



Full wwPDB EM Model Validation Report ⓘ

Apr 13, 2020 – 04:31 PM EDT

PDB ID : 6TB3
EMDB ID : EMD-10431
Title : yeast 80S ribosome in complex with the Not5 subunit of the CCR4-NOT complex
Authors : Buschauer, R.; Cheng, J.; Berninghausen, O.; Tesina, P.; Becker, T.; Beckmann, R.
Deposited on : 2019-10-31
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

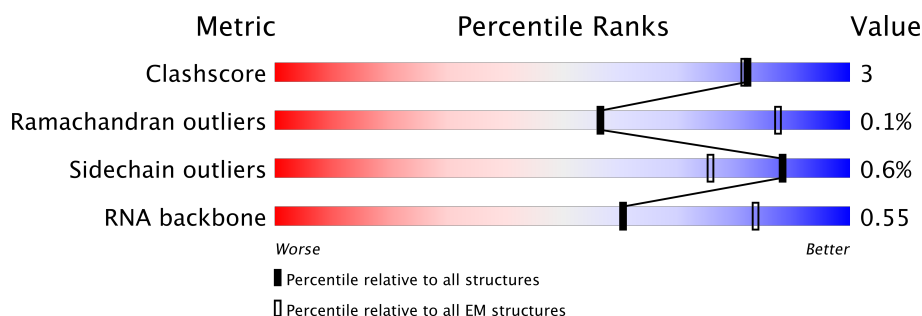
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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








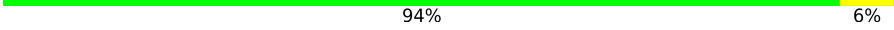

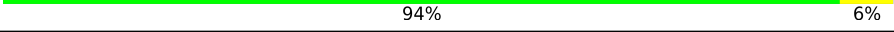



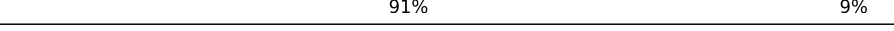
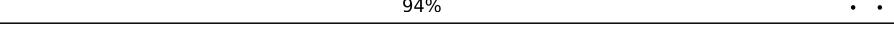


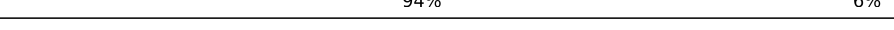

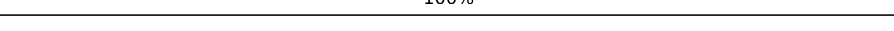
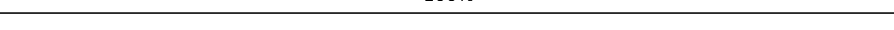
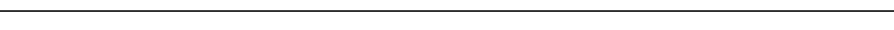

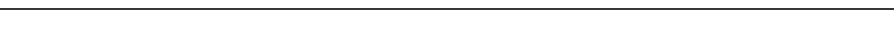
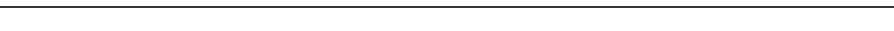


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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

Mol	Chain	Length	Quality of chain
1	2	1798	64% 28% 6% .
2	1	3	100%
3	P	206	89% 11%
4	Q	232	88% 9% .
5	E	117	85% 15%
6	R	216	93% 7%
7	A	222	95% 5%

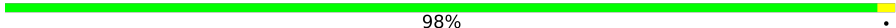



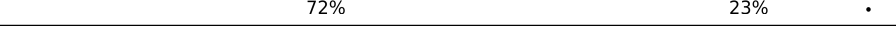
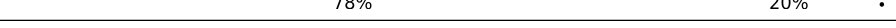

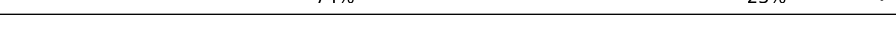
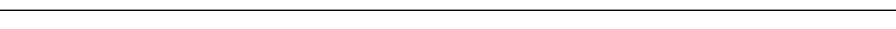
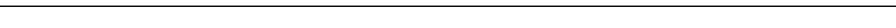









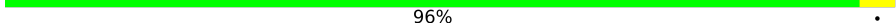
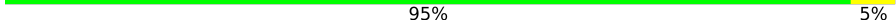
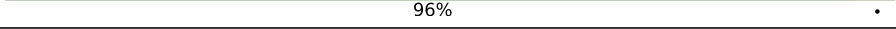



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Mol	Chain	Length	Quality of chain
8	S	258	 91% 9%
9	B	206	 90% 10%
10	T	228	 90% 10%
11	U	184	 88% 13%
12	V	187	 88% 12%
13	W	184	 94% 6%
14	C	92	 87% 13%
15	X	142	 94% 6%
16	D	121	 80% 18% .
17	Y	150	 91% 9%
18	Z	127	 89% 11%
19	F	141	 91% 9%
20	G	125	 94% . .
21	H	145	 90% 10%
22	I	143	 83% 17%
23	J	100	 94% 6%
24	n	75	 77% 23%
25	a	87	 100%
26	b	129	 100%
27	c	144	 99% .
28	d	134	 100%
29	K	82	 95% . .
30	e	97	 100%
31	f	81	 99% .
32	M	53	 89% 11%



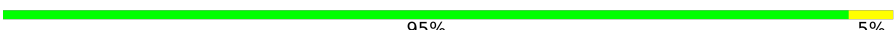

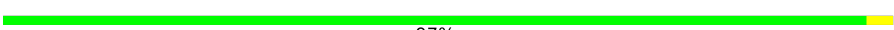





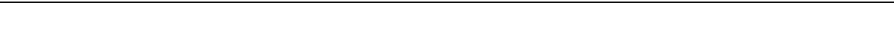

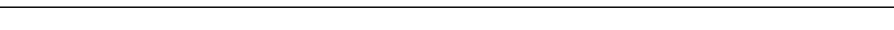
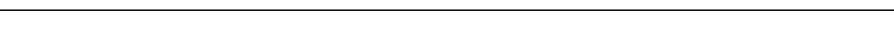


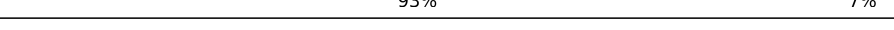
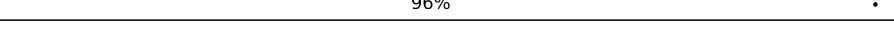







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Mol	Chain	Length	Quality of chain
33	g	60	 98% .
34	N	73	 84% 15% .
35	O	312	 89% 11%
36	L	63	 81% 19%
37	BQ	3223	 72% 23% .
38	BT	204	 78% 20% .
39	BR	121	 83% 14% .
40	BS	158	 74% 23% .
41	AW	251	 92% 8%
42	BA	386	 93% 7%
43	BE	361	 93% 6%
44	BI	294	 93% 7%
45	BM	175	 87% 7% 5%
46	BO	222	 94% 6%
47	AA	233	 93% 7%
48	AD	191	 90% 10%
49	BD	218	 91% 8%
50	AG	169	 92% 8%
51	AJ	193	 92% 8%
52	AM	136	 85% 15%
53	AQ	203	 96% .
54	AU	197	 95% 5%
55	AX	183	 96% .
56	BB	185	 91% 9%
57	BF	188	 88% 11% .


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Mol	Chain	Length	Quality of chain
58	BH	171	 89% 11%
59	BJ	159	 92% 8%
60	BL	100	 95% 5%
61	AB	136	 92% 8%
62	AE	126	 97% .
63	AH	121	 95% 5%
64	AK	125	 96% . .
65	AN	135	 93% 7%
66	AR	148	 90% 10%
67	AV	58	 91% 7% .
68	AY	96	 91% 9%
69	BC	109	 89% 11%
70	BG	127	 92% 8%
71	BK	106	 90% 10%
72	BN	112	 90% 9% .
73	BP	119	 93% 7%
74	AC	99	 96% .
75	AF	81	 89% 11%
76	AI	77	 88% 12%
77	AL	50	 86% 14%
78	AO	52	 90% 10%
79	AS	25	 92% 8%
80	AP	103	 93% 7%
81	AT	91	 92% 8%
82	BV	22	 73% 27%

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Mol	Chain	Length	Quality of chain
83	BW	112	 86% 13% •

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 205032 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 *Saccharomyces cerevisiae* S288C 18S ribosomal RNA (RDN18-1), rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	184	Total	C	N	O	S	0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	75	Total	C	N	O	P	0	0
			1624	728	298	523	75		

- Molecule 25 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 26 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 27 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 29 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 30 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 31 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 32 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 33 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 35 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 36 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 37 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BQ	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 38 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BT	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AW	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 42 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 43 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BI	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 45 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	BM	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 46 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BO	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 47 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AA	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 48 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 49 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BD	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 50 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AG	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 51 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AJ	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 52 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 53 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 54 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AU	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 55 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	AX	183	Total	C	N	O	0	0
			1416	879	284	253		

- Molecule 56 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BB	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 57 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BF	188	Total	C	N	O	0	0
			1515	932	323	260		

- Molecule 58 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BH	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 59 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BJ	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 60 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	BL	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 61 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AB	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 62 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	126	Total	C	N	O	S	0	0
			836	525	165	145	1		

- Molecule 63 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 64 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AK	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 65 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AN	135	Total	C	N	O		0	0
			1080	701	199	180			

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AR	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 67 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AV	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 68 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 69 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BG	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 71 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 72 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	BN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 73 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BP	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 74 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AC	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 75 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AF	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 76 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	AI	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 77 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AL	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 78 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AO	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 79 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AS	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 80 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AP	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 81 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 82 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	BV	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 83 is a protein called General negative regulator of transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BW	112	Total	C	N	O	S	0	0
			940	585	170	182	3		

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	BO	1	Total	Mg	0
			1	1	
84	AQ	1	Total	Mg	0
			1	1	
84	BA	3	Total	Mg	0
			3	3	
84	BN	1	Total	Mg	0
			1	1	
84	AW	2	Total	Mg	0
			2	2	
84	B	1	Total	Mg	0
			1	1	
84	BF	1	Total	Mg	0
			1	1	
84	BG	1	Total	Mg	0
			1	1	
84	BR	1	Total	Mg	0
			1	1	
84	BQ	220	Total	Mg	0
			220	220	
84	n	3	Total	Mg	0
			3	3	
84	AX	1	Total	Mg	0
			1	1	
84	2	89	Total	Mg	0
			89	89	
84	S	1	Total	Mg	0
			1	1	
84	AB	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

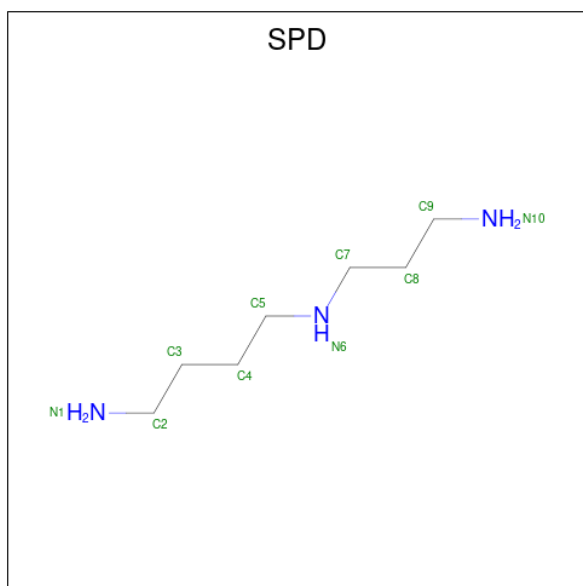
Mol	Chain	Residues	Atoms		AltConf
85	AP	1	Total	Zn	0
			1	1	
85	BN	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
85	AT	1	Total	Zn	0
			1	1	
85	N	1	Total	Zn	0
			1	1	
85	AO	1	Total	Zn	0
			1	1	
85	AF	1	Total	Zn	0
			1	1	
85	M	1	Total	Zn	0
			1	1	

- Molecule 86 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

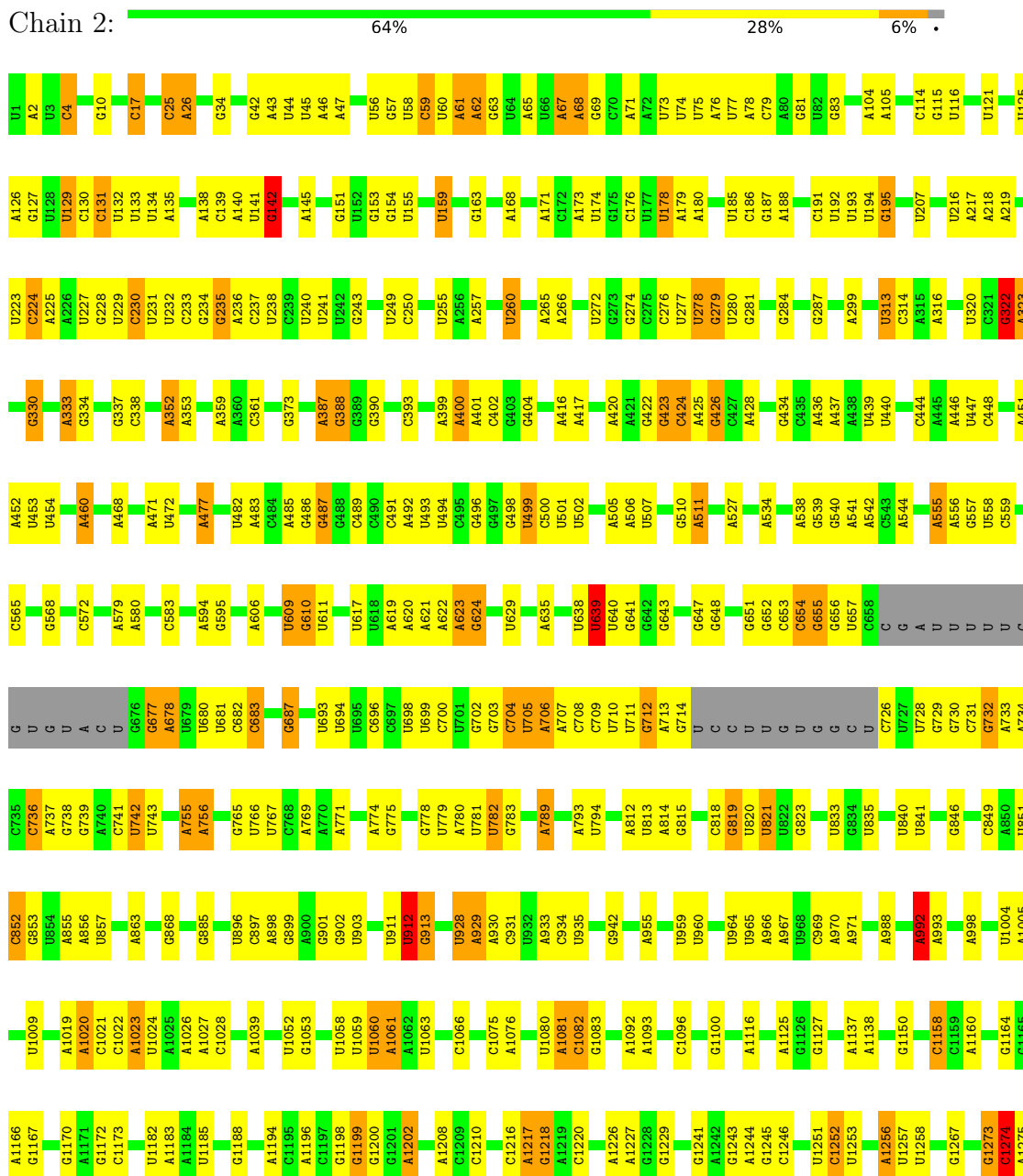


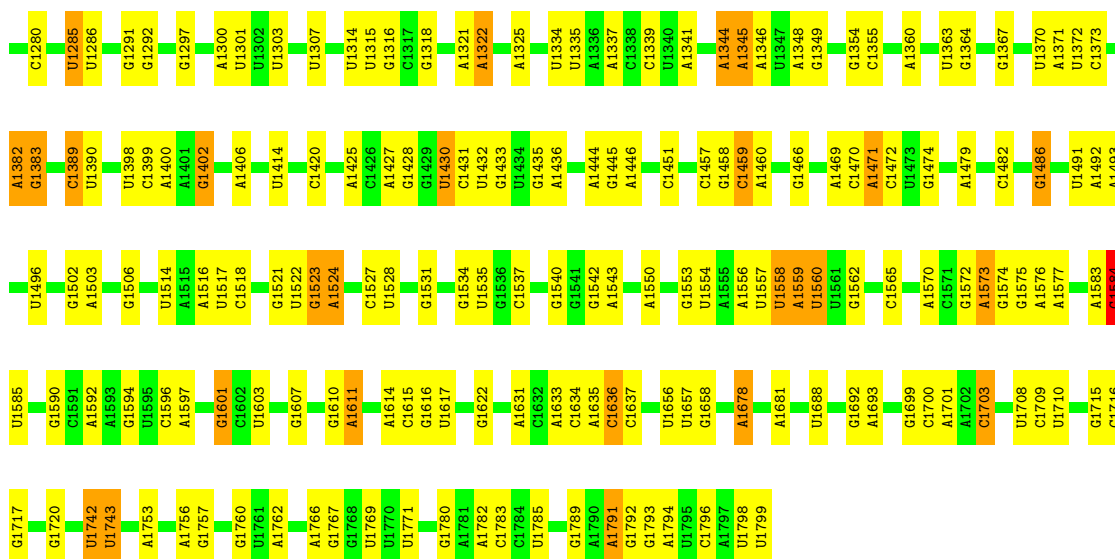
Mol	Chain	Residues	Atoms			AltConf
86	BQ	1	Total	C	N	0
			10	7	3	

3 Residue-property plots

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

- Molecule 1: *Saccharomyces cerevisiae* S288C 18S ribosomal RNA (RDN18-1), rRNA





- Molecule 2: mRNA

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: 40S ribosomal protein S0-A

Chain P: 89% 11%



- Molecule 4: 40S ribosomal protein S1-A

Chain Q: 88% 9%



- Molecule 5: 40S ribosomal protein S15

Chain E: 85% 15%



- Molecule 6: 40S ribosomal protein S2

Chain R: 93% 7%



- Molecule 7: 40S ribosomal protein S3

Chain A:  95% 5%




- Molecule 8: 40S ribosomal protein S4-A

Chain S:  91% 9%



- Molecule 9: 40S ribosomal protein S5

Chain B:  90% 10%




- Molecule 10: 40S ribosomal protein S6-A

Chain T:  90% 10%




- Molecule 11: 40S ribosomal protein S7-A

Chain U:  88% 13%



- Molecule 12: 40S ribosomal protein S8

Chain V:  88% 12%




- Molecule 13: 40S ribosomal protein S9-A

Chain W:  94% 6%



- Molecule 14: 40S ribosomal protein S10-A

Chain C:  87% 13%




- Molecule 15: 40S ribosomal protein S11-A

Chain X:  94% 6%



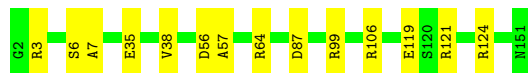
- Molecule 16: 40S ribosomal protein S12

Chain D:  80% 18%




- Molecule 17: 40S ribosomal protein S13

Chain Y:  91% 9%



- Molecule 18: 40S ribosomal protein S14-B

Chain Z:  89% 11%



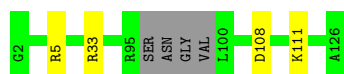
- Molecule 19: 40S ribosomal protein S16-A

Chain F:  91% 9%




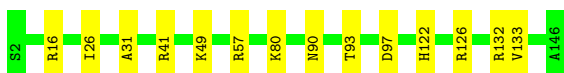
- Molecule 20: 40S ribosomal protein S17-B

Chain G:  94%




- Molecule 21: 40S ribosomal protein S18-A

Chain H:  90% 10%



- Molecule 22: 40S ribosomal protein S19-A

Chain I:  83% 17%




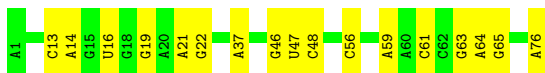
- Molecule 23: 40S ribosomal protein S20

Chain J:  94% 6%



- Molecule 24: tRNA

Chain n:  77% 23%



- Molecule 25: 40S ribosomal protein S21-A

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 40S ribosomal protein S22-A

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 40S ribosomal protein S23-A

Chain c:  99%



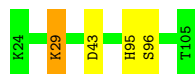
- Molecule 28: 40S ribosomal protein S24-A

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 40S ribosomal protein S25-A

Chain K:  95% ..



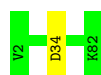
- Molecule 30: 40S ribosomal protein S26-B

Chain e:  100%


There are no outlier residues recorded for this chain.

- Molecule 31: 40S ribosomal protein S27-A

Chain f:  99% .



- Molecule 32: 40S ribosomal protein S29-A

Chain M:  89% 11%




- Molecule 33: 40S ribosomal protein S30-A

Chain g:  98% .




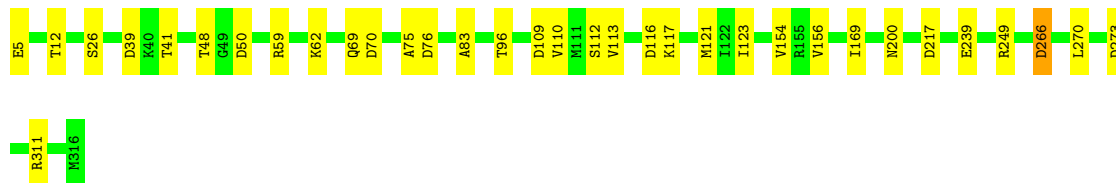
- Molecule 34: Ubiquitin-40S ribosomal protein S31

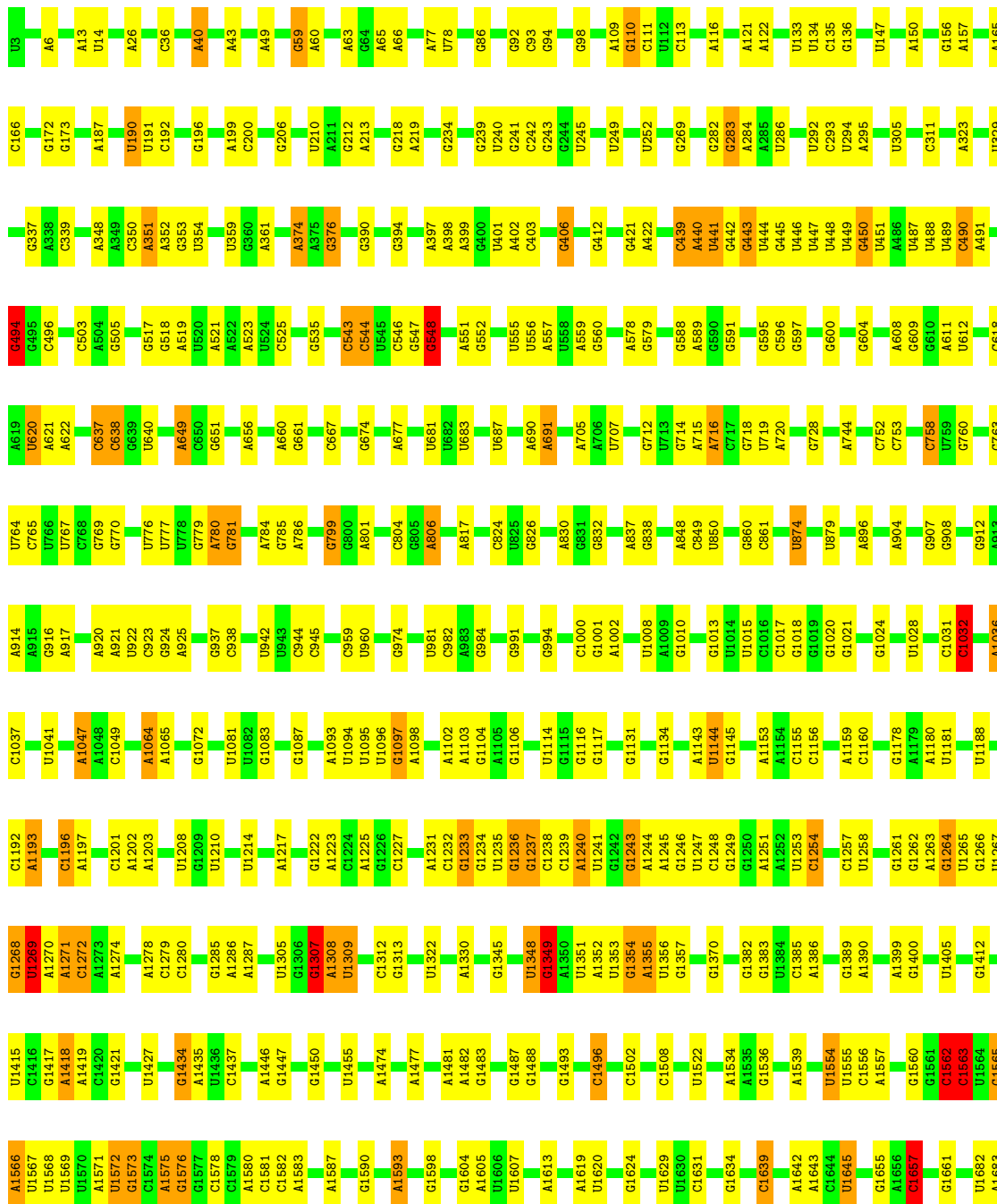
Chain N:  84% 15% .




- Molecule 35: Guanine nucleotide-binding protein subunit beta-like protein

Chain O:  89% 11%






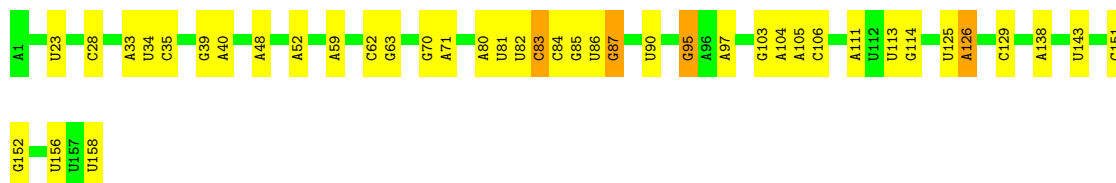
- Molecule 39: 5S rRNA

Chain BR:  83% 14%



- Molecule 40: 5.8S rRNA

Chain BS:  74% 23%



- Molecule 41: 60S ribosomal protein L2-A

Chain AW:  92% 8%



- Molecule 42: 60S ribosomal protein L3

Chain BA:  93% 7%



- Molecule 43: 60S ribosomal protein L4-A

Chain BE:  93% 6%



- Molecule 44: 60S ribosomal protein L5

Chain BI:  93% 7%



- Molecule 45: 60S ribosomal protein L6-B

Chain BM:  87% 7% 5%



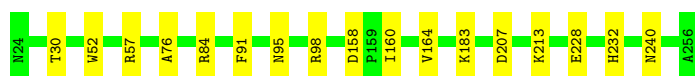
- Molecule 46: 60S ribosomal protein L7-A

Chain BO: 94% 6%



- Molecule 47: 60S ribosomal protein L8-A

Chain AA: 93% 7%



- Molecule 48: 60S ribosomal protein L9-A

Chain AD: 90% 10%



- Molecule 49: 60S ribosomal protein L10

Chain BD: 91% 8%



- Molecule 50: 60S ribosomal protein L11-B

Chain AG: 92% 8%



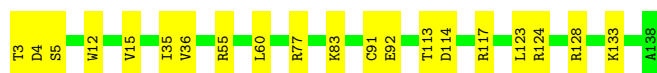
- Molecule 51: 60S ribosomal protein L13-A

Chain AJ: 92% 8%



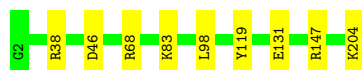
- Molecule 52: 60S ribosomal protein L14-A

Chain AM: 85% 15%



- Molecule 53: 60S ribosomal protein L15-A

Chain AQ: 96%



- Molecule 54: 60S ribosomal protein L16-A

Chain AU: 95%



- Molecule 55: 60S ribosomal protein L17-A

Chain AX: 96%



- Molecule 56: 60S ribosomal protein L18-A

Chain BB: 91%



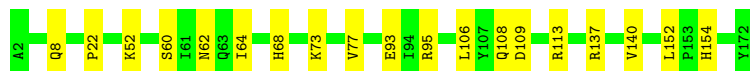
- Molecule 57: 60S ribosomal protein L19-A

Chain BF: 88%



- Molecule 58: 60S ribosomal protein L20-A

Chain BH: 89%



- Molecule 59: 60S ribosomal protein L21-A

Chain BJ: 92%



- Molecule 60: 60S ribosomal protein L22-A

Chain BL: 95% 5%



- Molecule 61: 60S ribosomal protein L23-A

Chain AB: 92% 8%



- Molecule 62: 60S ribosomal protein L24-A

Chain AE: 97% .



- Molecule 63: 60S ribosomal protein L25

Chain AH: 95% 5%



- Molecule 64: 60S ribosomal protein L26-A

Chain AK: 96% ..



- Molecule 65: 60S ribosomal protein L27-A

Chain AN: 93% 7%



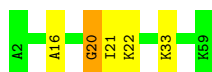
- Molecule 66: 60S ribosomal protein L28

Chain AR: 90% 10%



- Molecule 67: 60S ribosomal protein L29

Chain AV: 91% 7%



- Molecule 68: 60S ribosomal protein L30

Chain AY: 91% 9%



- Molecule 69: 60S ribosomal protein L31-A

Chain BC: 89% 11%



- Molecule 70: 60S ribosomal protein L32

Chain BG: 92% 8%



- Molecule 71: 60S ribosomal protein L33-A

Chain BK: 90% 10%



- Molecule 72: 60S ribosomal protein L34-A

Chain BN: 90% 9%



- Molecule 73: 60S ribosomal protein L35-A

Chain BP: 93% 7%



- Molecule 74: 60S ribosomal protein L36-A

Chain AC: 96%



- Molecule 75: 60S ribosomal protein L37-A

Chain AF: 89%



- Molecule 76: 60S ribosomal protein L38

Chain AI: 88%



- Molecule 77: 60S ribosomal protein L39

Chain AL: 86%



- Molecule 78: Ubiquitin-60S ribosomal protein L40

Chain AO: 90%



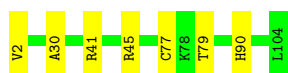
- Molecule 79: 60S ribosomal protein L41-B

Chain AS: 92%



- Molecule 80: 60S ribosomal protein L42-A

Chain AP: 93%



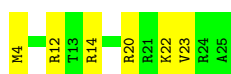
- Molecule 81: 60S ribosomal protein L43-A

Chain AT: 92% 8%



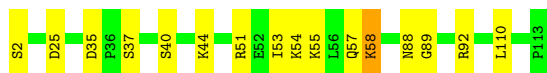
- Molecule 82: 60S ribosomal protein L41-A

Chain BV: 73% 27%



- Molecule 83: General negative regulator of transcription subunit 5

Chain BW: 86% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	176111	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (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, H2U, T6A, MG, 7MG, 2MG, 5MC, 1MA, M2G, SPD, 1MG

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	2	0.49	0/42211	0.93	63/65773 (0.1%)
2	l	0.50	0/72	0.79	0/110
3	P	0.33	0/1644	0.60	0/2249
4	Q	0.33	0/1823	0.71	1/2447 (0.0%)
5	E	0.33	0/936	0.64	0/1259
6	R	0.36	0/1656	0.64	0/2251
7	A	0.33	0/1754	0.66	1/2361 (0.0%)
8	S	0.33	0/2097	0.64	0/2823
9	B	0.32	0/1625	0.63	0/2197
10	T	0.32	0/1839	0.68	0/2460
11	U	0.33	0/1498	0.68	0/2019
12	V	0.33	0/1501	0.66	0/2006
13	W	0.32	0/1504	0.68	0/2016
14	C	0.35	0/769	0.61	0/1039
15	X	0.36	0/1168	0.64	0/1575
16	D	0.34	0/883	0.74	0/1199
17	Y	0.36	0/1215	0.69	0/1638
18	Z	0.35	0/934	0.71	0/1257
19	F	0.35	0/1125	0.68	1/1510 (0.1%)
20	G	0.31	0/957	0.64	0/1283
21	H	0.32	0/1207	0.69	0/1623
22	I	0.36	0/1130	0.69	1/1517 (0.1%)
23	J	0.33	0/807	0.63	0/1091
24	n	0.50	1/1577 (0.1%)	0.94	1/2457 (0.0%)
25	a	0.34	0/682	0.67	0/921
26	b	0.36	0/1038	0.65	0/1395
27	c	0.35	0/1139	0.68	0/1518
28	d	0.33	0/1087	0.64	0/1449
29	K	0.33	0/661	0.68	0/888
30	e	0.35	0/778	0.69	0/1042
31	f	0.32	0/620	0.60	0/838
32	M	0.33	0/452	0.69	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.33	0/480	0.80	1/639 (0.2%)
34	N	0.33	0/567	0.69	0/764
35	O	0.30	0/2436	0.62	0/3318
36	L	0.34	0/493	0.78	1/663 (0.2%)
37	BQ	0.57	0/77157	0.93	86/120295 (0.1%)
38	BT	0.42	0/1634	1.00	5/2195 (0.2%)
39	BR	0.50	0/2883	0.85	0/4491
40	BS	0.57	0/3746	0.89	0/5832
41	AW	0.40	0/1933	0.68	0/2598
42	BA	0.38	0/3146	0.65	2/4228 (0.0%)
43	BE	0.37	0/2800	0.63	0/3790
44	BI	0.36	0/2400	0.65	1/3239 (0.0%)
45	BM	0.35	0/1329	0.61	0/1794
46	BO	0.39	0/1821	0.61	0/2451
47	AA	0.35	0/1836	0.58	0/2481
48	AD	0.34	0/1529	0.61	0/2060
49	BD	0.35	0/1801	0.64	0/2416
50	AG	0.33	0/1367	0.71	1/1834 (0.1%)
51	AJ	0.38	0/1568	0.70	0/2106
52	AM	0.33	0/1068	0.68	0/1438
53	AQ	0.42	0/1757	0.72	0/2354
54	AU	0.38	0/1585	0.60	0/2128
55	AX	0.37	0/1439	0.67	0/1938
56	BB	0.36	0/1465	0.69	0/1965
57	BF	0.36	0/1532	0.72	1/2043 (0.0%)
58	BH	0.38	0/1473	0.62	0/1980
59	BJ	0.38	0/1296	0.61	0/1739
60	BL	0.37	0/812	0.61	0/1099
61	AB	0.35	0/1018	0.61	0/1369
62	AE	0.32	0/850	0.58	0/1152
63	AH	0.37	0/979	0.59	0/1321
64	AK	0.33	0/995	0.64	0/1329
65	AN	0.38	0/1106	0.62	0/1485
66	AR	0.37	0/1200	0.62	0/1607
67	AV	0.34	0/473	0.64	0/629
68	AY	0.35	0/745	0.58	0/1001
69	BC	0.36	0/890	0.63	0/1196
70	BG	0.36	0/1034	0.61	0/1385
71	BK	0.41	0/868	0.63	0/1168
72	BN	0.37	0/890	0.70	1/1189 (0.1%)
73	BP	0.34	0/978	0.65	0/1301
74	AC	0.33	0/772	0.66	0/1026
75	AF	0.41	0/660	0.74	0/875

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AI	0.32	0/618	0.64	0/826
77	AL	0.34	0/443	0.65	0/588
78	AO	0.36	0/416	0.72	1/553 (0.2%)
79	AS	0.34	0/230	0.79	0/296
80	AP	0.36	0/836	0.66	0/1104
81	AT	0.38	0/701	0.71	0/934
82	BV	0.31	0/208	0.98	0/267
83	BW	0.36	0/950	0.66	0/1260
All	All	0.47	1/219602 (0.0%)	0.83	168/322550 (0.1%)

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
11	U	0	1
12	V	0	1
16	D	0	2
19	F	0	1
34	N	0	1
35	O	0	2
38	BT	0	1
43	BE	0	2
47	AA	0	2
48	AD	0	1
52	AM	0	1
67	AV	0	1
69	BC	0	1
73	BP	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	61	C	O3'-P	7.05	1.69	1.61

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1254	C	N1-C2-O2	22.03	132.12	118.90
37	BQ	1254	C	N3-C2-O2	-19.43	108.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1234	G	N3-C2-N2	11.76	128.13	119.90
37	BQ	1254	C	C6-N1-C2	-10.62	116.05	120.30
37	BQ	1234	G	N1-C2-N2	-10.18	107.04	116.20
37	BQ	543	C	N3-C4-N4	10.08	125.06	118.00
1	2	654	C	C6-N1-C2	-9.77	116.39	120.30
37	BQ	637	C	C6-N1-C2	-9.72	116.41	120.30
1	2	224	C	C6-N1-C2	-9.15	116.64	120.30
37	BQ	2570	U	O4'-C1'-N1	-8.53	101.38	108.20
37	BQ	2496	C	N3-C2-O2	-8.40	116.02	121.90
37	BQ	543	C	C6-N1-C2	-8.39	116.94	120.30
38	BT	16	LEU	CA-CB-CG	8.28	134.34	115.30
24	n	61	C	P-O3'-C3'	8.04	129.35	119.70
37	BQ	543	C	C5-C4-N4	-7.86	114.70	120.20
38	BT	163	LEU	CA-CB-CG	7.86	133.38	115.30
37	BQ	1254	C	C5-C6-N1	7.79	124.89	121.00
50	AG	168	ASP	CB-CG-OD1	7.38	124.94	118.30
37	BQ	406	G	O4'-C1'-N9	7.14	113.91	108.20
37	BQ	2496	C	N1-C2-O2	7.08	123.15	118.90
1	2	1527	C	C2-N1-C1'	7.02	126.53	118.80
22	I	35	ASP	CB-CG-OD1	7.02	124.62	118.30
37	BQ	548	G	N1-C2-N2	-6.99	109.91	116.20
1	2	656	G	C4-N9-C1'	6.97	135.56	126.50
37	BQ	637	C	C5-C6-N1	6.90	124.45	121.00
1	2	736	C	C6-N1-C2	-6.85	117.56	120.30
37	BQ	3217	C	C2-N1-C1'	6.83	126.31	118.80
1	2	1458	G	C4-N9-C1'	6.76	135.29	126.50
38	BT	123	LEU	CA-CB-CG	6.75	130.84	115.30
1	2	555	A	C8-N9-C4	-6.70	103.12	105.80
37	BQ	1563	C	N3-C2-O2	-6.66	117.24	121.90
37	BQ	2570	U	C6-N1-C2	-6.62	117.03	121.00
37	BQ	505	G	O5'-P-OP1	-6.60	99.76	105.70
37	BQ	1254	C	C2-N1-C1'	6.58	126.04	118.80
37	BQ	656	A	N7-C8-N9	6.53	117.07	113.80
1	2	1389	C	C2-N1-C1'	6.41	125.85	118.80
1	2	656	G	C8-N9-C1'	-6.40	118.68	127.00
37	BQ	3217	C	N1-C2-O2	6.38	122.73	118.90
44	BI	230	ASP	CB-CG-OD1	6.37	124.04	118.30
37	BQ	2492	C	N3-C2-O2	-6.33	117.47	121.90
1	2	819	G	P-O3'-C3'	6.32	127.29	119.70
1	2	1285	U	N3-C2-O2	-6.32	117.77	122.20
57	BF	182	ASP	CB-CG-OD1	6.32	123.98	118.30
37	BQ	3181	C	N1-C2-O2	6.30	122.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1695	U	O4'-C1'-N1	6.29	113.24	108.20
1	2	260	U	C6-N1-C2	-6.28	117.23	121.00
1	2	1158	C	C6-N1-C2	-6.27	117.79	120.30
1	2	1258	U	C6-N1-C2	-6.25	117.25	121.00
37	BQ	1280	C	C6-N1-C2	-6.25	117.80	120.30
1	2	142	G	N3-C4-N9	-6.25	122.25	126.00
37	BQ	494	G	C8-N9-C1'	-6.24	118.88	127.00
1	2	224	C	N3-C4-N4	6.21	122.35	118.00
38	BT	128	LEU	CA-CB-CG	6.21	129.59	115.30
1	2	555	A	N7-C8-N9	6.18	116.89	113.80
1	2	322	G	P-O3'-C3'	6.15	127.08	119.70
1	2	1172	G	N7-C8-N9	6.13	116.16	113.10
37	BQ	1032	C	N1-C2-O2	-6.13	115.22	118.90
37	BQ	2489	C	N3-C2-O2	-6.09	117.64	121.90
1	2	1636	C	P-O3'-C3'	6.08	126.99	119.70
1	2	1258	U	N3-C2-O2	-6.07	117.95	122.20
19	F	39	VAL	C-N-CA	6.02	136.75	121.70
37	BQ	1355	A	P-O3'-C3'	6.01	126.92	119.70
37	BQ	2237	C	N3-C2-O2	-6.01	117.69	121.90
1	2	782	U	C6-N1-C2	-5.98	117.41	121.00
1	2	352	A	P-O3'-C3'	5.98	126.87	119.70
1	2	1256	A	P-O3'-C3'	5.95	126.84	119.70
1	2	1258	U	C5-C6-N1	5.93	125.66	122.70
1	2	782	U	N3-C2-O2	-5.92	118.06	122.20
1	2	992	A	O4'-C1'-N9	5.89	112.92	108.20
37	BQ	548	G	N3-C2-N2	5.88	124.02	119.90
37	BQ	2836	C	C2-N1-C1'	5.86	125.24	118.80
1	2	1458	G	C8-N9-C1'	-5.86	119.39	127.00
37	BQ	1578	C	C6-N1-C2	-5.85	117.96	120.30
33	g	3	LYS	CA-CB-CG	5.81	126.18	113.40
37	BQ	922	U	C2-N1-C1'	5.80	124.66	117.70
1	2	1307	U	N3-C2-O2	-5.80	118.14	122.20
1	2	142	G	N3-C2-N2	-5.79	115.84	119.90
1	2	928	U	P-O3'-C3'	5.78	126.64	119.70
37	BQ	2541	U	P-O3'-C3'	5.73	126.57	119.70
37	BQ	3217	C	N3-C2-O2	-5.67	117.93	121.90
1	2	1527	C	C6-N1-C2	-5.64	118.05	120.30
37	BQ	2870	C	N3-C2-O2	-5.62	117.97	121.90
1	2	224	C	N3-C2-O2	-5.62	117.97	121.90
1	2	639	U	P-O3'-C3'	5.60	126.42	119.70
37	BQ	3181	C	C2-N1-C1'	5.60	124.96	118.80
37	BQ	1280	C	N1-C2-O2	5.58	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	1604	G	C4-N9-C1'	5.57	133.74	126.50
1	2	1307	U	N1-C2-O2	5.56	126.69	122.80
42	BA	387	LEU	CB-CG-CD2	5.55	120.44	111.00
37	BQ	2531	C	C6-N1-C2	-5.54	118.08	120.30
72	BN	74	ARG	NE-CZ-NH1	5.53	123.07	120.30
37	BQ	1097	G	P-O3'-C3'	5.51	126.31	119.70
1	2	610	G	C4-N9-C1'	5.50	133.65	126.50
1	2	656	G	N3-C4-N9	5.49	129.30	126.00
37	BQ	2961	G	N7-C8-N9	5.49	115.85	113.10
78	AO	127	LEU	CB-CG-CD1	5.48	120.31	111.00
1	2	1274	C	P-O3'-C3'	5.46	126.25	119.70
7	A	218	LEU	CA-CB-CG	5.45	127.82	115.30
37	BQ	1661	G	N7-C8-N9	5.44	115.82	113.10
1	2	782	U	C5-C6-N1	5.43	125.42	122.70
37	BQ	1496	C	C6-N1-C2	-5.42	118.13	120.30
37	BQ	1233	G	N3-C2-N2	-5.41	116.11	119.90
37	BQ	1716	U	P-O3'-C3'	5.41	126.19	119.70
37	BQ	2407	C	C5-C6-N1	5.40	123.70	121.00
37	BQ	1576	G	C4-N9-C1'	5.40	133.52	126.50
37	BQ	1144	U	N3-C4-O4	5.39	123.18	119.40
1	2	313	U	P-O3'-C3'	5.39	126.17	119.70
37	BQ	1144	U	C5-C4-O4	-5.38	122.67	125.90
37	BQ	1563	C	C6-N1-C2	-5.38	118.15	120.30
37	BQ	3181	C	N3-C2-O2	-5.36	118.14	121.90
37	BQ	3165	A	O4'-C1'-N9	5.35	112.48	108.20
37	BQ	1349	G	C4-N9-C1'	5.35	133.46	126.50
1	2	400	A	P-O3'-C3'	5.34	126.11	119.70
1	2	1573	A	P-O3'-C3'	5.34	126.11	119.70
37	BQ	758	C	C6-N1-C2	-5.34	118.16	120.30
37	BQ	2112	U	P-O3'-C3'	5.34	126.11	119.70
1	2	1584	G	O4'-C1'-N9	5.33	112.46	108.20
37	BQ	1280	C	N3-C2-O2	-5.32	118.18	121.90
37	BQ	1036	A	N1-C6-N6	5.31	121.78	118.60
37	BQ	2374	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1560	U	N3-C2-O2	-5.29	118.50	122.20
37	BQ	1031	C	C6-N1-C2	-5.29	118.19	120.30
37	BQ	1562	C	N3-C2-O2	-5.29	118.20	121.90
37	BQ	1239	C	C6-N1-C2	-5.28	118.19	120.30
42	BA	387	LEU	CB-CG-CD1	-5.28	102.03	111.00
38	BT	90	LEU	CA-CB-CG	5.27	127.42	115.30
37	BQ	1657	C	C6-N1-C2	-5.25	118.20	120.30
37	BQ	3269	U	P-O3'-C3'	5.24	125.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BQ	2483	G	N9-C1'-C2'	-5.24	106.23	112.00
37	BQ	1064	A	P-O3'-C3'	5.23	125.97	119.70
1	2	1082	C	C2-N1-C1'	5.22	124.55	118.80
37	BQ	1724	U	O4'-C1'-N1	5.22	112.38	108.20
1	2	1172	G	C8-N9-C4	-5.21	104.31	106.40
37	BQ	1820	U	P-O3'-C3'	5.21	125.95	119.70
1	2	1023	A	P-O3'-C3'	5.21	125.95	119.70
37	BQ	2407	C	C6-N1-C2	-5.20	118.22	120.30
1	2	499	U	C6-N1-C2	-5.19	117.89	121.00
1	2	736	C	C2-N1-C1'	5.19	124.51	118.80
37	BQ	2101	C	C6-N1-C2	-5.17	118.23	120.30
37	BQ	2870	C	N1-C2-O2	5.17	122.00	118.90
1	2	699	U	C5-C6-N1	5.15	125.28	122.70
37	BQ	494	G	C4-N9-C1'	5.15	133.19	126.50
1	2	609	U	P-O3'-C3'	5.13	125.86	119.70
37	BQ	2492	C	N1-C2-O2	5.13	121.98	118.90
1	2	1560	U	C2-N1-C1'	5.12	123.85	117.70
1	2	387	A	P-O3'-C3'	5.11	125.84	119.70
37	BQ	1269	U	C2-N1-C1'	5.11	123.83	117.70
36	L	18	ARG	NE-CZ-NH2	5.10	122.85	120.30
37	BQ	1254	C	C2-N3-C4	5.09	122.45	119.90
37	BQ	1307	G	P-O3'-C3'	5.09	125.81	119.70
37	BQ	1562	C	N1-C2-O2	5.09	121.96	118.90
1	2	959	U	C2-N1-C1'	5.08	123.80	117.70
37	BQ	190	U	N3-C2-O2	-5.08	118.65	122.20
1	2	912	U	P-O3'-C3'	5.07	125.78	119.70
1	2	1791	A	P-O3'-C3'	5.06	125.78	119.70
1	2	1182	U	C2-N1-C1'	5.06	123.77	117.70
1	2	965	U	C2-N1-C1'	5.06	123.77	117.70
1	2	1458	G	N3-C4-N9	5.04	129.02	126.00
4	Q	213	ARG	NE-CZ-NH2	5.04	122.82	120.30
37	BQ	1565	G	C8-N9-C1'	-5.04	120.45	127.00
37	BQ	3218	A	P-O3'-C3'	5.04	125.75	119.70
1	2	1474	G	N9-C4-C5	5.03	107.41	105.40
37	BQ	1237	G	C4-N9-C1'	5.03	133.04	126.50
1	2	583	C	C6-N1-C2	-5.02	118.29	120.30
37	BQ	3217	C	C6-N1-C1'	-5.02	114.78	120.80
37	BQ	1554	U	P-O3'-C3'	5.02	125.72	119.70
1	2	1285	U	C6-N1-C2	-5.00	118.00	121.00
1	2	1592	A	N7-C8-N9	5.00	116.30	113.80

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	AA	30	THR	Peptide
47	AA	76	ALA	Peptide
48	AD	21	LYS	Peptide
52	AM	12	TRP	Peptide
67	AV	20	GLY	Peptide
69	BC	83	GLU	Peptide
43	BE	13	GLY	Peptide
43	BE	318	LEU	Peptide
73	BP	83	LYS	Peptide
38	BT	16	LEU	Peptide
16	D	110	GLY	Peptide
16	D	84	ASN	Peptide
19	F	40	GLU	Peptide
34	N	144	CYS	Peptide
35	O	116	ASP	Peptide
35	O	117	LYS	Peptide
11	U	64	VAL	Peptide
12	V	187	GLU	Sidechain

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	2	37739	0	18988	164	0
2	l	65	0	33	0	0
3	P	1603	0	1610	12	0
4	Q	1798	0	1890	15	0
5	E	916	0	941	12	0
6	R	1626	0	1715	10	0
7	A	1729	0	1812	6	0
8	S	2056	0	2140	16	0
9	B	1605	0	1669	13	0
10	T	1815	0	1894	17	0
11	U	1473	0	1555	13	0
12	V	1476	0	1501	16	0
13	W	1479	0	1556	6	0
14	C	752	0	719	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	X	1142	0	1209	4	0
16	D	875	0	878	13	0
17	Y	1192	0	1255	10	0
18	Z	923	0	948	12	0
19	F	1105	0	1166	8	0
20	G	948	0	990	4	0
21	H	1188	0	1218	13	0
22	I	1112	0	1124	15	0
23	J	797	0	863	5	0
24	n	1624	0	841	0	0
25	a	673	0	662	0	0
26	b	1021	0	1060	0	0
27	c	1121	0	1196	0	0
28	d	1073	0	1132	0	0
29	K	651	0	682	3	0
30	e	765	0	814	0	0
31	f	610	0	633	0	0
32	M	442	0	428	7	0
33	g	472	0	521	0	0
34	N	556	0	550	7	0
35	O	2383	0	2332	21	0
36	L	491	0	524	7	0
37	BQ	68931	0	34632	269	0
38	BT	1609	0	1701	25	0
39	BR	2579	0	1303	9	0
40	BS	3353	0	1695	15	0
41	AW	1899	0	1957	15	0
42	BA	3075	0	3142	21	0
43	BE	2748	0	2859	15	0
44	BI	2351	0	2294	13	0
45	BM	1307	0	1377	12	0
46	BO	1784	0	1862	10	0
47	AA	1804	0	1877	9	0
48	AD	1508	0	1572	15	0
49	BD	1764	0	1804	12	0
50	AG	1346	0	1370	9	0
51	AJ	1543	0	1608	11	0
52	AM	1053	0	1149	16	0
53	AQ	1720	0	1779	8	0
54	AU	1555	0	1659	8	0
55	AX	1416	0	1433	7	0
56	BB	1441	0	1543	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BF	1515	0	1606	16	0
58	BH	1437	0	1475	13	0
59	BJ	1272	0	1312	9	0
60	BL	796	0	812	3	0
61	AB	1003	0	1048	7	0
62	AE	836	0	706	3	0
63	AH	964	0	1025	3	0
64	AK	984	0	1075	8	0
65	AN	1080	0	1122	7	0
66	AR	1169	0	1211	14	0
67	AV	462	0	491	3	0
68	AY	737	0	792	6	0
69	BC	876	0	912	7	0
70	BG	1013	0	1077	10	0
71	BK	850	0	880	8	0
72	BN	880	0	942	9	0
73	BP	969	0	1078	5	0
74	AC	766	0	844	4	0
75	AF	645	0	645	9	0
76	AI	612	0	682	6	0
77	AL	436	0	475	9	0
78	AO	410	0	442	5	0
79	AS	229	0	273	2	0
80	AP	824	0	888	5	0
81	AT	694	0	734	7	0
82	BV	207	0	250	5	0
83	BW	940	0	973	10	0
84	2	89	0	0	0	0
84	AB	1	0	0	0	0
84	AQ	1	0	0	0	0
84	AW	2	0	0	0	0
84	AX	1	0	0	0	0
84	B	1	0	0	0	0
84	BA	3	0	0	0	0
84	BF	1	0	0	0	0
84	BG	1	0	0	0	0
84	BN	1	0	0	0	0
84	BO	1	0	0	0	0
84	BQ	220	0	0	0	0
84	BR	1	0	0	0	0
84	S	1	0	0	0	0
84	n	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AF	1	0	0	0	0
85	AO	1	0	0	0	0
85	AP	1	0	0	0	0
85	AT	1	0	0	0	0
85	BN	1	0	0	0	0
85	M	1	0	0	0	0
85	N	1	0	0	0	0
86	BQ	10	0	19	2	0
All	All	205032	0	151454	842	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 3.

All (842) 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)
83:BW:53:ILE:O	83:BW:57:GLN:HG3	1.69	0.92
67:AV:16:ALA:O	67:AV:20:GLY:HA3	1.75	0.85
38:BT:60:ARG:NH2	38:BT:166:ALA:O	2.10	0.85
37:BQ:687:U:OP2	51:AJ:36:ARG:NH2	2.13	0.81
37:BQ:2883:U:OP1	42:BA:10:ARG:NH2	2.14	0.80
16:D:34:THR:OG1	16:D:127:GLY:O	1.99	0.80
36:L:27:GLN:OE1	36:L:43:ASN:ND2	2.16	0.78
38:BT:20:SER:OG	38:BT:174:MET:SD	2.39	0.78
1:2:1339:C:O2'	1:2:1341:A:N7	2.18	0.77
37:BQ:2767:U:O2'	80:AP:30:ALA:O	2.03	0.76
38:BT:145:TYR:O	38:BT:149:THR:OG1	2.03	0.76
23:J:106:ILE:HG23	23:J:107:THR:HG23	1.68	0.75
37:BQ:2177:G:OP2	41:AW:128:ARG:NH1	2.20	0.75
37:BQ:1257:C:N4	37:BQ:1261:G:H22	1.85	0.74
37:BQ:2245:C:O2'	41:AW:220:GLY:O	2.05	0.74
37:BQ:1682:U:O4	60:BL:90:ARG:NH1	2.21	0.74
37:BQ:3181:C:O2'	54:AU:164[A]:SER:OG	2.05	0.74
37:BQ:1722:U:OP1	57:BF:100:ARG:NH1	2.20	0.73
1:2:159:U:O2'	10:T:87:ARG:NH1	2.22	0.73
37:BQ:1243:G:O2'	37:BQ:1271:A:O2'	2.06	0.73
37:BQ:1257:C:H42	37:BQ:1261:G:N2	1.86	0.72
37:BQ:560:G:OP1	52:AM:83:LYS:NZ	2.22	0.72
1:2:278:U:OP2	1:2:279:G:N2	2.23	0.72
23:J:80:GLU:OE1	32:M:44:ARG:NH1	2.22	0.72
51:AJ:4:SER:O	66:AR:44:ASN:ND2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BQ:1724:U:OP2	57:BF:128:LYS:NZ	2.19	0.72
37:BQ:838:G:O6	81:AT:4:ARG:NH2	2.23	0.72
1:2:1459:C:OP1	21:H:126:ARG:NH2	2.23	0.72
1:2:231:U:O2	1:2:235:G:N2	2.23	0.71
10:T:21:GLU:OE1	10:T:25:ARG:NH2	2.23	0.71
44:BI:206:GLN:NE2	44:BI:210:GLU:OE1	2.22	0.71
37:BQ:804:C:OP1	43:BE:98:ARG:NH1	2.23	0.71
1:2:1009:U:OP2	18:Z:129:LYS:NZ	2.23	0.71
37:BQ:1348:U:OP2	56:BB:38:ARG:NH2	2.23	0.71
8:S:100:ARG:NH2	8:S:121:TYR:O	2.23	0.71
37:BQ:3045:G:OP1	42:BA:19:ARG:NH2	2.25	0.70
37:BQ:1634:G:N7	65:AN:17:ARG:NH1	2.39	0.70
40:BS:95:G:OP2	75:AF:72:ARG:NH1	2.24	0.70
37:BQ:1106:G:OP1	67:AV:22:LYS:NZ	2.25	0.70
41:AW:27:ALA:O	41:AW:128:ARG:NH2	2.25	0.69
1:2:1502:G:N7	22:I:102:ARG:NH2	2.39	0.69
37:BQ:1778:G:O2'	37:BQ:1780:G:OP2	2.09	0.69
37:BQ:2457:G:N2	37:BQ:2486:A:C2	2.59	0.69
1:2:1435:G:O6	14:C:64:TYR:OH	2.07	0.69
37:BQ:714:G:HO2'	37:BQ:753:C:HO2'	1.40	0.69
49:BD:66:GLU:OE1	49:BD:69:ARG:NH2	2.25	0.69
47:AA:52:TRP:O	47:AA:57:ARG:NH1	2.26	0.69
37:BQ:1566:A:N1	37:BQ:1571:A:N6	2.40	0.69
3:P:92:HIS:HD1	3:P:202:TYR:HH	1.41	0.68
37:BQ:2219:A:OP2	74:AC:68:ARG:NH2	2.26	0.68
47:AA:95:ASN:OD1	47:AA:98:ARG:NH2	2.27	0.68
37:BQ:1846:C:OP1	37:BQ:1849:C:N4	2.24	0.68
37:BQ:2514:U:OP2	37:BQ:2586:G:N2	2.26	0.68
37:BQ:3187:A:OP1	48:AD:23:ARG:NH2	2.27	0.68
48:AD:47:LYS:NZ	52:AM:5:SER:O	2.24	0.68
44:BI:41:LYS:NZ	59:BJ:30:TYR:O	2.26	0.68
37:BQ:1383:G:O3'	43:BE:138:ARG:NH2	2.25	0.68
37:BQ:1493:G:O6	77:AL:2:ALA:N	2.27	0.68
37:BQ:2116:G:OP1	37:BQ:2118:C:N4	2.27	0.68
16:D:140:PHE:O	16:D:143:GLN:NE2	2.27	0.68
1:2:852:C:OP2	57:BF:173:ARG:NH2	2.28	0.67
37:BQ:1244:A:O2'	37:BQ:1247:U:OP1	2.07	0.67
72:BN:87:GLU:OE1	72:BN:91:ARG:NH1	2.28	0.67
38:BT:58:CYS:SG	38:BT:152:ARG:NH2	2.68	0.67
13:W:107:ARG:NH2	13:W:153:GLU:OE2	2.28	0.67
37:BQ:860:G:OP1	81:AT:17:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AV:16:ALA:O	67:AV:20:GLY:CA	2.43	0.66
44:BI:50:ARG:NH2	44:BI:72:ASP:OD2	2.27	0.66
37:BQ:3272:C:OP2	45:BM:78:ARG:NH1	2.28	0.66
1:2:1451:C:OP1	32:M:12:ARG:NH2	2.29	0.66
65:AN:22:LYS:NZ	65:AN:132:SER:O	2.27	0.66
37:BQ:496:C:OP1	70:BG:8:LYS:NZ	2.28	0.66
37:BQ:1196:C:OP1	37:BQ:1309:U:O2'	2.13	0.66
16:D:73:LYS:NZ	34:N:109:ASP:O	2.25	0.66
37:BQ:2852:C:N3	49:BD:158:LYS:NZ	2.44	0.66
37:BQ:1348:U:O2	37:BQ:1349:G:N2	2.28	0.66
37:BQ:3214:U:OP2	52:AM:128:ARG:NH1	2.27	0.66
1:2:1584:G:N2	1:2:1611:A:OP2	2.27	0.66
37:BQ:1474:A:O2'	69:BC:57:GLN:OE1	2.14	0.66
37:BQ:1598:G:OP2	72:BN:31:ARG:NH2	2.29	0.66
3:P:27:ARG:NH2	3:P:43:ASP:O	2.29	0.66
1:2:1558:U:OP2	1:2:1559:A:O2'	2.12	0.65
1:2:460:A:HO2'	8:S:27:TYR:HH	1.44	0.65
66:AR:6:THR:HG22	66:AR:8:THR:H	1.61	0.65
69:BC:4:LEU:O	69:BC:79:ARG:NH2	2.29	0.65
17:Y:99:ARG:NH2	17:Y:119:GLU:OE1	2.29	0.65
37:BQ:3050:U:O2'	62:AE:16:GLY:O	2.14	0.65
37:BQ:618:C:OP1	55:AX:173:ARG:NH2	2.30	0.65
11:U:133:THR:OG1	11:U:155:ASP:OD1	2.15	0.65
44:BI:120:LYS:O	44:BI:248:ARG:NH2	2.30	0.65
1:2:771:A:OP1	13:W:9:SER:OG	2.14	0.64
57:BF:182:ASP:OD1	57:BF:183:ALA:N	2.30	0.64
37:BQ:2895:G:O2'	78:AO:100:TYR:O	2.15	0.64
1:2:125:U:OP1	10:T:201:GLN:NE2	2.30	0.64
54:AU:54[A]:TYR:OH	54:AU:73[A]:PHE:O	2.15	0.64
37:BQ:2307:G:O2'	37:BQ:2310:U:OP2	2.16	0.64
37:BQ:1565:G:N2	37:BQ:1575:A:C5	2.65	0.64
39:BR:50:U:O3'	44:BI:224:LYS:NZ	2.31	0.64
1:2:898:A:N1	1:2:911:U:O2'	2.27	0.64
8:S:129:VAL:HG12	8:S:139:VAL:HG12	1.79	0.64
37:BQ:1693:C:O2'	37:BQ:1772:U:O2'	2.15	0.64
34:N:141:CYS:SG	34:N:142:GLY:N	2.71	0.64
8:S:103:TYR:O	8:S:182:TYR:OH	2.16	0.64
1:2:992:A:O2'	1:2:1785:U:O2	2.16	0.64
11:U:15:GLU:OE1	11:U:19:GLN:NE2	2.30	0.64
37:BQ:799:G:HO2'	51:AJ:18:TRP:HE1	1.45	0.63
39:BR:85:G:O3'	46:BO:218:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:57:SER:OG	9:B:167:ARG:NH2	2.32	0.63
61:AB:14:SER:O	61:AB:81:GLN:NE2	2.31	0.63
11:U:38:LEU:HA	11:U:41:LEU:HD23	1.80	0.63
61:AB:104:ASN:OD1	61:AB:108:GLU:N	2.32	0.63
1:2:868:G:OP1	17:Y:121:ARG:NH1	2.29	0.63
83:BW:25:ASP:OD1	83:BW:92:ARG:NH1	2.31	0.63
9:B:63:GLN:NE2	9:B:64:VAL:O	2.31	0.63
1:2:1300:A:OP1	6:R:99:LYS:NZ	2.32	0.63
1:2:237:C:O2'	1:2:238:U:O4'	2.15	0.62
37:BQ:1793:C:OP2	81:AT:49:ARG:NH2	2.32	0.62
37:BQ:283:G:OP1	80:AP:45:ARG:NH1	2.31	0.62
49:BD:61:SER:OG	49:BD:63:GLU:OE1	2.16	0.62
1:2:1562:G:OP1	22:I:89:ARG:NH2	2.33	0.62
18:Z:88:GLY:O	18:Z:92:LYS:NZ	2.29	0.62
39:BR:44:C:OP2	50:AG:137:ARG:NH2	2.33	0.62
9:B:63:GLN:NE2	9:B:66:GLN:OE1	2.32	0.62
37:BQ:2355:G:OP1	55:AX:141:SER:OG	2.13	0.62
4:Q:70:LEU:HD23	4:Q:82:ARG:HE	1.64	0.62
37:BQ:718:G:OP1	66:AR:117:ARG:NH2	2.32	0.62
37:BQ:649:A:OP2	37:BQ:2868:U:O2'	2.17	0.61
22:I:16:ASN:OD1	22:I:56:LYS:NZ	2.32	0.61
1:2:219:A:OP1	10:T:227:ARG:NH2	2.33	0.61
37:BQ:86:G:O2'	37:BQ:98:G:O6	2.16	0.61
37:BQ:640:U:OP1	66:AR:21:ARG:NH2	2.33	0.61
37:BQ:40:A:OP1	86:BQ:3621:SPD:N10	2.27	0.61
9:B:92:ARG:NH2	9:B:169:ASN:OD1	2.34	0.61
37:BQ:2948:C:OP1	42:BA:244:ARG:NH2	2.32	0.61
37:BQ:1565:G:C2	37:BQ:1575:A:N6	2.68	0.61
37:BQ:3268:A:OP1	45:BM:46:ARG:NH1	2.32	0.61
37:BQ:443:G:O6	37:BQ:490:C:N4	2.32	0.61
13:W:18:PRO:O	13:W:23:ARG:NH2	2.34	0.61
1:2:207:U:O2	12:V:178:ARG:NH1	2.33	0.61
1:2:154:G:OP1	10:T:2:LYS:NZ	2.34	0.61
1:2:789:A:OP1	8:S:108:ARG:NH2	2.34	0.61
37:BQ:3227:A:O3'	52:AM:133:LYS:NZ	2.34	0.61
44:BI:163:LEU:HD21	44:BI:175:HIS:CG	2.36	0.61
76:AI:2:ALA:N	76:AI:51:LEU:O	2.34	0.60
37:BQ:1193:A:OP1	54:AU:49[A]:ARG:NH2	2.34	0.60
37:BQ:3373:U:OP2	69:BC:102:LYS:NZ	2.26	0.60
1:2:897:C:O2	18:Z:41:ARG:NH2	2.35	0.60
62:AE:86:SER:O	62:AE:89:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1382:A:O2'	1:2:1383:G:OP1	2.17	0.60
1:2:44:U:OP2	1:2:437:A:N6	2.34	0.60
1:2:1534:G:OP1	21:H:57:ARG:NH2	2.35	0.60
1:2:1019:A:OP1	17:Y:106:ARG:NH1	2.34	0.60
1:2:1594:G:OP2	1:2:1596:C:N4	2.35	0.60
37:BQ:1811:G:N7	65:AN:64:LYS:NZ	2.48	0.60
37:BQ:837:A:OP2	81:AT:4:ARG:NH1	2.35	0.60
48:AD:137:SER:OG	48:AD:143:GLU:OE1	2.13	0.60
37:BQ:519:A:N7	43:BE:360:LYS:NZ	2.49	0.60
45:BM:82:ARG:NH1	71:BK:106:ASN:OD1	2.35	0.60
1:2:61:A:O2'	1:2:62:A:O4'	2.19	0.59
37:BQ:1727:G:OP1	81:AT:44:LYS:NZ	2.33	0.59
65:AN:17:ARG:NH2	65:AN:18:TYR:OH	2.36	0.59
37:BQ:3042:U:OP2	37:BQ:3092:C:N4	2.34	0.59
37:BQ:1631:C:OP2	65:AN:48:ARG:NH2	2.35	0.59
37:BQ:2478:C:OP2	37:BQ:2480:A:N6	2.35	0.59
3:P:79:ARG:NH2	3:P:164:ASN:O	2.35	0.59
1:2:472:U:O2'	1:2:769:A:N3	2.31	0.59
56:BB:36:LEU:O	56:BB:40:THR:OG1	2.20	0.59
73:BP:30:GLU:OE2	73:BP:34:GLN:NE2	2.36	0.59
37:BQ:1257:C:H42	37:BQ:1261:G:H22	1.41	0.59
1:2:195:G:N7	12:V:137:LYS:NZ	2.44	0.59
38:BT:41:TYR:O	38:BT:200:ASN:ND2	2.36	0.59
29:K:95:HIS:ND1	29:K:96:SER:O	2.36	0.59
37:BQ:2800:G:O6	66:AR:42:ARG:NH2	2.35	0.59
39:BR:28:C:OP1	50:AG:137:ARG:NH1	2.36	0.59
1:2:955:A:OP1	17:Y:3:ARG:NE	2.36	0.58
37:BQ:1779:C:N4	57:BF:88:ARG:O	2.36	0.58
4:Q:175:GLU:O	4:Q:187:LYS:NZ	2.36	0.58
37:BQ:2898:G:N7	78:AO:125:LYS:NZ	2.50	0.58
8:S:98:ASN:ND2	8:S:116:ASP:OD1	2.36	0.58
50:AG:10:ARG:NH2	50:AG:151:SER:O	2.35	0.58
3:P:53:THR:HG22	3:P:161:PRO:HG2	1.85	0.58
23:J:70:THR:OG1	23:J:72:ASN:OD1	2.22	0.58
29:K:29:LYS:HE2	83:BW:110:LEU:HA	1.84	0.58
1:2:930:A:O2'	4:Q:111:ARG:NH1	2.36	0.58
37:BQ:439:C:OP1	70:BG:2:ALA:N	2.36	0.58
1:2:1482:C:O2'	19:F:72:GLY:O	2.15	0.58
1:2:1020:A:OP2	17:Y:106:ARG:NH2	2.36	0.58
1:2:1334:U:O3'	23:J:85:ARG:NH2	2.36	0.58
37:BQ:1243:G:N2	37:BQ:1271:A:OP1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:141:THR:OG1	8:S:143:ASP:OD1	2.18	0.58
37:BQ:1619:A:OP1	82:BV:14:ARG:NH1	2.36	0.58
37:BQ:2854:U:OP2	49:BD:3:ARG:NH2	2.36	0.58
1:2:1116:A:OP1	79:AS:17:ARG:NH2	2.37	0.58
37:BQ:1231:A:O2'	37:BQ:1261:G:O2'	2.12	0.58
37:BQ:2476:C:N4	37:BQ:2477:G:O6	2.37	0.58
35:O:5:GLU:OE1	35:O:249:ARG:NH1	2.37	0.58
10:T:163:THR:OG1	10:T:165:GLY:O	2.21	0.58
1:2:163:G:N2	1:2:163:G:OP2	2.32	0.57
11:U:24:PHE:HE1	11:U:77:LEU:HD11	1.68	0.57
1:2:1681:A:N6	1:2:1720:G:O2'	2.37	0.57
1:2:142:G:H22	1:2:173:A:H2	1.51	0.57
38:BT:151:VAL:HG21	38:BT:166:ALA:HB3	1.86	0.57
37:BQ:2374:C:N4	37:BQ:2941:A:O4'	2.37	0.57
37:BQ:2504:U:O2'	37:BQ:2505:U:OP1	2.13	0.57
37:BQ:2568:C:O2'	37:BQ:2569:A:O4'	2.21	0.57
21:H:126:ARG:HB3	21:H:133:VAL:HG12	1.86	0.57
1:2:911:U:OP2	4:Q:8:ARG:NH2	2.36	0.57
35:O:48:THR:OG1	35:O:50:ASP:OD1	2.18	0.57
1:2:655:G:C2	1:2:678:A:N6	2.73	0.57
1:2:1220:C:OP1	14:C:48:SER:OG	2.17	0.57
37:BQ:3275:U:O2'	71:BK:99:ARG:NH1	2.38	0.57
37:BQ:596:C:N3	37:BQ:608:A:O2'	2.36	0.57
37:BQ:212:G:OP2	64:AK:2:ALA:N	2.37	0.57
37:BQ:2468:A:O2'	37:BQ:2477:G:N2	2.38	0.57
1:2:1022:C:O2'	1:2:1125:A:N1	2.36	0.56
38:BT:66:CYS:SG	38:BT:67:ILE:N	2.78	0.56
83:BW:51:ARG:O	83:BW:55:LYS:HG3	2.04	0.56
1:2:885:G:N2	18:Z:123:SER:O	2.38	0.56
5:E:18:ARG:NH1	21:H:90:ASN:O	2.38	0.56
37:BQ:2455:U:N3	37:BQ:2483:G:O2'	2.38	0.56
36:L:31:GLU:OE2	36:L:37:SER:N	2.36	0.56
4:Q:129:THR:OG1	4:Q:179:SER:O	2.23	0.56
1:2:1565:C:OP1	21:H:41:ARG:NH1	2.36	0.56
1:2:388:G:OP1	1:2:423:G:O2'	2.23	0.56
37:BQ:351:A:N6	77:AL:37:TYR:O	2.38	0.56
50:AG:26:SER:OG	50:AG:27:GLY:N	2.36	0.56
9:B:47:SER:OG	9:B:49:GLU:OE1	2.23	0.56
37:BQ:2256:A:H8	37:BQ:2256:A:H3'	1.71	0.56
37:BQ:440:A:N7	37:BQ:441:U:O2'	2.35	0.56
68:AY:9:SER:OG	68:AY:10:ILE:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BF:105:LEU:HD22	57:BF:135:LYS:HG3	1.88	0.55
37:BQ:3184:A:OP2	54:AU:12[A]:LYS:NZ	2.36	0.55
6:R:226:THR:OG1	6:R:228:ASN:OD1	2.23	0.55
49:BD:21:ARG:O	49:BD:24:ARG:NH2	2.39	0.55
37:BQ:2269:U:OP1	83:BW:55:LYS:HE3	2.05	0.55
14:C:35:ILE:HG22	14:C:37:THR:H	1.71	0.55
37:BQ:2138:A:HO2'	75:AF:2:GLY:N	2.04	0.55
58:BH:22:PRO:O	59:BJ:146:ASN:ND2	2.37	0.55
37:BQ:1203:A:N3	37:BQ:2855:U:O2'	2.33	0.55
37:BQ:2681:U:O2	50:AG:20:ASN:ND2	2.40	0.55
4:Q:207:LEU:O	4:Q:210:ILE:HD11	2.04	0.55
13:W:59:LEU:HD22	13:W:69:ARG:HA	1.87	0.55
37:BQ:1322:U:O2	58:BH:108:GLN:NE2	2.35	0.55
37:BQ:3308:C:N3	55:AX:69:ARG:NH1	2.54	0.55
37:BQ:1940:G:H21	37:BQ:3362:A:H8	1.55	0.55
37:BQ:595:G:OP2	46:BO:30:ARG:NH2	2.40	0.55
1:2:1066:C:O2'	4:Q:148:ASN:OD1	2.17	0.55
1:2:1173:C:OP1	21:H:132:ARG:NH2	2.40	0.55
37:BQ:1831:U:O2'	40:BS:114:G:OP1	2.13	0.55
1:2:1075:C:O2'	5:E:13:LYS:O	127.30	0.55
58:BH:93:GLU:OE2	58:BH:137:ARG:N	2.38	0.55
1:2:1360:A:HO2'	22:I:2:PRO:N	2.04	0.55
1:2:929:A:OP1	1:2:931:C:N4	2.39	0.55
37:BQ:824:C:O2'	37:BQ:1534:A:N3	2.39	0.55
37:BQ:2185:G:O2'	37:BQ:2314:U:OP2	2.23	0.55
49:BD:140:THR:HG21	49:BD:148:VAL:HG11	1.88	0.55
37:BQ:2969:A:N7	41:AW:215:ASN:ND2	2.55	0.55
37:BQ:1382:G:OP2	43:BE:188:ARG:NH1	2.38	0.55
37:BQ:394:G:N1	37:BQ:397:A:OP2	2.40	0.55
4:Q:69:CYS:SG	18:Z:114:ARG:NH1	2.80	0.55
1:2:129:U:O2'	1:2:131:C:N4	2.39	0.55
1:2:821:U:N3	1:2:852:C:O2	2.39	0.55
37:BQ:3214:U:O4	52:AM:124:ARG:NH1	2.39	0.55
83:BW:54:LYS:O	83:BW:58:LYS:HD3	2.07	0.55
21:H:90:ASN:N	21:H:97:ASP:OD1	2.40	0.55
22:I:109:GLU:OE2	22:I:122:ARG:NE	2.40	0.55
43:BE:292:SER:OG	43:BE:294:GLU:OE1	2.25	0.54
37:BQ:1572:U:O2'	37:BQ:1573:G:O4'	2.25	0.54
1:2:1280:C:OP1	32:M:44:ARG:NH2	2.40	0.54
35:O:26:SER:OG	35:O:75:ALA:O	2.24	0.54
37:BQ:2525:G:O2'	37:BQ:2526:C:OP2	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1198:G:OP1	1:2:1199:G:O2'	2.15	0.54
20:G:33:ARG:NE	35:O:109:ASP:OD2	2.40	0.54
37:BQ:284:A:OP2	80:AP:41:ARG:NH1	2.38	0.54
37:BQ:1114:U:OP1	66:AR:23:GLY:N	2.41	0.54
83:BW:53:ILE:O	83:BW:57:GLN:CG	2.50	0.54
37:BQ:1593:A:OP1	72:BN:60:ARG:NH1	2.41	0.54
5:E:86:VAL:HG22	5:E:87:PRO:HD2	1.89	0.54
11:U:87:ASP:O	11:U:88:ARG:NH1	2.41	0.54
1:2:1656:U:HO2'	37:BQ:2292:U:HO2'	1.56	0.54
71:BK:49:ILE:HD11	71:BK:71:VAL:HG22	1.90	0.54
43:BE:286:VAL:HG11	56:BB:31:LYS:HE3	1.89	0.54
44:BI:64:ILE:HG13	44:BI:109:THR:HG21	1.90	0.54
37:BQ:2901:G:O2'	37:BQ:3024:A:N1	2.38	0.54
10:T:163:THR:HB	10:T:168:THR:HG22	1.89	0.54
48:AD:9:GLN:HB3	48:AD:52:LEU:HD11	1.89	0.53
37:BQ:544:C:O2	37:BQ:548:G:N2	2.40	0.53
11:U:98:ILE:HG12	11:U:121:VAL:HG21	1.90	0.53
52:AM:15:VAL:HG23	52:AM:35:ILE:HD13	1.89	0.53
37:BQ:113:C:OP1	53:AQ:147:ARG:NE	2.41	0.53
37:BQ:1156:C:OP2	46:BO:94:LYS:NZ	2.37	0.53
37:BQ:1815:U:O2'	37:BQ:1816:A:OP2	2.23	0.53
35:O:41:THR:HG22	35:O:62:LYS:HG2	1.90	0.53
43:BE:266:THR:HG23	43:BE:267:VAL:HG13	1.89	0.53
37:BQ:1345:G:N2	43:BE:307:GLN:OE1	2.39	0.53
40:BS:97:A:OP1	73:BP:67:ARG:NH2	2.42	0.53
37:BQ:1257:C:N3	37:BQ:1261:G:N1	2.54	0.53
37:BQ:2256:A:C8	37:BQ:2256:A:H3'	2.43	0.53
1:2:1617:U:O2'	36:L:21:SER:O	2.27	0.53
52:AM:123:LEU:HD22	54:AU:190[A]:VAL:HG23	1.91	0.53
37:BQ:2631:U:OP2	59:BJ:4:SER:OG	2.26	0.53
37:BQ:2137:U:OP2	37:BQ:2142:A:N6	2.36	0.53
11:U:150:GLN:HB3	11:U:181:ILE:HG22	1.89	0.53
42:BA:349:LYS:NZ	42:BA:352:GLU:OE1	2.41	0.53
37:BQ:674:G:O6	56:BB:56:LYS:NZ	2.41	0.53
12:V:11:ARG:NH1	12:V:15:GLY:O	2.41	0.53
46:BO:80:GLN:OE1	59:BJ:136:ARG:NH1	2.40	0.53
12:V:4:SER:OG	12:V:6:ASP:OD1	2.23	0.53
1:2:1303:U:O2'	1:2:1322:A:OP2	2.27	0.53
37:BQ:1562:C:O2'	37:BQ:1563:C:O5'	2.26	0.53
19:F:129:PHE:O	19:F:137:ARG:NH1	2.41	0.53
37:BQ:744:A:OP1	56:BB:66:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BT:193:LEU:O	38:BT:196:LYS:NZ	2.41	0.53
1:2:151:G:N3	10:T:13:GLN:NE2	2.55	0.52
1:2:59:C:O2'	1:2:60:U:O4'	2.26	0.52
1:2:655:G:N3	1:2:678:A:C6	2.77	0.52
8:S:112:HIS:NE2	8:S:237:SER:OG	2.42	0.52
12:V:138:ASN:OD1	12:V:141:ARG:NH2	2.40	0.52
42:BA:74:GLU:OE1	42:BA:283:TYR:OH	2.16	0.52
1:2:68:A:OP1	10:T:171:LYS:NZ	2.32	0.52
47:AA:91:PHE:O	47:AA:95:ASN:ND2	2.43	0.52
37:BQ:1134:G:O2'	37:BQ:2642:A:N3	2.30	0.52
38:BT:107:TYR:OH	38:BT:140:HIS:O	2.27	0.52
76:AI:7:ASP:N	76:AI:7:ASP:OD1	2.43	0.52
68:AY:30:THR:HG23	68:AY:91:SER:HB2	1.92	0.52
8:S:193:GLY:O	8:S:211:LYS:N	2.42	0.52
37:BQ:904:A:OP2	75:AF:30:GLN:NE2	2.43	0.52
52:AM:36:VAL:HG11	52:AM:55:ARG:HH21	1.75	0.52
37:BQ:1565:G:N3	37:BQ:1575:A:N6	2.57	0.52
37:BQ:374:A:HO2'	37:BQ:376:G:H8	1.56	0.52
4:Q:72:ASP:OD1	18:Z:114:ARG:NH2	2.43	0.52
1:2:1060:U:H3'	1:2:1061:A:H5''	1.92	0.52
47:AA:207:ASP:N	47:AA:207:ASP:OD1	2.43	0.52
1:2:105:A:O3'	12:V:8:ARG:NH1	2.42	0.52
1:2:629:U:OP2	1:2:969:C:N4	2.37	0.52
37:BQ:591:G:O2'	45:BM:17:ALA:O	2.25	0.52
37:BQ:1613:A:OP1	76:AI:2:ALA:N	2.42	0.52
37:BQ:2945:G:O2'	37:BQ:2948:C:OP2	2.25	0.52
16:D:34:THR:HG21	16:D:128:ALA:HB2	1.92	0.52
37:BQ:3002:C:OP1	42:BA:26:ARG:NH2	2.42	0.51
58:BH:8:GLN:HB3	58:BH:64:ILE:HD11	1.93	0.51
35:O:12:THR:HG22	35:O:311:ARG:HG2	1.92	0.51
1:2:333:A:OP2	12:V:31:ARG:NH2	2.38	0.51
37:BQ:945:C:OP1	70:BG:36:LYS:NZ	2.43	0.51
37:BQ:1385:C:HO2'	45:BM:2:THR:N	2.08	0.51
38:BT:181:ASN:O	38:BT:185:MET:N	2.31	0.51
37:BQ:359:U:HO2'	75:AF:16:HIS:HD1	1.58	0.51
57:BF:105:LEU:HD23	57:BF:138:LEU:HD23	1.92	0.51
37:BQ:2491:A:OP1	38:BT:207:LYS:NZ	2.22	0.51
5:E:123:TYR:OH	21:H:122:HIS:NE2	2.29	0.51
53:AQ:68:ARG:HA	53:AQ:98:LEU:HD21	1.91	0.51
44:BI:54:ARG:NH1	44:BI:147:ASP:O	2.42	0.51
37:BQ:1370:G:OP1	66:AR:16:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:967:A:OP2	17:Y:124:ARG:NH2	2.42	0.51
41:AW:130:SER:OG	41:AW:174:ARG:NH2	2.44	0.51
45:BM:87:THR:HG22	45:BM:89:THR:H	1.76	0.51
37:BQ:1565:G:N2	37:BQ:1575:A:N7	2.58	0.51
38:BT:158:GLN:NE2	38:BT:161:LYS:O	2.43	0.51
8:S:148:ARG:NH1	10:T:201:GLN:OE1	2.40	0.51
40:BS:156:U:OP2	47:AA:84:ARG:NH2	2.44	0.51
37:BQ:1214:U:OP2	58:BH:137:ARG:NH2	2.44	0.51
37:BQ:1729:A:O4'	68:AY:52:ARG:NH1	2.42	0.51
16:D:26:ASP:OD1	16:D:29:LYS:NZ	2.44	0.51
1:2:322:G:O2'	1:2:323:A:OP2	2.29	0.51
1:2:704:C:N4	1:2:732:G:O2'	2.44	0.51
1:2:849:C:OP1	57:BF:162:ARG:NH1	2.43	0.51
55:AX:126:ARG:NH2	55:AX:140:GLU:OE2	2.44	0.51
70:BG:96:ILE:HG21	70:BG:105:ARG:HG2	1.94	0.51
37:BQ:361:A:O3'	75:AF:45:ARG:NH2	2.44	0.51
37:BQ:1645:U:O2'	82:BV:12:ARG:NH2	2.44	0.51
49:BD:76:MET:SD	49:BD:148:VAL:HG12	2.51	0.50
37:BQ:1021:G:N2	37:BQ:1032:C:O2	2.45	0.50
37:BQ:1210:U:OP1	48:AD:62:ARG:NH1	2.44	0.50
5:E:34:VAL:HG23	5:E:41:VAL:HG12	1.93	0.50
71:BK:35:VAL:HG23	71:BK:40:ASP:HB2	1.93	0.50
51:AJ:126:PHE:O	73:BP:114:ARG:NH2	2.42	0.50
1:2:1584:G:O2'	1:2:1585:U:OP2	2.29	0.50
47:AA:228:GLU:O	47:AA:232:HIS:ND1	2.41	0.50
80:AP:77:CYS:SG	80:AP:79:THR:OG1	2.56	0.50
1:2:853:G:OP2	57:BF:173:ARG:NH1	2.44	0.50
37:BQ:1639:C:OP2	72:BN:74:ARG:NH2	2.37	0.50
37:BQ:938:C:OP2	66:AR:26:ARG:NH1	2.43	0.50
38:BT:122:ARG:HG3	38:BT:123:LEU:HD12	1.93	0.50
42:BA:211:GLN:NE2	42:BA:283:TYR:O	2.44	0.50
37:BQ:1565:G:C2	37:BQ:1575:A:C6	2.99	0.50
19:F:64:ASP:OD1	19:F:64:ASP:N	2.44	0.50
21:H:16:ARG:NH1	50:AG:111:ASP:OD1	2.45	0.50
37:BQ:1624:G:O6	37:BQ:1819:U:O4	2.30	0.50
37:BQ:799:G:O2'	51:AJ:18:TRP:NE1	2.40	0.50
1:2:1556:A:O2'	1:2:1560:U:OP2	2.24	0.50
1:2:852:C:OP1	57:BF:176:ARG:NH2	2.45	0.50
48:AD:120:ASP:OD2	48:AD:124:ARG:NH2	2.43	0.50
37:BQ:353:G:O6	75:AF:55:ARG:NH1	2.45	0.50
58:BH:60:SER:OG	58:BH:62:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1596:C:OP1	32:M:16:LYS:NZ	2.41	0.50
1:2:1471:A:OP1	9:B:185:ARG:NH2	2.44	0.50
37:BQ:1145:G:O2'	70:BG:45:ARG:O	2.25	0.50
37:BQ:348:A:N3	37:BQ:352:A:O2'	2.44	0.50
37:BQ:63:A:N3	37:BQ:78:U:O2'	2.39	0.49
1:2:1274:C:OP1	1:2:1428:G:OP2	2.31	0.49
7:A:23:GLU:OE1	7:A:27:ARG:NE	2.46	0.49
61:AB:10:LYS:NZ	61:AB:56:ASP:OD1	2.28	0.49
64:AK:74:TYR:CZ	64:AK:77:LYS:HE2	2.47	0.49
57:BF:13:SER:OG	57:BF:38:ARG:NH2	2.45	0.49
37:BQ:412:G:OP1	55:AX:62:ARG:NH1	2.45	0.49
4:Q:82:ARG:NH2	4:Q:188:LEU:O	2.44	0.49
16:D:33:ARG:NH2	16:D:99:GLU:O	2.42	0.49
34:N:123:ASN:ND2	34:N:144:CYS:SG	2.85	0.49
12:V:57:ALA:HB2	12:V:177:GLY:HA2	1.94	0.49
37:BQ:3260:G:OP2	52:AM:128:ARG:NH2	2.45	0.49
43:BE:35:VAL:HG21	43:BE:244:LEU:HD21	1.94	0.49
15:X:109:VAL:HG12	15:X:137:PHE:HB2	1.93	0.49
61:AB:15:LEU:HD23	61:AB:53:SER:HB3	1.94	0.49
37:BQ:2464:U:O2	38:BT:39:LYS:NZ	2.33	0.49
37:BQ:874:U:N3	37:BQ:2978:U:OP1	2.40	0.49
1:2:1253:U:H5''	34:N:130:VAL:HG23	1.94	0.49
1:2:1081:A:O2'	1:2:1083:G:N7	2.44	0.49
1:2:284:G:N7	10:T:188:ARG:NH1	2.61	0.49
37:BQ:3304:U:O2'	42:BA:334:ARG:NH2	2.45	0.49
37:BQ:2256:A:C3'	37:BQ:2256:A:C8	2.95	0.49
1:2:1601:G:OP1	22:I:86:ARG:NH1	2.41	0.49
69:BC:77:ARG:HD2	69:BC:89:LEU:HD13	1.95	0.49
38:BT:107:TYR:OH	38:BT:138:VAL:HG11	2.13	0.49
1:2:655:G:N3	1:2:678:A:N6	2.61	0.49
1:2:912:U:OP1	1:2:913:G:O2'	2.24	0.49
56:BB:176:ARG:NH1	66:AR:46:ASP:OD2	2.45	0.49
37:BQ:1655:G:OP1	72:BN:40:THR:OG1	2.26	0.49
52:AM:60:LEU:HD13	58:BH:152:LEU:HD11	1.94	0.49
35:O:123:ILE:HG21	35:O:169:ILE:HG21	1.95	0.49
1:2:330:G:OP2	12:V:172:ARG:NH1	2.46	0.49
1:2:4:C:OP2	6:R:200:SER:OG	2.31	0.48
1:2:67:A:N6	1:2:83:G:O2'	2.46	0.48
74:AC:21:THR:OG1	74:AC:21:THR:O	2.30	0.48
37:BQ:1907:C:O2	42:BA:240:ARG:NH2	2.45	0.48
37:BQ:3244:A:OP1	42:BA:97:ARG:NH2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:896:U:OP1	4:Q:26:ARG:NH2	2.46	0.48
1:2:705:U:O2'	1:2:706:A:O5'	2.21	0.48
5:E:75:PRO:HA	5:E:93:VAL:HG23	1.94	0.48
1:2:1402:G:OP2	20:G:5:ARG:NH1	2.46	0.48
37:BQ:147:U:O4	47:AA:183:LYS:NZ	2.39	0.48
37:BQ:449:U:O2'	37:BQ:450:G:N2	2.46	0.48
37:BQ:3243:A:H4'	42:BA:95:THR:HG22	1.93	0.48
37:BQ:1240:A:H61	37:BQ:1244:A:H5''	1.78	0.48
37:BQ:1236:G:N2	37:BQ:1272:C:OP1	2.47	0.48
1:2:1603:U:OP2	19:F:132:LYS:NZ	2.46	0.48
7:A:20:GLU:OE2	7:A:76:ARG:NE	2.40	0.48
10:T:180:THR:HG23	10:T:183:ARG:H	1.77	0.48
1:2:1202:A:N6	1:2:1457:C:O5'	2.46	0.48
1:2:1188:G:O2'	1:2:1430:U:OP1	2.26	0.48
37:BQ:1008:U:O2'	49:BD:35:ASP:OD2	2.25	0.48
16:D:84:ASN:O	16:D:86:VAL:N	2.47	0.48
11:U:45:SER:OG	11:U:46:ILE:N	2.47	0.48
76:AI:26:LYS:HD2	76:AI:78:LEU:HD12	1.96	0.48
64:AK:77:LYS:NZ	77:AL:31:THR:HG21	2.29	0.48
65:AN:23:VAL:HG12	65:AN:45:GLY:HA3	1.95	0.48
59:BJ:68:THR:OG1	59:BJ:71:SER:OG	2.21	0.48
37:BQ:2538:U:O2	37:BQ:2542:U:N3	2.47	0.48
39:BR:52:G:O2'	39:BR:53:U:OP1	2.27	0.48
5:E:61:ARG:NH2	5:E:88:GLU:OE2	2.46	0.48
3:P:180:GLU:OE1	3:P:191:ARG:NH2	2.40	0.48
1:2:511:A:H5''	13:W:172:VAL:HG13	1.95	0.48
69:BC:51:LEU:HB3	69:BC:55:LEU:HD23	1.95	0.48
37:BQ:3070:A:OP1	57:BF:62:ARG:NH2	2.42	0.48
59:BJ:17:ARG:NH2	59:BJ:23:GLY:O	2.46	0.48
37:BQ:1047:A:N3	37:BQ:2633:U:O2'	2.46	0.48
37:BQ:1900:A:O2'	37:BQ:1906:G:N7	2.47	0.48
37:BQ:912:G:OP2	41:AW:9:ARG:NH1	2.44	0.48
40:BS:83:C:O2	64:AK:51:ARG:NH2	2.47	0.48
3:P:30:GLN:HE22	3:P:149:LEU:HD13	1.78	0.48
40:BS:95:G:O2'	75:AF:81:GLY:O	2.29	0.48
35:O:83:ALA:HB1	35:O:110:VAL:HG23	1.94	0.48
3:P:2:SER:OG	3:P:3:LEU:N	2.47	0.48
63:AH:82:LEU:HD11	63:AH:135:ILE:HD11	1.96	0.48
45:BM:175:LYS:O	52:AM:117:ARG:NH2	2.47	0.48
37:BQ:2505:U:O2'	37:BQ:2506:U:OP1	2.31	0.48
1:2:712:G:O6	1:2:726:C:O2'	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BQ:1820:U:OP2	82:BV:12:ARG:NE	2.47	0.47
37:BQ:294:U:H4'	74:AC:77:LEU:HD23	1.94	0.47
83:BW:88:ASN:OD1	83:BW:89:GLY:N	2.47	0.47
6:R:195:ASP:N	6:R:195:ASP:OD1	2.43	0.47
61:AB:10:LYS:NZ	61:AB:53:SER:OG	2.47	0.47
37:BQ:98:G:N7	51:AJ:13:HIS:NE2	2.62	0.47
37:BQ:1244:A:O2'	37:BQ:1249:G:O6	2.32	0.47
37:BQ:94:G:OP1	86:BQ:3621:SPD:N1	2.47	0.47
8:S:45:ILE:HA	8:S:61:VAL:HG11	1.96	0.47
42:BA:10:ARG:HH12	42:BA:14:LEU:HD21	1.79	0.47
37:BQ:3111:U:OP1	48:AD:184:LYS:NZ	2.44	0.47
34:N:121:CYS:SG	34:N:122:SER:N	2.87	0.47
35:O:112:SER:HB3	35:O:154:VAL:HG22	1.96	0.47
43:BE:59:GLN:OE1	75:AF:55:ARG:NH2	2.47	0.47
37:BQ:1657:C:O2'	37:BQ:1797:A:OP2	2.28	0.47
37:BQ:801:A:OP1	66:AR:27:LYS:NZ	2.26	0.47
16:D:35:ALA:O	16:D:40:GLY:N	2.45	0.47
1:2:652:G:N2	1:2:683:C:OP2	2.48	0.47
42:BA:83:PRO:O	42:BA:165:GLN:NE2	2.47	0.47
1:2:393:C:OP2	12:V:2:GLY:N	2.48	0.47
41:AW:14:SER:OG	41:AW:15:ILE:N	2.47	0.47
37:BQ:2193:U:H5'	37:BQ:2194:G:H5'	1.96	0.47
37:BQ:3275:U:N3	37:BQ:3277:U:O4'	2.48	0.47
48:AD:23:ARG:HE	48:AD:39:LYS:HA	1.79	0.47
37:BQ:2842:U:OP1	37:BQ:2844:C:N4	2.42	0.47
37:BQ:3052:G:OP1	62:AE:34:SER:OG	2.31	0.47
37:BQ:781:G:OP1	56:BB:151:ARG:NE	2.48	0.47
37:BQ:638:C:OP1	70:BG:21:HIS:NE2	2.45	0.47
35:O:156:VAL:HG12	35:O:169:ILE:HG22	1.97	0.47
35:O:266:ASP:N	35:O:266:ASP:OD1	2.42	0.47
71:BK:15:SER:OG	71:BK:16:TYR:N	2.47	0.47
14:C:24:LYS:O	14:C:39:ASN:ND2	2.47	0.47
1:2:655:G:C2	1:2:678:A:C6	3.03	0.47
40:BS:52:A:OP1	77:AL:21:ARG:NH1	2.46	0.47
46:BO:83:LEU:HD11	46:BO:116:PHE:HB3	1.97	0.47
37:BQ:292:U:OP2	53:AQ:68:ARG:NH1	2.46	0.47
37:BQ:2981:U:OP2	42:BA:244:ARG:NH1	2.48	0.47
40:BS:40:A:OP2	40:BS:103:G:N1	2.44	0.47
21:H:41:ARG:NH2	22:I:36:ILE:O	2.48	0.47
22:I:108:LEU:HA	22:I:111:ILE:HG22	1.97	0.47
22:I:13:ASP:N	22:I:13:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:487:G:C6	1:2:501:U:N3	2.82	0.46
37:BQ:1764:U:H3'	37:BQ:1765:U:H4'	1.96	0.46
37:BQ:2538:U:O2'	37:BQ:2541:U:N3	2.47	0.46
37:BQ:2613:U:O2'	37:BQ:2805:G:OP2	2.22	0.46
20:G:108:ASP:HA	20:G:111:LYS:HG2	1.97	0.46
54:AU:126[A]:VAL:O	58:BH:154:HIS:NE2	2.43	0.46
37:BQ:683:U:OP1	53:AQ:204:LYS:NZ	2.46	0.46
1:2:1344:A:O2'	1:2:1345:A:OP1	2.22	0.46
1:2:1436:A:OP2	7:A:27:ARG:NH2	2.45	0.46
37:BQ:1565:G:N3	37:BQ:1575:A:C6	2.83	0.46
3:P:31:VAL:HG12	3:P:33:GLN:H	1.79	0.46
4:Q:129:THR:OG1	4:Q:130:SER:N	2.47	0.46
11:U:10:SER:OG	11:U:11:GLN:N	2.49	0.46
1:2:428:A:N3	1:2:440:U:O2'	2.27	0.46
1:2:1127:G:OP1	79:AS:11:ARG:NH1	2.49	0.46
37:BQ:1354:G:N3	45:BM:8:LYS:NZ	2.63	0.46
37:BQ:196:G:N1	37:BQ:199:A:OP2	2.48	0.46
37:BQ:2553:U:C5	72:BN:95:ILE:HG22	2.50	0.46
37:BQ:439:C:O2'	37:BQ:440:A:OP1	2.32	0.46
40:BS:103:G:OP2	40:BS:105:A:O2'	2.33	0.46
38:BT:206:VAL:HG12	38:BT:214:PHE:HE1	1.80	0.46
12:V:20:GLN:NE2	12:V:22:ARG:O	2.48	0.46
37:BQ:1739:U:HO2'	72:BN:56:THR:HG1	1.52	0.46
37:BQ:716:A:OP1	37:BQ:752:C:O2'	2.33	0.46
37:BQ:779:G:OP1	56:BB:185:LYS:NZ	2.48	0.46
1:2:477:A:O3'	20:G:33:ARG:NH2	99.49	0.46
41:AW:137:ILE:HD11	41:AW:149:ARG:HB2	1.96	0.46
37:BQ:1116:G:N2	37:BQ:2817:A:O4'	2.49	0.46
38:BT:206:VAL:HG12	38:BT:214:PHE:CE1	2.51	0.46
17:Y:87:ASP:OD1	17:Y:87:ASP:N	2.49	0.46
58:BH:77:VAL:HG11	58:BH:106:LEU:HD22	1.98	0.46
37:BQ:2908:G:O2'	78:AO:114:LYS:NZ	2.44	0.46
22:I:86:ARG:NH1	22:I:90:PRO:O	2.48	0.46
35:O:200:ASN:ND2	35:O:239:GLU:OE2	2.49	0.46
1:2:1292:G:H21	3:P:111:ILE:HD11	1.79	0.46
1:2:1550:A:OP2	5:E:42:ARG:NH2	2.47	0.46
37:BQ:3115:C:OP1	48:AD:62:ARG:NH2	2.49	0.46
40:BS:71:A:O2'	64:AK:52:ARG:NH2	2.49	0.46
46:BO:110:ARG:O	46:BO:113:SER:OG	2.27	0.46
1:2:821:U:O4	1:2:852:C:N3	2.49	0.46
48:AD:130:ASP:OD1	48:AD:130:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:89:ASP:N	13:W:89:ASP:OD1	2.48	0.46
52:AM:3:THR:OG1	52:AM:4:ASP:N	2.49	0.45
37:BQ:1188:U:OP1	37:BQ:1210:U:O2'	2.29	0.45
35:O:270:LEU:HD21	35:O:273:ASP:HB2	1.98	0.45
15:X:22:ASN:HB3	15:X:25:VAL:HG22	1.97	0.45
37:BQ:691:A:N1	40:BS:28:C:O2'	2.42	0.45
1:2:1610:G:N7	19:F:14:LYS:NZ	2.62	0.45
58:BH:95:ARG:HB2	58:BH:140:VAL:HG23	1.98	0.45
37:BQ:1412:G:OP1	70:BG:105:ARG:NH1	2.46	0.45
1:2:460:A:O2'	8:S:27:TYR:OH	2.18	0.45
1:2:1335:U:OP1	23:J:85:ARG:NH1	2.50	0.45
81:AT:8:VAL:O	81:AT:11:THR:OG1	2.32	0.45
49:BD:47:PRO:O	49:BD:172:GLY:N	2.49	0.45
37:BQ:110:G:OP2	51:AJ:73:ARG:NH1	2.43	0.45
37:BQ:2196:C:O2'	37:BQ:2270:A:N3	2.39	0.45
37:BQ:439:C:O2'	37:BQ:494:G:N2	2.43	0.45
5:E:41:VAL:HG22	5:E:84:ILE:HD13	1.99	0.45
1:2:10:G:O2'	6:R:94:GLN:OE1	2.34	0.45
1:2:1553:G:N1	1:2:1556:A:OP2	2.49	0.45
37:BQ:1390:A:N6	37:BQ:1418:A:O2'	2.49	0.45
38:BT:107:TYR:CZ	38:BT:138:VAL:HG11	2.52	0.45
5:E:34:VAL:HG21	5:E:45:PHE:HB2	1.98	0.45
1:2:451:A:N6	1:2:453:U:O2	2.49	0.45
41:AW:108:PRO:HG2	81:AT:86:LEU:HD13	1.98	0.45
54:AU:189[A]:ASP:N	54:AU:189[A]:ASP:OD1	2.50	0.45
16:D:34:THR:HA	16:D:37:VAL:HG22	1.98	0.45
9:B:31:GLU:OE1	9:B:35:GLN:NE2	2.50	0.45
37:BQ:93:C:OP2	37:BQ:2764:C:O2'	2.28	0.45
10:T:71:THR:OG1	10:T:72:ARG:N	2.49	0.45
1:2:623:A:O2'	1:2:624:G:OP1	2.20	0.45
57:BF:7:GLN:NE2	57:BF:35:ALA:O	2.50	0.45
46:BO:74:SER:OG	46:BO:75:TYR:N	2.50	0.45
5:E:19:GLY:N	21:H:93:THR:O	2.48	0.45
34:N:133:ALA:HB3	34:N:140:TYR:HB3	1.99	0.45
1:2:1742:U:O2'	1:2:1743:U:OP1	2.31	0.45
1:2:793:A:H5''	1:2:794:U:H5'	1.99	0.45
37:BQ:2540:A:N3	37:BQ:2541:U:N3	2.65	0.45
40:BS:143:U:OP1	53:AQ:38:ARG:NH2	2.49	0.45
3:P:147:THR:O	3:P:162:CYS:N	2.46	0.45
8:S:11:ARG:NH2	8:S:21:ASP:O	2.47	0.45
51:AJ:43:ALA:O	51:AJ:47:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BD:54:SER:OG	49:BD:130:ASP:O	2.34	0.45
60:BL:20:SER:HA	60:BL:23:THR:HG22	1.98	0.45
37:BQ:651:G:O2'	37:BQ:1435:A:OP1	2.33	0.45
58:BH:68:HIS:O	58:BH:73:LYS:NZ	2.50	0.44
37:BQ:1802:C:OP1	82:BV:4:MET:N	2.50	0.44
37:BQ:1920:U:O2'	37:BQ:1932:A:N7	2.45	0.44
37:BQ:2468:A:O2'	37:BQ:2478:C:O2	2.24	0.44
16:D:31:VAL:HA	16:D:34:THR:HG22	1.99	0.44
17:Y:56:ASP:OD1	17:Y:57:ALA:N	2.50	0.44
7:A:55:THR:HA	7:A:58:VAL:HG12	1.99	0.44
39:BR:101:G:N7	58:BH:52:LYS:NZ	2.63	0.44
40:BS:126:A:O2'	40:BS:129:C:N4	2.50	0.44
60:BL:56:VAL:HG12	60:BL:65:VAL:HG22	1.99	0.44
70:BG:23:ASP:OD1	70:BG:23:ASP:N	2.50	0.44
46:BO:47:ARG:NH1	46:BO:183:ASP:OD2	2.49	0.44
37:BQ:2772:C:H4'	37:BQ:2773:C:H5'	1.99	0.44
37:BQ:806:A:N3	37:BQ:2812:C:O2'	2.40	0.44
16:D:28:LEU:HA	16:D:31:VAL:HG22	1.99	0.44
6:R:108:ASN:OD1	6:R:108:ASN:N	2.49	0.44
1:2:447:U:O2'	8:S:27:TYR:O	2.33	0.44
19:F:50:GLU:OE2	19:F:82:ARG:NH2	2.48	0.44
7:A:32:GLU:OE2	7:A:65:ARG:NH2	2.49	0.44
50:AG:22:SER:OG	50:AG:22:SER:O	2.36	0.44
42:BA:14:LEU:HA	42:BA:17:LEU:HD13	1.99	0.44
37:BQ:591:G:N2	37:BQ:612:U:OP1	2.48	0.44
14:C:50:THR:HG21	14:C:57:THR:CG2	2.47	0.44
12:V:48:THR:OG1	12:V:52:ASN:O	2.27	0.44
15:X:27:THR:OG1	15:X:28:SER:N	2.50	0.44
75:AF:58:THR:OG1	75:AF:59:THR:N	2.51	0.44
38:BT:33:GLU:OE1	38:BT:35:GLN:NE2	2.47	0.44
1:2:755:A:O2'	1:2:756:A:OP1	2.34	0.44
37:BQ:1493:G:N2	37:BQ:1493:G:OP2	2.48	0.44
37:BQ:760:G:O2'	37:BQ:770:G:N2	2.46	0.44
3:P:28:ASN:OD1	3:P:46:HIS:NE2	2.48	0.44
1:2:1252:C:OP2	34:N:118:ARG:NE	2.46	0.44
1:2:229:U:OP2	1:2:230:C:N4	2.39	0.44
58:BH:109:ASP:OD2	58:BH:113:ARG:NH1	2.51	0.44
37:BQ:1268:G:O2'	37:BQ:1269:U:O2	2.36	0.44
37:BQ:3154:C:N3	37:BQ:3157:U:O4	2.51	0.44
37:BQ:2584:G:O2'	47:AA:240:ASN:OD1	2.36	0.43
37:BQ:406:G:OP1	37:BQ:1415:U:O2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:144:GLU:N	22:I:144:GLU:OE2	2.51	0.43
4:Q:168:ILE:HG12	4:Q:197:ILE:HD12	2.00	0.43
4:Q:5:LYS:NZ	18:Z:51:ASP:OD2	2.51	0.43
22:I:38:LYS:O	22:I:39:THR:OG1	2.35	0.43
8:S:100:ARG:HG2	8:S:102:VAL:HG13	2.00	0.43
17:Y:35:GLU:HA	17:Y:38:VAL:HG22	2.00	0.43
1:2:17:C:O2'	1:2:1137:A:N1	2.39	0.43
1:2:1611:A:O2'	9:B:95:ASN:O	2.35	0.43
1:2:647:G:H22	1:2:687:G:H1	1.66	0.43
41:AW:95:SER:O	41:AW:100:ASN:ND2	2.45	0.43
40:BS:70:G:O2'	40:BS:87:G:N2	2.52	0.43
1:2:1553:G:O2'	32:M:14:TYR:OH	2.26	0.43
1:2:1681:A:H2	1:2:1720:G:H21	1.66	0.43
1:2:639:U:OP1	11:U:112:ARG:NH2	2.49	0.43
7:A:74:GLN:NE2	7:A:79:TYR:O	2.45	0.43
37:BQ:293:C:O2'	74:AC:76:ARG:O	2.26	0.43
64:AK:77:LYS:NZ	77:AL:31:THR:CG2	2.81	0.43
44:BI:77:ALA:O	44:BI:108:ARG:NH1	2.49	0.43
37:BQ:3139:A:OP1	42:BA:274:SER:OG	2.29	0.43
37:BQ:728:G:H5''	56:BB:43:PRO:HB2	2.01	0.43
18:Z:31:THR:HG22	18:Z:38:THR:HA	1.99	0.43
1:2:25:C:H5'	1:2:26:A:H5'	2.01	0.43
37:BQ:1307:G:O2'	37:BQ:1308:A:OP2	2.25	0.43
37:BQ:2206:G:O2'	37:BQ:2208:A:N6	2.43	0.43
37:BQ:3110:C:O3'	48:AD:155:SER:OG	2.28	0.43
37:BQ:620:U:OP1	55:AX:167:ARG:NH2	2.51	0.43
50:AG:36:VAL:HG22	50:AG:120:ILE:HD12	2.00	0.43
42:BA:163:HIS:ND1	42:BA:164:THR:O	2.51	0.43
57:BF:68:GLN:OE1	57:BF:71:ARG:NH2	2.49	0.43
37:BQ:59:G:H2'	40:BS:33:A:H2'	2.01	0.43
5:E:90:ILE:HD11	5:E:112:LEU:HD21	2.01	0.43
1:2:487:G:N1	1:2:501:U:C2	2.87	0.43
71:BK:16:TYR:OH	71:BK:89:LEU:O	2.33	0.43
83:BW:57:GLN:HB3	83:BW:57:GLN:HE21	1.58	0.43
3:P:150:ASP:OD2	3:P:165:ARG:NH2	2.51	0.43
71:BK:37:THR:HG23	71:BK:40:ASP:H	1.82	0.43
37:BQ:2162:U:OP1	41:AW:234:LYS:NZ	2.50	0.43
38:BT:185:MET:HA	38:BT:187:VAL:HG13	2.01	0.43
35:O:69:GLN:N	35:O:83:ALA:O	2.47	0.43
18:Z:29:HIS:HB3	18:Z:41:ARG:HA	2.01	0.43
41:AW:142:ASP:OD1	41:AW:142:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BQ:3116:G:OP1	37:BQ:3116:G:N2	2.52	0.43
37:BQ:3140:G:N7	42:BA:28:ARG:NH2	2.65	0.43
37:BQ:661:G:N7	66:AR:25:HIS:ND1	2.64	0.43
37:BQ:769:G:O2'	51:AJ:168:ARG:NH1	2.50	0.43
42:BA:10:ARG:NH1	42:BA:14:LEU:HD21	2.33	0.43
37:BQ:1385:C:O2	45:BM:2:THR:N	2.51	0.43
37:BQ:3174:A:OP1	71:BK:97:SER:OG	2.24	0.43
16:D:36:LEU:HB3	16:D:41:LEU:HD13	2.01	0.43
22:I:136:ALA:HA	22:I:139:THR:HG22	2.00	0.43
35:O:76:ASP:OD1	35:O:76:ASP:N	2.51	0.43
4:Q:110:LEU:O	4:Q:114:VAL:HG12	2.19	0.43
50:AG:15:GLU:OE2	50:AG:132:ASN:ND2	2.51	0.42
64:AK:77:LYS:HZ3	77:AL:31:THR:HG21	1.84	0.42
80:AP:2:VAL:N	80:AP:90:HIS:O	2.52	0.42
43:BE:237:GLN:O	43:BE:246:ARG:NH1	2.52	0.42
21:H:26:ILE:HG13	21:H:31:ALA:HB2	2.00	0.42
41:AW:114:SER:N	41:AW:165:VAL:O	2.51	0.42
56:BB:131:ALA:HB1	56:BB:135:GLN:H	1.84	0.42
69:BC:36:ILE:HD12	69:BC:59:ILE:HD11	2.00	0.42
49:BD:182:LEU:HA	49:BD:185:ARG:HG2	2.00	0.42
36:L:11:LYS:NZ	36:L:51:ASN:OD1	2.52	0.42
35:O:96:THR:O	35:O:96:THR:OG1	2.32	0.42
1:2:1678:A:OP1	12:V:59:ARG:NH1	2.52	0.42
1:2:334:G:O6	12:V:5:ARG:NH2	2.52	0.42
43:BE:328:ASN:OD1	46:BO:48:ASN:ND2	2.52	0.42
44:BI:234:ASP:N	44:BI:234:ASP:OD1	2.52	0.42
49:BD:169:LYS:NZ	59:BJ:158:THR:OG1	2.52	0.42
39:BR:7:G:OP1	44:BI:33:ARG:NH1	2.51	0.42
1:2:1267:G:OP1	1:2:1435:G:N2	2.52	0.42
1:2:1420:C:OP1	32:M:54:LYS:NZ	2.50	0.42
53:AQ:119:TYR:OH	53:AQ:131:GLU:OE1	2.29	0.42
37:BQ:1405:U:OP2	70:BG:59:SER:OG	2.35	0.42
14:C:72:GLY:O	14:C:76:LEU:HD23	2.19	0.42
19:F:95:LYS:O	35:O:59:ARG:NH1	2.48	0.42
53:AQ:46:ASP:N	53:AQ:46:ASP:OD1	2.53	0.42
37:BQ:2553:U:C4	72:BN:95:ILE:HG22	2.54	0.42
73:BP:76:GLN:O	73:BP:81:ARG:NH2	2.47	0.42
22:I:65:ILE:HG12	22:I:71:VAL:HG22	2.01	0.42
35:O:83:ALA:HB2	35:O:113:VAL:HB	2.00	0.42
15:X:132:SER:O	15:X:136:ARG:NH1	2.51	0.42
1:2:1482:C:N4	1:2:1524:A:OP2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:651:G:O6	1:2:652:G:N1	2.52	0.42
47:AA:160:ILE:O	47:AA:164:VAL:HG13	2.19	0.42
52:AM:113:THR:OG1	52:AM:114:ASP:N	2.52	0.42
9:B:130:ILE:HA	9:B:133:VAL:HG22	2.02	0.42
43:BE:261:VAL:HG23	43:BE:262:TRP:CD1	2.55	0.42
39:BR:72:A:O2'	39:BR:74:C:OP1	2.33	0.42
21:H:49:LYS:NZ	21:H:80:LYS:O	2.52	0.42
1:2:58:U:O2'	1:2:451:A:N3	2.49	0.42
1:2:896:U:O2	18:Z:41:ARG:NH1	2.53	0.42
48:AD:22:SER:OG	48:AD:39:LYS:NZ	2.52	0.42
37:BQ:784:A:OP2	56:BB:69:ARG:NH1	2.52	0.42
43:BE:27:SER:O	43:BE:279:HIS:NE2	2.44	0.42
45:BM:54:TYR:HA	45:BM:65:VAL:HG12	2.01	0.42
39:BR:5:G:OP2	44:BI:27:LYS:NZ	2.53	0.42
38:BT:15:GLU:OE2	38:BT:181:ASN:ND2	2.47	0.42
1:2:1615:C:OP1	9:B:81:ARG:NH2	2.53	0.42
1:2:742:U:O2	11:U:107:ARG:NH2	2.49	0.42
48:AD:93:VAL:HG13	78:AO:78:ILE:HG21	2.01	0.42
9:B:94:THR:HG22	9:B:114:ILE:HG13	2.01	0.42
42:BA:66:LYS:O	42:BA:70:ARG:NH2	2.53	0.42
36:L:19:THR:HG22	36:L:20:GLY:H	1.84	0.42
35:O:39:ASP:OD1	35:O:41:THR:OG1	2.38	0.42
52:AM:91:CYS:SG	52:AM:92:GLU:N	2.92	0.42
42:BA:35:ASP:OD1	42:BA:36:ASP:N	2.53	0.42
37:BQ:2525:G:O5'	41:AW:37:ARG:NH1	2.52	0.42
83:BW:35:ASP:O	83:BW:37:SER:N	2.53	0.42
35:O:217:ASP:N	35:O:217:ASP:OD1	2.52	0.42
6:R:139:ILE:HD12	6:R:218:ILE:HB	2.01	0.42
1:2:623:A:H3'	1:2:624:G:H5''	2.02	0.41
48:AD:41:ILE:HD13	48:AD:71:VAL:HB	2.02	0.41
37:BQ:1613:A:OP1	76:AI:51:LEU:N	2.45	0.41
10:T:2:LYS:HB3	10:T:108:VAL:HG22	2.02	0.41
1:2:424:C:O2'	1:2:426:G:OP1	2.21	0.41
51:AJ:107:GLU:N	51:AJ:107:GLU:OE1	2.46	0.41
38:BT:174:MET:HB3	38:BT:177:ASP:HB2	2.02	0.41
1:2:322:G:O2'	12:V:10:LYS:NZ	2.53	0.41
1:2:174:U:H3	1:2:266:A:H62	1.68	0.41
69:BC:44:MET:O	69:BC:77:ARG:NH1	2.53	0.41
11:U:40:PRO:HB3	57:BF:185:LEU:HD11	2.03	0.41
73:BP:102:GLU:N	73:BP:102:GLU:OE1	2.46	0.41
37:BQ:3319:U:O2'	37:BQ:3320:A:OP1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:37:VAL:HG21	22:I:100:ILE:HD11	2.01	0.41
1:2:1027:A:OP1	1:2:1789:G:O2'	2.35	0.41
48:AD:173:ARG:NH1	78:AO:125:LYS:O	2.46	0.41
68:AY:12:GLN:OE1	68:AY:12:GLN:N	2.52	0.41
1:2:1406:A:OP2	9:B:80:LYS:NZ	2.54	0.41
37:BQ:2722:U:O2'	59:BJ:88:ARG:O	2.32	0.41
37:BQ:3043:C:OP1	61:AB:45:ARG:NE	2.54	0.41
37:BQ:36:C:OP2	53:AQ:83:LYS:NZ	2.42	0.41
38:BT:205:VAL:HG13	38:BT:213:ALA:HA	2.03	0.41
29:K:43:ASP:N	29:K:43:ASP:OD1	2.52	0.41
36:L:36:THR:OG1	36:L:37:SER:N	2.53	0.41
6:R:81:MET:HB2	6:R:101:VAL:HG13	2.03	0.41
1:2:487:G:N1	1:2:501:U:N3	2.67	0.41
45:BM:176:PHE:O	52:AM:113:THR:OG1	2.24	0.41
37:BQ:2208:A:H2	37:BQ:2236:G:H22	1.68	0.41
37:BQ:2727:A:OP2	37:BQ:2728:G:N2	2.49	0.41
1:2:1523:G:OP2	1:2:1523:G:N2	2.43	0.41
1:2:1597:A:OP2	32:M:32:ARG:NH2	2.54	0.41
1:2:1471:A:HO2'	9:B:102:ARG:HH12	1.67	0.41
56:BB:27:LYS:HA	56:BB:30:VAL:HG12	2.02	0.41
6:R:147:ASN:O	6:R:147:ASN:ND2	2.54	0.41
61:AB:38:ALA:HB3	61:AB:59:MET:HB2	2.01	0.41
63:AH:62:VAL:HG23	63:AH:63:ILE:HG13	2.03	0.41
76:AI:32:ASN:OD1	76:AI:33:LYS:N	2.48	0.41
41:AW:127:ALA:HB2	41:AW:134:VAL:HG23	2.02	0.41
37:BQ:1522:U:OP2	63:AH:121:LYS:NZ	2.47	0.41
37:BQ:525:C:OP2	52:AM:77:ARG:NH2	2.49	0.41
14:C:46:LEU:O	14:C:50:THR:HG23	2.21	0.41
1:2:1217:A:O3'	14:C:44:LYS:NZ	2.50	0.41
1:2:1692:G:N1	1:2:1710:U:N3	2.68	0.41
1:2:178:U:OP1	10:T:191:ARG:NH2	2.49	0.41
44:BI:236:LEU:HA	44:BI:239:ILE:HG12	2.03	0.41
82:BV:20:ARG:HA	82:BV:23:VAL:HG12	2.02	0.41
6:R:116:LYS:HG2	6:R:127:ALA:HB3	2.03	0.41
8:S:112:HIS:NE2	8:S:237:SER:O	2.54	0.41
11:U:163:ASP:N	11:U:163:ASP:OD1	2.53	0.41
18:Z:16:VAL:HG12	18:Z:80:HIS:HB2	2.03	0.41
1:2:1218:G:N2	1:2:1444:A:OP2	2.29	0.41
1:2:420:A:OP1	10:T:96:SER:OG	2.20	0.41
1:2:657:U:C2	1:2:677:G:C2	3.09	0.41
51:AJ:162:ASN:N	51:AJ:162:ASN:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AR:130:VAL:HG11	66:AR:145:VAL:HG11	2.01	0.41
68:AY:17:VAL:HG11	68:AY:92:ILE:HD12	2.03	0.41
17:Y:6:SER:OG	17:Y:7:ALA:N	2.54	0.41
18:Z:107:ARG:NH1	36:L:60:GLU:OE2	2.54	0.41
16:D:108:ARG:O	16:D:110:GLY:N	2.54	0.41
1:2:1585:U:OP1	19:F:125:GLU:N	2.45	0.40
57:BF:43:LYS:O	57:BF:47:ASN:ND2	2.54	0.40
37:BQ:1389:G:OP1	70:BG:104:ASN:ND2	2.48	0.40
37:BQ:3163:A:N6	37:BQ:3288:G:O6	2.54	0.40
1:2:1486:G:N2	1:2:1522:U:O4	2.55	0.40
1:2:1699:G:C6	1:2:1703:C:N3	2.89	0.40
37:BQ:942:U:OP1	37:BQ:1434:G:C8	2.74	0.40
10:T:14:LYS:HB3	10:T:124:LEU:HD21	2.02	0.40
77:AL:24:PRO:HD2	77:AL:27:ILE:HD12	2.02	0.40
37:BQ:2799:A:O2'	66:AR:42:ARG:NH1	2.54	0.40
37:BQ:1312:C:O2'	54:AU:83[A]:ALA:O	2.39	0.40
43:BE:326:ARG:O	46:BO:41:ARG:NH2	2.52	0.40
35:O:70:ASP:OD1	35:O:83:ALA:HB3	2.21	0.40
1:2:1273:G:H4'	1:2:1274:C:H3'	2.03	0.40
1:2:322:G:HO2'	1:2:323:A:P	2.45	0.40
59:BJ:91:LEU:HD12	59:BJ:96:ILE:HD11	2.04	0.40
45:BM:76:LEU:N	45:BM:138:GLN:OE1	2.54	0.40
37:BQ:354:U:O2'	77:AL:40:LYS:NZ	2.50	0.40
37:BQ:707:U:OP1	37:BQ:780:A:O2'	2.24	0.40
38:BT:136:THR:O	38:BT:138:VAL:N	2.54	0.40
12:V:162:ALA:O	37:BQ:3352:U:O2'	2.34	0.40
1:2:1183:A:N3	1:2:1210:C:O2'	2.39	0.40
1:2:1297:G:N2	1:2:1300:A:OP2	2.41	0.40
64:AK:77:LYS:HZ3	77:AL:31:THR:CG2	2.34	0.40
65:AN:5:LEU:HD11	68:AY:35:ARG:HD2	2.03	0.40
56:BB:125:ASP:N	56:BB:125:ASP:OD1	2.54	0.40
72:BN:79:SER:OG	72:BN:80:ARG:NH1	2.53	0.40
37:BQ:1264:G:N2	37:BQ:1265:U:O4	2.53	0.40
37:BQ:1427:U:OP2	66:AR:4:ARG:NH1	2.46	0.40
37:BQ:1447:G:OP1	55:AX:65:SER:OG	2.29	0.40
37:BQ:2454:G:O5'	37:BQ:2484:A:N6	2.55	0.40
37:BQ:2504:U:HO2'	37:BQ:2505:U:P	2.35	0.40
38:BT:38:LEU:HD21	38:BT:167:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
4	Q	222/232 (96%)	202 (91%)	20 (9%)	0	100	100
5	E	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
6	R	214/216 (99%)	195 (91%)	19 (9%)	0	100	100
7	A	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	S	256/258 (99%)	237 (93%)	19 (7%)	0	100	100
9	B	204/206 (99%)	186 (91%)	18 (9%)	0	100	100
10	T	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
11	U	182/184 (99%)	171 (94%)	11 (6%)	0	100	100
12	V	183/187 (98%)	174 (95%)	9 (5%)	0	100	100
13	W	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
14	C	90/92 (98%)	75 (83%)	15 (17%)	0	100	100
15	X	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
16	D	119/121 (98%)	93 (78%)	23 (19%)	3 (2%)	6	21
17	Y	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
18	Z	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
19	F	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	24	57
20	G	117/125 (94%)	111 (95%)	6 (5%)	0	100	100
21	H	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
22	I	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
23	J	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
25	a	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
26	b	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
27	c	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	24	57
28	d	132/134 (98%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	K	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
30	e	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
31	f	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
32	M	51/53 (96%)	51 (100%)	0	0	100	100
33	g	58/60 (97%)	51 (88%)	7 (12%)	0	100	100
34	N	71/73 (97%)	50 (70%)	21 (30%)	0	100	100
35	O	310/312 (99%)	276 (89%)	34 (11%)	0	100	100
36	L	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
38	BT	202/204 (99%)	140 (69%)	62 (31%)	0	100	100
41	AW	249/251 (99%)	234 (94%)	15 (6%)	0	100	100
42	BA	384/386 (100%)	358 (93%)	26 (7%)	0	100	100
43	BE	359/361 (99%)	331 (92%)	27 (8%)	1 (0%)	43	75
44	BI	292/294 (99%)	276 (94%)	16 (6%)	0	100	100
45	BM	163/175 (93%)	154 (94%)	9 (6%)	0	100	100
46	BO	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
47	AA	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
48	AD	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
49	BD	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
50	AG	167/169 (99%)	156 (93%)	10 (6%)	1 (1%)	27	60
51	AJ	191/193 (99%)	174 (91%)	16 (8%)	1 (0%)	31	65
52	AM	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
53	AQ	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
54	AU	195/197 (99%)	192 (98%)	3 (2%)	0	100	100
55	AX	181/183 (99%)	170 (94%)	11 (6%)	0	100	100
56	BB	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
57	BF	186/188 (99%)	184 (99%)	2 (1%)	0	100	100
58	BH	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
59	BJ	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
60	BL	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
61	AB	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
62	AE	124/126 (98%)	112 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	AH	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
64	AK	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
65	AN	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
66	AR	146/148 (99%)	134 (92%)	12 (8%)	0	100	100
67	AV	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	9	30
68	AY	94/96 (98%)	94 (100%)	0	0	100	100
69	BC	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
70	BG	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
71	BK	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
72	BN	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
73	BP	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
74	AC	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
75	AF	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
76	AI	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
77	AL	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
78	AO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
79	AS	23/25 (92%)	23 (100%)	0	0	100	100
80	AP	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
81	AT	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
82	BV	20/22 (91%)	18 (90%)	2 (10%)	0	100	100
83	BW	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
All	All	11310/11490 (98%)	10528 (93%)	773 (7%)	9 (0%)	56	84

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	D	85	LYS
16	D	126	TRP
16	D	109	GLU
43	BE	4	PRO
67	AV	21	ILE
19	F	41	PRO
50	AG	8	PRO
51	AJ	61	PRO
27	c	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	200 (100%)	0	100	100
5	E	95/98 (97%)	95 (100%)	0	100	100
6	R	175/175 (100%)	173 (99%)	2 (1%)	76	93
7	A	182/182 (100%)	180 (99%)	2 (1%)	76	93
8	S	220/220 (100%)	218 (99%)	2 (1%)	81	95
9	B	172/173 (99%)	171 (99%)	1 (1%)	87	96
10	T	189/195 (97%)	188 (100%)	1 (0%)	90	97
11	U	163/165 (99%)	163 (100%)	0	100	100
12	V	148/149 (99%)	148 (100%)	0	100	100
13	W	156/157 (99%)	154 (99%)	2 (1%)	71	92
14	C	77/85 (91%)	77 (100%)	0	100	100
15	X	126/127 (99%)	125 (99%)	1 (1%)	83	95
16	D	88/98 (90%)	88 (100%)	0	100	100
17	Y	127/127 (100%)	126 (99%)	1 (1%)	83	95
18	Z	90/96 (94%)	89 (99%)	1 (1%)	76	93
19	F	117/117 (100%)	117 (100%)	0	100	100
20	G	101/113 (89%)	101 (100%)	0	100	100
21	H	127/128 (99%)	127 (100%)	0	100	100
22	I	115/115 (100%)	114 (99%)	1 (1%)	81	95
23	J	93/93 (100%)	93 (100%)	0	100	100
25	a	71/74 (96%)	71 (100%)	0	100	100
26	b	110/110 (100%)	110 (100%)	0	100	100
27	c	119/119 (100%)	119 (100%)	0	100	100
28	d	112/112 (100%)	112 (100%)	0	100	100
29	K	67/73 (92%)	66 (98%)	1 (2%)	67	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	e	82/83 (99%)	82 (100%)	0	100	100
31	f	70/70 (100%)	69 (99%)	1 (1%)	69	91
32	M	47/47 (100%)	47 (100%)	0	100	100
33	g	50/51 (98%)	50 (100%)	0	100	100
34	N	56/63 (89%)	55 (98%)	1 (2%)	62	88
35	O	250/257 (97%)	248 (99%)	2 (1%)	83	95
36	L	55/56 (98%)	55 (100%)	0	100	100
38	BT	185/185 (100%)	179 (97%)	6 (3%)	42	76
41	AW	190/193 (98%)	190 (100%)	0	100	100
42	BA	321/322 (100%)	318 (99%)	3 (1%)	81	95
43	BE	288/288 (100%)	287 (100%)	1 (0%)	93	98
44	BI	241/243 (99%)	241 (100%)	0	100	100
45	BM	139/154 (90%)	138 (99%)	1 (1%)	85	96
46	BO	186/186 (100%)	186 (100%)	0	100	100
47	AA	187/191 (98%)	185 (99%)	2 (1%)	76	93
48	AD	168/171 (98%)	168 (100%)	0	100	100
49	BD	185/185 (100%)	184 (100%)	1 (0%)	90	97
50	AG	145/147 (99%)	145 (100%)	0	100	100
51	AJ	154/154 (100%)	151 (98%)	3 (2%)	60	87
52	AM	107/107 (100%)	107 (100%)	0	100	100
53	AQ	175/175 (100%)	175 (100%)	0	100	100
54	AU	160/160 (100%)	159 (99%)	1 (1%)	87	96
55	AX	138/145 (95%)	138 (100%)	0	100	100
56	BB	150/150 (100%)	149 (99%)	1 (1%)	85	96
57	BF	152/153 (99%)	150 (99%)	2 (1%)	71	92
58	BH	155/155 (100%)	155 (100%)	0	100	100
59	BJ	135/136 (99%)	134 (99%)	1 (1%)	85	96
60	BL	87/87 (100%)	87 (100%)	0	100	100
61	AB	104/104 (100%)	104 (100%)	0	100	100
62	AE	56/108 (52%)	56 (100%)	0	100	100
63	AH	104/105 (99%)	103 (99%)	1 (1%)	78	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AK	108/108 (100%)	107 (99%)	1 (1%)	81	95
65	AN	112/115 (97%)	111 (99%)	1 (1%)	81	95
66	AR	117/118 (99%)	117 (100%)	0	100	100
67	AV	46/46 (100%)	45 (98%)	1 (2%)	55	85
68	AY	81/81 (100%)	81 (100%)	0	100	100
69	BC	92/96 (96%)	92 (100%)	0	100	100
70	BG	107/109 (98%)	107 (100%)	0	100	100
71	BK	90/90 (100%)	90 (100%)	0	100	100
72	BN	95/95 (100%)	94 (99%)	1 (1%)	76	93
73	BP	104/104 (100%)	104 (100%)	0	100	100
74	AC	80/81 (99%)	80 (100%)	0	100	100
75	AF	67/67 (100%)	67 (100%)	0	100	100
76	AI	68/68 (100%)	66 (97%)	2 (3%)	45	79
77	AL	45/45 (100%)	45 (100%)	0	100	100
78	AO	45/47 (96%)	45 (100%)	0	100	100
79	AS	22/23 (96%)	22 (100%)	0	100	100
80	AP	87/88 (99%)	87 (100%)	0	100	100
81	AT	71/71 (100%)	71 (100%)	0	100	100
82	BV	20/20 (100%)	19 (95%)	1 (5%)	27	60
83	BW	109/109 (100%)	105 (96%)	4 (4%)	37	71
All	All	9498/9691 (98%)	9445 (99%)	53 (1%)	88	96

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	39	THR
6	R	111	VAL
7	A	76	ARG
7	A	178	ARG
8	S	69	HIS
8	S	211	LYS
9	B	156	ARG
10	T	98	ARG
13	W	179	ARG
13	W	180	LYS

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Mol	Chain	Res	Type
15	X	67	ARG
17	Y	64	ARG
18	Z	136	ARG
22	I	140	LEU
29	K	29	LYS
31	f	34	ASP
34	N	138	ARG
35	O	121	MET
35	O	266	ASP
38	BT	16	LEU
38	BT	26	ARG
38	BT	60	ARG
38	BT	63	MET
38	BT	118	LYS
38	BT	161	LYS
42	BA	332	ARG
42	BA	369	ARG
42	BA	387	LEU
43	BE	98	ARG
45	BM	8	LYS
47	AA	158	ASP
47	AA	213	LYS
49	BD	185	ARG
51	AJ	21	ARG
51	AJ	58	VAL
51	AJ	104	ARG
54	AU	117[A]	ARG
56	BB	12	ARG
57	BF	164	LEU
57	BF	173	ARG
59	BJ	83	ARG
63	AH	56	ARG
64	AK	74	TYR
65	AN	3	LYS
67	AV	33	LYS
72	BN	106	LYS
76	AI	9	LYS
76	AI	63	LYS
82	BV	22	LYS
83	BW	2	SER
83	BW	40	SER
83	BW	44	LYS

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Mol	Chain	Res	Type
83	BW	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
9	B	63	GLN
9	B	66	GLN
21	H	25	ASN
36	L	43	ASN
38	BT	40	ASN
38	BT	197	ASN
41	AW	7	ASN
83	BW	57	GLN
83	BW	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1798 (98%)	472 (26%)	39 (2%)
2	1	2/3 (66%)	0	0
24	n	74/75 (98%)	16 (21%)	0
37	BQ	3220/3223 (99%)	654 (20%)	35 (1%)
39	BR	120/121 (99%)	11 (9%)	1 (0%)
40	BS	157/158 (99%)	28 (17%)	1 (0%)
All	All	5341/5378 (99%)	1181 (22%)	76 (1%)

All (1181) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A

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Mol	Chain	Res	Type
1	2	56	U
1	2	57	G
1	2	59	C
1	2	61	A
1	2	62	A
1	2	63	G
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	78	A
1	2	79	C
1	2	81	G
1	2	104	A
1	2	114	C
1	2	115	G
1	2	116	U
1	2	121	U
1	2	126	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	138	A
1	2	140	A
1	2	141	U
1	2	142	G
1	2	145	A
1	2	153	G
1	2	155	U
1	2	159	U
1	2	168	A
1	2	171	A

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Mol	Chain	Res	Type
1	2	176	C
1	2	178	U
1	2	179	A
1	2	180	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	216	U
1	2	217	A
1	2	218	A
1	2	223	U
1	2	224	C
1	2	225	A
1	2	227	U
1	2	228	G
1	2	230	C
1	2	232	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	240	U
1	2	241	U
1	2	243	G
1	2	249	U
1	2	250	C
1	2	255	U
1	2	257	A
1	2	260	U
1	2	265	A
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G

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Mol	Chain	Res	Type
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	322	G
1	2	323	A
1	2	330	G
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	373	G
1	2	388	G
1	2	390	G
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	417	A
1	2	422	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	436	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	452	A
1	2	454	U
1	2	460	A

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Mol	Chain	Res	Type
1	2	468	A
1	2	471	A
1	2	477	A
1	2	482	U
1	2	483	A
1	2	485	A
1	2	486	G
1	2	487	G
1	2	489	C
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	496	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	527	A
1	2	534	A
1	2	538	A
1	2	540	G
1	2	541	A
1	2	542	A
1	2	544	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	568	G
1	2	572	C
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	606	A

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Mol	Chain	Res	Type
1	2	610	G
1	2	611	U
1	2	617	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G
1	2	643	G
1	2	648	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	677	G
1	2	678	A
1	2	680	U
1	2	681	U
1	2	682	C
1	2	683	C
1	2	687	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	698	U
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G

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Mol	Chain	Res	Type
1	2	713	A
1	2	714	G
1	2	728	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	737	A
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	789	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	833	U
1	2	835	U
1	2	840	U
1	2	841	U

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Mol	Chain	Res	Type
1	2	846	G
1	2	851	U
1	2	852	C
1	2	855	A
1	2	856	A
1	2	857	U
1	2	863	A
1	2	899	G
1	2	901	G
1	2	902	G
1	2	903	U
1	2	912	U
1	2	913	G
1	2	929	A
1	2	933	A
1	2	934	C
1	2	935	U
1	2	942	G
1	2	960	U
1	2	964	U
1	2	966	A
1	2	970	A
1	2	971	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	998	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1063	U

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Mol	Chain	Res	Type
1	2	1076	A
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1100	G
1	2	1138	A
1	2	1150	G
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1166	A
1	2	1167	G
1	2	1170	G
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1208	A
1	2	1216	C
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1251	U
1	2	1252	C
1	2	1256	A
1	2	1257	U
1	2	1274	C
1	2	1275	A
1	2	1285	U
1	2	1286	U
1	2	1291	G

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Mol	Chain	Res	Type
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1325	A
1	2	1337	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1373	C
1	2	1382	A
1	2	1383	G
1	2	1389	C
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1414	U
1	2	1425	A
1	2	1427	A
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1445	G
1	2	1446	A
1	2	1459	C
1	2	1460	A
1	2	1466	G

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Mol	Chain	Res	Type
1	2	1469	A
1	2	1470	C
1	2	1471	A
1	2	1472	C
1	2	1479	A
1	2	1486	G
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1503	A
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1528	U
1	2	1531	G
1	2	1535	U
1	2	1537	C
1	2	1540	G
1	2	1542	G
1	2	1543	A
1	2	1554	U
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1570	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1575	G
1	2	1576	A
1	2	1577	A
1	2	1583	A
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1607	G

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Mol	Chain	Res	Type
1	2	1611	A
1	2	1614	A
1	2	1616	G
1	2	1622	G
1	2	1631	A
1	2	1634	C
1	2	1635	A
1	2	1636	C
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1678	A
1	2	1688	U
1	2	1693	A
1	2	1700	C
1	2	1701	A
1	2	1703	C
1	2	1708	U
1	2	1709	C
1	2	1715	G
1	2	1716	C
1	2	1717	G
1	2	1743	U
1	2	1753	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1771	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1798	U
1	2	1799	U
24	n	13	C

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Mol	Chain	Res	Type
24	n	14	A
24	n	16	H2U
24	n	19	G
24	n	21	A
24	n	22	G
24	n	37	T6A
24	n	46	7MG
24	n	47	H2U
24	n	48	5MC
24	n	56	C
24	n	59	A
24	n	63	G
24	n	64	A
24	n	65	G
24	n	76	A
37	BQ	6	A
37	BQ	13	A
37	BQ	14	U
37	BQ	26	A
37	BQ	40	A
37	BQ	43	A
37	BQ	49	A
37	BQ	59	G
37	BQ	60	A
37	BQ	65	A
37	BQ	66	A
37	BQ	77	A
37	BQ	92	G
37	BQ	109	A
37	BQ	110	G
37	BQ	111	C
37	BQ	116	A
37	BQ	121	A
37	BQ	122	A
37	BQ	133	U
37	BQ	134	U
37	BQ	135	C
37	BQ	136	G
37	BQ	150	A
37	BQ	156	G
37	BQ	157	A
37	BQ	165	A

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Mol	Chain	Res	Type
37	BQ	166	C
37	BQ	172	G
37	BQ	173	G
37	BQ	187	A
37	BQ	190	U
37	BQ	191	U
37	BQ	192	C
37	BQ	200	C
37	BQ	206	G
37	BQ	210	U
37	BQ	213	A
37	BQ	218	G
37	BQ	219	A
37	BQ	234	G
37	BQ	240	U
37	BQ	241	G
37	BQ	242	C
37	BQ	243	G
37	BQ	245	U
37	BQ	249	U
37	BQ	252	U
37	BQ	269	G
37	BQ	283	G
37	BQ	286	U
37	BQ	295	A
37	BQ	305	U
37	BQ	311	C
37	BQ	323	A
37	BQ	329	U
37	BQ	337	G
37	BQ	339	C
37	BQ	350	C
37	BQ	351	A
37	BQ	374	A
37	BQ	376	G
37	BQ	390	G
37	BQ	398	A
37	BQ	399	A
37	BQ	401	U
37	BQ	402	A
37	BQ	403	C
37	BQ	421	G

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Mol	Chain	Res	Type
37	BQ	422	A
37	BQ	439	C
37	BQ	440	A
37	BQ	441	U
37	BQ	442	G
37	BQ	443	G
37	BQ	444	U
37	BQ	445	G
37	BQ	446	U
37	BQ	447	U
37	BQ	448	U
37	BQ	450	G
37	BQ	451	U
37	BQ	487	U
37	BQ	488	U
37	BQ	489	U
37	BQ	490	C
37	BQ	491	A
37	BQ	494	G
37	BQ	503	C
37	BQ	517	G
37	BQ	518	G
37	BQ	521	A
37	BQ	523	A
37	BQ	535	G
37	BQ	543	C
37	BQ	544	C
37	BQ	546	C
37	BQ	547	G
37	BQ	548	G
37	BQ	551	A
37	BQ	552	G
37	BQ	555	U
37	BQ	556	U
37	BQ	557	A
37	BQ	559	A
37	BQ	578	A
37	BQ	579	G
37	BQ	589	A
37	BQ	597	G
37	BQ	600	G
37	BQ	604	G

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Mol	Chain	Res	Type
37	BQ	609	G
37	BQ	611	A
37	BQ	620	U
37	BQ	621	A
37	BQ	622	A
37	BQ	637	C
37	BQ	638	C
37	BQ	649	A
37	BQ	660	A
37	BQ	667	C
37	BQ	677	A
37	BQ	681	U
37	BQ	690	A
37	BQ	691	A
37	BQ	705	A
37	BQ	712	G
37	BQ	715	A
37	BQ	716	A
37	BQ	719	U
37	BQ	720	A
37	BQ	758	C
37	BQ	763	G
37	BQ	764	U
37	BQ	765	C
37	BQ	767	U
37	BQ	776	U
37	BQ	777	U
37	BQ	780	A
37	BQ	781	G
37	BQ	785	G
37	BQ	786	A
37	BQ	799	G
37	BQ	806	A
37	BQ	817	A
37	BQ	826	G
37	BQ	830	A
37	BQ	832	G
37	BQ	848	A
37	BQ	849	C
37	BQ	850	U
37	BQ	861	C
37	BQ	874	U

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Mol	Chain	Res	Type
37	BQ	879	U
37	BQ	896	A
37	BQ	907	G
37	BQ	908	G
37	BQ	914	A
37	BQ	916	G
37	BQ	917	A
37	BQ	920	A
37	BQ	921	A
37	BQ	923	C
37	BQ	924	G
37	BQ	925	A
37	BQ	937	G
37	BQ	944	C
37	BQ	959	C
37	BQ	960	U
37	BQ	974	G
37	BQ	981	U
37	BQ	982	C
37	BQ	984	G
37	BQ	991	G
37	BQ	994	G
37	BQ	1000	C
37	BQ	1001	G
37	BQ	1002	A
37	BQ	1010	G
37	BQ	1013	G
37	BQ	1015	U
37	BQ	1017	C
37	BQ	1018	G
37	BQ	1020	G
37	BQ	1024	G
37	BQ	1028	U
37	BQ	1032	C
37	BQ	1036	A
37	BQ	1037	C
37	BQ	1041	U
37	BQ	1047	A
37	BQ	1049	C
37	BQ	1064	A
37	BQ	1065	A
37	BQ	1072	G

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Mol	Chain	Res	Type
37	BQ	1081	U
37	BQ	1083	G
37	BQ	1087	G
37	BQ	1093	A
37	BQ	1094	U
37	BQ	1095	U
37	BQ	1096	U
37	BQ	1097	G
37	BQ	1098	A
37	BQ	1102	A
37	BQ	1103	A
37	BQ	1104	G
37	BQ	1117	G
37	BQ	1131	G
37	BQ	1143	A
37	BQ	1144	U
37	BQ	1153	A
37	BQ	1155	C
37	BQ	1159	A
37	BQ	1160	C
37	BQ	1178	G
37	BQ	1180	A
37	BQ	1181	U
37	BQ	1192	C
37	BQ	1193	A
37	BQ	1196	C
37	BQ	1197	A
37	BQ	1201	C
37	BQ	1202	A
37	BQ	1208	U
37	BQ	1217	A
37	BQ	1222	G
37	BQ	1223	A
37	BQ	1225	A
37	BQ	1227	C
37	BQ	1232	C
37	BQ	1233	G
37	BQ	1235	U
37	BQ	1236	G
37	BQ	1237	G
37	BQ	1238	C
37	BQ	1240	A

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Mol	Chain	Res	Type
37	BQ	1241	U
37	BQ	1243	G
37	BQ	1245	A
37	BQ	1246	G
37	BQ	1248	C
37	BQ	1251	A
37	BQ	1253	U
37	BQ	1254	C
37	BQ	1258	U
37	BQ	1262	G
37	BQ	1263	A
37	BQ	1264	G
37	BQ	1266	G
37	BQ	1267	U
37	BQ	1268	G
37	BQ	1269	U
37	BQ	1270	A
37	BQ	1271	A
37	BQ	1272	C
37	BQ	1274	A
37	BQ	1278	A
37	BQ	1279	C
37	BQ	1285	G
37	BQ	1286	A
37	BQ	1287	A
37	BQ	1305	U
37	BQ	1307	G
37	BQ	1308	A
37	BQ	1309	U
37	BQ	1313	G
37	BQ	1330	A
37	BQ	1348	U
37	BQ	1349	G
37	BQ	1351	U
37	BQ	1352	A
37	BQ	1353	U
37	BQ	1354	G
37	BQ	1356	U
37	BQ	1357	G
37	BQ	1386	A
37	BQ	1399	A
37	BQ	1400	G

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Mol	Chain	Res	Type
37	BQ	1417	G
37	BQ	1418	A
37	BQ	1419	A
37	BQ	1421	G
37	BQ	1434	G
37	BQ	1437	C
37	BQ	1446	A
37	BQ	1450	G
37	BQ	1455	U
37	BQ	1477	A
37	BQ	1481	A
37	BQ	1482	A
37	BQ	1483	G
37	BQ	1487	G
37	BQ	1488	G
37	BQ	1496	C
37	BQ	1502	C
37	BQ	1508	C
37	BQ	1536	G
37	BQ	1539	A
37	BQ	1555	U
37	BQ	1556	C
37	BQ	1557	A
37	BQ	1560	G
37	BQ	1562	C
37	BQ	1563	C
37	BQ	1566	A
37	BQ	1567	U
37	BQ	1568	U
37	BQ	1569	U
37	BQ	1572	U
37	BQ	1573	G
37	BQ	1575	A
37	BQ	1576	G
37	BQ	1580	A
37	BQ	1581	C
37	BQ	1582	C
37	BQ	1583	A
37	BQ	1587	A
37	BQ	1590	G
37	BQ	1593	A
37	BQ	1605	A

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Mol	Chain	Res	Type
37	BQ	1607	U
37	BQ	1620	U
37	BQ	1629	U
37	BQ	1639	C
37	BQ	1642	A
37	BQ	1643	A
37	BQ	1645	U
37	BQ	1657	C
37	BQ	1683	A
37	BQ	1716	U
37	BQ	1717	U
37	BQ	1724	U
37	BQ	1725	C
37	BQ	1736	G
37	BQ	1741	A
37	BQ	1750	A
37	BQ	1751	G
37	BQ	1760	A
37	BQ	1761	C
37	BQ	1765	U
37	BQ	1766	G
37	BQ	1770	G
37	BQ	1775	G
37	BQ	1778	G
37	BQ	1780	G
37	BQ	1794	G
37	BQ	1797	A
37	BQ	1808	G
37	BQ	1814	A
37	BQ	1816	A
37	BQ	1819	U
37	BQ	1820	U
37	BQ	1821	U
37	BQ	1835	A
37	BQ	1839	A
37	BQ	1840	U
37	BQ	1841	A
37	BQ	1842	A
37	BQ	1846	C
37	BQ	1849	C
37	BQ	1866	C
37	BQ	1867	A

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Mol	Chain	Res	Type
37	BQ	1879	A
37	BQ	1880	U
37	BQ	1881	A
37	BQ	1893	A
37	BQ	1906	G
37	BQ	1952	G
37	BQ	1953	G
37	BQ	1954	G
37	BQ	2101	C
37	BQ	2102	U
37	BQ	2107	A
37	BQ	2111	G
37	BQ	2112	U
37	BQ	2113	A
37	BQ	2114	C
37	BQ	2121	G
37	BQ	2122	G
37	BQ	2131	A
37	BQ	2140	U
37	BQ	2144	A
37	BQ	2158	A
37	BQ	2169	G
37	BQ	2171	G
37	BQ	2176	U
37	BQ	2201	G
37	BQ	2204	C
37	BQ	2205	U
37	BQ	2206	G
37	BQ	2207	A
37	BQ	2209	U
37	BQ	2210	G
37	BQ	2222	A
37	BQ	2223	A
37	BQ	2225	U
37	BQ	2228	A
37	BQ	2235	C
37	BQ	2244	A
37	BQ	2249	G
37	BQ	2250	G
37	BQ	2255	A
37	BQ	2256	A
37	BQ	2257	C

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Mol	Chain	Res	Type
37	BQ	2272	G
37	BQ	2273	G
37	BQ	2274	U
37	BQ	2281	A
37	BQ	2282	U
37	BQ	2288	G
37	BQ	2306	C
37	BQ	2307	G
37	BQ	2308	C
37	BQ	2310	U
37	BQ	2313	A
37	BQ	2314	U
37	BQ	2315	G
37	BQ	2334	U
37	BQ	2335	G
37	BQ	2336	U
37	BQ	2373	A
37	BQ	2374	C
37	BQ	2375	G
37	BQ	2385	G
37	BQ	2388	U
37	BQ	2393	G
37	BQ	2397	A
37	BQ	2402	A
37	BQ	2403	G
37	BQ	2404	A
37	BQ	2411	U
37	BQ	2419	A
37	BQ	2435	G
37	BQ	2437	G
37	BQ	2439	A
37	BQ	2440	G
37	BQ	2443	A
37	BQ	2445	A
37	BQ	2450	G
37	BQ	2453	U
37	BQ	2454	G
37	BQ	2455	U
37	BQ	2456	A
37	BQ	2457	G
37	BQ	2458	A
37	BQ	2459	A

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Mol	Chain	Res	Type
37	BQ	2460	U
37	BQ	2461	A
37	BQ	2463	G
37	BQ	2467	G
37	BQ	2468	A
37	BQ	2472	U
37	BQ	2474	G
37	BQ	2475	G
37	BQ	2477	G
37	BQ	2479	C
37	BQ	2480	A
37	BQ	2486	A
37	BQ	2487	U
37	BQ	2488	A
37	BQ	2490	C
37	BQ	2491	A
37	BQ	2493	U
37	BQ	2495	C
37	BQ	2497	U
37	BQ	2498	U
37	BQ	2499	U
37	BQ	2501	U
37	BQ	2503	G
37	BQ	2505	U
37	BQ	2506	U
37	BQ	2514	U
37	BQ	2515	A
37	BQ	2526	C
37	BQ	2531	C
37	BQ	2532	U
37	BQ	2537	U
37	BQ	2538	U
37	BQ	2539	C
37	BQ	2540	A
37	BQ	2541	U
37	BQ	2542	U
37	BQ	2543	U
37	BQ	2544	U
37	BQ	2548	C
37	BQ	2549	G
37	BQ	2552	C
37	BQ	2554	A

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Mol	Chain	Res	Type
37	BQ	2561	A
37	BQ	2569	A
37	BQ	2570	U
37	BQ	2571	U
37	BQ	2572	C
37	BQ	2573	G
37	BQ	2581	U
37	BQ	2585	G
37	BQ	2589	G
37	BQ	2593	A
37	BQ	2594	C
37	BQ	2606	G
37	BQ	2607	G
37	BQ	2614	G
37	BQ	2652	U
37	BQ	2656	A
37	BQ	2674	A
37	BQ	2677	G
37	BQ	2678	A
37	BQ	2689	A
37	BQ	2691	A
37	BQ	2694	A
37	BQ	2696	A
37	BQ	2704	A
37	BQ	2714	G
37	BQ	2719	U
37	BQ	2728	G
37	BQ	2729	U
37	BQ	2737	C
37	BQ	2740	A
37	BQ	2752	U
37	BQ	2753	G
37	BQ	2755	C
37	BQ	2772	C
37	BQ	2773	C
37	BQ	2777	G
37	BQ	2778	G
37	BQ	2788	C
37	BQ	2796	G
37	BQ	2800	G
37	BQ	2801	A
37	BQ	2803	A

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Mol	Chain	Res	Type
37	BQ	2810	C
37	BQ	2814	G
37	BQ	2817	A
37	BQ	2818	U
37	BQ	2821	C
37	BQ	2834	G
37	BQ	2842	U
37	BQ	2844	C
37	BQ	2845	A
37	BQ	2849	C
37	BQ	2859	U
37	BQ	2860	U
37	BQ	2867	C
37	BQ	2871	G
37	BQ	2872	A
37	BQ	2875	U
37	BQ	2876	C
37	BQ	2887	A
37	BQ	2898	G
37	BQ	2899	C
37	BQ	2911	A
37	BQ	2923	U
37	BQ	2927	C
37	BQ	2933	A
37	BQ	2935	U
37	BQ	2936	A
37	BQ	2938	G
37	BQ	2942	C
37	BQ	2947	G
37	BQ	2957	G
37	BQ	2971	A
37	BQ	2972	G
37	BQ	2983	C
37	BQ	2992	U
37	BQ	2996	U
37	BQ	2997	G
37	BQ	3012	A
37	BQ	3056	U
37	BQ	3059	G
37	BQ	3078	U
37	BQ	3079	U
37	BQ	3086	A

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Mol	Chain	Res	Type
37	BQ	3092	C
37	BQ	3101	G
37	BQ	3104	U
37	BQ	3109	G
37	BQ	3116	G
37	BQ	3119	U
37	BQ	3122	A
37	BQ	3129	A
37	BQ	3130	A
37	BQ	3131	U
37	BQ	3138	U
37	BQ	3139	A
37	BQ	3142	A
37	BQ	3143	C
37	BQ	3151	U
37	BQ	3154	C
37	BQ	3155	U
37	BQ	3156	U
37	BQ	3157	U
37	BQ	3158	G
37	BQ	3164	C
37	BQ	3165	A
37	BQ	3170	A
37	BQ	3173	G
37	BQ	3174	A
37	BQ	3175	U
37	BQ	3176	G
37	BQ	3179	U
37	BQ	3181	C
37	BQ	3186	A
37	BQ	3187	A
37	BQ	3196	U
37	BQ	3207	U
37	BQ	3209	A
37	BQ	3217	C
37	BQ	3218	A
37	BQ	3219	G
37	BQ	3227	A
37	BQ	3228	C
37	BQ	3229	G
37	BQ	3243	A
37	BQ	3245	A

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Mol	Chain	Res	Type
37	BQ	3247	G
37	BQ	3259	U
37	BQ	3263	G
37	BQ	3269	U
37	BQ	3270	U
37	BQ	3273	A
37	BQ	3276	G
37	BQ	3281	U
37	BQ	3287	U
37	BQ	3288	G
37	BQ	3289	G
37	BQ	3294	A
37	BQ	3295	A
37	BQ	3303	G
37	BQ	3304	U
37	BQ	3307	A
37	BQ	3313	U
37	BQ	3316	A
37	BQ	3317	U
37	BQ	3318	G
37	BQ	3319	U
37	BQ	3320	A
37	BQ	3335	A
37	BQ	3341	U
37	BQ	3345	G
37	BQ	3351	U
37	BQ	3352	U
37	BQ	3353	G
37	BQ	3354	U
37	BQ	3355	U
37	BQ	3356	G
37	BQ	3369	G
37	BQ	3375	A
37	BQ	3378	C
37	BQ	3382	U
37	BQ	3383	G
37	BQ	3386	G
37	BQ	3389	U
37	BQ	3390	G
39	BR	7	G
39	BR	53	U
39	BR	54	U

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Mol	Chain	Res	Type
39	BR	55	A
39	BR	65	G
39	BR	73	C
39	BR	76	A
39	BR	99	G
39	BR	102	A
39	BR	112	G
39	BR	121	U
40	BS	23	U
40	BS	34	U
40	BS	35	C
40	BS	39	G
40	BS	48	A
40	BS	59	A
40	BS	62	C
40	BS	63	G
40	BS	80	A
40	BS	81	U
40	BS	82	U
40	BS	83	C
40	BS	84	C
40	BS	85	G
40	BS	86	U
40	BS	87	G
40	BS	90	U
40	BS	95	G
40	BS	104	A
40	BS	106	C
40	BS	111	A
40	BS	113	U
40	BS	125	U
40	BS	126	A
40	BS	138	A
40	BS	151	C
40	BS	152	G
40	BS	158	U

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	77	U

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Mol	Chain	Res	Type
1	2	139	C
1	2	141	U
1	2	224	C
1	2	278	U
1	2	280	U
1	2	313	U
1	2	322	G
1	2	352	A
1	2	387	A
1	2	400	A
1	2	539	G
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	640	U
1	2	705	U
1	2	711	U
1	2	755	A
1	2	765	G
1	2	819	G
1	2	912	U
1	2	928	U
1	2	1023	A
1	2	1226	A
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1344	A
1	2	1382	A
1	2	1430	U
1	2	1471	A
1	2	1573	A
1	2	1633	A
1	2	1636	C
1	2	1742	U
1	2	1791	A
37	BQ	13	A
37	BQ	239	G
37	BQ	282	G
37	BQ	439	C
37	BQ	588	G

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Mol	Chain	Res	Type
37	BQ	637	C
37	BQ	715	A
37	BQ	763	G
37	BQ	849	C
37	BQ	916	G
37	BQ	1064	A
37	BQ	1097	G
37	BQ	1307	G
37	BQ	1355	A
37	BQ	1554	U
37	BQ	1562	C
37	BQ	1716	U
37	BQ	1815	U
37	BQ	1820	U
37	BQ	2101	C
37	BQ	2112	U
37	BQ	2249	G
37	BQ	2504	U
37	BQ	2505	U
37	BQ	2525	G
37	BQ	2537	U
37	BQ	2541	U
37	BQ	3078	U
37	BQ	3121	U
37	BQ	3218	A
37	BQ	3228	C
37	BQ	3269	U
37	BQ	3316	A
37	BQ	3319	U
37	BQ	3350	C
39	BR	52	G
40	BS	85	G

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	7MG	n	46	24	22,26,27	3.88	11 (50%)	28,39,42	1.74	8 (28%)
24	5MC	n	48	24	15,22,23	2.96	5 (33%)	19,32,35	1.27	1 (5%)
24	T6A	n	37	24,84	24,34,35	2.50	6 (25%)	24,49,52	2.44	7 (29%)
24	M2G	n	26	24	20,27,28	3.62	7 (35%)	22,40,43	2.06	5 (22%)
24	1MA	n	58	24	15,25,26	4.31	3 (20%)	15,37,40	3.30	2 (13%)
24	H2U	n	16	24	18,21,22	3.51	3 (16%)	21,30,33	2.03	5 (23%)
24	2MG	n	10	24	19,26,27	4.28	7 (36%)	21,38,41	1.90	7 (33%)
24	H2U	n	47	24	18,21,22	3.62	3 (16%)	21,30,33	2.04	5 (23%)
24	1MG	n	9	24	18,26,27	3.66	6 (33%)	19,39,42	1.50	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	7MG	n	46	24	-	0/7/37/38	0/3/3/3
24	5MC	n	48	24	-	2/5/25/26	0/2/2/2
24	T6A	n	37	24,84	-	2/15/41/42	0/3/3/3
24	M2G	n	26	24	-	0/7/29/30	0/3/3/3
24	1MA	n	58	24	-	0/3/25/26	0/3/3/3
24	H2U	n	16	24	-	0/7/38/39	0/2/2/2
24	2MG	n	10	24	-	0/5/27/28	0/3/3/3
24	H2U	n	47	24	-	6/7/38/39	0/2/2/2
24	1MG	n	9	24	-	0/3/25/26	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	10	2MG	C2-N2	12.80	1.44	1.34
24	n	47	H2U	C2-N1	12.60	1.53	1.35
24	n	16	H2U	C2-N1	12.10	1.52	1.35
24	n	58	1MA	C4-N3	11.00	1.50	1.35
24	n	46	7MG	C4-N3	9.85	1.46	1.34
24	n	58	1MA	C2-N3	8.90	1.46	1.30
24	n	58	1MA	C6-C5	8.58	1.54	1.41
24	n	10	2MG	C4-N3	8.51	1.49	1.35
24	n	26	M2G	C4-N3	8.39	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	9	1MG	C4-N3	8.39	1.48	1.35
24	n	37	T6A	C6-N6	8.06	1.50	1.36
24	n	9	1MG	C2-N3	7.72	1.46	1.34
24	n	46	7MG	C6-C5	7.44	1.51	1.41
24	n	9	1MG	C6-C5	7.42	1.53	1.41
24	n	26	M2G	C6-C5	7.02	1.53	1.41
24	n	10	2MG	C6-C5	6.89	1.53	1.41
24	n	48	5MC	C4-N3	6.76	1.44	1.35
24	n	46	7MG	C6-N1	6.62	1.44	1.33
24	n	47	H2U	C2-N3	6.57	1.49	1.38
24	n	16	H2U	C2-N3	6.51	1.49	1.38
24	n	26	M2G	C2-N2	6.46	1.45	1.34
24	n	46	7MG	C2-N1	6.19	1.46	1.35
24	n	46	7MG	C2-N3	6.18	1.46	1.35
24	n	26	M2G	C6-N1	5.93	1.43	1.33
24	n	37	T6A	C10-N6	5.83	1.49	1.37
24	n	10	2MG	C6-N1	5.62	1.42	1.33
24	n	9	1MG	C2-N2	5.57	1.45	1.33
24	n	26	M2G	C2-N1	5.55	1.44	1.34
24	n	46	7MG	C2-N2	5.42	1.44	1.33
24	n	16	H2U	C4-N3	5.22	1.46	1.37
24	n	48	5MC	C2-N3	5.16	1.48	1.38
24	n	47	H2U	C4-N3	5.16	1.46	1.37
24	n	26	M2G	C2-N3	4.97	1.45	1.33
24	n	48	5MC	C5-C4	4.93	1.49	1.41
24	n	37	T6A	C10-N11	4.79	1.45	1.35
24	n	48	5MC	C4-N4	4.40	1.45	1.34
24	n	10	2MG	C2-N3	3.76	1.46	1.34
24	n	9	1MG	C6-N1	3.59	1.43	1.38
24	n	48	5MC	C6-C5	3.45	1.49	1.40
24	n	10	2MG	C2-N1	3.04	1.44	1.34
24	n	46	7MG	C4-N9	2.63	1.43	1.38
24	n	46	7MG	O6-C6	-2.38	1.18	1.24
24	n	46	7MG	C5-N7	2.38	1.44	1.39
24	n	37	T6A	C2-N3	2.34	1.35	1.32
24	n	46	7MG	C8-N9	2.34	1.51	1.45
24	n	10	2MG	O6-C6	-2.30	1.18	1.24
24	n	9	1MG	O6-C6	-2.29	1.18	1.24
24	n	26	M2G	O6-C6	-2.28	1.18	1.24
24	n	37	T6A	C5-C4	-2.23	1.35	1.40
24	n	46	7MG	C5-C4	2.15	1.43	1.39
24	n	37	T6A	O10-C10	-2.09	1.19	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	58	1MA	C1'-N9-C4	12.17	148.03	126.64
24	n	16	H2U	C4-N3-C2	-7.17	119.84	125.79
24	n	37	T6A	N6-C10-N11	7.07	123.63	113.76
24	n	47	H2U	C4-N3-C2	-6.97	120.01	125.79
24	n	26	M2G	C1'-N9-C4	5.58	136.44	126.64
24	n	37	T6A	N3-C2-N1	-5.48	120.11	128.68
24	n	37	T6A	C2-N1-C6	4.33	120.30	116.59
24	n	26	M2G	C2-N3-C4	4.18	120.03	115.28
24	n	26	M2G	N1-C2-N2	4.11	121.35	117.19
24	n	46	7MG	C6-C5-C4	3.92	119.41	115.20
24	n	48	5MC	C2-N3-C4	3.89	120.71	116.02
24	n	10	2MG	C2-N3-C4	3.85	119.65	115.28
24	n	9	1MG	C2-N3-C4	3.83	119.73	115.36
24	n	47	H2U	N3-C2-N1	3.72	120.58	116.65
24	n	10	2MG	CM2-N2-C2	-3.66	119.17	123.59
24	n	37	T6A	N6-C6-N1	3.66	123.62	118.72
24	n	9	1MG	C1'-N9-C4	-3.65	120.23	126.64
24	n	10	2MG	N3-C2-N1	-3.54	120.63	126.23
24	n	37	T6A	O10-C10-N6	-3.32	118.01	123.62
24	n	46	7MG	N1-C2-N3	-3.31	120.22	125.42
24	n	46	7MG	C5-C4-N3	-3.28	121.14	126.49
24	n	16	H2U	N3-C2-N1	3.10	119.93	116.65
24	n	10	2MG	N2-C2-N1	3.10	119.94	116.96
24	n	26	M2G	C6-N1-C2	2.96	119.70	116.18
24	n	46	7MG	C6-N1-C2	2.94	120.61	115.93
24	n	16	H2U	C5-C4-N3	2.87	119.88	116.65
24	n	46	7MG	C5-C4-N9	2.83	110.42	106.44
24	n	47	H2U	C5-C6-N1	2.76	120.72	111.61
24	n	10	2MG	C5-C6-N1	-2.70	119.74	123.43
24	n	26	M2G	C5-C6-N1	-2.67	119.78	123.43
24	n	37	T6A	C12-N11-C10	-2.63	119.94	122.75
24	n	47	H2U	C5-C4-N3	2.61	119.58	116.65
24	n	58	1MA	C2-N3-C4	2.60	119.83	116.58
24	n	10	2MG	N2-C2-N3	2.57	119.43	116.96
24	n	16	H2U	C5-C6-N1	2.53	119.95	111.61
24	n	10	2MG	C6-N1-C2	2.43	119.54	115.18
24	n	16	H2U	O2-C2-N1	-2.43	120.05	123.11
24	n	46	7MG	N7-C8-N9	2.38	106.78	103.38
24	n	37	T6A	O10-C10-N11	-2.34	118.36	122.62
24	n	9	1MG	N2-C2-N1	2.34	121.41	118.47
24	n	47	H2U	O2-C2-N1	-2.29	120.23	123.11
24	n	46	7MG	C4-C5-N7	2.14	110.25	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	46	7MG	C2-N3-C4	2.03	119.49	113.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	n	48	5MC	O4'-C4'-C5'-O5'
24	n	48	5MC	C3'-C4'-C5'-O5'
24	n	47	H2U	O4'-C4'-C5'-O5'
24	n	47	H2U	C3'-C4'-C5'-O5'
24	n	47	H2U	O4'-C1'-N1-C6
24	n	47	H2U	C2'-C1'-N1-C6
24	n	47	H2U	O4'-C1'-N1-C2
24	n	47	H2U	C2'-C1'-N1-C2
24	n	37	T6A	C3'-C4'-C5'-O5'
24	n	37	T6A	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 335 ligands modelled in this entry, 334 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	SPD	BQ	3621	-	9,9,9	0.30	0	8,8,8	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPD	BQ	3621	-	-	6/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	BQ	3621	SPD	C3-C4-C5-N6
86	BQ	3621	SPD	N6-C7-C8-C9
86	BQ	3621	SPD	C2-C3-C4-C5
86	BQ	3621	SPD	C7-C8-C9-N10
86	BQ	3621	SPD	C4-C5-N6-C7
86	BQ	3621	SPD	C8-C7-N6-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	BQ	3621	SPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	BQ	2
12	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BQ	1955:U	O3'	2093:A	P	26.76
1	V	123:LYS	C	135:LYS	N	21.11
1	BQ	451:U	O3'	486:A	P	9.87