



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:38 PM BST

PDB ID : 3JAP
EMDB ID: : EMD-3048
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 4.90 Å(reported)
Based on PDB ID : 2D74, 3J81, 4U1C, 3CW2, 4U1D, 4U1E

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

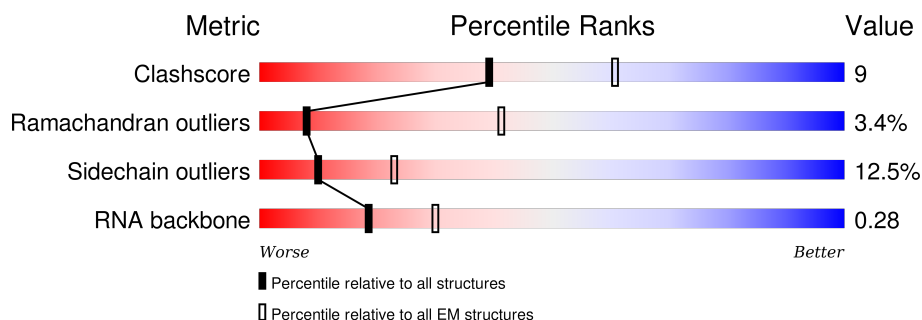
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

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




























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

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

Mol	Chain	Length	Quality of chain
1	1	75	28% 45% 27%
2	2	1781	26% 51% 23%
3	3	25	• 52% 44%
4	A	254	59% 19% • 18%
5	B	255	66% 20% • 13%
6	C	259	59% 23% • 16%
7	D	237	65% 24% • 6%
8	E	261	70% 27% •


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Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	588	
44	p	652	
45	q	347	
46	r	31	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 98333 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 Met-tRNAi (U31:A39 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 20 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S		
			433	271	88	73	1	0	0

- Molecule 35 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 36 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	550	Total	C	N	O	S	0	0
			4189	2667	721	794	7		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	634	Total	C	N	O	S	0	0
			4899	3121	826	940	12		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	31	Total	C	N	O	S	0	0
			277	177	48	50	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

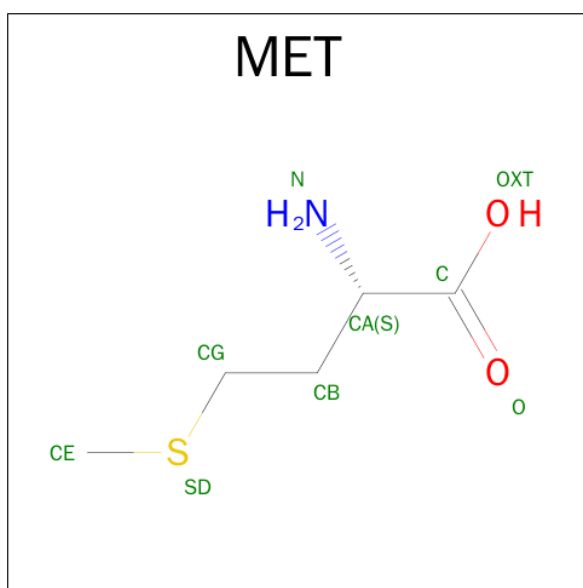
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	80	Total	Mg	0
			80	80	
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

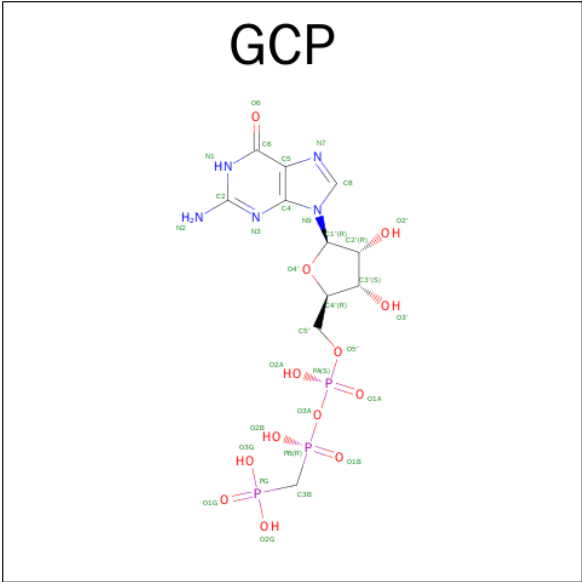
Mol	Chain	Residues	Atoms		AltConf
49	b	1	Total	Zn	0
			1	1	
49	a	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

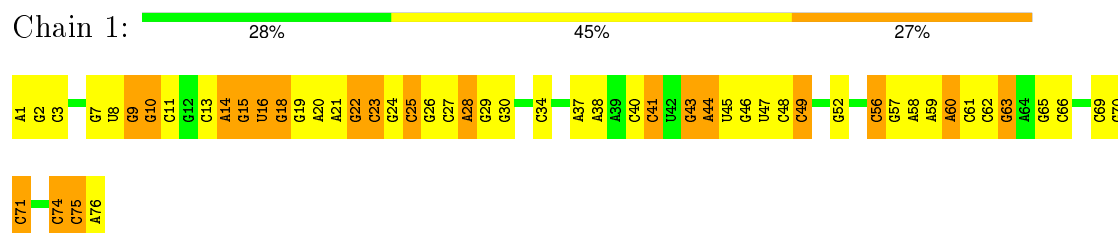


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

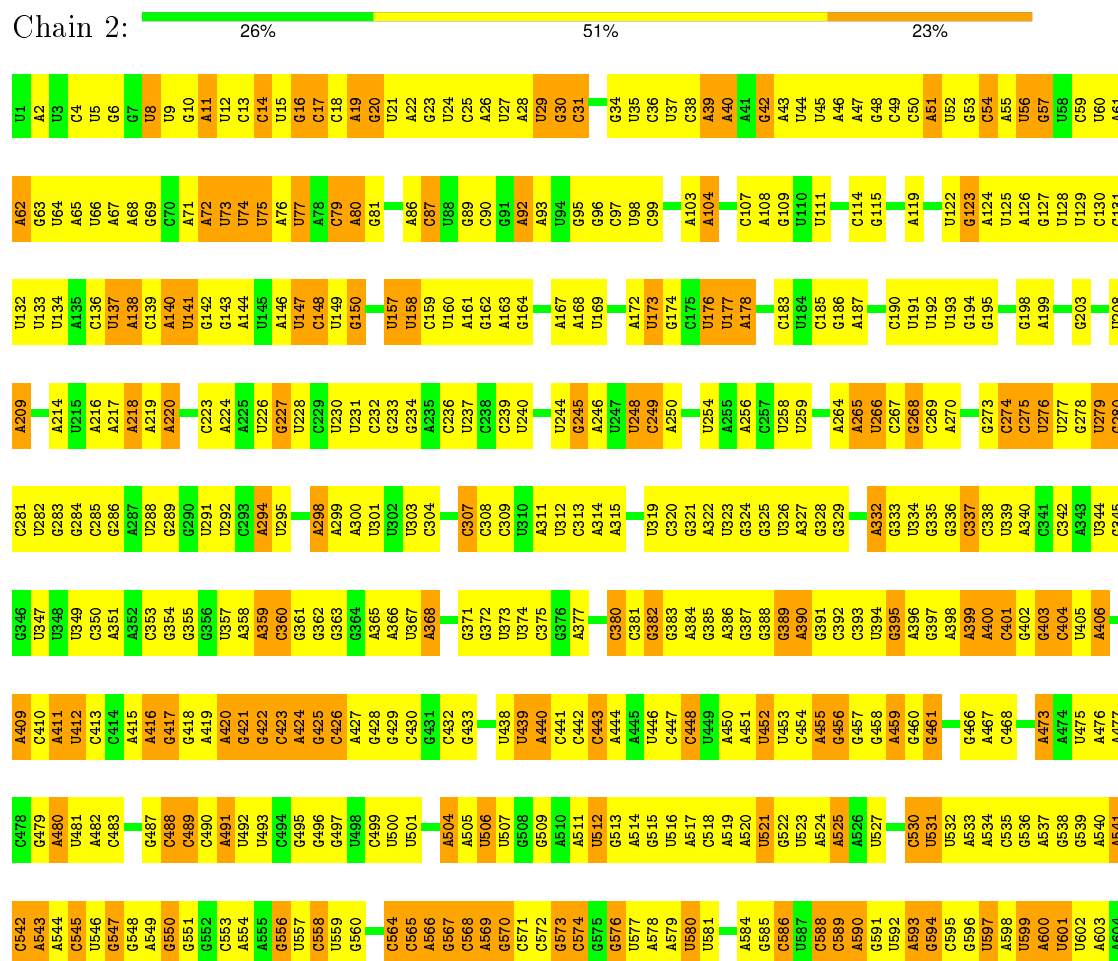
3 Residue-property plots

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

• Molecule 1: Met-tRNAi (U31:A39 variant)

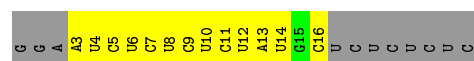


• Molecule 2: 18S rRNA

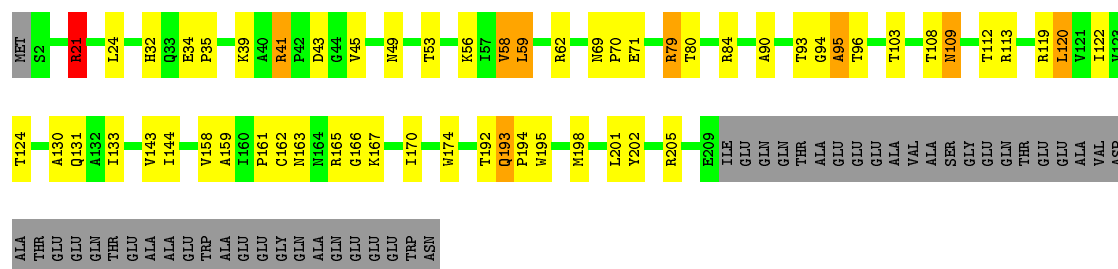


U1619	A1557	C1480	A1420	G1357	U1288	C1221	A1159	U1084	C1032	A966	A897	U827	G761	G688	A605
G1620	U1558	A1451	U1421	C1358	U1289	A1222	C1160	C1095	C1033	U967	G898	A828	A762	G688	G606
C1621	U1559	A1452	A1422	A1359	G1290	A1223	C1161	U1096	G1034	C968	A904	U829	G763	G692	U607
C1622	G1560	C1483	A1423	C1360	G1291	U1224	A1162	U1097		A969	A905	U830	U764	U693	U608
C1623	C1561	G1494	C1424	U1361	A1292	A1225	G1163	U1098	A1038	A970	A906	U831	U765	U694	G609
U1624	A1495	A1425	U1362	U1362	G1293	A1226	G1164	C1099	A1039	G971	U907	U832	U766	U695	U610
U1625	C1486	G1426	G1363	G1363	G1294	G1227	A1165	G1100	G1040	C974	U908	U833	U767	C696	U611
U1626	U1487	G1427	C1364	C1364	A1295	G1228	C1166	G1101	G1041	G975	U909	U834	C768	C697	G612
G1627	U1565	G1428	C1365	C1365	G1296	A1229	U1167	U1102	A1042	G976	C909	U835		U698	G613
U1628	C1489	C1429	G1366	G1366	U1297	U1230	G1168	U1103	U1043	A977	U910	G836	G772	C700	G615
C1629	A1490	U1430	G1367	G1367	G1298	U1231	G1169	U1104	C1044	A978	U911	A814	C773	C700	G616
G1630	A1491	G1431	U1368	U1368	A1299	G1232	A1170	G1106	G1045		U912	U838	C774	G701	U617
A1631	C1492	U1432	U1300	G1370	U1301	G1236	C1172	G1107	G1046		U913	U839	C775	G702	U618
C1632	G1493	G1433	U1302	G1371	U1302	A1237	C1173	G1108	G1047	U981	A914	U840	G776	G703	A618
A1633	U1494	A1434	U1303		U1303	G1237	U1174	G1109	U1048	A982	U915	C841	G777	C704	A619
C1634	U1495	U1435	G1303		G1303	G1240	G1175	G1110	G1049	G983	U916	U842	C778	C705	A620
G1635	G1496	G1436	U1304	C1374	U1304	G1243	C1176	G1111	G1050	G984		U843	C779	A706	A621
G1636	G1497	G1437	U1305	U1375	U1305	A1244	G1177	G1112	G1051	G985	U919	G844	A779	A622	A622
C1637	A1575	C1498	C1438	U1376	U1306	G1245	G1178	G1113	G1052	G986	U920	G845	A780	G623	G623
C1638	U1576	C1499	C1439	C1377	G1307	G1247	G1179	G1114	U1053	A987	G921	A846	A781	C716	G624
G1640	U1577	G1500	U1440	U1378	U1308			U1115	U1054		A922	C847	G782	C717	G630
G1643	U1580	A1503	G1443	G1381	A1311	G1254	A1182	G1116	U1055	A991	A923	C848	A783	U712	G631
C1644	A1581	G1504	A1444	A1382	A1312	U1250	U1184	G1117	U1056	A992	G924	U851	U784	C714	U632
U1648	G1582	G1505	C1445	G1383	U1313	C1251	U1185	U1118	U1057	A993	C925	G852	U785	U715	U633
G1651	U1583	U1506	G1446	G1384	U1314		U1186	G1119	U1058	A994	U927	U853	C786	C716	U634
G1652	A1584	U1507	U1447	G1385	G1315	G1254	G1187	A1123	A1061	A997	C930	A854	A788	C717	U635
C1653	A1585		U1448	A1386	A1316	A1255	A1188	G1124	U1062	U998	U931	A855	U789	U718	U638
U1654	G1586	C1499	G1449	C1387	G1317	U1256	C1189	G1125	G1063	C999	A932	G857	A790	G720	U639
U1655	C1587	U1512	U1450	U1388	A1318	U1257	U1190	G1126	A1064	A1000	C933	A858	U793	U721	U640
G1656	U1588	A1513	G1451	U1389	U1319	U1258	C1191	C1127	C1065	U1003	U934	U859	U794	G722	G641
U1659	C1589	A1514	G1452	U1390	A1320	U1259	A1192	U1128	C1066	U1004	G935	A861	A795	G723	G642
G1660	U1590	U1515	G1453	C1391	C1321	U1260	C1193	G1129	C1067	C1005	C936	U862	C797	G724	U643
G1661	U1593	U1516	G1454	G1392	C1322	U1261	C1194		A1068	C1006	G937	U863	A798	G725	G644
C1662	U1594	U1517	G1455	G1393	G1323	G1262	C1196	A1132	C1069	C1007	A938	A864		G726	U645
U1667	C1597	U1518	G1456	U1396	A1324	G1263	C1197	G1133	U1070	U1008	A940	G865	A803	G727	U646
G1670	U1598	U1520	A1458	C1397	A1328	G1266	G1198	U1135	G1072	C1009	G941	G866	U804	A728	U647
C1671	A1599	G1521	C1459	A1398	G1267	G1267	G1199	A1136	G1073	C1009	G942	G867	A805	G729	U648
U1672	C1600	A1522	A1460	A1399	C1332	U1268	G1200	A1137	C1074	U1011	A943		A806	C731	U649
C1673	A1523	A1461	G1461	G1400	U1333	G1269	A1201	A1138	A1075	A1012	U944	U872	G809	G732	U651
U1674	U1528	G1462	C1463	C1401	U1334	U1270	A1202	G1139	C1076	G1013	U945	G873	A733	C652	C652
C1675	G1529	C1463	C1463	C1402	U1335	U1271	A1203	G1140	C1077	U1014	U946	G874	A734	C653	C653
U1675	U1533	U1465	A1404	A1404	C1337	G1272	C1204	U1141	U1078	C1015	G947	G875	A811	C735	G654
G1676	G1534	U1466	U1466	U1405	C1338	A1273	U1205	A1142	U1079	U1016	C948	G876	U812	C736	G655
G1677	C1535	C1468	A1467	U1406	U1339	U1274	U1207	U1143	A1080	U1017	C949	G877	A813	A737	U656
U1678	U1536	U1469	A1468	A1407	A1340	G1275	G1145	U1144	C1081	A1018	A950	G878	G814	G738	C657
A1679	G1537	C1470	G1440	A1409	A1340	G1276	C1208	G1146	G1082	A1019	A951	C879	G815	C	C
U1680	U1538	U1471	U1411	G1440	A1343	G1277	C1209	A1146	A1083	C1020	G952		A816	C741	G676
U1681	G1539	G1472	U1412	U1411	C1344	C1278	A1210	G1149	G1084	C1021	G953	A883	C817	C742	G677
C1682	U1540	A1473	U1413	A1345	A1345	G1280	G1212	A1150	A1086	U1022	G956	G894	G818	U743	U678
G1683	C1613	G1474	U1414	A1347	U1281	U1281	U1213	A1087	U1023	A1024	U957	U885	U819	U744	U679
U1684	U1544	G1475	A1415	G1348	C1283	U1284	G1214	G1153	U1068	A1025	U958	U887	U821	U745	U681
U1685	G1476	G1476	G1416	G1416	U1284	U1284	C1215	G1154	U1089	A1026	U959	U888	G822	A753	
U1686	C1477	G1477	G1417	U1352	U1285	U1285	A1216	C1155	A1090	C1027		G894	G823	A754	A684
A1687	U1555	A1478	C1418	U1353	A1286	A1286	A1156	C1156	A1091	U1030	A962	U895	U824	A755	A685
C1688	U1556	C1479	A1419	U1353	A1287	G1287	G1218	C1157	A1092	U1031	A965	C896	C826	A760	C687

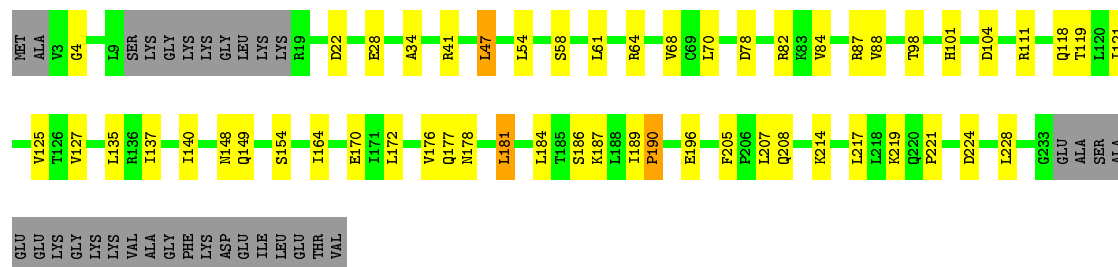
- Molecule 3: mRNA



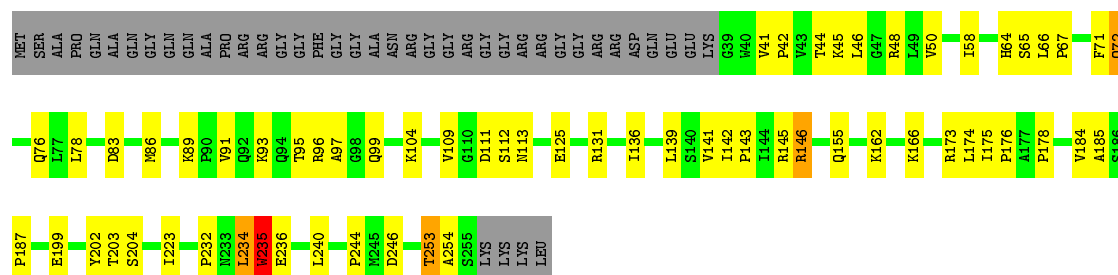
- Molecule 4: uS2



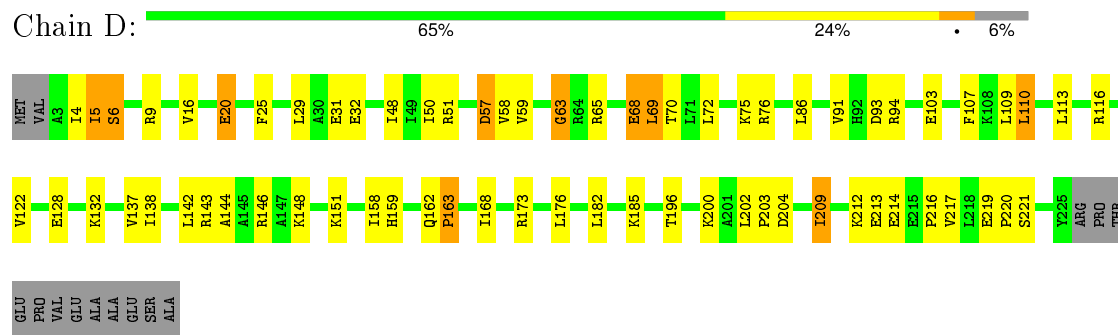
- Molecule 5: eS1



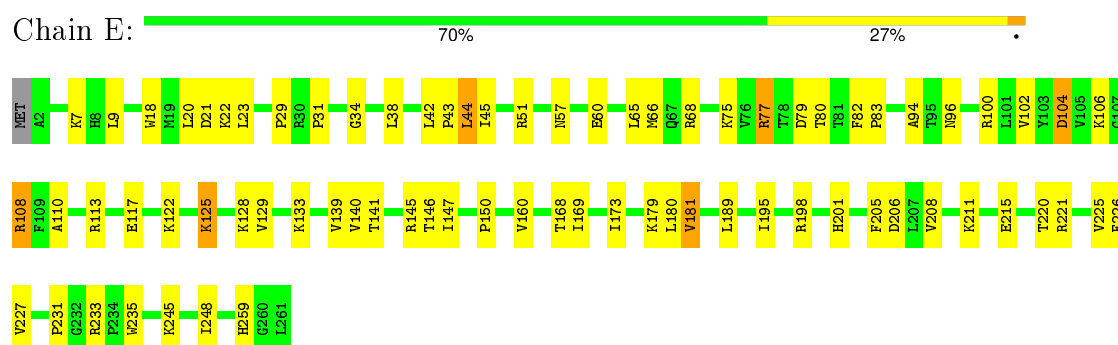
- Molecule 6: uS5



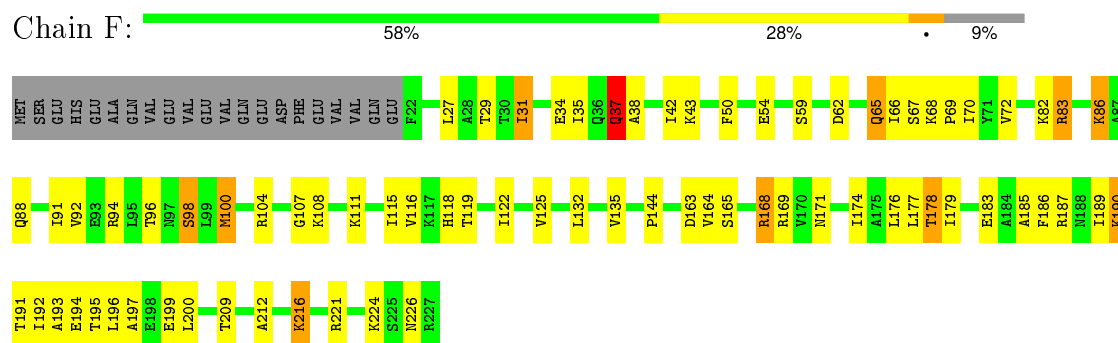
- Molecule 7: uS3



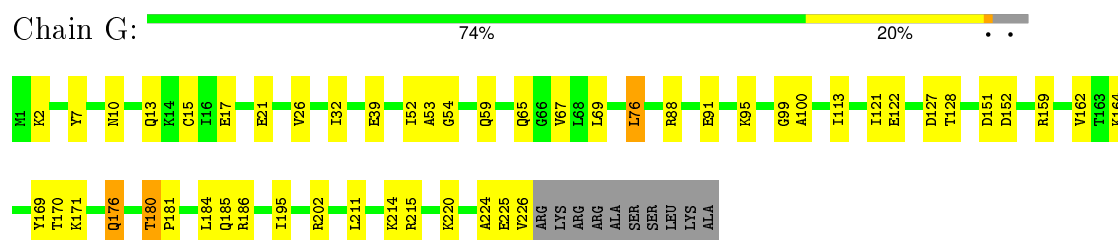
- Molecule 8: eS4



- Molecule 9: uS7

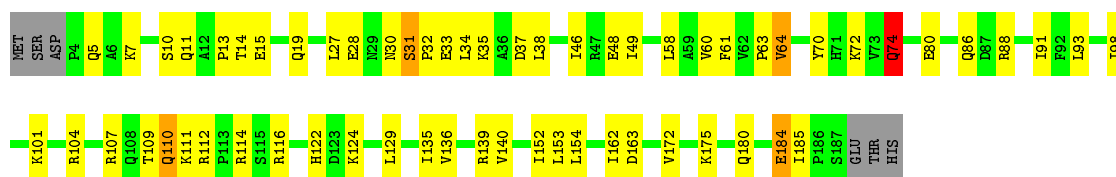


- Molecule 10: eS6

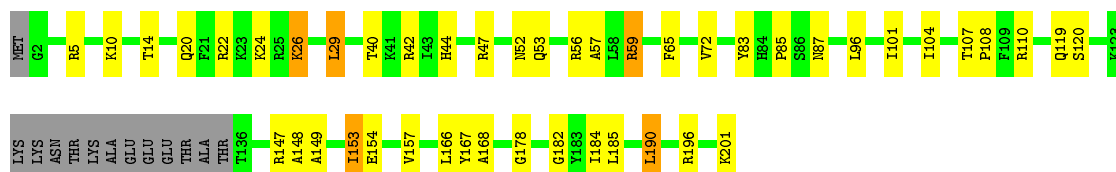


- Molecule 11: eS7

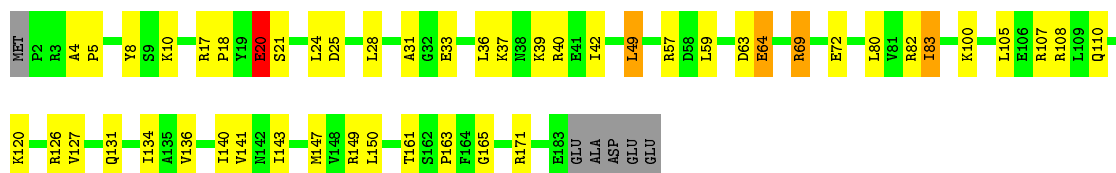




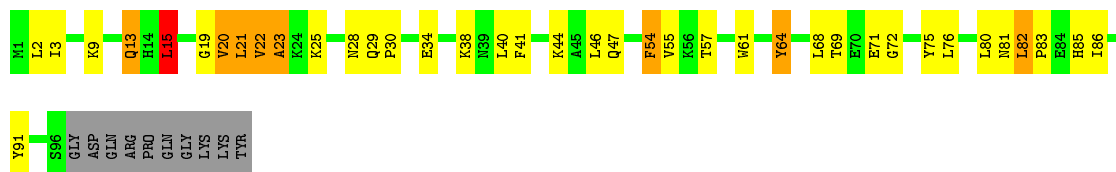
• Molecule 12: eS8



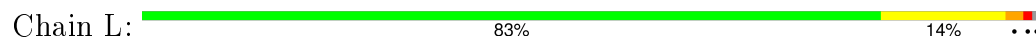
• Molecule 13: uS4



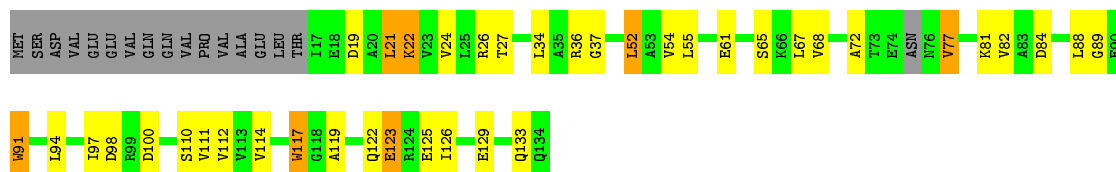
• Molecule 14: eS10



• Molecule 15: uS17



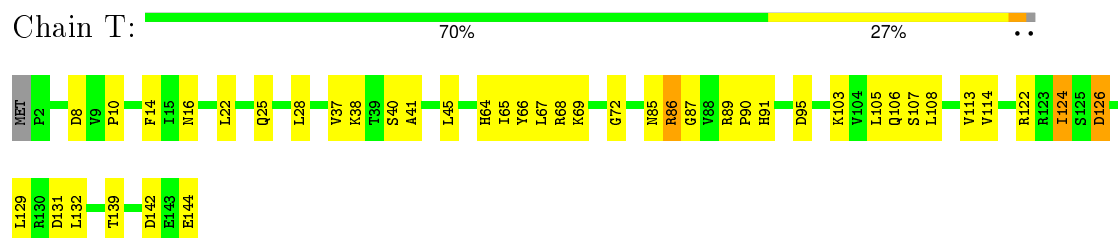
• Molecule 16: eS12



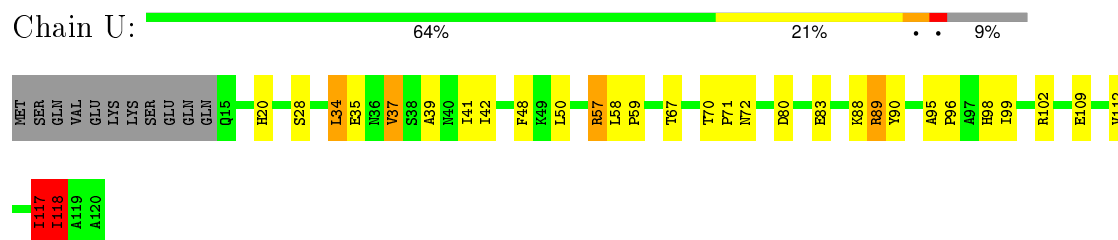
- Molecule 22: uS13



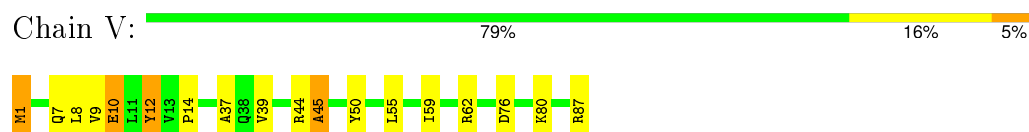
- Molecule 23: eS19



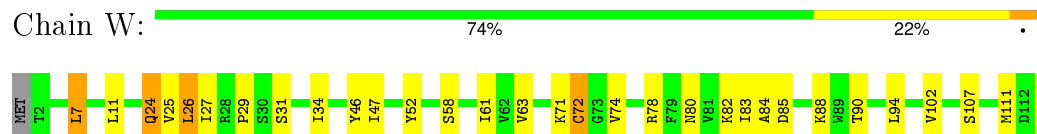
- Molecule 24: uS10



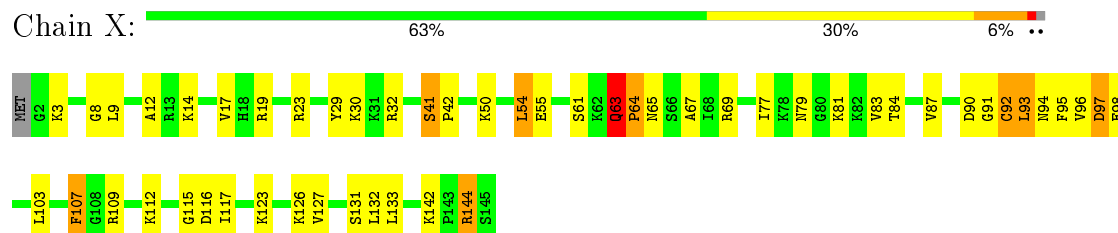
- Molecule 25: eS21




- Molecule 26: uS8



- Molecule 27: uS12



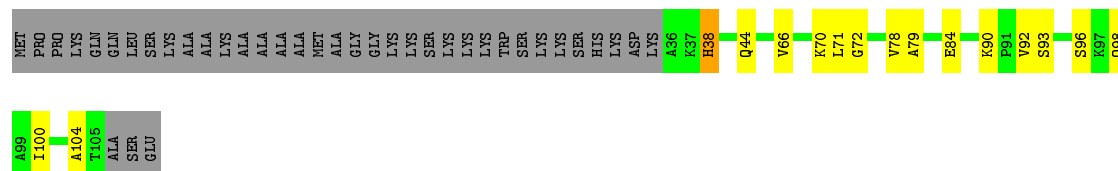
- Molecule 28: eS24

Chain Y: 



- Molecule 29: eS25

Chain Z: 



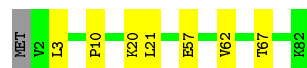
- Molecule 30: eS26

Chain a: 




- Molecule 31: eS27

Chain b: 




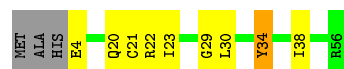
- Molecule 32: eS28

Chain c: 



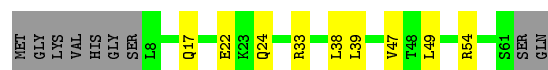
- Molecule 33: uS14

Chain d: 

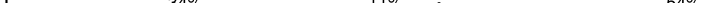


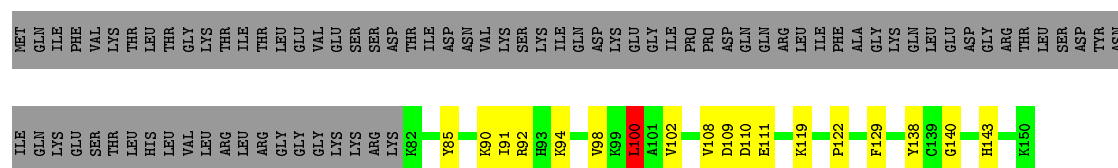
- Molecule 34: eS30

Chain e: 

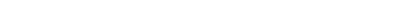


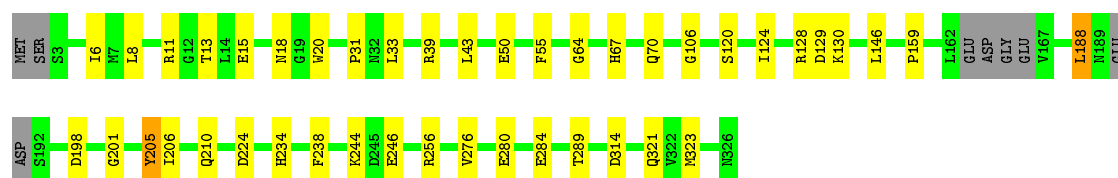
- Molecule 35: eS31

Chain f:  34% 11% 54%



- Molecule 36: RACK1

Chain g:  84% 13% •



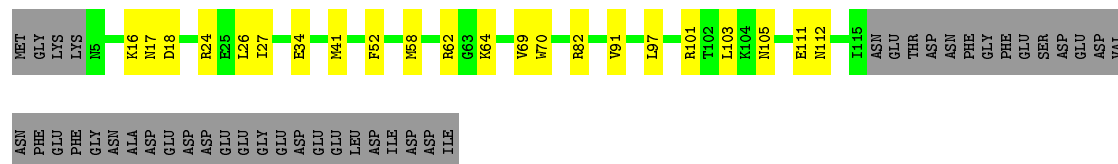
- Molecule 37: eL41

Chain h: 88% 12%



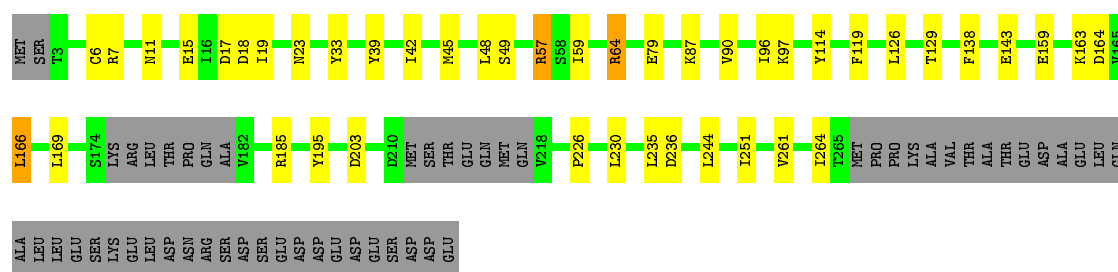
- Molecule 38: eIF1A

Chain i: 58% 14% 27%



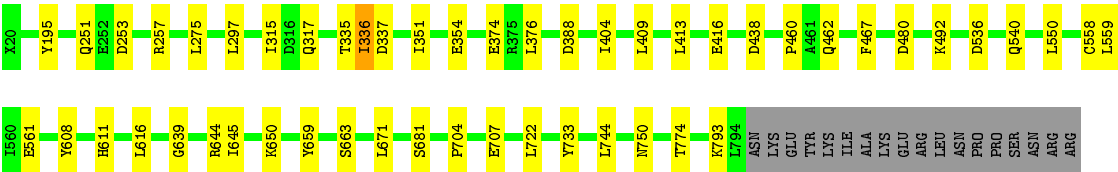
- Molecule 39: eIF2 alpha

Chain j:  67% 13% • 18%



- Molecule 40: eIF2 gamma

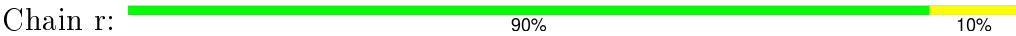
Chain k: 69% 6% 25%



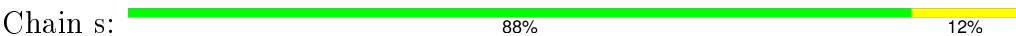
• Molecule 45: eIF3i



• Molecule 46: eIF3b



• Molecule 47: eIF3g



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	21401	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (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: GCP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.38	1/1797 (0.1%)	0.69	0/2799
10	G	0.41	0/1835	0.72	1/2451 (0.0%)
11	H	0.42	0/1507	0.71	0/2028
12	I	0.41	0/1515	0.73	2/2029 (0.1%)
13	J	0.40	0/1495	0.75	1/2001 (0.0%)
14	K	0.48	0/831	0.77	1/1123 (0.1%)
15	L	0.41	0/1276	0.63	0/1718
16	M	0.46	0/891	0.80	1/1201 (0.1%)
17	N	0.41	0/1210	0.77	0/1628
18	O	0.38	0/953	0.68	0/1279
19	P	0.42	0/946	0.71	1/1273 (0.1%)
2	2	0.27	0/42269	0.69	7/65862 (0.0%)
20	Q	0.43	0/1125	0.71	0/1510
21	R	0.43	0/969	0.77	1/1299 (0.1%)
22	S	0.43	0/1212	0.78	0/1629
23	T	0.40	0/1129	0.72	0/1520
24	U	0.40	0/857	0.73	0/1158
25	V	0.36	0/696	0.66	0/938
26	W	0.39	0/1039	0.74	1/1399 (0.1%)
27	X	0.40	0/1137	0.75	2/1516 (0.1%)
28	Y	0.40	0/1075	0.69	0/1433
29	Z	0.44	0/567	0.69	0/762
3	3	0.30	0/317	0.69	0/489
30	a	0.36	0/791	0.67	0/1059
31	b	0.38	0/619	0.65	0/837
32	c	0.38	0/489	0.71	0/655
33	d	0.41	0/457	0.62	0/607
34	e	0.40	0/440	0.73	0/586
35	f	0.49	0/559	0.73	1/747 (0.1%)
36	g	0.41	0/2521	0.64	1/3431 (0.0%)
37	h	0.36	0/234	0.75	0/300
38	i	0.39	0/894	0.70	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	j	0.47	0/2034	0.77	2/2737 (0.1%)
4	A	0.42	0/1666	0.78	2/2279 (0.1%)
40	k	0.47	0/3079	0.70	1/4157 (0.0%)
41	l	0.47	0/1051	0.76	1/1402 (0.1%)
42	m	0.41	0/724	0.75	1/968 (0.1%)
43	o	0.49	0/3796	0.80	0/5128
44	p	0.49	0/4602	0.76	2/6226 (0.0%)
45	q	0.50	0/2757	0.67	0/3733
46	r	0.49	0/282	0.74	0/373
47	s	0.47	0/426	0.64	0/571
5	B	0.40	0/1793	0.72	2/2414 (0.1%)
6	C	0.39	0/1659	0.69	0/2252
7	D	0.42	0/1769	0.72	1/2378 (0.0%)
8	E	0.38	0/2122	0.67	0/2861
9	F	0.41	0/1628	0.75	0/2198
All	All	0.38	1/103040 (0.0%)	0.71	32/148132 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	X	0	1
28	Y	0	1
41	l	0	1
9	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.88	1.49	1.61

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	685	A	C2'-C3'-O3'	8.09	127.30	109.50
12	I	29	LEU	CA-CB-CG	7.26	132.00	115.30
39	j	166	LEU	CA-CB-CG	6.66	130.62	115.30
41	l	191	LEU	CA-CB-CG	6.50	130.25	115.30
26	W	26	LEU	CA-CB-CG	6.10	129.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1157	C	C4'-C3'-O3'	5.95	124.91	113.00
19	P	56	LEU	CA-CB-CG	5.90	128.87	115.30
44	p	550	LEU	CA-CB-CG	5.81	128.67	115.30
2	2	1491	A	C2'-C3'-O3'	5.74	122.88	113.70
12	I	190	LEU	CA-CB-CG	5.71	128.44	115.30
5	B	181	LEU	CA-CB-CG	5.70	128.40	115.30
27	X	9	LEU	CA-CB-CG	5.70	128.40	115.30
7	D	110	LEU	CA-CB-CG	5.67	128.35	115.30
13	J	49	LEU	CA-CB-CG	5.64	128.28	115.30
2	2	279	U	C2'-C3'-O3'	5.63	122.71	113.70
42	m	76	GLU	N-CA-C	-5.63	95.81	111.00
44	p	376	LEU	CA-CB-CG	5.61	128.21	115.30
39	j	126	LEU	CA-CB-CG	5.60	128.19	115.30
2	2	700	C	C2'-C3'-O3'	5.55	122.59	113.70
5	B	184	LEU	CA-CB-CG	5.54	128.04	115.30
2	2	704	C	N1-C1'-C2'	5.48	121.12	114.00
10	G	76	LEU	CA-CB-CG	5.42	127.76	115.30
35	f	100	LEU	CA-CB-CG	5.33	127.56	115.30
4	A	59	LEU	CA-CB-CG	5.24	127.36	115.30
2	2	1430	U	C2'-C3'-O3'	5.23	122.07	113.70
21	R	53	TYR	CB-CA-C	5.15	120.69	110.40
36	g	188	LEU	CA-CB-CG	5.15	127.14	115.30
4	A	201	LEU	CA-CB-CG	5.13	127.10	115.30
27	X	93	LEU	CA-CB-CG	5.06	126.94	115.30
14	K	15	LEU	CA-CB-CG	5.05	126.92	115.30
16	M	21	LEU	CA-CB-CG	5.03	126.87	115.30
40	k	462	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	191	THR	Peptide
27	X	63	GLN	Peptide
28	Y	29	HIS	Peptide
41	l	158	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1607	0	815	48	0
2	2	37797	0	19016	882	0
3	3	287	0	149	2	0
4	A	1626	0	1633	20	0
5	B	1769	0	1829	13	0
6	C	1629	0	1710	26	0
7	D	1744	0	1826	24	0
8	E	2078	0	2157	24	0
9	F	1609	0	1679	30	0
10	G	1812	0	1911	23	0
11	H	1483	0	1579	18	0
12	I	1489	0	1504	19	0
13	J	1471	0	1554	16	0
14	K	809	0	810	17	0
15	L	1248	0	1311	10	0
16	M	885	0	917	17	0
17	N	1187	0	1251	18	0
18	O	942	0	979	18	0
19	P	927	0	971	17	0
20	Q	1105	0	1170	19	0
21	R	959	0	1006	17	0
22	S	1193	0	1217	22	0
23	T	1110	0	1124	18	0
24	U	845	0	913	13	0
25	V	687	0	682	7	0
26	W	1021	0	1056	14	0
27	X	1119	0	1198	20	0
28	Y	1061	0	1111	11	0
29	Z	558	0	585	7	0
30	a	779	0	831	0	0
31	b	609	0	630	0	0
32	c	487	0	528	0	0
33	d	446	0	436	0	0
34	e	433	0	470	0	0
35	f	546	0	557	0	0
36	g	2466	0	2406	0	0
37	h	233	0	284	0	0
38	i	884	0	891	0	0
39	j	2006	0	2066	0	0
40	k	3034	0	3195	0	0
41	l	1036	0	1079	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	m	716	0	742	0	0
43	o	4189	0	3874	0	0
44	p	4899	0	4599	0	0
45	q	2693	0	2609	0	0
46	r	277	0	273	0	0
47	s	418	0	411	0	0
48	2	80	0	0	0	0
48	k	1	0	0	0	0
49	a	1	0	0	0	0
49	b	1	0	0	0	0
49	f	1	0	0	0	0
49	l	1	0	0	0	0
50	k	8	0	8	0	0
51	k	32	0	14	0	0
All	All	98333	0	79566	1306	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 9.

All (1306) 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)
2:2:567:G:H22	2:2:573:G:N2	1.34	1.24
2:2:567:G:N2	2:2:573:G:H22	1.36	1.23
2:2:480:A:N1	2:2:506:U:O4	1.89	1.05
2:2:1292:U:O4	2:2:1321:A:N1	1.89	1.05
1:1:18:G:H1'	1:1:58:A:N1	1.71	1.04
2:2:991:A:N1	2:2:1011:U:O4	1.92	1.02
2:2:299:A:H2'	2:2:300:A:C8	1.94	1.01
1:1:14:A:H3'	1:1:15:G:C5'	1.91	1.01
2:2:1396:U:H3'	2:2:1397:C:H5'	1.41	1.01
1:1:14:A:C2'	1:1:15:G:H5''	1.91	1.00
1:1:18:G:H1'	1:1:58:A:C2	1.97	1.00
2:2:420:A:H2	2:2:421:G:H8	1.07	0.97
1:1:14:A:C3'	1:1:15:G:H5''	1.93	0.97
2:2:991:A:N6	2:2:1011:U:H3	1.65	0.94
2:2:763:G:H1	2:2:772:G:H1	1.14	0.94
2:2:420:A:H2	2:2:421:G:C8	1.85	0.94
2:2:1266:G:H1	2:2:1440:U:H3	1.14	0.94
2:2:420:A:C2	2:2:421:G:H8	1.87	0.93
2:2:1583:U:C4	2:2:1609:A:N1	2.36	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:157:U:H4'	2:2:158:U:OP1	1.69	0.92
1:1:15:G:H2'	1:1:16:U:O4'	1.72	0.90
2:2:1292:U:C4	2:2:1321:A:N1	2.40	0.88
1:1:14:A:C3'	1:1:15:G:C5'	2.48	0.88
2:2:40:A:H62	2:2:466:G:H21	1.21	0.88
2:2:1583:U:O4	2:2:1609:A:N1	2.06	0.88
2:2:1402:C:H2'	2:2:1403:G:H8	1.39	0.88
2:2:480:A:N1	2:2:506:U:C4	2.41	0.87
2:2:1670:G:H2'	2:2:1671:G:C8	2.10	0.87
2:2:645:U:H3	2:2:688:G:H1	1.23	0.86
2:2:1289:U:H2'	2:2:1290:G:C8	2.10	0.86
2:2:991:A:H61	2:2:1011:U:H3	0.90	0.86
2:2:1402:C:H2'	2:2:1403:G:C8	2.11	0.86
8:E:106:LYS:HB3	8:E:108:ARG:HE	1.43	0.84
1:1:14:A:O2'	1:1:15:G:H5''	1.79	0.83
2:2:763:G:H22	2:2:772:G:H22	1.27	0.83
2:2:1292:U:O4	2:2:1321:A:C6	2.32	0.82
2:2:1774:A:H2'	2:2:1775:G:C8	2.14	0.81
2:2:709:C:H2'	2:2:710:U:H4'	1.62	0.81
2:2:20:G:H4'	2:2:570:G:N7	1.96	0.80
2:2:1391:C:H42	2:2:1403:G:H1	1.30	0.80
2:2:394:U:H3'	2:2:395:G:H8	1.46	0.80
15:L:54:ILE:HG23	15:L:55:ASP:H	1.48	0.78
19:P:30:THR:O	19:P:34:VAL:HG23	1.84	0.78
2:2:1085:A:H2'	2:2:1086:A:C8	2.19	0.78
2:2:1332:C:H42	2:2:1416:G:H1	1.31	0.78
6:C:50:VAL:HG12	6:C:76:GLN:HE21	1.49	0.77
1:1:37:A:H2'	1:1:38:A:C8	2.19	0.76
2:2:1108:G:H1	2:2:1135:U:H3	1.29	0.76
2:2:732:G:H1'	2:2:734:A:H61	1.51	0.75
2:2:97:C:H2'	2:2:98:U:C6	2.21	0.75
1:1:74:C:H4'	1:1:75:C:O5'	1.86	0.75
2:2:1583:U:O2	2:2:1583:U:H2'	1.86	0.75
2:2:1559:U:H2'	2:2:1560:G:H8	1.53	0.74
2:2:1292:U:O4	2:2:1321:A:C2	2.41	0.74
2:2:420:A:C2	2:2:421:G:C8	2.70	0.74
2:2:591:G:H2'	2:2:592:U:O4'	1.86	0.74
1:1:28:A:H2'	1:1:29:G:C8	2.23	0.74
2:2:1017:U:H2'	2:2:1017:U:O2	1.86	0.74
9:F:118:HIS:O	9:F:122:ILE:HG12	1.89	0.73
2:2:419:A:H3'	2:2:420:A:H8	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:925:A:H4'	2:2:1015:C:H4'	1.70	0.73
5:B:149:GLN:HE22	5:B:154:SER:HB3	1.54	0.73
2:2:480:A:C6	2:2:506:U:O4	2.42	0.73
2:2:771:A:H3'	2:2:772:G:H8	1.54	0.72
2:2:17:C:H2'	2:2:18:C:C6	2.24	0.72
19:P:108:ARG:HB2	19:P:109:PRO:HD3	1.72	0.72
6:C:142:ILE:HG13	6:C:143:PRO:HD2	1.72	0.71
6:C:111:ASP:CG	6:C:112:SER:H	1.94	0.71
2:2:1157:C:N4	2:2:1162:A:H61	1.86	0.71
2:2:452:U:O2	2:2:452:U:H2'	1.89	0.71
2:2:360:C:C2	2:2:383:G:N2	2.58	0.71
2:2:1768:U:H2'	2:2:1769:U:C6	2.24	0.71
5:B:186:SER:O	5:B:190:PRO:HD3	1.89	0.71
25:V:1:MET:HA	25:V:10:GLU:HB2	1.71	0.71
2:2:642:G:N2	2:2:692:C:C2	2.59	0.71
2:2:1671:G:H2'	2:2:1672:C:C6	2.26	0.70
2:2:15:U:H2'	2:2:16:G:O4'	1.89	0.70
2:2:1670:G:H2'	2:2:1671:G:H8	1.57	0.70
2:2:1290:G:H1	2:2:1323:G:H22	1.38	0.70
7:D:6:SER:HB2	7:D:9:ARG:HB2	1.73	0.70
2:2:1044:C:H42	2:2:1072:G:H1	1.39	0.70
2:2:804:U:O2	2:2:804:U:H2'	1.92	0.70
2:2:39:A:H2	2:2:466:G:H22	1.37	0.70
2:2:952:G:H2'	2:2:953:G:C8	2.27	0.70
26:W:11:LEU:HD12	26:W:74:VAL:HG23	1.74	0.70
1:1:14:A:H3'	1:1:15:G:H5'	1.73	0.69
12:I:166:LEU:HB3	12:I:184:ILE:HD11	1.73	0.69
2:2:1413:U:H2'	2:2:1413:U:O2	1.92	0.69
2:2:567:G:H1	2:2:573:G:H1	0.84	0.69
2:2:1320:A:H2	4:A:131:GLN:NE2	1.90	0.69
2:2:399:A:C6	12:I:26:LYS:HG3	2.27	0.69
2:2:1221:C:H2'	2:2:1222:A:C8	2.27	0.69
2:2:394:U:H3'	2:2:395:G:C8	2.28	0.69
2:2:51:A:H61	2:2:439:U:H3	1.38	0.68
2:2:1176:C:H4'	2:2:1188:A:H61	1.56	0.68
2:2:419:A:H3'	2:2:420:A:C8	2.28	0.68
2:2:1198:G:H4'	2:2:1199:G:O5'	1.93	0.68
2:2:946:U:HO2'	2:2:947:G:H8	1.41	0.68
13:J:31:ALA:HA	13:J:36:LEU:HD12	1.76	0.68
18:O:81:ILE:HB	18:O:115:ILE:HG22	1.76	0.68
10:G:162:VAL:HG21	10:G:171:LYS:HZ2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:137:VAL:HB	7:D:185:LYS:HB2	1.73	0.68
2:2:1206:C:H42	2:2:1454:C:H41	1.40	0.68
2:2:30:G:H4'	27:X:131:SER:HB2	1.75	0.68
2:2:993:G:C6	2:2:1009:C:N4	2.62	0.67
2:2:1774:A:H2'	2:2:1775:G:H8	1.57	0.67
1:1:9:G:H21	1:1:43:G:H3'	1.57	0.67
2:2:703:G:N2	2:2:736:C:C2	2.62	0.67
2:2:399:A:H4'	2:2:400:A:H5''	1.77	0.67
2:2:1217:G:N2	2:2:1442:A:OP2	2.27	0.67
2:2:1380:A:H2'	2:2:1381:G:C8	2.30	0.67
2:2:1207:A:H2'	2:2:1207:A:N3	2.09	0.67
4:A:70:PRO:HB2	4:A:94:GLY:HA3	1.77	0.66
2:2:894:G:H1	2:2:916:U:H3	1.43	0.66
2:2:1157:C:H4'	2:2:1158:C:OP1	1.95	0.66
1:1:26:G:C2	1:1:27:C:N3	2.63	0.66
2:2:1221:C:H2'	2:2:1222:A:H8	1.61	0.66
2:2:1198:G:H2'	2:2:1198:G:N3	2.11	0.66
2:2:29:U:O2	2:2:29:U:H2'	1.96	0.66
2:2:337:C:H5''	12:I:10:LYS:HG3	1.77	0.66
2:2:771:A:H3'	2:2:772:G:C8	2.31	0.66
2:2:1344:A:H2'	2:2:1347:A:N6	2.10	0.66
2:2:1293:G:H21	2:2:1320:A:H8	1.44	0.66
2:2:999:C:H2'	2:2:1000:A:H3'	1.78	0.66
2:2:984:G:H1	2:2:1015:C:H5	1.44	0.66
2:2:459:A:H3'	2:2:460:G:H8	1.61	0.66
20:Q:22:VAL:HG12	20:Q:65:ILE:HG12	1.78	0.66
2:2:1492:C:H42	2:2:1511:G:H1	1.44	0.66
1:1:26:G:C6	1:1:27:C:N4	2.64	0.65
2:2:992:A:H3'	2:2:993:G:H5''	1.79	0.65
2:2:867:G:H1	2:2:959:U:H3	1.43	0.65
2:2:1285:U:H2'	2:2:1286:A:O4'	1.96	0.65
2:2:147:U:H5''	2:2:148:C:H5	1.61	0.65
2:2:1115:A:H62	2:2:1129:G:H21	1.44	0.65
13:J:64:GLU:HA	13:J:69:ARG:HD2	1.79	0.65
2:2:1775:G:H1	2:2:1782:C:H42	1.45	0.65
2:2:1564:U:H5'	22:S:39:GLY:HA3	1.78	0.65
2:2:1161:C:N3	2:2:1614:G:C2	2.65	0.65
2:2:480:A:C2	2:2:506:U:O4	2.49	0.64
2:2:922:A:H2'	2:2:923:A:C8	2.32	0.64
2:2:444:A:H8	2:2:524:A:H5''	1.63	0.64
2:2:873:C:H2'	2:2:874:G:C8	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:763:G:O6	2:2:772:G:O6	2.14	0.64
2:2:1583:U:O4	2:2:1609:A:C6	2.51	0.64
2:2:763:G:H22	2:2:772:G:N2	1.93	0.64
2:2:803:A:C4	2:2:804:U:H6	2.15	0.64
2:2:597:U:O2	2:2:597:U:H2'	1.97	0.64
2:2:443:C:H1'	2:2:444:A:C2	2.32	0.64
2:2:1437:C:H2'	2:2:1438:C:C6	2.33	0.64
8:E:31:PRO:HG3	8:E:43:PRO:HG3	1.78	0.64
7:D:58:VAL:O	7:D:65:ARG:HB3	1.97	0.64
7:D:69:LEU:HA	7:D:72:LEU:HD12	1.79	0.64
2:2:930:C:H3'	2:2:931:U:H5''	1.79	0.64
2:2:410:C:H2'	2:2:410:C:O2	1.98	0.64
2:2:1050:G:N2	2:2:1067:C:C2	2.66	0.64
2:2:1292:U:C4	2:2:1321:A:C2	2.86	0.63
2:2:991:A:N1	2:2:1011:U:C4	2.66	0.63
2:2:601:U:H5''	27:X:32:ARG:HH21	1.63	0.63
1:1:28:A:H2'	1:1:29:G:H8	1.61	0.63
2:2:1159:A:H2'	2:2:1160:C:C6	2.33	0.63
2:2:1380:A:H2'	2:2:1381:G:H8	1.63	0.63
2:2:1601:U:H2'	2:2:1602:U:C6	2.33	0.63
24:U:39:ALA:O	24:U:42:ILE:HG22	1.98	0.63
2:2:267:C:H3'	10:G:186:ARG:HH22	1.63	0.63
2:2:1540:G:C5'	23:T:87:GLY:HA3	2.29	0.63
2:2:566:A:C6	2:2:567:G:H1'	2.34	0.63
2:2:107:C:H2'	2:2:108:A:C8	2.33	0.63
2:2:823:G:C6	2:2:848:C:N3	2.66	0.63
2:2:409:A:H3'	2:2:410:C:C6	2.34	0.63
27:X:63:GLN:HB3	27:X:64:PRO:CD	2.29	0.63
2:2:1267:G:H1	2:2:1439:C:H42	1.45	0.62
2:2:55:A:H3'	2:2:402:G:H1	1.64	0.62
2:2:1043:U:C2	2:2:1044:C:H5	2.17	0.62
10:G:2:LYS:HG3	10:G:17:GLU:HG3	1.80	0.62
2:2:1408:A:O2'	2:2:1409:A:C8	2.52	0.62
2:2:530:C:H3'	2:2:531:U:H5''	1.80	0.62
2:2:480:A:H61	2:2:506:U:H3	1.47	0.62
2:2:826:C:H2'	2:2:827:U:C6	2.34	0.62
2:2:1073:G:C6	2:2:1074:C:N4	2.68	0.62
10:G:67:VAL:HB	10:G:99:GLY:HA2	1.82	0.62
2:2:703:G:C2	2:2:736:C:N3	2.68	0.62
2:2:1772:G:H2'	2:2:1773:U:O4'	1.99	0.62
22:S:68:ARG:O	22:S:72:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:86:LEU:HD23	22:S:86:LEU:H	1.64	0.62
16:M:34:LEU:HD13	16:M:36:ARG:HH21	1.64	0.62
4:A:130:ALA:HA	4:A:133:ILE:HD12	1.82	0.62
7:D:48:ILE:HB	7:D:86:LEU:HD23	1.82	0.62
2:2:1475:G:H1	2:2:1528:C:H42	1.46	0.62
2:2:588:C:HO2'	2:2:589:C:H6	1.46	0.62
2:2:1439:C:H2'	2:2:1440:U:H6	1.63	0.61
2:2:1132:A:O2'	2:2:1133:C:O4'	2.18	0.61
23:T:126:ASP:HA	23:T:129:LEU:HD12	1.82	0.61
2:2:360:C:N3	2:2:383:G:C2	2.69	0.61
1:1:25:C:H2'	1:1:26:G:C8	2.35	0.61
5:B:87:ARG:HB3	5:B:101:HIS:HB2	1.82	0.61
2:2:107:C:H5''	2:2:382:G:O2'	2.00	0.61
2:2:274:C:N4	2:2:275:C:N4	2.49	0.61
2:2:29:U:O2	2:2:30:G:N7	2.32	0.61
2:2:491:A:N3	2:2:491:A:H2'	2.15	0.61
16:M:129:GLU:HA	16:M:133:GLN:HB2	1.83	0.61
2:2:1788:A:C2	2:2:1789:A:C6	2.89	0.61
12:I:57:ALA:HB2	12:I:178:GLY:HA2	1.83	0.61
23:T:67:LEU:HB3	23:T:68:ARG:HD2	1.83	0.61
2:2:1294:G:H2'	2:2:1295:A:H5'	1.82	0.61
2:2:1083:A:H2'	2:2:1084:G:O4'	2.01	0.61
2:2:1559:U:H2'	2:2:1560:G:C8	2.36	0.60
27:X:63:GLN:C	27:X:65:ASN:H	2.05	0.60
2:2:1540:G:H5''	23:T:87:GLY:HA3	1.83	0.60
2:2:1639:C:H2'	2:2:1640:G:C8	2.36	0.60
2:2:363:G:N2	2:2:380:C:C2	2.68	0.60
2:2:1338:C:H42	2:2:1383:G:H1	1.49	0.60
2:2:1295:A:H2'	2:2:1296:G:O4'	2.02	0.60
2:2:952:G:H2'	2:2:953:G:H8	1.65	0.60
2:2:599:U:O2	2:2:599:U:H2'	2.00	0.60
2:2:779:A:H1'	2:2:781:A:H62	1.67	0.60
10:G:32:ILE:HG23	10:G:53:ALA:HA	1.84	0.60
13:J:141:VAL:HG12	13:J:143:ILE:H	1.67	0.60
18:O:61:MET:HG3	18:O:104:ALA:HB2	1.83	0.59
2:2:403:G:N2	2:2:404:C:C2	2.69	0.59
1:1:3:C:H42	1:1:70:G:H1	1.48	0.59
1:1:25:C:H2'	1:1:26:G:H8	1.65	0.59
2:2:760:A:C2	2:2:761:G:H1'	2.38	0.59
2:2:815:G:H2'	2:2:816:A:H8	1.66	0.59
8:E:45:ILE:HG13	8:E:80:THR:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:732:G:H1'	2:2:734:A:N6	2.16	0.59
27:X:50:LYS:HB3	27:X:77:ILE:HD12	1.85	0.59
1:1:18:G:C1'	1:1:58:A:C2	2.81	0.59
14:K:3:ILE:HG12	14:K:41:PHE:HB2	1.83	0.59
16:M:19:ASP:HA	16:M:22:LYS:HE3	1.84	0.59
2:2:393:C:H2'	2:2:394:U:O4'	2.03	0.59
2:2:1462:G:C6	2:2:1463:C:N4	2.71	0.59
12:I:83:TYR:HD2	12:I:101:ILE:HD13	1.68	0.59
16:M:88:LEU:HA	16:M:91:TRP:HD1	1.67	0.59
2:2:866:G:OP1	17:N:3:ARG:HA	2.01	0.59
2:2:1157:C:H42	2:2:1162:A:H61	1.50	0.58
2:2:1043:U:H3'	2:2:1043:U:O2	2.03	0.58
2:2:79:C:H3'	2:2:80:A:H8	1.68	0.58
2:2:16:G:H21	2:2:1137:A:H62	1.51	0.58
2:2:1133:C:H2'	2:2:1134:U:O4'	2.03	0.58
2:2:1651:C:H2'	2:2:1652:G:O4'	2.03	0.58
2:2:476:A:H2'	2:2:477:A:H8	1.67	0.58
12:I:85:PRO:HB3	15:L:12:ALA:HB2	1.85	0.58
2:2:444:A:C8	2:2:524:A:H5''	2.39	0.58
2:2:597:U:O2	2:2:597:U:C2'	2.51	0.58
2:2:865:G:H5''	17:N:2:GLY:HA2	1.84	0.58
16:M:52:LEU:HB3	16:M:114:VAL:HB	1.85	0.58
2:2:291:U:H2'	2:2:292:U:C6	2.38	0.58
2:2:1229:A:H2'	2:2:1230:U:O4'	2.03	0.58
2:2:590:A:H2'	2:2:591:G:C8	2.39	0.58
11:H:140:VAL:HB	26:W:52:TYR:HB3	1.85	0.58
2:2:1499:C:H42	2:2:1504:G:H1	1.52	0.58
2:2:1620:G:N2	2:2:1621:C:C2	2.70	0.58
2:2:1215:C:C2	2:2:1446:G:N2	2.71	0.58
2:2:1047:G:H1	2:2:1069:C:H42	1.50	0.58
2:2:1332:C:N4	2:2:1416:G:H1	1.99	0.58
16:M:24:VAL:HG21	16:M:52:LEU:HG	1.86	0.58
2:2:550:G:H1	2:2:572:C:H42	1.52	0.58
2:2:42:G:H1	2:2:432:C:H42	1.52	0.58
2:2:923:A:H2'	2:2:924:G:C8	2.39	0.58
2:2:817:C:H42	2:2:852:G:H1	1.52	0.57
2:2:887:U:H2'	2:2:888:U:C6	2.38	0.57
2:2:309:C:H42	2:2:355:G:H1	1.52	0.57
2:2:108:A:H2'	2:2:109:G:C8	2.38	0.57
16:M:88:LEU:HA	16:M:91:TRP:CD1	2.39	0.57
2:2:448:C:N4	2:2:456:G:O6	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:34:GLY:HA3	8:E:83:PRO:HG2	1.84	0.57
1:1:14:A:C2'	1:1:15:G:C5'	2.75	0.57
2:2:1396:U:H3'	2:2:1397:C:C5'	2.27	0.57
2:2:1782:C:H2'	2:2:1783:U:C6	2.39	0.57
2:2:698:U:H2'	2:2:699:U:C6	2.39	0.57
2:2:1472:G:H2'	2:2:1473:A:C8	2.40	0.57
12:I:167:TYR:HB3	12:I:185:LEU:HD12	1.86	0.57
2:2:619:A:H2'	2:2:620:A:C8	2.39	0.57
2:2:360:C:H2'	2:2:361:G:H8	1.69	0.57
1:1:49:C:H42	1:1:65:G:H1	1.52	0.57
2:2:208:U:H2'	2:2:209:A:O4'	2.05	0.57
2:2:813:A:H61	2:2:856:U:H3	1.52	0.57
2:2:245:G:H2'	2:2:246:A:C8	2.39	0.57
2:2:107:C:H2'	2:2:108:A:H8	1.68	0.57
2:2:1038:A:H4'	25:V:62:ARG:HH12	1.70	0.57
26:W:102:VAL:HB	26:W:113:HIS:HB3	1.85	0.57
27:X:67:ALA:HB3	27:X:69:ARG:HE	1.69	0.57
2:2:545:C:H42	2:2:591:G:H1	1.53	0.57
2:2:1651:C:H42	2:2:1745:G:H1	1.51	0.57
2:2:617:U:H3'	2:2:618:A:H5''	1.86	0.57
2:2:598:A:H2'	2:2:599:U:H6	1.69	0.57
21:R:28:PHE:O	21:R:32:LYS:HB2	2.05	0.57
2:2:1603:G:N2	2:2:1604:C:C2	2.72	0.57
26:W:27:ILE:HB	26:W:61:ILE:HB	1.87	0.57
2:2:57:G:H1	2:2:90:C:H42	1.53	0.57
1:1:18:G:H4'	1:1:60:A:C2	2.40	0.56
2:2:823:G:N1	2:2:848:C:C2	2.73	0.56
2:2:1062:U:H3'	2:2:1063:G:H8	1.69	0.56
2:2:363:G:C2	2:2:380:C:C2	2.93	0.56
12:I:107:THR:N	12:I:108:PRO:HD2	2.19	0.56
2:2:992:A:H3'	2:2:993:G:C5'	2.35	0.56
2:2:548:G:H1	2:2:588:C:H5	1.53	0.56
4:A:56:LYS:HZ1	4:A:159:ALA:HB3	1.70	0.56
2:2:1097:U:H1'	26:W:71:LYS:HD2	1.85	0.56
1:1:2:G:H1	1:1:71:C:H42	1.53	0.56
2:2:780:A:H8	28:Y:8:ARG:HB3	1.70	0.56
2:2:423:C:O2	2:2:427:A:N6	2.38	0.56
2:2:524:A:H2'	2:2:525:A:C8	2.41	0.56
2:2:266:U:H2'	2:2:267:C:H6	1.71	0.56
1:1:10:G:C6	1:1:11:C:N4	2.73	0.56
2:2:1344:A:H2'	2:2:1347:A:H62	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:702:G:H1	2:2:736:C:H42	1.54	0.56
2:2:1482:G:H21	2:2:1604:C:H1'	1.69	0.56
2:2:267:C:H5''	10:G:186:ARG:HH12	1.70	0.56
2:2:634:A:H2'	2:2:635:A:O4'	2.05	0.56
25:V:39:VAL:HA	25:V:45:ALA:HA	1.87	0.56
2:2:1140:G:H2'	2:2:1141:A:C8	2.41	0.56
24:U:57:ARG:HG3	24:U:89:ARG:HG2	1.87	0.56
28:Y:37:LYS:HA	28:Y:40:LEU:HD12	1.86	0.56
2:2:1232:G:H1	2:2:1251:C:H42	1.54	0.56
2:2:1174:U:O2	2:2:1174:U:H2'	2.06	0.56
15:L:99:ARG:HD3	27:X:8:GLY:O	2.05	0.56
2:2:1158:C:H5'	2:2:1159:A:H5''	1.86	0.56
2:2:1155:C:H42	2:2:1620:G:H1	1.53	0.56
2:2:412:U:O2	2:2:412:U:H2'	2.05	0.56
2:2:566:A:H3'	2:2:567:G:H5''	1.88	0.55
2:2:1043:U:C2	2:2:1044:C:C5	2.94	0.55
2:2:558:C:H2'	2:2:558:C:O2	2.05	0.55
6:C:136:ILE:HA	6:C:139:LEU:HD12	1.87	0.55
2:2:337:C:H2'	2:2:338:C:C6	2.41	0.55
12:I:168:ALA:HB2	12:I:184:ILE:HD12	1.89	0.55
2:2:1161:C:C2	2:2:1614:G:N2	2.75	0.55
6:C:175:ILE:HB	6:C:202:TYR:HB2	1.87	0.55
2:2:40:A:N6	2:2:466:G:H21	1.99	0.55
2:2:395:G:H22	2:2:397:G:H3'	1.71	0.55
11:H:30:ASN:HB2	11:H:34:LEU:HB2	1.89	0.55
2:2:638:U:H5	11:H:101:LYS:H	1.54	0.55
10:G:211:LEU:O	10:G:214:LYS:HG2	2.06	0.55
9:F:86:LYS:HD3	9:F:94:ARG:HH12	1.72	0.55
2:2:1226:A:H5'	2:2:1228:G:O4'	2.06	0.55
1:1:2:G:C6	1:1:3:C:N4	2.74	0.55
6:C:184:VAL:HB	6:C:202:TYR:HA	1.88	0.55
2:2:1671:G:C2	2:2:1672:C:C2	2.95	0.55
13:J:39:LYS:HA	13:J:42:ILE:HD12	1.88	0.55
2:2:1174:U:C2'	2:2:1174:U:O2	2.55	0.55
2:2:1320:A:H4'	2:2:1321:A:OP1	2.06	0.55
2:2:30:G:H2'	2:2:31:C:C6	2.42	0.55
2:2:1380:A:P	24:U:59:PRO:HA	2.46	0.55
1:1:10:G:N2	1:1:11:C:C2	2.75	0.55
2:2:703:G:C2	2:2:736:C:C2	2.95	0.54
2:2:865:G:H2'	2:2:866:G:C8	2.41	0.54
27:X:103:LEU:HB3	27:X:126:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:617:U:H3'	2:2:618:A:C5'	2.38	0.54
2:2:440:A:H2'	2:2:441:C:C6	2.42	0.54
2:2:1267:G:H1	2:2:1439:C:N4	2.05	0.54
2:2:273:G:C6	2:2:274:C:N4	2.76	0.54
2:2:1464:G:N2	2:2:1465:C:C2	2.75	0.54
2:2:1711:G:H3'	2:2:1712:A:C8	2.42	0.54
2:2:823:G:C2	2:2:848:C:O2	2.61	0.54
2:2:835:U:H2'	2:2:836:G:O4'	2.07	0.54
6:C:48:ARG:HE	6:C:254:ALA:H	1.55	0.54
2:2:1557:A:H1'	22:S:134:ARG:HB3	1.90	0.54
2:2:1052:G:H1	2:2:1065:C:H42	1.56	0.54
2:2:843:A:H2'	2:2:844:G:C8	2.43	0.54
8:E:179:LYS:HA	8:E:231:PRO:HD3	1.88	0.54
2:2:1671:G:C6	2:2:1672:C:N4	2.76	0.54
28:Y:8:ARG:HH22	28:Y:28:LEU:HD13	1.73	0.54
13:J:140:ILE:HD13	28:Y:65:GLY:HA3	1.88	0.54
18:O:30:VAL:HG12	18:O:39:ILE:HB	1.90	0.54
2:2:804:U:C2'	2:2:804:U:O2	2.55	0.54
2:2:1306:U:H3'	2:2:1307:G:H8	1.72	0.54
2:2:1315:G:N2	2:2:1316:C:C2	2.76	0.54
2:2:223:C:H2'	2:2:224:A:C8	2.43	0.54
2:2:8:U:H3	2:2:1138:A:N6	2.04	0.54
2:2:993:G:C2	2:2:1009:C:N3	2.76	0.54
7:D:32:GLU:HG3	7:D:57:ASP:HB3	1.88	0.54
6:C:234:LEU:HD11	25:V:14:PRO:HD2	1.90	0.54
6:C:72:GLN:NE2	6:C:72:GLN:H	2.06	0.54
7:D:209:ILE:HG22	21:R:38:ILE:HG23	1.90	0.54
2:2:1466:U:H2'	2:2:1467:A:O4'	2.08	0.53
2:2:1775:G:H1	2:2:1782:C:N4	2.05	0.53
2:2:617:U:O4	2:2:1086:A:N6	2.40	0.53
2:2:1338:C:C2	2:2:1384:G:C2	2.96	0.53
2:2:473:A:N6	2:2:593:A:OP1	2.41	0.53
2:2:163:A:H2'	2:2:164:G:C8	2.43	0.53
2:2:613:C:H42	2:2:1106:G:H1	1.56	0.53
18:O:80:HIS:CD2	18:O:114:ARG:HB2	2.43	0.53
28:Y:18:LEU:HB2	28:Y:20:ARG:HG2	1.90	0.53
2:2:1480:C:O4'	2:2:1480:C:O2	2.26	0.53
2:2:1062:U:H3'	2:2:1063:G:C8	2.44	0.53
2:2:829:U:H2'	2:2:830:U:O4'	2.09	0.53
4:A:53:THR:HG22	4:A:161:PRO:HG2	1.89	0.53
2:2:28:A:N1	2:2:596:G:O6	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1588:G:N2	2:2:1589:C:C2	2.77	0.53
2:2:1399:A:P	21:R:60:ARG:HH12	2.31	0.53
2:2:1003:U:O2	2:2:1003:U:H2'	2.09	0.53
2:2:1086:A:H2'	2:2:1087:A:C8	2.44	0.53
2:2:1270:G:N2	2:2:1438:C:C2	2.77	0.53
26:W:85:ASP:HA	26:W:88:LYS:HE3	1.90	0.53
2:2:1258:U:N3	2:2:1259:U:H5	2.06	0.53
2:2:12:U:H2'	2:2:13:C:C6	2.44	0.53
2:2:405:U:H2'	2:2:406:A:C8	2.43	0.53
2:2:421:G:H3'	2:2:422:G:C8	2.43	0.53
2:2:763:G:N2	2:2:772:G:H22	2.02	0.53
2:2:403:G:N1	2:2:404:C:C4	2.76	0.53
1:1:2:G:C2	1:1:3:C:N3	2.77	0.53
2:2:1258:U:H2'	2:2:1259:U:H5'	1.90	0.53
2:2:737:A:HO2'	2:2:738:G:H8	1.56	0.53
4:A:21:ARG:HD2	4:A:24:LEU:HD13	1.91	0.53
2:2:1120:C:H42	2:2:1125:G:H1	1.56	0.53
2:2:387:G:N3	2:2:387:G:H2'	2.23	0.52
2:2:1044:C:N4	2:2:1072:G:H1	2.06	0.52
2:2:803:A:C4	2:2:804:U:C6	2.97	0.52
2:2:30:G:C6	2:2:31:C:N4	2.77	0.52
2:2:1161:C:N4	2:2:1614:G:C6	2.77	0.52
2:2:599:U:O2	2:2:599:U:C2'	2.57	0.52
2:2:865:G:H2'	2:2:866:G:H8	1.74	0.52
1:1:10:G:C2	1:1:11:C:C4	2.98	0.52
4:A:35:PRO:HG3	25:V:87:ARG:HH21	1.74	0.52
2:2:914:A:H5''	2:2:914:A:H8	1.74	0.52
2:2:925:A:H3'	2:2:926:C:H6	1.73	0.52
2:2:1512:U:O4'	2:2:1512:U:O2	2.26	0.52
2:2:409:A:H3'	2:2:410:C:H6	1.75	0.52
2:2:1727:C:H2'	2:2:1728:A:O4'	2.09	0.52
20:Q:115:THR:HB	20:Q:119:ALA:HA	1.91	0.52
12:I:154:GLU:HB3	12:I:157:VAL:HG23	1.91	0.52
11:H:31:SER:HB2	11:H:32:PRO:HD3	1.92	0.52
2:2:567:G:N2	2:2:568:C:C2	2.77	0.52
2:2:1781:C:H2'	2:2:1782:C:C6	2.44	0.52
9:F:27:LEU:HB2	9:F:31:ILE:HD11	1.91	0.52
2:2:488:C:H2'	2:2:489:C:H5	1.73	0.52
4:A:124:THR:HG22	4:A:174:TRP:HE1	1.74	0.52
23:T:14:PHE:HA	23:T:139:THR:HG21	1.90	0.52
2:2:1240:G:H5'	19:P:77:ARG:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:91:ASP:HB3	22:S:95:GLY:H	1.75	0.52
2:2:1363:G:N2	2:2:1364:C:C2	2.78	0.52
9:F:98:SER:HB3	9:F:178:THR:HG21	1.91	0.52
2:2:711:G:H1	2:2:727:C:H42	1.56	0.52
2:2:18:C:H4'	2:2:1136:A:H61	1.73	0.52
27:X:107:PHE:HA	27:X:123:LYS:HD2	1.90	0.52
29:Z:90:LYS:HE2	29:Z:104:ALA:HA	1.91	0.52
29:Z:66:VAL:HG22	29:Z:72:GLY:HA2	1.90	0.52
2:2:173:U:H3'	2:2:174:G:H8	1.73	0.52
2:2:1290:G:H22	2:2:1323:G:N2	2.08	0.52
2:2:1215:C:N3	2:2:1446:G:C2	2.78	0.52
12:I:107:THR:HG22	12:I:110:ARG:HH21	1.75	0.52
2:2:1203:A:H2'	2:2:1204:C:C6	2.44	0.52
20:Q:127:LYS:HA	20:Q:134:ALA:HA	1.89	0.52
2:2:1585:A:H2'	2:2:1586:G:H8	1.75	0.52
5:B:47:LEU:HD23	18:O:37:GLU:HG2	1.91	0.52
2:2:1583:U:H3	2:2:1609:A:H61	1.56	0.52
2:2:1206:C:H42	2:2:1454:C:N4	2.06	0.52
2:2:548:G:H2'	2:2:549:A:O4'	2.09	0.52
13:J:105:LEU:HA	13:J:108:ARG:HD3	1.91	0.52
2:2:40:A:H62	2:2:466:G:N2	2.01	0.52
2:2:1560:G:N2	2:2:1561:C:C2	2.78	0.52
2:2:1586:G:H1	2:2:1606:U:H3	1.58	0.52
11:H:109:THR:O	11:H:110:GLN:HG2	2.10	0.52
2:2:1298:G:H2'	2:2:1299:A:C8	2.45	0.52
2:2:1423:A:H1'	6:C:97:ALA:HB1	1.92	0.52
2:2:421:G:N3	2:2:421:G:H2'	2.24	0.51
2:2:530:C:H3'	2:2:531:U:C5'	2.40	0.51
5:B:137:ILE:HD12	5:B:172:LEU:HD22	1.92	0.51
17:N:62:GLN:HB2	17:N:65:VAL:HB	1.92	0.51
21:R:84:TYR:O	21:R:85:VAL:HB	2.10	0.51
2:2:28:A:H2'	2:2:29:U:O4'	2.09	0.51
2:2:1073:G:C2	2:2:1074:C:C4	2.99	0.51
2:2:1469:A:H62	2:2:1536:U:H3	1.56	0.51
2:2:1446:G:H2'	2:2:1446:G:N3	2.25	0.51
2:2:1171:G:H2'	2:2:1172:C:O4'	2.09	0.51
2:2:1468:C:H4'	2:2:1538:G:H21	1.74	0.51
2:2:74:U:H4'	2:2:75:U:OP1	2.09	0.51
28:Y:53:ASP:HB3	28:Y:96:LEU:HD21	1.91	0.51
2:2:1245:C:O2	2:2:1245:C:O4'	2.27	0.51
1:1:9:G:N2	1:1:43:G:H3'	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1578:C:H2'	2:2:1579:C:C6	2.46	0.51
2:2:1126:G:N2	2:2:1127:C:C2	2.79	0.51
2:2:838:U:H2'	2:2:839:U:O4'	2.11	0.51
2:2:1377:C:H2'	2:2:1377:C:O2	2.08	0.51
2:2:1603:G:N1	2:2:1604:C:C4	2.78	0.51
27:X:63:GLN:HB3	27:X:64:PRO:HD2	1.92	0.51
13:J:110:GLN:HE22	13:J:126:ARG:HB2	1.75	0.51
4:A:49:ASN:HA	21:R:109:LEU:HD11	1.91	0.51
2:2:360:C:H2'	2:2:361:G:C8	2.46	0.51
2:2:1154:G:N2	2:2:1622:C:C2	2.77	0.51
2:2:52:U:H2'	2:2:53:G:H8	1.76	0.51
2:2:1484:G:H3'	2:2:1485:A:H8	1.75	0.51
2:2:762:A:H2'	2:2:762:A:N3	2.24	0.51
2:2:1362:U:H5''	2:2:1363:G:H8	1.74	0.51
2:2:481:U:H3	2:2:504:A:H61	1.57	0.51
6:C:232:PRO:HA	6:C:235:TRP:CD2	2.46	0.51
9:F:82:LYS:HG2	9:F:83:ARG:H	1.75	0.51
29:Z:93:SER:HB3	29:Z:100:ILE:HD12	1.91	0.51
2:2:1432:U:H2'	2:2:1432:U:O2	2.10	0.51
2:2:1058:C:O4'	2:2:1058:C:O2	2.27	0.51
2:2:1400:G:H4'	21:R:4:VAL:HG13	1.92	0.51
2:2:452:U:O2	2:2:452:U:C2'	2.55	0.51
4:A:58:VAL:O	4:A:62:ARG:HG3	2.11	0.51
2:2:1417:G:C6	2:2:1418:C:N4	2.79	0.51
2:2:360:C:C2	2:2:383:G:C2	2.99	0.51
2:2:455:A:H2'	2:2:456:G:O4'	2.11	0.51
2:2:429:G:N2	2:2:430:C:C2	2.79	0.51
9:F:190:LYS:HD2	9:F:195:THR:HG22	1.93	0.51
14:K:82:LEU:HD12	14:K:86:ILE:HG21	1.92	0.51
16:M:37:GLY:O	16:M:111:VAL:HB	2.11	0.51
7:D:5:ILE:HG21	7:D:9:ARG:HH11	1.75	0.51
2:2:778:G:H2'	2:2:779:A:H8	1.75	0.51
18:O:80:HIS:HD2	18:O:114:ARG:HB2	1.74	0.51
2:2:140:A:H2	2:2:265:A:H4'	1.76	0.51
22:S:3:LEU:H	29:Z:78:VAL:HG11	1.76	0.50
21:R:3:ARG:H	21:R:3:ARG:NE	2.09	0.50
16:M:117:TRP:HA	16:M:117:TRP:CE3	2.46	0.50
2:2:1413:U:C2'	2:2:1413:U:O2	2.59	0.50
2:2:815:G:H2'	2:2:816:A:C8	2.46	0.50
2:2:1497:G:C2	2:2:1507:C:O2	2.64	0.50
2:2:1143:U:H2'	2:2:1144:U:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1176:C:H42	2:2:1460:G:H1	1.58	0.50
2:2:218:A:H2'	2:2:219:A:H8	1.76	0.50
2:2:8:U:N3	2:2:1138:A:N6	2.59	0.50
2:2:1043:U:O2	2:2:1043:U:C2'	2.60	0.50
2:2:1185:U:H2'	2:2:1186:U:O4'	2.12	0.50
2:2:1149:G:H2'	2:2:1766:G:N3	2.27	0.50
11:H:58:LEU:HD21	11:H:88:ARG:HH11	1.77	0.50
2:2:21:U:H4'	13:J:18:PRO:HG3	1.93	0.50
2:2:163:A:H2'	2:2:164:G:H8	1.75	0.50
2:2:1679:A:C8	10:G:65:GLN:HG3	2.47	0.50
2:2:1452:G:H4'	19:P:81:ARG:HH21	1.77	0.50
8:E:125:LYS:HB2	8:E:226:PHE:CE2	2.47	0.50
2:2:249:C:H2'	2:2:250:A:H8	1.75	0.50
2:2:1432:U:O4	2:2:1434:A:N7	2.45	0.50
2:2:1417:G:C2	2:2:1418:C:N3	2.79	0.50
2:2:564:C:N4	2:2:576:G:C6	2.80	0.50
15:L:84:ILE:HB	15:L:111:VAL:CG2	2.42	0.50
2:2:1042:A:C4	2:2:1043:U:H6	2.29	0.50
9:F:65:GLN:HE22	9:F:68:LYS:HB2	1.77	0.50
2:2:605:A:C8	2:2:607:U:H2'	2.45	0.50
2:2:1594:C:O4'	2:2:1594:C:O2	2.27	0.50
2:2:39:A:H2'	2:2:39:A:N3	2.26	0.50
12:I:44:HIS:HB2	12:I:56:ARG:HB2	1.93	0.50
2:2:786:G:H2'	2:2:786:G:N3	2.27	0.50
2:2:1462:G:C2	2:2:1463:C:N3	2.79	0.50
2:2:1343:A:H4'	2:2:1344:A:OP1	2.12	0.50
13:J:82:ARG:HH21	13:J:149:ARG:HD3	1.77	0.50
2:2:1659:U:H2'	2:2:1660:G:C8	2.47	0.50
2:2:1117:G:H3'	2:2:1118:G:H8	1.77	0.49
22:S:57:ARG:HB2	22:S:60:GLU:HB2	1.94	0.49
2:2:840:U:O2	2:2:840:U:H2'	2.11	0.49
2:2:1768:U:H2'	2:2:1769:U:H6	1.74	0.49
2:2:531:U:H2'	2:2:532:U:O4'	2.12	0.49
16:M:68:VAL:HG21	16:M:111:VAL:HG21	1.93	0.49
9:F:144:PRO:HD3	9:F:216:LYS:HE3	1.93	0.49
2:2:1192:A:H1'	2:2:1281:U:H4'	1.94	0.49
2:2:1195:A:H4'	2:2:1196:C:H5''	1.94	0.49
2:2:884:G:H2'	2:2:885:U:C6	2.47	0.49
2:2:859:U:O4'	11:H:114:ARG:HD2	2.12	0.49
2:2:395:G:N2	2:2:397:G:H3'	2.26	0.49
2:2:930:C:H3'	2:2:931:U:C5'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:266:U:H2'	2:2:267:C:C6	2.47	0.49
20:Q:87:LYS:HA	20:Q:90:VAL:HG22	1.94	0.49
2:2:1389:A:H61	2:2:1405:U:H3	1.60	0.49
2:2:50:C:H2'	2:2:423:C:H41	1.77	0.49
1:1:23:C:H2'	1:1:24:G:C8	2.46	0.49
13:J:17:ARG:HB3	13:J:20:GLU:HG3	1.93	0.49
17:N:94:LYS:O	17:N:98:VAL:HG23	2.11	0.49
2:2:1756:U:H2'	2:2:1757:C:C6	2.48	0.49
2:2:1671:G:C6	2:2:1672:C:C4	3.01	0.49
2:2:570:G:H21	2:2:570:G:P	2.35	0.49
2:2:1539:G:H21	2:2:1568:A:H62	1.58	0.49
14:K:80:LEU:HB3	14:K:82:LEU:HD23	1.94	0.49
2:2:71:A:H3'	2:2:72:A:H5''	1.93	0.49
2:2:805:A:C2	2:2:806:A:C5	3.00	0.49
2:2:1600:C:H2'	2:2:1601:U:C6	2.46	0.49
2:2:1602:U:H2'	2:2:1603:G:H8	1.77	0.49
2:2:1073:G:C2	2:2:1074:C:N3	2.81	0.49
2:2:1793:U:HO2'	2:2:1795:A:H2	1.60	0.49
2:2:419:A:C3'	2:2:420:A:H8	2.24	0.49
2:2:1583:U:C2'	2:2:1583:U:O2	2.56	0.49
2:2:1558:U:O2	2:2:1558:U:O4'	2.30	0.49
2:2:14:C:H42	2:2:1139:G:H1	1.60	0.49
2:2:1165:A:N1	2:2:1577:U:O4	2.45	0.49
14:K:80:LEU:O	14:K:81:ASN:HB3	2.12	0.49
2:2:1736:U:H2'	2:2:1737:C:C6	2.48	0.49
2:2:1714:C:H2'	2:2:1715:G:O4'	2.13	0.49
2:2:698:U:H1'	11:H:107:ARG:HG2	1.94	0.49
2:2:248:U:H3'	2:2:249:C:H5'	1.94	0.49
2:2:1075:A:H2'	2:2:1076:C:O4'	2.13	0.49
14:K:15:LEU:HD22	14:K:68:LEU:HD11	1.95	0.49
2:2:176:U:H3'	2:2:177:U:H2'	1.94	0.49
2:2:387:G:C8	2:2:422:G:N2	2.80	0.49
2:2:1162:A:H2'	2:2:1163:G:O4'	2.12	0.49
2:2:1454:C:O2	2:2:1454:C:O4'	2.28	0.49
2:2:365:A:H2'	2:2:366:A:C8	2.48	0.49
2:2:56:U:O4'	2:2:56:U:O2	2.31	0.49
12:I:42:ARG:HE	12:I:59:ARG:HD2	1.78	0.49
27:X:91:GLY:O	27:X:93:LEU:N	2.46	0.49
2:2:642:G:C2	2:2:692:C:N3	2.81	0.49
2:2:1170:A:H2'	2:2:1171:G:C8	2.48	0.49
18:O:85:ALA:HB2	18:O:94:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:162:G:H2'	2:2:163:A:H8	1.78	0.49
2:2:1393:G:O6	2:2:1401:C:N4	2.45	0.48
2:2:162:G:H2'	2:2:163:A:C8	2.48	0.48
5:B:135:LEU:HD23	5:B:217:LEU:HA	1.93	0.48
21:R:9:VAL:HG22	21:R:50:ILE:HG13	1.95	0.48
11:H:63:PRO:O	11:H:64:VAL:HB	2.13	0.48
2:2:1486:G:H3'	2:2:1513:A:H61	1.78	0.48
6:C:111:ASP:CG	6:C:112:SER:N	2.63	0.48
26:W:11:LEU:HD13	26:W:72:CYS:HB3	1.94	0.48
2:2:1161:C:C2	2:2:1614:G:C2	3.01	0.48
2:2:1788:A:H2'	2:2:1789:A:C8	2.48	0.48
2:2:886:A:C5	2:2:887:U:C5	3.01	0.48
7:D:107:PHE:O	7:D:110:LEU:HG	2.13	0.48
2:2:1243:A:N3	2:2:1243:A:H2'	2.28	0.48
2:2:946:U:O2'	2:2:947:G:H8	1.93	0.48
2:2:1381:G:H2'	2:2:1382:A:C8	2.48	0.48
2:2:273:G:H1	2:2:281:C:H42	1.60	0.48
2:2:1786:G:H2'	2:2:1787:G:O4'	2.13	0.48
2:2:844:G:H2'	2:2:845:G:O4'	2.13	0.48
11:H:28:GLU:HB3	11:H:35:LYS:HE3	1.94	0.48
2:2:325:G:H2'	2:2:326:U:C6	2.49	0.48
24:U:58:LEU:HD21	24:U:90:TYR:HD1	1.78	0.48
2:2:1671:G:C5	2:2:1672:C:C4	3.01	0.48
2:2:644:C:H2'	2:2:645:U:O4'	2.14	0.48
2:2:1085:A:H2'	2:2:1086:A:H8	1.73	0.48
2:2:701:U:H2'	2:2:702:G:O4'	2.13	0.48
1:1:13:C:H42	1:1:22:G:H1	1.61	0.48
2:2:1231:U:H2'	2:2:1232:G:H8	1.78	0.48
2:2:1605:G:H2'	2:2:1606:U:C6	2.48	0.48
2:2:1679:A:H5'	2:2:1680:U:C6	2.48	0.48
2:2:1502:G:H4'	23:T:41:ALA:HB2	1.93	0.48
22:S:115:ARG:O	22:S:119:ILE:HG13	2.14	0.48
9:F:135:VAL:HA	9:F:200:LEU:HD21	1.95	0.48
2:2:1091:A:H2'	2:2:1091:A:N3	2.28	0.48
2:2:1156:A:O2'	2:2:1158:C:OP1	2.30	0.48
2:2:1068:A:H2'	2:2:1069:C:O4'	2.13	0.48
2:2:1464:G:C6	2:2:1465:C:N4	2.81	0.48
2:2:1106:G:H2'	2:2:1107:G:N3	2.28	0.48
2:2:488:C:H2'	2:2:489:C:C5	2.48	0.48
6:C:89:LYS:HG3	6:C:104:LYS:HB3	1.95	0.48
2:2:298:A:H2'	2:2:299:A:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:867:G:H22	2:2:959:U:H3	1.61	0.48
2:2:1651:C:N4	2:2:1745:G:H1	2.11	0.48
2:2:1277:G:C2	2:2:1278:C:C2	3.02	0.48
2:2:639:U:H2'	2:2:640:G:O4'	2.14	0.48
23:T:86:ARG:HH11	23:T:89:ARG:HB3	1.78	0.48
6:C:178:PRO:HG3	13:J:57:ARG:HE	1.78	0.48
2:2:1287:G:H8	2:2:1287:G:O5'	1.97	0.48
2:2:566:A:H3'	2:2:567:G:C5'	2.43	0.48
2:2:1292:U:H2'	4:A:109:ASN:HD21	1.78	0.48
2:2:392:C:H5''	2:2:399:A:C2	2.49	0.48
2:2:1050:G:C2	2:2:1067:C:C2	3.01	0.48
2:2:1357:G:H1	2:2:1364:C:H42	1.59	0.48
5:B:58:SER:HA	5:B:61:LEU:HD12	1.94	0.48
2:2:1771:C:C2	2:2:1787:G:N2	2.81	0.48
2:2:141:U:H2'	2:2:142:G:H8	1.79	0.48
2:2:444:A:H61	2:2:460:G:N2	2.12	0.48
2:2:410:C:H2'	2:2:411:A:O4'	2.14	0.48
2:2:1746:G:H2'	2:2:1747:A:C8	2.49	0.48
14:K:13:GLN:HA	14:K:80:LEU:HD21	1.94	0.48
22:S:112:ASP:O	22:S:116:LEU:HG	2.13	0.48
23:T:105:LEU:HA	23:T:108:LEU:HD12	1.95	0.48
2:2:1504:G:H2'	2:2:1505:G:O4'	2.14	0.48
16:M:89:GLY:HA2	16:M:94:LEU:HD13	1.96	0.48
15:L:14:GLN:HB3	15:L:54:ILE:HG12	1.96	0.47
10:G:32:ILE:HD12	10:G:100:ALA:HA	1.95	0.47
2:2:1204:C:H5''	2:2:1205:U:C5	2.49	0.47
2:2:323:U:H2'	2:2:324:G:C8	2.48	0.47
2:2:940:A:C2	2:2:975:G:H5'	2.49	0.47
1:1:74:C:H4'	1:1:75:C:C5'	2.45	0.47
2:2:642:G:C2	2:2:692:C:C2	3.02	0.47
1:1:3:C:N4	1:1:70:G:H1	2.12	0.47
23:T:113:VAL:HG23	23:T:114:VAL:HG23	1.95	0.47
2:2:1209:C:H2'	2:2:1210:A:H8	1.79	0.47
2:2:877:G:H2'	2:2:878:G:C8	2.49	0.47
2:2:642:G:N1	2:2:692:C:C4	2.83	0.47
2:2:877:G:H1	2:2:949:C:H42	1.62	0.47
28:Y:129:ALA:O	28:Y:133:ASN:HB2	2.14	0.47
2:2:453:U:C2	8:E:66:MET:HG3	2.49	0.47
22:S:49:LYS:HG3	22:S:81:ILE:HD11	1.95	0.47
2:2:444:A:H1'	2:2:524:A:H5''	1.95	0.47
7:D:72:LEU:HA	14:K:20:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1389:A:H4'	21:R:28:PHE:HE2	1.78	0.47
1:1:10:G:C2	1:1:11:C:N3	2.82	0.47
2:2:1586:G:C2	2:2:1587:C:C2	3.02	0.47
2:2:646:G:H2'	2:2:647:G:O4'	2.14	0.47
2:2:1571:A:H4'	2:2:1572:G:O5'	2.14	0.47
2:2:1014:U:H3'	2:2:1015:C:H5'	1.96	0.47
2:2:1137:A:H2'	2:2:1138:A:C8	2.50	0.47
2:2:832:U:H5'	2:2:833:G:H5''	1.96	0.47
2:2:597:U:C2	2:2:598:A:C8	3.02	0.47
16:M:21:LEU:O	16:M:24:VAL:HG22	2.15	0.47
2:2:1497:G:C6	2:2:1507:C:N3	2.82	0.47
2:2:805:A:H2	2:2:806:A:C5	2.33	0.47
2:2:1631:A:H5''	2:2:1631:A:C8	2.49	0.47
2:2:1182:A:C8	19:P:100:LYS:HD2	2.50	0.47
2:2:862:A:H2'	2:2:864:A:C8	2.50	0.47
21:R:4:VAL:C	21:R:5:ARG:HE	2.17	0.47
5:B:187:LYS:O	5:B:190:PRO:HD2	2.14	0.47
2:2:1127:C:H2'	2:2:1128:U:O4'	2.15	0.47
2:2:142:G:H2'	2:2:143:G:C8	2.50	0.47
26:W:24:GLN:HA	26:W:63:VAL:O	2.15	0.47
5:B:88:VAL:HG22	5:B:98:THR:HG22	1.97	0.47
22:S:117:LYS:HE2	22:S:128:PHE:HB2	1.97	0.47
2:2:1628:U:C2	2:2:1630:C:N4	2.83	0.47
16:M:123:GLU:HA	16:M:126:ILE:HD12	1.96	0.47
13:J:59:LEU:HD21	13:J:72:GLU:HB2	1.97	0.47
13:J:21:SER:HA	13:J:24:LEU:HD12	1.97	0.47
8:E:128:LYS:HB2	8:E:140:VAL:HB	1.96	0.47
11:H:49:ILE:HG23	11:H:175:LYS:HG3	1.96	0.47
2:2:520:A:H2'	2:2:521:U:O4'	2.15	0.47
1:1:29:G:H1	1:1:41:C:H42	1.62	0.47
2:2:223:C:H2'	2:2:224:A:H8	1.80	0.47
2:2:325:G:C2	2:2:342:C:O2	2.68	0.47
2:2:323:U:H2'	2:2:324:G:H8	1.80	0.47
24:U:117:ILE:HG22	24:U:118:ILE:HG13	1.97	0.47
2:2:1711:G:N3	2:2:1711:G:H2'	2.29	0.47
2:2:1116:U:H2'	2:2:1117:G:O4'	2.15	0.47
2:2:373:U:H2'	2:2:374:U:C6	2.50	0.47
9:F:37:GLN:HB3	9:F:38:ALA:H	1.54	0.47
2:2:417:G:H8	10:G:59:GLN:NE2	2.13	0.47
8:E:129:VAL:HG22	8:E:139:VAL:HG23	1.97	0.47
2:2:394:U:H2'	2:2:394:U:O2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:702:G:H1	2:2:736:C:N4	2.13	0.47
2:2:601:U:H2'	2:2:602:U:C6	2.50	0.47
2:2:1482:G:C6	2:2:1483:C:N4	2.83	0.47
2:2:1240:G:OP2	19:P:77:ARG:HD3	2.15	0.47
18:O:63:ALA:O	18:O:67:VAL:HG23	2.15	0.47
4:A:79:ARG:HH11	4:A:79:ARG:HB2	1.79	0.47
2:2:730:G:N3	2:2:730:G:H2'	2.30	0.47
2:2:97:C:O2	2:2:424:A:O2'	2.33	0.46
1:1:9:G:N2	1:1:43:G:H5''	2.30	0.46
2:2:1475:G:H1	2:2:1528:C:N4	2.13	0.46
2:2:391:G:H5'	2:2:1727:C:O2'	2.15	0.46
2:2:810:A:C2	2:2:857:G:H1'	2.50	0.46
2:2:1317:G:H2'	2:2:1318:A:C8	2.51	0.46
26:W:46:TYR:CZ	26:W:130:TYR:HA	2.50	0.46
2:2:976:A:H2'	2:2:977:A:O4'	2.14	0.46
2:2:1043:U:O2	2:2:1043:U:C3'	2.63	0.46
1:1:9:G:H1'	1:1:44:A:C8	2.50	0.46
2:2:409:A:H3'	2:2:410:C:C5	2.50	0.46
2:2:410:C:O2	2:2:410:C:C2'	2.63	0.46
2:2:1540:G:C6	2:2:1566:C:N3	2.83	0.46
2:2:328:G:H2'	2:2:329:G:H8	1.79	0.46
2:2:1611:U:OP1	9:F:171:ASN:HB3	2.15	0.46
2:2:334:U:H2'	2:2:335:G:C8	2.50	0.46
20:Q:117:LEU:H	20:Q:117:LEU:HD23	1.79	0.46
2:2:1798:A:N3	2:2:1798:A:H2'	2.30	0.46
2:2:825:U:H2'	2:2:826:C:H4'	1.97	0.46
2:2:778:G:H5'	2:2:780:A:H2	1.79	0.46
2:2:1464:G:C2	2:2:1465:C:C4	3.04	0.46
2:2:1617:C:H2'	2:2:1618:C:H6	1.79	0.46
2:2:984:G:H22	2:2:1015:C:H5	1.64	0.46
2:2:338:C:H2'	2:2:339:U:C6	2.50	0.46
2:2:339:U:H2'	2:2:340:A:H8	1.81	0.46
2:2:390:A:H2'	2:2:391:G:O4'	2.16	0.46
19:P:77:ARG:HB3	19:P:102:PHE:HE2	1.80	0.46
23:T:105:LEU:HD22	23:T:122:ARG:HD3	1.96	0.46
2:2:1263:G:O5'	2:2:1263:G:H8	1.99	0.46
2:2:1017:U:C2'	2:2:1017:U:O2	2.58	0.46
2:2:28:A:N3	2:2:29:U:H1'	2.30	0.46
2:2:1343:A:H2'	2:2:1344:A:C8	2.50	0.46
2:2:1619:U:H2'	2:2:1620:G:H8	1.81	0.46
2:2:50:C:O2	2:2:429:G:C2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:365:A:H2'	2:2:366:A:H8	1.80	0.46
9:F:185:ALA:CB	9:F:192:ILE:HG12	2.45	0.46
11:H:154:LEU:HB2	11:H:185:ILE:HG13	1.97	0.46
24:U:48:PHE:HB3	24:U:50:LEU:HG	1.98	0.46
17:N:87:ASP:N	17:N:87:ASP:OD1	2.49	0.46
2:2:1673:C:C2	2:2:1725:G:N2	2.84	0.46
6:C:46:LEU:O	6:C:50:VAL:HG23	2.15	0.46
2:2:444:A:H8	2:2:524:A:C5'	2.25	0.46
2:2:1464:G:N1	2:2:1465:C:C4	2.84	0.46
4:A:41:ARG:HB2	4:A:45:VAL:O	2.15	0.46
23:T:66:TYR:HA	23:T:124:ILE:HG12	1.96	0.46
2:2:1457:C:H5'	22:S:131:LEU:HD21	1.98	0.46
2:2:609:G:H8	2:2:612:G:H21	1.63	0.46
2:2:1288:U:H2'	2:2:1289:U:C6	2.51	0.46
2:2:925:A:H3'	2:2:926:C:C6	2.50	0.46
2:2:1073:G:N2	2:2:1074:C:C2	2.83	0.46
2:2:52:U:H2'	2:2:53:G:C8	2.50	0.46
2:2:1031:G:C2	2:2:1032:C:C2	3.04	0.46
9:F:43:LYS:HE2	20:Q:54:LEU:HD23	1.97	0.46
2:2:119:A:H1'	2:2:396:A:C4	2.51	0.46
4:A:193:GLN:HA	4:A:194:PRO:HD3	1.78	0.46
2:2:1412:U:O4'	2:2:1412:U:O2	2.33	0.46
2:2:220:A:H61	2:2:839:U:H3	1.64	0.46
1:1:62:C:H2'	1:1:63:G:H8	1.81	0.46
28:Y:122:GLY:HA2	28:Y:125:ILE:HD12	1.97	0.46
2:2:1162:A:N1	2:2:1580:U:O4	2.49	0.46
2:2:1206:C:N4	2:2:1454:C:H41	2.08	0.46
2:2:599:U:H2'	2:2:600:A:C8	2.51	0.46
2:2:1499:C:C2	2:2:1505:G:N2	2.84	0.46
2:2:1620:G:N1	2:2:1621:C:C4	2.84	0.46
2:2:1306:U:H3'	2:2:1307:G:C8	2.50	0.46
2:2:1315:G:OP2	21:R:7:LYS:HB2	2.16	0.46
2:2:1637:C:H42	2:2:1761:A:H61	1.64	0.46
2:2:294:A:C2	2:2:295:U:C2	3.04	0.46
6:C:95:THR:HG22	6:C:96:ARG:H	1.80	0.46
2:2:994:A:H61	2:2:1007:G:H1	1.64	0.46
23:T:22:LEU:HD22	23:T:28:LEU:HD23	1.98	0.46
5:B:176:VAL:C	5:B:178:ASN:H	2.19	0.46
10:G:7:TYR:HD1	10:G:113:ILE:HG23	1.81	0.46
2:2:1333:U:H2'	2:2:1334:U:O4'	2.16	0.46
2:2:1269:G:C2	2:2:1439:C:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:944:U:H2'	2:2:945:U:C6	2.51	0.46
2:2:1588:G:N1	2:2:1589:C:C4	2.83	0.46
2:2:842:U:H2'	2:2:843:A:C8	2.50	0.46
19:P:77:ARG:HB3	19:P:102:PHE:CE2	2.51	0.46
2:2:1577:U:H2'	2:2:1578:C:C6	2.51	0.46
18:O:24:ASN:HA	18:O:55:SER:HB3	1.98	0.46
19:P:111:MET:SD	22:S:119:ILE:HG21	2.56	0.46
1:1:56:C:H2'	1:1:57:G:O4'	2.16	0.46
20:Q:38:LEU:HD21	23:T:10:PRO:HA	1.97	0.46
27:X:87:VAL:HG13	27:X:132:LEU:HD11	1.98	0.46
2:2:1338:C:N4	2:2:1383:G:H1	2.11	0.45
2:2:1659:U:H2'	2:2:1660:G:H8	1.81	0.45
19:P:111:MET:CE	22:S:119:ILE:HG12	2.47	0.45
5:B:176:VAL:HG12	5:B:177:GLN:H	1.80	0.45
2:2:541:A:H3'	2:2:542:C:H3'	1.98	0.45
2:2:797:C:H2'	2:2:798:A:C8	2.50	0.45
2:2:993:G:N1	2:2:1009:C:C4	2.84	0.45
1:1:11:C:H42	1:1:24:G:H1	1.63	0.45
14:K:83:PRO:HG2	14:K:86:ILE:HD13	1.98	0.45
2:2:541:A:H2	2:2:543:A:H1'	1.80	0.45
22:S:35:ILE:HD12	22:S:38:VAL:HG21	1.98	0.45
2:2:1393:G:N2	2:2:1402:C:C2	2.85	0.45
2:2:1204:C:H5''	2:2:1205:U:H5	1.81	0.45
2:2:1484:G:H3'	2:2:1485:A:C8	2.51	0.45
17:N:114:ARG:O	17:N:118:ILE:HG12	2.15	0.45
2:2:1284:U:O4'	2:2:1284:U:O2	2.34	0.45
2:2:178:A:H61	10:G:202:ARG:NH2	2.15	0.45
2:2:1288:U:H2'	2:2:1289:U:H6	1.81	0.45
2:2:1334:U:H2'	2:2:1335:A:H8	1.81	0.45
8:E:104:ASP:HB3	8:E:110:ALA:HB2	1.98	0.45
9:F:119:THR:HG21	9:F:196:LEU:HD22	1.97	0.45
2:2:1496:G:H5''	23:T:72:GLY:HA3	1.99	0.45
2:2:967:U:C4	2:2:968:C:C4	3.04	0.45
24:U:34:LEU:O	24:U:37:VAL:HG12	2.16	0.45
2:2:332:A:C6	2:2:333:G:C6	3.04	0.45
2:2:28:A:C2	2:2:29:U:H1'	2.52	0.45
2:2:970:A:H3'	2:2:971:G:H8	1.82	0.45
2:2:1178:G:C2	2:2:1179:C:C2	3.04	0.45
2:2:1179:C:H42	2:2:1456:G:H1	1.64	0.45
10:G:10:ASN:HB3	10:G:128:THR:HA	1.99	0.45
21:R:59:LYS:O	21:R:62:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:547:G:H1	2:2:589:C:H42	1.63	0.45
20:Q:78:VAL:HA	20:Q:81:ILE:HD12	1.99	0.45
2:2:48:G:C2	2:2:49:C:C2	3.05	0.45
4:A:90:ALA:HA	4:A:95:ALA:HB3	1.98	0.45
2:2:92:A:H5'	2:2:93:A:H5''	1.99	0.45
2:2:1100:G:H8	2:2:1100:G:H5''	1.81	0.45
6:C:146:ARG:HB2	6:C:146:ARG:HH11	1.82	0.45
2:2:389:G:O2'	2:2:390:A:O4'	2.34	0.45
2:2:564:C:C2	2:2:576:G:C2	3.04	0.45
2:2:878:G:C6	2:2:879:C:N4	2.85	0.45
2:2:22:A:H2'	2:2:23:G:O4'	2.17	0.45
5:B:121:ILE:HD13	5:B:164:ILE:HG21	1.99	0.45
8:E:94:ALA:C	8:E:96:ASN:H	2.20	0.45
9:F:176:LEU:HB3	9:F:212:ALA:HB1	1.99	0.45
2:2:442:C:C2	2:2:461:G:C2	3.04	0.45
2:2:1153:G:H2'	2:2:1154:G:O4'	2.16	0.45
4:A:120:LEU:HD11	4:A:144:ILE:HD12	1.99	0.45
16:M:54:VAL:HB	16:M:112:VAL:HB	1.98	0.45
2:2:1673:C:C2	2:2:1725:G:C2	3.05	0.45
2:2:1270:G:H2'	2:2:1271:U:C6	2.51	0.45
20:Q:69:VAL:HG21	20:Q:81:ILE:HG12	1.99	0.45
2:2:1171:G:C6	2:2:1172:C:C4	3.05	0.45
2:2:1467:A:H4'	2:2:1539:G:H4'	1.97	0.45
2:2:1643:G:C6	2:2:1644:C:N4	2.84	0.45
2:2:362:G:C2	2:2:381:C:C2	3.05	0.45
15:L:3:THR:HA	15:L:82:ARG:HH21	1.80	0.45
2:2:803:A:C8	26:W:107:SER:HA	2.51	0.45
2:2:1462:G:N2	2:2:1463:C:C2	2.85	0.45
2:2:1588:G:H1	2:2:1604:C:H42	1.65	0.45
2:2:550:G:H1	2:2:572:C:N4	2.14	0.45
2:2:1171:G:H1	2:2:1465:C:H42	1.63	0.45
18:O:31:THR:HG22	18:O:38:THR:HA	1.99	0.45
8:E:100:ARG:HH22	8:E:122:LYS:HA	1.82	0.45
2:2:340:A:H4'	12:I:87:ASN:ND2	2.32	0.44
7:D:65:ARG:HA	7:D:68:GLU:HG3	1.99	0.44
2:2:477:A:H2	2:2:509:G:H22	1.65	0.44
2:2:1586:G:C6	2:2:1587:C:C4	3.06	0.44
2:2:564:C:N3	2:2:576:G:C2	2.85	0.44
18:O:89:THR:HB	18:O:128:LYS:HG3	1.99	0.44
9:F:115:ILE:HG23	9:F:193:ALA:HB2	1.99	0.44
2:2:1268:U:O4'	2:2:1268:U:O2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:30:G:C2	2:2:31:C:C2	3.05	0.44
2:2:1367:G:H5''	23:T:69:LYS:HD3	1.99	0.44
7:D:59:VAL:HG13	7:D:63:GLY:HA2	2.00	0.44
2:2:1655:U:H4'	2:2:1656:G:O5'	2.17	0.44
14:K:21:LEU:HG	14:K:46:LEU:HD21	2.00	0.44
13:J:80:LEU:O	13:J:83:ILE:HG22	2.17	0.44
2:2:1300:U:H2'	2:2:1301:U:O4'	2.17	0.44
2:2:480:A:N6	2:2:506:U:H3	2.15	0.44
2:2:1462:G:C2	2:2:1463:C:C4	3.05	0.44
2:2:1497:G:C2	2:2:1507:C:C2	3.05	0.44
10:G:88:ARG:HB2	10:G:91:GLU:HB2	1.99	0.44
2:2:1075:A:C2	2:2:1076:C:C2	3.05	0.44
17:N:71:ILE:HA	17:N:74:ILE:HD12	1.98	0.44
2:2:1272:G:N7	2:2:1428:U:H3'	2.32	0.44
2:2:385:G:H2'	2:2:386:A:C8	2.53	0.44
2:2:1494:U:H2'	2:2:1495:U:H6	1.83	0.44
14:K:69:THR:HG23	14:K:72:GLY:H	1.82	0.44
2:2:1145:G:H3'	2:2:1146:A:H8	1.81	0.44
2:2:6:G:H1	2:2:18:C:H42	1.64	0.44
2:2:1175:G:C5	2:2:1462:G:C6	3.05	0.44
7:D:137:VAL:HG22	7:D:151:LYS:HG2	2.00	0.44
2:2:1620:G:C6	2:2:1621:C:N4	2.86	0.44
2:2:14:C:C2	2:2:1140:G:C2	3.06	0.44
2:2:1363:G:C6	2:2:1364:C:N4	2.86	0.44
2:2:1605:G:H2'	2:2:1606:U:H6	1.82	0.44
2:2:1606:U:O3'	20:Q:73:GLY:HA3	2.17	0.44
25:V:37:ALA:HA	25:V:50:TYR:HB3	1.99	0.44
9:F:100:MET:HG3	9:F:107:GLY:O	2.18	0.44
2:2:1286:A:N6	2:2:1328:A:O4'	2.51	0.44
2:2:1437:C:H2'	2:2:1438:C:H6	1.81	0.44
7:D:25:PHE:CE2	7:D:50:ILE:HG12	2.52	0.44
20:Q:77:GLN:O	20:Q:81:ILE:HG13	2.17	0.44
2:2:429:G:N1	2:2:430:C:C4	2.85	0.44
2:2:1679:A:H2	2:2:1718:G:H21	1.65	0.44
2:2:1367:G:H5''	23:T:69:LYS:HB3	2.00	0.44
28:Y:34:ASN:CG	28:Y:35:VAL:H	2.20	0.44
17:N:35:GLU:HA	17:N:38:ILE:HG12	1.99	0.44
2:2:1441:U:H4'	2:2:1444:A:H1'	1.99	0.44
2:2:268:G:C2	2:2:269:C:C2	3.06	0.44
20:Q:29:ILE:HB	20:Q:36:ILE:HD12	1.99	0.44
2:2:930:C:H5''	2:2:931:U:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:602:U:H2'	2:2:603:A:C8	2.53	0.44
1:1:10:G:N1	1:1:11:C:C4	2.86	0.44
2:2:1045:G:H2'	2:2:1046:G:O4'	2.17	0.44
26:W:90:THR:HG23	26:W:94:LEU:HD12	2.00	0.44
2:2:567:G:N1	2:2:568:C:C4	2.85	0.44
2:2:1154:G:C6	2:2:1155:C:C4	3.06	0.44
8:E:173:ILE:HD11	8:E:235:TRP:CE2	2.53	0.44
2:2:77:U:H5	10:G:159:ARG:HD2	1.82	0.44
2:2:1123:A:H2'	2:2:1124:A:C8	2.53	0.44
7:D:142:LEU:C	7:D:144:ALA:H	2.19	0.44
2:2:1208:C:H6	2:2:1208:C:O5'	2.01	0.44
1:1:30:G:C2	1:1:41:C:C2	3.05	0.44
2:2:1136:A:O3'	2:2:1137:A:H4'	2.18	0.44
2:2:450:A:H2'	2:2:452:U:C6	2.52	0.44
2:2:1171:G:C2	2:2:1172:C:C2	3.06	0.44
14:K:82:LEU:HD13	14:K:83:PRO:HD2	2.00	0.44
2:2:877:G:H2'	2:2:878:G:H8	1.82	0.44
2:2:10:G:C6	2:2:1631:A:C2	3.06	0.44
2:2:374:U:H2'	2:2:375:C:C6	2.52	0.44
14:K:54:PHE:HA	14:K:72:GLY:HA3	1.99	0.44
2:2:1279:C:C2	2:2:1427:G:C2	3.06	0.44
2:2:283:G:O6	10:G:185:GLN:HG3	2.18	0.44
6:C:173:ARG:HB3	6:C:204:SER:HB2	2.00	0.44
2:2:403:G:C2	2:2:404:C:C2	3.04	0.44
2:2:1482:G:C2	2:2:1483:C:N3	2.86	0.44
27:X:61:SER:HB2	27:X:116:ASP:HB2	2.00	0.44
2:2:1583:U:O4	2:2:1609:A:C2	2.69	0.43
2:2:1670:G:C2	2:2:1671:G:C5	3.05	0.43
2:2:1155:C:N4	2:2:1620:G:H1	2.16	0.43
2:2:1038:A:O2'	2:2:1039:G:H8	2.01	0.43
21:R:32:LYS:HD3	21:R:47:ARG:HD3	1.99	0.43
1:1:22:G:N2	1:1:23:C:C2	2.86	0.43
17:N:64:LYS:HG3	17:N:70:LYS:HD2	1.99	0.43
11:H:70:TYR:O	11:H:74:GLN:N	2.49	0.43
14:K:22:VAL:HB	14:K:23:ALA:H	1.62	0.43
27:X:109:ARG:HB3	27:X:112:LYS:HB2	2.00	0.43
24:U:28:SER:HB2	24:U:112:VAL:HG23	1.99	0.43
2:2:1015:C:O4'	2:2:1015:C:O2	2.35	0.43
2:2:1492:C:N4	2:2:1511:G:H1	2.12	0.43
1:1:65:G:N2	1:1:66:C:C2	2.86	0.43
2:2:1141:A:H2'	2:2:1142:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1192:A:H2'	2:2:1192:A:N3	2.33	0.43
27:X:42:PRO:HA	27:X:81:LYS:HD2	2.00	0.43
20:Q:125:GLU:HA	20:Q:126:PRO:HD2	1.81	0.43
2:2:1236:G:H1	2:2:1247:C:H42	1.65	0.43
17:N:101:HIS:CE1	17:N:105:ASN:HD21	2.36	0.43
2:2:1136:A:H1'	2:2:1137:A:H1'	2.01	0.43
2:2:1175:G:C2	2:2:1176:C:C2	3.07	0.43
2:2:1482:G:N2	2:2:1483:C:C2	2.87	0.43
2:2:275:C:H1'	2:2:276:U:C5	2.53	0.43
2:2:280:G:C2	2:2:281:C:C2	3.07	0.43
2:2:1537:G:H3'	2:2:1538:G:H5'	2.00	0.43
9:F:190:LYS:HB3	9:F:195:THR:HG22	2.00	0.43
6:C:174:LEU:HD23	6:C:203:THR:HG22	2.00	0.43
2:2:935:G:C2	2:2:936:C:C2	3.07	0.43
22:S:126:ARG:HD3	22:S:133:VAL:HA	2.00	0.43
2:2:573:G:C2	2:2:574:C:C2	3.07	0.43
2:2:18:C:H4'	2:2:1136:A:N6	2.34	0.43
2:2:1126:G:N1	2:2:1127:C:C4	2.87	0.43
2:2:176:U:H2'	2:2:177:U:C6	2.53	0.43
9:F:119:THR:HG23	9:F:197:ALA:HB2	2.01	0.43
27:X:23:ARG:HB3	27:X:29:TYR:CE2	2.53	0.43
7:D:51:ARG:HB3	7:D:91:VAL:HG22	1.99	0.43
24:U:99:ILE:HA	24:U:102:ARG:HD2	1.99	0.43
5:B:34:ALA:HB3	5:B:41:ARG:HA	2.01	0.43
2:2:1261:U:H2'	2:2:1262:G:C8	2.53	0.43
2:2:846:A:H8	2:2:846:A:O5'	2.01	0.43
2:2:512:U:O4'	2:2:512:U:O2	2.33	0.43
2:2:339:U:H2'	2:2:340:A:C8	2.53	0.43
2:2:57:G:H1	2:2:90:C:N4	2.17	0.43
2:2:1497:G:C2	2:2:1498:C:C2	3.06	0.43
8:E:20:LEU:HD11	8:E:29:PRO:HD3	2.00	0.43
8:E:44:LEU:HD12	8:E:82:PHE:HB3	2.00	0.43
2:2:1157:C:C5	2:2:1580:U:C5	3.07	0.43
2:2:460:G:H2'	2:2:461:G:O4'	2.19	0.43
2:2:598:A:N3	2:2:598:A:H2'	2.34	0.43
2:2:89:G:H2'	2:2:90:C:O4'	2.19	0.43
2:2:1031:G:C6	2:2:1032:C:C4	3.07	0.43
2:2:1179:C:N4	2:2:1456:G:H1	2.16	0.43
8:E:140:VAL:HG22	8:E:146:THR:HG22	1.99	0.43
2:2:1637:C:H2'	2:2:1638:C:O4'	2.19	0.43
18:O:87:GLY:HA2	18:O:92:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:55:LEU:HB3	25:V:59:ILE:HD11	2.01	0.43
6:C:64:HIS:CD2	6:C:244:PRO:HD3	2.52	0.43
11:H:61:PHE:HA	11:H:93:LEU:O	2.18	0.43
16:M:72:ALA:O	16:M:77:VAL:HA	2.18	0.43
2:2:18:C:H2'	2:2:19:A:H8	1.84	0.43
2:2:1418:C:H3'	2:2:1419:A:H8	1.83	0.43
10:G:180:THR:HG22	10:G:181:PRO:HD2	2.01	0.43
15:L:67:ARG:NH2	15:L:129:ARG:HA	2.34	0.43
2:2:1673:C:N3	2:2:1725:G:C2	2.86	0.43
2:2:1560:G:N1	2:2:1561:C:C4	2.86	0.43
2:2:30:G:N2	2:2:31:C:C2	2.87	0.43
2:2:1295:A:C6	2:2:1296:G:C5	3.07	0.43
2:2:1154:G:C2	2:2:1622:C:C2	3.07	0.43
2:2:89:G:C6	2:2:90:C:C4	3.06	0.43
2:2:48:G:C6	2:2:49:C:C4	3.06	0.43
2:2:481:U:H3	2:2:504:A:N6	2.16	0.43
2:2:1178:G:H2'	2:2:1179:C:C6	2.54	0.43
18:O:20:PHE:HD2	18:O:27:PHE:HB2	1.84	0.43
2:2:1033:C:C2	2:2:1101:G:C2	3.06	0.43
2:2:1014:U:C3'	2:2:1015:C:H5'	2.49	0.43
2:2:30:G:C2	2:2:31:C:N3	2.87	0.43
2:2:546:U:H2'	2:2:547:G:C8	2.54	0.43
10:G:32:ILE:HG12	10:G:54:GLY:H	1.84	0.43
8:E:45:ILE:CG1	8:E:80:THR:HB	2.49	0.43
2:2:326:U:H2'	2:2:327:A:C8	2.54	0.43
9:F:185:ALA:HB2	9:F:192:ILE:HG12	1.99	0.43
24:U:70:THR:HA	24:U:71:PRO:HD3	1.92	0.43
2:2:168:A:H5''	10:G:176:GLN:HG2	1.99	0.43
20:Q:12:LYS:H	20:Q:83:GLN:HE22	1.65	0.43
8:E:211:LYS:HG2	8:E:215:GLU:HA	2.00	0.43
2:2:687:C:H6	2:2:687:C:H5''	1.84	0.43
2:2:1460:G:C2	2:2:1461:C:C2	3.06	0.43
2:2:380:C:O2'	2:2:755:A:N1	2.52	0.43
2:2:1153:G:N2	2:2:1623:C:C2	2.87	0.43
18:O:30:VAL:HG11	18:O:71:CYS:SG	2.58	0.43
2:2:1497:G:C6	2:2:1498:C:C4	3.07	0.43
2:2:685:A:H2'	2:2:686:C:C6	2.53	0.43
2:2:1651:C:C2	2:2:1746:G:C2	3.07	0.42
2:2:620:A:O5'	2:2:620:A:H8	2.02	0.42
6:C:162:LYS:HE2	6:C:175:ILE:HG12	2.01	0.42
14:K:15:LEU:O	14:K:19:GLY:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:82:LYS:O	26:W:84:ALA:N	2.52	0.42
2:2:623:G:C2	2:2:624:C:C2	3.07	0.42
2:2:150:G:H21	10:G:13:GLN:HE22	1.66	0.42
2:2:446:U:OP2	8:E:57:ASN:HB2	2.18	0.42
19:P:90:ILE:HG23	19:P:108:ARG:HA	2.00	0.42
1:1:9:G:H22	1:1:43:G:H5"	1.83	0.42
2:2:1437:C:C2	2:2:1438:C:C5	3.08	0.42
2:2:1620:G:C2	2:2:1621:C:C2	3.07	0.42
2:2:1154:G:C2	2:2:1622:C:N3	2.86	0.42
21:R:9:VAL:CG2	21:R:50:ILE:HG13	2.48	0.42
2:2:1145:G:H3'	2:2:1146:A:C8	2.55	0.42
8:E:181:VAL:HG23	8:E:227:VAL:HA	2.00	0.42
9:F:92:VAL:O	9:F:96:THR:HG23	2.18	0.42
2:2:425:G:N2	2:2:426:C:C2	2.87	0.42
2:2:700:C:H2'	2:2:701:U:C6	2.54	0.42
27:X:63:GLN:C	27:X:65:ASN:N	2.70	0.42
2:2:1717:A:H2'	2:2:1718:G:O4'	2.18	0.42
2:2:328:G:H2'	2:2:329:G:C8	2.54	0.42
2:2:1012:A:H3'	2:2:1013:G:H8	1.84	0.42
7:D:202:LEU:HA	7:D:203:PRO:HD3	1.93	0.42
17:N:47:PRO:HA	17:N:50:ILE:HD12	2.00	0.42
2:2:1222:A:N1	2:2:1259:U:O4	2.53	0.42
2:2:945:U:O2'	2:2:946:U:H5'	2.20	0.42
2:2:977:A:N6	2:2:1023:U:H3	2.16	0.42
2:2:367:U:H3'	2:2:368:A:C8	2.54	0.42
2:2:137:U:HO2'	2:2:138:A:H8	1.60	0.42
19:P:17:TYR:HH	19:P:33:PHE:HZ	1.64	0.42
2:2:725:U:O5'	2:2:725:U:H6	2.03	0.42
1:1:38:A:O2'	2:2:1000:A:O5'	2.35	0.42
2:2:16:G:C6	2:2:17:C:N3	2.87	0.42
2:2:594:G:H2'	2:2:595:C:O4'	2.19	0.42
2:2:1481:A:H61	2:2:1589:C:H1'	1.84	0.42
2:2:1499:C:C2	2:2:1505:G:C2	3.07	0.42
2:2:1315:G:N1	2:2:1316:C:C4	2.87	0.42
14:K:28:ASN:H	14:K:40:LEU:HD21	1.85	0.42
6:C:66:LEU:HA	6:C:67:PRO:HD3	1.86	0.42
2:2:775:G:C6	2:2:785:C:N4	2.88	0.42
15:L:133:LYS:HG2	15:L:134:THR:HG23	2.01	0.42
2:2:1257:U:O4'	2:2:1257:U:O2	2.38	0.42
2:2:947:G:C2	2:2:948:C:C2	3.08	0.42
2:2:1602:U:H2'	2:2:1603:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1419:A:H5'	7:D:159:HIS:HB3	2.01	0.42
22:S:119:ILE:H	22:S:119:ILE:HG13	1.76	0.42
11:H:135:ILE:HG23	11:H:152:ILE:HG23	2.01	0.42
16:M:27:THR:HG21	16:M:119:ALA:H	1.84	0.42
28:Y:57:VAL:HB	28:Y:60:PHE:CE1	2.55	0.42
2:2:1517:U:H2'	2:2:1518:U:C6	2.54	0.42
9:F:165:SER:OG	9:F:168:ARG:HB3	2.19	0.42
2:2:703:G:H3'	2:2:704:C:H3'	2.01	0.42
2:2:244:U:H2'	2:2:245:G:H3'	2.02	0.42
19:P:107:ILE:HG23	19:P:111:MET:HB2	2.01	0.42
4:A:41:ARG:HH11	4:A:41:ARG:HB2	1.85	0.42
2:2:61:A:H2'	2:2:62:A:C8	2.55	0.42
2:2:1490:A:O2'	2:2:1491:A:C8	2.71	0.42
2:2:1016:U:H2'	2:2:1016:U:O2	2.19	0.42
2:2:299:A:H2'	2:2:300:A:H8	1.71	0.42
2:2:392:C:H42	2:2:404:C:H42	1.68	0.42
2:2:550:G:H5'	2:2:580:U:O2	2.20	0.42
11:H:49:ILE:HG21	11:H:172:VAL:HA	2.00	0.42
17:N:146:ALA:HA	17:N:149:LEU:HD12	2.02	0.42
11:H:46:ILE:HG12	11:H:60:VAL:HG12	2.02	0.42
22:S:4:VAL:HG23	29:Z:79:ALA:HA	2.02	0.42
2:2:974:C:O2	2:2:974:C:H2'	2.19	0.42
2:2:568:C:H2'	2:2:569:A:H5'	2.01	0.42
2:2:1322:C:H2'	2:2:1323:G:C8	2.55	0.42
2:2:1462:G:H2'	2:2:1463:C:C6	2.54	0.42
2:2:1589:C:H42	2:2:1603:G:H1	1.67	0.42
2:2:532:U:H4'	28:Y:33:ALA:HB2	2.02	0.42
2:2:588:C:O2'	2:2:589:C:H6	2.01	0.42
2:2:760:A:H3'	2:2:761:G:H8	1.85	0.42
26:W:113:HIS:CG	26:W:114:GLU:N	2.88	0.42
2:2:1389:A:C8	2:2:1389:A:H5''	2.55	0.42
10:G:225:GLU:HB3	10:G:226:VAL:H	1.67	0.42
6:C:41:VAL:HA	6:C:42:PRO:HD3	1.89	0.42
2:2:1222:A:H2'	2:2:1223:A:O4'	2.20	0.42
8:E:42:LEU:HA	8:E:43:PRO:HD3	1.89	0.42
2:2:547:G:H2'	2:2:548:G:O4'	2.20	0.42
2:2:556:G:C2	2:2:558:C:C2	3.07	0.42
9:F:144:PRO:HD2	9:F:169:ARG:CG	2.50	0.42
24:U:58:LEU:HB2	24:U:88:LYS:HB2	2.02	0.42
2:2:335:G:O6	12:I:5:ARG:HB3	2.19	0.42
2:2:981:U:H5'	2:2:982:A:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:162:GLN:N	7:D:163:PRO:HD2	2.35	0.42
2:2:958:U:O2	2:2:958:U:O4'	2.36	0.42
2:2:1212:G:C2	2:2:1449:C:C2	3.08	0.41
2:2:585:G:C2	2:2:586:C:C2	3.08	0.41
23:T:89:ARG:HA	23:T:90:PRO:HD3	1.82	0.41
2:2:1643:G:C2	2:2:1644:C:N3	2.88	0.41
12:I:65:PHE:HA	12:I:182:GLY:O	2.20	0.41
2:2:77:U:C5	10:G:159:ARG:HD2	2.55	0.41
9:F:179:ILE:O	9:F:183:GLU:HG2	2.20	0.41
2:2:610:U:H2'	2:2:611:U:O4'	2.20	0.41
2:2:633:G:N3	2:2:633:G:H2'	2.35	0.41
2:2:1560:G:C2	2:2:1561:C:C2	3.09	0.41
2:2:1588:G:C2	2:2:1589:C:C2	3.08	0.41
27:X:142:LYS:HG2	27:X:144:ARG:H	1.86	0.41
2:2:280:G:C6	2:2:281:C:C4	3.08	0.41
2:2:1168:G:H21	2:2:1574:A:H62	1.67	0.41
2:2:42:G:H1	2:2:432:C:N4	2.18	0.41
2:2:89:G:C2	2:2:90:C:C2	3.08	0.41
2:2:249:C:H2'	2:2:250:A:C8	2.53	0.41
2:2:327:A:H2'	2:2:328:G:C8	2.55	0.41
2:2:416:A:H1'	2:2:417:G:C2	2.55	0.41
6:C:185:ALA:HA	6:C:203:THR:OG1	2.21	0.41
2:2:1016:U:C2'	2:2:1016:U:O2	2.68	0.41
22:S:87:ASN:HB2	22:S:99:HIS:CD2	2.54	0.41
2:2:651:U:H3'	2:2:652:C:C6	2.56	0.41
16:M:55:LEU:HD12	16:M:65:SER:HB2	2.02	0.41
2:2:1672:C:H2'	2:2:1673:C:C6	2.56	0.41
2:2:944:U:H2'	2:2:945:U:H6	1.84	0.41
2:2:598:A:N3	2:2:599:U:C6	2.88	0.41
2:2:1154:G:C2	2:2:1155:C:C2	3.09	0.41
2:2:53:G:C2	2:2:54:C:C2	3.07	0.41
2:2:1191:C:H3'	2:2:1192:A:H5''	2.01	0.41
2:2:812:U:H4'	15:L:156:PHE:HA	2.01	0.41
29:Z:96:SER:O	29:Z:98:GLN:N	2.45	0.41
2:2:122:U:H2'	2:2:123:G:O4'	2.20	0.41
15:L:66:ILE:HD13	15:L:128:CYS:HB3	2.02	0.41
19:P:115:TYR:N	19:P:115:TYR:CD1	2.88	0.41
2:2:1416:G:H5''	2:2:1416:G:C8	2.55	0.41
2:2:1558:U:H3'	2:2:1559:U:C6	2.55	0.41
2:2:524:A:O2'	2:2:525:A:O4'	2.39	0.41
9:F:29:THR:HG21	20:Q:29:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1073:G:N1	2:2:1074:C:C4	2.88	0.41
2:2:1505:G:C6	2:2:1506:U:C2	3.08	0.41
2:2:1712:A:H2'	2:2:1713:G:C8	2.55	0.41
2:2:11:A:H2'	2:2:12:U:H5'	2.02	0.41
2:2:1682:U:H2'	2:2:1683:G:H8	1.85	0.41
9:F:96:THR:HG22	9:F:116:VAL:HG21	2.02	0.41
22:S:27:ASN:O	22:S:29:VAL:N	2.53	0.41
13:J:163:PRO:C	13:J:165:GLY:H	2.23	0.41
8:E:160:VAL:HG11	8:E:169:ILE:HG12	2.02	0.41
2:2:1400:G:C2	2:2:1401:C:C2	3.08	0.41
2:2:1449:C:O2'	2:2:1450:U:H5'	2.20	0.41
2:2:1153:G:C2	2:2:1623:C:C2	3.09	0.41
2:2:353:C:H2'	2:2:354:G:O4'	2.19	0.41
2:2:50:C:N4	2:2:428:G:H1	2.17	0.41
21:R:83:GLN:HB2	21:R:84:TYR:H	1.68	0.41
13:J:4:ALA:HA	13:J:5:PRO:HD3	1.95	0.41
2:2:1617:C:H2'	2:2:1618:C:C6	2.55	0.41
2:2:38:C:C2	2:2:39:A:C8	3.09	0.41
2:2:1379:U:O3'	24:U:59:PRO:HA	2.21	0.41
2:2:429:G:C2	2:2:430:C:C2	3.08	0.41
2:2:71:A:C3'	2:2:72:A:H5''	2.51	0.41
10:G:181:PRO:HA	10:G:184:LEU:HD12	2.03	0.41
17:N:37:ILE:HG12	17:N:54:LEU:HD11	2.02	0.41
21:R:22:PRO:O	21:R:23:LYS:HB2	2.20	0.41
2:2:1675:C:H2'	2:2:1676:A:O4'	2.20	0.41
20:Q:29:ILE:HG22	20:Q:65:ILE:HD12	2.01	0.41
2:2:1620:G:C2	2:2:1621:C:C4	3.09	0.41
2:2:1038:A:O2'	2:2:1039:G:C8	2.70	0.41
12:I:107:THR:N	12:I:108:PRO:CD	2.83	0.41
2:2:1577:U:H2'	2:2:1578:C:H6	1.85	0.41
2:2:72:A:H4'	2:2:73:U:OP1	2.20	0.41
8:E:122:LYS:HD2	8:E:145:ARG:HH21	1.84	0.41
7:D:138:ILE:HG23	7:D:182:LEU:HD21	2.02	0.41
7:D:20:GLU:HG3	14:K:61:TRP:CG	2.55	0.41
2:2:1088:U:H2'	2:2:1089:C:C6	2.56	0.41
20:Q:29:ILE:HD12	20:Q:36:ILE:HB	2.01	0.41
2:2:49:C:H2'	2:2:50:C:O4'	2.21	0.41
2:2:1422:A:H2'	2:2:1423:A:O4'	2.21	0.41
2:2:940:A:H2	2:2:975:G:H5'	1.85	0.41
2:2:878:G:C2	2:2:879:C:C2	3.08	0.41
17:N:30:SER:HB2	17:N:67:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:45:LYS:HE3	6:C:253:THR:HG23	2.03	0.41
2:2:1420:A:H2'	2:2:1421:U:C6	2.56	0.41
3:3:3:A:H3'	3:3:3:A:N3	2.36	0.41
1:1:58:A:O5'	1:1:58:A:H8	2.03	0.41
2:2:16:G:C5	2:2:17:C:C4	3.09	0.41
2:2:1157:C:C5	2:2:1580:U:H5	2.39	0.41
2:2:392:C:N4	2:2:404:C:H42	2.18	0.41
2:2:400:A:O2'	2:2:401:C:H4'	2.21	0.41
2:2:595:C:H2'	2:2:596:G:O4'	2.21	0.41
2:2:1787:G:H2'	2:2:1788:A:H8	1.86	0.41
2:2:476:A:H2'	2:2:477:A:C8	2.53	0.41
7:D:209:ILE:HB	21:R:38:ILE:O	2.21	0.41
2:2:564:C:H4'	2:2:565:C:O5'	2.21	0.41
22:S:35:ILE:HG13	22:S:35:ILE:H	1.65	0.41
27:X:41:SER:HA	27:X:42:PRO:HD3	1.89	0.41
2:2:1012:A:H3'	2:2:1013:G:C8	2.56	0.41
19:P:17:TYR:CD1	19:P:18:LYS:HB2	2.55	0.41
2:2:1005:C:H3'	2:2:1006:C:H6	1.86	0.41
2:2:1562:U:H2'	2:2:1563:C:O4'	2.21	0.41
11:H:153:LEU:HD23	11:H:184:GLU:HB3	2.02	0.41
2:2:303:U:H2'	2:2:304:C:C6	2.56	0.41
2:2:1040:G:OP1	4:A:32:HIS:HB2	2.21	0.41
3:3:14:U:H6	3:3:14:U:O5'	2.04	0.41
19:P:52:LYS:HB2	19:P:53:PRO:HD3	2.02	0.41
4:A:162:CYS:SG	4:A:163:ASN:N	2.93	0.41
17:N:23:PRO:HG3	17:N:61:THR:HG21	2.03	0.41
27:X:92:CYS:HA	27:X:95:PHE:CD2	2.55	0.41
2:2:947:G:C6	2:2:948:C:C4	3.09	0.41
2:2:1482:G:C2	2:2:1483:C:C2	3.09	0.41
2:2:1603:G:C2	2:2:1604:C:C2	3.09	0.41
2:2:309:C:N4	2:2:355:G:H1	2.16	0.41
2:2:354:G:H2'	2:2:355:G:H8	1.86	0.41
2:2:556:G:H1	2:2:586:C:H42	1.69	0.41
2:2:1363:G:H2'	2:2:1363:G:N3	2.36	0.41
9:F:68:LYS:HA	9:F:69:PRO:HD3	1.89	0.41
2:2:1471:U:OP1	9:F:192:ILE:HG13	2.21	0.41
2:2:1636:G:C6	2:2:1637:C:N3	2.89	0.41
2:2:1244:G:H22	2:2:1247:C:H5	1.69	0.41
2:2:1033:C:C2	2:2:1101:G:N2	2.89	0.41
14:K:30:PRO:HA	14:K:38:LYS:HG3	2.03	0.41
2:2:1582:G:C8	20:Q:122:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1625:U:H2'	2:2:1626:U:O4'	2.21	0.41
2:2:1400:G:C6	2:2:1401:C:C4	3.09	0.40
2:2:1009:C:N4	2:2:1010:G:C6	2.89	0.40
2:2:1482:G:O2'	2:2:1483:C:H5''	2.21	0.40
18:O:27:PHE:HA	18:O:43:THR:HG22	2.03	0.40
9:F:125:VAL:HG21	29:Z:92:VAL:HG21	2.03	0.40
2:2:514:A:H62	2:2:536:G:H21	1.69	0.40
2:2:96:G:C2	2:2:97:C:C2	3.09	0.40
4:A:58:VAL:HG22	18:O:111:ARG:HD3	85.94	0.40
2:2:425:G:C2	2:2:426:C:C2	3.09	0.40
2:2:630:G:C5	2:2:631:U:C4	3.09	0.40
2:2:104:A:N6	2:2:307:C:O4'	2.55	0.40
2:2:86:A:H2'	2:2:87:C:C6	2.56	0.40
24:U:20:HIS:HB2	24:U:95:ALA:O	2.21	0.40
19:P:39:ALA:HA	19:P:42:ARG:HD3	2.02	0.40
2:2:337:C:H2'	2:2:338:C:H6	1.84	0.40
2:2:1115:A:H62	2:2:1129:G:N2	2.17	0.40
2:2:1050:G:N1	2:2:1067:C:C4	2.90	0.40
2:2:1154:G:N1	2:2:1155:C:C2	2.88	0.40
2:2:1621:C:H2'	2:2:1622:C:C6	2.57	0.40
7:D:29:LEU:HB3	7:D:32:GLU:HB2	2.04	0.40
2:2:1022:A:H5''	2:2:1126:G:H4'	2.02	0.40
17:N:98:VAL:HG11	17:N:115:LEU:HB2	2.03	0.40
2:2:325:G:C2	2:2:342:C:C2	3.10	0.40
2:2:977:A:H2'	2:2:978:A:O4'	2.21	0.40
17:N:37:ILE:HG23	17:N:50:ILE:HG21	2.02	0.40
26:W:7:LEU:HA	26:W:34:ILE:HG12	2.04	0.40
17:N:81:ALA:HA	17:N:82:PRO:HD3	1.95	0.40
2:2:284:G:C2	2:2:285:C:C2	3.09	0.40
18:O:88:GLY:HA2	18:O:122:PRO:HG3	2.04	0.40
2:2:1291:G:H2'	2:2:1292:U:O4'	2.21	0.40
2:2:96:G:C6	2:2:97:C:C4	3.10	0.40
2:2:337:C:C5'	12:I:10:LYS:HG3	2.49	0.40
2:2:1604:C:C6	2:2:1604:C:H5''	2.56	0.40
2:2:1474:C:H2'	2:2:1475:G:H8	1.86	0.40
2:2:50:C:H42	2:2:428:G:H1	1.69	0.40
6:C:175:ILE:HA	6:C:176:PRO:HD3	1.96	0.40
2:2:1464:G:C2	2:2:1465:C:N3	2.89	0.40
22:S:89:GLN:C	22:S:91:ASP:H	2.24	0.40
8:E:125:LYS:O	8:E:141:THR:HA	2.22	0.40
2:2:1005:C:H5''	2:2:1006:C:H5	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:13:VAL:HB	18:O:77:THR:H	1.86	0.40
9:F:35:ILE:HG23	20:Q:53:LEU:HD21	2.03	0.40
2:2:357:U:H2'	2:2:359:A:H8	1.86	0.40
2:2:98:U:H2'	2:2:99:C:C6	2.57	0.40
7:D:50:ILE:HD11	7:D:86:LEU:HD22	2.03	0.40
2:2:1619:U:H2'	2:2:1620:G:C8	2.57	0.40
2:2:551:G:C2	2:2:572:C:C2	3.10	0.40
2:2:888:U:O2	2:2:987:A:H4'	2.21	0.40
2:2:1315:G:C2	2:2:1316:C:C2	3.10	0.40
2:2:1586:G:H22	2:2:1606:U:H3	1.70	0.40
2:2:1178:G:C6	2:2:1179:C:C4	3.10	0.40
2:2:941:G:C2	2:2:942:C:C2	3.09	0.40
2:2:776:G:C2	2:2:777:C:C2	3.10	0.40
2:2:227:G:O6	2:2:236:C:N3	2.55	0.40
23:T:38:LYS:C	23:T:40:SER:H	2.25	0.40
2:2:347:U:H4'	12:I:14:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	206/254 (81%)	170 (82%)	27 (13%)	9 (4%)	3	34
5	B	218/255 (86%)	185 (85%)	25 (12%)	8 (4%)	4	39
6	C	215/259 (83%)	186 (86%)	22 (10%)	7 (3%)	5	42
7	D	221/237 (93%)	196 (89%)	16 (7%)	9 (4%)	3	35
8	E	258/261 (99%)	225 (87%)	28 (11%)	5 (2%)	10	53
9	F	204/227 (90%)	169 (83%)	28 (14%)	7 (3%)	5	41
10	G	224/236 (95%)	197 (88%)	23 (10%)	4 (2%)	11	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	182/190 (96%)	157 (86%)	15 (8%)	10 (6%)	2	29
12	I	184/201 (92%)	160 (87%)	15 (8%)	9 (5%)	3	31
13	J	180/188 (96%)	154 (86%)	19 (11%)	7 (4%)	4	37
14	K	94/106 (89%)	81 (86%)	7 (7%)	6 (6%)	2	25
15	L	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	3	33
16	M	113/134 (84%)	85 (75%)	21 (19%)	7 (6%)	2	26
17	N	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	26	71
18	O	125/137 (91%)	102 (82%)	16 (13%)	7 (6%)	2	28
19	P	115/142 (81%)	96 (84%)	13 (11%)	6 (5%)	2	30
20	Q	139/143 (97%)	108 (78%)	20 (14%)	11 (8%)	1	19
21	R	116/136 (85%)	101 (87%)	13 (11%)	2 (2%)	11	56
22	S	143/146 (98%)	111 (78%)	21 (15%)	11 (8%)	1	19
23	T	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
24	U	104/117 (89%)	84 (81%)	16 (15%)	4 (4%)	4	38
25	V	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	3	32
26	W	127/130 (98%)	112 (88%)	10 (8%)	5 (4%)	4	37
27	X	142/145 (98%)	117 (82%)	14 (10%)	11 (8%)	1	19
28	Y	132/135 (98%)	118 (89%)	7 (5%)	7 (5%)	2	30
29	Z	68/108 (63%)	50 (74%)	17 (25%)	1 (2%)	13	58
30	a	96/119 (81%)	81 (84%)	11 (12%)	4 (4%)	3	35
31	b	79/82 (96%)	61 (77%)	15 (19%)	3 (4%)	4	38
32	c	60/67 (90%)	51 (85%)	6 (10%)	3 (5%)	3	31
33	d	51/56 (91%)	33 (65%)	15 (29%)	3 (6%)	2	27
34	e	52/63 (82%)	45 (86%)	6 (12%)	1 (2%)	10	53
35	f	67/150 (45%)	48 (72%)	9 (13%)	10 (15%)	0	5
36	g	312/326 (96%)	257 (82%)	45 (14%)	10 (3%)	5	42
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	92 (84%)	14 (13%)	3 (3%)	6	45
39	j	243/304 (80%)	205 (84%)	32 (13%)	6 (2%)	7	47
40	k	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	13	58
41	l	120/285 (42%)	100 (83%)	16 (13%)	4 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	m	88/108 (82%)	76 (86%)	10 (11%)	2 (2%)	8	49
43	o	451/588 (77%)	417 (92%)	31 (7%)	3 (1%)	26	71
44	p	554/652 (85%)	497 (90%)	45 (8%)	12 (2%)	8	50
45	q	340/347 (98%)	302 (89%)	33 (10%)	5 (2%)	13	58
46	r	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
47	s	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
All	All	7149/8360 (86%)	6131 (86%)	778 (11%)	240 (3%)	8	41

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	95	ALA
4	A	166	GLY
6	C	141	VAL
6	C	235	TRP
7	D	216	PRO
7	D	220	PRO
8	E	245	LYS
10	G	69	LEU
11	H	14	THR
11	H	31	SER
11	H	64	VAL
11	H	74	GLN
12	I	22	ARG
12	I	147	ARG
15	L	105	LYS
20	Q	97	VAL
21	R	85	VAL
22	S	19	ASN
22	S	27	ASN
22	S	28	VAL
22	S	82	PRO
22	S	91	ASP
24	U	96	PRO
26	W	83	ILE
27	X	12	ALA
27	X	64	PRO
27	X	90	ASP
27	X	92	CYS
28	Y	30	PRO

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Mol	Chain	Res	Type
34	e	47	VAL
35	f	94	LYS
39	j	48	LEU
40	k	129	LYS
43	o	63	LYS
44	p	460	PRO
44	p	558	CYS
4	A	21	ARG
5	B	148	ASN
5	B	214	LYS
5	B	221	PRO
5	B	224	ASP
6	C	253	THR
7	D	221	SER
9	F	66	ILE
10	G	122	GLU
11	H	10	SER
11	H	136	VAL
11	H	163	ASP
12	I	40	THR
12	I	52	ASN
12	I	153	ILE
13	J	136	VAL
14	K	22	VAL
14	K	54	PHE
14	K	64	TYR
15	L	7	VAL
16	M	82	VAL
16	M	84	ASP
16	M	110	SER
17	N	3	ARG
18	O	124	ASP
20	Q	39	VAL
20	Q	40	GLN
20	Q	122	ARG
22	S	7	GLU
22	S	83	ALA
22	S	145	ARG
25	V	12	TYR
25	V	45	ALA
26	W	78	ARG
27	X	115	GLY

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Mol	Chain	Res	Type
28	Y	4	ALA
30	a	13	LYS
30	a	59	TYR
33	d	23	ILE
35	f	100	LEU
35	f	102	VAL
36	g	130	LYS
39	j	57	ARG
40	k	495	ILE
40	k	507	LYS
41	l	200	GLY
45	q	329	PHE
4	A	39	LYS
4	A	109	ASN
5	B	54	LEU
5	B	190	PRO
5	B	207	LEU
6	C	187	PRO
7	D	163	PRO
8	E	205	PHE
9	F	37	GLN
9	F	59	SER
9	F	190	LYS
12	I	120	SER
13	J	20	GLU
13	J	134	ILE
13	J	150	LEU
14	K	23	ALA
15	L	4	GLU
15	L	30	LYS
15	L	55	ASP
16	M	98	ASP
18	O	18	ARG
18	O	40	ALA
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
19	P	108	ARG
19	P	109	PRO
20	Q	14	LYS
20	Q	27	GLY
20	Q	115	THR

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Mol	Chain	Res	Type
20	Q	116	LEU
21	R	5	ARG
22	S	8	GLN
25	V	9	VAL
26	W	29	PRO
26	W	58	SER
27	X	3	LYS
27	X	41	SER
27	X	54	LEU
27	X	97	ASP
28	Y	36	SER
31	b	21	LEU
35	f	111	GLU
35	f	122	PRO
35	f	140	GLY
35	f	143	HIS
36	g	106	GLY
36	g	120	SER
36	g	201	GLY
36	g	205	TYR
38	i	17	ASN
38	i	64	LYS
39	j	49	SER
39	j	64	ARG
39	j	138	PHE
40	k	127	ARG
40	k	497	GLU
41	l	159	ARG
42	m	85	ARG
44	p	492	LYS
44	p	536	ASP
44	p	639	GLY
45	q	291	GLY
6	C	44	THR
6	C	65	SER
6	C	155	GLN
7	D	143	ARG
8	E	77	ARG
8	E	150	PRO
8	E	195	ILE
9	F	65	GLN
9	F	67	SER

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Mol	Chain	Res	Type
11	H	13	PRO
11	H	110	GLN
12	I	148	ALA
13	J	120	LYS
13	J	171	ARG
14	K	25	LYS
16	M	81	LYS
18	O	42	VAL
19	P	90	ILE
24	U	89	ARG
25	V	10	GLU
26	W	72	CYS
29	Z	38	HIS
32	c	35	ASP
32	c	49	ARG
33	d	34	TYR
35	f	110	ASP
36	g	31	PRO
36	g	50	GLU
41	l	129	LEU
41	l	219	SER
42	m	74	MET
43	o	394	ASN
44	p	337	ASP
44	p	650	LYS
44	p	774	THR
45	q	162	SER
4	A	103	THR
4	A	158	VAL
4	A	195	TRP
4	A	202	TYR
5	B	4	GLY
7	D	196	THR
11	H	98	ILE
12	I	149	ALA
13	J	147	MET
16	M	77	VAL
18	O	91	SER
19	P	100	LYS
20	Q	74	HIS
22	S	14	ILE
22	S	90	LYS

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Mol	Chain	Res	Type
28	Y	31	ASN
28	Y	64	TYR
30	a	36	ILE
31	b	62	VAL
35	f	90	LYS
35	f	98	VAL
36	g	15	GLU
38	i	16	LYS
39	j	226	PRO
43	o	335	THR
44	p	351	ILE
44	p	645	ILE
44	p	704	PRO
7	D	63	GLY
7	D	219	GLU
9	F	100	MET
10	G	152	ASP
10	G	224	ALA
12	I	59	ARG
15	L	3	THR
16	M	122	GLN
28	Y	67	GLY
20	Q	33	GLY
24	U	118	ILE
30	a	64	LEU
19	P	48	GLY
24	U	117	ILE
27	X	63	GLN
27	X	96	VAL
45	q	50	GLY
45	q	239	PRO
15	L	54	ILE
31	b	10	PRO
32	c	24	GLY
33	d	29	GLY
36	g	159	PRO
7	D	217	VAL
14	K	82	LEU
20	Q	73	GLY
36	g	64	GLY
40	k	210	VAL
44	p	336	ILE

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Mol	Chain	Res	Type
28	Y	5	ILE

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	
4	A	174/211 (82%)	147 (84%)	27 (16%)	3	23
5	B	198/228 (87%)	174 (88%)	24 (12%)	6	32
6	C	176/203 (87%)	153 (87%)	23 (13%)	5	29
7	D	185/196 (94%)	152 (82%)	33 (18%)	2	17
8	E	223/224 (100%)	186 (83%)	37 (17%)	3	20
9	F	174/194 (90%)	140 (80%)	34 (20%)	2	13
10	G	192/200 (96%)	174 (91%)	18 (9%)	11	44
11	H	164/170 (96%)	138 (84%)	26 (16%)	3	22
12	I	147/159 (92%)	133 (90%)	14 (10%)	11	43
13	J	153/158 (97%)	135 (88%)	18 (12%)	6	34
14	K	88/96 (92%)	70 (80%)	18 (20%)	1	12
15	L	136/137 (99%)	128 (94%)	8 (6%)	24	63
16	M	93/109 (85%)	82 (88%)	11 (12%)	6	34
17	N	127/128 (99%)	108 (85%)	19 (15%)	3	24
18	O	96/104 (92%)	88 (92%)	8 (8%)	14	51
19	P	100/119 (84%)	83 (83%)	17 (17%)	2	19
20	Q	117/119 (98%)	99 (85%)	18 (15%)	3	23
21	R	109/124 (88%)	91 (84%)	18 (16%)	3	20
22	S	128/129 (99%)	105 (82%)	23 (18%)	2	16
23	T	117/118 (99%)	97 (83%)	20 (17%)	2	18
24	U	96/107 (90%)	83 (86%)	13 (14%)	5	28
25	V	73/73 (100%)	66 (90%)	7 (10%)	10	43
26	W	110/111 (99%)	102 (93%)	8 (7%)	17	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	X	119/120 (99%)	102 (86%)	17 (14%)	4	27
28	Y	108/109 (99%)	102 (94%)	6 (6%)	26	65
29	Z	60/88 (68%)	55 (92%)	5 (8%)	14	51
30	a	83/100 (83%)	71 (86%)	12 (14%)	4	26
31	b	71/72 (99%)	67 (94%)	4 (6%)	26	65
32	c	54/59 (92%)	48 (89%)	6 (11%)	8	36
33	d	46/48 (96%)	39 (85%)	7 (15%)	3	24
34	e	47/55 (86%)	39 (83%)	8 (17%)	2	19
35	f	57/133 (43%)	48 (84%)	9 (16%)	3	22
36	g	265/272 (97%)	231 (87%)	34 (13%)	5	30
37	h	23/23 (100%)	20 (87%)	3 (13%)	5	30
38	i	93/130 (72%)	74 (80%)	19 (20%)	1	12
39	j	224/274 (82%)	185 (83%)	39 (17%)	2	18
40	k	332/449 (74%)	306 (92%)	26 (8%)	16	53
41	l	119/246 (48%)	103 (87%)	16 (13%)	5	29
42	m	77/96 (80%)	64 (83%)	13 (17%)	2	19
43	o	411/444 (93%)	364 (89%)	47 (11%)	7	35
44	p	507/536 (95%)	469 (92%)	38 (8%)	17	55
45	q	297/301 (99%)	280 (94%)	17 (6%)	25	64
46	r	30/30 (100%)	27 (90%)	3 (10%)	9	41
47	s	43/43 (100%)	37 (86%)	6 (14%)	4	28
All	All	6242/7045 (89%)	5465 (88%)	777 (12%)	10	31

All (777) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	ARG
4	A	34	GLU
4	A	41	ARG
4	A	43	ASP
4	A	58	VAL
4	A	59	LEU
4	A	69	ASN
4	A	71	GLU
4	A	79	ARG

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Mol	Chain	Res	Type
4	A	80	THR
4	A	84	ARG
4	A	93	THR
4	A	96	THR
4	A	108	THR
4	A	112	THR
4	A	113	ARG
4	A	119	ARG
4	A	120	LEU
4	A	122	ILE
4	A	143	VAL
4	A	165	ARG
4	A	167	LYS
4	A	170	ILE
4	A	192	THR
4	A	193	GLN
4	A	198	MET
4	A	205	ARG
5	B	22	ASP
5	B	28	GLU
5	B	47	LEU
5	B	64	ARG
5	B	68	VAL
5	B	70	LEU
5	B	78	ASP
5	B	82	ARG
5	B	84	VAL
5	B	104	ASP
5	B	111	ARG
5	B	118	GLN
5	B	119	THR
5	B	125	VAL
5	B	127	VAL
5	B	140	ILE
5	B	170	GLU
5	B	181	LEU
5	B	189	ILE
5	B	196	GLU
5	B	205	PHE
5	B	208	GLN
5	B	219	LYS
5	B	228	LEU

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Mol	Chain	Res	Type
6	C	58	ILE
6	C	71	PHE
6	C	72	GLN
6	C	78	LEU
6	C	83	ASP
6	C	86	MET
6	C	91	VAL
6	C	93	LYS
6	C	99	GLN
6	C	109	VAL
6	C	113	ASN
6	C	125	GLU
6	C	131	ARG
6	C	145	ARG
6	C	146	ARG
6	C	166	LYS
6	C	199	GLU
6	C	223	ILE
6	C	234	LEU
6	C	235	TRP
6	C	236	GLU
6	C	240	LEU
6	C	246	ASP
7	D	4	ILE
7	D	5	ILE
7	D	6	SER
7	D	16	VAL
7	D	20	GLU
7	D	31	GLU
7	D	57	ASP
7	D	68	GLU
7	D	69	LEU
7	D	70	THR
7	D	75	LYS
7	D	76	ARG
7	D	93	ASP
7	D	94	ARG
7	D	103	GLU
7	D	109	LEU
7	D	113	LEU
7	D	116	ARG
7	D	122	VAL

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Mol	Chain	Res	Type
7	D	128	GLU
7	D	132	LYS
7	D	146	ARG
7	D	148	LYS
7	D	158	ILE
7	D	168	ILE
7	D	173	ARG
7	D	176	LEU
7	D	200	LYS
7	D	204	ASP
7	D	209	ILE
7	D	212	LYS
7	D	213	GLU
7	D	214	GLU
8	E	7	LYS
8	E	9	LEU
8	E	18	TRP
8	E	21	ASP
8	E	22	LYS
8	E	23	LEU
8	E	38	LEU
8	E	44	LEU
8	E	51	ARG
8	E	60	GLU
8	E	65	LEU
8	E	68	ARG
8	E	75	LYS
8	E	77	ARG
8	E	79	ASP
8	E	102	VAL
8	E	104	ASP
8	E	108	ARG
8	E	113	ARG
8	E	117	GLU
8	E	125	LYS
8	E	133	LYS
8	E	147	ILE
8	E	168	THR
8	E	180	LEU
8	E	181	VAL
8	E	189	LEU
8	E	198	ARG

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Mol	Chain	Res	Type
8	E	201	HIS
8	E	206	ASP
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	233	ARG
8	E	248	ILE
8	E	259	HIS
9	F	31	ILE
9	F	34	GLU
9	F	37	GLN
9	F	42	ILE
9	F	50	PHE
9	F	54	GLU
9	F	62	ASP
9	F	70	ILE
9	F	72	VAL
9	F	83	ARG
9	F	86	LYS
9	F	88	GLN
9	F	91	ILE
9	F	98	SER
9	F	104	ARG
9	F	108	LYS
9	F	111	LYS
9	F	132	LEU
9	F	163	ASP
9	F	164	VAL
9	F	168	ARG
9	F	174	ILE
9	F	177	LEU
9	F	178	THR
9	F	186	PHE
9	F	187	ARG
9	F	189	ILE
9	F	194	GLU
9	F	199	GLU
9	F	209	THR
9	F	216	LYS
9	F	221	ARG
9	F	224	LYS

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Mol	Chain	Res	Type
9	F	226	ASN
10	G	15	CYS
10	G	21	GLU
10	G	26	VAL
10	G	39	GLU
10	G	52	ILE
10	G	76	LEU
10	G	95	LYS
10	G	121	ILE
10	G	127	ASP
10	G	151	ASP
10	G	164	LYS
10	G	169	TYR
10	G	170	THR
10	G	176	GLN
10	G	180	THR
10	G	195	ILE
10	G	215	ARG
10	G	220	LYS
11	H	5	GLN
11	H	7	LYS
11	H	11	GLN
11	H	15	GLU
11	H	19	GLN
11	H	27	LEU
11	H	33	GLU
11	H	37	ASP
11	H	38	LEU
11	H	48	GLU
11	H	72	LYS
11	H	74	GLN
11	H	80	GLU
11	H	86	GLN
11	H	91	ILE
11	H	104	ARG
11	H	111	LYS
11	H	112	ARG
11	H	116	ARG
11	H	122	HIS
11	H	124	LYS
11	H	129	LEU
11	H	139	ARG

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Mol	Chain	Res	Type
11	H	162	ILE
11	H	180	GLN
11	H	184	GLU
12	I	20	GLN
12	I	24	LYS
12	I	26	LYS
12	I	29	LEU
12	I	47	ARG
12	I	53	GLN
12	I	72	VAL
12	I	96	LEU
12	I	104	ILE
12	I	119	GLN
12	I	153	ILE
12	I	190	LEU
12	I	196	ARG
12	I	201	LYS
13	J	8	TYR
13	J	10	LYS
13	J	20	GLU
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	40	ARG
13	J	49	LEU
13	J	63	ASP
13	J	64	GLU
13	J	69	ARG
13	J	83	ILE
13	J	100	LYS
13	J	107	ARG
13	J	127	VAL
13	J	131	GLN
13	J	161	THR
14	K	2	LEU
14	K	9	LYS
14	K	13	GLN
14	K	15	LEU
14	K	20	VAL
14	K	21	LEU
14	K	29	GLN

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Mol	Chain	Res	Type
14	K	34	GLU
14	K	44	LYS
14	K	47	GLN
14	K	55	VAL
14	K	57	THR
14	K	64	TYR
14	K	71	GLU
14	K	75	TYR
14	K	76	LEU
14	K	85	HIS
14	K	91	TYR
15	L	5	LEU
15	L	10	GLU
15	L	36	LYS
15	L	55	ASP
15	L	80	MET
15	L	84	ILE
15	L	118	GLN
15	L	124	THR
16	M	22	LYS
16	M	26	ARG
16	M	52	LEU
16	M	61	GLU
16	M	67	LEU
16	M	91	TRP
16	M	97	ILE
16	M	100	ASP
16	M	117	TRP
16	M	123	GLU
16	M	125	GLU
17	N	3	ARG
17	N	16	ILE
17	N	20	ARG
17	N	27	LYS
17	N	53	LEU
17	N	64	LYS
17	N	70	LYS
17	N	83	GLU
17	N	84	ILE
17	N	86	GLU
17	N	88	LEU
17	N	96	VAL

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Mol	Chain	Res	Type
17	N	99	ARG
17	N	100	LYS
17	N	107	LYS
17	N	112	LYS
17	N	121	ARG
17	N	125	LEU
17	N	141	TYR
18	O	29	HIS
18	O	49	LYS
18	O	65	GLN
18	O	92	LYS
18	O	102	LEU
18	O	110	LEU
18	O	114	ARG
18	O	121	VAL
19	P	13	LYS
19	P	21	ASP
19	P	25	LEU
19	P	56	LEU
19	P	57	MET
19	P	71	GLU
19	P	72	LYS
19	P	76	VAL
19	P	79	HIS
19	P	82	ASN
19	P	85	ILE
19	P	101	VAL
19	P	106	GLU
19	P	108	ARG
19	P	111	MET
19	P	122	THR
19	P	123	TYR
20	Q	13	LYS
20	Q	28	LEU
20	Q	37	THR
20	Q	38	LEU
20	Q	45	ARG
20	Q	46	PHE
20	Q	47	LYS
20	Q	68	LYS
20	Q	74	HIS
20	Q	82	ARG

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Mol	Chain	Res	Type
20	Q	83	GLN
20	Q	89	LEU
20	Q	100	GLN
20	Q	105	LEU
20	Q	132	ARG
20	Q	137	ARG
20	Q	139	GLN
20	Q	143	ARG
21	R	3	ARG
21	R	5	ARG
21	R	6	THR
21	R	9	VAL
21	R	10	LYS
21	R	28	PHE
21	R	33	ARG
21	R	37	GLU
21	R	45	ARG
21	R	47	ARG
21	R	48	ASN
21	R	63	LYS
21	R	82	ASP
21	R	83	GLN
21	R	100	LEU
21	R	102	VAL
21	R	103	ASP
21	R	117	LEU
22	S	6	GLN
22	S	20	THR
22	S	25	ASN
22	S	35	ILE
22	S	52	VAL
22	S	54	LEU
22	S	57	ARG
22	S	73	MET
22	S	78	HIS
22	S	84	TRP
22	S	86	LEU
22	S	91	ASP
22	S	97	ASP
22	S	99	HIS
22	S	105	LEU
22	S	111	ASP

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Mol	Chain	Res	Type
22	S	114	GLU
22	S	115	ARG
22	S	120	ARG
22	S	122	HIS
22	S	126	ARG
22	S	136	GLN
22	S	144	ARG
23	T	8	ASP
23	T	16	ASN
23	T	25	GLN
23	T	37	VAL
23	T	45	LEU
23	T	64	HIS
23	T	65	ILE
23	T	85	ASN
23	T	86	ARG
23	T	91	HIS
23	T	95	ASP
23	T	103	LYS
23	T	106	GLN
23	T	107	SER
23	T	124	ILE
23	T	126	ASP
23	T	131	ASP
23	T	132	LEU
23	T	142	ASP
23	T	144	GLU
24	U	34	LEU
24	U	35	GLU
24	U	37	VAL
24	U	41	ILE
24	U	57	ARG
24	U	67	THR
24	U	72	ASN
24	U	80	ASP
24	U	83	GLU
24	U	98	HIS
24	U	109	GLU
24	U	117	ILE
24	U	118	ILE
25	V	1	MET
25	V	7	GLN

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Mol	Chain	Res	Type
25	V	8	LEU
25	V	12	TYR
25	V	44	ARG
25	V	76	ASP
25	V	80	LYS
26	W	7	LEU
26	W	24	GLN
26	W	25	VAL
26	W	26	LEU
26	W	31	SER
26	W	47	ILE
26	W	80	ASN
26	W	111	MET
27	X	14	LYS
27	X	17	VAL
27	X	19	ARG
27	X	30	LYS
27	X	54	LEU
27	X	55	GLU
27	X	79	ASN
27	X	83	VAL
27	X	84	THR
27	X	94	ASN
27	X	97	ASP
27	X	98	GLU
27	X	107	PHE
27	X	117	ILE
27	X	127	VAL
27	X	133	LEU
27	X	144	ARG
28	Y	8	ARG
28	Y	13	ILE
28	Y	35	VAL
28	Y	84	LYS
28	Y	99	LYS
28	Y	121	THR
29	Z	38	HIS
29	Z	44	GLN
29	Z	70	LYS
29	Z	71	LEU
29	Z	84	GLU
30	a	12	LYS

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Mol	Chain	Res	Type
30	a	15	ARG
30	a	19	LYS
30	a	28	ARG
30	a	30	VAL
30	a	34	LYS
30	a	38	ARG
30	a	46	GLU
30	a	53	LEU
30	a	64	LEU
30	a	69	ASN
30	a	75	ILE
31	b	3	LEU
31	b	20	LYS
31	b	57	GLU
31	b	67	THR
32	c	9	LEU
32	c	31	GLU
32	c	43	ASN
32	c	49	ARG
32	c	54	LEU
32	c	65	ARG
33	d	4	GLU
33	d	20	GLN
33	d	21	CYS
33	d	22	ARG
33	d	30	LEU
33	d	34	TYR
33	d	38	ILE
34	e	17	GLN
34	e	22	GLU
34	e	24	GLN
34	e	33	ARG
34	e	38	LEU
34	e	39	LEU
34	e	49	LEU
34	e	54	ARG
35	f	85	TYR
35	f	91	ILE
35	f	92	ARG
35	f	100	LEU
35	f	108	VAL
35	f	109	ASP

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Mol	Chain	Res	Type
35	f	119	LYS
35	f	129	PHE
35	f	138	TYR
36	g	6	ILE
36	g	8	LEU
36	g	11	ARG
36	g	13	THR
36	g	18	ASN
36	g	20	TRP
36	g	33	LEU
36	g	39	ARG
36	g	43	LEU
36	g	55	PHE
36	g	67	HIS
36	g	70	GLN
36	g	124	ILE
36	g	128	ARG
36	g	129	ASP
36	g	146	LEU
36	g	188	LEU
36	g	198	ASP
36	g	205	TYR
36	g	206	ILE
36	g	210	GLN
36	g	224	ASP
36	g	234	HIS
36	g	238	PHE
36	g	244	LYS
36	g	246	GLU
36	g	256	ARG
36	g	276	VAL
36	g	280	GLU
36	g	284	GLU
36	g	289	THR
36	g	314	ASP
36	g	321	GLN
36	g	323	MET
37	h	5	TRP
37	h	9	ARG
37	h	12	ARG
38	i	18	ASP
38	i	24	ARG

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Mol	Chain	Res	Type
38	i	26	LEU
38	i	27	ILE
38	i	34	GLU
38	i	41	MET
38	i	52	PHE
38	i	58	MET
38	i	62	ARG
38	i	69	VAL
38	i	70	TRP
38	i	82	ARG
38	i	91	VAL
38	i	97	LEU
38	i	101	ARG
38	i	103	LEU
38	i	105	ASN
38	i	111	GLU
38	i	112	ASN
39	j	6	CYS
39	j	7	ARG
39	j	11	ASN
39	j	15	GLU
39	j	17	ASP
39	j	18	ASP
39	j	19	ILE
39	j	23	ASN
39	j	33	TYR
39	j	39	TYR
39	j	42	ILE
39	j	45	MET
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	79	GLU
39	j	87	LYS
39	j	90	VAL
39	j	96	ILE
39	j	97	LYS
39	j	114	TYR
39	j	119	PHE
39	j	129	THR
39	j	143	GLU
39	j	159	GLU

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Mol	Chain	Res	Type
39	j	163	LYS
39	j	164	ASP
39	j	166	LEU
39	j	169	LEU
39	j	185	ARG
39	j	195	TYR
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	236	ASP
39	j	244	LEU
39	j	251	ILE
39	j	261	VAL
39	j	264	ILE
40	k	130	ASP
40	k	132	LEU
40	k	224	CYS
40	k	228	GLN
40	k	236	ILE
40	k	253	LEU
40	k	257	GLU
40	k	291	ILE
40	k	307	ARG
40	k	332	ASP
40	k	354	GLU
40	k	359	ILE
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	406	LEU
40	k	426	ILE
40	k	432	ILE
40	k	438	ARG
40	k	440	LEU
40	k	443	VAL
40	k	462	LEU
40	k	495	ILE
40	k	502	SER
40	k	508	HIS
40	k	512	ILE
41	l	131	TYR
41	l	135	LEU

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Mol	Chain	Res	Type
41	l	141	ILE
41	l	157	LYS
41	l	159	ARG
41	l	161	PRO
41	l	166	LEU
41	l	167	ARG
41	l	171	LYS
41	l	172	THR
41	l	177	ILE
41	l	189	GLU
41	l	213	ILE
41	l	229	TYR
41	l	246	LEU
41	l	257	MET
42	m	22	THR
42	m	39	LEU
42	m	40	THR
42	m	62	PHE
42	m	65	ASN
42	m	68	ILE
42	m	71	ASP
42	m	74	MET
42	m	87	LYS
42	m	92	MET
42	m	98	LEU
42	m	103	ILE
42	m	104	LYS
43	o	6	PHE
43	o	9	GLU
43	o	16	ASP
43	o	39	ARG
43	o	41	ARG
43	o	73	HIS
43	o	79	ILE
43	o	104	ILE
43	o	109	THR
43	o	114	LEU
43	o	120	ASP
43	o	151	ILE
43	o	154	TRP
43	o	168	LEU
43	o	169	LEU

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Mol	Chain	Res	Type
43	o	170	ARG
43	o	183	VAL
43	o	186	THR
43	o	188	HIS
43	o	190	CYS
43	o	199	PHE
43	o	211	ASP
43	o	223	ASN
43	o	235	ARG
43	o	265	HIS
43	o	268	LYS
43	o	278	THR
43	o	279	LEU
43	o	282	TYR
43	o	284	GLU
43	o	298	LEU
43	o	303	TRP
43	o	329	PHE
43	o	351	MET
43	o	354	LEU
43	o	365	GLU
43	o	387	LEU
43	o	407	LEU
43	o	415	THR
43	o	416	TYR
43	o	420	TYR
43	o	424	LEU
43	o	426	ASP
43	o	443	VAL
43	o	476	ASP
43	o	478	VAL
43	o	480	ILE
44	p	195	TYR
44	p	251	GLN
44	p	253	ASP
44	p	257	ARG
44	p	275	LEU
44	p	297	LEU
44	p	315	ILE
44	p	317	GLN
44	p	335	THR
44	p	336	ILE

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Mol	Chain	Res	Type
44	p	354	GLU
44	p	374	GLU
44	p	388	ASP
44	p	404	ILE
44	p	409	LEU
44	p	413	LEU
44	p	416	GLU
44	p	438	ASP
44	p	462	GLN
44	p	467	PHE
44	p	480	ASP
44	p	540	GLN
44	p	559	LEU
44	p	561	GLU
44	p	608	TYR
44	p	611	HIS
44	p	616	LEU
44	p	644	ARG
44	p	659	TYR
44	p	663	SER
44	p	671	LEU
44	p	681	SER
44	p	707	GLU
44	p	722	LEU
44	p	733	TYR
44	p	744	LEU
44	p	750	ASN
44	p	793	LYS
45	q	7	THR
45	q	40	LEU
45	q	47	THR
45	q	49	ASP
45	q	79	TRP
45	q	80	ASP
45	q	100	GLU
45	q	101	PHE
45	q	108	PHE
45	q	135	GLU
45	q	138	LYS
45	q	157	THR
45	q	193	ASP
45	q	201	ASP

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Mol	Chain	Res	Type
45	q	264	THR
45	q	308	TYR
45	q	329	PHE
46	r	704	LEU
46	r	708	GLU
46	r	725	GLU
47	s	58	TYR
47	s	61	GLU
47	s	82	ARG
47	s	85	ARG
47	s	86	ASN
47	s	96	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	30	GLN
4	A	33	GLN
4	A	46	ASN
4	A	109	ASN
4	A	131	GLN
4	A	140	ASN
5	B	101	HIS
5	B	148	ASN
5	B	183	GLN
6	C	64	HIS
6	C	72	GLN
6	C	76	GLN
6	C	87	ASN
6	C	92	GLN
6	C	99	GLN
6	C	194	GLN
6	C	225	ASN
6	C	233	ASN
8	E	69	HIS
8	E	188	ASN
9	F	37	GLN
9	F	65	GLN
9	F	81	ASN
9	F	105	ASN
9	F	172	GLN
9	F	188	ASN

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Mol	Chain	Res	Type
10	G	4	ASN
10	G	10	ASN
10	G	13	GLN
11	H	19	GLN
11	H	110	GLN
12	I	53	GLN
15	L	8	GLN
15	L	118	GLN
17	N	36	GLN
17	N	49	GLN
17	N	58	HIS
17	N	105	ASN
18	O	80	HIS
20	Q	83	GLN
21	R	48	ASN
22	S	13	HIS
22	S	21	ASN
22	S	25	ASN
22	S	75	ASN
22	S	99	HIS
23	T	43	ASN
24	U	72	ASN
25	V	33	GLN
25	V	70	ASN
26	W	24	GLN
27	X	22	ASN
27	X	48	HIS
27	X	79	ASN
31	b	51	GLN
33	d	10	HIS
33	d	41	GLN
36	g	161	ASN
38	i	37	GLN
38	i	44	ASN
38	i	60	HIS
38	i	85	GLN
40	k	98	GLN
40	k	248	GLN
40	k	415	GLN
40	k	508	HIS
41	l	176	ASN
41	l	190	HIS

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Mol	Chain	Res	Type
41	l	243	ASN
42	m	67	ASN
42	m	79	GLN
43	o	32	HIS
43	o	194	GLN
43	o	209	HIS
43	o	216	GLN
43	o	242	GLN
43	o	254	HIS
43	o	299	HIS
43	o	348	HIS
43	o	403	GLN
44	p	582	GLN
44	p	683	GLN
45	q	9	HIS
45	q	195	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	32 (43%)	7 (9%)
2	2	1778/1781 (99%)	879 (49%)	146 (8%)
3	3	13/25 (52%)	11 (84%)	1 (7%)
All	All	1865/1881 (99%)	922 (49%)	154 (8%)

All (922) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	G
1	1	10	G
1	1	14	A
1	1	15	G
1	1	16	U
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	25	C

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Mol	Chain	Res	Type
1	1	28	A
1	1	34	C
1	1	40	C
1	1	41	C
1	1	44	A
1	1	45	U
1	1	46	G
1	1	48	C
1	1	49	C
1	1	52	G
1	1	56	C
1	1	59	A
1	1	60	A
1	1	61	C
1	1	63	G
1	1	69	C
1	1	71	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	9	U
2	2	11	A
2	2	14	C
2	2	16	G
2	2	17	C
2	2	19	A
2	2	20	G
2	2	24	U
2	2	25	C
2	2	26	A
2	2	27	U
2	2	29	U
2	2	30	G
2	2	31	C
2	2	34	G
2	2	35	U
2	2	36	C
2	2	37	U
2	2	39	A

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Mol	Chain	Res	Type
2	2	40	A
2	2	42	G
2	2	43	A
2	2	44	U
2	2	45	U
2	2	47	A
2	2	51	A
2	2	54	C
2	2	56	U
2	2	57	G
2	2	59	C
2	2	60	U
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	81	G
2	2	87	C
2	2	92	A
2	2	95	G
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	123	G
2	2	124	A
2	2	125	U
2	2	127	G
2	2	128	U
2	2	129	U
2	2	131	C

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Mol	Chain	Res	Type
2	2	132	U
2	2	133	U
2	2	134	U
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	141	U
2	2	144	A
2	2	146	A
2	2	147	U
2	2	148	C
2	2	149	U
2	2	150	G
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	169	U
2	2	172	A
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	183	C
2	2	185	C
2	2	186	G
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	193	U
2	2	194	G
2	2	195	G
2	2	198	G
2	2	199	A
2	2	203	G
2	2	209	A
2	2	214	A

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Mol	Chain	Res	Type
2	2	217	A
2	2	218	A
2	2	220	A
2	2	226	U
2	2	227	G
2	2	228	U
2	2	230	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	237	U
2	2	239	C
2	2	240	U
2	2	245	G
2	2	248	U
2	2	249	C
2	2	254	U
2	2	256	A
2	2	259	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	268	G
2	2	270	A
2	2	274	C
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	288	U
2	2	289	G
2	2	294	A
2	2	298	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A

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Mol	Chain	Res	Type
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	319	U
2	2	320	C
2	2	321	G
2	2	322	A
2	2	332	A
2	2	336	G
2	2	337	C
2	2	345	G
2	2	349	U
2	2	350	C
2	2	351	A
2	2	358	A
2	2	359	A
2	2	360	C
2	2	368	A
2	2	371	G
2	2	372	G
2	2	377	A
2	2	380	C
2	2	382	G
2	2	384	A
2	2	388	G
2	2	389	G
2	2	390	A
2	2	395	G
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	403	G
2	2	404	C
2	2	406	A
2	2	409	A
2	2	411	A
2	2	412	U
2	2	413	C
2	2	415	A
2	2	416	A

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Mol	Chain	Res	Type
2	2	417	G
2	2	418	G
2	2	420	A
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	426	C
2	2	433	G
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	447	C
2	2	448	C
2	2	452	U
2	2	454	C
2	2	455	A
2	2	456	G
2	2	457	G
2	2	458	G
2	2	459	A
2	2	461	G
2	2	467	A
2	2	468	C
2	2	473	A
2	2	475	U
2	2	479	G
2	2	480	A
2	2	482	A
2	2	483	C
2	2	487	G
2	2	488	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	497	G

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Mol	Chain	Res	Type
2	2	499	C
2	2	500	U
2	2	501	U
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	511	A
2	2	512	U
2	2	513	G
2	2	515	G
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	521	U
2	2	522	G
2	2	523	U
2	2	525	A
2	2	527	U
2	2	530	C
2	2	531	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	550	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	559	U

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Mol	Chain	Res	Type
2	2	560	G
2	2	564	C
2	2	565	C
2	2	566	A
2	2	567	G
2	2	568	C
2	2	569	A
2	2	570	G
2	2	571	C
2	2	573	G
2	2	574	C
2	2	576	G
2	2	577	U
2	2	578	A
2	2	579	A
2	2	580	U
2	2	581	U
2	2	584	A
2	2	586	C
2	2	589	C
2	2	590	A
2	2	593	A
2	2	594	G
2	2	597	U
2	2	599	U
2	2	600	A
2	2	601	U
2	2	605	A
2	2	610	U
2	2	612	G
2	2	613	C
2	2	614	A
2	2	615	G
2	2	616	U
2	2	617	U
2	2	618	A
2	2	619	A
2	2	621	A
2	2	622	A
2	2	624	C
2	2	634	A
2	2	638	U

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Mol	Chain	Res	Type
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	681	U
2	2	684	A
2	2	685	A
2	2	686	C
2	2	687	C
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	700	C
2	2	701	U
2	2	702	G
2	2	703	G
2	2	704	C
2	2	705	U
2	2	706	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	713	A
2	2	714	C
2	2	715	U
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	723	G

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Mol	Chain	Res	Type
2	2	725	U
2	2	727	C
2	2	729	G
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	735	C
2	2	736	C
2	2	738	G
2	2	741	C
2	2	742	U
2	2	743	U
2	2	744	U
2	2	745	U
2	2	753	A
2	2	755	A
2	2	762	A
2	2	763	G
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	774	A
2	2	775	G
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	783	C
2	2	784	U
2	2	785	C
2	2	788	A
2	2	790	A
2	2	793	U
2	2	794	U
2	2	796	G
2	2	803	A
2	2	805	A
2	2	806	A
2	2	809	G

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Mol	Chain	Res	Type
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	832	U
2	2	834	U
2	2	836	G
2	2	837	G
2	2	839	U
2	2	840	U
2	2	841	C
2	2	845	G
2	2	847	C
2	2	851	C
2	2	855	A
2	2	856	U
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	864	A
2	2	872	U
2	2	875	G
2	2	883	A
2	2	885	U
2	2	886	A
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	904	A
2	2	905	A

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Mol	Chain	Res	Type
2	2	907	U
2	2	908	U
2	2	910	U
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	919	U
2	2	920	U
2	2	925	A
2	2	927	U
2	2	930	C
2	2	931	U
2	2	932	A
2	2	934	U
2	2	936	C
2	2	938	A
2	2	939	A
2	2	941	G
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	957	U
2	2	958	U
2	2	959	U
2	2	962	A
2	2	965	A
2	2	970	A
2	2	978	A
2	2	981	U
2	2	982	A
2	2	983	G
2	2	987	A
2	2	991	A
2	2	992	A
2	2	993	G
2	2	994	A
2	2	995	U
2	2	996	G

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Mol	Chain	Res	Type
2	2	998	U
2	2	999	C
2	2	1000	A
2	2	1003	U
2	2	1004	A
2	2	1007	G
2	2	1008	U
2	2	1009	C
2	2	1012	A
2	2	1013	G
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1022	A
2	2	1023	U
2	2	1024	A
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1042	A
2	2	1043	U
2	2	1046	G
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U

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Mol	Chain	Res	Type
2	2	1064	A
2	2	1065	C
2	2	1066	C
2	2	1069	C
2	2	1070	U
2	2	1075	A
2	2	1076	C
2	2	1077	C
2	2	1079	U
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1086	A
2	2	1089	C
2	2	1090	A
2	2	1091	A
2	2	1092	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1098	U
2	2	1099	G
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1107	G
2	2	1108	G
2	2	1110	G
2	2	1111	G
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1117	G
2	2	1118	G
2	2	1123	A
2	2	1125	G
2	2	1133	C
2	2	1135	U
2	2	1136	A
2	2	1137	A
2	2	1138	A

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Mol	Chain	Res	Type
2	2	1145	G
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1163	G
2	2	1164	G
2	2	1166	G
2	2	1168	G
2	2	1169	G
2	2	1172	C
2	2	1174	U
2	2	1175	G
2	2	1176	C
2	2	1184	U
2	2	1185	U
2	2	1186	U
2	2	1188	A
2	2	1189	C
2	2	1190	U
2	2	1191	C
2	2	1192	A
2	2	1193	A
2	2	1195	A
2	2	1196	C
2	2	1197	G
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1218	A

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Mol	Chain	Res	Type
2	2	1224	U
2	2	1225	A
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1237	A
2	2	1240	G
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1247	C
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1260	G
2	2	1268	U
2	2	1272	G
2	2	1273	C
2	2	1275	U
2	2	1282	U
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1286	A
2	2	1287	G
2	2	1292	U
2	2	1294	G
2	2	1295	A
2	2	1296	G
2	2	1298	G
2	2	1300	U
2	2	1303	G
2	2	1305	C
2	2	1306	U
2	2	1309	U
2	2	1311	A
2	2	1312	A
2	2	1313	U
2	2	1314	U

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Mol	Chain	Res	Type
2	2	1315	G
2	2	1316	C
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1332	C
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1340	A
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1346	U
2	2	1347	A
2	2	1348	G
2	2	1352	U
2	2	1353	G
2	2	1357	G
2	2	1358	C
2	2	1359	A
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1374	C
2	2	1376	U
2	2	1377	C
2	2	1380	A
2	2	1381	G
2	2	1383	G
2	2	1386	A
2	2	1387	C
2	2	1388	U
2	2	1389	A
2	2	1390	U

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Mol	Chain	Res	Type
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1408	A
2	2	1409	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1417	G
2	2	1418	C
2	2	1419	A
2	2	1420	A
2	2	1423	A
2	2	1425	A
2	2	1426	G
2	2	1428	U
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1433	G
2	2	1434	A
2	2	1435	U
2	2	1442	A
2	2	1444	A
2	2	1448	U
2	2	1449	C
2	2	1450	U
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A
2	2	1459	C
2	2	1461	C
2	2	1465	C
2	2	1466	U
2	2	1467	A
2	2	1469	A
2	2	1470	C

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Mol	Chain	Res	Type
2	2	1471	U
2	2	1476	G
2	2	1478	G
2	2	1479	C
2	2	1480	C
2	2	1481	A
2	2	1482	G
2	2	1484	G
2	2	1487	U
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1496	G
2	2	1498	C
2	2	1499	C
2	2	1501	A
2	2	1504	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1528	C
2	2	1529	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1537	G
2	2	1538	G
2	2	1540	G
2	2	1544	G
2	2	1554	A
2	2	1555	U
2	2	1557	A

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Mol	Chain	Res	Type
2	2	1558	U
2	2	1559	U
2	2	1566	C
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1574	A
2	2	1575	A
2	2	1578	C
2	2	1579	C
2	2	1580	U
2	2	1581	A
2	2	1582	G
2	2	1583	U
2	2	1584	A
2	2	1588	G
2	2	1590	A
2	2	1593	U
2	2	1594	C
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1608	G
2	2	1611	U
2	2	1612	A
2	2	1613	C
2	2	1614	G
2	2	1616	C
2	2	1631	A
2	2	1632	C
2	2	1633	A
2	2	1634	C
2	2	1635	C
2	2	1636	G
2	2	1637	C
2	2	1638	C
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C

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Mol	Chain	Res	Type
2	2	1667	U
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1719	A
2	2	1725	G
2	2	1728	A
2	2	1730	A
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U
2	2	1753	A
2	2	1754	A
2	2	1758	G
2	2	1763	A
2	2	1764	A
2	2	1765	G
2	2	1766	G

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Mol	Chain	Res	Type
2	2	1767	U
2	2	1768	U
2	2	1778	G
2	2	1779	A
2	2	1781	C
2	2	1782	C
2	2	1786	G
2	2	1787	G
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1794	C
2	2	1795	A
2	2	1796	U
2	2	1797	U
2	2	1798	A
3	3	4	U
3	3	5	C
3	3	6	U
3	3	7	C
3	3	8	U
3	3	9	C
3	3	10	U
3	3	11	C
3	3	12	U
3	3	13	A
3	3	16	C

All (154) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	43	G
1	1	44	A
1	1	47	U
1	1	48	C
1	1	59	A
1	1	74	C
2	2	42	G
2	2	46	A
2	2	66	U
2	2	68	A

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Mol	Chain	Res	Type
2	2	72	A
2	2	73	U
2	2	74	U
2	2	103	A
2	2	115	G
2	2	126	A
2	2	129	U
2	2	130	C
2	2	131	C
2	2	133	U
2	2	134	U
2	2	140	A
2	2	157	U
2	2	177	U
2	2	186	G
2	2	190	C
2	2	193	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	248	U
2	2	258	U
2	2	265	A
2	2	277	U
2	2	278	G
2	2	279	U
2	2	294	A
2	2	312	U
2	2	320	C
2	2	321	G
2	2	344	U
2	2	349	U
2	2	368	A
2	2	388	G
2	2	389	G
2	2	403	G
2	2	451	A
2	2	473	A
2	2	497	G
2	2	517	A
2	2	538	G
2	2	540	A

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Mol	Chain	Res	Type
2	2	542	C
2	2	554	A
2	2	564	C
2	2	570	G
2	2	588	C
2	2	589	C
2	2	593	A
2	2	600	A
2	2	617	U
2	2	620	A
2	2	654	G
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	704	C
2	2	721	U
2	2	736	C
2	2	781	A
2	2	793	U
2	2	810	A
2	2	811	A
2	2	826	C
2	2	828	A
2	2	854	A
2	2	855	A
2	2	860	U
2	2	896	C
2	2	907	U
2	2	938	A
2	2	946	U
2	2	956	G
2	2	986	G
2	2	995	U
2	2	998	U
2	2	1010	G
2	2	1030	U
2	2	1038	A
2	2	1056	U
2	2	1080	A
2	2	1089	C
2	2	1092	A

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Mol	Chain	Res	Type
2	2	1095	C
2	2	1096	U
2	2	1099	G
2	2	1107	G
2	2	1110	G
2	2	1117	G
2	2	1136	A
2	2	1157	C
2	2	1188	A
2	2	1192	A
2	2	1194	C
2	2	1195	A
2	2	1196	C
2	2	1198	G
2	2	1202	A
2	2	1206	C
2	2	1225	A
2	2	1226	A
2	2	1283	C
2	2	1314	U
2	2	1315	G
2	2	1320	A
2	2	1343	A
2	2	1345	A
2	2	1360	C
2	2	1363	G
2	2	1375	U
2	2	1389	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1416	G
2	2	1419	A
2	2	1423	A
2	2	1425	A
2	2	1430	U
2	2	1445	C
2	2	1455	C
2	2	1457	C
2	2	1465	C
2	2	1479	C
2	2	1481	A

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Mol	Chain	Res	Type
2	2	1482	G
2	2	1489	C
2	2	1491	A
2	2	1533	U
2	2	1534	G
2	2	1571	A
2	2	1579	C
2	2	1580	U
2	2	1604	C
2	2	1613	C
2	2	1655	U
2	2	1678	G
2	2	1763	A
2	2	1765	G
2	2	1766	G
2	2	1792	A
3	3	10	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 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	$\# Z > 2$
50	MET	k	601	-	5,7,8	0.39	0	4,7,9	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	GCP	k	603	48	29,34,34	1.85	7 (24%)	32,54,54	1.75	5 (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
50	MET	k	601	-	-	0/4/6/8	0/0/0/0
51	GCP	k	603	48	-	0/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O3G	-2.58	1.48	1.54
51	k	603	GCP	PB-O2B	2.06	1.61	1.56
51	k	603	GCP	PG-O2G	2.67	1.61	1.54
51	k	603	GCP	PB-O3A	3.06	1.61	1.58
51	k	603	GCP	C5-C4	3.50	1.48	1.40
51	k	603	GCP	C6-C5	4.13	1.49	1.41
51	k	603	GCP	PG-O1G	5.09	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C5-C6-N1	-4.11	118.16	123.52
51	k	603	GCP	N3-C2-N1	-3.80	122.38	127.56
51	k	603	GCP	C6-C5-C4	-3.20	117.20	120.86
51	k	603	GCP	O4'-C1'-N9	2.39	112.62	108.11
51	k	603	GCP	C6-N1-C2	5.62	122.46	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.