



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:46 AM UTC

PDB ID : 6W2T / pdb_00006w2t
EMDB ID : EMD-21530
Title : Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES)
bound to the small ribosomal subunit in the closed state (Class 2)
Authors : Neupane, R.; Pisareva, V.; Rodriguez, C.F.; Pisarev, A.; Fernandez, I.S.
Deposited on : 2020-03-08
Resolution : 3.36 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

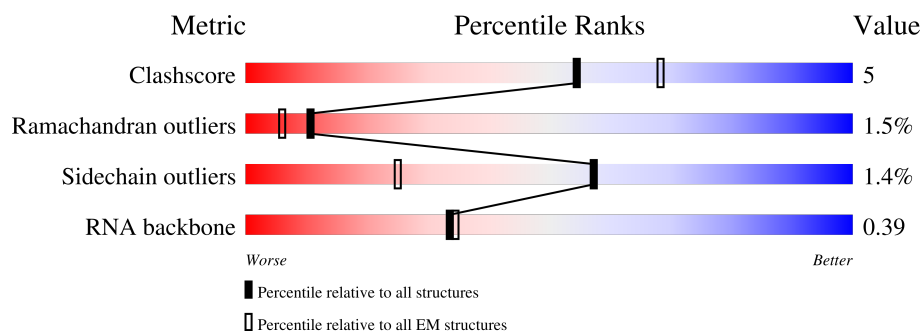
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.36 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.



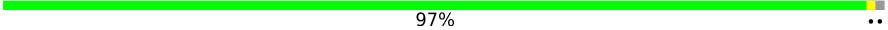
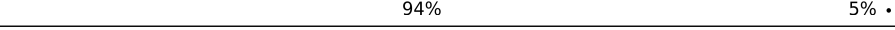
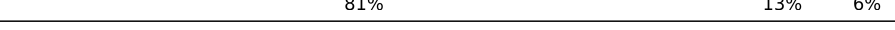
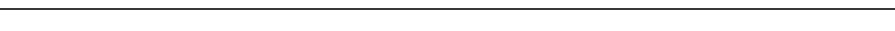
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 of 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	70% 26% .
2	B	295	63% 10% 26%
3	C	264	76% . 19%
4	D	255	78% 8% . 13%
5	F	263	95% .
6	H	249	89% 6% 5%
7	I	194	85% 10% . 5%

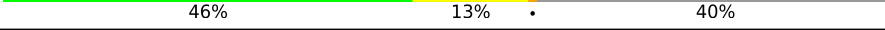
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Mol	Chain	Length	Quality of chain
8	J	208	 89% 9% .
9	K	194	 86% 9% . 5%
10	M	158	 86% . 9%
11	O	151	 97% ..
12	P	151	 83% 7% 10%
13	W	83	 90% 10%
14	X	130	 88% 9% ..
15	Y	143	 89% 9% ..
16	Z	134	 87% 5% 7%
17	b	115	 78% 9% . 12%
18	c	84	 94% 5% .
19	f	133	 39% . 57%
20	E	281	 73% 7% . 19%
21	G	204	 81% 13% 6%
22	L	149	 58% 7% 36%
23	N	132	 73% 16% 11%
24	Q	145	 58% 19% . 21%
25	R	172	 79% . 17%
26	S	135	 87% 11% .
27	T	152	 86% 9% 5%
28	U	145	 87% 10% .
29	V	119	 75% 9% 16%
30	i	125	 50% 10% 40%
31	d	69	 80% 10% 10%
32	e	56	 80% 18% .

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Mol	Chain	Length	Quality of chain
33	g	156	
34	h	317	
35	3	462	
36	4	364	
37	6	218	
38	7	607	
39	8	374	
40	1	1362	
41	2	913	
42	9	558	
43	5	363	
44	A	377	

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 109778 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 protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	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 3 is a protein called eS1.

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

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	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

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

- Molecule 5 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	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 6 is a protein called eS6.

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

- Molecule 7 is a protein called eS7.

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

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	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 9 is a protein called uS4.

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

- Molecule 10 is a protein called uS17.

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

- Molecule 11 is a protein called uS15.

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

- Molecule 12 is a protein called uS11.

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

- Molecule 13 is a protein called eS21.

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

- Molecule 14 is a protein called uS8.

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

- Molecule 15 is a protein called uS12.

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

- Molecule 16 is a protein called eS24.

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

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called eS27.

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

- Molecule 19 is a protein called eS30.

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

- Molecule 20 is a protein called uS3.

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

- Molecule 21 is a protein called uS7.

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

- Molecule 22 is a protein called eS10.

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

- Molecule 23 is a protein called eS12.

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

- Molecule 24 is a protein called uS19.

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

- Molecule 25 is a protein called uS9.

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

- Molecule 26 is a protein called eS17.

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

- Molecule 27 is a protein called uS13.

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

- Molecule 28 is a protein called eS19.

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

- Molecule 29 is a protein called uS10.

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

- Molecule 30 is a protein called eS25.

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

- Molecule 31 is a protein called eS28.

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

- Molecule 32 is a protein called eS29.

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

- Molecule 33 is a protein called eS31.

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

- Molecule 34 is a protein called RACK1.

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

- Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	3	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1	534	Total	C	N	O	S	0	0
			4377	2770	778	808	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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 42 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	356	Total	C	N	O	S	0	0
			2867	1804	500	548	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 44 is a RNA chain called CrPV 5'-UTR IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	A	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
A	569	U	C	conflict	GB 8895506
A	570	U	C	conflict	GB 8895506
A	571	U	A	conflict	GB 8895506
A	572	U	C	conflict	GB 8895506
A	574	U	C	conflict	GB 8895506
A	575	U	G	conflict	GB 8895506
A	729	G	-	expression tag	GB 8895506
A	730	G	-	expression tag	GB 8895506
A	731	A	-	expression tag	GB 8895506
A	732	U	-	expression tag	GB 8895506
A	733	C	-	expression tag	GB 8895506

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	a	1	Total	Mg	0
			1	1	

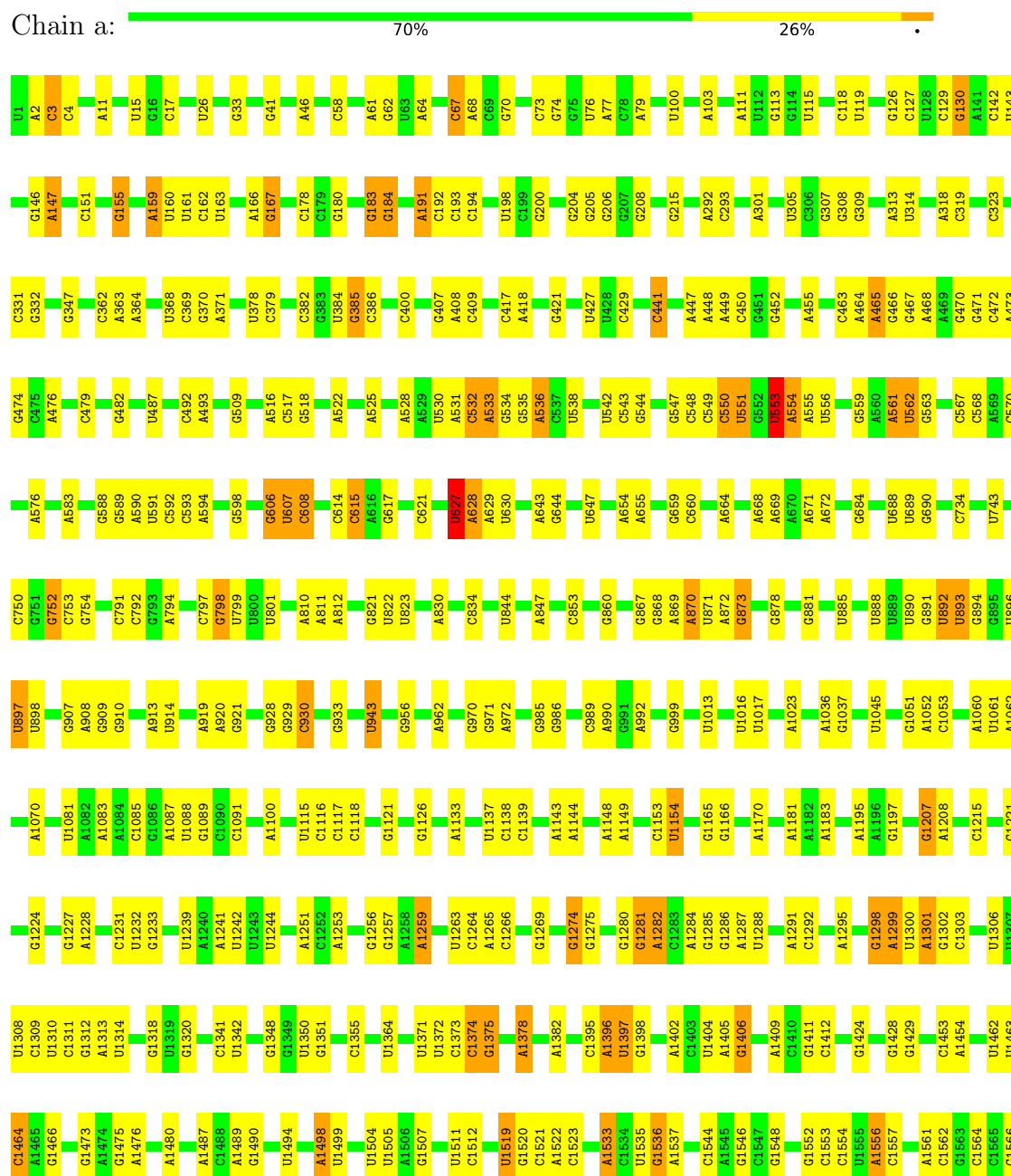
- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

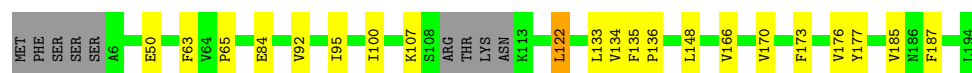


Chain H:  89% 6% 5%



• Molecule 7: eS7

Chain I:  85% 10% 5%



• Molecule 8: eS8

Chain J:  89% 9% .



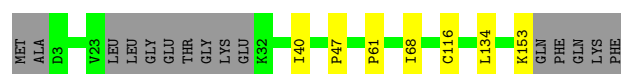
• Molecule 9: uS4

Chain K:  86% 9% . 5%

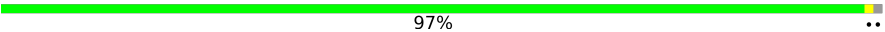


• Molecule 10: uS17

Chain M:  86% . 9%



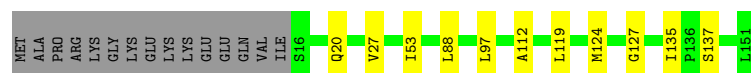
• Molecule 11: uS15

Chain O:  97% ..



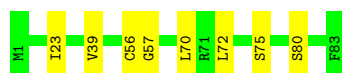
• Molecule 12: uS11

Chain P:  83% 7% 10%



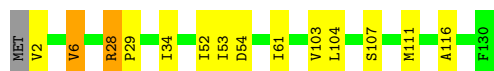
• Molecule 13: eS21

Chain W:  90% 10%



- Molecule 14: uS8

Chain X: 88% 9% ..



- Molecule 15: uS12

Chain Y: 89% 9% ..



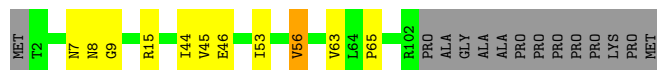
- Molecule 16: eS24

Chain Z: 87% 5% 7%



- Molecule 17: eS26

Chain b: 78% 9% 12%



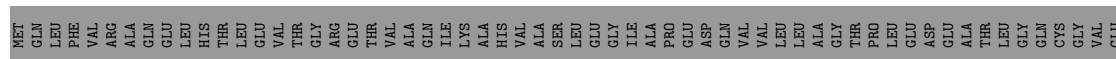
- Molecule 18: eS27

Chain c: 94% 5% .



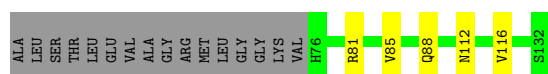
- Molecule 19: eS30

Chain f: 39% 57%



- Molecule 20: uS3

Chain E: 73% 7% 19%





- Molecule 27: uS13

Chain T: 86% 9% 5%



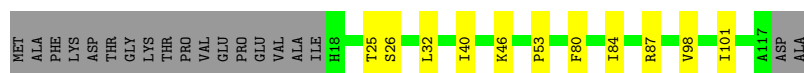
- Molecule 28: eS19

Chain U: 87% 10% 3%



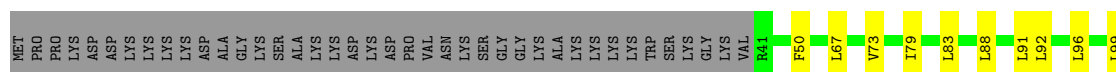
- Molecule 29: uS10

Chain V: 75% 9% 16%



- Molecule 30: eS25

Chain i: 50% 10% 40%



- Molecule 31: eS28

Chain d: 80% 10% 10%

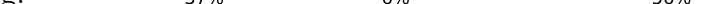


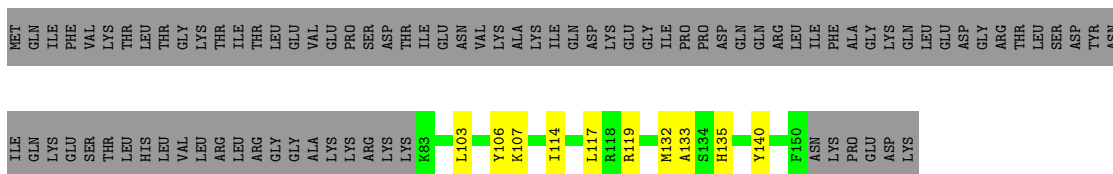
- Molecule 32: eS29

Chain e: 80% 18% 2%



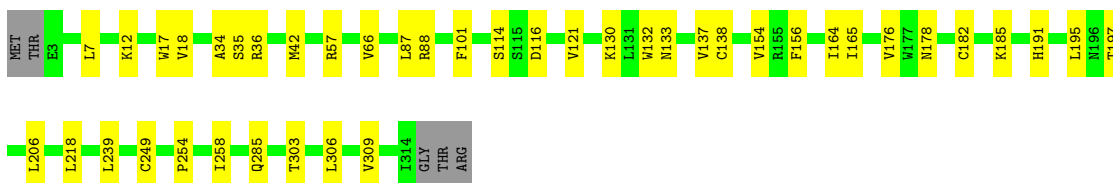
- Molecule 33: eS31

Chain g: 

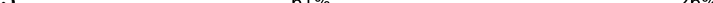


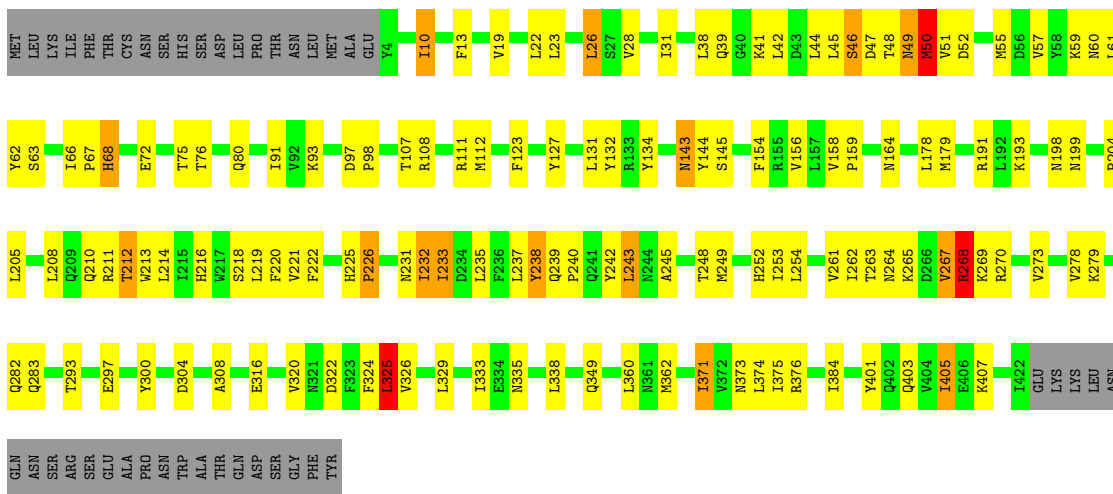
- Molecule 34: RACK1

Chain h: 85% 13%

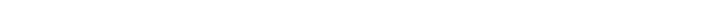


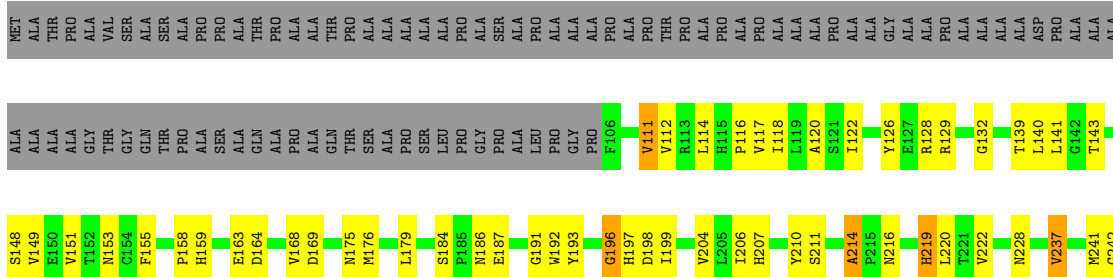
- Molecule 35: Eukaryotic translation initiation factor 3 subunit E

Chain 3:  61% 26% . . 9%



- Molecule 36: Eukaryotic translation initiation factor 3 subunit F

Chain 4:  48% 24% . 25%





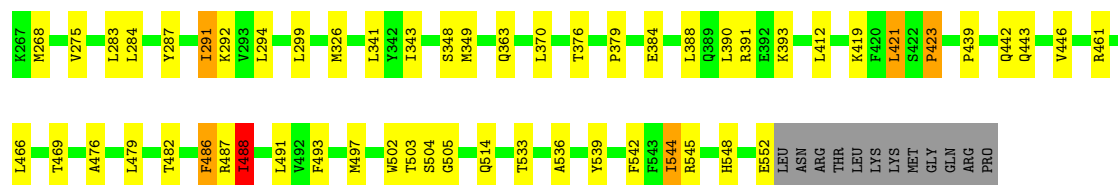
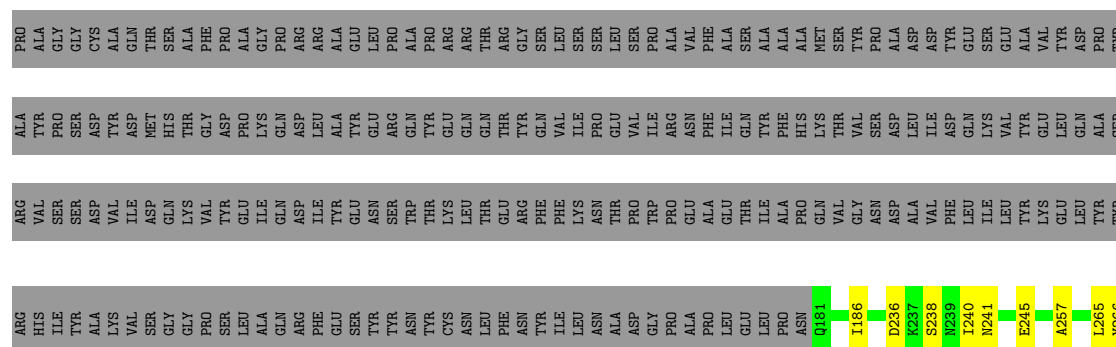
• Molecule 37: Eukaryotic translation initiation factor 3 subunit K

Chain 6: 86% 12%



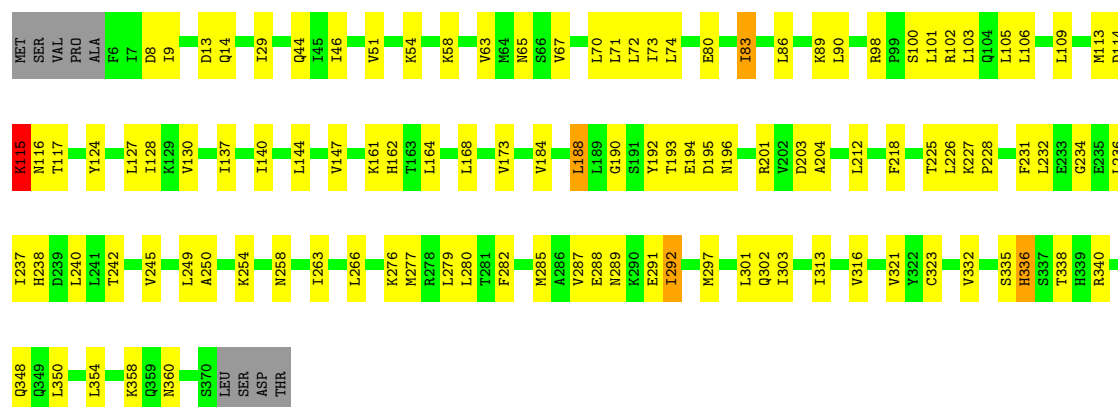
• Molecule 38: Eukaryotic translation initiation factor 3 subunit L

Chain 7: 51% 10% 39%



• Molecule 39: Eukaryotic translation initiation factor 3 subunit M

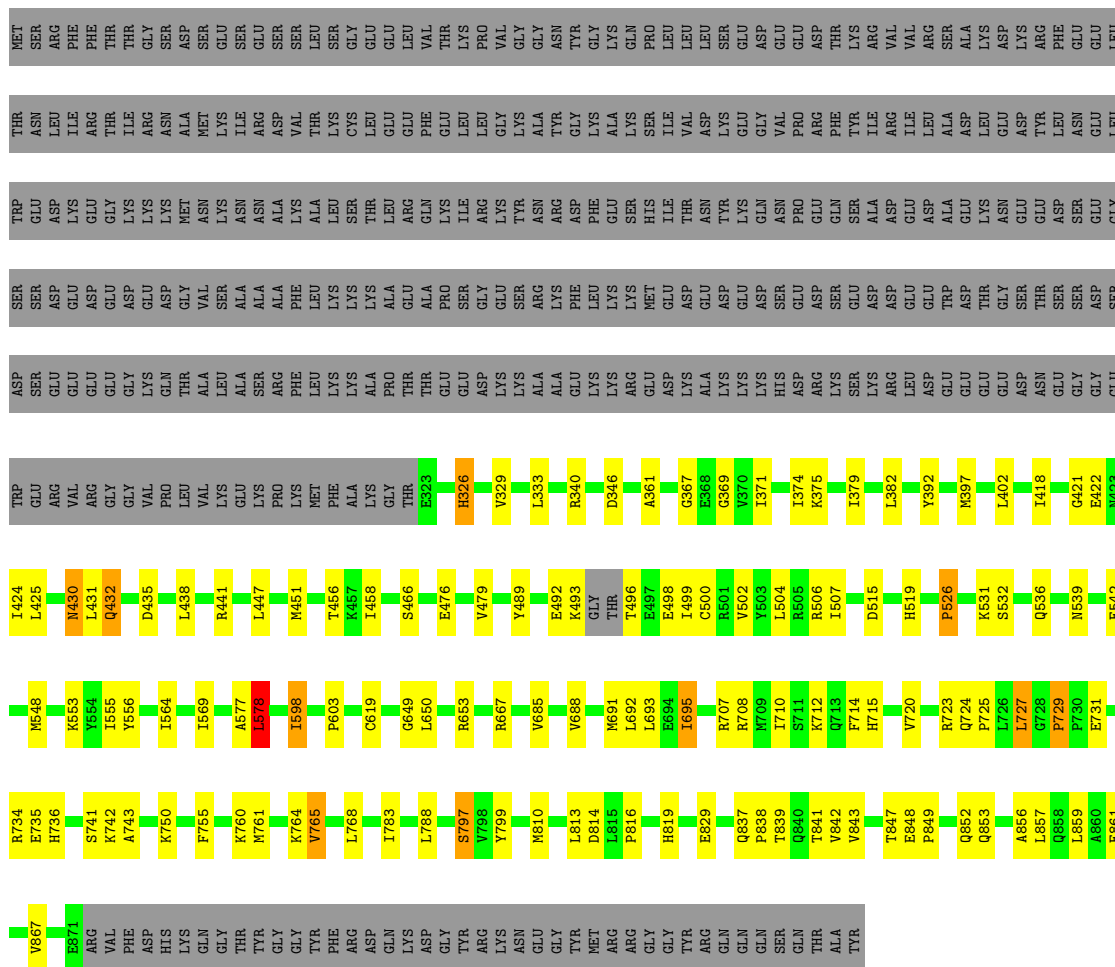
Chain 8: 68% 28%



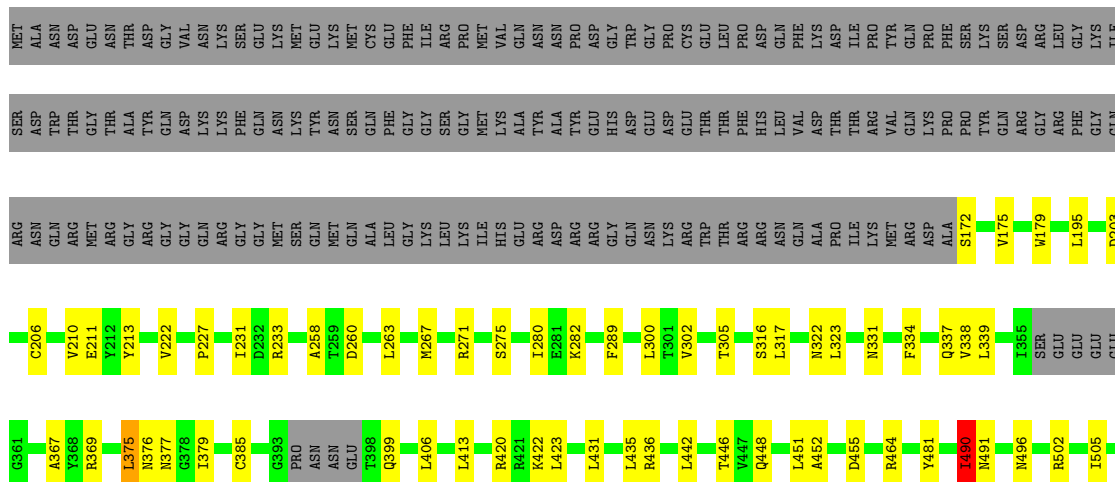
Chain 1: 29% 10% 61%

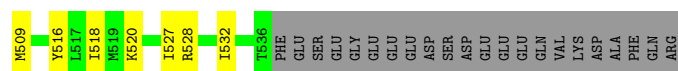


Chain 2: 46% 13% . 40%



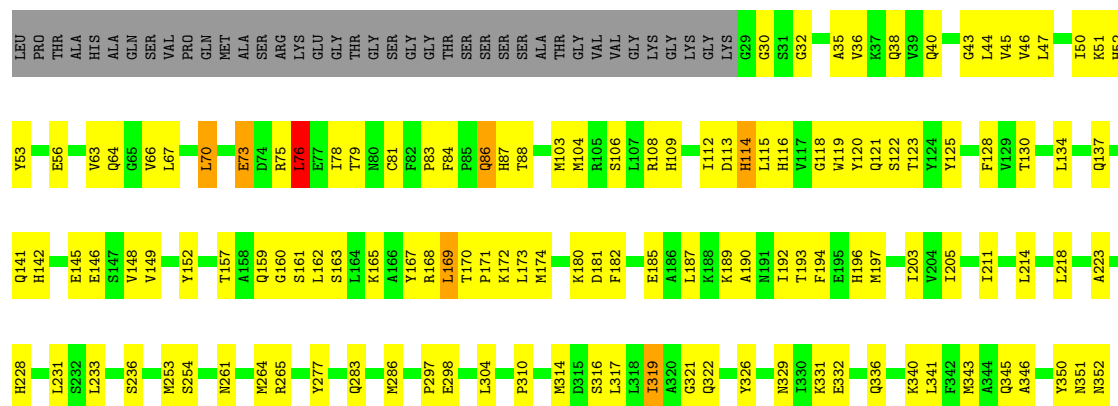
Chain 9: 51% 12% 36%





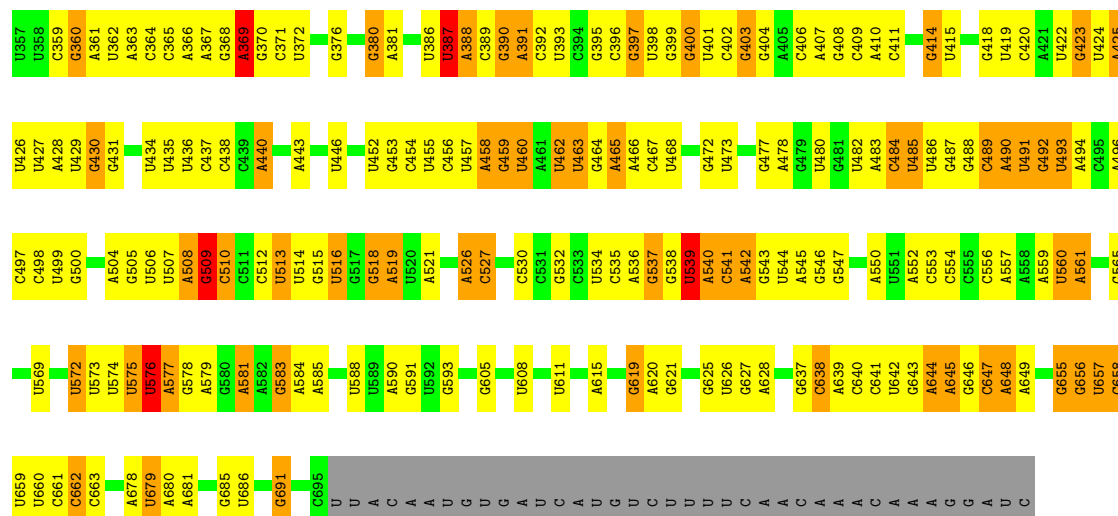
• Molecule 43: Eukaryotic translation initiation factor 3 subunit H

Chain 5: 54% 33% 11%



• Molecule 44: CrPV 5'-UTR IRES

Chain A: 36% 37% 15% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23444	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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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	0.37	0/40505	0.69	15/63112 (0.0%)
2	B	1.05	0/1743	1.51	2/2370 (0.1%)
3	C	1.05	0/1756	1.48	0/2350
4	D	1.05	0/1754	1.45	0/2370
5	F	1.04	0/2114	1.38	0/2843
6	H	1.05	0/1946	1.50	0/2590
7	I	1.06	0/1510	1.50	2/2022 (0.1%)
8	J	1.04	0/1715	1.44	0/2287
9	K	1.03	0/1550	1.57	0/2069
10	M	1.04	0/1195	1.32	0/1597
11	O	1.04	0/1226	1.62	0/1649
12	P	1.06	0/1029	1.50	0/1380
13	W	1.08	0/641	1.54	0/858
14	X	1.05	0/1051	1.51	0/1406
15	Y	1.06	0/1116	1.45	0/1490
16	Z	1.03	0/1028	1.42	0/1366
17	b	1.05	0/830	1.44	0/1112
18	c	1.05	0/665	1.38	0/891
19	f	1.04	0/462	1.56	0/607
20	E	1.07	0/1796	1.49	0/2417
21	G	1.07	0/1521	1.61	0/2046
22	L	1.02	0/834	1.48	0/1125
23	N	1.06	0/918	1.52	1/1233 (0.1%)
24	Q	1.05	0/974	1.45	2/1301 (0.2%)
25	R	1.06	0/1146	1.47	0/1534
26	S	1.06	1/1082 (0.1%)	1.52	0/1452
27	T	1.05	0/1208	1.50	0/1618
28	U	1.05	0/1115	1.61	0/1493
29	V	1.07	0/805	1.44	0/1081
30	i	1.08	0/604	1.56	0/810
31	d	1.10	0/490	1.39	0/656
32	e	1.02	0/470	1.37	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	1.04	0/567	1.36	0/753
34	h	1.09	0/2486	1.38	0/3384
35	3	1.07	2/3538 (0.1%)	1.55	7/4786 (0.1%)
36	4	1.10	1/2149 (0.0%)	1.56	5/2920 (0.2%)
37	6	1.09	1/1772 (0.1%)	1.57	1/2396 (0.0%)
38	7	1.05	0/3185	1.57	7/4296 (0.2%)
39	8	1.10	3/2963 (0.1%)	1.59	6/3998 (0.2%)
40	1	1.05	0/4460	1.54	0/6034
41	2	1.07	0/4522	1.48	6/6102 (0.1%)
42	9	1.05	0/2921	1.43	0/3957
43	5	1.03	0/2675	1.51	1/3609 (0.0%)
44	A	0.41	2/8053 (0.0%)	0.78	12/12543 (0.1%)
All	All	0.84	10/116090 (0.0%)	1.20	67/166536 (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
5	F	0	1
14	X	0	1
15	Y	0	1
21	G	0	2
34	h	0	1
35	3	0	12
36	4	0	7
37	6	0	1
39	8	0	3
40	1	0	4
41	2	0	5
42	9	0	2
43	5	0	2
All	All	0	42

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	368	ILE	CG1-CD1	-8.59	1.18	1.51
39	8	9	ILE	CG1-CD1	-7.31	1.23	1.51
37	6	131	ILE	CG1-CD1	-7.22	1.23	1.51
44	A	509	G	C1'-N9	-6.52	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	3	371	ILE	CG1-CD1	-5.85	1.28	1.51
44	A	576	U	C1'-N1	5.65	1.56	1.48
35	3	384	ILE	CG1-CD1	-5.40	1.30	1.51
39	8	46	ILE	CG1-CD1	-5.05	1.32	1.51
26	S	94	GLU	N-CA	5.03	1.49	1.46
39	8	73	ILE	CG1-CD1	-5.03	1.32	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	688	U	C2'-C3'-O3'	10.10	124.65	109.50
37	6	131	ILE	CB-CG1-CD1	9.77	134.31	113.80
44	A	679	U	C2'-C3'-O3'	9.62	123.92	109.50
44	A	655	G	C4'-C3'-O3'	8.79	122.58	109.40
35	3	384	ILE	CB-CG1-CD1	8.57	131.80	113.80
35	3	371	ILE	CB-CG1-CD1	8.10	130.80	113.80
7	I	65	PRO	CA-C-N	8.05	125.31	120.24
7	I	65	PRO	C-N-CA	8.05	125.31	120.24
39	8	9	ILE	CB-CG1-CD1	7.88	130.35	113.80
1	a	1664	A	C4'-C3'-O3'	7.61	120.81	109.40
1	a	553	U	C2'-C3'-O3'	7.58	120.87	109.50
39	8	140	ILE	CB-CG1-CD1	-7.19	98.70	113.80
1	a	870	A	C4'-C3'-O3'	7.15	120.12	109.40
44	A	425	A	C2'-C3'-O3'	7.01	120.02	109.50
1	a	465	A	C2'-C3'-O3'	6.61	119.41	109.50
1	a	627	U	C2'-C3'-O3'	6.60	119.40	109.50
38	7	488	ILE	CB-CG1-CD1	6.43	127.30	113.80
44	A	387	U	C2'-C3'-O3'	6.42	119.12	109.50
1	a	752	G	C2'-C3'-O3'	6.38	119.07	109.50
41	2	603	PRO	N-CA-C	6.34	118.44	110.70
39	8	46	ILE	CB-CG1-CD1	6.29	127.01	113.80
44	A	657	U	C4'-C3'-O3'	6.10	118.55	109.40
38	7	486	PHE	CA-C-N	6.03	132.56	121.70
38	7	486	PHE	C-N-CA	6.03	132.56	121.70
1	a	166	A	C2'-C3'-O3'	6.01	122.72	113.70
38	7	186	ILE	CB-CG1-CD1	5.96	126.31	113.80
38	7	544	ILE	CB-CG1-CD1	5.85	126.09	113.80
35	3	268	ARG	CA-C-N	5.84	132.21	121.70
35	3	268	ARG	C-N-CA	5.84	132.21	121.70
41	2	765	VAL	CA-C-N	5.81	130.24	121.40
41	2	765	VAL	C-N-CA	5.81	130.24	121.40
39	8	237	ILE	CB-CG1-CD1	5.77	125.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	244	PRO	N-CA-CB	-5.70	97.26	103.25
1	a	1137	U	C2'-C3'-O3'	5.58	122.06	113.70
1	a	1637	A	C4'-C3'-O3'	5.58	117.76	109.40
35	3	405	ILE	CB-CG1-CD1	5.56	125.47	113.80
44	A	485	U	C2'-C3'-O3'	5.56	122.04	113.70
24	Q	38	SER	CA-C-N	5.55	127.98	120.65
24	Q	38	SER	C-N-CA	5.55	127.98	120.65
1	a	532	C	C2'-C3'-O3'	5.52	121.98	113.70
44	A	518	G	C4'-C3'-O3'	5.51	117.67	109.40
35	3	50	MET	CA-C-N	5.44	131.77	121.97
35	3	50	MET	C-N-CA	5.44	131.77	121.97
36	4	228	ASN	CA-C-N	5.42	126.10	120.03
36	4	228	ASN	C-N-CA	5.42	126.10	120.03
38	7	275	VAL	CA-C-N	5.42	126.11	119.99
38	7	275	VAL	C-N-CA	5.42	126.11	119.99
39	8	137	ILE	CB-CG1-CD1	-5.37	102.51	113.80
1	a	1395	C	C3'-C2'-O2'	5.22	118.53	110.70
44	A	539	U	N1-C1'-C2'	5.19	119.78	112.00
41	2	729	PRO	N-CA-C	5.18	117.02	110.70
1	a	1824	A	C2'-C3'-O3'	5.18	121.47	113.70
23	N	34	GLY	CA-C-O	-5.16	117.85	121.88
2	B	166	LYS	CA-C-N	5.15	124.86	119.92
2	B	166	LYS	C-N-CA	5.15	124.86	119.92
44	A	508	A	C2'-C3'-O3'	5.15	117.22	109.50
43	5	203	ILE	CA-C-O	-5.12	116.25	120.80
36	4	199	ILE	CB-CG1-CD1	5.10	124.51	113.80
44	A	369	A	C2'-C3'-O3'	5.10	121.35	113.70
44	A	619	G	C2'-C3'-O3'	5.09	117.13	109.50
36	4	368	ILE	CB-CG1-CD1	5.07	124.45	113.80
44	A	485	U	C3'-C2'-O2'	5.05	118.27	110.70
1	a	1264	C	C4'-C3'-O3'	5.04	116.96	109.40
39	8	115	LYS	CB-CA-C	5.02	120.42	110.42
1	a	1824	A	C3'-C2'-O2'	5.01	118.21	110.70
41	2	422	GLU	CA-C-N	5.00	128.76	121.31
41	2	422	GLU	C-N-CA	5.00	128.76	121.31

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	1	165	ARG	Peptide
40	1	416	GLU	Peptide

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Mol	Chain	Res	Type	Group
40	1	477	HIS	Peptide
40	1	514	MET	Peptide
41	2	496	THR	Peptide
41	2	649	GLY	Peptide
41	2	650	LEU	Peptide
41	2	693	LEU	Peptide
41	2	741	SER	Peptide
35	3	143	ASN	Peptide
35	3	22	LEU	Peptide
35	3	23	LEU	Peptide
35	3	237	LEU	Peptide
35	3	249	MET	Peptide
35	3	268	ARG	Peptide
35	3	279	LYS	Peptide
35	3	325	LEU	Peptide
35	3	49	ASN	Peptide
35	3	50	MET	Peptide
35	3	60	ASN	Peptide
35	3	61	LEU	Peptide
36	4	132	GLY	Peptide
36	4	186	ASN	Peptide
36	4	214	ALA	Peptide
36	4	241	MET	Peptide
36	4	242	GLY	Peptide
36	4	243	VAL	Peptide
36	4	279	PRO	Peptide
43	5	169	LEU	Peptide
43	5	304	LEU	Peptide
37	6	204	LYS	Peptide
39	8	115	LYS	Peptide
39	8	117	THR	Peptide
39	8	218	PHE	Peptide
42	9	375	LEU	Peptide
42	9	490	ILE	Peptide
5	F	155	LYS	Peptide
21	G	129	GLY	Peptide
21	G	130	ARG	Peptide
14	X	54	ASP	Peptide
15	Y	61	GLN	Peptide
34	h	36	ARG	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	131	0
2	B	1706	0	1698	21	0
3	C	1729	0	1803	7	0
4	D	1717	0	1812	22	0
5	F	2072	0	2175	6	0
6	H	1923	0	2089	10	0
7	I	1488	0	1582	11	0
8	J	1686	0	1772	12	0
9	K	1525	0	1640	12	0
10	M	1175	0	1249	4	0
11	O	1202	0	1289	2	0
12	P	1016	0	1039	9	0
13	W	634	0	629	6	0
14	X	1034	0	1080	8	0
15	Y	1098	0	1167	5	0
16	Z	1011	0	1083	3	0
17	b	816	0	867	9	0
18	c	651	0	672	4	0
19	f	457	0	502	3	0
20	E	1768	0	1866	12	0
21	G	1499	0	1540	12	0
22	L	810	0	836	5	0
23	N	908	0	939	13	0
24	Q	956	0	1002	17	0
25	R	1128	0	1195	3	0
26	S	1068	0	1121	9	0
27	T	1190	0	1249	5	0
28	U	1097	0	1130	8	0
29	V	795	0	862	7	0
30	i	598	0	656	9	0
31	d	488	0	514	4	0
32	e	459	0	452	7	0
33	g	555	0	567	6	0
34	h	2429	0	2386	21	0
35	3	3465	0	3446	84	0
36	4	2111	0	2105	75	0
37	6	1737	0	1706	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	7	3109	0	3084	47	0
39	8	2918	0	2950	65	0
40	1	4377	0	4433	97	0
41	2	4446	0	4446	102	0
42	9	2867	0	2838	44	0
43	5	2624	0	2592	109	0
44	A	7205	0	3626	58	0
45	a	1	0	0	0	0
46	b	1	0	0	0	0
All	All	109778	0	89993	996	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (996) 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)
40:1:42:THR:CG2	40:1:81:VAL:HG21	1.44	1.45
41:2:710:ILE:HB	41:2:714:PHE:CE2	1.61	1.35
41:2:438:LEU:CD2	41:2:493:LYS:HD3	1.56	1.35
41:2:438:LEU:HD21	41:2:493:LYS:CD	1.71	1.19
4:D:141:LEU:HD11	4:D:238:LYS:NZ	1.55	1.19
40:1:42:THR:HG21	40:1:81:VAL:HG21	1.18	1.17
41:2:438:LEU:HD21	41:2:493:LYS:HD3	1.10	1.07
40:1:42:THR:HG22	40:1:81:VAL:HG21	1.18	1.06
4:D:141:LEU:CD1	4:D:238:LYS:HZ1	1.70	1.04
40:1:42:THR:HG21	40:1:81:VAL:CG2	1.87	1.04
4:D:141:LEU:CD1	4:D:238:LYS:NZ	2.21	1.03
40:1:42:THR:CG2	40:1:81:VAL:CG2	2.37	1.02
40:1:42:THR:O	42:9:528:ARG:NH2	1.93	1.01
41:2:438:LEU:CG	41:2:493:LYS:HD3	1.90	1.00
41:2:710:ILE:HB	41:2:714:PHE:HE2	1.00	0.98
4:D:141:LEU:HD11	4:D:238:LYS:HZ2	1.26	0.96
41:2:712:LYS:HA	41:2:715:HIS:HD2	1.29	0.95
41:2:438:LEU:CD2	41:2:493:LYS:CD	2.36	0.93
41:2:710:ILE:O	41:2:714:PHE:HD2	1.54	0.90
17:b:56:VAL:HG12	17:b:56:VAL:O	1.72	0.88
44:A:365:C:H42	44:A:458:A:H2	1.21	0.85
42:9:435:LEU:HD11	42:9:490:ILE:HG22	1.59	0.85
41:2:492:GLU:O	41:2:493:LYS:HG3	1.82	0.80
41:2:710:ILE:CB	41:2:714:PHE:HE2	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:322:VAL:HG21	40:1:383:VAL:HA	1.65	0.78
36:4:279:PRO:HA	36:4:280:ASN:HB2	1.66	0.77
12:P:124:MET:O	17:b:56:VAL:CG1	2.32	0.77
40:1:278:LYS:O	40:1:282:VAL:HG23	1.85	0.76
43:5:130:THR:O	43:5:134:LEU:HB2	1.86	0.76
1:a:1753:C:O2	1:a:1780:G:N2	2.19	0.75
41:2:432:GLN:O	41:2:432:GLN:NE2	2.18	0.75
1:a:1396:A:O2'	1:a:1398:G:N7	2.19	0.75
35:3:268:ARG:N	35:3:269:LYS:HB3	2.03	0.74
40:1:42:THR:HG22	40:1:81:VAL:CG2	2.10	0.73
41:2:438:LEU:HG	41:2:493:LYS:HD3	1.70	0.73
44:A:509:G:C6	44:A:510:C:C5	2.77	0.73
35:3:349:GLN:HB2	41:2:829:GLU:HB3	1.71	0.72
4:D:141:LEU:HD13	4:D:238:LYS:HZ1	1.55	0.71
40:1:277:ASN:O	40:1:281:THR:HG23	1.90	0.71
44:A:365:C:N4	44:A:458:A:H2	1.86	0.71
1:a:1533:A:H2	1:a:1536:G:N3	1.89	0.71
39:8:292:ILE:HG12	39:8:332:VAL:HG22	1.73	0.71
39:8:358:LYS:HG3	43:5:352:ASN:HD21	1.57	0.70
41:2:438:LEU:HD23	41:2:493:LYS:HZ3	1.57	0.69
44:A:576:U:C5	44:A:577:A:H2'	2.27	0.69
1:a:1091:C:HO2'	14:X:2:VAL:N	1.91	0.69
35:3:158:VAL:HG22	35:3:159:PRO:HD2	1.73	0.69
41:2:710:ILE:O	41:2:714:PHE:CD2	2.42	0.68
44:A:397:G:H2'	44:A:398:U:O4'	1.93	0.68
43:5:66:VAL:HA	43:5:119:TRP:HA	1.76	0.68
40:1:343:ASP:CB	41:2:714:PHE:HE1	2.06	0.68
35:3:335:ASN:HA	35:3:338:LEU:HB3	1.75	0.67
41:2:438:LEU:CD2	41:2:493:LYS:CE	2.72	0.67
24:Q:37:TYR:OH	24:Q:45:LEU:HD12	1.94	0.67
35:3:375:ILE:HG21	38:7:466:LEU:HD21	1.76	0.67
41:2:867:VAL:HG12	41:2:867:VAL:O	1.94	0.67
1:a:627:U:H4'	1:a:628:A:O5'	1.94	0.67
41:2:432:GLN:HE21	41:2:432:GLN:C	2.01	0.67
41:2:438:LEU:CD2	41:2:493:LYS:NZ	2.58	0.67
41:2:710:ILE:CB	41:2:714:PHE:CE2	2.58	0.67
35:3:55:MET:SD	35:3:59:LYS:NZ	2.67	0.67
44:A:360:G:H1	44:A:463:U:H3	1.44	0.66
43:5:142:HIS:HA	43:5:174:MET:HE1	1.78	0.66
36:4:168:VAL:HG21	36:4:206:ILE:HG23	1.78	0.66
44:A:509:G:N1	44:A:510:C:C5	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:553:U:O2'	1:a:554:A:O5'	2.13	0.65
12:P:124:MET:O	17:b:56:VAL:HG13	1.96	0.65
40:1:343:ASP:OD2	41:2:714:PHE:CZ	2.49	0.65
8:J:101:ILE:HD12	8:J:190:LEU:HD11	1.78	0.65
36:4:373:LYS:HB3	38:7:544:ILE:HG21	1.79	0.65
39:8:212:LEU:HD21	39:8:263:ILE:HG21	1.79	0.65
40:1:3:ALA:N	44:A:583:G:HO2'	1.95	0.64
42:9:267:MET:HE1	42:9:451:LEU:HD21	1.79	0.64
43:5:44:LEU:HD21	43:5:214:LEU:HD21	1.80	0.64
40:1:237:LEU:HD11	40:1:253:VAL:HG12	1.79	0.64
39:8:13:ASP:HA	39:8:14:GLN:C	2.23	0.64
41:2:685:VAL:HA	41:2:688:VAL:HG12	1.80	0.63
1:a:534:G:O6	1:a:550:C:N4	2.31	0.63
44:A:493:U:OP1	44:A:516:U:N3	2.31	0.63
35:3:50:MET:O	35:3:52:ASP:N	2.30	0.63
44:A:402:C:H3'	44:A:403:G:H5'	1.80	0.63
43:5:297:PRO:HA	43:5:298:GLU:HB2	1.81	0.63
2:B:65:ILE:HD12	2:B:178:LEU:HD21	1.81	0.62
35:3:268:ARG:H	35:3:269:LYS:HB3	1.63	0.62
38:7:348:SER:HA	38:7:349:MET:CB	2.29	0.62
40:1:42:THR:O	42:9:528:ARG:CZ	2.47	0.62
1:a:1599:U:O2	1:a:1600:G:N1	2.32	0.62
40:1:11:ALA:HB2	40:1:34:VAL:HG21	1.80	0.62
40:1:341:LEU:HA	40:1:345:ASP:HB2	1.79	0.62
35:3:218:SER:CB	35:3:232:ILE:HG12	2.29	0.62
35:3:108:ARG:NH2	35:3:134:TYR:OH	2.32	0.62
40:1:19:LEU:HD21	40:1:57:LEU:HD21	1.81	0.62
29:V:46:LYS:HG3	29:V:101:ILE:HD11	1.82	0.62
44:A:492:G:H3'	44:A:516:U:H3	1.64	0.62
1:a:1397:U:H2'	1:a:1397:U:O2	2.00	0.61
17:b:56:VAL:O	17:b:56:VAL:CG1	2.46	0.61
35:3:243:LEU:HB2	35:3:248:THR:HG22	1.82	0.61
1:a:3:C:O2	9:K:18:ARG:NH2	2.33	0.61
42:9:271:ARG:NH2	42:9:491:ASN:O	2.34	0.61
43:5:76:LEU:O	43:5:76:LEU:HD12	2.01	0.61
39:8:124:TYR:CD2	39:8:164:LEU:HD13	2.35	0.61
41:2:438:LEU:HD23	41:2:493:LYS:NZ	2.16	0.61
4:D:211:LYS:O	4:D:215:LEU:HG	2.00	0.61
34:h:133:ASN:HD22	34:h:137:VAL:HB	1.66	0.61
35:3:39:GLN:HE22	35:3:55:MET:HE1	1.65	0.61
38:7:240:ILE:HG13	38:7:257:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:9:172:SER:N	42:9:275:SER:HG	1.98	0.61
1:a:1259:A:N6	1:a:1519:U:OP1	2.33	0.61
40:1:403:LEU:HD22	40:1:439:LEU:HD21	1.83	0.61
40:1:529:VAL:HG12	43:5:233:LEU:HD21	1.82	0.61
44:A:365:C:N4	44:A:458:A:C2	2.66	0.61
36:4:159:HIS:CE1	36:4:168:VAL:HG22	2.36	0.60
41:2:712:LYS:HA	41:2:715:HIS:CD2	2.21	0.60
41:2:438:LEU:CD2	41:2:493:LYS:HZ3	2.14	0.60
40:1:348:ILE:HA	40:1:351:LYS:HB2	1.84	0.60
41:2:438:LEU:HD23	41:2:493:LYS:CE	2.31	0.60
36:4:336:PRO:HB3	43:5:350:TYR:O	2.02	0.60
41:2:735:GLU:HB3	41:2:750:LYS:HB3	1.84	0.60
21:G:201:LYS:HA	21:G:204:ARG:HD3	1.84	0.60
35:3:220:PHE:HB2	35:3:325:LEU:HB2	1.84	0.59
35:3:233:ILE:O	35:3:238:TYR:HB2	2.03	0.59
36:4:112:VAL:HG23	36:4:255:LEU:HD13	1.84	0.59
41:2:783:ILE:HD13	41:2:813:LEU:HD22	1.83	0.59
43:5:187:LEU:HA	43:5:190:ALA:HB3	1.84	0.59
21:G:154:LEU:HD13	21:G:177:LEU:HD21	1.84	0.59
1:a:191:A:N6	1:a:208:G:O2'	2.35	0.59
41:2:515:ASP:O	41:2:519:HIS:N	2.33	0.59
36:4:126:TYR:O	36:4:129:ARG:NE	2.30	0.59
42:9:406:LEU:HD21	42:9:442:LEU:HD11	1.85	0.59
42:9:435:LEU:HD11	42:9:490:ILE:CG2	2.32	0.59
1:a:860:G:N3	14:X:107:SER:OG	2.33	0.59
40:1:479:ASP:HA	40:1:505:ALA:HB2	1.85	0.59
36:4:141:LEU:HB3	36:4:187:GLU:HB3	1.85	0.59
40:1:383:VAL:HG13	40:1:388:LYS:HG2	1.85	0.59
22:L:11:ILE:HD11	22:L:40:VAL:HG11	1.83	0.58
35:3:158:VAL:HG21	35:3:164:ASN:HB3	1.86	0.58
42:9:258:ALA:HB1	42:9:263:LEU:HD13	1.84	0.58
24:Q:81:ARG:NH2	24:Q:117:GLY:O	2.36	0.58
41:2:367:GLY:HA2	41:2:371:ILE:HD11	1.83	0.58
27:T:33:ILE:HD12	27:T:71:MET:HE1	1.85	0.58
36:4:116:PRO:HG2	36:4:269:VAL:HG21	1.86	0.58
43:5:125:TYR:CD2	43:5:128:PHE:HB2	2.38	0.58
36:4:304:SER:O	39:8:348:GLN:NE2	2.35	0.58
40:1:343:ASP:HB2	41:2:714:PHE:HE1	1.68	0.58
1:a:1298:G:N3	1:a:1298:G:H2'	2.18	0.58
36:4:283:ILE:O	43:5:161:SER:OG	2.22	0.58
44:A:402:C:H3'	44:A:403:G:C5'	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1016:U:H2'	1:a:1016:U:O2	2.02	0.58
1:a:1473:G:O2'	1:a:1475:G:N2	2.36	0.58
17:b:7:ASN:O	17:b:9:GLY:N	2.37	0.58
38:7:348:SER:HA	38:7:349:MET:HB3	1.86	0.58
33:g:107:LYS:HB2	33:g:117:LEU:HD21	1.86	0.57
35:3:131:LEU:HG	35:3:159:PRO:HD3	1.85	0.57
40:1:512:GLN:O	40:1:514:MET:N	2.35	0.57
43:5:108:ARG:HD3	43:5:113:ASP:HA	1.86	0.57
7:I:100:ILE:HD11	7:I:122:LEU:HA	1.86	0.57
36:4:369:ALA:HA	36:4:373:LYS:HE2	1.84	0.57
43:5:180:LYS:HD3	43:5:319:ILE:HD13	1.85	0.57
15:Y:61:GLN:O	15:Y:63:ASN:N	2.37	0.57
39:8:195:ASP:HA	39:8:196:ASN:C	2.29	0.57
41:2:438:LEU:HD21	41:2:493:LYS:CE	2.32	0.57
12:P:124:MET:O	17:b:56:VAL:HG11	2.04	0.57
1:a:1464:C:OP2	26:S:63:ARG:NH2	2.37	0.57
35:3:49:ASN:HA	35:3:50:MET:HB2	1.87	0.57
41:2:761:MET:HE2	41:2:768:LEU:HG	1.86	0.57
43:5:350:TYR:O	43:5:352:ASN:N	2.38	0.57
39:8:242:THR:HG23	39:8:258:ASN:HB3	1.87	0.56
41:2:379:ILE:HD11	41:2:447:LEU:HD13	1.88	0.56
43:5:170:THR:O	43:5:173:LEU:HB2	2.04	0.56
43:5:261:ASN:O	43:5:265:ARG:HG2	2.05	0.56
29:V:32:LEU:HD21	29:V:87:ARG:HG2	1.87	0.56
36:4:269:VAL:HG22	43:5:47:LEU:HD21	1.88	0.56
4:D:141:LEU:CD2	4:D:238:LYS:HZ1	2.17	0.56
41:2:476:GLU:HA	41:2:479:VAL:HG12	1.86	0.56
35:3:263:THR:HG22	35:3:335:ASN:HB2	1.87	0.56
21:G:20:PHE:CZ	21:G:69:VAL:HG11	2.40	0.56
35:3:221:VAL:HG13	35:3:225:HIS:HB2	1.87	0.56
40:1:273:ALA:HB2	40:1:306:MET:HE1	1.88	0.56
36:4:122:ILE:HG12	36:4:193:TYR:CE1	2.41	0.55
39:8:192:TYR:O	39:8:193:THR:OG1	2.21	0.55
40:1:469:ARG:HA	40:1:472:VAL:HG12	1.88	0.55
42:9:379:ILE:HG21	42:9:505:ILE:HD12	1.87	0.55
36:4:140:LEU:HD22	36:4:220:LEU:CD1	2.36	0.55
40:1:216:THR:HG23	40:1:224:GLU:HB2	1.87	0.55
20:E:16:ILE:HD11	32:e:36:LEU:HD23	1.88	0.55
21:G:102:LEU:HD22	30:i:110:THR:HG21	1.89	0.55
35:3:55:MET:HE2	35:3:324:PHE:HA	1.89	0.55
36:4:365:GLN:HA	43:5:329:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:7:539:TYR:HA	38:7:542:PHE:CD2	2.41	0.55
40:1:270:GLN:HE22	40:1:309:ASN:HD22	1.54	0.55
1:a:534:G:C2	1:a:551:U:O2	2.59	0.55
35:3:240:PRO:O	35:3:253:ILE:HG12	2.06	0.55
38:7:245:GLU:HA	38:7:439:PRO:HG2	1.88	0.55
2:B:70:ASN:HB2	4:D:274:MET:HE2	1.87	0.55
16:Z:110:ARG:NH2	16:Z:114:MET:SD	2.79	0.55
36:4:364:THR:O	36:4:368:ILE:HG12	2.06	0.55
43:5:173:LEU:HD21	43:5:180:LYS:NZ	2.22	0.55
38:7:488:ILE:HG22	38:7:491:LEU:HB2	1.87	0.55
1:a:1397:U:O2	1:a:1397:U:C2'	2.55	0.55
4:D:233:LEU:HD12	4:D:233:LEU:O	2.07	0.55
38:7:545:ARG:NH2	43:5:322:GLN:HE22	2.04	0.55
41:2:816:PRO:HA	41:2:819:HIS:HB2	1.88	0.55
42:9:222:VAL:HG21	42:9:422:LYS:O	2.07	0.55
42:9:280:ILE:HB	42:9:516:TYR:HB2	1.87	0.55
42:9:316:SER:O	42:9:322:ASN:ND2	2.39	0.55
38:7:421:LEU:HB3	38:7:443:GLN:HG2	1.89	0.55
42:9:305:THR:OG1	42:9:436:ARG:O	2.23	0.55
43:5:86:GLN:O	43:5:88:THR:OG1	2.23	0.55
42:9:420:ARG:NH2	42:9:464:ARG:O	2.40	0.54
40:1:44:GLN:H	40:1:47:HIS:HD2	1.54	0.54
40:1:229:HIS:HB3	40:1:259:LEU:HD11	1.89	0.54
43:5:141:GLN:HE22	43:5:168:ARG:HA	1.72	0.54
43:5:173:LEU:HD21	43:5:180:LYS:HZ1	1.72	0.54
38:7:370:LEU:HA	38:7:412:LEU:HD21	1.90	0.54
40:1:55:LEU:HD13	40:1:93:TYR:HB2	1.89	0.54
41:2:493:LYS:HG3	41:2:498:GLU:OE2	2.06	0.54
36:4:360:LEU:HA	36:4:363:LEU:HB2	1.89	0.54
39:8:80:GLU:HA	39:8:83:ILE:HG22	1.88	0.54
40:1:343:ASP:OD2	41:2:714:PHE:HZ	1.89	0.54
1:a:301:A:N3	8:J:73:THR:HG21	2.22	0.54
16:Z:35:VAL:HG23	16:Z:40:ILE:HD11	1.89	0.54
1:a:1698:C:H2'	1:a:1698:C:O2	2.06	0.54
2:B:19:LEU:HD11	26:S:106:LEU:HD21	1.89	0.54
37:6:15:LEU:HD13	37:6:45:GLU:HB3	1.89	0.54
43:5:340:LYS:HA	43:5:343:MET:HE2	1.90	0.54
35:3:262:ILE:HG12	35:3:267:VAL:HG11	1.90	0.54
37:6:48:LEU:HD13	37:6:84:LEU:HB3	1.89	0.54
10:M:47:PRO:HG2	10:M:116:CYS:SG	2.48	0.53
34:h:178:ASN:O	34:h:182:CYS:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:210:ARG:HG2	40:1:212:HIS:CD2	2.43	0.53
39:8:44:GLN:HG2	39:8:72:LEU:HD21	1.90	0.53
39:8:201:ARG:NH1	39:8:236:LEU:HD21	2.23	0.53
40:1:42:THR:HB	42:9:528:ARG:HH12	1.74	0.53
43:5:137:GLN:HG3	43:5:169:LEU:HD23	1.90	0.53
3:C:86:LEU:HB3	3:C:98:THR:HB	1.91	0.53
14:X:53:ILE:HD13	18:c:24:LEU:HD11	1.90	0.53
42:9:260:ASP:HB3	42:9:448:GLN:HG2	1.89	0.53
43:5:119:TRP:HE1	43:5:137:GLN:HB3	1.73	0.53
4:D:273:LEU:HA	4:D:276:THR:HG22	1.89	0.53
36:4:158:PRO:HG3	43:5:109:HIS:HB3	1.91	0.53
1:a:4:C:O2'	9:K:18:ARG:NH1	2.42	0.53
1:a:407:G:H2'	1:a:407:G:N3	2.24	0.53
26:S:98:VAL:HG13	26:S:98:VAL:O	2.08	0.53
43:5:122:SER:HB3	43:5:123:THR:HA	1.90	0.53
1:a:896:U:H2'	1:a:897:U:O4'	2.08	0.53
5:F:44:LEU:HD13	5:F:72:ILE:HD11	1.91	0.53
23:N:31:LEU:C	23:N:31:LEU:HD12	2.34	0.53
36:4:118:ILE:O	36:4:122:ILE:HG13	2.09	0.53
43:5:145:GLU:HG2	43:5:174:MET:HE2	1.89	0.53
43:5:79:THR:HG21	43:5:112:ILE:HD13	1.91	0.53
6:H:2:LYS:HD3	6:H:15:LEU:HD11	1.90	0.53
25:R:53:GLU:OE1	25:R:85:ARG:NH2	2.42	0.53
41:2:500:CYS:HB3	41:2:555:ILE:HD11	1.91	0.53
43:5:45:VAL:HG21	43:5:78:ILE:HB	1.91	0.53
26:S:31:ASN:HA	26:S:34:VAL:HG12	1.91	0.52
30:i:91:LEU:HD13	30:i:96:LEU:HD12	1.91	0.52
40:1:525:ALA:CA	43:5:345:GLN:HE22	2.21	0.52
41:2:326:HIS:HA	41:2:329:VAL:HG22	1.91	0.52
1:a:1300:U:H2'	1:a:1300:U:O2	2.09	0.52
35:3:405:ILE:HG12	36:4:360:LEU:HD11	1.91	0.52
41:2:432:GLN:NE2	41:2:432:GLN:HA	2.24	0.52
43:5:190:ALA:HA	43:5:193:THR:HA	1.92	0.52
39:8:227:LYS:N	39:8:228:PRO:HD3	2.25	0.52
43:5:122:SER:CB	43:5:123:THR:HA	2.40	0.52
34:h:17:TRP:CE3	34:h:303:THR:HG22	2.45	0.52
35:3:46:SER:HA	35:3:216:HIS:CD2	2.44	0.52
38:7:536:ALA:HA	38:7:539:TYR:HB3	1.92	0.52
39:8:276:LYS:O	39:8:279:LEU:HG	2.10	0.52
44:A:656:G:O2'	44:A:658:C:OP2	2.25	0.52
41:2:418:ILE:HG23	41:2:441:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:560:U:O2'	44:A:561:A:O5'	2.24	0.52
1:a:536:A:N3	1:a:536:A:H2'	2.23	0.52
8:J:165:GLN:HE22	8:J:195:LEU:HD11	1.74	0.52
43:5:316:SER:HA	43:5:319:ILE:HD12	1.92	0.52
38:7:238:SER:HA	38:7:423:PRO:HB2	1.92	0.52
41:2:361:ALA:HB1	41:2:367:GLY:HA2	1.91	0.52
41:2:432:GLN:NE2	41:2:432:GLN:CA	2.73	0.52
44:A:415:U:O2	44:A:430:G:N2	2.43	0.52
39:8:103:LEU:HD13	39:8:127:LEU:HD13	1.92	0.52
40:1:445:GLN:HA	40:1:448:GLN:HE22	1.75	0.52
8:J:61:ASP:O	8:J:78:ILE:N	2.43	0.51
1:a:1118:C:O2	1:a:1118:C:O4'	2.28	0.51
35:3:219:LEU:HD11	35:3:324:PHE:CE1	2.44	0.51
10:M:40:ILE:HD11	10:M:68:ILE:HG12	1.91	0.51
35:3:208:LEU:HD22	35:3:243:LEU:HB3	1.91	0.51
39:8:263:ILE:HG22	39:8:266:LEU:HD22	1.92	0.51
43:5:181:ASP:HB2	43:5:185:GLU:HB2	1.91	0.51
21:G:40:ALA:HB1	21:G:45:TYR:CG	2.46	0.51
36:4:159:HIS:ND1	36:4:168:VAL:HG22	2.26	0.51
44:A:368:G:H2'	44:A:369:A:O4'	2.10	0.51
4:D:144:SER:HB3	4:D:149:THR:HG23	1.92	0.51
38:7:341:LEU:HD22	38:7:343:ILE:HB	1.92	0.51
39:8:212:LEU:CD2	39:8:263:ILE:HG21	2.40	0.51
1:a:549:C:N4	1:a:550:C:C4	2.79	0.51
1:a:823:U:O2	1:a:823:U:O4'	2.29	0.51
36:4:347:LEU:HD23	43:5:346:ALA:HB1	1.92	0.51
1:a:553:U:HO2'	1:a:554:A:C5'	2.22	0.51
36:4:339:VAL:N	36:4:340:PRO:HD3	2.26	0.51
41:2:867:VAL:O	41:2:867:VAL:CG1	2.58	0.51
42:9:210:VAL:HG13	42:9:367:ALA:HB2	1.93	0.51
43:5:159:GLN:N	43:5:160:GLY:HA3	2.25	0.51
29:V:40:ILE:HD11	29:V:53:PRO:HD3	1.93	0.51
39:8:51:VAL:O	39:8:89:LYS:NZ	2.43	0.51
42:9:399:GLN:HE22	42:9:455:ASP:HB3	1.76	0.51
42:9:446:THR:HG21	42:9:490:ILE:HD11	1.93	0.51
42:9:490:ILE:HG13	42:9:491:ASN:H	1.76	0.51
23:N:79:VAL:HG12	23:N:80:ASP:H	1.75	0.51
40:1:80:GLN:O	42:9:175:VAL:HB	2.11	0.51
43:5:103:MET:O	43:5:106:SER:OG	2.27	0.51
44:A:423:G:H2'	44:A:423:G:N3	2.26	0.51
4:D:135:GLY:HA2	4:D:165:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:393:TRP:HB3	40:1:403:LEU:HD11	1.93	0.50
40:1:372:ASN:HA	40:1:375:VAL:HB	1.93	0.50
43:5:310:PRO:HA	43:5:314:MET:HE3	1.94	0.50
3:C:62:LEU:HD23	3:C:91:VAL:HG21	1.91	0.50
20:E:115:VAL:HG11	20:E:142:LEU:HD21	1.94	0.50
39:8:204:ALA:HB1	39:8:240:LEU:HD11	1.93	0.50
40:1:302:LEU:HG	40:1:306:MET:HE3	1.92	0.50
41:2:492:GLU:O	41:2:493:LYS:CG	2.57	0.50
14:X:111:MET:HE3	14:X:116:ALA:HA	1.93	0.50
37:6:87:CYS:HA	38:7:446:VAL:HG13	1.93	0.50
44:A:491:U:H2'	44:A:492:G:O4'	2.11	0.50
1:a:1589:A:N3	1:a:1653:U:O2'	2.42	0.50
42:9:300:LEU:HD11	42:9:331:ASN:HD22	1.76	0.50
29:V:98:VAL:HA	29:V:101:ILE:HD12	1.94	0.50
36:4:114:LEU:HD12	36:4:118:ILE:HB	1.92	0.50
38:7:545:ARG:HH21	43:5:322:GLN:HE22	1.59	0.50
40:1:226:GLN:HA	40:1:230:LEU:HD23	1.93	0.50
40:1:318:MET:O	40:1:322:VAL:HG22	2.11	0.50
1:a:155:G:H4'	6:H:15:LEU:HD13	1.93	0.50
39:8:225:THR:HG23	39:8:226:LEU:HG	1.94	0.50
41:2:504:LEU:HA	41:2:507:ILE:HG12	1.94	0.50
44:A:519:A:N6	44:A:575:U:O4	2.45	0.50
34:h:206:LEU:HD12	34:h:218:LEU:HD12	1.93	0.50
35:3:123:PHE:O	35:3:127:TYR:HB2	2.11	0.50
39:8:63:VAL:HG11	39:8:98:ARG:HB3	1.93	0.50
44:A:535:C:H2'	44:A:536:A:H8	1.76	0.50
35:3:19:VAL:HG21	35:3:45:LEU:HA	1.92	0.50
35:3:335:ASN:HA	35:3:338:LEU:CB	2.40	0.50
36:4:372:GLU:O	36:4:375:VAL:HB	2.12	0.50
37:6:165:LEU:HD13	37:6:169:GLN:HB3	1.94	0.50
1:a:183:G:O2'	1:a:184:G:O5'	2.30	0.49
1:a:1139:C:O2	1:a:1139:C:O4'	2.30	0.49
35:3:320:VAL:HA	35:3:329:LEU:HD11	1.93	0.49
41:2:438:LEU:HD21	41:2:493:LYS:NZ	2.26	0.49
1:a:1351:G:O2'	1:a:1378:A:N1	2.38	0.49
14:X:52:ILE:HG22	14:X:61:ILE:HG12	1.93	0.49
36:4:112:VAL:HG22	36:4:149:VAL:HB	1.94	0.49
43:5:170:THR:HB	43:5:171:PRO:HD2	1.93	0.49
18:c:59:CYS:SG	41:2:340:ARG:NH2	2.86	0.49
21:G:73:THR:O	21:G:89:THR:HG21	2.11	0.49
35:3:76:THR:O	35:3:80:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:6:45:GLU:HB2	38:7:294:LEU:HD23	1.92	0.49
38:7:469:THR:HG23	38:7:514:GLN:HG2	1.94	0.49
43:5:162:LEU:HD21	43:5:165:LYS:HB3	1.95	0.49
44:A:581:A:N3	44:A:581:A:H2'	2.28	0.49
34:h:87:LEU:HB2	34:h:101:PHE:HB2	1.95	0.49
43:5:30:GLY:HA3	43:5:38:GLN:HB2	1.94	0.49
43:5:122:SER:HA	43:5:152:TYR:O	2.12	0.49
1:a:1808:U:H2'	1:a:1809:A:C8	2.47	0.49
35:3:97:ASP:N	35:3:98:PRO:HD2	2.27	0.49
37:6:80:THR:HG21	38:7:326:MET:C	2.37	0.49
20:E:105:LEU:HB2	20:E:122:VAL:HG21	1.94	0.49
22:L:15:LEU:HD22	22:L:49:MET:HE1	1.94	0.49
40:1:306:MET:O	40:1:310:LEU:N	2.45	0.49
40:1:400:PRO:HB3	40:1:446:ILE:HG21	1.95	0.49
34:h:154:VAL:HB	34:h:165:ILE:HD11	1.94	0.49
36:4:361:ALA:HB1	43:5:332:GLU:HB2	1.94	0.49
40:1:75:LYS:HG2	40:1:86:LEU:HD11	1.94	0.49
40:1:329:ILE:HG21	40:1:371:ILE:HB	1.94	0.49
43:5:185:GLU:HB3	43:5:189:LYS:HE2	1.94	0.49
1:a:142:C:O4'	1:a:142:C:O2	2.30	0.49
1:a:1398:G:O2'	34:h:88:ARG:NH2	2.46	0.49
22:L:59:LYS:HB3	22:L:70:TYR:HB2	1.95	0.49
34:h:17:TRP:HB2	34:h:303:THR:HA	1.93	0.49
25:R:57:LEU:HD11	25:R:115:TYR:CD2	2.48	0.49
35:3:213:TRP:HA	35:3:216:HIS:CD2	2.48	0.49
36:4:140:LEU:HD22	36:4:220:LEU:HD11	1.94	0.49
43:5:50:ILE:HG12	43:5:152:TYR:CE2	2.48	0.49
5:F:183:VAL:HG11	5:F:220:THR:HG21	1.95	0.49
24:Q:51:ARG:NH2	24:Q:55:SER:OG	2.45	0.49
29:V:80:PHE:HB3	32:e:52:PHE:HB3	1.95	0.49
32:e:39:CYS:SG	32:e:42:CYS:SG	3.11	0.49
1:a:1037:G:H4'	1:a:1845:A:H4'	1.95	0.48
23:N:69:CYS:SG	23:N:76:LEU:HD11	2.53	0.48
35:3:225:HIS:N	35:3:226:PRO:HD2	2.29	0.48
40:1:428:VAL:N	40:1:429:PRO:HD2	2.29	0.48
42:9:490:ILE:HG13	42:9:491:ASN:N	2.29	0.48
19:f:85:VAL:HA	19:f:88:GLN:HE21	1.78	0.48
29:V:25:THR:HG22	29:V:84:ILE:HD11	1.96	0.48
35:3:75:THR:HG21	35:3:143:ASN:HB3	1.95	0.48
43:5:173:LEU:HD11	43:5:180:LYS:HD2	1.94	0.48
1:a:1780:G:H2'	1:a:1781:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:HB3	2:B:173:LEU:HD11	1.95	0.48
24:Q:17:TYR:HB3	24:Q:25:LEU:HD11	1.96	0.48
36:4:204:VAL:HA	36:4:207:HIS:HB2	1.93	0.48
40:1:101:THR:HG22	40:1:149:TRP:HB3	1.94	0.48
43:5:67:LEU:HD12	43:5:78:ILE:HD11	1.96	0.48
39:8:101:LEU:HD12	39:8:102:ARG:N	2.28	0.48
43:5:118:GLY:HA3	43:5:148:VAL:O	2.14	0.48
43:5:167:TYR:OH	43:5:196:HIS:O	2.30	0.48
30:i:73:VAL:HG12	30:i:79:ILE:HD11	1.94	0.48
35:3:10:ILE:HG13	35:3:204:PRO:HB3	1.96	0.48
36:4:184:SER:HB2	43:5:52:HIS:HE2	1.77	0.48
36:4:272:ILE:HG23	43:5:43:GLY:HA3	1.95	0.48
36:4:287:SER:HA	43:5:341:LEU:HD11	1.95	0.48
41:2:685:VAL:HG13	41:2:708:ARG:HG2	1.96	0.48
44:A:389:C:H2'	44:A:390:G:O4'	2.13	0.48
1:a:1556:A:N6	32:e:12:ARG:O	2.46	0.48
11:O:25:TRP:CD2	18:c:82:LYS:HD3	2.48	0.48
36:4:265:GLU:HA	43:5:50:ILE:HG21	1.96	0.48
40:1:484:ILE:HG22	40:1:485:ASP:HB2	1.96	0.48
1:a:1757:G:H1'	1:a:1776:G:H1	1.79	0.48
40:1:451:GLU:O	40:1:454:ARG:HG2	2.14	0.48
42:9:213:TYR:HA	42:9:339:LEU:HD12	1.95	0.48
1:a:293:C:H2'	1:a:293:C:O2	2.14	0.48
9:K:61:LEU:HD13	9:K:94:LEU:HB3	1.96	0.48
37:6:11:VAL:HG21	37:6:32:TYR:CG	2.48	0.48
43:5:104:MET:O	43:5:108:ARG:HG2	2.12	0.48
1:a:986:G:C8	12:P:137:SER:O	2.67	0.48
17:b:45:VAL:HG11	17:b:53:ILE:HD13	1.96	0.48
35:3:243:LEU:O	35:3:282:GLN:NE2	2.47	0.48
43:5:197:MET:HE1	43:5:326:TYR:HB3	1.95	0.48
43:5:314:MET:HA	43:5:314:MET:HE2	1.96	0.48
44:A:574:U:H2'	44:A:575:U:C6	2.48	0.48
1:a:921:G:C6	14:X:28:ARG:HD2	2.48	0.47
1:a:1298:G:O2'	1:a:1299:A:C8	2.67	0.47
10:M:40:ILE:CD1	10:M:61:PRO:HB2	2.44	0.47
28:U:28:LEU:O	28:U:30:VAL:N	2.47	0.47
39:8:282:PHE:O	39:8:285:MET:HE2	2.14	0.47
43:5:172:LYS:HB3	43:5:194:PHE:HA	1.95	0.47
1:a:159:A:N1	1:a:467:G:O2'	2.35	0.47
24:Q:50:ARG:HB3	24:Q:54:HIS:HB3	1.96	0.47
34:h:42:MET:HB3	34:h:57:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:156:VAL:HG11	35:3:191:ARG:CZ	2.43	0.47
43:5:264:MET:HE1	43:5:321:GLY:CA	2.44	0.47
29:V:26:SER:OG	29:V:32:LEU:HB2	2.15	0.47
39:8:277:MET:HG3	39:8:301:LEU:HD22	1.96	0.47
40:1:284:TRP:CZ2	40:1:426:GLN:HB3	2.50	0.47
41:2:727:LEU:HB3	41:2:729:PRO:HD2	1.95	0.47
35:3:208:LEU:HA	35:3:243:LEU:HD22	1.96	0.47
38:7:363:GLN:HA	38:7:419:LYS:HD3	1.96	0.47
40:1:43:TRP:CH2	40:1:45:LYS:HD2	2.49	0.47
41:2:598:ILE:O	41:2:598:ILE:HG23	2.15	0.47
41:2:839:THR:HB	41:2:841:THR:HG23	1.96	0.47
42:9:385:CYS:HB3	42:9:452:ALA:HA	1.95	0.47
1:a:919:A:OP2	11:O:64:ARG:NH2	2.47	0.47
33:g:133:ALA:HB1	33:g:135:HIS:CD2	2.50	0.47
35:3:212:THR:HG22	35:3:216:HIS:CE1	2.49	0.47
38:7:476:ALA:HA	38:7:479:LEU:HD12	1.96	0.47
1:a:853:C:O4'	1:a:853:C:O2	2.32	0.47
34:h:121:VAL:HG21	34:h:165:ILE:CD1	2.43	0.47
36:4:282:VAL:HG13	36:4:285:LEU:HB2	1.95	0.47
43:5:157:THR:HG21	43:5:163:SER:HA	1.97	0.47
1:a:1722:G:C6	1:a:1813:A:N6	2.83	0.47
1:a:1737:G:OP1	6:H:94:ARG:NH2	2.48	0.47
2:B:173:LEU:HD12	26:S:91:LEU:HD13	1.97	0.47
20:E:74:GLN:HE22	20:E:81:GLU:HB2	1.80	0.47
34:h:18:VAL:HA	34:h:35:SER:HA	1.97	0.47
38:7:284:LEU:HD13	38:7:299:LEU:HD13	1.97	0.47
38:7:376:THR:O	38:7:461:ARG:NH1	2.48	0.47
40:1:514:MET:N	40:1:515:PRO:CD	2.78	0.47
44:A:513:U:O2'	44:A:514:U:O4'	2.29	0.47
1:a:1300:U:O2	1:a:1300:U:C2'	2.62	0.47
2:B:30:LEU:HD13	2:B:38:ILE:CD1	2.45	0.47
28:U:75:MET:HA	28:U:78:ILE:HG22	1.96	0.47
34:h:12:LYS:HD3	34:h:306:LEU:HD21	1.97	0.47
37:6:121:LEU:HD11	37:6:128:LEU:HD11	1.97	0.47
38:7:241:ASN:HB3	38:7:423:PRO:HG3	1.97	0.47
38:7:482:THR:HG21	38:7:493:PHE:HD1	1.79	0.47
39:8:350:LEU:C	39:8:350:LEU:HD12	2.40	0.47
44:A:644:A:H2	44:A:661:C:H42	1.61	0.47
1:a:198:U:H2'	1:a:200:G:N7	2.29	0.47
15:Y:140:ARG:HD2	15:Y:141:PRO:HD2	1.97	0.47
24:Q:56:LEU:O	24:Q:60:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:8:98:ARG:O	39:8:101:LEU:HG	2.14	0.47
44:A:399:G:C6	44:A:400:G:C6	3.02	0.47
1:a:873:G:H22	10:M:153:LYS:HD3	1.80	0.47
4:D:200:ARG:O	9:K:54:ARG:NH2	2.48	0.47
5:F:188:ASN:HD22	5:F:220:THR:HG23	1.79	0.47
1:a:561:A:H2'	1:a:562:U:O4'	2.15	0.46
12:P:20:GLN:HG3	12:P:27:VAL:HG22	1.98	0.46
26:S:24:LEU:HD22	26:S:54:VAL:HG11	1.97	0.46
35:3:270:ARG:HD2	35:3:273:VAL:HB	1.97	0.46
41:2:731:GLU:HB3	41:2:755:PHE:CZ	2.49	0.46
43:5:170:THR:OG1	43:5:173:LEU:HD23	2.15	0.46
43:5:180:LYS:CD	43:5:319:ILE:HD13	2.44	0.46
44:A:387:U:H4'	44:A:388:A:OP1	2.15	0.46
1:a:929:G:H2'	1:a:930:C:O4'	2.14	0.46
28:U:60:THR:HG23	28:U:75:MET:HE2	1.97	0.46
39:8:285:MET:HE1	39:8:336:HIS:HA	1.98	0.46
40:1:87:GLU:HA	40:1:173:LEU:CD1	2.44	0.46
41:2:852:GLN:HE22	43:5:254:SER:HB3	1.81	0.46
1:a:160:U:O2	1:a:468:A:O2'	2.32	0.46
35:3:204:PRO:O	35:3:208:LEU:HG	2.16	0.46
40:1:470:ALA:HA	40:1:473:ASP:HB2	1.96	0.46
24:Q:33:LEU:HD21	24:Q:87:PRO:HD2	1.96	0.46
30:i:73:VAL:HG21	30:i:88:LEU:HD21	1.97	0.46
36:4:117:VAL:HG11	43:5:51:LYS:HD3	1.97	0.46
36:4:192:TRP:O	36:4:219:HIS:HA	2.14	0.46
42:9:280:ILE:HD11	42:9:518:ILE:HD11	1.96	0.46
27:T:73:ASN:HB3	27:T:76:GLN:HE21	1.79	0.46
35:3:254:LEU:HD13	35:3:283:GLN:NE2	2.31	0.46
35:3:403:GLN:O	35:3:407:LYS:HB2	2.15	0.46
36:4:266:ARG:NH1	43:5:228:HIS:O	2.49	0.46
37:6:47:ASN:HB3	37:6:69:ILE:HG23	1.96	0.46
39:8:263:ILE:HA	39:8:266:LEU:HB2	1.97	0.46
42:9:435:LEU:CD1	42:9:490:ILE:HG22	2.39	0.46
43:5:36:VAL:HA	43:5:146:GLU:HA	1.98	0.46
43:5:336:GLN:HE21	43:5:340:LYS:HG3	1.80	0.46
40:1:297:HIS:NE2	40:1:329:ILE:HD11	2.30	0.46
41:2:577:ALA:HB1	41:2:619:CYS:SG	2.55	0.46
41:2:691:MET:HE3	41:2:691:MET:HA	1.96	0.46
43:5:52:HIS:CG	43:5:83:PRO:HG3	2.50	0.46
1:a:928:G:H1	1:a:1013:U:H3	1.62	0.46
1:a:1568:C:OP1	28:U:96:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:MET:HE3	13:W:39:VAL:CG2	2.46	0.46
36:4:273:MET:HB3	43:5:218:LEU:HD13	1.98	0.46
38:7:265:LEU:HA	38:7:268:MET:HE2	1.96	0.46
39:8:161:LYS:HA	39:8:164:LEU:HD12	1.96	0.46
43:5:64:GLN:O	43:5:83:PRO:HA	2.16	0.46
44:A:437:C:H2'	44:A:437:C:O2	2.16	0.46
44:A:512:C:H3'	44:A:513:U:H5'	1.96	0.46
43:5:63:VAL:HG13	43:5:119:TRP:CE3	2.51	0.46
43:5:81:CYS:HB2	43:5:120:TYR:CE1	2.51	0.46
43:5:261:ASN:O	43:5:264:MET:HB3	2.15	0.46
39:8:236:LEU:HD23	39:8:238:HIS:CE1	2.51	0.46
40:1:138:GLN:O	40:1:142:ASP:HB2	2.16	0.46
40:1:455:LEU:HA	40:1:458:LEU:HB2	1.98	0.46
40:1:478:CYS:HB3	40:1:502:ARG:HD2	1.97	0.46
41:2:553:LYS:HE2	41:2:569:ILE:HD12	1.98	0.46
1:a:607:U:H3'	1:a:608:C:C5'	2.46	0.46
1:a:1207:G:O2'	1:a:1837:G:N2	2.49	0.46
8:J:36:THR:HG23	8:J:96:LEU:HB2	1.98	0.46
41:2:430:ASN:N	41:2:430:ASN:HD22	2.14	0.46
42:9:334:PHE:CZ	42:9:338:VAL:HG11	2.51	0.46
44:A:459:G:O2'	44:A:460:U:O4'	2.34	0.46
1:a:371:A:OP2	8:J:10:LYS:HB2	2.15	0.45
39:8:86:LEU:O	39:8:102:ARG:NH1	2.49	0.45
40:1:481:GLN:HE22	40:1:498:ASN:C	2.24	0.45
41:2:755:PHE:HB3	41:2:760:LYS:HB2	1.97	0.45
4:D:141:LEU:HD13	4:D:238:LYS:NZ	2.19	0.45
7:I:84:GLU:HG3	7:I:92:VAL:HG12	1.98	0.45
37:6:151:GLN:HB2	38:7:505:GLY:HA3	1.98	0.45
38:7:545:ARG:HA	38:7:548:HIS:HB3	1.98	0.45
40:1:424:LEU:HD23	40:1:424:LEU:N	2.31	0.45
41:2:843:VAL:HG22	41:2:847:THR:HB	1.98	0.45
43:5:253:MET:HG2	43:5:331:LYS:HD2	1.97	0.45
1:a:130:G:N3	1:a:130:G:H2'	2.31	0.45
1:a:1239:U:O2	1:a:1241:A:H8	1.99	0.45
1:a:1662:U:O4	1:a:1663:A:N6	2.49	0.45
28:U:27:LYS:HD2	28:U:110:LEU:HD13	1.99	0.45
35:3:219:LEU:HD11	35:3:324:PHE:CZ	2.51	0.45
36:4:300:GLN:HB2	40:1:532:LYS:HG3	1.98	0.45
39:8:71:LEU:HA	39:8:74:LEU:HD13	1.99	0.45
40:1:256:ILE:O	40:1:260:PHE:HB2	2.16	0.45
40:1:472:VAL:HG23	40:1:484:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:432:GLN:NE2	41:2:432:GLN:C	2.73	0.45
42:9:406:LEU:CD2	42:9:442:LEU:HD11	2.45	0.45
1:a:146:G:O2'	1:a:147:A:O5'	2.30	0.45
5:F:173:ILE:HD11	5:F:235:TRP:CE3	2.51	0.45
8:J:130:THR:N	8:J:131:PRO:CD	2.78	0.45
20:E:134:CYS:SG	20:E:135:GLU:N	2.90	0.45
35:3:41:LYS:HA	35:3:44:LEU:HG	1.98	0.45
35:3:254:LEU:HD11	35:3:293:THR:HG22	1.97	0.45
39:8:287:VAL:HG12	39:8:288:GLU:HB2	1.99	0.45
40:1:210:ARG:HB3	40:1:212:HIS:CG	2.51	0.45
41:2:456:THR:HB	41:2:667:ARG:HD2	1.97	0.45
42:9:179:TRP:CG	42:9:532:ILE:HG22	2.50	0.45
44:A:638:C:O2'	44:A:639:A:N7	2.47	0.45
35:3:38:LEU:HD12	35:3:39:GLN:N	2.31	0.45
35:3:143:ASN:HA	35:3:145:SER:N	2.32	0.45
40:1:303:SER:OG	40:1:321:ARG:NH1	2.50	0.45
42:9:435:LEU:HA	42:9:442:LEU:HD22	1.98	0.45
44:A:386:U:C4	44:A:403:G:N3	2.84	0.45
15:Y:51:VAL:HG13	15:Y:70:VAL:CG2	2.47	0.45
35:3:131:LEU:HD11	35:3:158:VAL:HA	1.98	0.45
35:3:193:LYS:HZ3	35:3:235:LEU:HD21	1.82	0.45
35:3:297:GLU:HA	35:3:300:TYR:HB3	1.97	0.45
36:4:191:GLY:HA2	36:4:210:TYR:CE1	2.51	0.45
16:Z:79:LEU:HD21	16:Z:96:LEU:HD21	1.99	0.45
35:3:261:VAL:HA	35:3:265:LYS:HB2	1.98	0.45
38:7:533:THR:HA	38:7:536:ALA:HB3	1.99	0.45
44:A:537:G:O2'	44:A:540:A:N1	2.49	0.45
1:a:962:A:H4'	44:A:691:G:O6	2.16	0.45
19:f:112:ASN:HA	19:f:116:VAL:HG12	1.98	0.45
36:4:111:VAL:HG13	36:4:148:SER:HA	1.98	0.45
36:4:116:PRO:HG3	36:4:259:TYR:CE2	2.52	0.45
35:3:304:ASP:HB3	35:3:308:ALA:HB2	1.98	0.45
36:4:298:ARG:HD3	39:8:360:ASN:OD1	2.17	0.45
39:8:323:CYS:HA	40:1:517:GLU:HB3	1.99	0.45
44:A:454:C:H2'	44:A:455:U:C6	2.51	0.45
21:G:39:ILE:HG23	21:G:68:ILE:HD13	1.99	0.45
36:4:175:ASN:O	36:4:179:LEU:HG	2.16	0.45
36:4:364:THR:HG22	41:2:859:LEU:CD1	2.46	0.45
38:7:486:PHE:H	38:7:487:ARG:C	2.25	0.45
39:8:184:VAL:O	39:8:188:LEU:HD23	2.16	0.45
41:2:707:ARG:HA	41:2:707:ARG:NE	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:553:U:HO2'	1:a:554:A:P	2.39	0.44
1:a:1221:G:O2'	1:a:1676:U:O2	2.27	0.44
24:Q:54:HIS:HB3	24:Q:57:LEU:HB2	1.98	0.44
24:Q:87:PRO:HA	24:Q:90:VAL:HG23	1.99	0.44
39:8:70:LEU:HD13	39:8:105:LEU:HD11	1.97	0.44
42:9:302:VAL:HG11	42:9:323:LEU:HB3	1.97	0.44
40:1:403:LEU:CD2	40:1:439:LEU:HD21	2.46	0.44
41:2:379:ILE:HA	41:2:382:LEU:HD12	1.99	0.44
41:2:688:VAL:HG22	41:2:692:LEU:HD12	2.00	0.44
1:a:118:C:H2'	1:a:119:U:O4'	2.18	0.44
9:K:47:LYS:HG3	9:K:102:ILE:HD11	2.00	0.44
36:4:273:MET:SD	43:5:218:LEU:HB2	2.58	0.44
40:1:306:MET:O	40:1:309:ASN:N	2.51	0.44
41:2:710:ILE:HB	41:2:714:PHE:CD2	2.36	0.44
42:9:211:GLU:HB2	42:9:339:LEU:HD21	1.99	0.44
43:5:277:TYR:OH	44:A:535:C:OP1	2.27	0.44
43:5:283:GLN:HA	43:5:286:MET:HE3	1.99	0.44
34:h:130:LYS:NZ	34:h:138:CYS:SG	2.73	0.44
35:3:211:ARG:NH1	35:3:242:TYR:O	2.50	0.44
36:4:207:HIS:CE1	36:4:219:HIS:NE2	2.86	0.44
36:4:347:LEU:O	36:4:351:ILE:HG13	2.16	0.44
41:2:504:LEU:HD13	41:2:564:ILE:HG23	1.99	0.44
41:2:536:GLN:HG3	41:2:539:ASN:HB2	1.99	0.44
42:9:282:LYS:HE2	42:9:509:MET:HA	2.00	0.44
1:a:1556:A:C5	32:e:13:LYS:HA	2.53	0.44
2:B:50:ASN:HD22	2:B:53:ARG:HD2	1.82	0.44
9:K:130:ILE:HG12	9:K:135:ILE:HD11	2.00	0.44
20:E:34:TYR:OH	20:E:37:VAL:HG13	2.18	0.44
23:N:19:GLN:HE22	23:N:88:TRP:CG	2.36	0.44
35:3:373:ASN:HA	35:3:376:ARG:HG2	2.00	0.44
39:8:90:LEU:HD21	39:8:102:ARG:HD2	1.98	0.44
40:1:323:LEU:CD1	40:1:424:LEU:HD22	2.48	0.44
42:9:431:LEU:HD22	42:9:481:TYR:OH	2.17	0.44
2:B:119:PRO:HG2	2:B:142:LEU:HD11	2.00	0.44
27:T:66:ARG:O	27:T:69:THR:OG1	2.28	0.44
40:1:147:THR:HA	40:1:150:VAL:HG22	2.00	0.44
1:a:1088:U:H4'	1:a:1089:G:OP2	2.17	0.44
17:b:45:VAL:HG11	17:b:53:ILE:CD1	2.47	0.44
35:3:193:LYS:NZ	35:3:235:LEU:HD21	2.33	0.44
35:3:278:VAL:HA	35:3:283:GLN:HG2	1.99	0.44
41:2:542:GLU:N	41:2:542:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:578:LEU:N	41:2:619:CYS:SG	2.91	0.44
2:B:2:SER:HA	2:B:59:LEU:HD13	2.00	0.44
3:C:190:PRO:HG3	40:1:17:GLU:HB3	2.00	0.44
34:h:191:HIS:CG	34:h:195:LEU:HD21	2.53	0.44
36:4:336:PRO:HG3	43:5:352:ASN:HB2	1.99	0.44
36:4:371:ASN:HD21	43:5:264:MET:HG2	1.82	0.44
41:2:857:LEU:O	41:2:861:GLU:N	2.36	0.44
35:3:210:GLN:HA	35:3:213:TRP:HB2	2.00	0.44
36:4:369:ALA:O	36:4:373:LYS:HB2	2.18	0.44
38:7:236:ASP:O	38:7:240:ILE:HG12	2.18	0.44
1:a:1232:U:H2'	1:a:1233:G:C8	2.53	0.43
1:a:1664:A:H4'	1:a:1665:G:OP1	2.18	0.43
4:D:141:LEU:CD1	4:D:238:LYS:HZ2	2.04	0.43
24:Q:68:PRO:HB2	24:Q:69:PRO:HD2	1.99	0.43
35:3:218:SER:HB2	35:3:232:ILE:HG12	1.99	0.43
36:4:120:ALA:HA	43:5:44:LEU:HD22	1.99	0.43
40:1:78:CYS:SG	40:1:86:LEU:HG	2.58	0.43
43:5:46:VAL:O	43:5:50:ILE:HG13	2.17	0.43
44:A:380:G:C4	44:A:440:A:C2	3.06	0.43
1:a:142:C:H1'	6:H:180:VAL:HG11	2.00	0.43
1:a:798:G:H2'	7:I:107:LYS:O	2.18	0.43
1:a:1282:A:N7	23:N:102:LYS:NZ	2.66	0.43
2:B:60:LEU:HD22	2:B:159:ILE:HG21	1.99	0.43
5:F:256:LEU:O	5:F:260:GLN:HG2	2.18	0.43
35:3:158:VAL:CG2	35:3:159:PRO:HD2	2.44	0.43
38:7:266:TYR:CB	38:7:283:LEU:HD13	2.48	0.43
41:2:810:MET:O	41:2:814:ASP:N	2.45	0.43
43:5:70:LEU:HD13	43:5:115:LEU:HD13	2.00	0.43
1:a:1280:G:H2'	1:a:1281:G:C8	2.54	0.43
1:a:1533:A:OP2	21:G:164:ARG:NH2	2.51	0.43
24:Q:75:VAL:HG22	24:Q:93:MET:HB3	2.00	0.43
42:9:206:CYS:HA	42:9:369:ARG:HB3	1.99	0.43
43:5:211:ILE:O	43:5:214:LEU:N	2.52	0.43
44:A:462:U:C4	44:A:463:U:C4	3.06	0.43
44:A:560:U:HO2'	44:A:561:A:P	2.42	0.43
1:a:533:A:H2'	1:a:534:G:H8	1.84	0.43
6:H:49:VAL:CG2	6:H:115:LYS:HB3	2.48	0.43
20:E:59:LEU:HA	20:E:66:ILE:HG12	1.99	0.43
31:d:35:MET:SD	42:9:435:LEU:HD13	2.58	0.43
36:4:246:ARG:NH1	36:4:247:THR:OG1	2.51	0.43
37:6:211:SER:HA	37:6:214:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:87:GLU:HA	40:1:173:LEU:HD13	2.00	0.43
42:9:195:LEU:HD22	42:9:502:ARG:HD2	2.01	0.43
43:5:40:GLN:HB2	43:5:75:ARG:HD3	2.01	0.43
1:a:193:C:H2'	1:a:194:C:C6	2.54	0.43
1:a:1100:A:OP1	26:S:129:LYS:NZ	2.48	0.43
1:a:1405:A:H2'	1:a:1406:G:O4'	2.19	0.43
2:B:70:ASN:CB	4:D:274:MET:HE2	2.49	0.43
3:C:62:LEU:HD21	3:C:96:CYS:SG	2.58	0.43
4:D:212:LYS:HA	4:D:215:LEU:HD12	1.99	0.43
4:D:250:TYR:N	13:W:23:ILE:HD11	2.33	0.43
14:X:6:VAL:HG12	14:X:34:ILE:HD11	1.99	0.43
36:4:155:PHE:CG	36:4:176:MET:HE2	2.53	0.43
37:6:23:PRO:HG2	37:6:57:ASN:HD22	1.84	0.43
39:8:354:LEU:HD21	43:5:352:ASN:CG	2.43	0.43
43:5:104:MET:HB3	43:5:114:HIS:HB2	2.01	0.43
13:W:72:LEU:O	13:W:75:SER:OG	2.32	0.43
21:G:103:LEU:HD11	30:i:67:LEU:HD22	2.00	0.43
24:Q:22:LEU:HD11	24:Q:109:PRO:HB3	2.00	0.43
38:7:552:GLU:HA	43:5:192:ILE:HA	2.00	0.43
44:A:509:G:O6	44:A:510:C:C5	2.72	0.43
2:B:63:ARG:HA	2:B:185:MET:HE1	2.00	0.43
33:g:119:ARG:NE	33:g:132:MET:SD	2.92	0.43
35:3:26:LEU:HB2	35:3:68:HIS:CE1	2.54	0.43
37:6:48:LEU:HD22	37:6:84:LEU:HD13	2.00	0.43
37:6:115:GLN:N	37:6:115:GLN:OE1	2.52	0.43
40:1:403:LEU:HA	40:1:406:ARG:HB3	2.00	0.43
43:5:119:TRP:CZ3	43:5:121:GLN:HB3	2.53	0.43
44:A:464:G:C2	44:A:465:A:C2	3.06	0.43
44:A:526:A:O2'	44:A:527:C:OP1	2.26	0.43
1:a:791:C:H2'	1:a:792:C:O4'	2.19	0.43
31:d:40:ARG:NH1	31:d:61:SER:O	2.52	0.43
35:3:198:ASN:N	35:3:199:ASN:HA	2.32	0.43
37:6:125:MET:HB3	37:6:128:LEU:HG	2.00	0.43
41:2:691:MET:HE2	41:2:788:LEU:HD12	1.99	0.43
42:9:520:LYS:HA	42:9:527:ILE:HA	2.01	0.43
43:5:36:VAL:HG11	43:5:168:ARG:CZ	2.49	0.43
3:C:31:TYR:CE2	3:C:49:VAL:HG11	2.54	0.43
22:L:64:TRP:HB3	32:e:23:VAL:HA	2.01	0.43
30:i:50:PHE:CZ	30:i:83:LEU:HD21	2.53	0.43
33:g:133:ALA:HB3	33:g:140:TYR:HB3	2.01	0.43
44:A:484:C:N4	44:A:491:U:O4	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:493:U:OP1	44:A:516:U:C4	2.72	0.43
1:a:183:G:C2'	1:a:183:G:N3	2.82	0.43
1:a:562:U:H2'	1:a:563:G:C8	2.54	0.43
2:B:132:GLN:HB3	2:B:133:PRO:HD3	2.01	0.43
9:K:113:GLN:O	9:K:117:LEU:HB2	2.19	0.43
20:E:137:VAL:HG13	20:E:185:LYS:HB2	2.01	0.43
35:3:38:LEU:HD12	35:3:38:LEU:C	2.44	0.43
36:4:139:THR:HA	36:4:192:TRP:HA	1.99	0.43
1:a:1154:U:O4	4:D:227:ARG:HD2	2.18	0.42
1:a:1597:C:H4'	1:a:1603:G:C6	2.54	0.42
9:K:46:VAL:HG11	9:K:106:LEU:CD1	2.49	0.42
1:a:167:G:OP1	6:H:8:PRO:HB3	2.19	0.42
1:a:1813:A:C6	1:a:1814:G:C5	3.07	0.42
24:Q:54:HIS:ND1	24:Q:57:LEU:HD13	2.35	0.42
39:8:83:ILE:CG1	39:8:106:LEU:HD21	2.49	0.42
39:8:100:SER:HA	39:8:103:LEU:HD12	2.01	0.42
39:8:109:LEU:HG	39:8:114:ASP:HB3	2.00	0.42
40:1:80:GLN:HA	40:1:83:ILE:HD11	2.02	0.42
41:2:402:LEU:HD23	41:2:402:LEU:HA	1.93	0.42
42:9:227:PRO:O	42:9:337:GLN:NE2	2.48	0.42
1:a:130:G:N3	1:a:130:G:C2'	2.82	0.42
1:a:151:C:O2'	6:H:132:ARG:NH1	2.51	0.42
2:B:124:VAL:HG13	2:B:130:ASP:HB2	2.01	0.42
7:I:135:PHE:HB3	7:I:136:PRO:HD3	2.01	0.42
12:P:119:LEU:O	12:P:124:MET:HB2	2.19	0.42
23:N:19:GLN:HE22	23:N:88:TRP:CD1	2.37	0.42
28:U:62:ARG:NH1	28:U:66:LEU:HD11	2.35	0.42
36:4:216:ASN:HD21	36:4:237:VAL:HG21	1.83	0.42
38:7:284:LEU:HA	38:7:287:TYR:HB3	2.01	0.42
38:7:461:ARG:HA	38:7:502:TRP:HE1	1.84	0.42
41:2:392:TYR:HB2	41:2:458:ILE:HD13	2.00	0.42
41:2:848:GLU:HB3	41:2:849:PRO:HD3	2.01	0.42
9:K:126:ALA:O	9:K:130:ILE:HG13	2.19	0.42
35:3:278:VAL:O	35:3:283:GLN:HB3	2.20	0.42
35:3:371:ILE:O	35:3:375:ILE:HG12	2.19	0.42
39:8:288:GLU:C	39:8:292:ILE:HG22	2.44	0.42
39:8:301:LEU:O	39:8:302:GLN:HG3	2.20	0.42
41:2:451:MET:SD	41:2:479:VAL:HG23	2.60	0.42
41:2:723:ARG:HG2	41:2:724:GLN:H	1.82	0.42
43:5:75:ARG:HH12	43:5:205:ILE:HB	1.84	0.42
44:A:541:C:H2'	44:A:542:A:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:576:U:O2	44:A:576:U:O4'	2.37	0.42
1:a:1808:U:H2'	1:a:1809:A:H8	1.84	0.42
1:a:1865:C:O2	1:a:1865:C:O4'	2.38	0.42
2:B:3:GLY:HA3	13:W:80:SER:HB3	2.00	0.42
23:N:24:THR:HA	23:N:27:ILE:HG12	2.02	0.42
32:e:15:GLY:O	32:e:19:ARG:NH1	2.53	0.42
35:3:178:LEU:HB2	35:3:179:MET:HE2	2.00	0.42
38:7:390:LEU:HD23	38:7:393:LYS:HD2	2.01	0.42
39:8:193:THR:HG22	39:8:194:GLU:HB2	2.00	0.42
40:1:43:TRP:CZ3	40:1:45:LYS:HD2	2.54	0.42
40:1:175:HIS:CD2	40:1:228:MET:HB3	2.55	0.42
41:2:371:ILE:O	41:2:375:LYS:N	2.50	0.42
41:2:421:GLY:HA2	41:2:431:LEU:H	1.84	0.42
41:2:499:ILE:O	41:2:502:VAL:HG12	2.19	0.42
44:A:539:U:O2	44:A:539:U:C2'	2.67	0.42
44:A:647:C:H3'	44:A:648:A:C5'	2.50	0.42
7:I:133:LEU:HD21	7:I:176:VAL:HG11	2.00	0.42
36:4:207:HIS:CE1	36:4:250:VAL:HG11	2.55	0.42
36:4:329:MET:HA	36:4:332:VAL:HG22	2.00	0.42
39:8:254:LYS:O	39:8:258:ASN:ND2	2.53	0.42
39:8:313:ILE:HA	39:8:316:VAL:HG22	2.01	0.42
40:1:78:CYS:SG	40:1:78:CYS:O	2.78	0.42
40:1:499:TYR:CD1	40:1:503:GLU:HG3	2.55	0.42
41:2:526:PRO:HB2	41:2:531:LYS:HE2	2.01	0.42
41:2:755:PHE:HB3	41:2:760:LYS:CB	2.50	0.42
41:2:799:TYR:CZ	41:2:837:GLN:HB2	2.55	0.42
44:A:662:C:H2'	44:A:663:C:C5	2.54	0.42
1:a:615:C:O2'	19:f:81:ARG:NH2	2.53	0.42
23:N:71:GLU:CG	33:g:114:ILE:HG21	2.49	0.42
37:6:151:GLN:NE2	37:6:195:SER:HB2	2.34	0.42
39:8:250:ALA:HB1	39:8:280:LEU:HD11	2.01	0.42
44:A:414:G:H2'	44:A:414:G:N3	2.34	0.42
44:A:644:A:H1'	44:A:645:A:C6	2.55	0.42
1:a:1504:U:H2'	1:a:1505:U:O4'	2.19	0.42
1:a:1536:G:H2'	1:a:1537:A:C8	2.54	0.42
2:B:57:LYS:HD3	13:W:70:LEU:HD12	2.01	0.42
15:Y:123:VAL:HG12	15:Y:124:LYS:HG3	2.02	0.42
34:h:130:LYS:HE3	34:h:132:TRP:CZ2	2.55	0.42
41:2:695:ILE:HD11	41:2:788:LEU:HD22	2.01	0.42
43:5:32:GLY:HA3	43:5:36:VAL:HG13	2.00	0.42
1:a:1546:G:H5'	25:R:18:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:68:LYS:HB3	15:Y:91:LEU:HD22	2.02	0.42
21:G:25:THR:HG21	21:G:46:ALA:HB2	2.02	0.42
34:h:114:SER:HA	34:h:156:PHE:HD2	1.84	0.42
35:3:42:LEU:CD1	35:3:219:LEU:HD13	2.50	0.42
39:8:63:VAL:HG21	39:8:98:ARG:HB3	2.02	0.42
40:1:421:GLU:O	40:1:424:LEU:HG	2.19	0.42
41:2:424:ILE:HG22	41:2:425:LEU:HD12	2.02	0.42
43:5:350:TYR:CD2	43:5:350:TYR:C	2.97	0.42
1:a:907:G:H2'	1:a:908:A:C8	2.55	0.42
1:a:1227:G:C2	1:a:1228:A:C8	3.08	0.42
4:D:141:LEU:HD21	4:D:238:LYS:NZ	2.35	0.42
8:J:153:LYS:HA	8:J:156:ALA:HB2	2.01	0.42
23:N:85:LEU:HA	23:N:88:TRP:CE3	2.55	0.42
23:N:92:CYS:HB2	23:N:103:VAL:HA	2.01	0.42
35:3:226:PRO:HB3	35:3:264:ASN:CG	2.45	0.42
37:6:195:SER:HA	38:7:503:THR:HG22	2.02	0.42
38:7:421:LEU:HD23	38:7:421:LEU:O	2.19	0.42
43:5:44:LEU:HD23	43:5:47:LEU:HD12	2.02	0.42
1:a:1280:G:H2'	1:a:1281:G:H8	1.85	0.41
12:P:53:ILE:HG23	12:P:88:LEU:HD22	2.02	0.41
34:h:164:ILE:HD11	34:h:185:LYS:HD3	2.02	0.41
36:4:128:ARG:NE	43:5:79:THR:HG22	2.35	0.41
36:4:163:GLU:HA	36:4:164:ASP:HA	1.80	0.41
36:4:219:HIS:C	36:4:220:LEU:HD12	2.45	0.41
40:1:483:ARG:HD2	40:1:483:ARG:N	2.34	0.41
1:a:606:G:N3	1:a:606:G:H2'	2.36	0.41
35:3:107:THR:O	35:3:111:ARG:HD3	2.20	0.41
36:4:249:GLY:N	39:8:8:ASP:OD1	2.44	0.41
39:8:190:GLY:HA2	39:8:231:PHE:CG	2.55	0.41
39:8:249:LEU:HB3	39:8:254:LYS:HG3	2.03	0.41
39:8:282:PHE:HZ	39:8:340:ARG:HB2	1.84	0.41
40:1:208:ILE:HG13	40:1:211:HIS:NE2	2.35	0.41
1:a:427:U:O2	1:a:427:U:O4'	2.38	0.41
1:a:522:A:O2'	9:K:131:ARG:NH1	2.53	0.41
1:a:1613:G:OP2	24:Q:39:ALA:N	2.52	0.41
1:a:1757:G:C2	1:a:1758:G:C5	3.09	0.41
17:b:44:ILE:HD12	17:b:65:PRO:HG2	2.00	0.41
30:i:50:PHE:CE1	30:i:83:LEU:HD21	2.55	0.41
36:4:141:LEU:HB3	36:4:187:GLU:CB	2.50	0.41
38:7:266:TYR:HB2	38:7:283:LEU:HD13	2.01	0.41
39:8:234:GLY:HA2	39:8:240:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:8:297:MET:O	39:8:301:LEU:HG	2.20	0.41
40:1:250:PHE:CZ	41:2:720:VAL:HG21	2.56	0.41
42:9:231:ILE:HG22	42:9:233:ARG:HG3	2.03	0.41
1:a:441:C:OP2	8:J:2:GLY:N	2.53	0.41
1:a:534:G:C2	1:a:535:G:C8	3.08	0.41
1:a:1566:G:O2'	1:a:1567:G:N2	2.53	0.41
6:H:52:ILE:HD11	6:H:109:LEU:HD22	2.02	0.41
8:J:36:THR:HG21	8:J:179:PRO:HB2	2.03	0.41
8:J:165:GLN:NE2	8:J:195:LEU:HD11	2.36	0.41
18:c:59:CYS:SG	18:c:59:CYS:O	2.78	0.41
24:Q:53:GLN:HE21	24:Q:54:HIS:CD2	2.38	0.41
31:d:10:LYS:HD2	31:d:61:SER:OG	2.20	0.41
31:d:14:VAL:HG22	31:d:30:VAL:HG21	2.03	0.41
34:h:34:ALA:HB1	34:h:66:VAL:HG12	2.01	0.41
36:4:331:LEU:HD23	40:1:531:ALA:HB3	2.01	0.41
36:4:363:LEU:HA	38:7:533:THR:HG21	2.01	0.41
41:2:725:PRO:HG3	41:2:734:ARG:HB2	2.01	0.41
42:9:302:VAL:HG11	42:9:323:LEU:CB	2.51	0.41
43:5:64:GLN:O	43:5:120:TYR:CZ	2.73	0.41
43:5:137:GLN:HB2	43:5:149:VAL:HG21	2.02	0.41
9:K:84:ILE:HG13	9:K:86:VAL:HG23	2.02	0.41
44:A:391:A:C2	44:A:401:U:O2	2.74	0.41
1:a:892:U:H2'	1:a:893:U:H5''	2.02	0.41
1:a:1374:C:O2'	1:a:1375:G:P	2.79	0.41
2:B:173:LEU:HD12	26:S:91:LEU:CD1	2.50	0.41
14:X:28:ARG:CB	14:X:29:PRO:HD3	2.50	0.41
36:4:140:LEU:HD21	36:4:151:VAL:HG21	2.03	0.41
36:4:153:ASN:N	36:4:187:GLU:OE2	2.49	0.41
36:4:158:PRO:CG	43:5:109:HIS:HB3	2.51	0.41
36:4:196:GLY:N	36:4:222:VAL:O	2.54	0.41
38:7:341:LEU:HD12	38:7:384:GLU:C	2.46	0.41
38:7:497:MET:SD	38:7:504:SER:OG	2.76	0.41
40:1:404:CYS:HB2	40:1:459:VAL:HA	2.02	0.41
40:1:408:THR:HA	40:1:411:LEU:HB2	2.02	0.41
41:2:829:GLU:N	41:2:838:PRO:O	2.46	0.41
43:5:134:LEU:HG	43:5:169:LEU:HD11	2.02	0.41
43:5:182:PHE:CE1	43:5:317:LEU:HG	2.56	0.41
1:a:67:C:C6	6:H:162:LEU:HD12	2.55	0.41
20:E:135:GLU:HB3	20:E:187:LYS:HB3	2.03	0.41
26:S:17:ILE:HD11	26:S:54:VAL:HA	2.02	0.41
35:3:108:ARG:NH2	35:3:112:MET:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:316:GLU:HB3	35:3:333:ILE:HG23	2.02	0.41
36:4:251:MET:HG3	39:8:67:VAL:HG11	2.02	0.41
39:8:316:VAL:HG12	39:8:321:VAL:O	2.20	0.41
40:1:144:LEU:HD13	41:2:466:SER:HB2	2.03	0.41
40:1:428:VAL:HA	40:1:431:LEU:HD12	2.03	0.41
41:2:783:ILE:CD1	41:2:813:LEU:HD22	2.49	0.41
43:5:50:ILE:HG22	43:5:50:ILE:O	2.20	0.41
44:A:371:C:C4	44:A:372:U:C4	3.09	0.41
44:A:489:C:O2	44:A:489:C:O4'	2.37	0.41
1:a:943:U:O2'	12:P:135:ILE:O	2.38	0.41
1:a:1286:G:O6	23:N:36:ARG:HB3	2.20	0.41
1:a:1498:A:OP2	20:E:27:ARG:NH2	2.44	0.41
1:a:1590:C:H5'	28:U:82:ARG:HD2	2.02	0.41
2:B:30:LEU:HD13	2:B:38:ILE:HD12	2.03	0.41
3:C:181:LEU:HA	3:C:184:VAL:HG22	2.02	0.41
20:E:21:LEU:HD11	20:E:48:ILE:HD11	2.03	0.41
24:Q:34:MET:HA	24:Q:37:TYR:CE2	2.56	0.41
28:U:127:GLY:O	28:U:131:LEU:HD23	2.20	0.41
35:3:13:PHE:CE2	35:3:205:LEU:HD23	2.56	0.41
35:3:48:THR:HG21	35:3:72:GLU:HG2	2.01	0.41
35:3:401:TYR:O	35:3:405:ILE:HG13	2.21	0.41
36:4:207:HIS:CE1	36:4:219:HIS:CE1	3.09	0.41
1:a:378:U:H2'	1:a:379:C:O4'	2.21	0.41
1:a:407:G:N3	1:a:407:G:C2'	2.84	0.41
1:a:1016:U:O2	1:a:1016:U:C2'	2.68	0.41
1:a:1411:G:H2'	1:a:1412:C:O4'	2.21	0.41
4:D:236:PHE:O	4:D:237:ALA:HB3	2.21	0.41
7:I:63:PHE:HA	7:I:95:ILE:O	2.20	0.41
13:W:56:CYS:SG	13:W:57:GLY:N	2.93	0.41
34:h:197:THR:HG21	34:h:239:LEU:H	1.86	0.41
34:h:249:CYS:CB	34:h:258:ILE:HG22	2.51	0.41
35:3:50:MET:HG3	35:3:178:LEU:HD13	2.02	0.41
35:3:91:ILE:HG23	35:3:91:ILE:O	2.21	0.41
35:3:231:ASN:O	35:3:235:LEU:HD23	2.21	0.41
37:6:48:LEU:HG	38:7:292:LYS:HG3	2.02	0.41
38:7:376:THR:HA	38:7:379:PRO:HD2	2.03	0.41
39:8:29:ILE:HG13	39:8:54:LYS:HB3	2.03	0.41
40:1:469:ARG:HA	40:1:472:VAL:CG1	2.50	0.41
40:1:485:ASP:HB3	41:2:797:SER:HA	2.01	0.41
41:2:556:TYR:CE1	41:2:564:ILE:HB	2.56	0.41
42:9:175:VAL:HG13	42:9:179:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5:73:GLU:O	43:5:73:GLU:HG2	2.20	0.41
43:5:310:PRO:HB3	43:5:314:MET:CG	2.51	0.41
1:a:385:G:O2'	8:J:10:LYS:NZ	2.49	0.41
1:a:1274:G:N3	1:a:1274:G:H5'	2.35	0.41
1:a:1561:A:H2'	1:a:1562:C:O4'	2.22	0.41
1:a:1728:U:H2'	1:a:1729:U:O4'	2.21	0.41
6:H:223:LYS:HA	6:H:226:GLU:HB3	2.02	0.41
35:3:39:GLN:NE2	35:3:55:MET:HE1	2.34	0.41
35:3:269:LYS:HG3	35:3:269:LYS:O	2.20	0.41
38:7:388:LEU:HA	38:7:391:ARG:HB3	2.02	0.41
39:8:288:GLU:N	39:8:289:ASN:HA	2.36	0.41
41:2:382:LEU:HD23	41:2:397:MET:HE1	2.02	0.41
41:2:493:LYS:CG	41:2:498:GLU:OE2	2.68	0.41
43:5:67:LEU:HA	43:5:81:CYS:HB3	2.03	0.41
43:5:253:MET:SD	43:5:331:LYS:HB3	2.61	0.41
1:a:1624:U:O2	1:a:1624:U:O4'	2.38	0.40
9:K:63:LEU:HD23	9:K:63:LEU:HA	1.94	0.40
12:P:97:LEU:HD11	12:P:112:ALA:HB1	2.03	0.40
24:Q:90:VAL:HG21	24:Q:112:ILE:HD11	2.03	0.40
35:3:38:LEU:CD1	35:3:252:HIS:HE2	2.33	0.40
35:3:132:TYR:HA	35:3:159:PRO:HG3	2.03	0.40
36:4:210:TYR:O	36:4:214:ALA:N	2.48	0.40
39:8:128:ILE:HG12	39:8:168:LEU:HD21	2.03	0.40
40:1:390:LEU:HD11	40:1:410:VAL:HG13	2.01	0.40
1:a:1597:C:H4'	1:a:1603:G:O6	2.22	0.40
2:B:180:GLN:HB2	2:B:195:TRP:CE3	2.56	0.40
4:D:146:GLU:HB2	4:D:149:THR:HG22	2.01	0.40
7:I:100:ILE:HG23	7:I:100:ILE:O	2.21	0.40
7:I:134:VAL:HG12	7:I:173:PHE:CE2	2.56	0.40
21:G:72:LEU:HD22	21:G:112:LEU:HD11	2.03	0.40
23:N:68:LEU:HD21	33:g:106:TYR:CD1	2.55	0.40
34:h:254:PRO:HA	34:h:285:GLN:HA	2.01	0.40
35:3:66:ILE:HB	35:3:67:PRO:HD3	2.03	0.40
36:4:117:VAL:HG22	43:5:47:LEU:HB3	2.02	0.40
39:8:101:LEU:HD12	39:8:101:LEU:C	2.46	0.40
39:8:245:VAL:HG12	39:8:258:ASN:HD21	1.86	0.40
41:2:333:LEU:HD22	41:2:374:ILE:HG13	2.03	0.40
43:5:297:PRO:HA	43:5:298:GLU:CB	2.49	0.40
44:A:572:U:C4	44:A:573:U:C4	3.09	0.40
1:a:1036:A:N3	1:a:1844:U:O2'	2.51	0.40
1:a:1301:A:N3	1:a:1301:A:H3'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:133:LEU:HD23	7:I:133:LEU:HA	1.97	0.40
7:I:177:TYR:CD2	7:I:185:VAL:HG21	2.57	0.40
20:E:67:ARG:NE	22:L:93:THR:O	2.47	0.40
35:3:143:ASN:N	35:3:144:TYR:HB2	2.36	0.40
37:6:55:GLN:HE21	38:7:442:GLN:HG2	1.87	0.40
37:6:80:THR:HG21	38:7:326:MET:HA	2.02	0.40
37:6:148:ILE:HG22	37:6:149:THR:HG23	2.03	0.40
39:8:162:HIS:HE2	39:8:203:ASP:CG	2.30	0.40
1:a:76:U:O2	1:a:76:U:H2'	2.21	0.40
2:B:36:GLN:O	2:B:53:ARG:NH1	2.54	0.40
7:I:170:VAL:HG13	7:I:187:PHE:HB2	2.03	0.40
27:T:48:ALA:O	27:T:50:ILE:N	2.55	0.40
30:i:92:LEU:CD1	30:i:99:LEU:HB2	2.52	0.40
40:1:211:HIS:HB2	44:A:490:A:H4'	2.03	0.40
41:2:506:ARG:CG	41:2:548:MET:HE1	2.51	0.40
44:A:526:A:H2'	44:A:527:C:H5''	2.03	0.40
1:a:812:A:N3	5:F:12:VAL:HG12	2.37	0.40
1:a:1511:U:H2'	1:a:1512:C:C6	2.56	0.40
3:C:134:LEU:HD23	3:C:218:LEU:HB2	2.04	0.40
21:G:102:LEU:HD13	30:i:110:THR:HG22	2.03	0.40
23:N:38:ALA:HA	23:N:110:VAL:HB	2.02	0.40
27:T:68:ILE:HG23	27:T:72:GLN:HE22	1.87	0.40
36:4:196:GLY:HA2	36:4:197:HIS:HA	1.92	0.40
39:8:67:VAL:HA	39:8:70:LEU:HD12	2.02	0.40
39:8:144:LEU:HA	39:8:147:VAL:HB	2.03	0.40
40:1:276:TYR:HA	40:1:279:VAL:HG12	2.04	0.40
40:1:454:ARG:HG3	40:1:458:LEU:HD13	2.03	0.40
40:1:483:ARG:O	40:1:491:LEU:HG	2.22	0.40
41:2:853:GLN:HA	41:2:856:ALA:HB3	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	
2	B	215/295 (73%)	206 (96%)	8 (4%)	1 (0%)	24	52
3	C	211/264 (80%)	187 (89%)	23 (11%)	1 (0%)	24	52
4	D	219/255 (86%)	202 (92%)	16 (7%)	1 (0%)	24	52
5	F	260/263 (99%)	240 (92%)	20 (8%)	0	100	100
6	H	235/249 (94%)	219 (93%)	16 (7%)	0	100	100
7	I	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
8	J	204/208 (98%)	188 (92%)	12 (6%)	4 (2%)	6	24
9	K	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
10	M	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
11	O	147/151 (97%)	138 (94%)	9 (6%)	0	100	100
12	P	134/151 (89%)	120 (90%)	13 (10%)	1 (1%)	18	46
13	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
14	X	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	44
15	Y	139/143 (97%)	129 (93%)	6 (4%)	4 (3%)	3	18
16	Z	122/134 (91%)	114 (93%)	8 (7%)	0	100	100
17	b	99/115 (86%)	88 (89%)	7 (7%)	4 (4%)	2	14
18	c	81/84 (96%)	74 (91%)	6 (7%)	1 (1%)	10	33
19	f	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
20	E	226/281 (80%)	211 (93%)	14 (6%)	1 (0%)	30	58
21	G	189/204 (93%)	166 (88%)	18 (10%)	5 (3%)	4	20
22	L	94/149 (63%)	86 (92%)	7 (7%)	1 (1%)	11	36
23	N	115/132 (87%)	94 (82%)	19 (16%)	2 (2%)	7	27
24	Q	113/145 (78%)	95 (84%)	15 (13%)	3 (3%)	4	20
25	R	140/172 (81%)	136 (97%)	3 (2%)	1 (1%)	18	46
26	S	130/135 (96%)	110 (85%)	18 (14%)	2 (2%)	8	29
27	T	142/152 (93%)	132 (93%)	7 (5%)	3 (2%)	5	23
28	U	139/145 (96%)	130 (94%)	7 (5%)	2 (1%)	9	30
29	V	98/119 (82%)	88 (90%)	10 (10%)	0	100	100
30	i	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
31	d	60/69 (87%)	54 (90%)	6 (10%)	0	100	100
32	e	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
33	g	66/156 (42%)	52 (79%)	14 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	310/317 (98%)	278 (90%)	32 (10%)	0	100	100
35	3	417/462 (90%)	315 (76%)	86 (21%)	16 (4%)	2	14
36	4	270/364 (74%)	219 (81%)	45 (17%)	6 (2%)	5	23
37	6	213/218 (98%)	182 (85%)	31 (15%)	0	100	100
38	7	370/607 (61%)	316 (85%)	52 (14%)	2 (0%)	24	52
39	8	363/374 (97%)	283 (78%)	71 (20%)	9 (2%)	4	20
40	1	532/1362 (39%)	429 (81%)	85 (16%)	18 (3%)	3	16
41	2	543/913 (60%)	424 (78%)	104 (19%)	15 (3%)	4	19
42	9	350/558 (63%)	317 (91%)	28 (8%)	5 (1%)	9	30
43	5	322/363 (89%)	255 (79%)	53 (16%)	14 (4%)	2	13
All	All	8160/10782 (76%)	7106 (87%)	931 (11%)	123 (2%)	11	29

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Y	61	GLN
17	b	8	ASN
24	Q	18	ARG
25	R	17	LYS
26	S	99	ASP
27	T	100	ALA
28	U	29	LYS
35	3	26	LEU
35	3	50	MET
35	3	51	VAL
35	3	63	SER
35	3	238	TYR
35	3	245	ALA
35	3	325	LEU
36	4	244	PRO
36	4	338	ILE
39	8	335	SER
39	8	336	HIS
40	1	42	THR
40	1	513	SER
41	2	653	ARG
41	2	742	LYS
41	2	842	VAL

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Mol	Chain	Res	Type
42	9	376	ASN
42	9	490	ILE
43	5	73	GLU
43	5	86	GLN
43	5	351	ASN
2	B	44	ASP
3	C	190	PRO
4	D	237	ALA
14	X	28	ARG
21	G	132	GLY
21	G	134	VAL
24	Q	70	MET
27	T	49	ASP
35	3	28	VAL
35	3	46	SER
35	3	93	LYS
35	3	322	ASP
38	7	423	PRO
39	8	116	ASN
40	1	79	GLN
40	1	122	GLN
41	2	326	HIS
41	2	489	TYR
42	9	203	ASP
42	9	377	ASN
43	5	53	TYR
43	5	76	LEU
43	5	87	HIS
8	J	123	ARG
8	J	142	SER
15	Y	86	PRO
17	b	46	GLU
18	c	50	ALA
21	G	43	GLU
26	S	92	ASP
35	3	62	TYR
36	4	198	ASP
36	4	262	TYR
39	8	113	MET
40	1	167	ASN
40	1	168	SER
40	1	484	ILE

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Mol	Chain	Res	Type
40	1	515	PRO
41	2	435	ASP
41	2	578	LEU
41	2	743	ALA
42	9	289	PHE
43	5	35	ALA
43	5	56	GLU
43	5	114	HIS
43	5	116	HIS
43	5	223	ALA
8	J	86	SER
20	E	43	PRO
35	3	47	ASP
35	3	68	HIS
39	8	58	LYS
39	8	232	LEU
40	1	43	TRP
40	1	344	MET
40	1	421	GLU
8	J	94	LYS
15	Y	60	LYS
17	b	63	VAL
22	L	95	ARG
23	N	101	ARG
35	3	154	PHE
36	4	169	ASP
36	4	196	GLY
40	1	214	GLN
40	1	368	ILE
40	1	506	PRO
41	2	727	LEU
43	5	70	LEU
24	Q	118	GLU
28	U	86	GLY
39	8	115	LYS
39	8	130	VAL
39	8	173	VAL
40	1	418	PRO
41	2	346	ASP
41	2	764	LYS
43	5	319	ILE
23	N	100	PRO

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Mol	Chain	Res	Type
40	1	267	PRO
41	2	369	GLY
41	2	598	ILE
43	5	84	PHE
15	Y	62	PRO
21	G	21	GLY
27	T	74	PRO
35	3	57	VAL
38	7	291	ILE
40	1	7	ARG
41	2	765	VAL
12	P	127	GLY
17	b	56	VAL
21	G	128	ILE
40	1	422	PRO
41	2	526	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	
2	B	180/246 (73%)	178 (99%)	2 (1%)	65	73
3	C	194/231 (84%)	194 (100%)	0	100	100
4	D	186/205 (91%)	182 (98%)	4 (2%)	45	63
5	F	223/224 (100%)	221 (99%)	2 (1%)	70	75
6	H	180/218 (83%)	177 (98%)	3 (2%)	53	67
7	I	165/174 (95%)	161 (98%)	4 (2%)	43	62
8	J	178/180 (99%)	177 (99%)	1 (1%)	78	79
9	K	161/168 (96%)	159 (99%)	2 (1%)	63	72
10	M	111/142 (78%)	110 (99%)	1 (1%)	70	75
11	O	130/131 (99%)	130 (100%)	0	100	100
12	P	106/119 (89%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	W	68/68 (100%)	68 (100%)	0	100	100
14	X	112/113 (99%)	109 (97%)	3 (3%)	39	60
15	Y	113/114 (99%)	112 (99%)	1 (1%)	70	75
16	Z	107/115 (93%)	106 (99%)	1 (1%)	70	75
17	b	89/99 (90%)	88 (99%)	1 (1%)	65	73
18	c	75/76 (99%)	75 (100%)	0	100	100
19	f	47/106 (44%)	47 (100%)	0	100	100
20	E	190/232 (82%)	185 (97%)	5 (3%)	40	61
21	G	158/170 (93%)	158 (100%)	0	100	100
22	L	87/125 (70%)	86 (99%)	1 (1%)	65	73
23	N	99/108 (92%)	99 (100%)	0	100	100
24	Q	105/130 (81%)	101 (96%)	4 (4%)	29	55
25	R	117/140 (84%)	117 (100%)	0	100	100
26	S	119/121 (98%)	117 (98%)	2 (2%)	53	67
27	T	125/132 (95%)	124 (99%)	1 (1%)	73	76
28	U	111/116 (96%)	111 (100%)	0	100	100
29	V	92/107 (86%)	92 (100%)	0	100	100
30	i	66/103 (64%)	65 (98%)	1 (2%)	57	68
31	d	55/62 (89%)	54 (98%)	1 (2%)	51	66
32	e	48/49 (98%)	47 (98%)	1 (2%)	47	64
33	g	61/140 (44%)	60 (98%)	1 (2%)	55	67
34	h	271/275 (98%)	267 (98%)	4 (2%)	57	68
35	3	384/423 (91%)	369 (96%)	15 (4%)	28	54
36	4	239/282 (85%)	232 (97%)	7 (3%)	37	60
37	6	190/193 (98%)	190 (100%)	0	100	100
38	7	342/544 (63%)	339 (99%)	3 (1%)	70	75
39	8	327/335 (98%)	320 (98%)	7 (2%)	47	64
40	1	490/1245 (39%)	479 (98%)	11 (2%)	45	63
41	2	494/812 (61%)	487 (99%)	7 (1%)	59	69
42	9	320/496 (64%)	315 (98%)	5 (2%)	55	67
43	5	293/320 (92%)	290 (99%)	3 (1%)	68	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7208/9389 (77%)	7104 (99%)	104 (1%)	57 69

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	128	GLN
2	B	180	GLN
4	D	102	LEU
4	D	141	LEU
4	D	213	LEU
4	D	248	TYR
5	F	49	ARG
5	F	220	THR
6	H	52	ILE
6	H	127	THR
6	H	202	ASN
7	I	50	GLU
7	I	122	LEU
7	I	148	LEU
7	I	166	VAL
8	J	153	LYS
9	K	131	ARG
9	K	144	ILE
10	M	134	LEU
14	X	6	VAL
14	X	103	VAL
14	X	104	LEU
15	Y	112	VAL
16	Z	117	VAL
17	b	15	ARG
20	E	26	THR
20	E	42	THR
20	E	59	LEU
20	E	66	ILE
20	E	137	VAL
22	L	83	LEU
24	Q	25	LEU
24	Q	37	TYR
24	Q	57	LEU
24	Q	80	LEU
26	S	78	ARG
26	S	114	LEU

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Mol	Chain	Res	Type
27	T	44	VAL
30	i	109	TYR
31	d	36	ASP
32	e	25	SER
33	g	103	LEU
34	h	7	LEU
34	h	116	ASP
34	h	176	VAL
34	h	309	VAL
35	3	10	ILE
35	3	31	ILE
35	3	212	THR
35	3	214	LEU
35	3	222	PHE
35	3	226	PRO
35	3	232	ILE
35	3	233	ILE
35	3	239	GLN
35	3	243	LEU
35	3	267	VAL
35	3	326	VAL
35	3	360	LEU
35	3	362	MET
35	3	374	LEU
36	4	111	VAL
36	4	143	THR
36	4	211	SER
36	4	219	HIS
36	4	237	VAL
36	4	244	PRO
36	4	339	VAL
38	7	291	ILE
38	7	421	LEU
38	7	488	ILE
39	8	65	ASN
39	8	83	ILE
39	8	188	LEU
39	8	291	GLU
39	8	292	ILE
39	8	303	ILE
39	8	338	THR
40	1	34	VAL

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Mol	Chain	Res	Type
40	1	42	THR
40	1	113	LEU
40	1	145	LEU
40	1	167	ASN
40	1	212	HIS
40	1	237	LEU
40	1	303	SER
40	1	324	LEU
40	1	424	LEU
40	1	520	ARG
41	2	430	ASN
41	2	432	GLN
41	2	532	SER
41	2	578	LEU
41	2	695	ILE
41	2	736	HIS
41	2	797	SER
42	9	317	LEU
42	9	375	LEU
42	9	413	LEU
42	9	423	LEU
42	9	496	ASN
43	5	76	LEU
43	5	231	LEU
43	5	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	141	ASN
3	C	157	GLN
3	C	179	ASN
3	C	186	ASN
3	C	202	GLN
5	F	50	ASN
5	F	112	HIS
5	F	161	GLN
5	F	232	ASN
6	H	202	ASN
7	I	44	ASN
7	I	168	HIS

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Mol	Chain	Res	Type
8	J	52	ASN
8	J	84	ASN
8	J	155	ASN
8	J	165	GLN
9	K	143	ASN
9	K	177	ASN
10	M	18	GLN
10	M	100	ASN
10	M	121	GLN
10	M	141	ASN
11	O	69	ASN
11	O	90	HIS
14	X	16	ASN
14	X	24	GLN
14	X	92	ASN
15	Y	127	ASN
16	Z	89	HIS
16	Z	106	GLN
16	Z	124	ASN
17	b	43	ASN
19	f	88	GLN
20	E	56	GLN
20	E	57	ASN
20	E	74	GLN
21	G	79	HIS
21	G	83	ASN
21	G	101	HIS
21	G	110	GLN
21	G	118	ASN
22	L	7	ASN
22	L	32	HIS
24	Q	41	GLN
24	Q	53	GLN
24	Q	79	HIS
25	R	48	GLN
26	S	48	ASN
27	T	76	GLN
27	T	101	ASN
28	U	85	ASN
29	V	47	ASN
30	i	64	ASN
31	d	26	GLN

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Mol	Chain	Res	Type
31	d	45	ASN
33	g	111	ASN
34	h	76	GLN
34	h	119	GLN
34	h	133	ASN
34	h	196	ASN
35	3	12	HIS
35	3	60	ASN
35	3	138	GLN
35	3	216	HIS
35	3	239	GLN
35	3	244	ASN
35	3	282	GLN
35	3	283	GLN
35	3	416	GLN
36	4	186	ASN
36	4	197	HIS
36	4	207	HIS
36	4	216	ASN
36	4	280	ASN
36	4	290	GLN
36	4	352	ASN
37	6	55	GLN
37	6	57	ASN
37	6	68	GLN
37	6	76	ASN
38	7	199	GLN
38	7	363	GLN
38	7	442	GLN
38	7	454	GLN
38	7	499	ASN
39	8	33	ASN
39	8	116	ASN
39	8	138	GLN
39	8	146	GLN
39	8	199	GLN
39	8	258	ASN
39	8	299	GLN
39	8	329	GLN
39	8	359	GLN
40	1	47	HIS
40	1	79	GLN

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Mol	Chain	Res	Type
40	1	80	GLN
40	1	159	GLN
40	1	187	GLN
40	1	226	GLN
40	1	309	ASN
40	1	381	GLN
40	1	448	GLN
40	1	481	GLN
41	2	377	ASN
41	2	399	GLN
41	2	430	ASN
41	2	467	GLN
41	2	522	GLN
41	2	579	HIS
41	2	648	GLN
41	2	678	ASN
41	2	715	HIS
41	2	717	GLN
41	2	837	GLN
41	2	852	GLN
42	9	236	HIS
42	9	322	ASN
42	9	333	ASN
42	9	496	ASN
42	9	511	GLN
43	5	58	GLN
43	5	100	GLN
43	5	111	ASN
43	5	137	GLN
43	5	141	GLN
43	5	237	ASN
43	5	255	GLN
43	5	271	GLN
43	5	282	GLN
43	5	283	GLN
43	5	322	GLN
43	5	336	GLN
43	5	345	GLN
43	5	348	GLN
43	5	351	ASN
43	5	352	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1684/1697 (99%)	405 (24%)	0
44	A	338/377 (89%)	176 (52%)	23 (6%)
All	All	2022/2074 (97%)	581 (28%)	23 (1%)

All (581) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A
1	a	3	C
1	a	11	A
1	a	15	U
1	a	17	C
1	a	26	U
1	a	33	G
1	a	41	G
1	a	46	A
1	a	58	C
1	a	61	A
1	a	62	G
1	a	64	A
1	a	67	C
1	a	68	A
1	a	70	G
1	a	73	C
1	a	74	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	126	G
1	a	127	C
1	a	129	C
1	a	130	G
1	a	143	U
1	a	147	A
1	a	155	G
1	a	159	A
1	a	161	U

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Mol	Chain	Res	Type
1	a	162	C
1	a	163	U
1	a	167	G
1	a	178	C
1	a	180	G
1	a	183	G
1	a	184	G
1	a	191	A
1	a	192	C
1	a	204	G
1	a	205	G
1	a	206	G
1	a	215	G
1	a	292	A
1	a	305	U
1	a	307	G
1	a	308	G
1	a	309	G
1	a	313	A
1	a	314	U
1	a	318	A
1	a	319	C
1	a	323	C
1	a	331	C
1	a	332	G
1	a	347	G
1	a	362	C
1	a	363	A
1	a	364	A
1	a	368	U
1	a	369	C
1	a	370	G
1	a	382	C
1	a	384	U
1	a	385	G
1	a	386	C
1	a	400	C
1	a	408	A
1	a	409	C
1	a	417	C
1	a	418	A
1	a	421	G

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Mol	Chain	Res	Type
1	a	429	C
1	a	441	C
1	a	447	A
1	a	448	A
1	a	449	A
1	a	450	C
1	a	452	G
1	a	455	A
1	a	463	C
1	a	464	A
1	a	465	A
1	a	466	G
1	a	470	G
1	a	471	G
1	a	472	C
1	a	473	A
1	a	474	G
1	a	476	A
1	a	479	C
1	a	482	G
1	a	487	U
1	a	492	C
1	a	493	A
1	a	509	G
1	a	516	A
1	a	517	C
1	a	518	G
1	a	525	A
1	a	528	A
1	a	530	U
1	a	531	A
1	a	532	C
1	a	533	A
1	a	536	A
1	a	538	U
1	a	542	U
1	a	543	C
1	a	544	G
1	a	547	G
1	a	548	C
1	a	550	C
1	a	551	U

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Mol	Chain	Res	Type
1	a	553	U
1	a	554	A
1	a	555	A
1	a	556	U
1	a	559	G
1	a	561	A
1	a	562	U
1	a	567	C
1	a	568	C
1	a	570	C
1	a	576	A
1	a	583	A
1	a	588	G
1	a	589	G
1	a	590	A
1	a	591	U
1	a	592	C
1	a	593	C
1	a	594	A
1	a	598	G
1	a	606	G
1	a	607	U
1	a	608	C
1	a	614	C
1	a	615	C
1	a	617	G
1	a	621	C
1	a	627	U
1	a	628	A
1	a	629	A
1	a	630	U
1	a	643	A
1	a	644	G
1	a	647	U
1	a	654	A
1	a	655	A
1	a	659	G
1	a	660	C
1	a	664	A
1	a	668	A
1	a	669	A
1	a	671	A

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Mol	Chain	Res	Type
1	a	672	A
1	a	684	G
1	a	689	U
1	a	690	G
1	a	734	C
1	a	743	U
1	a	750	C
1	a	752	G
1	a	753	C
1	a	754	G
1	a	794	A
1	a	797	C
1	a	798	G
1	a	799	U
1	a	801	U
1	a	810	A
1	a	811	A
1	a	821	G
1	a	822	U
1	a	830	A
1	a	834	C
1	a	844	U
1	a	847	A
1	a	867	G
1	a	868	G
1	a	869	A
1	a	870	A
1	a	871	U
1	a	872	A
1	a	873	G
1	a	878	G
1	a	881	G
1	a	885	U
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	909	G

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Mol	Chain	Res	Type
1	a	910	G
1	a	913	A
1	a	914	U
1	a	920	A
1	a	930	C
1	a	933	G
1	a	943	U
1	a	956	G
1	a	970	G
1	a	971	G
1	a	972	A
1	a	985	G
1	a	989	C
1	a	990	A
1	a	992	A
1	a	999	G
1	a	1017	U
1	a	1023	A
1	a	1045	U
1	a	1051	G
1	a	1052	A
1	a	1053	C
1	a	1060	A
1	a	1061	U
1	a	1062	A
1	a	1070	A
1	a	1081	U
1	a	1083	A
1	a	1085	C
1	a	1087	A
1	a	1115	U
1	a	1116	C
1	a	1117	C
1	a	1121	G
1	a	1126	G
1	a	1133	A
1	a	1138	C
1	a	1143	A
1	a	1144	A
1	a	1148	A
1	a	1149	A
1	a	1153	C

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Mol	Chain	Res	Type
1	a	1154	U
1	a	1165	G
1	a	1166	G
1	a	1170	A
1	a	1181	A
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	1224	G
1	a	1231	C
1	a	1242	U
1	a	1244	U
1	a	1251	A
1	a	1253	A
1	a	1256	G
1	a	1257	G
1	a	1259	A
1	a	1263	U
1	a	1265	A
1	a	1266	C
1	a	1269	G
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	1287	A
1	a	1288	U
1	a	1291	A
1	a	1292	C
1	a	1295	A
1	a	1298	G
1	a	1299	A
1	a	1301	A
1	a	1302	G
1	a	1303	C
1	a	1306	U
1	a	1308	U

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Mol	Chain	Res	Type
1	a	1309	C
1	a	1310	U
1	a	1311	C
1	a	1312	G
1	a	1313	A
1	a	1314	U
1	a	1318	G
1	a	1320	G
1	a	1341	C
1	a	1342	U
1	a	1348	G
1	a	1350	U
1	a	1355	C
1	a	1364	U
1	a	1371	U
1	a	1372	U
1	a	1373	C
1	a	1374	C
1	a	1375	G
1	a	1378	A
1	a	1382	A
1	a	1396	A
1	a	1397	U
1	a	1402	A
1	a	1404	U
1	a	1406	G
1	a	1409	A
1	a	1424	G
1	a	1428	G
1	a	1429	G
1	a	1453	C
1	a	1454	A
1	a	1462	U
1	a	1463	U
1	a	1464	C
1	a	1466	G
1	a	1476	A
1	a	1480	A
1	a	1487	A
1	a	1489	A
1	a	1490	G
1	a	1494	U

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Mol	Chain	Res	Type
1	a	1498	A
1	a	1499	U
1	a	1507	G
1	a	1519	U
1	a	1520	G
1	a	1521	C
1	a	1522	A
1	a	1523	C
1	a	1533	A
1	a	1535	U
1	a	1536	G
1	a	1544	C
1	a	1548	G
1	a	1552	G
1	a	1553	C
1	a	1554	C
1	a	1556	A
1	a	1557	C
1	a	1564	C
1	a	1567	G
1	a	1573	G
1	a	1574	C
1	a	1575	G
1	a	1578	U
1	a	1580	A
1	a	1585	U
1	a	1588	A
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	1638	G
1	a	1639	G
1	a	1648	G
1	a	1654	G
1	a	1661	A
1	a	1664	A
1	a	1665	G

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Mol	Chain	Res	Type
1	a	1671	G
1	a	1695	A
1	a	1698	C
1	a	1699	A
1	a	1713	C
1	a	1721	U
1	a	1722	G
1	a	1724	A
1	a	1726	G
1	a	1748	G
1	a	1753	C
1	a	1757	G
1	a	1758	G
1	a	1774	C
1	a	1775	U
1	a	1777	G
1	a	1783	C
1	a	1784	G
1	a	1805	G
1	a	1815	A
1	a	1823	A
1	a	1824	A
1	a	1825	A
1	a	1831	A
1	a	1836	G
1	a	1837	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
44	A	359	C
44	A	360	G
44	A	361	A
44	A	362	U
44	A	363	A
44	A	364	C
44	A	366	A

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Mol	Chain	Res	Type
44	A	367	A
44	A	369	A
44	A	370	G
44	A	376	G
44	A	380	G
44	A	381	A
44	A	387	U
44	A	388	A
44	A	390	G
44	A	391	A
44	A	392	C
44	A	393	U
44	A	395	G
44	A	396	C
44	A	397	G
44	A	400	G
44	A	403	G
44	A	404	G
44	A	406	C
44	A	407	A
44	A	408	G
44	A	409	C
44	A	410	A
44	A	411	C
44	A	414	G
44	A	418	G
44	A	419	U
44	A	420	C
44	A	422	U
44	A	423	G
44	A	424	U
44	A	425	A
44	A	426	U
44	A	427	U
44	A	428	A
44	A	429	U
44	A	430	G
44	A	431	G
44	A	434	U
44	A	435	U
44	A	436	U
44	A	438	C

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Mol	Chain	Res	Type
44	A	440	A
44	A	443	A
44	A	446	U
44	A	452	U
44	A	453	G
44	A	457	U
44	A	458	A
44	A	459	G
44	A	460	U
44	A	462	U
44	A	463	U
44	A	465	A
44	A	466	A
44	A	467	C
44	A	468	U
44	A	472	G
44	A	473	U
44	A	477	G
44	A	478	A
44	A	480	U
44	A	482	U
44	A	483	A
44	A	484	C
44	A	485	U
44	A	486	U
44	A	487	G
44	A	488	G
44	A	489	C
44	A	490	A
44	A	491	U
44	A	492	G
44	A	493	U
44	A	494	A
44	A	496	A
44	A	497	C
44	A	498	C
44	A	499	U
44	A	500	G
44	A	504	A
44	A	505	G
44	A	506	U
44	A	507	U

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Mol	Chain	Res	Type
44	A	508	A
44	A	509	G
44	A	510	C
44	A	513	U
44	A	515	G
44	A	516	U
44	A	518	G
44	A	519	A
44	A	521	A
44	A	527	C
44	A	530	C
44	A	532	G
44	A	534	U
44	A	537	G
44	A	538	G
44	A	539	U
44	A	540	A
44	A	541	C
44	A	542	A
44	A	543	G
44	A	544	U
44	A	545	A
44	A	546	G
44	A	547	G
44	A	550	A
44	A	552	A
44	A	553	C
44	A	554	C
44	A	556	C
44	A	557	A
44	A	559	A
44	A	560	U
44	A	561	A
44	A	565	G
44	A	569	U
44	A	572	U
44	A	575	U
44	A	576	U
44	A	577	A
44	A	578	G
44	A	579	A
44	A	581	A

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Mol	Chain	Res	Type
44	A	583	G
44	A	584	A
44	A	585	A
44	A	588	U
44	A	590	A
44	A	591	G
44	A	593	G
44	A	605	G
44	A	608	U
44	A	611	U
44	A	615	A
44	A	619	G
44	A	620	A
44	A	621	G
44	A	625	G
44	A	626	U
44	A	627	G
44	A	628	A
44	A	637	G
44	A	638	C
44	A	640	C
44	A	641	C
44	A	642	U
44	A	643	G
44	A	644	A
44	A	645	A
44	A	646	G
44	A	647	C
44	A	648	A
44	A	649	A
44	A	656	G
44	A	657	U
44	A	658	C
44	A	659	U
44	A	660	U
44	A	662	C
44	A	678	A
44	A	679	U
44	A	680	A
44	A	681	A
44	A	685	G
44	A	686	U

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Mol	Chain	Res	Type
44	A	691	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	A	369	A
44	A	387	U
44	A	409	C
44	A	419	U
44	A	425	A
44	A	428	A
44	A	456	C
44	A	465	A
44	A	485	U
44	A	508	A
44	A	518	G
44	A	526	A
44	A	559	A
44	A	561	A
44	A	578	G
44	A	619	G
44	A	626	U
44	A	642	U
44	A	644	A
44	A	655	G
44	A	656	G
44	A	657	U
44	A	679	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	a	15

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	834:C	O3'	841:G	P	19.31
1	a	697:G	O3'	729:C	P	19.00
1	a	756:C	O3'	788:G	P	16.00
1	a	323:C	O3'	329:G	P	15.98
1	a	130:G	O3'	141:A	P	15.87
1	a	1761:U	O3'	1771:G	P	15.37
1	a	1417:C	O3'	1423:C	P	15.01
1	a	225:G	O3'	287:U	P	7.13
1	a	745:C	O3'	749:U	P	6.54
1	a	1432:U	O3'	1438:A	P	4.95
1	a	886:A	O3'	887:U	P	4.63
1	a	903:A	O3'	904:A	P	4.52
1	a	798:G	O3'	799:U	P	3.46
1	a	902:G	O3'	903:A	P	3.40
1	a	736:C	O3'	743:U	P	3.18

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21530. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.