ILE:HB	8:I:92:VAL:HG12	2.02	0.42
23:L:71:LEU:HG	23:L:76:ILE:HG12	2.02	0.42
36:1:338:ILE:HA	36:1:341:LEU:HB2	2.01	0.41
36:1:499:TYR:CE2	36:1:503:GLU:HG2	2.54	0.41
39:4:272:ILE:HG23	40:5:43:GLY:HA3	2.02	0.41
39:4:347:LEU:HD11	40:5:346:ALA:HB3	2.01	0.41
39:4:375:VAL:HB	40:5:318:LEU:HD21	2.01	0.41
43:8:280:LEU:HD21	43:8:300:GLU:HB3	2.02	0.41
3:B:24:HIS:CB	3:B:51:LEU:HD21	2.50	0.41
1:A:1334:G:O3'	21:E:183:GLY:HA3	2.20	0.41
11:M:10:TYR:OH	11:M:18:GLN:NE2	2.52	0.41
2:0:477:G:N2	2:0:478:A:N3	2.67	0.41
2:0:512:C:H3'	2:0:513:U:C5'	2.50	0.41
37:2:449:GLU:HG3	37:2:505:ARG:HD2	2.02	0.41
39:4:354:LEU:C	39:4:358:THR:HG23	2.41	0.41
41:6:174:MET:SD	41:6:187:ILE:HG12	2.60	0.41
42:7:284:LEU:HD22	42:7:299:LEU:HD22	2.03	0.41
38:3:401:TYR:O	38:3:405:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:G:C2	1:A:1228:A:C8	3.08	0.41
1:A:190:G:O2'	1:A:209:A:N6	2.53	0.41
6:F:111:VAL:O	6:F:111:VAL:HG23	2.20	0.41
36:1:90:VAL:HG21	36:1:165:ARG:HH22	1.84	0.41
36:1:526:MET:CB	40:5:237:ASN:OD1	2.66	0.41
40:5:218:LEU:O	40:5:222:SER:N	2.54	0.41
42:7:321:PHE:O	42:7:325:MET:HG2	2.20	0.41
42:7:479:LEU:HA	42:7:482:THR:HB	2.01	0.41
43:8:144:LEU:HD21	43:8:184:VAL:HG11	2.02	0.41
24:N:19:GLN:O	24:N:23:LYS:HG2	2.19	0.41
2:0:422:U:H3'	2:0:423:G:H4'	2.02	0.41
38:3:292:ILE:HG21	38:3:318:VAL:HB	2.02	0.41
39:4:269:VAL:CG2	40:5:47:LEU:HD21	2.49	0.41
42:7:218:ASN:HB3	42:7:219:PRO:HD3	2.03	0.41
42:7:231:LEU:O	42:7:235:VAL:HG22	2.19	0.41
1:A:318:A:N6	7:H:186:GLN:OE1	2.54	0.41
1:A:380:G:O6	9:J:178:ARG:NH1	2.50	0.41
1:A:30:C:O2'	1:A:596:U:OP1	2.37	0.41
6:F:191:ARG:HD3	6:F:245:ARG:HB3	2.03	0.41
27:S:76:GLU:O	27:S:80:ARG:HG2	2.21	0.41
2:0:454:C:H2'	2:0:455:U:C6	2.55	0.41
2:0:533:C:H2'	2:0:534:U:C6	2.55	0.41
2:0:603:A:H2'	2:0:604:C:C6	2.56	0.41
36:1:163:LEU:HG	36:1:164:LEU:HD22	2.01	0.41
39:4:240:SER:HA	39:4:241:MET:C	2.41	0.41
4:C:28:LYS:NZ	13:P:51:GLU:OE1	2.52	0.41
5:D:141:LEU:HD11	5:D:238:LYS:HE3	2.02	0.41
11:M:126:VAL:HG12	11:M:128:VAL:HG13	2.02	0.41
27:S:126:MET:HB2	27:S:128:PHE:CD1	2.55	0.41
1:A:1623:A:H5''	28:T:133:GLY:HA3	2.03	0.41
1:A:921:G:C6	15:X:28:ARG:HD2	2.55	0.41
2:0:363:A:N6	2:0:461:A:N1	2.69	0.41
36:1:229:HIS:O	36:1:232:THR:HG22	2.21	0.41
36:1:524:THR:OG1	36:1:525:ALA:N	2.53	0.41
36:1:526:MET:O	36:1:530:LEU:N	2.43	0.41
36:1:58:CYS:SG	36:1:63:LYS:O	2.78	0.41
37:2:710:ILE:C	37:2:714:PHE:CE2	2.94	0.41
40:5:349:GLU:O	40:5:350:TYR:C	2.59	0.41
1:A:1303:C:H2'	1:A:1304:U:O4'	2.20	0.41
21:E:126:ILE:HG21	21:E:134:CYS:HB3	2.02	0.41
28:T:73:ASN:HB3	28:T:76:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:142:ASP:O	36:1:146:LEU:HB3	2.21	0.41
36:1:175:HIS:CD2	36:1:228:MET:HB3	2.56	0.41
36:1:383:VAL:O	36:1:388:LYS:HG3	2.21	0.41
36:1:499:TYR:CZ	40:5:242:ASN:HB3	2.56	0.41
38:3:49:ASN:HA	38:3:50:MET:CB	2.44	0.41
1:A:506:G:OP1	17:Z:108:LYS:NZ	2.46	0.41
3:B:38:ILE:HD11	3:B:150:THR:HG22	2.03	0.41
15:X:53:ILE:N	15:X:60:LYS:O	2.52	0.41
39:4:269:VAL:O	39:4:273:MET:HG2	2.20	0.41
39:4:359:TYR:CE2	39:4:363:LEU:HD12	2.55	0.41
39:4:125:SER:CA	40:5:111:ASN:HD21	2.31	0.41
40:5:272:GLN:NE2	40:5:275:HIS:ND1	2.69	0.41
41:6:85:CYS:O	41:6:89:ILE:HG13	2.21	0.41
42:7:200:TYR:O	42:7:204:THR:OG1	2.39	0.41
1:A:69:C:OP2	7:H:164:LYS:NZ	2.50	0.41
3:B:119:PRO:HG2	3:B:142:LEU:HD11	2.02	0.41
21:E:162:ASP:N	21:E:163:PRO:CD	2.83	0.41
36:1:331:ILE:CA	36:1:434:ASN:HD21	2.34	0.41
37:2:806:THR:C	37:2:807:LEU:HD23	2.42	0.41
37:2:853:GLN:HA	37:2:856:ALA:HB3	2.01	0.41
39:4:276:CYS:SG	40:5:211:ILE:HG23	2.61	0.41
39:4:365:GLN:CG	40:5:329:ASN:CB	2.97	0.41
1:A:295:C:H2'	1:A:296:U:O4'	2.20	0.41
26:R:33:LYS:NZ	26:R:36:GLY:O	2.43	0.41
25:Q:18:ARG:HD2	28:T:88:LYS:HG2	2.02	0.41
2:0:511:C:H2'	2:0:512:C:C6	2.56	0.41
36:1:204:HIS:O	36:1:208:ILE:HG12	2.21	0.41
36:1:241:ILE:HG21	36:1:282:VAL:HG22	2.03	0.41
37:2:549:GLU:HG3	37:2:572:HIS:HB2	2.02	0.41
36:1:524:THR:HG22	39:4:335:VAL:CG2	2.51	0.41
41:6:84:LEU:HA	41:6:87:CYS:SG	2.61	0.41
1:A:1650:A:H2'	1:A:1651:A:O4'	2.21	0.41
1:A:203:G:H2'	1:A:204:G:C8	2.55	0.41
1:A:628:A:N6	21:E:178:ARG:HB3	2.35	0.41
28:T:27:ALA:O	28:T:31:THR:OG1	2.39	0.41
28:T:86:ARG:CB	28:T:98:VAL:HG23	2.52	0.41
16:Y:51:VAL:HG13	16:Y:70:VAL:HG22	2.02	0.41
36:1:526:MET:HA	40:5:237:ASN:N	2.36	0.40
42:7:244:LEU:HD21	42:7:254:GLU:HB3	2.04	0.40
42:7:341:LEU:HD11	42:7:384:GLU:HB3	2.03	0.40
1:A:1724:A:C2	1:A:1811:C:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:376:G:O2'	2:0:447:A:N6	2.53	0.40
37:2:710:ILE:CB	37:2:714:PHE:HE2	2.08	0.40
37:2:691:MET:HE3	37:2:788:LEU:HD11	2.02	0.40
37:2:745:LYS:NZ	37:2:807:LEU:HD21	2.36	0.40
39:4:350:ASN:O	40:5:343:MET:SD	2.80	0.40
39:4:117:VAL:HG21	40:5:51:LYS:HB2	2.03	0.40
1:A:166:A:H2'	1:A:167:G:C8	2.56	0.40
1:A:878:G:C6	1:A:879:C:C4	3.10	0.40
3:B:132:GLN:HB3	3:B:133:PRO:HD3	2.02	0.40
10:K:50:LEU:HD13	10:K:105:PHE:CE2	2.57	0.40
21:E:72:VAL:CG1	23:L:20:VAL:HG22	2.51	0.40
17:Z:23:MET:SD	17:Z:23:MET:N	2.94	0.40
2:0:421:A:H2'	2:0:422:U:C4'	2.51	0.40
36:1:530:LEU:HD23	40:5:230:LEU:O	2.22	0.40
40:5:185:GLU:HB3	40:5:189:LYS:HE3	2.02	0.40
42:7:353:THR:CG2	42:7:354:THR:HA	2.51	0.40
43:8:251:SER:HB3	43:8:254:LYS:HG2	2.03	0.40
39:4:251:MET:HB3	43:8:67:VAL:HG11	2.04	0.40
43:8:83:ILE:O	43:8:87:CYS:SG	2.80	0.40
1:A:1149:A:H2'	1:A:1149:A:N3	2.36	0.40
1:A:1240:A:OP1	25:Q:100:LYS:NZ	2.54	0.40
1:A:1700:C:C2	1:A:1834:A:N6	2.90	0.40
6:F:256:LEU:HA	6:F:259:LYS:HB3	2.03	0.40
9:J:38:ILE:HD11	9:J:81:VAL:HG23	2.03	0.40
24:N:51:VAL:HB	24:N:77:ILE:HB	2.02	0.40
2:0:537:G:H1'	2:0:538:G:N1	2.37	0.40
36:1:331:ILE:C	36:1:434:ASN:HD21	2.25	0.40
36:1:58:CYS:SG	36:1:67:ALA:N	2.95	0.40
38:3:162:ASP:O	38:3:166:LEU:HB2	2.22	0.40
39:4:295:ALA:O	39:4:299:ILE:HG12	2.21	0.40
39:4:279:PRO:HG2	40:5:206:LYS:O	2.22	0.40
41:6:58:PRO:HB3	41:6:93:HIS:NE2	2.37	0.40
42:7:481:LEU:HG	42:7:482:THR:N	2.37	0.40
43:8:115:LYS:HB2	43:8:116:ASN:HB3	2.03	0.40
1:A:1162:C:H2'	1:A:1163:C:O4'	2.21	0.40
1:A:905:C:H2'	1:A:906:U:O4'	2.22	0.40
27:S:20:TYR:O	27:S:24:LEU:HG	2.20	0.40
1:A:681:U:H4'	16:Y:9:THR:HG22	2.03	0.40
36:1:452:PHE:HA	36:1:455:LEU:HB3	2.03	0.40
39:4:285:LEU:O	39:4:289:LEU:HG	2.22	0.40
40:5:50:ILE:O	40:5:53:TYR:HD1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:397:LYS:O	42:7:408:VAL:HG21	2.21	0.40
42:7:492:VAL:HA	42:7:495:HIS:CD2	2.56	0.40
1:A:1556:A:N3	1:A:1556:A:H2'	2.36	0.40
1:A:193:C:H2'	1:A:194:C:C6	2.57	0.40
1:A:929:G:H2'	1:A:930:C:O4'	2.22	0.40
3:B:30:LEU:HD21	3:B:35:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	31	71
4	C	211/264 (80%)	189 (90%)	21 (10%)	1 (0%)	31	71
5	D	219/255 (86%)	201 (92%)	17 (8%)	1 (0%)	31	71
6	F	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
7	H	235/249 (94%)	216 (92%)	18 (8%)	1 (0%)	36	76
8	I	181/194 (93%)	160 (88%)	20 (11%)	1 (1%)	27	67
9	J	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	17	56
10	K	183/194 (94%)	170 (93%)	13 (7%)	0	100	100
11	M	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
12	O	147/151 (97%)	137 (93%)	9 (6%)	1 (1%)	24	64
13	P	134/151 (89%)	120 (90%)	14 (10%)	0	100	100
14	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
15	X	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	21	61
16	Y	139/143 (97%)	128 (92%)	7 (5%)	4 (3%)	5	26
17	Z	122/134 (91%)	115 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	b	99/115 (86%)	87 (88%)	10 (10%)	2 (2%)	8	37
19	c	81/84 (96%)	75 (93%)	5 (6%)	1 (1%)	14	51
20	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
21	E	226/281 (80%)	209 (92%)	17 (8%)	0	100	100
22	G	189/204 (93%)	165 (87%)	21 (11%)	3 (2%)	11	43
23	L	94/149 (63%)	83 (88%)	10 (11%)	1 (1%)	16	53
24	N	115/132 (87%)	96 (84%)	16 (14%)	3 (3%)	6	30
25	Q	113/145 (78%)	92 (81%)	17 (15%)	4 (4%)	4	22
26	R	140/172 (81%)	130 (93%)	9 (6%)	1 (1%)	24	64
27	S	130/135 (96%)	111 (85%)	17 (13%)	2 (2%)	11	45
28	T	142/152 (93%)	132 (93%)	8 (6%)	2 (1%)	12	47
29	U	139/145 (96%)	126 (91%)	12 (9%)	1 (1%)	24	64
30	V	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
31	a	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
32	d	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
33	e	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	9	39
34	g	66/156 (42%)	54 (82%)	9 (14%)	3 (4%)	3	16
35	h	310/317 (98%)	274 (88%)	34 (11%)	2 (1%)	27	67
36	1	532/1362 (39%)	430 (81%)	85 (16%)	17 (3%)	4	24
37	2	543/913 (60%)	428 (79%)	105 (19%)	10 (2%)	9	40
38	3	417/462 (90%)	333 (80%)	67 (16%)	17 (4%)	3	18
39	4	270/364 (74%)	217 (80%)	45 (17%)	8 (3%)	5	26
40	5	320/363 (88%)	255 (80%)	54 (17%)	11 (3%)	4	22
41	6	213/218 (98%)	179 (84%)	31 (15%)	3 (1%)	12	47
42	7	370/607 (61%)	301 (81%)	57 (15%)	12 (3%)	4	24
43	8	363/374 (97%)	290 (80%)	61 (17%)	12 (3%)	4	23
All	All	7808/10224 (76%)	6786 (87%)	893 (11%)	129 (2%)	14	42

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	94	LYS
15	X	28	ARG

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Mol	Chain	Res	Type
16	Y	61	GLN
22	G	134	VAL
24	N	57	ASP
26	R	17	LYS
27	S	99	ASP
34	g	124	ASP
36	1	167	ASN
36	1	168	SER
36	1	526	MET
36	1	530	LEU
36	1	531	ALA
37	2	651	LEU
38	3	51	VAL
38	3	93	LYS
39	4	338	ILE
40	5	211	ILE
40	5	212	ASN
40	5	241	LYS
42	7	423	PRO
43	8	57	ASP
43	8	335	SER
3	B	44	ASP
4	C	190	PRO
5	D	237	ALA
8	I	88	SER
9	J	123	ARG
22	G	167	LYS
25	Q	17	TYR
25	Q	70	MET
28	T	100	ALA
35	h	275	ILE
36	1	416	GLU
36	1	513	SER
37	2	435	ASP
37	2	653	ARG
37	2	742	LYS
37	2	743	ALA
38	3	26	LEU
38	3	48	THR
38	3	50	MET
38	3	62	TYR
38	3	224	ASN

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Mol	Chain	Res	Type
38	3	238	TYR
38	3	242	TYR
38	3	245	ALA
38	3	325	LEU
38	3	328	CYS
39	4	169	ASP
39	4	368	ILE
40	5	87	HIS
40	5	240	GLY
42	7	270	GLY
42	7	381	ARG
42	7	462	SER
43	8	43	ALA
43	8	114	ASP
43	8	116	ASN
7	H	169	PRO
16	Y	62	PRO
16	Y	86	PRO
18	b	47	ALA
27	S	120	THR
35	h	272	GLN
36	1	42	THR
36	1	43	TRP
36	1	223	PRO
36	1	522	GLN
38	3	27	SER
38	3	63	SER
38	3	200	SER
38	3	350	CYS
39	4	133	ALA
39	4	244	PRO
40	5	340	LYS
43	8	108	ASN
43	8	225	THR
22	G	51	HIS
24	N	29	ASP
28	T	74	PRO
29	U	115	LYS
33	e	7	TYR
34	g	126	CYS
36	1	221	ASN
36	1	347	ILE

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Mol	Chain	Res	Type
37	2	325	THR
37	2	422	GLU
40	5	73	GLU
40	5	162	LEU
40	5	203	ILE
42	7	221	ILE
42	7	289	GLN
42	7	348	SER
43	8	323	CYS
12	O	83	ASP
19	c	50	ALA
23	L	19	GLY
24	N	33	ARG
25	Q	124	LYS
34	g	86	THR
36	1	209	GLN
36	1	421	GLU
37	2	702	GLU
37	2	869	ASN
40	5	239	LEU
41	6	184	SER
42	7	427	ASN
42	7	489	GLN
43	8	130	VAL
16	Y	60	LYS
39	4	199	ILE
39	4	285	LEU
40	5	339	GLY
42	7	468	THR
43	8	34	SER
43	8	191	SER
39	4	116	PRO
41	6	58	PRO
41	6	99	ILE
18	b	56	VAL
25	Q	69	PRO
36	1	436	ILE
42	7	212	ILE
42	7	382	ILE
37	2	564	ILE
38	3	291	PRO
43	8	118	PRO

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Mol	Chain	Res	Type
36	1	506	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	180/246 (73%)	177 (98%)	3 (2%)	63	88
4	C	194/231 (84%)	191 (98%)	3 (2%)	67	89
5	D	186/205 (91%)	183 (98%)	3 (2%)	65	89
6	F	223/224 (100%)	222 (100%)	1 (0%)	92	97
7	H	207/218 (95%)	203 (98%)	4 (2%)	60	87
8	I	165/174 (95%)	162 (98%)	3 (2%)	62	87
9	J	178/180 (99%)	178 (100%)	0	100	100
10	K	161/168 (96%)	161 (100%)	0	100	100
11	M	130/142 (92%)	128 (98%)	2 (2%)	67	89
12	O	130/131 (99%)	128 (98%)	2 (2%)	67	89
13	P	106/119 (89%)	105 (99%)	1 (1%)	81	93
14	W	68/68 (100%)	67 (98%)	1 (2%)	67	89
15	X	112/113 (99%)	109 (97%)	3 (3%)	48	81
16	Y	113/114 (99%)	112 (99%)	1 (1%)	81	93
17	Z	107/115 (93%)	106 (99%)	1 (1%)	81	93
18	b	89/99 (90%)	87 (98%)	2 (2%)	55	84
19	c	75/76 (99%)	75 (100%)	0	100	100
20	f	47/106 (44%)	47 (100%)	0	100	100
21	E	190/232 (82%)	189 (100%)	1 (0%)	90	96
22	G	158/170 (93%)	156 (99%)	2 (1%)	71	91
23	L	87/125 (70%)	86 (99%)	1 (1%)	76	92
24	N	99/108 (92%)	96 (97%)	3 (3%)	44	79
25	Q	105/130 (81%)	101 (96%)	4 (4%)	36	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	R	117/140 (84%)	116 (99%)	1 (1%)	81	93
27	S	119/121 (98%)	119 (100%)	0	100	100
28	T	125/132 (95%)	123 (98%)	2 (2%)	65	89
29	U	111/116 (96%)	109 (98%)	2 (2%)	62	87
30	V	92/107 (86%)	92 (100%)	0	100	100
31	a	66/103 (64%)	66 (100%)	0	100	100
32	d	55/62 (89%)	55 (100%)	0	100	100
33	e	48/49 (98%)	48 (100%)	0	100	100
34	g	61/140 (44%)	58 (95%)	3 (5%)	27	66
35	h	271/275 (98%)	268 (99%)	3 (1%)	76	92
36	1	490/1245 (39%)	476 (97%)	14 (3%)	45	80
37	2	494/812 (61%)	477 (97%)	17 (3%)	40	76
38	3	384/423 (91%)	375 (98%)	9 (2%)	53	84
39	4	239/282 (85%)	233 (98%)	6 (2%)	50	82
40	5	293/320 (92%)	283 (97%)	10 (3%)	40	76
41	6	190/193 (98%)	188 (99%)	2 (1%)	76	92
42	7	342/544 (63%)	335 (98%)	7 (2%)	58	86
43	8	327/335 (98%)	319 (98%)	8 (2%)	52	83
All	All	6934/8893 (78%)	6809 (98%)	125 (2%)	64	87

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	38	ILE
3	B	128	GLN
3	B	142	LEU
4	C	51	ARG
4	C	78	GLU
4	C	178	THR
5	D	117	ARG
5	D	213	LEU
5	D	248	TYR
6	F	51	LYS
7	H	98	ARG
7	H	163	ASN
7	H	171	THR

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Mol	Chain	Res	Type
7	H	201	LYS
8	I	82	GLU
8	I	113	LYS
8	I	143	ARG
11	M	69	ARG
11	M	101	ARG
12	O	67	THR
12	O	76	LYS
13	P	150	ARG
14	W	13	VAL
15	X	86	LEU
15	X	103	VAL
15	X	104	LEU
16	Y	99	GLU
17	Z	10	ARG
18	b	15	ARG
18	b	51	ARG
21	E	76	ARG
22	G	104	THR
22	G	142	SER
23	L	14	LEU
24	N	18	LEU
24	N	83	LYS
24	N	97	GLU
25	Q	13	ARG
25	Q	30	TYR
25	Q	37	TYR
25	Q	50	ARG
26	R	105	LYS
28	T	25	LYS
28	T	114	LEU
29	U	33	TRP
29	U	41	LYS
34	g	97	LYS
34	g	138	ARG
34	g	144	CYS
35	h	134	THR
35	h	156	PHE
35	h	221	LEU
36	1	41	ARG
36	1	75	LYS
36	1	163	LEU

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Mol	Chain	Res	Type
36	1	198	CYS
36	1	238	ASP
36	1	264	LYS
36	1	268	LYS
36	1	288	ASN
36	1	301	HIS
36	1	327	LEU
36	1	371	ILE
36	1	373	ASP
36	1	413	TRP
36	1	499	TYR
37	2	346	ASP
37	2	379	ILE
37	2	439	ARG
37	2	462	THR
37	2	531	LYS
37	2	578	LEU
37	2	608	LEU
37	2	616	LEU
37	2	668	ARG
37	2	669	ARG
37	2	674	HIS
37	2	723	ARG
37	2	738	VAL
37	2	776	ARG
37	2	807	LEU
37	2	848	GLU
37	2	862	LYS
38	3	7	THR
38	3	17	HIS
38	3	102	ARG
38	3	163	ARG
38	3	214	LEU
38	3	232	ILE
38	3	267	VAL
38	3	274	LEU
38	3	418	LEU
39	4	114	LEU
39	4	200	THR
39	4	232	SER
39	4	250	VAL
39	4	264	THR

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Mol	Chain	Res	Type
39	4	276	CYS
40	5	70	LEU
40	5	163	SER
40	5	168	ARG
40	5	197	MET
40	5	230	LEU
40	5	244	GLN
40	5	285	ASN
40	5	313	ARG
40	5	351	ASN
40	5	352	ASN
41	6	87	CYS
41	6	183	GLU
42	7	254	GLU
42	7	304	MET
42	7	350	PHE
42	7	390	LEU
42	7	447	PHE
42	7	481	LEU
42	7	483	GLU
43	8	72	LEU
43	8	75	GLU
43	8	86	LEU
43	8	149	LYS
43	8	165	LEU
43	8	210	ARG
43	8	225	THR
43	8	291	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	141	ASN
3	B	169	HIS
4	C	43	ASN
4	C	157	GLN
4	C	179	ASN
5	D	267	GLN
5	D	272	HIS
7	H	4	ASN
8	I	114	GLN
9	J	64	ASN

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Mol	Chain	Res	Type
9	J	99	ASN
9	J	116	HIS
9	J	165	GLN
9	J	167	GLN
11	M	18	GLN
11	M	121	GLN
14	W	35	ASN
15	X	15	ASN
15	X	16	ASN
17	Z	94	HIS
18	b	43	ASN
19	c	26	GLN
20	f	88	GLN
20	f	117	ASN
21	E	226	GLN
22	G	29	GLN
22	G	118	ASN
24	N	55	ASN
25	Q	41	GLN
25	Q	103	ASN
26	R	97	GLN
27	S	31	ASN
27	S	83	ASN
28	T	72	GLN
28	T	76	GLN
28	T	105	ASN
29	U	63	HIS
33	e	10	HIS
36	1	82	ASN
36	1	167	ASN
36	1	207	GLN
36	1	236	GLN
36	1	288	ASN
36	1	434	ASN
36	1	442	GLN
36	1	448	GLN
36	1	498	ASN
37	2	386	ASN
37	2	487	GLN
37	2	539	ASN
37	2	715	HIS
37	2	724	GLN

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Mol	Chain	Res	Type
37	2	837	GLN
37	2	854	ASN
37	2	869	ASN
37	2	870	ASN
38	3	103	GLN
38	3	244	ASN
38	3	282	GLN
38	3	302	ASN
38	3	377	ASN
39	4	352	ASN
40	5	58	GLN
40	5	111	ASN
40	5	137	GLN
40	5	261	ASN
40	5	272	GLN
40	5	273	GLN
40	5	279	GLN
40	5	328	GLN
40	5	336	GLN
40	5	345	GLN
40	5	351	ASN
41	6	25	ASN
41	6	151	GLN
42	7	239	ASN
42	7	241	ASN
42	7	243	GLN
42	7	289	GLN
42	7	364	ASN
42	7	489	GLN
42	7	548	HIS
43	8	116	ASN
43	8	259	ASN
43	8	355	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1682/1697 (99%)	406 (24%)	26 (1%)
2	0	338/377 (89%)	186 (55%)	20 (5%)
All	All	2020/2074 (97%)	592 (29%)	46 (2%)

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	C
1	A	4	C
1	A	17	C
1	A	33	G
1	A	41	G
1	A	44	U
1	A	46	A
1	A	58	C
1	A	64	A
1	A	67	C
1	A	68	A
1	A	73	C
1	A	74	G
1	A	75	G
1	A	77	A
1	A	79	A
1	A	100	U
1	A	103	A
1	A	111	A
1	A	113	G
1	A	115	U
1	A	124	U
1	A	126	G
1	A	127	C
1	A	130	G
1	A	142	C
1	A	143	U
1	A	147	A
1	A	160	U
1	A	161	U
1	A	162	C
1	A	163	U
1	A	164	A
1	A	166	A
1	A	167	G
1	A	178	C
1	A	183	G
1	A	184	G
1	A	191	A
1	A	192	C
1	A	201	C
1	A	202	G
1	A	205	G

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Mol	Chain	Res	Type
1	A	206	G
1	A	215	G
1	A	292	A
1	A	307	G
1	A	309	G
1	A	317	C
1	A	319	C
1	A	323	C
1	A	331	C
1	A	332	G
1	A	333	G
1	A	335	G
1	A	347	G
1	A	362	C
1	A	364	A
1	A	367	U
1	A	368	U
1	A	369	C
1	A	370	G
1	A	382	C
1	A	385	G
1	A	386	C
1	A	400	C
1	A	407	G
1	A	408	A
1	A	409	C
1	A	417	C
1	A	418	A
1	A	421	G
1	A	429	C
1	A	434	G
1	A	436	G
1	A	441	C
1	A	447	A
1	A	448	A
1	A	449	A
1	A	450	C
1	A	455	A
1	A	463	C
1	A	464	A
1	A	465	A
1	A	466	G

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Mol	Chain	Res	Type
1	A	470	G
1	A	471	G
1	A	472	C
1	A	473	A
1	A	474	G
1	A	482	G
1	A	487	U
1	A	492	C
1	A	493	A
1	A	517	C
1	A	518	G
1	A	525	A
1	A	530	U
1	A	531	A
1	A	532	C
1	A	533	A
1	A	534	G
1	A	536	A
1	A	537	C
1	A	541	U
1	A	543	C
1	A	544	G
1	A	547	G
1	A	550	C
1	A	551	U
1	A	554	A
1	A	555	A
1	A	556	U
1	A	559	G
1	A	560	A
1	A	561	A
1	A	562	U
1	A	568	C
1	A	576	A
1	A	583	A
1	A	587	A
1	A	588	G
1	A	589	G
1	A	590	A
1	A	591	U
1	A	593	C
1	A	598	G

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Mol	Chain	Res	Type
1	A	606	G
1	A	607	U
1	A	608	C
1	A	609	U
1	A	614	C
1	A	615	C
1	A	627	U
1	A	628	A
1	A	629	A
1	A	631	U
1	A	643	A
1	A	644	G
1	A	655	A
1	A	658	U
1	A	660	C
1	A	664	A
1	A	668	A
1	A	669	A
1	A	671	A
1	A	672	A
1	A	673	G
1	A	675	U
1	A	684	G
1	A	689	U
1	A	690	G
1	A	696	G
1	A	732	U
1	A	734	C
1	A	744	G
1	A	745	C
1	A	750	C
1	A	752	G
1	A	753	C
1	A	754	G
1	A	789	G
1	A	810	A
1	A	811	A
1	A	821	G
1	A	822	U
1	A	823	U
1	A	827	A
1	A	830	A

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Mol	Chain	Res	Type
1	A	834	C
1	A	844	U
1	A	847	A
1	A	852	G
1	A	869	A
1	A	870	A
1	A	871	U
1	A	872	A
1	A	873	G
1	A	874	G
1	A	878	G
1	A	881	G
1	A	884	C
1	A	886	A
1	A	888	U
1	A	890	U
1	A	891	G
1	A	892	U
1	A	893	U
1	A	894	G
1	A	897	U
1	A	898	U
1	A	913	A
1	A	917	U
1	A	918	U
1	A	920	A
1	A	921	G
1	A	922	A
1	A	933	G
1	A	938	A
1	A	943	U
1	A	947	G
1	A	952	G
1	A	956	G
1	A	965	U
1	A	970	G
1	A	971	G
1	A	972	A
1	A	978	G
1	A	988	C
1	A	990	A
1	A	992	A

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Mol	Chain	Res	Type
1	A	999	G
1	A	1002	U
1	A	1008	A
1	A	1017	U
1	A	1023	A
1	A	1045	U
1	A	1050	A
1	A	1060	A
1	A	1061	U
1	A	1062	A
1	A	1083	A
1	A	1085	C
1	A	1087	A
1	A	1088	U
1	A	1100	A
1	A	1114	U
1	A	1115	U
1	A	1116	C
1	A	1117	C
1	A	1120	U
1	A	1121	G
1	A	1126	G
1	A	1133	A
1	A	1138	C
1	A	1144	A
1	A	1148	A
1	A	1153	C
1	A	1154	U
1	A	1183	A
1	A	1195	A
1	A	1197	G
1	A	1207	G
1	A	1208	A
1	A	1215	C
1	A	1221	G
1	A	1224	G
1	A	1225	U
1	A	1230	C
1	A	1235	G
1	A	1242	U
1	A	1244	U
1	A	1251	A

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Mol	Chain	Res	Type
1	A	1253	A
1	A	1256	G
1	A	1257	G
1	A	1258	A
1	A	1259	A
1	A	1264	C
1	A	1269	G
1	A	1271	C
1	A	1274	G
1	A	1275	G
1	A	1281	G
1	A	1282	A
1	A	1284	A
1	A	1285	G
1	A	1286	G
1	A	1287	A
1	A	1288	U
1	A	1291	A
1	A	1293	A
1	A	1295	A
1	A	1296	U
1	A	1298	G
1	A	1299	A
1	A	1301	A
1	A	1302	G
1	A	1303	C
1	A	1305	C
1	A	1307	U
1	A	1308	U
1	A	1311	C
1	A	1312	G
1	A	1314	U
1	A	1315	U
1	A	1342	U
1	A	1349	G
1	A	1350	U
1	A	1354	G
1	A	1364	U
1	A	1365	G
1	A	1371	U
1	A	1372	U
1	A	1378	A

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Mol	Chain	Res	Type
1	A	1396	A
1	A	1397	U
1	A	1402	A
1	A	1403	C
1	A	1406	G
1	A	1412	C
1	A	1424	G
1	A	1428	G
1	A	1429	G
1	A	1440	C
1	A	1447	G
1	A	1449	G
1	A	1452	A
1	A	1453	C
1	A	1454	A
1	A	1459	G
1	A	1462	U
1	A	1463	U
1	A	1466	G
1	A	1475	G
1	A	1478	U
1	A	1479	G
1	A	1480	A
1	A	1489	A
1	A	1490	G
1	A	1494	U
1	A	1495	G
1	A	1498	A
1	A	1506	A
1	A	1507	G
1	A	1508	A
1	A	1509	U
1	A	1512	C
1	A	1519	U
1	A	1520	G
1	A	1521	C
1	A	1533	A
1	A	1536	G
1	A	1543	U
1	A	1544	C
1	A	1548	G
1	A	1552	G

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Mol	Chain	Res	Type
1	A	1553	C
1	A	1554	C
1	A	1556	A
1	A	1557	C
1	A	1560	U
1	A	1564	C
1	A	1573	G
1	A	1574	C
1	A	1575	G
1	A	1580	A
1	A	1588	A
1	A	1593	C
1	A	1600	G
1	A	1601	A
1	A	1604	G
1	A	1606	G
1	A	1619	A
1	A	1621	U
1	A	1622	U
1	A	1623	A
1	A	1637	A
1	A	1639	G
1	A	1641	A
1	A	1648	G
1	A	1654	G
1	A	1661	A
1	A	1665	G
1	A	1671	G
1	A	1680	G
1	A	1683	C
1	A	1695	A
1	A	1697	A
1	A	1698	C
1	A	1704	C
1	A	1715	A
1	A	1721	U
1	A	1722	G
1	A	1725	U
1	A	1726	G
1	A	1750	C
1	A	1753	C
1	A	1757	G

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Mol	Chain	Res	Type
1	A	1759	G
1	A	1775	U
1	A	1776	G
1	A	1777	G
1	A	1779	G
1	A	1782	G
1	A	1783	C
1	A	1784	G
1	A	1788	A
1	A	1800	A
1	A	1805	G
1	A	1809	A
1	A	1823	A
1	A	1824	A
1	A	1825	A
1	A	1826	G
1	A	1831	A
1	A	1836	G
1	A	1838	U
1	A	1849	G
1	A	1851	A
1	A	1861	G
1	A	1862	G
1	A	1863	A
1	A	1864	U
1	A	1865	C
1	A	1869	A
2	0	359	C
2	0	360	G
2	0	361	A
2	0	362	U
2	0	363	A
2	0	364	C
2	0	365	C
2	0	366	A
2	0	367	A
2	0	368	G
2	0	370	G
2	0	377	U
2	0	380	G
2	0	381	A
2	0	384	G

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Mol	Chain	Res	Type
2	0	385	A
2	0	386	U
2	0	387	U
2	0	388	A
2	0	391	A
2	0	392	C
2	0	393	U
2	0	395	G
2	0	396	C
2	0	397	G
2	0	400	G
2	0	403	G
2	0	404	G
2	0	406	C
2	0	407	A
2	0	408	G
2	0	409	C
2	0	410	A
2	0	411	C
2	0	412	A
2	0	417	A
2	0	418	G
2	0	419	U
2	0	420	C
2	0	422	U
2	0	423	G
2	0	425	A
2	0	426	U
2	0	427	U
2	0	428	A
2	0	429	U
2	0	430	G
2	0	431	G
2	0	433	G
2	0	434	U
2	0	435	U
2	0	436	U
2	0	443	A
2	0	446	U
2	0	451	U
2	0	452	U
2	0	453	G

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Mol	Chain	Res	Type
2	0	454	C
2	0	455	U
2	0	457	U
2	0	458	A
2	0	460	U
2	0	461	A
2	0	462	U
2	0	463	U
2	0	464	G
2	0	465	A
2	0	466	A
2	0	467	C
2	0	468	U
2	0	471	A
2	0	472	G
2	0	473	U
2	0	478	A
2	0	480	U
2	0	481	G
2	0	482	U
2	0	483	A
2	0	484	C
2	0	485	U
2	0	486	U
2	0	487	G
2	0	488	G
2	0	489	C
2	0	490	A
2	0	491	U
2	0	492	G
2	0	493	U
2	0	494	A
2	0	496	A
2	0	497	C
2	0	498	C
2	0	499	U
2	0	500	G
2	0	504	A
2	0	506	U
2	0	507	U
2	0	508	A
2	0	509	G

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Mol	Chain	Res	Type
2	0	513	U
2	0	515	G
2	0	516	U
2	0	518	G
2	0	519	A
2	0	520	U
2	0	526	A
2	0	527	C
2	0	532	G
2	0	534	U
2	0	537	G
2	0	538	G
2	0	539	U
2	0	540	A
2	0	541	C
2	0	542	A
2	0	543	G
2	0	545	A
2	0	546	G
2	0	550	A
2	0	552	A
2	0	553	C
2	0	557	A
2	0	559	A
2	0	560	U
2	0	561	A
2	0	562	U
2	0	567	U
2	0	568	U
2	0	569	U
2	0	570	U
2	0	572	U
2	0	575	U
2	0	576	U
2	0	577	A
2	0	580	G
2	0	581	A
2	0	582	A
2	0	583	G
2	0	584	A
2	0	586	A
2	0	587	A

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Mol	Chain	Res	Type
2	0	588	U
2	0	590	A
2	0	591	G
2	0	593	G
2	0	603	A
2	0	605	G
2	0	612	G
2	0	614	C
2	0	619	G
2	0	620	A
2	0	621	G
2	0	624	G
2	0	625	G
2	0	626	U
2	0	627	G
2	0	628	A
2	0	633	A
2	0	637	G
2	0	638	C
2	0	640	C
2	0	641	C
2	0	642	U
2	0	643	G
2	0	644	A
2	0	645	A
2	0	646	G
2	0	647	C
2	0	649	A
2	0	654	A
2	0	656	G
2	0	657	U
2	0	658	C
2	0	659	U
2	0	660	U
2	0	662	C
2	0	663	C
2	0	670	G
2	0	678	A
2	0	679	U
2	0	680	A
2	0	682	G
2	0	684	A

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Mol	Chain	Res	Type
2	0	685	G
2	0	686	U
2	0	692	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	110	U
1	A	166	A
1	A	205	G
1	A	304	C
1	A	407	G
1	A	463	C
1	A	465	A
1	A	500	A
1	A	532	C
1	A	553	U
1	A	555	A
1	A	561	A
1	A	606	G
1	A	627	U
1	A	688	U
1	A	752	G
1	A	753	C
1	A	870	A
1	A	887	U
1	A	912	C
1	A	1137	U
1	A	1295	A
1	A	1395	C
1	A	1664	A
1	A	1783	C
1	A	1824	A
2	0	369	A
2	0	387	U
2	0	406	C
2	0	416	U
2	0	425	A
2	0	429	U
2	0	456	C
2	0	480	U
2	0	484	C

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Mol	Chain	Res	Type
2	0	485	U
2	0	496	A
2	0	508	A
2	0	518	G
2	0	526	A
2	0	559	A
2	0	560	U
2	0	581	A
2	0	619	G
2	0	655	G
2	0	656	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	15
40	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	697:G	O3'	729:C	P	18.10
1	A	834:C	O3'	841:G	P	17.97
1	A	130:G	O3'	141:A	P	17.73
1	A	756:C	O3'	788:G	P	15.69
1	A	323:C	O3'	329:G	P	15.54
1	A	1417:C	O3'	1423:C	P	14.83
1	A	1761:U	O3'	1771:G	P	14.63
1	A	225:G	O3'	287:U	P	8.35
1	A	886:A	O3'	887:U	P	8.27
1	A	745:C	O3'	749:U	P	7.26
1	A	1432:U	O3'	1438:A	P	5.45
1	A	903:A	O3'	904:A	P	5.12
1	A	798:G	O3'	799:U	P	4.14
1	A	902:G	O3'	903:A	P	3.79
1	A	736:C	O3'	743:U	P	3.40
1	5	243:LEU	C	244:GLN	N	3.13