



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:14 AM UTC

PDB ID : 8RW1 / pdb_00008rw1
EMDB ID : EMD-19541
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-02-02
Resolution : 3.35 Å (reported)
Based on initial model : 6FYX

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

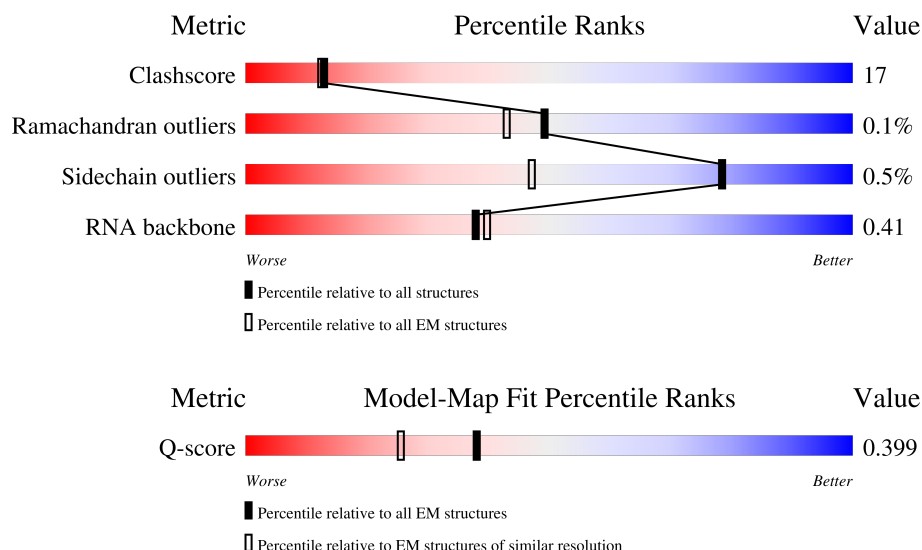
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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.



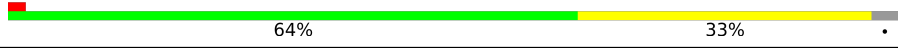
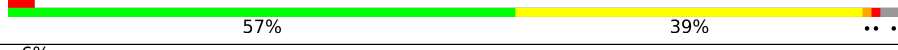
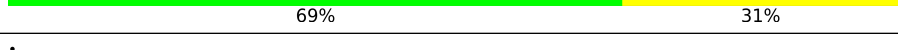
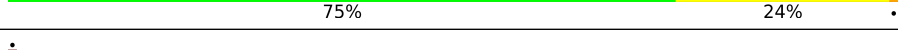
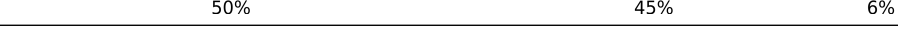
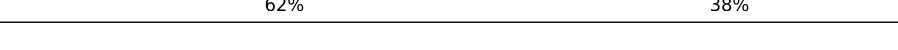
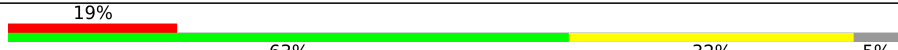
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1798	
2	A	254	
3	B	255	

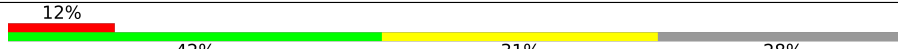
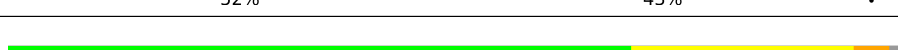
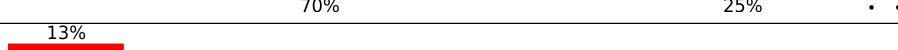
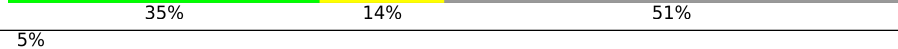
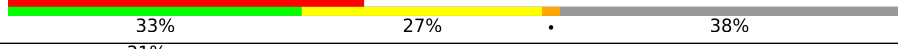
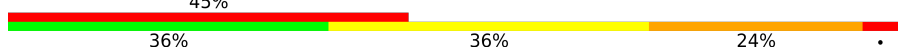
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	

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Mol	Chain	Length	Quality of chain
29	T	144	
30	U	117	
31	Z	108	
32	c	67	
33	d	56	
34	f	150	
35	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	527	
41	l	285	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 86000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total	C	N	O	P	0	0
			38190	17073	6722	12597	1798		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	225	Total	C	N	O	S	0	0
			1796	1135	330	328	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 5 is a protein called 40S ribosomal protein S4.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 7 is a protein called 40S ribosomal protein S7.

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

- Molecule 8 is a protein called 40S ribosomal protein S8.

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

- Molecule 9 is a protein called KLLA0E23673p.

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

- Molecule 10 is a protein called KLLA0A10483p.

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

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 13 is a protein called 40S ribosomal protein S21.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called KLLA0B11231p.

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

- Molecule 16 is a protein called 40S ribosomal protein S24.

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

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	102	Total	C	N	O	S	0	0
			797	492	168	132	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

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

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 20 is a protein called 40S ribosomal protein L41-A.

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

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 22 is a protein called KLLA0D10659p.

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

- Molecule 23 is a protein called KLLA0B08173p.

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

- Molecule 24 is a protein called 40S ribosomal protein S12.

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

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 29 is a protein called KLLA0A07194p.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 35 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	95	Total	C	N	O	S	0	0
			764	474	142	143	5		

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total	C	N	O	P	0	0
			536	242	84	184	26		

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	267	Total	C	N	O	S	0	0
			2139	1366	355	407	11		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total	C	N	O	S	0	0
			3596	2279	633	666	18		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			190	124	32	34		

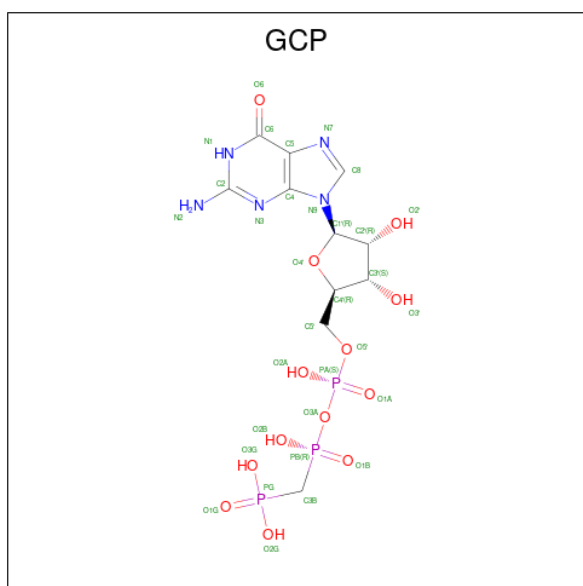
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	2	112	Total	Mg	0
			112	112	
42	T	1	Total	Mg	0
			1	1	
42	i	1	Total	Mg	0
			1	1	
42	3	1	Total	Mg	0
			1	1	

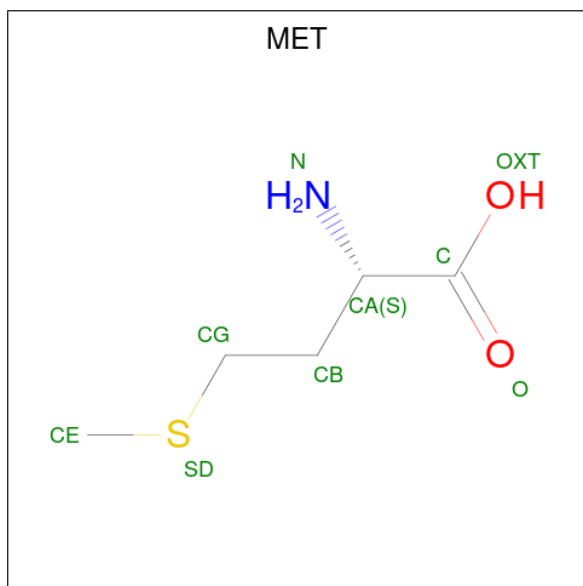
- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 44 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



- Molecule 45 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



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

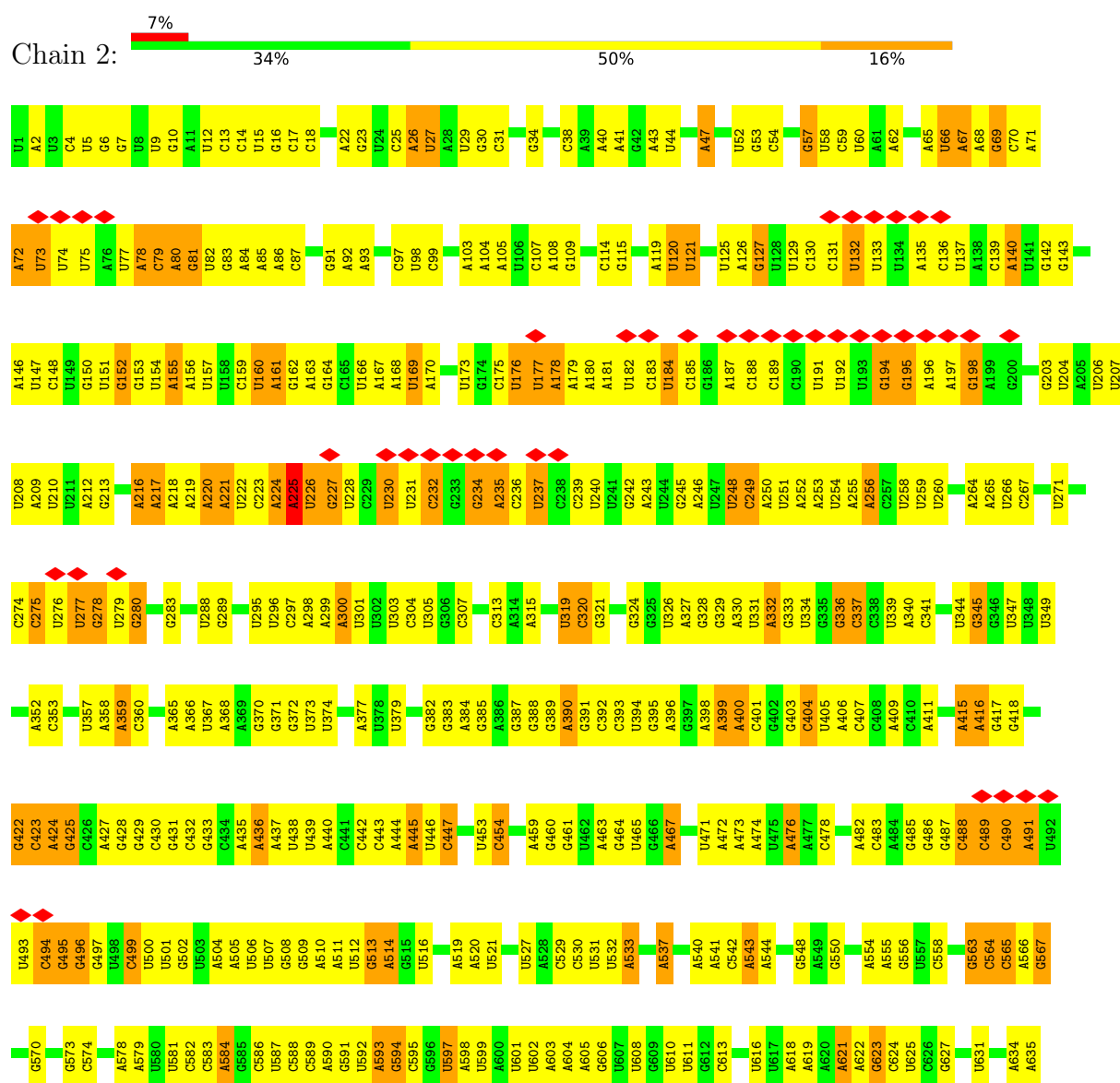
- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	2	3	Total	O	0
			3	3	

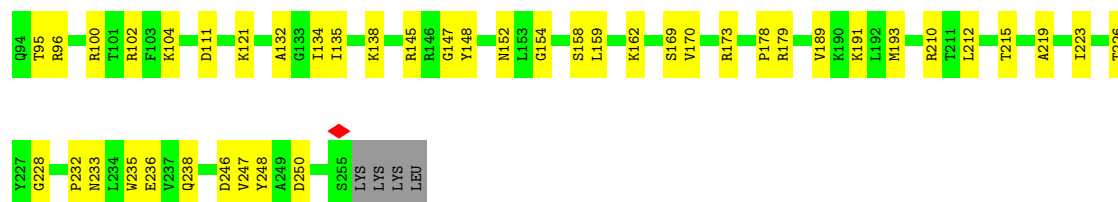
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

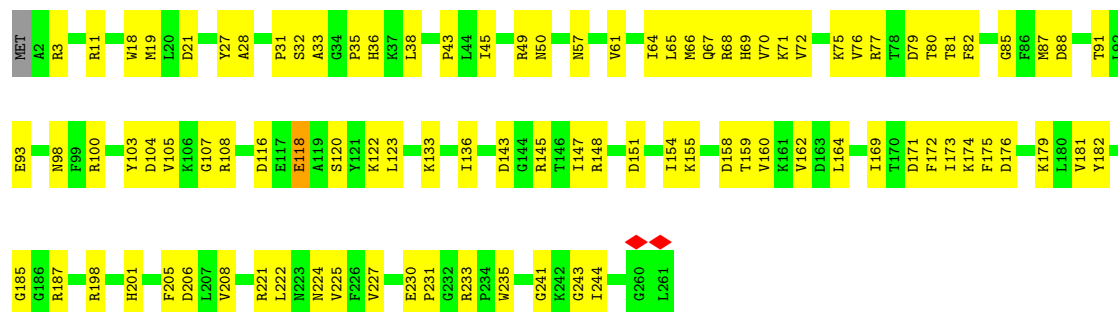
• Molecule 1: 18S ribosomal RNA



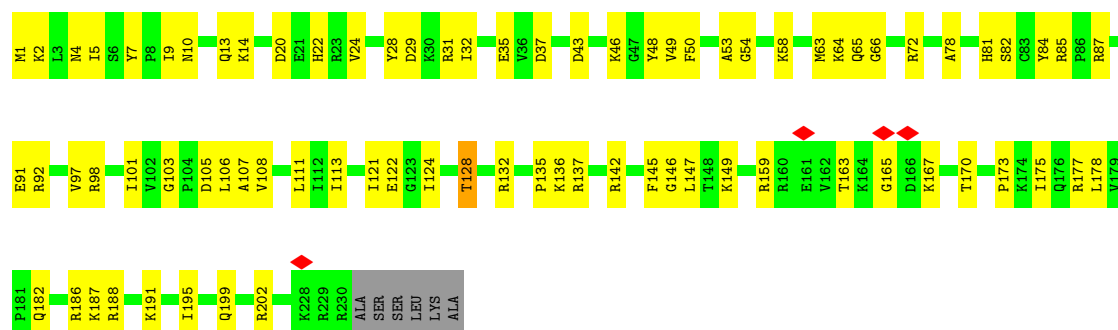
G1538	G1539	G1540	A1541	G1544	U1549	U1550	U1551	U1552	A1553	A1554	U1555	U1556	A1557	U1558	U1559	U1560	G1561	U1562	C1563	U1564	U1565	C1566	A1567	A1568	C1569	G1570	A1571	G1572	G1573	U1577	C1578	C1579	G1580	A1581	G1582	U1583	A1584	A1585	G1586	C1587	G1588	C1589	A1590	A1591	G1592	U1593	C1594	A1595	U1596	C1597	A1598	G1599	C1600	U1601	U1602	G1603			
C1470	A1471	G1472	A1473	G1476	A1477	G1478	C1479	C1480	C1481	G1482	U1483	A1484	U1485	G1486	U1487	A1488	C1489	A1490	A1491	C1492	U1493	U1494	C1498	A1499	C1499	G1500	A1501	G1502	A1503	U1506	C1507	U1508	G1509	U1580	G1580	U1581	U1582	U1583	A1584	A1585	G1586	C1587	U1588	C1589	A1590	U1520	A1591	G1592	U1593	C1594	A1595	U1596	C1597	A1598	G1599	C1600	U1601	U1602	G1603
U1396	C1397	G1400	C1401	G1402	G1403	A1404	U1405	C1406	G1407	A1408	A1409	G1410	U1411	U1412	U1413	U1414	A1415	G1416	C1424	A1425	G1426	G1427	U1428	C1429	U1430	G1431	A1434	C1437	C1438	A1442	G1443	A1444	G1445	G1446	U1447	U1448	U1449	U1450	G1451	C1455	C1456	C1457	A1458	G1459	G1460	C1463	G1464	A1465	U1466	A1467	U1468	A1469							
A1324	G1329	A1330	C1331	C1332	U1333	U1334	A1335	A1336	C1337	C1338	U1339	A1340	A1343	A1344	A1345	U1346	A1347	G1348	G1349	G1350	U1351	U1352	G1353	C1354	G1354	U1355	G1356	G1357	U1358	A1359	G1360	U1361	G1362	G1363	G1366	G1367	U1368	U1369	G1370	U1373	C1374	U1375	U1379	A1380	G1381	A1382	A1386	C1387	U1388	A1389	U1390	U1391	A1392	C1392	G1392				
G1254	A1255	U1256	U1257	U1258	U1259	G1260	U1261	G1262	G1263	G1266	U1267	U1268	G1269	G1272	C1273	A1274	U1275	G1276	C1279	G1280	C1283	U1284	G1287	U1288	U1289	G1290	G1291	U1292	G1293	G1294	A1295	G1296	U1297	G1298	A1299	U1300	U1301	U1302	U1306	U1309	U1313	U1314	G1315	C1316	G1317	U1318	U1319	A1320	U1321	C1322	G1323								
A1188	C1189	B8N1190	C1191	U1192	A1193	C1194	A1195	C1196	G1197	G1198	G1199	G1200	A1201	A1202	A1203	C1204	U1205	C1206	A1207	C1208	C1209	A1210	G1211	G1212	U1213	A1216	G1217	G1218	G1219	A1220	U1224	A1225	A1226	G1227	G1228	A1229	U1230	C1234	A1235	G1236	A1237	U1238	U1239	G1240	A1241	G1242	A1243	G1244	U1245	C1246	C1247	U1248	U1249	U1250	C1251				
A1112	G1113	U1114	U1115	U1116	G1121	A1124	U1125	G1126	G1129	A1130	A1131	A1132	A1136	A1137	A1141	A1142	U1143	U1144	G1145	A1146	C1147	G1148	G1149	A1150	A1151	G1152	C1155	A1156	C1157	C1158	A1159	C1160	A1161	A1162	G1163	G1164	A1165	G1166	U1167	G1168	G1169	A1170	G1171	C1172	C1173	A1182	A1183	U1184	U1185	U1186	G1187								
A1038	G1039	G1040	G1041	A1042	U1043	C1044	G1047	U1048	G1049	G1050	U1051	G1052	U1055	U1056	U1057	C1058	U1059	U1060	A1061	U1062	C1066	C1069	U1070	G1071	G1072	G1073	C1074	A1075	G1076	C1077	U1078	U1079	A1080	C1081	G1082	A1085	A1086	A1087	U1088	A1091	A1092	C1095	U1096	G1099	G1100	G1101	U1102	G1106	G1107	G1108									
A965	A969	A970	G971	A972	G975	A976	A977	A978	A982	G983	G984	G985	G986	A987	U988	C989	G990	A991	U995	G996	A997	U998	U1003	C1006	G1007	U1008	C1009	G1010	U1011	A1012	G1013	U1014	C1015	U1016	U1017	A1018	C1021	A1022	A1025	A1026	C1027	U1028	A1029	U1030	G1031	C1032	C1033	G1034	A1035	C1036	U1037								
C896	A897	G898	A899	G900	G901	U902	G903	A904	G912	G913	A914	U915	U916	U917	A918	G919	U920	G921	A922	U923	G924	A925	C926	U927	A928	A929	U930	U931	A932	C933	G934	A935	A938	U939	A940	G941	U944	U945	U946	G947	C948	C949	A950	A951	G952	U953	A954	C955	U956	C957	U958	A959	U960	A961					
U830	U831	U832	G833	U834	U835	G836	G837	U838	U839	U840	A841	U842	A843	A846	C847	G852	U853	A854	U855	U856	U857	U860	A861	A862	U863	A864	G865	G866	A867	U868	A869	G870	G871	U872	C873	G874	G875	G876	G877	G878	C882	A883	G884	U885	A886	U887	U888	C889	G892	U893	A894	U895							
U698	U699	U700	U701	G702	G703	C704	U705	A706	A707	C708	C709	U710	U711	U712	U713	C714	U715	C716	C717	U718	U719	A720	U721	G722	G723	G724	U725	G726	C727	A728	G729	U730	C731	G732	A733	A734	C735	C736	A737	G738	U739	A740	C741	U742	U743	U748	U749	U750	G751	A753	A754	A755	U758	U759	A760	G761			
A762	G765	U766	A769	U770	A771	G772	A773	A774	G775	G778	A779	U780	U781	U782	G783	G786	A787	U788	U789	A790	U791	A792	G793	U794	A798	G801	A802	U803	A806	U807	G808	G809	G810	A811	U812	A813	G814	A816	C817	G818	G819	U820	U821	G822	G823	U824	A825	U826	C827	U828	U829								
U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895



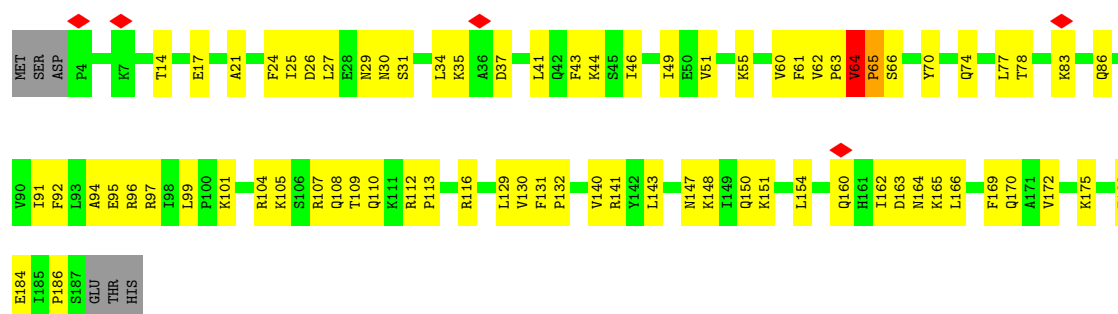
• Molecule 5: 40S ribosomal protein S4



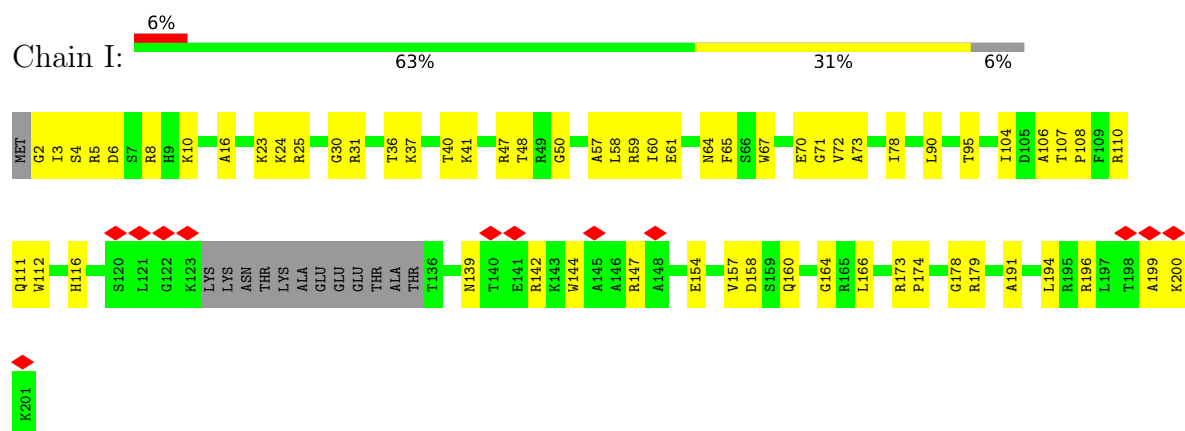
• Molecule 6: Small ribosomal subunit protein eS6



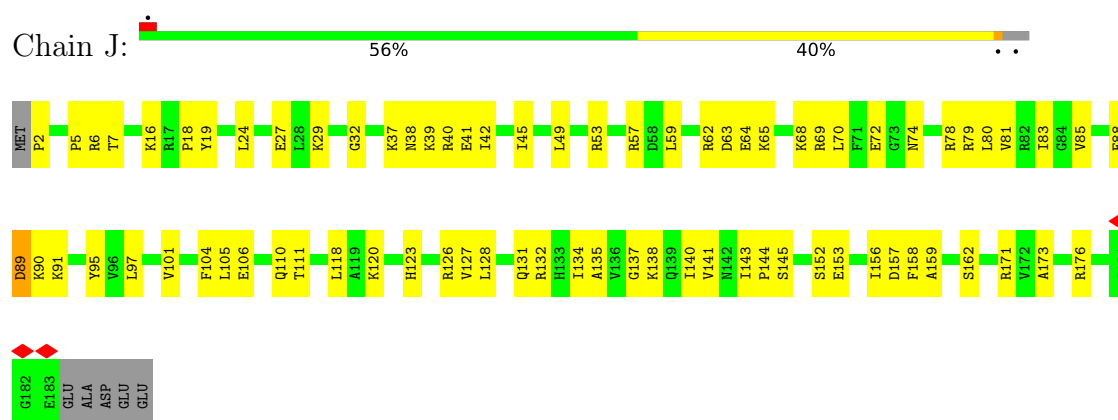
• Molecule 7: 40S ribosomal protein S7



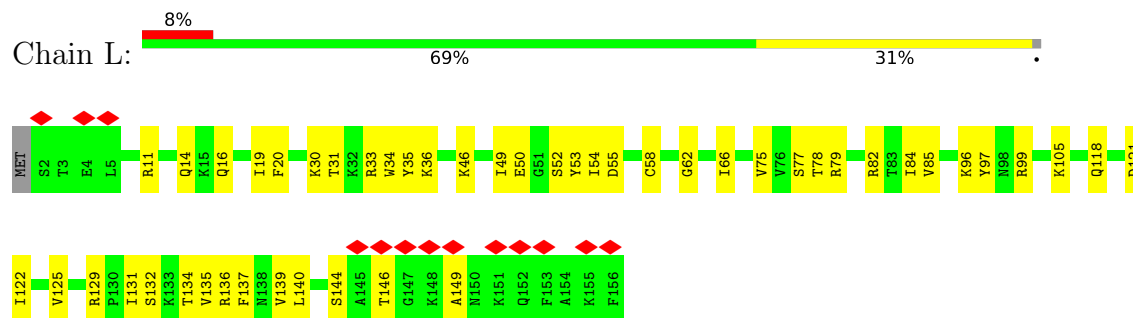
• Molecule 8: 40S ribosomal protein S8



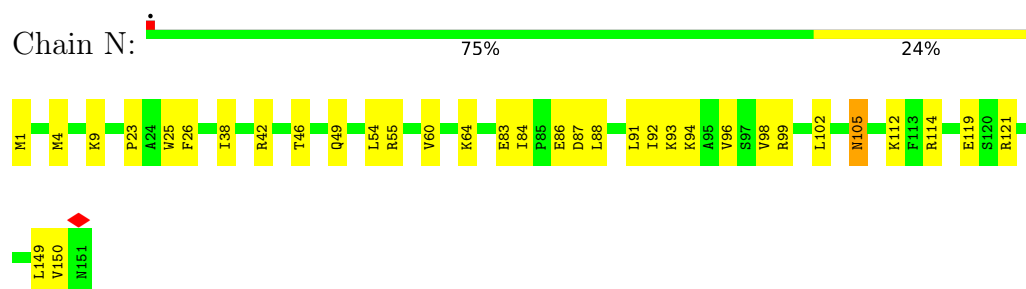
• Molecule 9: KLLA0E23673p



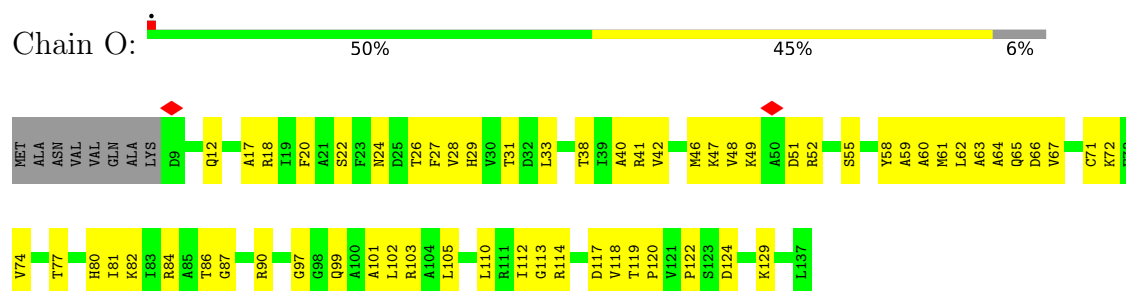
• Molecule 10: KLLA0A10483p



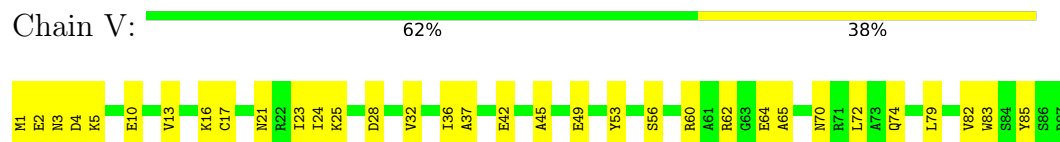
• Molecule 11: KLLA0F18040p



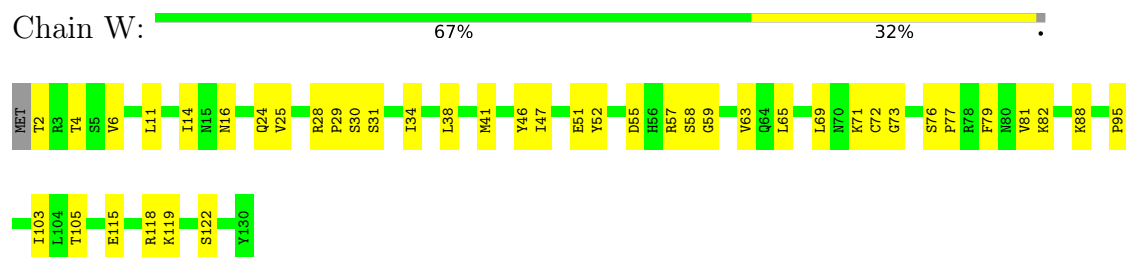
• Molecule 12: Small ribosomal subunit protein uS11



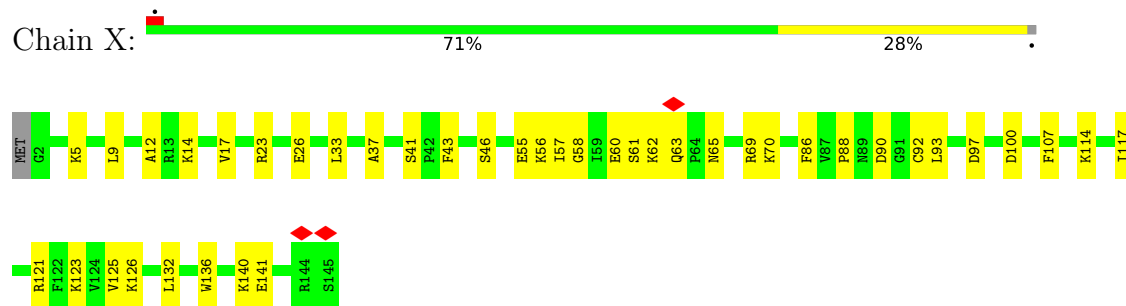
- Molecule 13: 40S ribosomal protein S21



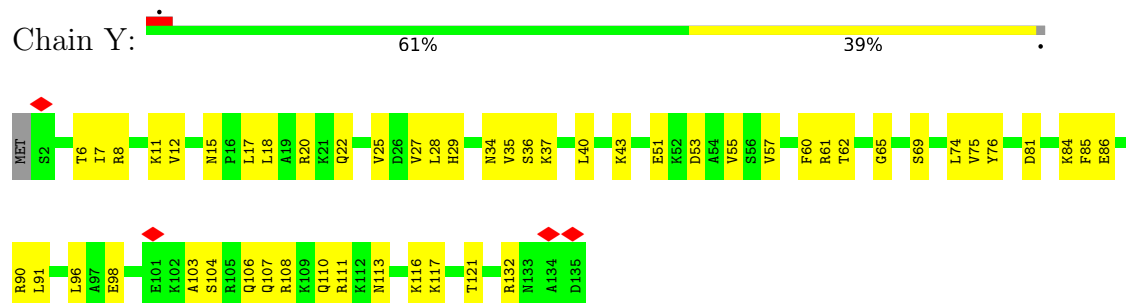
- Molecule 14: Small ribosomal subunit protein uS8



- Molecule 15: KLLA0B11231p

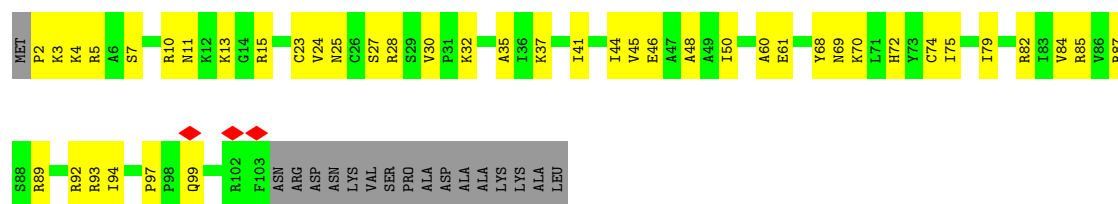


- Molecule 16: 40S ribosomal protein S24



- Molecule 17: 40S ribosomal protein S26

Chain a: 



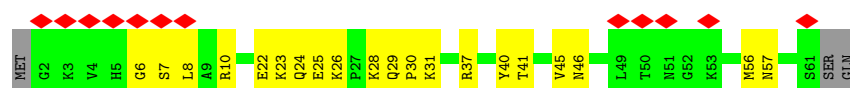
- Molecule 18: 40S ribosomal protein S27

Chain b: 



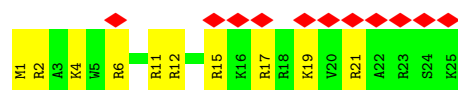
- Molecule 19: 40S ribosomal protein S30

Chain e: 



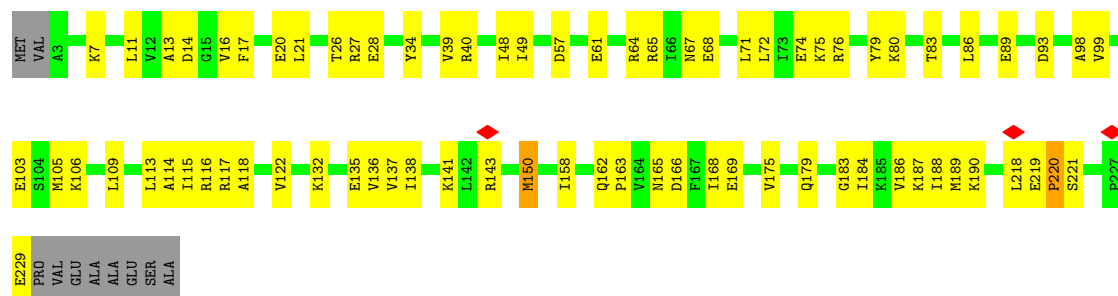
- Molecule 20: 40S ribosomal protein L41-A

Chain h: 



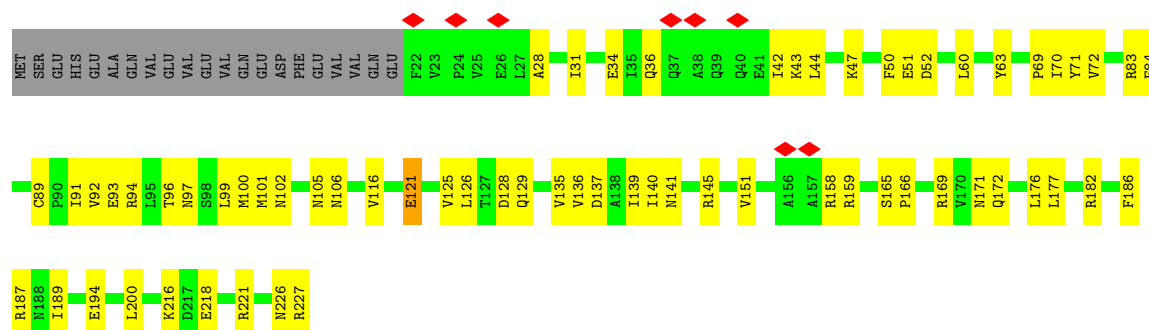
- Molecule 21: 40S ribosomal protein S3

Chain D: 

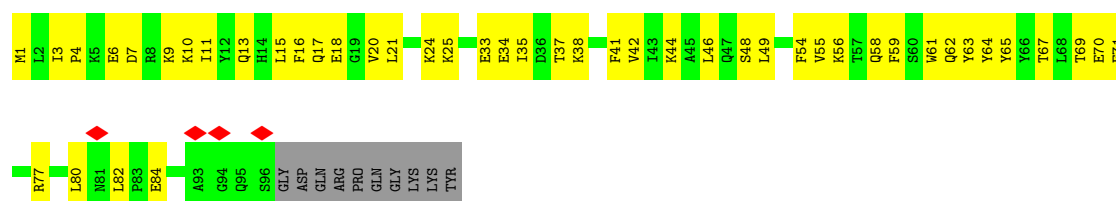


- Molecule 22: KLLA0D10659p

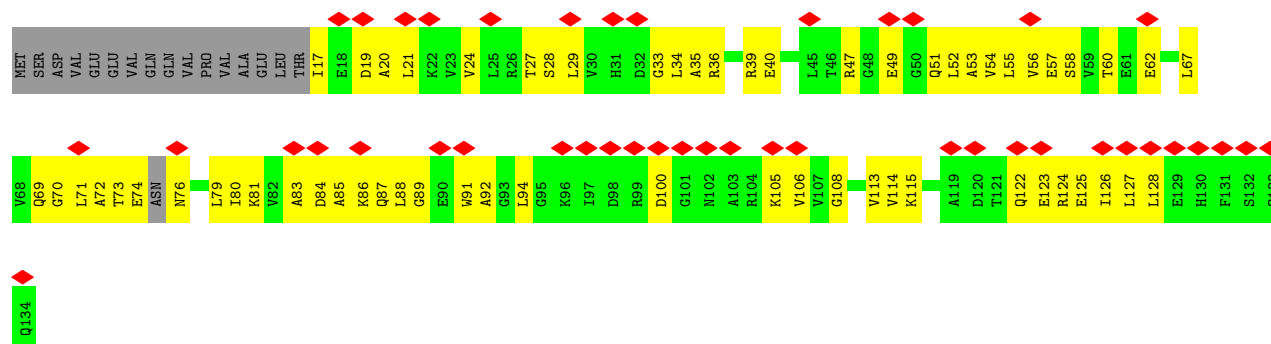
Chain F: 



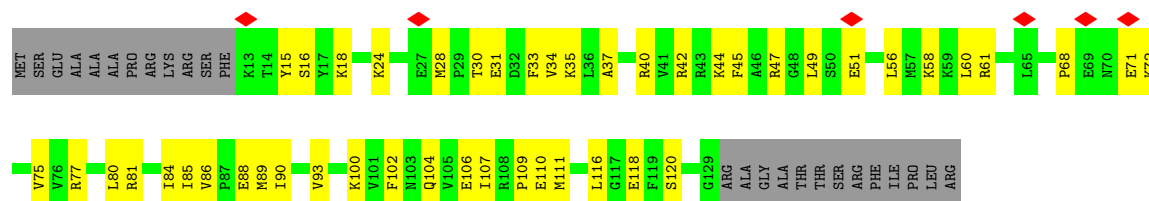
• Molecule 23: KLLA0B08173p



• Molecule 24: 40S ribosomal protein S12

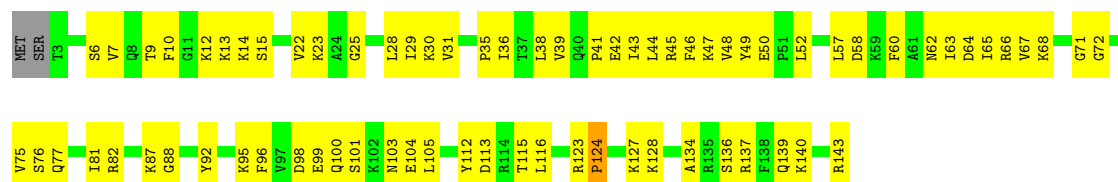


• Molecule 25: KLLA0F07843p

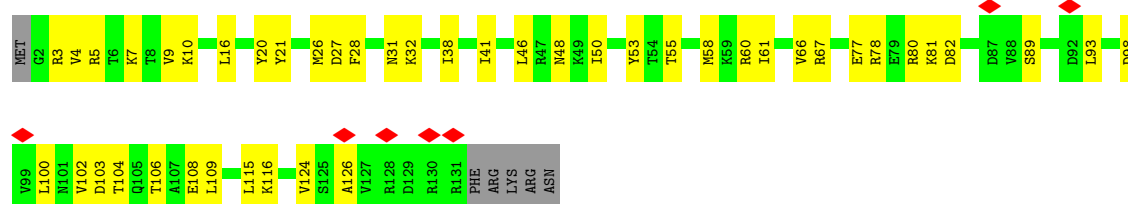


• Molecule 26: Small ribosomal subunit protein uS9

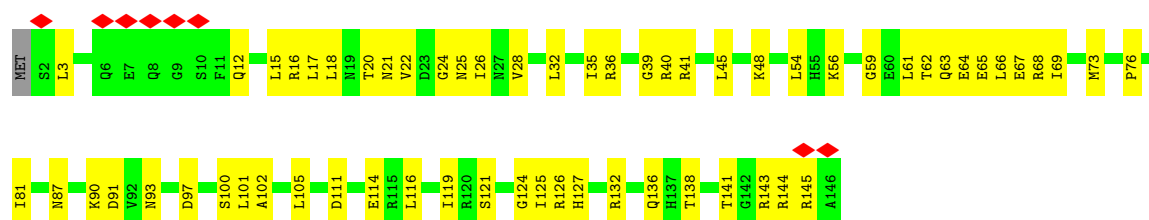




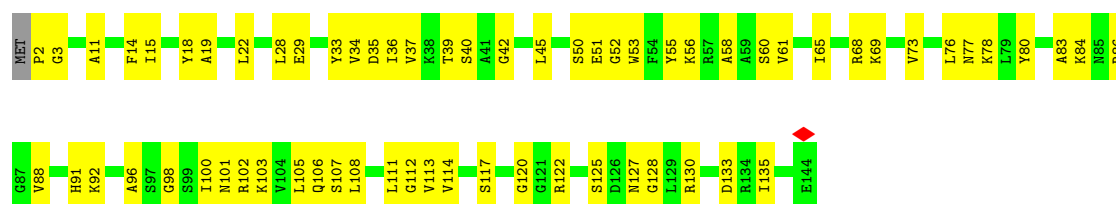
• Molecule 27: KLLA0B01474p



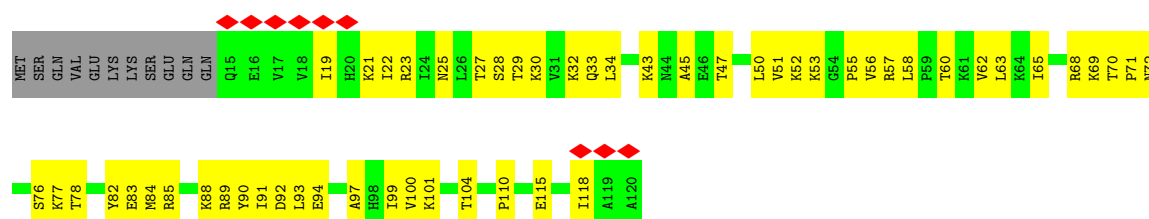
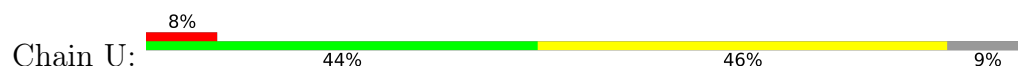
• Molecule 28: KLLA0B01562p



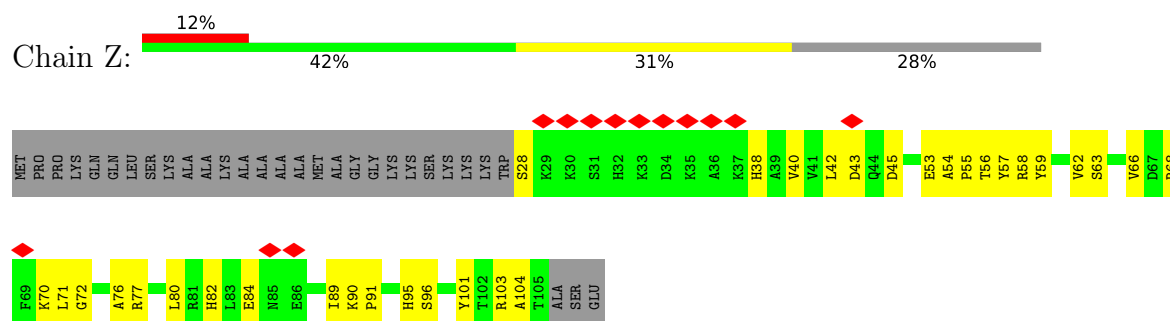
• Molecule 29: KLLA0A07194p



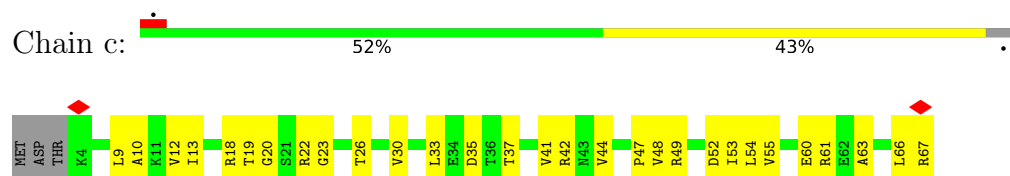
• Molecule 30: Small ribosomal subunit protein uS10



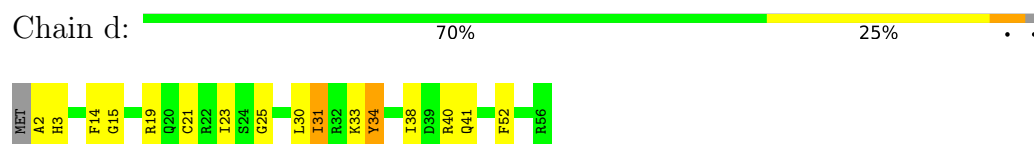
- Molecule 31: 40S ribosomal protein S25



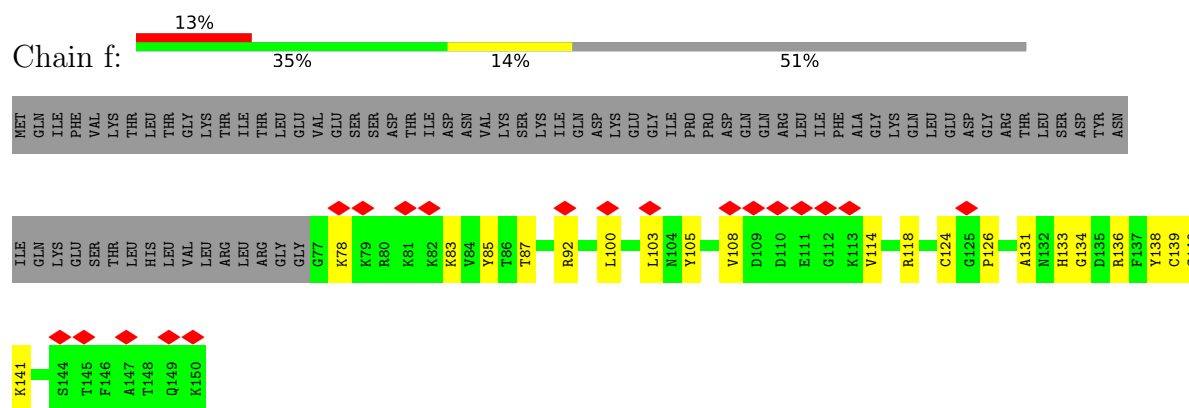
- Molecule 32: Small ribosomal subunit protein eS28



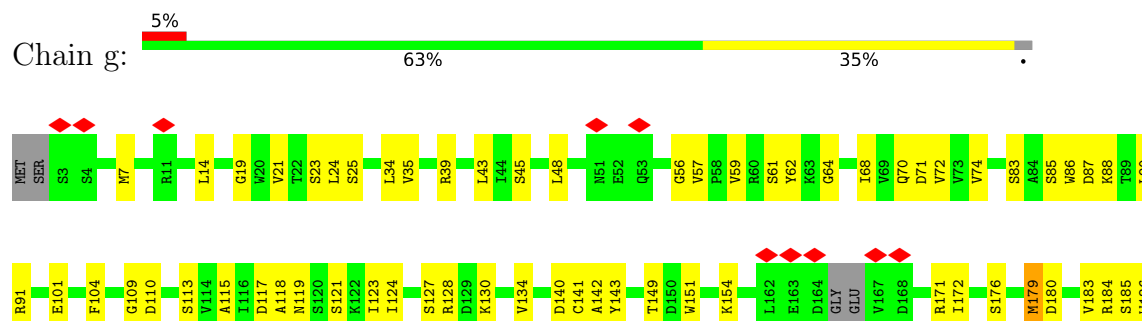
- Molecule 33: Small ribosomal subunit protein uS14

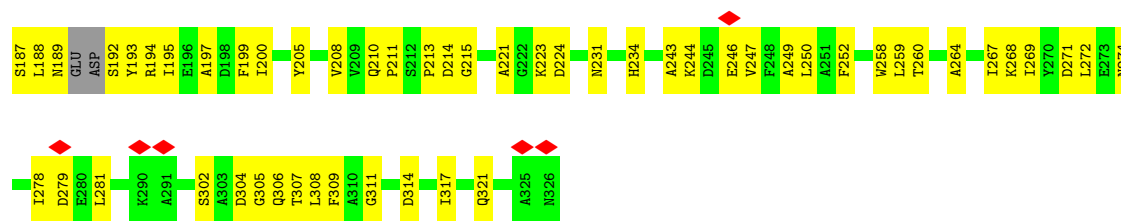


- Molecule 34: Small ribosomal subunit protein eS31

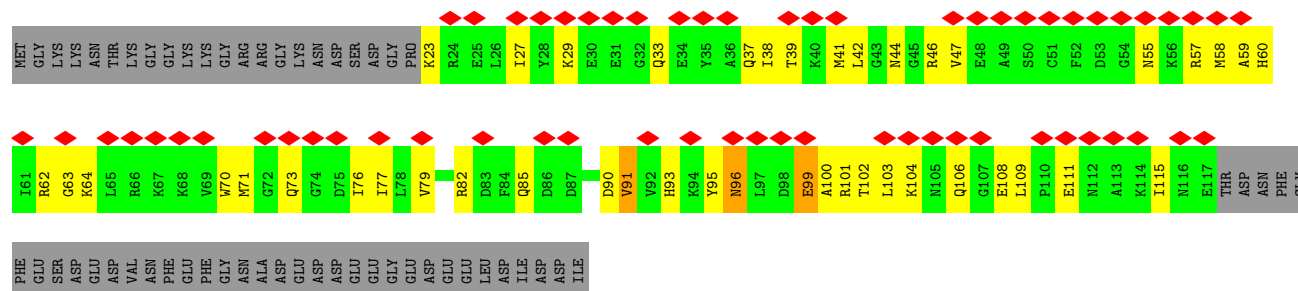
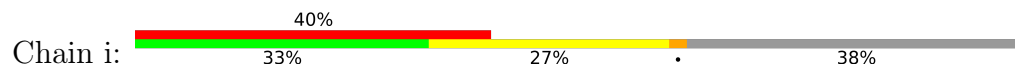


- Molecule 35: KLLA0E12277p

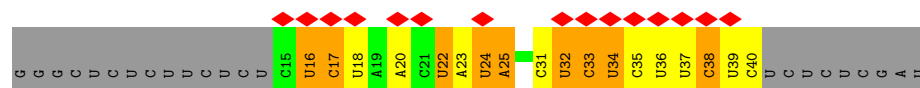
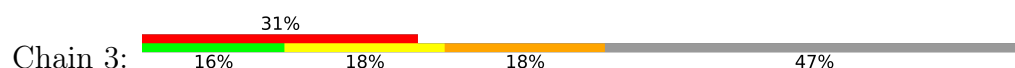




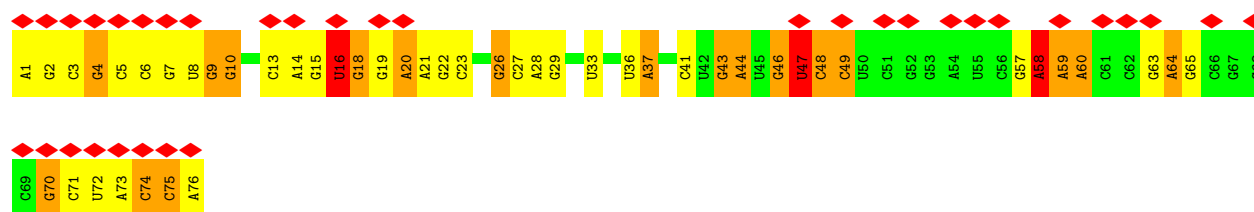
• Molecule 36: Eukaryotic translation initiation factor 1A



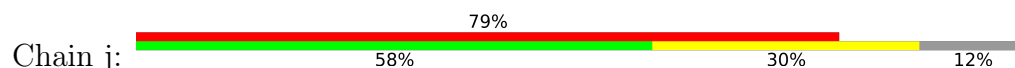
• Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')



• Molecule 38: Met-tRNA_i

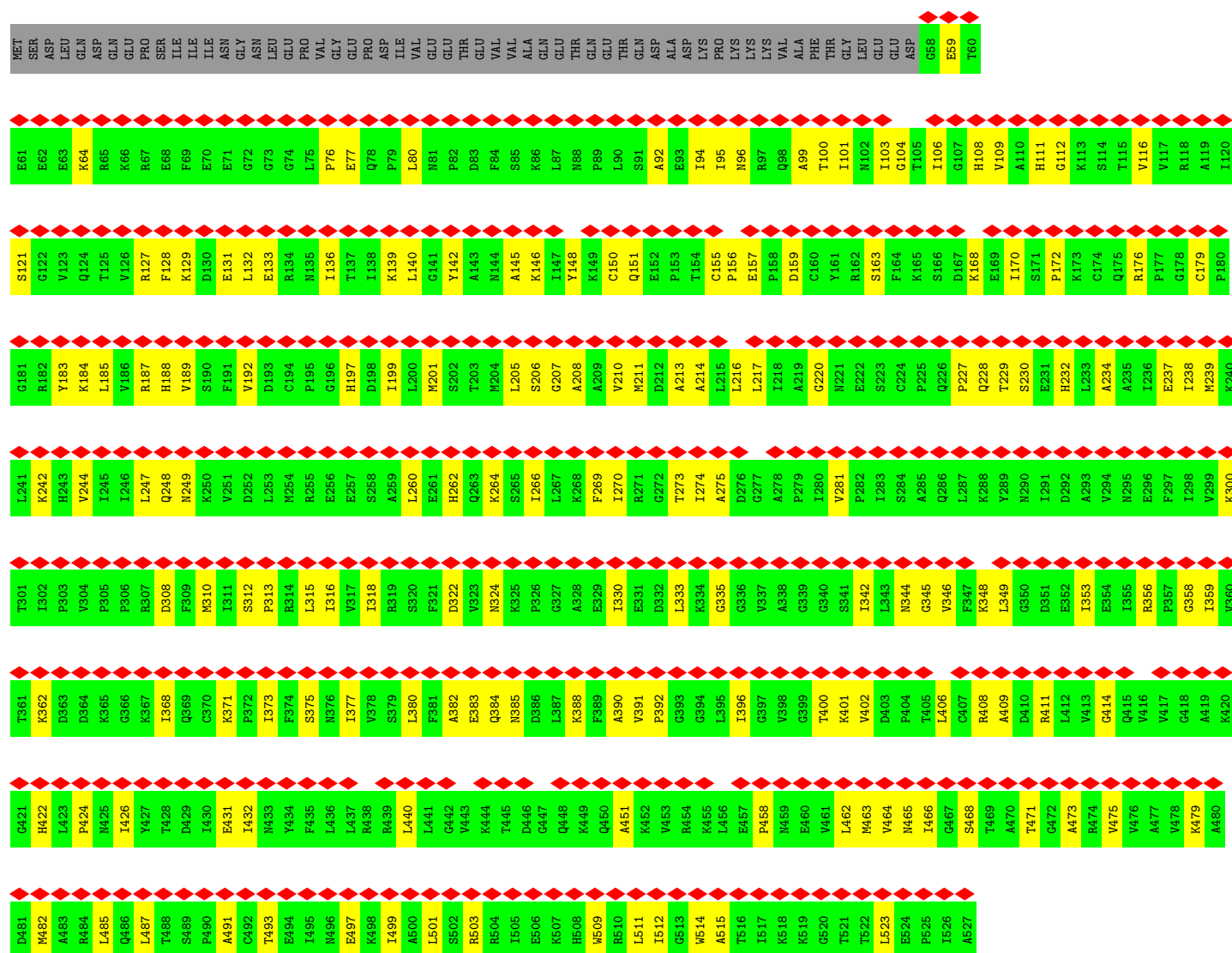
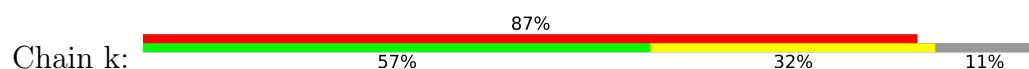


• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

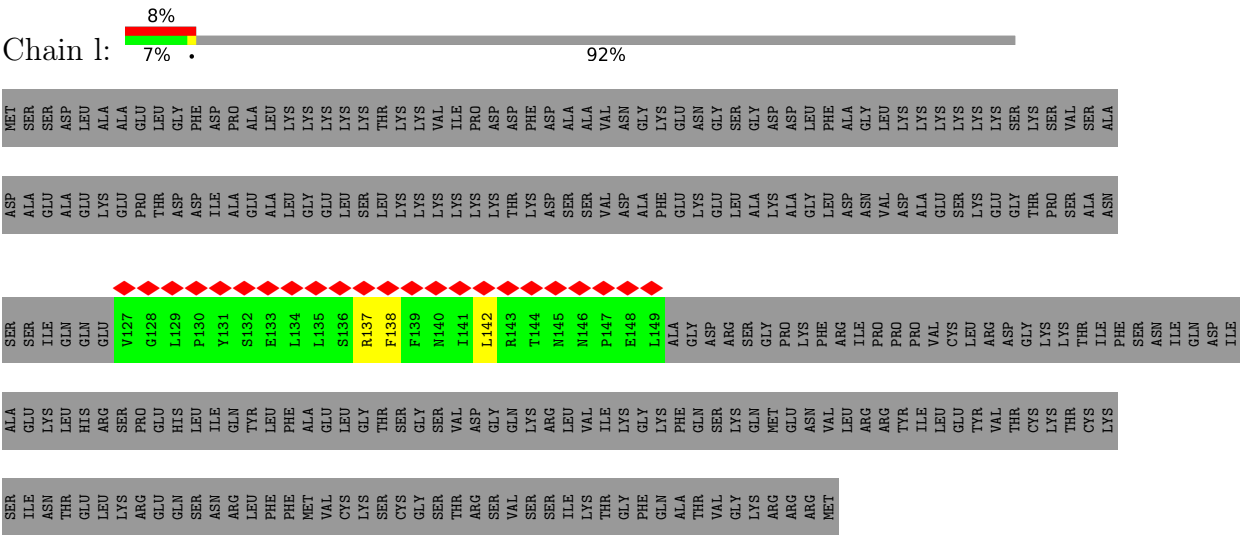




• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma



● Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66519	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.868	Depositor
Minimum map value	-0.475	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 5MC, B8N, RIA, GCP, M2G, 1MA, 2MG, PSU, MG, MA6, 1MG, ZN, 7MG, T6A

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.16	0/42410	0.31	4/66079 (0.0%)
2	A	0.19	0/1742	0.44	2/2383 (0.1%)
3	B	0.20	0/1820	0.46	1/2448 (0.0%)
4	C	0.20	0/1678	0.37	0/2277
5	E	0.19	0/2122	0.45	0/2861
6	G	0.14	0/1855	0.36	0/2479
7	H	0.20	0/1507	0.58	2/2028 (0.1%)
8	I	0.18	0/1515	0.44	0/2029
9	J	0.20	0/1495	0.45	1/2001 (0.0%)
10	L	0.19	0/1276	0.44	0/1718
11	N	0.17	0/1218	0.39	0/1638
12	O	0.21	0/966	0.51	0/1297
13	V	0.19	0/696	0.43	0/938
14	W	0.22	0/1039	0.42	0/1399
15	X	0.16	0/1137	0.37	0/1516
16	Y	0.19	0/1075	0.43	0/1433
17	a	0.22	0/810	0.52	0/1087
18	b	0.17	0/619	0.42	0/837
19	e	0.20	0/480	0.49	0/640
20	h	0.20	0/234	0.41	0/300
21	D	0.18	0/1800	0.42	0/2421
22	F	0.18	0/1628	0.45	0/2198
23	K	0.21	0/831	0.60	0/1123
24	M	0.17	0/891	0.50	0/1201
25	P	0.17	0/942	0.48	0/1269
26	Q	0.22	0/1125	0.57	2/1510 (0.1%)
27	R	0.17	0/1044	0.42	0/1402
28	S	0.17	0/1208	0.48	0/1624
29	T	0.22	0/1129	0.51	0/1520
30	U	0.18	0/857	0.48	0/1158
31	Z	0.18	0/603	0.49	0/814
32	c	0.17	0/501	0.41	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.18	0/473	0.40	0/629
34	f	0.13	0/597	0.43	0/795
35	g	0.15	0/2523	0.40	0/3434
36	i	0.20	0/773	0.53	0/1031
37	3	0.09	0/595	0.20	0/920
38	1	0.17	0/1529	0.27	0/2376
39	j	0.16	0/2171	0.47	0/2924
40	k	0.14	0/3657	0.41	0/4946
41	l	0.21	0/194	0.44	0/263
All	All	0.17	0/90765	0.38	12/131619 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	65	PRO	N-CA-C	-8.35	102.94	114.80
1	2	225	A	C4'-C3'-O3'	6.78	123.17	113.00
2	A	35	PRO	CA-N-CD	-6.75	102.55	112.00
1	2	225	A	N9-C1'-C2'	-6.63	102.05	112.00
9	J	2	PRO	CA-N-CD	-6.36	103.10	112.00
1	2	225	A	C2'-C3'-O3'	-6.04	104.64	113.70
1	2	225	A	C3'-C2'-O2'	6.02	119.73	110.70
7	H	64	VAL	N-CA-C	5.97	121.77	108.88
26	Q	124	PRO	CA-C-N	5.86	132.07	120.94
26	Q	124	PRO	C-N-CA	5.86	132.07	120.94
2	A	35	PRO	N-CD-CG	-5.58	94.83	103.20
3	B	23	PRO	CA-N-CD	-5.37	104.48	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	38190	0	19213	961	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1702	0	1695	72	0
3	B	1796	0	1874	68	0
4	C	1648	0	1727	51	0
5	E	2078	0	2157	79	0
6	G	1832	0	1919	72	0
7	H	1483	0	1579	72	0
8	I	1489	0	1504	57	0
9	J	1471	0	1554	65	0
10	L	1248	0	1311	46	0
11	N	1195	0	1263	31	0
12	O	955	0	987	66	0
13	V	687	0	682	34	0
14	W	1021	0	1056	42	0
15	X	1119	0	1198	38	0
16	Y	1061	0	1111	47	0
17	a	797	0	835	41	0
18	b	609	0	630	20	0
19	e	472	0	508	21	0
20	h	233	0	284	9	0
21	D	1774	0	1855	67	0
22	F	1609	0	1679	59	0
23	K	809	0	810	46	0
24	M	885	0	917	53	0
25	P	923	0	960	47	0
26	Q	1105	0	1170	73	0
27	R	1033	0	1082	43	0
28	S	1189	0	1211	53	0
29	T	1110	0	1124	55	0
30	U	845	0	913	44	0
31	Z	594	0	590	35	0
32	c	499	0	536	23	0
33	d	461	0	448	22	0
34	f	584	0	600	20	0
35	g	2469	0	2403	92	0
36	i	764	0	763	48	0
37	3	536	0	277	10	0
38	1	1639	0	853	36	0
39	j	2139	0	2205	78	0
40	k	3596	0	3713	127	0
41	l	190	0	191	3	0
42	2	112	0	0	0	0
42	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	T	1	0	0	0	0
42	i	1	0	0	0	0
43	a	1	0	0	0	0
43	b	1	0	0	0	0
43	f	1	0	0	0	0
44	k	32	0	13	1	0
45	k	8	0	8	2	0
46	2	3	0	0	0	0
All	All	86000	0	67408	2504	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 17.

All (2504) 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)
3:B:2:ALA:N	12:O:49:LYS:HE3	1.60	1.16
24:M:67:LEU:O	24:M:71:LEU:HD13	1.50	1.10
1:2:824:U:H3	1:2:847:C:N4	1.54	1.04
12:O:51:ASP:HB2	39:j:89:ARG:HH12	1.21	1.00
1:2:1586:G:H1	1:2:1606:U:H3	1.05	0.95
1:2:1355:U:H3	1:2:1366:G:H1	1.10	0.94
1:2:975:G:H1	1:2:1022:A:HO2'	1.17	0.93
3:B:2:ALA:N	12:O:49:LYS:CE	2.36	0.89
3:B:2:ALA:N	12:O:49:LYS:HA	1.88	0.89
35:g:258:TRP:HB3	35:g:269:ILE:HD11	1.52	0.88
1:2:824:U:H3	1:2:847:C:H42	0.88	0.88
12:O:49:LYS:O	39:j:89:ARG:NH1	2.08	0.86
12:O:51:ASP:HB2	39:j:89:ARG:NH1	1.90	0.86
1:2:65:A:H2	1:2:84:A:H62	1.26	0.84
1:2:1338:C:O2'	1:2:1340:A:N7	2.10	0.84
38:1:47:H2U:H5''	38:1:47:H2U:H61	1.57	0.84
1:2:485:G:H1	1:2:500:U:H3	0.87	0.83
40:k:356:ARG:HG3	40:k:424:PRO:HG2	1.57	0.83
1:2:521:U:H5''	16:Y:37:LYS:HG3	1.61	0.83
12:O:60:ALA:HB1	12:O:101:ALA:HB2	1.60	0.83
8:I:196:ARG:HH12	10:L:11:ARG:HA	1.45	0.82
1:2:1213:U:HO2'	33:d:2:ALA:N	1.78	0.82
35:g:171:ARG:HH12	35:g:192:SER:HA	1.45	0.82
35:g:259:LEU:HG	35:g:272:LEU:HD21	1.60	0.81
1:2:658:C:H2'	1:2:659:G:H8	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1171:G:OP1	28:S:144:ARG:NH1	2.09	0.80
14:W:24:GLN:HG3	18:b:7:LEU:HD11	1.63	0.80
12:O:51:ASP:CB	39:j:89:ARG:HH12	1.95	0.80
24:M:72:ALA:HB2	24:M:79:LEU:HD11	1.64	0.79
30:U:34:LEU:HD21	30:U:89:ARG:HG3	1.64	0.79
12:O:24:ASN:HA	12:O:55:SER:HB3	1.65	0.79
1:2:1460:G:N7	28:S:143:ARG:NH2	2.32	0.78
1:2:565:C:OP2	36:i:62:ARG:NH1	2.16	0.78
1:2:1675:C:H5''	8:I:59:ARG:HH12	1.48	0.78
21:D:105:MET:HE1	21:D:184:ILE:HD13	1.66	0.78
1:2:635:A:H5''	14:W:31:SER:HB3	1.66	0.78
3:B:181:LEU:HA	3:B:184:LEU:HB3	1.64	0.78
15:X:70:LYS:HG2	15:X:93:LEU:HD22	1.65	0.78
1:2:236:C:H5''	1:2:237:U:H5'	1.66	0.78
1:2:566:A:OP1	15:X:70:LYS:NZ	2.18	0.77
1:2:995:U:H3	1:2:1007:G:H1	1.31	0.77
1:2:1095:C:OP2	14:W:71:LYS:NZ	2.18	0.77
36:i:62:ARG:HG3	36:i:90:ASP:HB3	1.67	0.77
1:2:520:A:N3	16:Y:34:ASN:ND2	2.31	0.77
9:J:53:ARG:NH1	9:J:97:LEU:O	2.18	0.77
21:D:116:ARG:HH21	21:D:150:MET:HE1	1.49	0.76
1:2:1531:C:OP2	31:Z:77:ARG:NH2	2.17	0.76
22:F:125:VAL:HG12	31:Z:58:ARG:HH22	1.51	0.76
35:g:179:MET:HA	35:g:205:TYR:HB2	1.67	0.76
1:2:824:U:O2	1:2:847:C:N3	2.19	0.76
26:Q:67:VAL:HG11	26:Q:81:ILE:HG23	1.68	0.76
1:2:760:A:N1	1:2:789:U:C4	2.55	0.75
7:H:63:PRO:HB2	7:H:65:PRO:HD3	1.68	0.75
27:R:93:LEU:HD11	27:R:100:LEU:HB3	1.69	0.75
1:2:1170:A:H2'	1:2:1171:G:C8	2.22	0.75
1:2:52:U:O4	1:2:423:C:N4	2.19	0.75
5:E:100:ARG:NH1	5:E:118:GLU:OE2	2.19	0.75
9:J:70:LEU:O	9:J:74:ASN:ND2	2.19	0.75
26:Q:63:ILE:HD12	26:Q:92:TYR:HE2	1.50	0.75
39:j:147:LEU:O	39:j:151:ASP:N	2.19	0.75
2:A:56:LYS:NZ	13:V:70:ASN:OD1	2.16	0.74
1:2:1290:G:H1	1:2:1323:G:H22	1.32	0.74
1:2:1661:G:H1	1:2:1736:U:H3	1.33	0.74
4:C:238:GLN:HE21	13:V:13:VAL:HG21	1.52	0.74
26:Q:99:GLU:O	26:Q:103:ASN:ND2	2.21	0.74
35:g:171:ARG:HE	35:g:187:SER:HB2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:59:LEU:HD12	9:J:69:ARG:HA	1.68	0.74
13:V:64:GLU:HG2	18:b:3:LEU:HD23	1.70	0.74
16:Y:55:VAL:HG22	16:Y:75:VAL:HG22	1.68	0.74
22:F:94:ARG:NH2	22:F:171:ASN:OD1	2.21	0.74
30:U:23:ARG:HG3	30:U:92:ASP:HB3	1.70	0.73
29:T:22:LEU:HD23	29:T:28:LEU:HD22	1.70	0.73
1:2:642:G:O6	1:2:692:C:N4	2.21	0.73
24:M:56:VAL:HG11	24:M:85:ALA:HB2	1.69	0.73
28:S:132:ARG:HD2	28:S:136:GLN:HE21	1.54	0.73
1:2:809:G:N2	7:H:108:GLN:OE1	2.22	0.73
1:2:353:C:H5''	8:I:16:ALA:HB2	1.71	0.73
1:2:225:A:O2'	1:2:226:U:H5'	1.89	0.72
26:Q:143:ARG:NH2	38:1:33:U:OP2	2.22	0.72
26:Q:98:ASP:OD1	26:Q:99:GLU:N	2.22	0.72
1:2:1254:G:O6	24:M:39:ARG:NH1	2.22	0.72
34:f:139:CYS:SG	34:f:140:GLY:N	2.62	0.72
22:F:218:GLU:HG2	39:j:45:MET:HE2	1.70	0.72
18:b:18:LYS:O	18:b:29:ARG:NH2	2.22	0.72
4:C:100:ARG:HG2	4:C:100:ARG:HH11	1.55	0.72
1:2:701:U:O2	1:2:738:G:N2	2.23	0.71
40:k:111:HIS:O	40:k:249:ASN:ND2	2.21	0.71
13:V:3:ASN:OD1	13:V:4:ASP:N	2.22	0.71
30:U:22:ILE:HG21	30:U:100:VAL:HG11	1.71	0.71
24:M:69:GLN:OE1	24:M:69:GLN:HA	1.89	0.71
29:T:77:ASN:HD21	29:T:98:GLY:HA2	1.54	0.71
4:C:71:PHE:CD2	4:C:135:ILE:HD12	2.24	0.71
35:g:210:GLN:NE2	35:g:211:PRO:O	2.23	0.71
15:X:60:GLU:OE2	36:i:60:HIS:NE2	2.23	0.71
29:T:50:SER:OG	29:T:51:GLU:OE2	2.08	0.71
1:2:150:G:O2'	6:G:13:GLN:NE2	2.24	0.71
1:2:899:A:H3'	1:2:900:G:H21	1.54	0.70
1:2:1345:A:OP2	1:2:1347:A:N6	2.23	0.70
27:R:31:ASN:HD22	27:R:55:THR:HG22	1.55	0.70
35:g:43:LEU:HD11	35:g:83:SER:HB3	1.72	0.70
1:2:66:U:H3	6:G:173:PRO:HD3	1.55	0.70
1:2:895:U:O2	12:O:41:ARG:NH1	2.24	0.70
13:V:42:GLU:OE1	13:V:42:GLU:N	2.20	0.70
21:D:228:THR:HG21	35:g:194:ARG:HB2	1.72	0.70
21:D:21:LEU:HD21	21:D:48:ILE:HD13	1.74	0.70
35:g:210:GLN:HE22	35:g:252:PHE:HB2	1.57	0.70
40:k:127:ARG:NH1	40:k:133:GLU:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1170:A:H2'	1:2:1171:G:H8	1.55	0.70
3:B:5:LYS:HG3	3:B:7:LYS:H	1.55	0.70
5:E:64:ILE:HD11	16:Y:18:LEU:HG	1.73	0.70
2:A:15:GLN:HE22	27:R:93:LEU:HD13	1.57	0.70
30:U:82:TYR:HB3	33:d:52:PHE:HB3	1.74	0.70
1:2:502:G:O2'	19:e:46:ASN:ND2	2.25	0.69
1:2:370:G:O3'	14:W:88:LYS:NZ	2.24	0.69
1:2:1124:A:H5''	20:h:15:ARG:NH1	2.07	0.69
1:2:531:U:OP1	9:J:132:ARG:NH2	2.24	0.69
1:2:1124:A:H5''	20:h:15:ARG:HH12	1.56	0.69
1:2:1617:C:O2	32:c:22:ARG:NH2	2.25	0.69
29:T:37:VAL:HG12	29:T:39:THR:H	1.56	0.69
30:U:70:THR:HG22	30:U:72:ASN:H	1.55	0.69
1:2:156:A:H2	1:2:418:G:H21	1.40	0.69
1:2:226:U:O2	1:2:833:G:O6	2.09	0.69
1:2:1592:G:OP2	1:2:1594:C:N4	2.26	0.69
29:T:76:LEU:HB3	29:T:101:ASN:HD22	1.58	0.69
1:2:139:C:N4	1:2:280:G:OP1	2.23	0.69
1:2:1519:G:O2'	1:2:1521:G:OP2	2.11	0.69
5:E:151:ASP:HB3	5:E:154:ILE:HG13	1.74	0.69
29:T:28:LEU:HB2	29:T:111:LEU:HD11	1.75	0.69
35:g:90:LEU:HB2	35:g:104:PHE:HB2	1.75	0.68
1:2:1670:G:H2'	1:2:1671:G:H8	1.57	0.68
7:H:77:LEU:HD22	7:H:92:PHE:HZ	1.59	0.68
40:k:473:ALA:HB1	40:k:485:LEU:HB3	1.76	0.68
9:J:41:GLU:O	9:J:45:ILE:HG12	1.92	0.68
1:2:1076:C:OP1	17:a:13:LYS:NZ	2.26	0.68
1:2:758:U:H5''	9:J:7:THR:HG21	1.76	0.68
24:M:47:ARG:HD3	34:f:126:PRO:HG2	1.76	0.68
1:2:251:U:OP1	5:E:133:LYS:NZ	2.27	0.68
1:2:554:A:N3	1:2:589:C:O2'	2.24	0.68
15:X:58:GLY:H	36:i:85:GLN:HE21	1.41	0.68
21:D:76:ARG:NH1	21:D:76:ARG:O	2.25	0.68
28:S:25:ASN:HB2	31:Z:40:VAL:HG21	1.76	0.68
1:2:162:G:OP2	1:2:162:G:N2	2.25	0.67
1:2:984:G:H1	1:2:1015:C:H5	1.42	0.67
1:2:1415:A:O2'	26:Q:128:LYS:NZ	2.27	0.67
1:2:1792:A:OP2	17:a:4:LYS:NZ	2.21	0.67
33:d:33:LYS:NZ	33:d:34:TYR:OH	2.24	0.67
1:2:1246:U:OP1	34:f:92:ARG:NH1	2.27	0.67
4:C:233:ASN:HB2	13:V:1:MET:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:50:PHE:CD2	22:F:69:PRO:HA	2.30	0.67
1:2:715:U:H3	1:2:723:G:H1	1.42	0.67
1:2:952:G:H2'	1:2:953:G:H8	1.57	0.67
8:I:191:ALA:HA	8:I:194:LEU:HD12	1.76	0.67
4:C:72:GLN:OE1	4:C:72:GLN:N	2.22	0.67
39:j:7:ARG:HD2	39:j:12:LYS:HG2	1.76	0.67
1:2:1182:A:N3	1:2:1209:C:O2'	2.24	0.67
29:T:18:TYR:HD1	29:T:135:ILE:HG21	1.59	0.67
4:C:152:ASN:ND2	13:V:2:GLU:O	2.28	0.67
6:G:32:ILE:HD11	6:G:63:MET:HE2	1.75	0.67
40:k:208:ALA:HA	40:k:211:MET:HE2	1.76	0.67
15:X:69:ARG:HB3	15:X:86:PHE:HE1	1.59	0.67
22:F:50:PHE:HD2	22:F:69:PRO:HA	1.59	0.67
25:P:118:GLU:OE2	25:P:118:GLU:N	2.21	0.67
1:2:779:A:O2'	1:2:781:A:N7	2.28	0.67
1:2:798:A:H4'	5:E:201:HIS:CE1	2.30	0.67
1:2:866:G:O6	1:2:961:C:N4	2.28	0.67
1:2:1464:G:O2'	1:2:1600:C:OP1	2.13	0.67
5:E:185:GLY:O	5:E:224:ASN:ND2	2.23	0.67
31:Z:38:HIS:HB3	31:Z:72:GLY:HA2	1.77	0.67
1:2:923:A:H2'	1:2:924:G:C8	2.30	0.67
1:2:1320:A:N6	2:A:135:GLU:OE2	2.28	0.67
2:A:175:TYR:OH	2:A:197:ILE:O	2.12	0.67
6:G:48:TYR:HB3	6:G:113:ILE:HD11	1.76	0.67
1:2:1480:C:OP2	1:2:1519:G:N2	2.26	0.66
8:I:57:ALA:HB2	8:I:178:GLY:HA2	1.76	0.66
32:c:41:VAL:HG13	32:c:63:ALA:HB3	1.74	0.66
12:O:51:ASP:CB	39:j:89:ARG:NH1	2.56	0.66
35:g:117:ASP:OD2	35:g:121:SER:OG	2.13	0.66
1:2:1443:G:N2	34:f:87:THR:O	2.29	0.66
7:H:74:GLN:O	7:H:78:THR:OG1	2.12	0.66
12:O:49:LYS:HE2	39:j:74:LEU:HD13	1.77	0.66
1:2:329:G:OP2	8:I:173:ARG:NH1	2.28	0.66
1:2:586:C:OP2	19:e:23:LYS:NZ	2.28	0.66
1:2:1332:C:O4'	21:D:162:GLN:NE2	2.27	0.66
1:2:1682:U:O2	1:2:1715:G:O6	2.13	0.66
25:P:37:ALA:O	25:P:42:ARG:NH1	2.29	0.66
26:Q:47:LYS:HB3	26:Q:82:ARG:HD2	1.76	0.66
11:N:105:ASN:HD22	11:N:105:ASN:C	2.01	0.66
36:i:76:ILE:HG21	36:i:100:ALA:HB2	1.77	0.66
1:2:1161:C:H4'	32:c:22:ARG:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:144:ARG:HB3	3:B:206:PRO:HB2	1.78	0.66
19:e:8:LEU:HD21	36:i:62:ARG:HH21	1.59	0.66
28:S:62:THR:OG1	28:S:64:GLU:OE2	2.13	0.66
40:k:458:PRO:HA	40:k:475:VAL:HB	1.76	0.66
14:W:41:MET:HE2	14:W:47:ILE:HD12	1.78	0.66
23:K:77:ARG:HD3	23:K:84:GLU:HA	1.77	0.66
1:2:404:C:O2'	6:G:92:ARG:O	2.14	0.66
1:2:1598:A:H2'	1:2:1599:G:H5''	1.78	0.66
25:P:90:ILE:HA	25:P:107:ILE:HG22	1.78	0.66
36:i:95:TYR:HB3	36:i:99:GLU:HG3	1.78	0.66
23:K:11:ILE:HD11	23:K:42:VAL:HG22	1.78	0.65
39:j:53:ARG:HA	39:j:88:ARG:HG3	1.78	0.65
1:2:12:U:H2'	1:2:13:C:C6	2.32	0.65
1:2:326:U:H2'	1:2:327:A:C8	2.31	0.65
12:O:42:VAL:HG12	12:O:67:VAL:HG13	1.78	0.65
1:2:437:A:H1'	1:2:464:G:H22	1.61	0.65
1:2:917:U:H2'	1:2:918:A:C8	2.30	0.65
1:2:142:G:H2'	1:2:143:G:C8	2.31	0.65
1:2:234:G:H2'	1:2:235:A:C8	2.30	0.65
1:2:787:A:C5	5:E:19:MET:HE1	2.31	0.65
30:U:22:ILE:HG13	30:U:118:ILE:HA	1.79	0.65
39:j:225:ALA:H	40:k:408:ARG:HE	1.43	0.65
40:k:431:GLU:HB3	40:k:482:MET:HE2	1.78	0.65
1:2:1606:U:OP1	26:Q:15:SER:OG	2.14	0.65
8:I:67:TRP:O	8:I:71:GLY:HA2	1.97	0.65
9:J:85:VAL:HG11	9:J:104:PHE:HD1	1.62	0.65
21:D:105:MET:HE1	21:D:184:ILE:HG21	1.79	0.65
26:Q:77:GLN:O	26:Q:81:ILE:HG13	1.97	0.65
1:2:543:A:O3'	19:e:31:LYS:NZ	2.30	0.65
4:C:145:ARG:NH1	13:V:10:GLU:OE2	2.30	0.65
1:2:530:C:O2	16:Y:62:THR:OG1	2.14	0.65
30:U:63:LEU:O	30:U:83:GLU:HA	1.96	0.65
1:2:97:C:H1'	1:2:425:G:H5'	1.78	0.64
1:2:447:C:OP1	5:E:49:ARG:NH2	2.25	0.64
1:2:1289:PSU:H2'	1:2:1290:G:C8	2.33	0.64
17:a:46:GLU:OE2	17:a:46:GLU:N	2.26	0.64
24:M:29:LEU:HD12	24:M:36:ARG:HH22	1.60	0.64
1:2:92:A:H5''	1:2:93:A:H5''	1.79	0.64
1:2:775:G:N7	16:Y:11:LYS:NZ	2.45	0.64
35:g:246:GLU:HB3	35:g:264:ALA:HB2	1.79	0.64
36:i:104:LYS:HZ2	36:i:111:GLU:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1121:G:N2	1:2:1124:A:OP2	2.31	0.64
1:2:1472:G:H2'	1:2:1473:A:C8	2.32	0.64
3:B:74:GLN:HE21	3:B:189:ILE:HG21	1.63	0.64
6:G:7:TYR:HE1	6:G:9:ILE:HB	1.61	0.64
14:W:6:VAL:HG22	14:W:34:ILE:HD11	1.78	0.64
24:M:125:GLU:HA	24:M:128:LEU:HG	1.79	0.64
35:g:307:THR:HG22	35:g:321:GLN:HG3	1.78	0.64
11:N:4:MET:SD	11:N:124:ARG:NH1	2.70	0.64
24:M:72:ALA:CB	24:M:79:LEU:HD13	2.28	0.64
27:R:27:ASP:OD2	35:g:39:ARG:NH2	2.28	0.64
1:2:23:G:O6	1:2:601:U:O2	2.14	0.64
24:M:70:GLY:O	24:M:73:THR:OG1	2.16	0.64
1:2:453:U:N1	5:E:66:MET:HE1	2.12	0.64
22:F:34:GLU:OE2	22:F:34:GLU:N	2.26	0.64
38:1:23:C:H4'	39:j:64:ARG:HH12	1.62	0.64
9:J:63:ASP:OD1	9:J:64:GLU:N	2.31	0.64
1:2:256:A:H1'	8:I:73:ALA:HB3	1.80	0.64
1:2:396:A:H4'	8:I:50:GLY:HA2	1.80	0.64
2:A:42:PRO:HB2	27:R:126:ALA:HB2	1.80	0.64
3:B:97:LEU:HB3	3:B:232:HIS:CD2	2.32	0.64
12:O:17:ALA:N	12:O:80:HIS:O	2.31	0.64
24:M:72:ALA:HB2	24:M:79:LEU:CD1	2.28	0.64
24:M:72:ALA:CB	24:M:79:LEU:CD1	2.76	0.64
25:P:34:VAL:HG22	25:P:45:PHE:HD2	1.62	0.64
1:2:1595:A:OP1	33:d:19:ARG:NH1	2.28	0.64
35:g:85:SER:OG	35:g:87:ASP:OD1	2.15	0.64
1:2:367:U:O4	1:2:368:A:N6	2.31	0.63
8:I:37:LYS:H	8:I:59:ARG:H	1.46	0.63
1:2:151:U:O2	6:G:4:ASN:ND2	2.29	0.63
1:2:897:A:N6	1:2:913:G:O2'	2.31	0.63
1:2:277:U:O5'	1:2:278:G:N2	2.31	0.63
11:N:88:LEU:O	11:N:92:ILE:HG13	1.99	0.63
28:S:41:ARG:NH2	29:T:36:ILE:O	2.31	0.63
36:i:96:ASN:C	36:i:96:ASN:HD22	2.06	0.63
39:j:211:MET:HE1	39:j:243:GLN:HE21	1.63	0.63
1:2:248:U:H3'	1:2:249:C:H5'	1.80	0.63
1:2:537:A:H5'	1:2:542:C:H41	1.64	0.63
1:2:864:A:OP1	14:W:28:ARG:NH2	2.32	0.63
4:C:100:ARG:HH12	4:C:102:ARG:HD2	1.63	0.63
9:J:140:ILE:HD11	16:Y:65:GLY:HA2	1.80	0.63
24:M:56:VAL:HG22	24:M:58:SER:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:122:GLN:O	24:M:125:GLU:HG2	1.99	0.63
40:k:112:GLY:HA3	44:k:601:GCP:H8	1.80	0.63
1:2:148:C:OP1	16:Y:121:THR:OG1	2.16	0.63
1:2:249:C:H2'	1:2:250:A:H8	1.64	0.63
1:2:1656:G:O6	1:2:1741:U:O2	2.17	0.63
12:O:12:GLN:OE1	12:O:77:THR:OG1	2.16	0.63
2:A:112:THR:HG22	2:A:114:SER:H	1.63	0.63
2:A:154:GLU:N	2:A:154:GLU:OE2	2.32	0.63
4:C:87:ASN:HB2	4:C:212:LEU:HD23	1.80	0.63
7:H:140:VAL:HB	14:W:52:TYR:HB3	1.80	0.63
3:B:87:ARG:HB2	3:B:101:HIS:HB2	1.81	0.63
24:M:35:ALA:HB3	24:M:113:VAL:HB	1.79	0.63
37:3:16:U:O2	37:3:17:C:N4	2.31	0.63
1:2:1594:C:O2'	1:2:1596:U:OP2	2.17	0.63
25:P:107:ILE:HG12	25:P:111:MET:HG3	1.81	0.63
40:k:312:SER:O	40:k:344:ASN:ND2	2.32	0.63
1:2:700:C:O2'	1:2:701:U:OP1	2.17	0.62
16:Y:84:LYS:HG3	16:Y:85:PHE:HD1	1.63	0.62
1:2:78:A:H2'	1:2:79:C:C6	2.33	0.62
1:2:1173:C:O2'	1:2:1195:A:N6	2.33	0.62
1:2:1645:U:H2'	1:2:1646:A:C8	2.34	0.62
10:L:131:ILE:HB	10:L:135:VAL:HG23	1.81	0.62
24:M:52:LEU:HB3	24:M:114:VAL:HB	1.80	0.62
1:2:917:U:H2'	1:2:918:A:H8	1.62	0.62
5:E:160:VAL:HG21	5:E:169:ILE:HG12	1.81	0.62
40:k:101:ILE:HB	40:k:189:VAL:HG12	1.80	0.62
40:k:108:HIS:HB3	40:k:111:HIS:CD2	2.34	0.62
1:2:1564:U:H5''	28:S:39:GLY:N	2.14	0.62
4:C:189:VAL:O	4:C:193:MET:HG2	2.00	0.62
1:2:152:G:OP1	6:G:2:LYS:NZ	2.33	0.62
7:H:163:ASP:OD1	7:H:164:ASN:N	2.33	0.62
9:J:18:PRO:HG2	9:J:19:TYR:HD1	1.65	0.62
25:P:45:PHE:HD1	25:P:49:LEU:HD21	1.64	0.62
28:S:126:ARG:NH1	28:S:132:ARG:O	2.33	0.62
1:2:686:C:H4'	14:W:118:ARG:HD2	1.81	0.62
2:A:74:VAL:HG22	2:A:96:THR:HB	1.81	0.62
7:H:162:ILE:HG23	7:H:165:LYS:HB2	1.80	0.62
29:T:61:VAL:O	29:T:65:ILE:HG13	1.99	0.62
1:2:938:A:H2'	1:2:939:A:C8	2.34	0.62
1:2:1033:C:OP1	11:N:9:LYS:NZ	2.28	0.62
11:N:86:GLU:N	11:N:86:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:81:VAL:O	14:W:122:SER:OG	2.17	0.62
15:X:69:ARG:HG3	15:X:117:ILE:HG12	1.79	0.62
26:Q:46:PHE:HA	26:Q:49:TYR:HD2	1.65	0.62
30:U:71:PRO:HB3	33:d:41:GLN:HG2	1.82	0.62
1:2:1038:A:O2'	1:2:1039:G:O5'	2.18	0.62
3:B:129:THR:OG1	3:B:179:SER:O	2.18	0.62
6:G:7:TYR:CE1	6:G:9:ILE:HB	2.35	0.62
7:H:62:VAL:CG1	7:H:63:PRO:HD2	2.29	0.62
11:N:105:ASN:O	11:N:105:ASN:ND2	2.19	0.62
15:X:61:SER:OG	15:X:62:LYS:N	2.32	0.62
1:2:1033:C:HO2'	14:W:2:THR:N	1.98	0.62
1:2:1198:G:N2	33:d:30:LEU:O	2.33	0.62
1:2:1279:C:O2'	30:U:70:THR:OG1	2.16	0.62
6:G:85:ARG:O	6:G:87:ARG:NH1	2.32	0.62
35:g:271:ASP:OD2	35:g:274:ASN:ND2	2.33	0.62
40:k:148:TYR:HB3	40:k:183:TYR:HB3	1.81	0.62
1:2:512:U:H2'	1:2:513:G:C8	2.34	0.61
1:2:554:A:C5	9:J:19:TYR:HE2	2.17	0.61
1:2:1159:A:H2'	1:2:1160:C:C6	2.34	0.61
1:2:1563:C:OP1	28:S:41:ARG:NH1	2.33	0.61
1:2:1746:G:H2'	1:2:1747:A:C8	2.35	0.61
6:G:78:ALA:HB2	6:G:92:ARG:HG3	1.81	0.61
7:H:151:LYS:HE3	7:H:184:GLU:HG3	1.82	0.61
21:D:7:LYS:HG2	30:U:27:THR:HG21	1.82	0.61
29:T:51:GLU:OE2	29:T:51:GLU:N	2.31	0.61
1:2:1522:A:H2'	1:2:1523:A:C8	2.35	0.61
5:E:158:ASP:OD1	5:E:174:LYS:HA	1.99	0.61
9:J:106:GLU:O	9:J:111:THR:OG1	2.17	0.61
28:S:16:ARG:NH1	28:S:21:ASN:OD1	2.33	0.61
1:2:1570:2MG:O6	31:Z:28:SER:N	2.33	0.61
2:A:119:ARG:NE	4:C:246:ASP:OD1	2.31	0.61
25:P:93:VAL:HG22	25:P:106:GLU:HG2	1.81	0.61
29:T:102:ARG:O	29:T:106:GLN:HG3	2.00	0.61
40:k:335:GLY:HA3	40:k:400:THR:O	2.00	0.61
1:2:1434:A:OP2	21:D:27:ARG:NH2	2.33	0.61
25:P:18:LYS:NZ	28:S:90:LYS:O	2.34	0.61
1:2:392:C:OP1	8:I:2:GLY:N	2.33	0.61
2:A:41:ARG:HG2	2:A:43:ASP:H	1.65	0.61
20:h:19:LYS:HA	20:h:19:LYS:HE3	1.82	0.61
1:2:1589:C:H2'	1:2:1590:A:H8	1.66	0.61
3:B:89:ASP:OD1	3:B:89:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:7:ILE:HD11	16:Y:25:VAL:HG13	1.80	0.61
23:K:10:LYS:O	23:K:13:GLN:NE2	2.34	0.61
38:1:20:A:N6	38:1:57:G:O2'	2.33	0.61
39:j:220:VAL:HG22	39:j:230:LEU:HD13	1.83	0.61
1:2:574:C:N4	15:X:65:ASN:OD1	2.31	0.61
1:2:752:A:H3'	5:E:187:ARG:HH21	1.66	0.61
1:2:983:G:H1	1:2:1016:U:H5	1.48	0.61
1:2:1056:U:O2'	1:2:1058:C:OP2	2.17	0.61
24:M:17:ILE:HG22	24:M:127:LEU:HD11	1.83	0.61
9:J:157:ASP:OD1	9:J:158:PHE:N	2.32	0.61
30:U:68:ARG:HH21	30:U:77:LYS:HG3	1.66	0.61
34:f:108:VAL:HA	34:f:114:VAL:HG12	1.83	0.61
5:E:65:LEU:HD22	5:E:70:VAL:HG21	1.83	0.61
39:j:20:VAL:HB	39:j:36:LEU:HD11	1.82	0.61
1:2:508:G:H2'	1:2:509:G:C8	2.35	0.61
1:2:1679:A:N6	1:2:1718:G:O2'	2.32	0.61
3:B:3:VAL:O	3:B:3:VAL:HG12	2.01	0.61
13:V:74:GLN:NE2	13:V:83:TRP:O	2.33	0.61
1:2:326:U:H2'	1:2:327:A:H8	1.66	0.60
1:2:1711:G:H3'	1:2:1712:A:C8	2.36	0.60
6:G:50:PHE:HE1	6:G:113:ILE:HD13	1.66	0.60
10:L:77:SER:HB3	10:L:85:VAL:HB	1.82	0.60
22:F:194:GLU:OE1	31:Z:63:SER:OG	2.18	0.60
39:j:170:LYS:HA	39:j:173:ILE:HD12	1.82	0.60
1:2:1131:A:H2'	1:2:1132:A:H8	1.67	0.60
24:M:122:GLN:O	24:M:126:ILE:HD12	2.01	0.60
40:k:108:HIS:HE1	40:k:227:PRO:HD2	1.65	0.60
25:P:81:ARG:NH2	25:P:120:SER:OG	2.27	0.60
29:T:39:THR:HA	29:T:100:ILE:HD12	1.82	0.60
30:U:100:VAL:O	30:U:104:THR:HG23	2.00	0.60
35:g:21:VAL:HG11	35:g:317:ILE:HD11	1.83	0.60
1:2:433:G:N2	1:2:436:A:OP2	2.32	0.60
1:2:1212:G:O2'	1:2:1243:A:N6	2.33	0.60
26:Q:113:ASP:OD1	26:Q:115:THR:OG1	2.19	0.60
1:2:529:C:O2	16:Y:61:ARG:NH2	2.35	0.60
1:2:1486:G:H3'	1:2:1513:A:H61	1.66	0.60
10:L:66:ILE:HG21	10:L:140:LEU:HD11	1.83	0.60
35:g:210:GLN:OE1	35:g:252:PHE:N	2.34	0.60
38:1:65:G:H8	38:1:65:G:OP1	1.84	0.60
38:1:75:C:H5''	38:1:76:A:H5''	1.84	0.60
1:2:12:U:OP1	4:C:89:LYS:NZ	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:513:G:O2'	1:2:514:A:OP1	2.20	0.60
1:2:1500:G:N7	29:T:102:ARG:NH2	2.49	0.60
21:D:179:GLN:OE1	21:D:179:GLN:N	2.34	0.60
1:2:703:G:H3'	1:2:704:C:H3'	1.83	0.60
5:E:175:PHE:HE1	5:E:198:ARG:HD2	1.66	0.60
15:X:125:VAL:HG12	15:X:126:LYS:HG3	1.83	0.60
21:D:109:LEU:HD11	21:D:115:ILE:HG12	1.83	0.60
1:2:395:G:N7	8:I:47:ARG:NH1	2.49	0.60
1:2:1035:A:H2'	1:2:1036:C:C6	2.37	0.60
1:2:1197:G:O3'	33:d:40:ARG:NH2	2.34	0.60
1:2:1502:G:H2'	1:2:1503:A:C8	2.37	0.60
3:B:33:LYS:O	3:B:98:THR:OG1	2.19	0.60
4:C:121:LYS:HG2	4:C:132:ALA:HB3	1.84	0.60
5:E:185:GLY:C	5:E:224:ASN:HD21	2.07	0.60
26:Q:39:VAL:HG12	26:Q:41:PRO:HD2	1.83	0.60
29:T:113:VAL:HA	29:T:128:GLY:HA3	1.83	0.60
31:Z:57:TYR:OH	31:Z:68:ARG:NH1	2.35	0.60
39:j:24:VAL:HG21	39:j:63:ILE:HG23	1.84	0.60
40:k:464:VAL:HG21	40:k:485:LEU:HD13	1.83	0.60
1:2:565:C:P	36:i:62:ARG:HH22	2.25	0.60
1:2:929:A:OP1	17:a:32:LYS:NZ	2.35	0.60
1:2:1472:G:H2'	1:2:1473:A:H8	1.67	0.60
23:K:84:GLU:N	23:K:84:GLU:OE2	2.35	0.60
27:R:9:VAL:HG23	27:R:50:ILE:HA	1.83	0.60
1:2:704:C:N4	1:2:735:C:O2	2.35	0.60
2:A:33:GLN:NE2	13:V:64:GLU:OE1	2.34	0.60
2:A:206:ASN:HB3	2:A:209:GLU:HG2	1.83	0.60
7:H:83:LYS:O	7:H:86:GLN:NE2	2.30	0.60
12:O:31:THR:HG22	12:O:38:THR:HA	1.83	0.60
17:a:23:CYS:HB3	17:a:28:ARG:H	1.67	0.60
19:e:10:ARG:NE	19:e:10:ARG:HA	2.16	0.60
1:2:103:A:H4'	1:2:105:A:C8	2.37	0.59
1:2:328:G:H2'	1:2:329:G:H8	1.67	0.59
1:2:1146:A:O2'	1:2:1634:C:OP2	2.20	0.59
23:K:71:GLU:CD	23:K:71:GLU:H	2.10	0.59
1:2:453:U:C2	5:E:66:MET:HE1	2.37	0.59
12:O:81:ILE:HD11	12:O:112:ILE:HD12	1.85	0.59
36:i:104:LYS:HE2	36:i:104:LYS:HA	1.83	0.59
38:1:74:C:H4'	38:1:75:C:O5'	2.03	0.59
1:2:646:G:H2'	1:2:647:G:H8	1.67	0.59
1:2:1198:G:H1	33:d:31:ILE:HD11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:169:GLU:HB3	21:D:190:LYS:HZ1	1.66	0.59
22:F:137:ASP:OD1	22:F:141:ASN:ND2	2.35	0.59
28:S:32:LEU:O	28:S:35:ILE:HG22	2.02	0.59
1:2:99:C:OP2	1:2:377:A:O2'	2.17	0.59
1:2:1670:G:H2'	1:2:1671:G:C8	2.37	0.59
2:A:179:ARG:HD2	2:A:183:ARG:HD2	1.84	0.59
25:P:72:LYS:HZ1	25:P:106:GLU:HG3	1.68	0.59
31:Z:90:LYS:HD2	31:Z:104:ALA:HA	1.84	0.59
40:k:380:LEU:HD11	40:k:390:ALA:HB2	1.85	0.59
1:2:1564:U:H5''	28:S:39:GLY:H	1.67	0.59
12:O:47:LYS:HD3	12:O:62:LEU:HB2	1.84	0.59
40:k:128:PHE:HE2	40:k:139:LYS:HD2	1.66	0.59
40:k:201:MET:HE2	40:k:511:LEU:HD21	1.85	0.59
1:2:339:U:H2'	1:2:340:A:H8	1.66	0.59
1:2:485:G:O6	1:2:500:U:O4	2.20	0.59
1:2:862:A:OP1	14:W:57:ARG:NH2	2.27	0.59
1:2:883:A:H4'	3:B:124:ASN:HD21	1.66	0.59
12:O:84:ARG:HG3	12:O:119:THR:HA	1.83	0.59
13:V:53:TYR:CE2	13:V:72:LEU:HB3	2.38	0.59
1:2:337:C:H1'	8:I:5:ARG:HB2	1.85	0.59
1:2:1088:U:OP1	17:a:89:ARG:NH1	2.36	0.59
1:2:1266:G:HO2'	1:2:1446:G:HO2'	1.51	0.59
1:2:1613:C:O2'	1:2:1614:G:OP2	2.19	0.59
2:A:26:ALA:HB1	2:A:149:LEU:HB2	1.84	0.59
24:M:72:ALA:HB1	24:M:79:LEU:HD13	1.83	0.59
1:2:345:G:P	10:L:79:ARG:HH22	2.26	0.59
1:2:563:G:N1	1:2:579:A:OP2	2.23	0.59
1:2:593:A:OP2	9:J:37:LYS:NZ	2.35	0.59
1:2:654:G:O6	1:2:676:U:O2	2.21	0.59
1:2:1332:C:H2'	1:2:1333:U:H6	1.68	0.59
10:L:75:VAL:HG13	10:L:84:ILE:HD11	1.85	0.59
11:N:99:ARG:NH2	11:N:119:GLU:OE1	2.36	0.59
2:A:59:LEU:HD22	13:V:79:LEU:HD21	1.83	0.59
3:B:104:ASP:OD1	3:B:105:PHE:N	2.36	0.59
12:O:49:LYS:HE3	12:O:49:LYS:HA	1.85	0.59
12:O:99:GLN:NE2	17:a:44:ILE:O	2.30	0.59
1:2:97:C:H2'	1:2:98:U:C6	2.38	0.58
1:2:196:A:N6	8:I:139:ASN:OD1	2.33	0.58
13:V:74:GLN:OE1	13:V:83:TRP:N	2.33	0.58
25:P:72:LYS:NZ	25:P:106:GLU:HG3	2.17	0.58
32:c:44:VAL:HG22	32:c:54:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:440:LEU:HD12	40:k:451:ALA:HB3	1.85	0.58
40:k:479:LYS:HD3	40:k:482:MET:HB3	1.84	0.58
1:2:152:G:H2'	1:2:153:G:H8	1.68	0.58
27:R:93:LEU:HB3	27:R:98:ASP:HA	1.84	0.58
27:R:103:ASP:OD1	27:R:104:THR:N	2.36	0.58
40:k:59:GLU:HB2	40:k:64:LYS:HE2	1.85	0.58
1:2:1158:C:O2'	26:Q:140:LYS:NZ	2.36	0.58
7:H:62:VAL:HG12	7:H:63:PRO:HD2	1.84	0.58
22:F:136:VAL:O	22:F:140:ILE:HG12	2.03	0.58
1:2:230:U:O2'	1:2:232:C:OP2	2.20	0.58
1:2:490:C:H2'	1:2:491:A:H4'	1.86	0.58
1:2:1469:A:OP1	22:F:187:ARG:NH2	2.35	0.58
1:2:1640:G:H5'	20:h:1:MET:HG3	1.86	0.58
4:C:50:VAL:HG21	4:C:73:ILE:HG23	1.86	0.58
4:C:232:PRO:HA	4:C:235:TRP:CE2	2.38	0.58
9:J:127:VAL:O	9:J:131:GLN:HG2	2.03	0.58
21:D:17:PHE:HE2	21:D:39:VAL:HG11	1.66	0.58
40:k:373:ILE:HD13	40:k:406:LEU:HD11	1.85	0.58
1:2:639:U:H2'	1:2:640:G:O4'	2.03	0.58
7:H:55:LYS:HD3	7:H:89:HIS:HE2	1.68	0.58
10:L:49:ILE:HG23	10:L:50:GLU:HG3	1.85	0.58
24:M:54:VAL:HG22	24:M:80:ILE:HB	1.85	0.58
27:R:28:PHE:HA	27:R:55:THR:HG21	1.85	0.58
40:k:228:GLN:OE1	40:k:232:HIS:NE2	2.37	0.58
40:k:313:PRO:HA	40:k:345:GLY:HA3	1.84	0.58
1:2:220:A:H2'	1:2:221:A:C8	2.38	0.58
1:2:658:C:H2'	1:2:659:G:C8	2.33	0.58
16:Y:86:GLU:OE2	16:Y:90:ARG:NH1	2.31	0.58
21:D:106:LYS:HG3	21:D:175:VAL:HG22	1.86	0.58
23:K:70:GLU:N	23:K:70:GLU:OE1	2.37	0.58
40:k:315:LEU:HD12	40:k:353:ILE:HD11	1.86	0.58
1:2:1355:U:O4	1:2:1366:G:O6	2.21	0.58
1:2:1480:C:O2'	26:Q:72:GLY:O	2.21	0.58
6:G:7:TYR:HD1	6:G:10:ASN:H	1.52	0.58
11:N:55:ARG:NH2	18:b:51:GLN:OE1	2.33	0.58
23:K:49:LEU:HB3	23:K:55:VAL:HG23	1.86	0.58
1:2:345:G:OP2	10:L:79:ARG:NH2	2.33	0.58
1:2:902:U:O2'	1:2:904:A:N7	2.36	0.58
20:h:2:ARG:HH21	20:h:4:LYS:HD2	1.69	0.58
35:g:14:LEU:HB2	35:g:317:ILE:HB	1.84	0.58
1:2:1571:A:H4'	1:2:1572:G:O5'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:45:ALA:HA	30:U:50:LEU:HD22	1.85	0.58
34:f:133:HIS:HE1	34:f:138:TYR:HB3	1.69	0.58
1:2:611:U:OP2	15:X:5:LYS:NZ	2.36	0.57
26:Q:98:ASP:OD1	26:Q:100:GLN:N	2.35	0.57
35:g:183:VAL:HB	35:g:199:PHE:HB2	1.85	0.57
1:2:1741:U:H2'	1:2:1742:A:C8	2.40	0.57
6:G:142:ARG:HD3	6:G:149:LYS:HA	1.86	0.57
12:O:58:TYR:HA	12:O:61:MET:HE3	1.85	0.57
16:Y:18:LEU:HB2	16:Y:20:ARG:HG2	1.86	0.57
16:Y:84:LYS:HG3	16:Y:85:PHE:CD1	2.39	0.57
24:M:51:GLN:NE2	24:M:76:ASN:OD1	2.37	0.57
35:g:171:ARG:NH1	35:g:189:ASN:OD1	2.37	0.57
1:2:38:C:O3'	9:J:6:ARG:NH2	2.36	0.57
1:2:166:U:H5''	6:G:135:PRO:HA	1.86	0.57
22:F:96:THR:HG22	22:F:116:VAL:HG21	1.84	0.57
24:M:28:SER:O	24:M:33:GLY:N	2.29	0.57
24:M:100:ASP:N	24:M:100:ASP:OD1	2.36	0.57
40:k:156:PRO:HG2	40:k:159:ASP:HB2	1.87	0.57
1:2:649:U:O2'	1:2:650:G:OP1	2.18	0.57
1:2:956:G:N2	18:b:51:GLN:HE21	2.02	0.57
1:2:1660:G:H2'	1:2:1661:G:H8	1.69	0.57
22:F:63:TYR:OH	32:c:49:ARG:NH1	2.37	0.57
25:P:51:GLU:OE1	25:P:51:GLU:N	2.32	0.57
28:S:63:GLN:NE2	28:S:67:GLU:OE2	2.38	0.57
35:g:208:VAL:HG11	35:g:249:ALA:HA	1.85	0.57
38:l:41:C:OP1	39:j:58:SER:OG	2.18	0.57
40:k:116:VAL:HG21	40:k:217:LEU:HD11	1.86	0.57
1:2:222:U:H2'	1:2:223:C:C6	2.39	0.57
5:E:32:SER:OG	5:E:81:THR:OG1	2.22	0.57
7:H:65:PRO:HD2	7:H:66:SER:H	1.69	0.57
17:a:75:ILE:O	17:a:79:ILE:HG12	2.04	0.57
25:P:86:VAL:HG22	25:P:89:MET:HE3	1.86	0.57
1:2:72:A:O2'	6:G:167:LYS:NZ	2.37	0.57
1:2:1765:G:H4'	1:2:1766:G:O5'	2.04	0.57
14:W:25:VAL:HG23	14:W:65:LEU:HD11	1.87	0.57
17:a:41:ILE:HG12	17:a:68:TYR:HD2	1.70	0.57
22:F:172:GLN:O	22:F:176:LEU:HD22	2.03	0.57
35:g:124:ILE:HD12	35:g:134:VAL:HG22	1.86	0.57
40:k:216:LEU:HD11	40:k:229:THR:HB	1.87	0.57
1:2:91:G:OP1	1:2:396:A:N6	2.36	0.57
1:2:857:G:OP1	7:H:116:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:922:A:H2'	1:2:923:A:C8	2.40	0.57
1:2:1469:A:H2	1:2:1472:G:N3	2.03	0.57
10:L:34:TRP:HH2	10:L:36:LYS:HD3	1.70	0.57
22:F:63:TYR:CD2	22:F:166:PRO:HB2	2.40	0.57
1:2:520:A:H2'	1:2:521:U:C6	2.40	0.57
1:2:683:C:H3'	1:2:684:A:H8	1.70	0.57
1:2:1228:G:N1	24:M:40:GLU:OE2	2.37	0.57
3:B:164:ILE:O	3:B:168:ILE:HG13	2.05	0.57
10:L:99:ARG:HB2	15:X:12:ALA:HB2	1.87	0.57
15:X:58:GLY:H	36:i:85:GLN:NE2	2.01	0.57
22:F:137:ASP:O	22:F:141:ASN:ND2	2.38	0.57
40:k:358:GLY:HA3	40:k:371:LYS:O	2.05	0.57
1:2:1162:A:N3	1:2:1611:U:O2'	2.30	0.57
28:S:40:ARG:HD3	29:T:45:LEU:HD11	1.87	0.57
1:2:1066:C:H5''	3:B:150:VAL:HG12	1.86	0.56
1:2:1315:G:OP1	27:R:7:LYS:N	2.34	0.56
1:2:1386:A:OP2	27:R:32:LYS:NZ	2.38	0.56
2:A:59:LEU:HB2	13:V:79:LEU:HD11	1.87	0.56
5:E:105:VAL:HB	5:E:243:GLY:HA2	1.86	0.56
7:H:101:LYS:N	7:H:101:LYS:HD2	2.20	0.56
40:k:375:SER:HB2	40:k:400:THR:OG1	2.05	0.56
1:2:1554:A:O2'	25:P:40:ARG:NH1	2.38	0.56
1:2:1648:U:H2'	1:2:1649:A:C8	2.40	0.56
2:A:15:GLN:NE2	27:R:93:LEU:HD13	2.19	0.56
7:H:65:PRO:CD	7:H:66:SER:H	2.16	0.56
21:D:65:ARG:HA	21:D:68:GLU:OE2	2.04	0.56
39:j:161:PRO:HG2	39:j:165:VAL:HG21	1.86	0.56
39:j:224:ALA:HB3	39:j:227:LEU:HB2	1.86	0.56
40:k:146:LYS:HG2	40:k:188:HIS:CE1	2.40	0.56
1:2:327:A:H2'	1:2:328:G:H8	1.70	0.56
1:2:890:A:H2'	1:2:891:A:H8	1.69	0.56
1:2:1240:G:OP1	25:P:77:ARG:NH1	2.37	0.56
3:B:2:ALA:N	12:O:49:LYS:HZ1	2.03	0.56
24:M:53:ALA:HB3	24:M:79:LEU:HG	1.88	0.56
24:M:105:LYS:HG2	24:M:106:VAL:HG23	1.87	0.56
26:Q:100:GLN:NE2	35:g:57:VAL:HG13	2.20	0.56
28:S:26:ILE:H	28:S:26:ILE:HD12	1.71	0.56
38:l:64:RIA:H2A	38:l:64:RIA:N3	2.20	0.56
39:j:7:ARG:HH21	39:j:10:GLU:C	2.13	0.56
1:2:78:A:O2'	1:2:79:C:OP1	2.23	0.56
1:2:867:G:OP1	11:N:121:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:143:ASP:HB2	5:E:145:ARG:HG3	1.87	0.56
1:2:590:A:H2'	1:2:591:G:C8	2.41	0.56
6:G:43:ASP:HA	6:G:46:LYS:HE3	1.87	0.56
8:I:116:HIS:O	8:I:147:ARG:NH1	2.38	0.56
26:Q:36:ILE:HD13	26:Q:52:LEU:HD11	1.87	0.56
1:2:1753:A:O5'	15:X:63:GLN:NE2	2.39	0.56
7:H:65:PRO:HD2	7:H:66:SER:N	2.21	0.56
14:W:14:ILE:HD13	14:W:25:VAL:HG21	1.87	0.56
19:e:41:THR:HA	19:e:45:VAL:HG22	1.88	0.56
33:d:15:GLY:O	33:d:19:ARG:NH1	2.38	0.56
1:2:79:C:H2'	1:2:80:A:C4	2.41	0.56
3:B:103:MET:HB3	3:B:215:VAL:HB	1.88	0.56
1:2:29:U:H2'	1:2:30:G:H8	1.70	0.56
1:2:1457:C:H5''	28:S:138:THR:HG21	1.86	0.56
6:G:159:ARG:HE	6:G:170:THR:HG21	1.71	0.56
7:H:30:ASN:HB2	7:H:34:LEU:HD12	1.88	0.56
39:j:205:LEU:HD21	40:k:330:ILE:HB	1.88	0.56
40:k:140:LEU:HD11	40:k:192:VAL:HB	1.87	0.56
1:2:554:A:C6	9:J:19:TYR:HE2	2.23	0.56
1:2:1559:U:H4'	1:2:1597:C:H4'	1.88	0.56
11:N:94:LYS:O	11:N:98:VAL:HG23	2.05	0.56
21:D:218:LEU:HG	21:D:221:SER:HB2	1.88	0.56
23:K:6:GLU:OE2	23:K:6:GLU:N	2.28	0.56
25:P:45:PHE:CD1	25:P:49:LEU:HD21	2.40	0.56
30:U:51:VAL:HG23	30:U:94:GLU:HB3	1.88	0.56
1:2:1380:A:HO2'	1:2:1381:G:H8	1.54	0.56
2:A:126:PRO:HG2	2:A:147:THR:HG22	1.88	0.56
7:H:64:VAL:HG11	7:H:94:ALA:HB1	1.88	0.56
30:U:25:ASN:OD1	30:U:115:GLU:HB3	2.06	0.56
1:2:108:A:H2'	1:2:109:G:C8	2.41	0.55
3:B:5:LYS:CG	3:B:7:LYS:HD2	2.35	0.55
13:V:17:CYS:HB2	13:V:56:SER:HB2	1.88	0.55
19:e:29:GLN:OE1	19:e:30:PRO:HD2	2.06	0.55
34:f:124:CYS:SG	34:f:141:LYS:HB3	2.46	0.55
38:1:64:RIA:O3A	38:1:65:G:OP1	2.17	0.55
1:2:44:U:OP2	1:2:436:A:N6	2.35	0.55
5:E:171:ASP:OD1	5:E:172:PHE:N	2.38	0.55
19:e:6:GLY:O	36:i:33:GLN:NE2	2.39	0.55
21:D:168:ILE:HD11	21:D:187:LYS:HB3	1.87	0.55
33:d:30:LEU:HD12	33:d:31:ILE:H	1.70	0.55
1:2:646:G:H2'	1:2:647:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1069:C:H4'	18:b:17:ARG:HE	1.70	0.55
1:2:1146:A:H2'	1:2:1147:C:C6	2.41	0.55
3:B:27:LYS:HG2	3:B:49:ASN:HA	1.88	0.55
7:H:99:LEU:HB2	7:H:112:ARG:HD2	1.87	0.55
10:L:78:THR:HG21	10:L:118:GLN:HA	1.89	0.55
17:a:60:ALA:O	17:a:61:GLU:HG2	2.06	0.55
24:M:86:LYS:HZ3	24:M:106:VAL:HA	1.71	0.55
1:2:324:G:OP1	10:L:134:THR:OG1	2.24	0.55
2:A:84:ARG:NH2	27:R:82:ASP:O	2.38	0.55
9:J:41:GLU:N	9:J:41:GLU:OE2	2.39	0.55
31:Z:62:VAL:HG12	31:Z:80:LEU:HD13	1.88	0.55
34:f:134:GLY:O	34:f:136:ARG:HG3	2.07	0.55
40:k:400:THR:OG1	40:k:401:LYS:N	2.36	0.55
1:2:347:U:HO2'	1:2:352:A:HO2'	1.54	0.55
1:2:548:G:H1	1:2:588:C:H5	1.53	0.55
10:L:16:GLN:HE22	10:L:33:ARG:HA	1.70	0.55
40:k:172:PRO:HD2	40:k:183:TYR:HB2	1.88	0.55
1:2:473:A:H5'	9:J:144:PRO:HD2	1.87	0.55
1:2:738:G:N1	1:2:739:G:O6	2.40	0.55
1:2:1187:G:O2'	1:2:1428:U:OP1	2.23	0.55
9:J:65:LYS:HA	9:J:70:LEU:HD21	1.87	0.55
22:F:63:TYR:HD2	22:F:166:PRO:HB2	1.72	0.55
40:k:157:GLU:OE1	40:k:300:LYS:NZ	2.40	0.55
1:2:1794:C:H6	17:a:7:SER:HB3	1.70	0.55
3:B:82:ARG:HG2	3:B:103:MET:HE3	1.88	0.55
30:U:84:MET:HE3	33:d:52:PHE:CE1	2.42	0.55
40:k:176:ARG:NH1	40:k:179:CYS:SG	2.80	0.55
1:2:169:U:N3	1:2:288:U:O2'	2.40	0.55
1:2:649:U:O4	1:2:685:A:N6	2.39	0.55
1:2:1332:C:H2'	1:2:1333:U:C6	2.42	0.55
5:E:11:ARG:HD3	5:E:21:ASP:O	2.06	0.55
1:2:1657:A:H2'	1:2:1658:A:H8	1.72	0.55
2:A:41:ARG:HD3	27:R:124:VAL:HG11	1.88	0.55
3:B:90:GLU:HG3	3:B:97:LEU:HD12	1.88	0.55
6:G:31:ARG:HB3	6:G:101:ILE:HD13	1.89	0.55
7:H:65:PRO:CD	7:H:66:SER:N	2.65	0.55
10:L:146:THR:HB	10:L:149:ALA:HB3	1.89	0.55
12:O:18:ARG:HA	12:O:82:LYS:HB2	1.89	0.55
1:2:1216:A:H4'	23:K:44:LYS:HE2	1.89	0.55
1:2:1522:A:N3	1:2:1588:G:O2'	2.38	0.55
3:B:2:ALA:N	12:O:49:LYS:NZ	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:70:GLU:N	8:I:70:GLU:OE2	2.39	0.55
13:V:79:LEU:HD23	13:V:82:VAL:HG11	1.88	0.55
22:F:50:PHE:HE2	22:F:70:ILE:H	1.53	0.55
1:2:339:U:H2'	1:2:340:A:C8	2.43	0.54
1:2:930:C:OP1	3:B:116:LYS:NZ	2.41	0.54
1:2:1302:U:O2'	1:2:1321:A:OP2	2.25	0.54
5:E:18:TRP:HH2	5:E:31:PRO:HD3	1.73	0.54
6:G:7:TYR:HD2	6:G:113:ILE:HG23	1.72	0.54
7:H:49:ILE:HD12	7:H:175:LYS:HG2	1.88	0.54
8:I:78:ILE:HD12	8:I:78:ILE:H	1.71	0.54
28:S:24:GLY:O	28:S:59:GLY:N	2.39	0.54
34:f:118:ARG:HG2	34:f:118:ARG:HH11	1.71	0.54
39:j:190:VAL:N	39:j:226:PRO:O	2.31	0.54
40:k:432:ILE:HD12	40:k:485:LEU:HD12	1.87	0.54
11:N:1:MET:SD	11:N:1:MET:N	2.67	0.54
40:k:128:PHE:CE1	40:k:129:LYS:HG3	2.42	0.54
1:2:555:A:H4'	19:e:56:MET:HG3	1.88	0.54
1:2:1280:G:O3'	30:U:76:SER:OG	2.26	0.54
1:2:1335:A:O3'	26:Q:123:ARG:NH2	2.41	0.54
6:G:84:TYR:OH	6:G:91:GLU:O	2.19	0.54
14:W:55:ASP:HB3	14:W:57:ARG:HB2	1.90	0.54
32:c:19:THR:OG1	32:c:20:GLY:N	2.39	0.54
35:g:115:ALA:HB3	35:g:124:ILE:HB	1.90	0.54
1:2:952:G:H2'	1:2:953:G:C8	2.41	0.54
1:2:1657:A:H2'	1:2:1658:A:C8	2.42	0.54
2:A:30:GLN:NE2	2:A:31:VAL:O	2.38	0.54
3:B:48:VAL:HG21	3:B:61:LEU:HD11	1.90	0.54
12:O:17:ALA:HB3	12:O:81:ILE:HA	1.89	0.54
13:V:1:MET:HG3	13:V:10:GLU:HG3	1.90	0.54
26:Q:13:LYS:HG3	26:Q:14:LYS:H	1.73	0.54
26:Q:45:ARG:HG2	26:Q:49:TYR:CE2	2.42	0.54
27:R:60:ARG:HH21	27:R:66:VAL:HG21	1.71	0.54
27:R:104:THR:O	27:R:108:GLU:HG3	2.06	0.54
1:2:57:G:OP1	16:Y:116:LYS:NZ	2.41	0.54
1:2:735:C:O2'	1:2:736:C:O5'	2.19	0.54
1:2:926:C:H2'	1:2:927:U:C6	2.43	0.54
9:J:159:ALA:O	9:J:162:SER:OG	2.26	0.54
21:D:28:GLU:HA	23:K:58:GLN:HE21	1.73	0.54
26:Q:127:LYS:HA	26:Q:134:ALA:HA	1.89	0.54
29:T:73:VAL:HG11	29:T:102:ARG:HG3	1.90	0.54
35:g:109:GLY:O	35:g:127:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:283:G:N7	6:G:188:ARG:NH1	2.56	0.54
1:2:1523:A:N3	1:2:1587:C:O2'	2.33	0.54
2:A:184:LEU:HD12	13:V:45:ALA:HB2	1.90	0.54
16:Y:103:ALA:O	16:Y:108:ARG:NH1	2.40	0.54
26:Q:60:PHE:HB2	26:Q:63:ILE:HB	1.89	0.54
28:S:45:LEU:HD21	28:S:81:ILE:HG12	1.88	0.54
36:i:76:ILE:HD12	36:i:77:ILE:H	1.72	0.54
1:2:787:A:OP2	5:E:108:ARG:NH2	2.28	0.54
1:2:1256:U:O2'	23:K:1:MET:O	2.26	0.54
2:A:17:LEU:HD11	2:A:54:TRP:HD1	1.72	0.54
4:C:147:GLY:N	4:C:158:SER:O	2.40	0.54
22:F:125:VAL:O	31:Z:58:ARG:NH1	2.41	0.54
35:g:151:TRP:HB2	35:g:179:MET:HE3	1.89	0.54
40:k:108:HIS:HD2	40:k:109:VAL:HG12	1.73	0.54
40:k:382:ALA:O	40:k:383:GLU:HG3	2.08	0.54
1:2:446:U:O2'	5:E:27:TYR:O	2.24	0.54
1:2:590:A:H5''	9:J:24:LEU:HD13	1.88	0.54
1:2:591:G:H2'	1:2:592:U:O4'	2.08	0.54
1:2:1712:A:H2'	1:2:1713:G:H8	1.73	0.54
26:Q:123:ARG:HB3	26:Q:124:PRO:HD2	1.90	0.54
27:R:5:ARG:O	27:R:10:LYS:NZ	2.40	0.54
34:f:131:ALA:N	34:f:138:TYR:O	2.38	0.54
1:2:334:U:O2'	10:L:129:ARG:NH1	2.40	0.54
10:L:16:GLN:HB2	10:L:19:ILE:HD13	1.89	0.54
28:S:97:ASP:N	28:S:97:ASP:OD1	2.39	0.54
32:c:60:GLU:OE1	32:c:60:GLU:N	2.40	0.54
1:2:387:G:OP2	1:2:422:G:O2'	2.26	0.54
1:2:1357:G:O2'	29:T:133:ASP:OD2	2.26	0.54
4:C:81:LEU:HD23	4:C:111:ASP:HB3	1.90	0.54
14:W:11:LEU:HD13	14:W:73:GLY:H	1.73	0.54
17:a:97:PRO:O	17:a:99:GLN:N	2.39	0.54
1:2:26:A:O2'	1:2:27:U:OP1	2.26	0.53
1:2:152:G:H4'	6:G:2:LYS:HZ2	1.72	0.53
1:2:245:G:H2'	1:2:246:A:C8	2.43	0.53
1:2:299:A:H2'	1:2:300:A:C8	2.43	0.53
1:2:476:A:OP2	19:e:28:LYS:NZ	2.42	0.53
12:O:103:ARG:NH1	17:a:48:ALA:O	2.38	0.53
26:Q:58:ASP:N	26:Q:58:ASP:OD1	2.40	0.53
31:Z:62:VAL:O	31:Z:66:VAL:HG22	2.07	0.53
39:j:8:PHE:CE2	39:j:109:HIS:HB2	2.43	0.53
40:k:100:THR:OG1	40:k:188:HIS:O	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:432:ILE:HG21	40:k:515:ALA:HB1	1.89	0.53
1:2:1034:G:H2'	1:2:1035:A:H8	1.73	0.53
21:D:105:MET:HB2	21:D:122:VAL:HG21	1.89	0.53
1:2:12:U:H2'	1:2:13:C:H6	1.73	0.53
1:2:97:C:H2'	1:2:98:U:H6	1.73	0.53
1:2:445:A:OP1	5:E:57:ASN:ND2	2.42	0.53
1:2:1159:A:H2'	1:2:1160:C:H6	1.73	0.53
2:A:190:ASP:OD1	2:A:191:ARG:N	2.41	0.53
4:C:159:LEU:HD22	4:C:226:THR:HG21	1.89	0.53
6:G:50:PHE:CE1	6:G:113:ILE:HD13	2.43	0.53
12:O:80:HIS:ND1	12:O:113:GLY:O	2.41	0.53
16:Y:106:GLN:O	16:Y:110:GLN:HG2	2.08	0.53
21:D:20:GLU:CD	21:D:76:ARG:HH21	2.16	0.53
26:Q:136:SER:OG	26:Q:137:ARG:N	2.42	0.53
32:c:12:VAL:HG12	32:c:30:VAL:HG12	1.90	0.53
35:g:117:ASP:OD1	35:g:118:ALA:N	2.42	0.53
35:g:193:TYR:C	35:g:194:ARG:HE	2.17	0.53
40:k:121:SER:HB3	40:k:145:ALA:HB2	1.89	0.53
21:D:221:SER:HB3	35:g:200:ILE:O	2.08	0.53
24:M:89:GLY:HA3	24:M:108:GLY:HA2	1.90	0.53
25:P:90:ILE:H	25:P:90:ILE:HD12	1.71	0.53
25:P:111:MET:HE2	28:S:119:ILE:HD11	1.90	0.53
39:j:47:LEU:HD12	39:j:48:LEU:H	1.73	0.53
1:2:1035:A:H2'	1:2:1036:C:H6	1.73	0.53
1:2:1336:A:H4'	26:Q:123:ARG:HH22	1.72	0.53
1:2:1590:A:H2'	1:2:1591:A:H8	1.73	0.53
1:2:1661:G:N2	1:2:1736:U:O2	2.38	0.53
38:1:64:RIA:H3A	38:1:65:G:C8	2.43	0.53
1:2:223:C:H2'	1:2:224:A:H5'	1.90	0.53
1:2:990:G:H21	1:2:1012:A:H62	1.57	0.53
1:2:1040:G:H2'	1:2:1041:G:C8	2.43	0.53
1:2:1240:G:O2'	1:2:1241:A:O5'	2.26	0.53
1:2:1251:C:H5''	34:f:105:TYR:OH	2.09	0.53
2:A:18:LEU:HG	2:A:23:HIS:CD2	2.43	0.53
6:G:7:TYR:CD2	6:G:113:ILE:HG23	2.44	0.53
7:H:91:ILE:HD12	7:H:172:VAL:HG21	1.90	0.53
34:f:100:LEU:HD13	34:f:103:LEU:HD21	1.89	0.53
1:2:485:G:N2	1:2:500:U:O2	2.33	0.53
1:2:1319:U:H2'	1:2:1321:A:H5'	1.91	0.53
3:B:144:ARG:HB2	3:B:208:GLN:HB3	1.91	0.53
7:H:14:THR:O	7:H:17:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:56:VAL:HG23	24:M:83:ALA:HA	1.90	0.53
26:Q:39:VAL:HG21	26:Q:48:VAL:HG11	1.91	0.53
1:2:556:G:O4'	19:e:57:ASN:ND2	2.42	0.53
1:2:817:C:H2'	1:2:818:G:C8	2.43	0.53
1:2:1143:U:H2'	1:2:1144:U:C6	2.44	0.53
1:2:1742:A:H3'	1:2:1743:G:H8	1.73	0.53
7:H:101:LYS:HD2	7:H:101:LYS:H	1.74	0.53
9:J:90:LYS:HB3	9:J:95:TYR:CG	2.44	0.53
12:O:81:ILE:HG21	12:O:102:LEU:HD12	1.89	0.53
21:D:93:ASP:N	21:D:93:ASP:OD1	2.39	0.53
31:Z:91:PRO:HA	31:Z:101:TYR:HD1	1.73	0.53
36:i:104:LYS:NZ	36:i:111:GLU:HA	2.23	0.53
40:k:230:SER:HB3	40:k:269:PHE:CZ	2.43	0.53
1:2:1498:C:OP1	29:T:122:ARG:NH2	2.37	0.53
1:2:1677:G:H21	1:2:1720:A:H62	1.57	0.53
9:J:135:ALA:HA	9:J:140:ILE:HA	1.91	0.53
28:S:69:ILE:O	28:S:73:MET:HG3	2.09	0.53
40:k:76:PRO:HD3	40:k:170:ILE:HD11	1.90	0.53
40:k:108:HIS:CE1	40:k:228:GLN:HB2	2.44	0.53
1:2:460:G:H2'	1:2:461:G:H8	1.74	0.53
1:2:855:A:P	7:H:97:ARG:HH21	2.32	0.53
1:2:1274:A:N3	21:D:141:LYS:NZ	2.46	0.53
1:2:1712:A:H2'	1:2:1713:G:C8	2.43	0.53
3:B:173:THR:O	3:B:177:GLN:HG3	2.09	0.53
5:E:198:ARG:HG3	5:E:208:VAL:HG12	1.91	0.53
12:O:58:TYR:O	12:O:62:LEU:HG	2.09	0.53
21:D:98:ALA:N	21:D:169:GLU:OE1	2.35	0.53
35:g:134:VAL:HB	35:g:143:TYR:HB2	1.89	0.53
1:2:760:A:N1	1:2:789:U:O4	2.42	0.52
1:2:1145:G:H2'	1:2:1146:A:C8	2.43	0.52
1:2:1647:G:H2'	1:2:1648:U:C6	2.44	0.52
1:2:1269:G:O2'	34:f:78:LYS:NZ	2.41	0.52
1:2:1290:G:H22	1:2:1323:G:N2	2.07	0.52
7:H:99:LEU:HD12	7:H:112:ARG:HG3	1.90	0.52
36:i:55:ASN:HB3	36:i:57:ARG:HG3	1.91	0.52
1:2:5:U:H2'	1:2:6:G:H8	1.74	0.52
1:2:303:U:OP1	10:L:136:ARG:NH1	2.42	0.52
1:2:1043:U:H2'	1:2:1044:C:C6	2.44	0.52
8:I:4:SER:HB2	8:I:24:LYS:HD2	1.91	0.52
22:F:28:ALA:HB3	26:Q:28:LEU:HB2	1.91	0.52
26:Q:9:THR:HG21	26:Q:88:GLY:HA2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:45:ASP:OD1	31:Z:45:ASP:N	2.40	0.52
40:k:94:ILE:HG23	40:k:391:VAL:HG21	1.91	0.52
1:2:223:C:C4	1:2:224:A:N7	2.77	0.52
1:2:367:U:O2'	1:2:602:U:O2'	2.20	0.52
2:A:16:LEU:HB3	2:A:172:LEU:HD11	1.91	0.52
8:I:111:GLN:OE1	8:I:111:GLN:N	2.39	0.52
21:D:158:ILE:HD12	21:D:163:PRO:HB2	1.92	0.52
22:F:126:LEU:HG	31:Z:58:ARG:HH21	1.75	0.52
35:g:86:TRP:HA	35:g:110:ASP:HB2	1.90	0.52
40:k:104:GLY:HA3	40:k:211:MET:SD	2.50	0.52
1:2:1357:G:H2'	1:2:1358:C:C6	2.45	0.52
15:X:14:LYS:HA	15:X:17:VAL:HG22	1.91	0.52
15:X:37:ALA:O	15:X:41:SER:OG	2.22	0.52
35:g:314:ASP:OD1	35:g:314:ASP:O	2.27	0.52
39:j:239:LYS:HD2	39:j:243:GLN:HG3	1.90	0.52
1:2:946:U:H2'	1:2:947:G:H8	1.73	0.52
1:2:1086:A:OP2	1:2:1086:A:H8	1.93	0.52
3:B:132:ASP:HB2	3:B:221:PRO:HB3	1.92	0.52
4:C:178:PRO:HG3	9:J:57:ARG:HD3	1.92	0.52
4:C:250:ASP:N	4:C:250:ASP:OD1	2.41	0.52
36:i:101:ARG:HH11	36:i:101:ARG:HG3	1.75	0.52
1:2:383:G:H2'	1:2:384:A:C8	2.44	0.52
1:2:1279:C:H4'	30:U:69:LYS:HB3	1.91	0.52
1:2:1586:G:O6	1:2:1606:U:O4	2.28	0.52
2:A:207:PRO:HA	2:A:210:ILE:HG22	1.91	0.52
4:C:148:TYR:OH	4:C:154:GLY:O	2.23	0.52
9:J:49:LEU:HB2	9:J:104:PHE:HE2	1.73	0.52
35:g:184:ARG:HH11	35:g:195:ILE:HD11	1.75	0.52
1:2:91:G:H2'	1:2:92:A:O4'	2.10	0.52
1:2:467:A:N1	1:2:593:A:O2'	2.40	0.52
4:C:170:VAL:HG11	4:C:215:THR:HA	1.91	0.52
4:C:228:GLY:HA2	13:V:23:ILE:HD11	1.92	0.52
15:X:86:PHE:CE2	15:X:88:PRO:HA	2.45	0.52
16:Y:20:ARG:NH2	16:Y:76:TYR:OH	2.43	0.52
40:k:142:TYR:CD2	45:k:602:MET:HB2	2.44	0.52
1:2:85:A:N3	1:2:147:U:O2'	2.43	0.52
1:2:833:G:H8	1:2:833:G:OP2	1.93	0.52
1:2:935:G:N7	17:a:15:ARG:NH1	2.58	0.52
1:2:1554:A:OP1	25:P:44:LYS:NZ	2.43	0.52
1:2:1590:A:H2'	1:2:1591:A:C8	2.45	0.52
1:2:1794:C:OP2	17:a:5:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:236:GLU:N	4:C:236:GLU:OE2	2.40	0.52
5:E:36:HIS:CG	5:E:85:GLY:HA3	2.45	0.52
1:2:471:U:O2'	1:2:769:A:N3	2.34	0.52
3:B:5:LYS:HG2	3:B:7:LYS:HD2	1.92	0.52
31:Z:95:HIS:ND1	31:Z:96:SER:O	2.39	0.52
39:j:222:LEU:HB2	40:k:330:ILE:HD11	1.91	0.52
1:2:1113:G:O2'	1:2:1129:G:O6	2.23	0.51
1:2:1291:G:H2'	1:2:1292:U:O2	2.09	0.51
12:O:63:ALA:O	12:O:67:VAL:HG22	2.10	0.51
16:Y:29:HIS:ND1	16:Y:29:HIS:O	2.43	0.51
23:K:35:ILE:HG23	23:K:37:THR:H	1.75	0.51
28:S:56:LYS:HD3	28:S:61:LEU:HB3	1.92	0.51
38:1:16:H2U:H4'	38:1:16:H2U:OP1	2.09	0.51
39:j:181:ALA:HB2	39:j:235:LEU:HD12	1.92	0.51
1:2:1293:G:H1	1:2:1302:U:H3	1.58	0.51
1:2:1349:G:H2'	1:2:1350:G:H8	1.74	0.51
1:2:1562:U:H2'	1:2:1563:C:C6	2.45	0.51
1:2:1774:A:H2'	1:2:1775:G:C8	2.46	0.51
1:2:1785:C:H2'	1:2:1786:G:H8	1.75	0.51
3:B:168:ILE:HG23	3:B:197:ILE:HD13	1.92	0.51
6:G:32:ILE:HD12	6:G:54:GLY:H	1.76	0.51
17:a:87:ARG:NH2	17:a:94:ILE:O	2.40	0.51
25:P:33:PHE:O	25:P:37:ALA:N	2.43	0.51
35:g:110:ASP:N	35:g:110:ASP:OD1	2.42	0.51
40:k:248:GLN:HE21	40:k:266:ILE:HD13	1.75	0.51
1:2:151:U:H5'	6:G:13:GLN:HE22	1.75	0.51
1:2:299:A:H2'	1:2:300:A:H8	1.76	0.51
1:2:801:G:OP2	7:H:105:LYS:NZ	2.43	0.51
1:2:1738:A:H2'	1:2:1739:U:C6	2.45	0.51
21:D:75:LYS:HE2	23:K:18:GLU:OE1	2.11	0.51
23:K:15:LEU:HD22	23:K:46:LEU:HD11	1.92	0.51
40:k:466:ILE:HA	40:k:499:ILE:HG12	1.91	0.51
1:2:78:A:C6	6:G:178:LEU:HD23	2.44	0.51
1:2:699:U:H2'	1:2:700:C:H6	1.74	0.51
1:2:922:A:H2'	1:2:923:A:H8	1.75	0.51
1:2:1168:G:N1	1:2:1573:7MG:OP2	2.43	0.51
1:2:1386:A:H5'	27:R:48:ASN:ND2	2.25	0.51
1:2:1480:C:H4'	26:Q:77:GLN:NE2	2.25	0.51
3:B:109:LYS:O	3:B:113:MET:HG2	2.09	0.51
25:P:90:ILE:HG12	25:P:109:PRO:HA	1.91	0.51
26:Q:10:PHE:HE2	26:Q:12:LYS:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:52:SER:HB2	39:j:62:LEU:HD22	1.91	0.51
1:2:627:G:OP1	11:N:124:ARG:NE	2.43	0.51
1:2:1160:C:H2'	1:2:1161:C:H6	1.75	0.51
3:B:180:THR:O	3:B:184:LEU:N	2.33	0.51
5:E:104:ASP:O	5:E:107:GLY:N	2.27	0.51
9:J:110:GLN:NE2	9:J:126:ARG:HB2	2.26	0.51
9:J:137:GLY:O	9:J:138:LYS:HG2	2.10	0.51
10:L:125:VAL:HG23	10:L:139:VAL:HA	1.92	0.51
39:j:27:ILE:HD11	39:j:63:ILE:HG21	1.92	0.51
1:2:154:U:OP2	16:Y:132:ARG:NH2	2.37	0.51
1:2:371:G:H1'	1:2:611:U:H3	1.76	0.51
1:2:460:G:H2'	1:2:461:G:C8	2.46	0.51
1:2:946:U:H2'	1:2:947:G:C8	2.46	0.51
1:2:1132:A:N3	1:2:1648:U:O2'	2.44	0.51
1:2:1250:U:H1'	34:f:133:HIS:CD2	2.45	0.51
1:2:1506:U:H2'	1:2:1507:C:C6	2.46	0.51
4:C:158:SER:OG	4:C:159:LEU:N	2.44	0.51
25:P:31:GLU:O	25:P:35:LYS:HG2	2.11	0.51
25:P:110:GLU:OE1	25:P:110:GLU:N	2.43	0.51
1:2:6:G:O6	4:C:210:ARG:NH2	2.43	0.51
1:2:989:C:H5	1:2:1013:G:H1	1.57	0.51
7:H:60:VAL:HG22	7:H:92:PHE:HA	1.93	0.51
8:I:104:ILE:HG22	8:I:106:ALA:H	1.75	0.51
1:2:638:U:H1'	1:2:639:U:C5	2.46	0.51
1:2:787:A:C4	5:E:19:MET:HE1	2.46	0.51
1:2:1335:A:C2	1:2:1414:G:C5	2.99	0.51
2:A:36:TYR:OH	13:V:70:ASN:ND2	2.30	0.51
3:B:67:GLU:HG3	3:B:83:LYS:HD3	1.93	0.51
13:V:32:VAL:HG12	13:V:60:ARG:HD2	1.92	0.51
26:Q:29:ILE:HA	26:Q:65:ILE:HB	1.92	0.51
40:k:108:HIS:ND1	40:k:228:GLN:HB2	2.25	0.51
40:k:308:ASP:HB2	40:k:310:MET:HE1	1.92	0.51
1:2:372:G:H5'	10:L:96:LYS:HG3	1.93	0.51
1:2:788:A:C2	1:2:789:U:H1'	2.46	0.51
1:2:1195:A:H4'	1:2:1196:C:H5''	1.93	0.51
1:2:1331:C:O2'	21:D:162:GLN:NE2	2.43	0.51
1:2:1645:U:H2'	1:2:1646:A:H8	1.74	0.51
4:C:104:LYS:HA	4:C:121:LYS:O	2.11	0.51
9:J:27:GLU:HB3	9:J:39:LYS:HD3	1.93	0.51
35:g:154:LYS:HG3	35:g:208:VAL:HG23	1.91	0.51
1:2:958:U:H2'	1:2:958:U:O2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1170:A:O3'	28:S:144:ARG:NH2	2.37	0.51
3:B:27:LYS:HD3	3:B:47:LEU:HG	1.92	0.51
11:N:83:GLU:OE1	11:N:83:GLU:N	2.43	0.51
14:W:24:GLN:HA	14:W:63:VAL:O	2.11	0.51
17:a:24:VAL:HG23	17:a:25:ASN:OD1	2.11	0.51
24:M:36:ARG:HE	24:M:94:LEU:HD12	1.76	0.51
39:j:16:ILE:O	39:j:17:ASP:HB3	2.09	0.51
1:2:126:A:O2'	1:2:127:G:H5'	2.10	0.50
1:2:157:U:O2'	1:2:159:C:OP2	2.25	0.50
1:2:208:U:H2'	1:2:209:A:H8	1.76	0.50
1:2:1490:A:O2'	1:2:1491:A:O4'	2.26	0.50
1:2:1771:C:H2'	1:2:1772:G:H8	1.75	0.50
10:L:55:ASP:HA	10:L:82:ARG:HH12	1.75	0.50
12:O:99:GLN:NE2	17:a:45:VAL:HA	2.26	0.50
15:X:107:PHE:CE1	15:X:123:LYS:HG3	2.46	0.50
19:e:7:SER:OG	19:e:10:ARG:NH1	2.44	0.50
21:D:162:GLN:O	21:D:166:ASP:N	2.38	0.50
36:i:95:TYR:CD2	36:i:103:LEU:HD11	2.47	0.50
39:j:212:SER:HB3	39:j:218:VAL:HB	1.93	0.50
40:k:197:HIS:ND1	40:k:199:ILE:HG22	2.26	0.50
40:k:348:LYS:HE2	40:k:388:LYS:HB3	1.93	0.50
1:2:1463:C:H5'	26:Q:139:GLN:HB3	1.93	0.50
1:2:1683:G:H2'	1:2:1684:C:C6	2.46	0.50
1:2:1774:A:H2'	1:2:1775:G:H8	1.76	0.50
1:2:23:G:O6	1:2:601:U:C2	2.65	0.50
1:2:1427:G:H2'	1:2:1428:U:C6	2.46	0.50
1:2:1577:U:H2'	1:2:1578:C:C6	2.47	0.50
5:E:31:PRO:HG3	5:E:43:PRO:HG3	1.93	0.50
5:E:45:ILE:HB	5:E:80:THR:HG22	1.93	0.50
12:O:71:CYS:SG	12:O:110:LEU:HD21	2.51	0.50
22:F:31:ILE:HB	22:F:36:GLN:NE2	2.27	0.50
25:P:18:LYS:NZ	28:S:90:LYS:HB3	2.26	0.50
26:Q:57:LEU:H	26:Q:57:LEU:HD12	1.75	0.50
35:g:188:LEU:HA	35:g:193:TYR:HA	1.94	0.50
40:k:330:ILE:HA	40:k:333:LEU:HG	1.93	0.50
1:2:206:U:H2'	1:2:207:U:C6	2.47	0.50
1:2:357:U:O2'	1:2:359:A:OP1	2.26	0.50
1:2:1405:U:H2'	1:2:1406:G:C8	2.46	0.50
22:F:31:ILE:HB	22:F:36:GLN:HE21	1.75	0.50
26:Q:13:LYS:HG2	26:Q:76:SER:HA	1.93	0.50
26:Q:22:VAL:HG12	26:Q:65:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:64:GLY:HA3	35:g:91:ARG:HH12	1.76	0.50
40:k:146:LYS:NZ	40:k:168:LYS:O	2.44	0.50
1:2:1069:C:H4'	18:b:17:ARG:NE	2.27	0.50
1:2:1152:G:P	17:a:82:ARG:HH21	2.35	0.50
1:2:1344:A:H5'	30:U:53:LYS:HE2	1.94	0.50
4:C:162:LYS:HD3	4:C:173:ARG:HH21	1.77	0.50
7:H:24:PHE:CE1	7:H:77:LEU:HD21	2.47	0.50
7:H:41:LEU:HG	7:H:70:TYR:CE1	2.47	0.50
9:J:68:LYS:HG2	9:J:72:GLU:OE2	2.12	0.50
16:Y:15:ASN:OD1	16:Y:17:LEU:HB2	2.12	0.50
21:D:65:ARG:O	21:D:68:GLU:HG2	2.11	0.50
35:g:39:ARG:HD2	35:g:68:ILE:HG23	1.93	0.50
38:1:36:U:H2'	38:1:37:T6A:C8	2.47	0.50
40:k:80:LEU:HG	40:k:388:LYS:HD2	1.94	0.50
40:k:471:THR:HG21	40:k:491:ALA:HB2	1.93	0.50
1:2:127:G:N2	6:G:195:ILE:HD12	2.26	0.50
1:2:327:A:H2'	1:2:328:G:C8	2.46	0.50
1:2:494:C:H3'	1:2:495:G:C8	2.47	0.50
1:2:1549:U:O4	25:P:40:ARG:NH2	2.45	0.50
2:A:94:GLY:H	2:A:185:ARG:HH12	1.59	0.50
6:G:7:TYR:HD2	6:G:113:ILE:CG2	2.25	0.50
12:O:29:HIS:CD2	12:O:41:ARG:HG3	2.46	0.50
13:V:4:ASP:OD1	13:V:5:LYS:N	2.45	0.50
15:X:41:SER:OG	15:X:43:PHE:O	2.29	0.50
15:X:69:ARG:HB3	15:X:86:PHE:CE1	2.43	0.50
18:b:21:LEU:HD23	18:b:26:GLN:OE1	2.10	0.50
22:F:42:ILE:HG12	22:F:71:TYR:CZ	2.46	0.50
23:K:9:LYS:HE2	23:K:9:LYS:HA	1.93	0.50
26:Q:22:VAL:HG12	26:Q:65:ILE:CD1	2.42	0.50
30:U:19:ILE:HG22	30:U:21:LYS:H	1.76	0.50
40:k:146:LYS:O	40:k:163:SER:HA	2.12	0.50
1:2:497:G:H1'	1:2:499:C:H41	1.76	0.50
1:2:855:A:N6	7:H:96:ARG:HB3	2.26	0.50
1:2:1259:U:O2'	1:2:1260:G:H8	1.95	0.50
1:2:1381:G:H2'	1:2:1382:A:C8	2.47	0.50
1:2:1617:C:H2'	1:2:1618:C:H6	1.77	0.50
18:b:75:GLU:CD	18:b:75:GLU:H	2.19	0.50
28:S:17:LEU:HD21	28:S:66:LEU:HD22	1.93	0.50
40:k:330:ILE:HG23	40:k:333:LEU:HD12	1.94	0.50
1:2:624:C:H2'	1:2:625:U:H6	1.77	0.50
1:2:1389:A:H2'	1:2:1390:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1396:U:H3'	1:2:1397:C:H5'	1.93	0.50
1:2:1593:U:H5'	1:2:1594:C:OP2	2.11	0.50
6:G:199:GLN:OE1	6:G:202:ARG:NH2	2.45	0.50
11:N:38:ILE:O	11:N:42:ARG:HG3	2.12	0.50
25:P:75:VAL:HG21	25:P:104:GLN:HE22	1.76	0.50
36:i:64:LYS:HD3	36:i:64:LYS:N	2.27	0.50
1:2:14:C:H5'	4:C:169:SER:OG	2.12	0.50
1:2:938:A:OP1	11:N:114:ARG:NH2	2.41	0.50
1:2:1234:C:C2	1:2:1235:A:C8	3.00	0.50
1:2:1793:U:C2	17:a:75:ILE:HD11	2.46	0.50
3:B:3:VAL:HG23	12:O:49:LYS:NZ	2.27	0.50
3:B:167:VAL:HA	3:B:170:GLU:OE1	2.11	0.50
4:C:83:ASP:C	4:C:83:ASP:OD1	2.55	0.50
21:D:162:GLN:O	21:D:165:ASN:N	2.41	0.50
27:R:16:LEU:HD22	27:R:38:ILE:HD11	1.93	0.50
30:U:50:LEU:HD11	30:U:99:ILE:HD12	1.94	0.50
38:1:63:G:H2'	38:1:64:RIA:H1A	1.94	0.50
40:k:207:GLY:HA2	40:k:210:VAL:HG12	1.93	0.50
40:k:348:LYS:HD2	40:k:349:LEU:H	1.77	0.50
1:2:221:A:OP2	1:2:832:U:H1'	2.11	0.49
1:2:1205:U:OP2	1:2:1206:C:O2'	2.22	0.49
1:2:1244:G:OP1	33:d:3:HIS:NE2	2.45	0.49
1:2:1279:C:H2'	1:2:1280:G:H8	1.77	0.49
1:2:1659:U:H2'	1:2:1660:G:C8	2.47	0.49
3:B:57:ALA:O	3:B:60:SER:N	2.45	0.49
7:H:21:ALA:O	7:H:25:ILE:HG12	2.11	0.49
10:L:34:TRP:CH2	10:L:36:LYS:HD3	2.46	0.49
17:a:74:CYS:SG	17:a:75:ILE:N	2.85	0.49
25:P:58:LYS:O	25:P:61:ARG:HG2	2.12	0.49
1:2:606:G:H21	1:2:613:C:H5''	1.76	0.49
1:2:623:G:H2'	1:2:624:C:C6	2.47	0.49
1:2:643:U:H2'	1:2:644:C:C6	2.47	0.49
1:2:1144:U:C2	1:2:1145:G:C8	3.01	0.49
1:2:1415:A:H2'	1:2:1416:G:O4'	2.12	0.49
5:E:179:LYS:NZ	5:E:230:GLU:OE1	2.38	0.49
8:I:67:TRP:O	8:I:71:GLY:CA	2.60	0.49
8:I:104:ILE:HB	8:I:166:LEU:HB2	1.94	0.49
8:I:139:ASN:O	8:I:142:ARG:HG2	2.12	0.49
10:L:97:TYR:O	10:L:99:ARG:HG2	2.13	0.49
19:e:24:GLN:OE1	19:e:25:GLU:N	2.45	0.49
22:F:159:ARG:HB2	22:F:226:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:101:SER:O	26:Q:105:LEU:HG	2.12	0.49
27:R:100:LEU:HD13	27:R:102:VAL:HG13	1.94	0.49
28:S:15:LEU:HB2	28:S:22:VAL:HG13	1.93	0.49
1:2:606:G:N2	1:2:613:C:H5''	2.27	0.49
1:2:840:U:C4	1:2:841:C:C4	3.00	0.49
1:2:1239:U:O3'	1:2:1240:G:N2	2.30	0.49
1:2:1336:A:H4'	26:Q:123:ARG:HH12	1.78	0.49
6:G:50:PHE:CD2	6:G:111:LEU:HD13	2.46	0.49
6:G:159:ARG:HH21	6:G:170:THR:HG21	1.76	0.49
9:J:18:PRO:HG2	9:J:19:TYR:CD1	2.45	0.49
16:Y:12:VAL:HA	16:Y:22:GLN:O	2.12	0.49
28:S:12:GLN:N	28:S:59:GLY:O	2.45	0.49
36:i:44:ASN:OD1	36:i:46:ARG:NE	2.45	0.49
1:2:324:G:OP1	10:L:132:SER:OG	2.30	0.49
1:2:603:A:H2'	1:2:604:A:O4'	2.12	0.49
1:2:852:G:H2'	1:2:853:U:C6	2.47	0.49
1:2:1318:A:H2'	1:2:1319:U:O4'	2.11	0.49
1:2:1604:C:H2'	1:2:1605:G:C8	2.47	0.49
1:2:1628:U:O2'	1:2:1762:C:O2'	2.25	0.49
3:B:5:LYS:HG3	3:B:7:LYS:HD2	1.94	0.49
4:C:83:ASP:OD2	4:C:134:ILE:HD12	2.12	0.49
29:T:52:GLY:HA2	29:T:55:TYR:HD1	1.77	0.49
31:Z:53:GLU:OE2	31:Z:53:GLU:N	2.45	0.49
33:d:21:CYS:C	33:d:23:ILE:H	2.20	0.49
35:g:68:ILE:O	35:g:86:TRP:N	2.44	0.49
39:j:247:ALA:O	39:j:251:ILE:HG23	2.13	0.49
1:2:924:G:H2'	1:2:925:A:H8	1.78	0.49
1:2:1029:A:OP1	17:a:3:LYS:NZ	2.37	0.49
1:2:1309:U:O2'	1:2:1400:G:O2'	2.28	0.49
10:L:58:CYS:HB3	10:L:62:GLY:H	1.77	0.49
15:X:43:PHE:HB3	15:X:46:SER:HB3	1.93	0.49
16:Y:15:ASN:HB3	16:Y:20:ARG:HG3	1.93	0.49
17:a:23:CYS:CB	17:a:28:ARG:H	2.26	0.49
23:K:56:LYS:HB2	23:K:67:THR:HG23	1.92	0.49
40:k:77:GLU:OE1	40:k:77:GLU:N	2.36	0.49
1:2:107:C:H2'	1:2:108:A:H8	1.77	0.49
1:2:182:U:H2'	1:2:183:C:H6	1.76	0.49
1:2:564:C:O5'	36:i:64:LYS:NZ	2.37	0.49
1:2:624:C:H2'	1:2:625:U:C6	2.48	0.49
1:2:1017:U:C2	1:2:1018:A:C8	3.00	0.49
1:2:1523:A:H4'	29:T:83:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:TYR:CE1	27:R:109:LEU:HB2	2.47	0.49
7:H:43:PHE:HE1	7:H:60:VAL:HB	1.77	0.49
7:H:51:VAL:HB	7:H:55:LYS:HB3	1.93	0.49
7:H:91:ILE:HG21	7:H:129:LEU:HD12	1.95	0.49
14:W:69:LEU:HD11	14:W:72:CYS:SG	2.52	0.49
17:a:85:ARG:HH11	17:a:85:ARG:HG3	1.78	0.49
29:T:53:TRP:HH2	29:T:100:ILE:HD13	1.76	0.49
40:k:408:ARG:HG3	40:k:408:ARG:HH11	1.76	0.49
1:2:812:U:O2'	1:2:814:G:OP1	2.28	0.49
4:C:84:GLU:HG2	4:C:191:LYS:NZ	2.27	0.49
11:N:87:ASP:N	11:N:87:ASP:OD1	2.46	0.49
27:R:77:GLU:OE1	27:R:80:ARG:NH2	2.46	0.49
31:Z:58:ARG:HG3	31:Z:103:ARG:HH21	1.77	0.49
39:j:8:PHE:HE2	39:j:109:HIS:HB2	1.78	0.49
1:2:415:A:H5'	1:2:416:A:C8	2.48	0.49
1:2:812:U:O2'	1:2:813:A:H4'	2.13	0.49
2:A:53:THR:HA	2:A:161:PRO:HD2	1.95	0.49
21:D:49:ILE:HG23	21:D:89:GLU:HG2	1.95	0.49
24:M:67:LEU:O	24:M:71:LEU:CD1	2.42	0.49
25:P:81:ARG:NH2	25:P:120:SER:O	2.46	0.49
28:S:36:ARG:HB2	28:S:102:ALA:HA	1.95	0.49
29:T:130:ARG:HA	29:T:133:ASP:OD2	2.12	0.49
36:i:59:ALA:HB1	36:i:91:VAL:HG23	1.95	0.49
36:i:70:TRP:CZ2	37:3:32:U:H1'	2.48	0.49
38:1:1:A:H2'	38:1:2:G:H8	1.78	0.49
1:2:258:U:H1'	8:I:179:ARG:HH21	1.78	0.49
1:2:390:A:HO2'	1:2:1728:A:HO2'	1.59	0.49
1:2:698:U:H2'	1:2:699:U:C6	2.48	0.49
1:2:1262:G:H2'	1:2:1263:G:O4'	2.13	0.49
1:2:1537:G:H4'	28:S:40:ARG:HH21	1.78	0.49
2:A:92:HIS:ND1	2:A:202:TYR:OH	2.43	0.49
16:Y:15:ASN:ND2	16:Y:18:LEU:HD12	2.28	0.49
21:D:71:LEU:HB3	23:K:20:VAL:HG21	1.93	0.49
21:D:162:GLN:HG2	21:D:163:PRO:CD	2.43	0.49
25:P:51:GLU:H	25:P:51:GLU:CD	2.21	0.49
25:P:88:GLU:OE1	25:P:88:GLU:N	2.46	0.49
38:1:64:RIA:H4A	38:1:64:RIA:OP2	2.13	0.49
1:2:17:C:H2'	1:2:18:C:C6	2.48	0.49
1:2:388:G:H2'	1:2:389:G:O4'	2.12	0.49
1:2:1559:U:H2'	1:2:1560:G:H8	1.77	0.49
1:2:1726:U:H2'	1:2:1727:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:133:TYR:CD1	3:B:221:PRO:HD3	2.47	0.49
5:E:162:VAL:HG12	5:E:164:LEU:H	1.78	0.49
6:G:64:LYS:HB2	6:G:97:VAL:HG21	1.95	0.49
7:H:44:LYS:HD2	7:H:63:PRO:HA	1.95	0.49
21:D:169:GLU:HB3	21:D:190:LYS:NZ	2.27	0.49
27:R:41:ILE:H	27:R:41:ILE:HD12	1.78	0.49
28:S:76:PRO:HB3	28:S:81:ILE:HD12	1.94	0.49
29:T:15:ILE:H	29:T:15:ILE:HD12	1.78	0.49
35:g:45:SER:O	35:g:59:VAL:N	2.42	0.49
1:2:277:U:P	1:2:278:G:H21	2.36	0.48
1:2:751:G:H2'	1:2:752:A:C8	2.48	0.48
1:2:1047:G:O3'	18:b:69:GLY:HA3	2.12	0.48
1:2:1143:U:HO2'	1:2:1300:U:HO2'	1.61	0.48
1:2:1201:A:N6	1:2:1455:C:OP1	2.45	0.48
6:G:14:LYS:HB2	6:G:124:ILE:HD11	1.94	0.48
13:V:49:GLU:OE1	13:V:49:GLU:HA	2.13	0.48
14:W:57:ARG:CD	18:b:26:GLN:HE21	2.26	0.48
21:D:99:VAL:O	21:D:103:GLU:HG2	2.13	0.48
22:F:145:ARG:HG2	32:c:55:VAL:HG11	1.94	0.48
1:2:442:C:O2'	1:2:444:A:H2	1.97	0.48
1:2:996:G:H1	1:2:1006:5MC:HN41	1.59	0.48
1:2:1650:C:H2'	1:2:1651:C:H6	1.78	0.48
7:H:43:PHE:CG	7:H:46:ILE:HD11	2.48	0.48
7:H:141:ARG:HB3	14:W:51:GLU:OE1	2.11	0.48
24:M:55:LEU:HD21	24:M:81:LYS:NZ	2.29	0.48
25:P:85:ILE:HG21	25:P:111:MET:HB3	1.96	0.48
35:g:88:LYS:HG2	35:g:109:GLY:C	2.38	0.48
1:2:93:A:O4'	5:E:3:ARG:NH1	2.47	0.48
1:2:824:U:H2'	1:2:825:U:C6	2.48	0.48
1:2:1038:A:H4'	13:V:62:ARG:HH21	1.78	0.48
1:2:1043:U:H5	1:2:1073:G:H1	1.61	0.48
1:2:1430:U:H4'	1:2:1431:G:O5'	2.11	0.48
1:2:1455:C:O2'	1:2:1456:G:H5'	2.13	0.48
1:2:1582:G:O2'	1:2:1608:G:O6	2.27	0.48
1:2:1711:G:H3'	1:2:1712:A:H8	1.78	0.48
28:S:65:GLU:OE2	28:S:68:ARG:NH1	2.45	0.48
29:T:40:SER:HB2	29:T:96:ALA:HA	1.95	0.48
35:g:68:ILE:HB	35:g:86:TRP:CG	2.48	0.48
39:j:50:GLU:HG3	39:j:50:GLU:O	2.13	0.48
40:k:409:ALA:HB3	40:k:411:ARG:HE	1.78	0.48
1:2:152:G:H2'	1:2:153:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:403:G:H2'	1:2:404:C:H6	1.78	0.48
1:2:433:G:N2	1:2:435:A:H3'	2.27	0.48
1:2:444:A:H62	1:2:461:G:H1'	1.78	0.48
1:2:1276:G:O3'	21:D:183:GLY:HA3	2.13	0.48
1:2:1380:A:H5''	30:U:60:THR:HG23	1.95	0.48
1:2:1386:A:N6	1:2:1409:A:N7	2.61	0.48
1:2:1737:C:H2'	1:2:1738:A:H8	1.77	0.48
2:A:107:PHE:HD2	2:A:135:GLU:HB3	1.78	0.48
2:A:175:TYR:HE1	2:A:195:TRP:CE3	2.32	0.48
12:O:29:HIS:CE1	12:O:38:THR:HB	2.48	0.48
28:S:121:SER:O	28:S:125:ILE:HG23	2.12	0.48
30:U:58:LEU:HD21	30:U:90:TYR:CD2	2.48	0.48
1:2:383:G:H2'	1:2:384:A:H8	1.79	0.48
23:K:54:PHE:O	23:K:69:THR:HG22	2.13	0.48
25:P:30:THR:O	25:P:34:VAL:HG23	2.13	0.48
30:U:30:LYS:HD3	30:U:33:GLN:OE1	2.13	0.48
30:U:43:LYS:O	30:U:47:THR:OG1	2.26	0.48
36:i:39:THR:O	36:i:73:GLN:NE2	2.46	0.48
1:2:248:U:OP1	10:L:34:TRP:NE1	2.34	0.48
1:2:753:A:H5''	5:E:187:ARG:HH22	1.78	0.48
1:2:1544:G:OP1	28:S:127:HIS:NE2	2.43	0.48
1:2:1578:C:H4'	26:Q:137:ARG:HB2	1.95	0.48
9:J:141:VAL:HG12	9:J:143:ILE:H	1.78	0.48
28:S:18:LEU:O	28:S:20:THR:HG23	2.13	0.48
39:j:7:ARG:HD3	39:j:7:ARG:N	2.29	0.48
1:2:17:C:O2'	1:2:1136:A:N1	2.40	0.48
1:2:965:A:OP2	11:N:124:ARG:NH1	2.46	0.48
1:2:1658:A:H2'	1:2:1659:U:C6	2.48	0.48
6:G:180:THR:HG22	6:G:182:GLN:H	1.78	0.48
6:G:195:ILE:O	6:G:199:GLN:HG2	2.14	0.48
8:I:112:TRP:O	8:I:116:HIS:HB2	2.12	0.48
16:Y:51:GLU:H	16:Y:51:GLU:CD	2.20	0.48
21:D:61:GLU:OE1	21:D:64:ARG:HD3	2.14	0.48
28:S:116:LEU:O	28:S:124:GLY:HA3	2.13	0.48
36:i:27:ILE:HD13	36:i:93:HIS:CD2	2.48	0.48
40:k:239:MET:HA	40:k:239:MET:HE3	1.94	0.48
40:k:462:LEU:HD21	40:k:501:LEU:HB3	1.95	0.48
1:2:336:G:O2'	8:I:10:LYS:NZ	2.46	0.48
1:2:773:C:H5''	5:E:21:ASP:OD1	2.14	0.48
1:2:834:U:H2'	1:2:835:U:C6	2.48	0.48
1:2:1240:G:H2'	1:2:1241:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1562:U:H2'	1:2:1563:C:H6	1.78	0.48
6:G:2:LYS:HB3	6:G:108:VAL:HG13	1.96	0.48
9:J:152:SER:O	9:J:152:SER:OG	2.31	0.48
22:F:189:ILE:HG21	31:Z:66:VAL:HG21	1.95	0.48
29:T:73:VAL:HG22	29:T:105:LEU:HD12	1.96	0.48
31:Z:91:PRO:HA	31:Z:101:TYR:CD1	2.48	0.48
41:l:138:PHE:O	41:l:142:LEU:HG	2.13	0.48
1:2:430:C:C2	1:2:431:G:C8	3.02	0.48
1:2:544:A:H2'	19:e:31:LYS:HD3	1.96	0.48
1:2:570:G:H5''	15:X:114:LYS:HD2	1.95	0.48
1:2:1125:G:H2'	1:2:1126:G:H8	1.79	0.48
2:A:195:TRP:CH2	2:A:197:ILE:HD11	2.48	0.48
3:B:203:ASP:OD1	3:B:204:ILE:N	2.46	0.48
7:H:99:LEU:O	7:H:112:ARG:NH1	2.46	0.48
17:a:93:ARG:CZ	17:a:93:ARG:HA	2.44	0.48
21:D:28:GLU:HG2	23:K:58:GLN:HG2	1.95	0.48
36:i:79:VAL:HG23	36:i:90:ASP:C	2.39	0.48
40:k:132:LEU:HB3	40:k:136:ILE:O	2.14	0.48
40:k:353:ILE:HB	40:k:377:ILE:HD11	1.96	0.48
40:k:499:ILE:HB	40:k:515:ALA:HB3	1.96	0.48
1:2:220:A:C6	1:2:840:U:C4	3.02	0.48
1:2:554:A:C5	9:J:19:TYR:CE2	2.99	0.48
1:2:894:G:H22	1:2:916:U:H3	1.62	0.48
4:C:100:ARG:HG2	4:C:100:ARG:NH1	2.26	0.48
6:G:58:LYS:HA	6:G:107:ALA:HB2	1.94	0.48
7:H:109:THR:OG1	7:H:110:GLN:N	2.46	0.48
7:H:143:LEU:HB2	7:H:147:ASN:OD1	2.13	0.48
26:Q:25:GLY:HA3	26:Q:64:ASP:HB3	1.96	0.48
40:k:99:ALA:HA	40:k:188:HIS:CD2	2.49	0.48
1:2:22:A:H2'	1:2:23:G:O4'	2.13	0.47
1:2:680:U:O2'	1:2:682:U:OP1	2.20	0.47
1:2:682:U:C4	1:2:683:C:H1'	2.49	0.47
2:A:11:SER:HA	27:R:115:LEU:HD23	1.94	0.47
5:E:159:THR:CG2	5:E:227:VAL:HB	2.44	0.47
6:G:24:VAL:HG13	6:G:28:TYR:HE1	1.79	0.47
7:H:61:PHE:HB3	7:H:95:GLU:HG2	1.95	0.47
8:I:90:LEU:HB3	8:I:95:THR:HB	1.96	0.47
16:Y:98:GLU:N	16:Y:98:GLU:OE1	2.46	0.47
19:e:10:ARG:HH22	36:i:82:ARG:HA	1.79	0.47
30:U:55:PRO:HA	30:U:91:ILE:HG13	1.96	0.47
40:k:359:ILE:H	40:k:359:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:362:LYS:HE3	40:k:368:ILE:HG22	1.96	0.47
1:2:399:A:H5''	8:I:25:ARG:HA	1.94	0.47
1:2:1227:G:O2'	34:f:100:LEU:HD23	2.14	0.47
1:2:1391:C:H2'	1:2:1392:G:H8	1.78	0.47
1:2:1584:A:H5''	26:Q:136:SER:HB2	1.95	0.47
1:2:1589:C:H2'	1:2:1590:A:C8	2.48	0.47
5:E:66:MET:HG3	5:E:67:GLN:N	2.29	0.47
5:E:159:THR:HG21	5:E:227:VAL:O	2.13	0.47
6:G:191:LYS:O	6:G:195:ILE:HG12	2.14	0.47
27:R:4:VAL:O	27:R:10:LYS:NZ	2.47	0.47
32:c:26:THR:HG23	32:c:44:VAL:HB	1.95	0.47
35:g:267:ILE:HB	35:g:281:LEU:HB2	1.96	0.47
36:i:42:LEU:HD12	36:i:46:ARG:HB3	1.96	0.47
39:j:74:LEU:HD11	39:j:86:SER:HB2	1.95	0.47
1:2:332:A:OP2	8:I:48:THR:OG1	2.33	0.47
1:2:1025:A:N7	1:2:1770:C:O2'	2.43	0.47
1:2:1079:U:H2'	1:2:1080:A:C8	2.49	0.47
1:2:1588:G:H2'	1:2:1589:C:C6	2.50	0.47
6:G:32:ILE:HG23	6:G:53:ALA:HA	1.96	0.47
12:O:22:SER:OG	12:O:24:ASN:O	2.31	0.47
13:V:24:ILE:HD11	13:V:56:SER:HA	1.96	0.47
18:b:49:HIS:HA	18:b:70:LYS:HA	1.95	0.47
21:D:143:ARG:NH2	37:3:38:C:O2	2.39	0.47
28:S:119:ILE:HG23	28:S:121:SER:H	1.78	0.47
35:g:101:GLU:OE1	35:g:101:GLU:N	2.47	0.47
39:j:244:LEU:HD22	39:j:268:PRO:HB3	1.96	0.47
1:2:17:C:H2'	1:2:18:C:H6	1.79	0.47
1:2:194:G:O6	1:2:195:G:O6	2.32	0.47
1:2:997:A:N6	1:2:1003:U:OP2	2.47	0.47
1:2:1169:G:C2	1:2:1170:A:C8	3.02	0.47
7:H:62:VAL:HG12	7:H:64:VAL:H	1.79	0.47
38:1:43:G:O2'	38:1:44:A:OP1	2.30	0.47
39:j:224:ALA:HB1	39:j:226:PRO:HD2	1.95	0.47
40:k:330:ILE:HG12	40:k:333:LEU:HD11	1.95	0.47
1:2:254:U:H2'	1:2:255:A:H8	1.79	0.47
1:2:453:U:O2'	1:2:454:C:O5'	2.32	0.47
1:2:643:U:H2'	1:2:644:C:H6	1.79	0.47
1:2:846:A:H2'	1:2:847:C:C6	2.49	0.47
1:2:885:U:H2'	1:2:886:A:H8	1.80	0.47
1:2:1201:A:HO2'	1:2:1205:U:H3	1.57	0.47
5:E:98:ASN:HD22	5:E:116:ASP:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:30:VAL:HG13	17:a:35:ALA:HB2	1.96	0.47
21:D:72:LEU:HD12	23:K:65:TYR:HD2	1.78	0.47
24:M:21:LEU:HD12	24:M:91:TRP:HH2	1.78	0.47
26:Q:99:GLU:OE2	35:g:61:SER:N	2.46	0.47
28:S:28:VAL:HG23	28:S:56:LYS:O	2.14	0.47
29:T:18:TYR:CD1	29:T:135:ILE:HG21	2.44	0.47
1:2:366:A:H2'	1:2:367:U:O4'	2.15	0.47
8:I:60:ILE:HD12	8:I:61:GLU:H	1.80	0.47
19:e:22:GLU:HA	19:e:22:GLU:OE2	2.15	0.47
25:P:110:GLU:HB2	28:S:119:ILE:HD13	1.96	0.47
29:T:34:VAL:O	29:T:35:ASP:HB3	2.14	0.47
29:T:105:LEU:HD13	29:T:122:ARG:HD2	1.96	0.47
33:d:21:CYS:SG	33:d:23:ILE:HB	2.55	0.47
35:g:19:GLY:HA3	35:g:39:ARG:HB2	1.96	0.47
1:2:155:A:N6	1:2:417:G:N7	2.63	0.47
1:2:206:U:O2	8:I:179:ARG:NH1	2.37	0.47
1:2:574:C:H41	15:X:65:ASN:CG	2.20	0.47
1:2:627:G:N1	1:2:969:A:OP2	2.27	0.47
1:2:863:U:C5	14:W:28:ARG:HD2	2.49	0.47
1:2:1100:G:O2'	14:W:4:THR:OG1	2.30	0.47
1:2:1555:U:O2'	1:2:1556:U:H2'	2.15	0.47
1:2:1610:U:H1'	22:F:101:MET:HE1	1.97	0.47
1:2:1794:C:N4	17:a:93:ARG:HH12	2.13	0.47
2:A:63:ILE:HD12	2:A:158:VAL:HG11	1.96	0.47
2:A:190:ASP:OD2	2:A:192:THR:OG1	2.32	0.47
3:B:227:SER:HA	3:B:230:SER:HB3	1.96	0.47
8:I:154:GLU:OE1	8:I:157:VAL:HG13	2.14	0.47
16:Y:18:LEU:HD13	16:Y:20:ARG:CZ	2.44	0.47
16:Y:18:LEU:HA	16:Y:85:PHE:HE2	1.80	0.47
22:F:43:LYS:HD3	22:F:47:LYS:C	2.40	0.47
29:T:28:LEU:H	29:T:111:LEU:HD21	1.78	0.47
35:g:149:THR:N	35:g:180:ASP:OD2	2.48	0.47
38:l:57:G:O6	39:j:172:TYR:OH	2.31	0.47
39:j:42:ILE:HG22	39:j:83:ILE:HD11	1.97	0.47
39:j:190:VAL:HB	39:j:226:PRO:HA	1.97	0.47
40:k:432:ILE:CG2	40:k:515:ALA:HB1	2.45	0.47
40:k:503:ARG:HD2	40:k:512:ILE:HD13	1.97	0.47
1:2:227:G:H2'	1:2:228:U:C6	2.50	0.47
1:2:841:C:H2'	1:2:842:U:C6	2.49	0.47
1:2:854:A:O2'	1:2:855:A:H3'	2.15	0.47
1:2:1043:U:H2'	1:2:1044:C:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1200:G:N7	1:2:1593:U:H2'	2.30	0.47
2:A:22:VAL:HG13	2:A:162:CYS:HB2	1.97	0.47
13:V:85:TYR:CD1	18:b:6:ASP:HB2	2.49	0.47
16:Y:35:VAL:HG11	16:Y:40:LEU:HD13	1.96	0.47
22:F:93:GLU:O	22:F:96:THR:OG1	2.29	0.47
24:M:124:ARG:HH11	24:M:128:LEU:HD21	1.79	0.47
31:Z:54:ALA:HB3	31:Z:55:PRO:HD3	1.97	0.47
31:Z:91:PRO:HB3	31:Z:101:TYR:HE1	1.80	0.47
1:2:565:C:P	36:i:62:ARG:HH12	2.33	0.47
1:2:1074:C:O2'	17:a:13:LYS:O	2.25	0.47
1:2:1588:G:OP1	29:T:91:HIS:HB2	2.15	0.47
1:2:1679:A:O2'	6:G:31:ARG:NH1	2.48	0.47
5:E:173:ILE:HD11	5:E:235:TRP:CD2	2.49	0.47
14:W:30:SER:OG	14:W:58:SER:O	2.31	0.47
17:a:11:ASN:O	17:a:11:ASN:ND2	2.48	0.47
20:h:17:ARG:HH11	20:h:21:ARG:HD3	1.80	0.47
22:F:92:VAL:O	22:F:96:THR:HG23	2.14	0.47
36:i:29:LYS:HB2	36:i:33:GLN:O	2.15	0.47
40:k:184:LYS:HD3	40:k:185:LEU:N	2.30	0.47
40:k:260:LEU:O	40:k:264:LYS:HG2	2.14	0.47
40:k:422:HIS:ND1	40:k:424:PRO:HD3	2.30	0.47
1:2:57:G:C4	1:2:91:G:N2	2.83	0.47
1:2:328:G:H2'	1:2:329:G:C8	2.47	0.47
1:2:1357:G:H2'	1:2:1358:C:H6	1.80	0.47
1:2:1513:A:O2'	1:2:1514:A:OP1	2.33	0.47
1:2:1737:C:H2'	1:2:1738:A:C8	2.50	0.47
1:2:1794:C:O2	17:a:92:ARG:HB3	2.15	0.47
2:A:49:ASN:O	2:A:53:THR:HG23	2.15	0.47
25:P:85:ILE:HD12	25:P:111:MET:HB3	1.96	0.47
29:T:35:ASP:O	29:T:35:ASP:OD1	2.34	0.47
33:d:31:ILE:HB	33:d:38:ILE:O	2.15	0.47
35:g:128:ARG:HD3	35:g:151:TRP:CE3	2.50	0.47
41:l:138:PHE:CZ	41:l:142:LEU:HD21	2.49	0.47
1:2:29:U:H2'	1:2:30:G:C8	2.48	0.46
1:2:176:U:H3'	1:2:177:U:H2'	1.97	0.46
1:2:532:U:H2'	1:2:533:A:H5''	1.97	0.46
1:2:811:A:H62	1:2:857:G:H2'	1.80	0.46
1:2:1101:G:OP1	14:W:76:SER:OG	2.30	0.46
1:2:1647:G:H2'	1:2:1648:U:H6	1.80	0.46
1:2:1773:U:H2'	1:2:1774:A:C8	2.51	0.46
7:H:55:LYS:HD3	7:H:89:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:20:PHE:O	12:O:27:PHE:N	2.37	0.46
31:Z:70:LYS:HG3	31:Z:71:LEU:HD12	1.97	0.46
34:f:118:ARG:HG2	34:f:118:ARG:NH1	2.31	0.46
35:g:308:LEU:HD12	35:g:309:PHE:N	2.30	0.46
38:1:28:A:H2'	38:1:29:G:C8	2.50	0.46
1:2:72:A:H1'	1:2:73:U:C5	2.50	0.46
1:2:861:A:O2'	1:2:962:A:N6	2.48	0.46
1:2:1274:A:O2'	21:D:141:LYS:HD3	2.15	0.46
1:2:1467:A:H2'	1:2:1468:C:C6	2.50	0.46
1:2:1469:A:C8	1:2:1538:G:H1'	2.50	0.46
1:2:1554:A:H1'	1:2:1558:U:OP2	2.15	0.46
2:A:66:ALA:HB2	13:V:37:ALA:HB2	1.96	0.46
3:B:144:ARG:HB2	3:B:208:GLN:CB	2.45	0.46
6:G:10:ASN:HA	6:G:128:THR:HG22	1.96	0.46
11:N:23:PRO:HG2	11:N:26:PHE:HB2	1.95	0.46
12:O:20:PHE:HE1	12:O:86:THR:HA	1.79	0.46
12:O:86:THR:HG23	12:O:90:ARG:HB2	1.98	0.46
21:D:26:THR:HA	21:D:34:TYR:HD2	1.79	0.46
23:K:13:GLN:O	23:K:17:GLN:HG2	2.14	0.46
23:K:20:VAL:O	23:K:21:LEU:HD23	2.16	0.46
39:j:47:LEU:HD12	39:j:48:LEU:N	2.29	0.46
40:k:148:TYR:HD1	40:k:185:LEU:HA	1.80	0.46
1:2:30:G:H2'	1:2:31:C:C6	2.50	0.46
1:2:108:A:H2'	1:2:109:G:H8	1.81	0.46
1:2:554:A:H2'	1:2:555:A:C8	2.51	0.46
1:2:1171:G:H21	29:T:88:VAL:HG21	1.81	0.46
1:2:1511:G:O2'	1:2:1513:A:N3	2.34	0.46
21:D:113:LEU:HD22	21:D:118:ALA:HB2	1.96	0.46
35:g:48:LEU:HA	35:g:56:GLY:HA2	1.97	0.46
35:g:179:MET:HG3	35:g:205:TYR:CD1	2.50	0.46
39:j:211:MET:HE2	39:j:211:MET:O	2.15	0.46
1:2:277:U:H4'	1:2:278:G:O5'	2.14	0.46
1:2:638:U:H2'	7:H:101:LYS:CE	2.45	0.46
1:2:916:U:O2	12:O:41:ARG:HD2	2.15	0.46
1:2:1106:G:O2'	1:2:1107:G:H5'	2.16	0.46
1:2:1637:5MC:N4	37:3:31:C:OP2	2.49	0.46
4:C:179:ARG:O	9:J:53:ARG:NH2	2.45	0.46
8:I:107:THR:O	8:I:110:ARG:N	2.49	0.46
17:a:41:ILE:HG12	17:a:68:TYR:CD2	2.50	0.46
18:b:20:LYS:HG2	18:b:21:LEU:N	2.30	0.46
1:2:181:A:H2'	1:2:182:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:197:A:C5	1:2:198:G:H1'	2.50	0.46
1:2:387:G:O3'	1:2:424:A:N6	2.49	0.46
1:2:391:G:OP1	1:2:1727:C:O2'	2.30	0.46
1:2:891:A:H2'	1:2:892:U:H6	1.80	0.46
1:2:1143:U:H2'	1:2:1144:U:H6	1.79	0.46
1:2:1319:U:H3'	2:A:101:ARG:HH21	1.81	0.46
1:2:1411:U:O2'	1:2:1414:G:OP1	2.23	0.46
1:2:1639:C:H2'	1:2:1640:G:C8	2.49	0.46
1:2:1651:C:H2'	1:2:1652:G:O4'	2.16	0.46
1:2:1691:A:H3'	1:2:1692:A:H4'	1.97	0.46
7:H:113:PRO:HG2	7:H:116:ARG:HG3	1.96	0.46
14:W:115:GLU:O	14:W:119:LYS:HG2	2.16	0.46
17:a:37:LYS:HB2	17:a:37:LYS:HE2	1.62	0.46
22:F:151:VAL:HG21	32:c:66:LEU:HD22	1.96	0.46
25:P:31:GLU:OE1	25:P:31:GLU:N	2.46	0.46
31:Z:55:PRO:C	31:Z:57:TYR:H	2.24	0.46
35:g:134:VAL:O	35:g:142:ALA:N	2.43	0.46
35:g:172:ILE:HB	35:g:188:LEU:HB2	1.98	0.46
39:j:251:ILE:O	39:j:255:ILE:HG12	2.15	0.46
1:2:169:U:OP1	1:2:266:U:O2'	2.27	0.46
1:2:224:A:C6	1:2:836:G:N1	2.84	0.46
1:2:1564:U:H2'	1:2:1565:U:C5	2.50	0.46
3:B:35:PRO:HA	3:B:232:HIS:CE1	2.51	0.46
5:E:64:ILE:HD12	16:Y:17:LEU:HD22	1.97	0.46
7:H:77:LEU:HD22	7:H:92:PHE:CZ	2.45	0.46
8:I:6:ASP:OD1	8:I:8:ARG:N	2.49	0.46
16:Y:62:THR:HG22	16:Y:69:SER:HB2	1.97	0.46
31:Z:55:PRO:O	31:Z:56:THR:OG1	2.29	0.46
35:g:23:SER:OG	35:g:71:ASP:HA	2.16	0.46
37:3:33:C:H2'	37:3:34:U:C5	2.51	0.46
39:j:44:GLY:HA3	39:j:83:ILE:HB	1.98	0.46
1:2:223:C:C2'	1:2:224:A:H5'	2.46	0.46
1:2:255:A:H2'	1:2:256:A:O4'	2.16	0.46
1:2:1061:A:H2'	1:2:1062:U:O4'	2.15	0.46
1:2:1349:G:OP1	26:Q:68:LYS:NZ	2.49	0.46
1:2:1471:U:H1'	22:F:105:ASN:HD22	1.81	0.46
1:2:1513:A:O3'	30:U:88:LYS:NZ	2.49	0.46
2:A:72:ASP:OD2	4:C:45:LYS:NZ	2.49	0.46
2:A:120:LEU:HD21	2:A:144:ILE:HD12	1.97	0.46
3:B:188:LEU:HD21	3:B:215:VAL:HG21	1.97	0.46
4:C:162:LYS:HD2	14:W:95:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:36:THR:HA	8:I:58:LEU:HA	1.98	0.46
8:I:40:THR:OG1	8:I:59:ARG:HD3	2.14	0.46
22:F:44:LEU:HD13	22:F:50:PHE:HZ	1.81	0.46
35:g:304:ASP:OD1	35:g:305:GLY:N	2.49	0.46
38:l:75:C:O2'	40:k:322:ASP:O	2.20	0.46
1:2:453:U:O2'	1:2:454:C:O4'	2.34	0.46
1:2:567:G:H4'	15:X:90:ASP:HA	1.97	0.46
1:2:883:A:H2'	1:2:884:G:C8	2.51	0.46
1:2:1717:A:H2'	1:2:1718:G:O4'	2.16	0.46
1:2:1771:C:H2'	1:2:1772:G:C8	2.51	0.46
12:O:118:VAL:O	12:O:118:VAL:HG22	2.15	0.46
14:W:24:GLN:HE22	18:b:5:GLN:N	2.14	0.46
16:Y:36:SER:O	16:Y:36:SER:OG	2.29	0.46
25:P:56:LEU:HD12	25:P:60:LEU:HD23	1.98	0.46
27:R:103:ASP:CG	27:R:104:THR:H	2.23	0.46
28:S:100:SER:HB3	28:S:105:LEU:HA	1.98	0.46
29:T:77:ASN:HD21	29:T:98:GLY:CA	2.24	0.46
32:c:42:ARG:HA	32:c:63:ALA:HB2	1.98	0.46
1:2:513:G:HO2'	1:2:514:A:P	2.39	0.46
1:2:1389:A:H2'	1:2:1390:U:H6	1.81	0.46
1:2:1488:A:H2'	1:2:1488:A:OP2	2.16	0.46
2:A:18:LEU:HA	2:A:23:HIS:CD2	2.51	0.46
2:A:167:LYS:HD3	2:A:204:TYR:HB3	1.97	0.46
3:B:97:LEU:HB3	3:B:232:HIS:HD2	1.78	0.46
11:N:46:THR:HG22	11:N:49:GLN:HG3	1.97	0.46
20:h:12:ARG:O	20:h:15:ARG:HB2	2.16	0.46
22:F:89:CYS:SG	22:F:94:ARG:HG3	2.56	0.46
34:f:83:LYS:HB3	34:f:85:TYR:HE1	1.80	0.46
35:g:25:SER:HB3	35:g:74:VAL:HG13	1.98	0.46
36:i:58:MET:C	36:i:58:MET:HE3	2.41	0.46
40:k:92:ALA:O	40:k:96:ASN:ND2	2.48	0.46
1:2:295:U:H2'	1:2:296:U:C6	2.51	0.46
1:2:297:C:H5''	5:E:38:LEU:HD23	1.97	0.46
1:2:319:U:H5''	1:2:320:C:H5''	1.96	0.46
1:2:332:A:H2'	1:2:333:G:C8	2.51	0.46
1:2:621:A:O2'	1:2:1031:G:H5'	2.16	0.46
1:2:700:C:HO2'	1:2:701:U:P	2.39	0.46
1:2:778:G:N2	16:Y:8:ARG:HH22	2.14	0.46
1:2:1349:G:H2'	1:2:1350:G:C8	2.51	0.46
1:2:1350:G:H2'	1:2:1351:U:C6	2.51	0.46
1:2:1646:A:H2'	1:2:1647:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:30:TYR:HD2	3:B:48:VAL:HG21	1.80	0.46
4:C:212:LEU:HD12	4:C:212:LEU:HA	1.69	0.46
5:E:122:LYS:HG2	5:E:123:LEU:N	2.31	0.46
10:L:54:ILE:HG23	10:L:55:ASP:N	2.31	0.46
16:Y:43:LYS:HB3	16:Y:43:LYS:HE3	1.66	0.46
30:U:58:LEU:HB2	30:U:88:LYS:HB2	1.97	0.46
35:g:24:LEU:HD22	35:g:34:LEU:HD11	1.98	0.46
39:j:36:LEU:HG	39:j:39:TYR:H	1.81	0.46
39:j:95:ILE:HG13	39:j:99:GLU:OE2	2.16	0.46
40:k:159:ASP:OD1	41:l:137:ARG:NH2	2.48	0.46
1:2:194:G:C2'	1:2:195:G:H5'	2.46	0.45
1:2:329:G:C6	1:2:330:A:C6	3.04	0.45
1:2:423:C:O2'	1:2:424:A:O5'	2.34	0.45
1:2:646:G:C6	1:2:688:G:C6	3.04	0.45
1:2:1373:U:H2'	1:2:1374:C:H6	1.80	0.45
1:2:1424:C:H3'	1:2:1425:A:H4'	1.97	0.45
1:2:1513:A:O2'	1:2:1515:U:OP2	2.34	0.45
11:N:140:LYS:HB3	11:N:140:LYS:HE2	1.80	0.45
13:V:16:LYS:HA	13:V:23:ILE:HA	1.97	0.45
14:W:34:ILE:O	14:W:38:LEU:HG	2.15	0.45
22:F:102:ASN:OD1	22:F:182:ARG:HD3	2.16	0.45
26:Q:41:PRO:O	26:Q:42:GLU:HG3	2.16	0.45
27:R:20:TYR:CD2	27:R:38:ILE:HD12	2.51	0.45
29:T:11:ALA:O	29:T:14:PHE:N	2.49	0.45
30:U:84:MET:HE3	33:d:52:PHE:CZ	2.51	0.45
1:2:203:G:H2'	1:2:204:U:O4'	2.16	0.45
1:2:379:U:C5	9:J:5:PRO:HB3	2.51	0.45
1:2:445:A:H5''	5:E:57:ASN:HD22	1.81	0.45
1:2:594:G:H2'	1:2:595:C:C6	2.52	0.45
1:2:1405:U:H2'	1:2:1406:G:H8	1.82	0.45
1:2:1622:C:H2'	1:2:1623:C:H6	1.82	0.45
1:2:1637:5MC:H2'	1:2:1638:C:O4'	2.16	0.45
5:E:206:ASP:HB3	5:E:222:LEU:HB2	1.98	0.45
7:H:62:VAL:CG1	7:H:63:PRO:CD	2.94	0.45
7:H:130:VAL:HB	7:H:169:PHE:CE2	2.51	0.45
9:J:134:ILE:HG23	9:J:156:ILE:HG23	1.97	0.45
12:O:61:MET:O	12:O:65:GLN:HG3	2.16	0.45
17:a:23:CYS:SG	17:a:74:CYS:N	2.89	0.45
29:T:112:GLY:O	29:T:125:SER:OG	2.27	0.45
35:g:71:ASP:OD1	35:g:72:VAL:N	2.48	0.45
39:j:123:LEU:HD22	39:j:127:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:136:ILE:HG21	40:k:197:HIS:HB2	1.97	0.45
1:2:5:U:H2'	1:2:6:G:C8	2.52	0.45
1:2:97:C:O2	1:2:424:A:O2'	2.34	0.45
1:2:107:C:H2'	1:2:108:A:C8	2.52	0.45
1:2:748:U:OP1	14:W:82:LYS:NZ	2.50	0.45
1:2:790:A:H2'	1:2:791:U:C6	2.52	0.45
1:2:1380:A:H1'	30:U:57:ARG:HG2	1.98	0.45
7:H:140:VAL:HG22	7:H:150:GLN:HG3	1.97	0.45
9:J:145:SER:O	9:J:145:SER:OG	2.31	0.45
12:O:47:LYS:NZ	12:O:66:ASP:OD2	2.49	0.45
12:O:51:ASP:OD1	12:O:51:ASP:O	2.35	0.45
26:Q:43:ILE:HG23	26:Q:44:LEU:HD23	1.99	0.45
28:S:3:LEU:HD22	31:Z:82:HIS:CD2	2.51	0.45
40:k:103:ILE:HG12	40:k:213:ALA:HB3	1.98	0.45
1:2:565:C:OP1	36:i:63:GLY:HA3	2.17	0.45
1:2:917:U:O3'	12:O:18:ARG:NH1	2.49	0.45
1:2:1366:G:C2	1:2:1367:G:C8	3.05	0.45
1:2:1741:U:H2'	1:2:1742:A:H8	1.78	0.45
1:2:1753:A:P	15:X:63:GLN:HE21	2.39	0.45
15:X:141:GLU:N	15:X:141:GLU:OE1	2.50	0.45
21:D:76:ARG:HD2	23:K:63:TYR:HD2	1.82	0.45
26:Q:50:GLU:OE2	26:Q:112:TYR:OH	2.25	0.45
1:2:67:A:C6	1:2:84:A:C8	3.04	0.45
1:2:80:A:H5''	1:2:81:G:C8	2.51	0.45
6:G:121:ILE:HG22	6:G:122:GLU:H	1.82	0.45
8:I:160:GLN:O	8:I:164:GLY:N	2.47	0.45
12:O:58:TYR:CZ	12:O:62:LEU:HD21	2.51	0.45
24:M:24:VAL:O	24:M:27:THR:HG22	2.16	0.45
29:T:117:SER:OG	29:T:120:GLY:O	2.34	0.45
36:i:102:THR:O	36:i:106:GLN:HG2	2.17	0.45
39:j:24:VAL:HB	39:j:65:VAL:HA	1.97	0.45
1:2:86:A:H2'	1:2:87:C:H6	1.82	0.45
1:2:147:U:H3	6:G:132:ARG:NH2	2.14	0.45
1:2:748:U:O2'	14:W:122:SER:O	2.25	0.45
1:2:1017:U:N3	1:2:1018:A:N7	2.64	0.45
1:2:1141:A:H5''	17:a:2:PRO:HB3	1.99	0.45
1:2:1469:A:H2'	1:2:1469:A:N3	2.32	0.45
1:2:1481:A:H4'	26:Q:71:GLY:HA2	1.99	0.45
1:2:1532:G:N7	31:Z:77:ARG:NH1	2.49	0.45
1:2:1577:U:H2'	1:2:1578:C:H6	1.81	0.45
4:C:40:TRP:CD1	4:C:72:GLN:NE2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ARG:NH2	5:E:122:LYS:HA	2.32	0.45
16:Y:81:ASP:HA	16:Y:84:LYS:HG2	1.99	0.45
24:M:34:LEU:HB3	24:M:36:ARG:HG3	1.98	0.45
24:M:57:GLU:CD	24:M:57:GLU:H	2.24	0.45
26:Q:92:TYR:CE1	26:Q:96:PHE:HD2	2.35	0.45
40:k:493:THR:HA	40:k:497:GLU:OE1	2.15	0.45
1:2:6:G:C6	4:C:210:ARG:NH2	2.84	0.45
1:2:155:A:H2'	1:2:156:A:O4'	2.16	0.45
1:2:510:A:H5'	9:J:173:ALA:HB2	1.98	0.45
1:2:824:U:H2'	1:2:825:U:H6	1.82	0.45
1:2:1247:C:C2	1:2:1248:U:C5	3.04	0.45
1:2:1481:A:H2'	1:2:1482:G:C8	2.52	0.45
1:2:1689:A:N6	1:2:1708:U:O2'	2.49	0.45
5:E:147:ILE:HG21	5:E:169:ILE:HG13	1.99	0.45
8:I:41:LYS:N	8:I:61:GLU:OE2	2.50	0.45
9:J:16:LYS:O	9:J:18:PRO:HD3	2.17	0.45
10:L:52:SER:O	10:L:52:SER:OG	2.33	0.45
10:L:99:ARG:HH21	14:W:79:PHE:HZ	1.64	0.45
12:O:80:HIS:ND1	12:O:114:ARG:HB2	2.31	0.45
22:F:52:ASP:OD1	22:F:52:ASP:O	2.34	0.45
24:M:71:LEU:CD1	24:M:71:LEU:N	2.80	0.45
36:i:109:LEU:HD23	36:i:109:LEU:H	1.82	0.45
40:k:247:LEU:HD23	40:k:281:VAL:HB	1.98	0.45
1:2:251:U:H2'	1:2:252:A:H8	1.82	0.45
1:2:829:U:H2'	1:2:830:U:O4'	2.17	0.45
1:2:1182:A:C5	25:P:100:LYS:HD2	2.52	0.45
2:A:71:GLU:OE1	2:A:71:GLU:N	2.50	0.45
2:A:108:THR:HG23	2:A:135:GLU:OE1	2.17	0.45
2:A:207:PRO:O	2:A:210:ILE:HG22	2.16	0.45
4:C:121:LYS:HG2	4:C:132:ALA:CB	2.46	0.45
7:H:27:LEU:HD13	7:H:34:LEU:HD13	1.97	0.45
8:I:196:ARG:O	8:I:200:LYS:HG2	2.17	0.45
14:W:57:ARG:C	14:W:59:GLY:H	2.25	0.45
21:D:168:ILE:HA	21:D:188:ILE:O	2.17	0.45
22:F:194:GLU:OE2	31:Z:59:TYR:OH	2.27	0.45
25:P:15:TYR:HD1	25:P:16:SER:N	2.14	0.45
32:c:9:LEU:HD12	32:c:33:LEU:HD12	1.99	0.45
32:c:10:ALA:HB1	32:c:30:VAL:HB	1.99	0.45
35:g:269:ILE:HG22	35:g:279:ASP:O	2.17	0.45
39:j:23:ASN:H	39:j:37:LEU:HD13	1.82	0.45
39:j:160:PRO:HG3	39:j:166:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:182:U:H2'	1:2:183:C:C6	2.52	0.45
1:2:195:G:O2'	1:2:196:A:H8	2.00	0.45
1:2:445:A:H2'	1:2:446:U:C6	2.52	0.45
1:2:1040:G:OP2	2:A:32:HIS:HE1	2.00	0.45
1:2:1486:G:O2'	1:2:1492:C:O2	2.33	0.45
2:A:79:ARG:NH1	2:A:164:ASN:O	2.48	0.45
5:E:79:ASP:OD2	5:E:82:PHE:HB2	2.16	0.45
8:I:3:ILE:O	8:I:30:GLY:N	2.50	0.45
9:J:153:GLU:O	9:J:156:ILE:HD12	2.16	0.45
14:W:6:VAL:HG21	14:W:29:PRO:HB2	1.99	0.45
16:Y:15:ASN:HD22	16:Y:22:GLN:HE21	1.65	0.45
22:F:135:VAL:HG22	22:F:200:LEU:HD13	1.97	0.45
26:Q:44:LEU:O	26:Q:47:LYS:HB2	2.17	0.45
27:R:78:ARG:HA	27:R:78:ARG:HD2	1.72	0.45
29:T:19:ALA:HB2	29:T:56:LYS:HA	1.99	0.45
30:U:56:VAL:O	30:U:89:ARG:HA	2.16	0.45
39:j:248:ILE:HA	39:j:251:ILE:HG12	1.98	0.45
40:k:346:VAL:HG22	40:k:392:PRO:HD3	1.99	0.45
1:2:14:C:H2'	1:2:15:U:C6	2.52	0.45
1:2:53:G:H2'	1:2:54:C:H6	1.81	0.45
1:2:70:C:C4	1:2:71:A:C2	3.05	0.45
1:2:399:A:H4'	1:2:400:A:H5''	1.98	0.45
1:2:860:U:P	11:N:64:LYS:HZ3	2.40	0.45
1:2:978:A:H4'	1:2:1784:G:N2	2.32	0.45
1:2:984:G:C4	1:2:985:G:C8	3.04	0.45
1:2:1243:A:H2'	1:2:1243:A:N3	2.31	0.45
5:E:65:LEU:HD12	5:E:80:THR:HA	1.99	0.45
5:E:103:TYR:O	5:E:182:TYR:OH	2.35	0.45
7:H:46:ILE:H	7:H:46:ILE:HD12	1.81	0.45
18:b:23:THR:HG22	18:b:24:LEU:H	1.81	0.45
23:K:16:PHE:CD1	23:K:16:PHE:C	2.95	0.45
23:K:38:LYS:HB2	23:K:41:PHE:CZ	2.52	0.45
24:M:21:LEU:HB3	24:M:91:TRP:CZ3	2.53	0.45
30:U:57:ARG:HG3	30:U:89:ARG:CD	2.47	0.45
38:1:59:A:O2'	38:1:60:A:O4'	2.34	0.45
39:j:17:ASP:OD1	39:j:17:ASP:C	2.60	0.45
39:j:202:LYS:O	39:j:205:LEU:HD12	2.17	0.45
40:k:408:ARG:HG3	40:k:408:ARG:NH1	2.31	0.45
1:2:478:C:O2'	9:J:120:LYS:NZ	2.42	0.44
1:2:1681:U:H2'	1:2:1682:U:O4'	2.16	0.44
3:B:57:ALA:O	3:B:61:LEU:HD22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:99:ASN:OD1	3:B:100:PHE:N	2.49	0.44
4:C:72:GLN:H	4:C:72:GLN:CD	2.22	0.44
16:Y:108:ARG:HG2	16:Y:111:ARG:HH22	1.83	0.44
23:K:16:PHE:C	23:K:16:PHE:HD1	2.25	0.44
27:R:93:LEU:HD21	27:R:100:LEU:HG	1.99	0.44
40:k:380:LEU:HD21	40:k:396:ILE:HD13	1.99	0.44
1:2:67:A:O2'	1:2:69:G:OP1	2.32	0.44
1:2:140:A:H61	6:G:187:LYS:HB2	1.82	0.44
1:2:387:G:C6	1:2:409:A:C6	3.06	0.44
1:2:406:A:H1'	1:2:1669:A:H2	1.81	0.44
1:2:446:U:H2'	1:2:447:C:O4'	2.17	0.44
1:2:891:A:H2'	1:2:892:U:C6	2.52	0.44
1:2:1447:U:H2'	1:2:1448:U:C6	2.51	0.44
1:2:1527:C:H2'	1:2:1528:C:C6	2.53	0.44
7:H:101:LYS:N	7:H:101:LYS:CD	2.81	0.44
7:H:101:LYS:H	7:H:101:LYS:CD	2.30	0.44
8:I:41:LYS:HA	8:I:59:ARG:O	2.17	0.44
10:L:14:GLN:CG	10:L:54:ILE:HG21	2.48	0.44
14:W:46:TYR:O	14:W:69:LEU:HB2	2.16	0.44
15:X:92:CYS:HG	15:X:136:TRP:CD1	2.35	0.44
23:K:34:GLU:N	23:K:34:GLU:OE2	2.50	0.44
24:M:87:GLN:O	24:M:91:TRP:CD1	2.70	0.44
40:k:234:ALA:O	40:k:238:ILE:HG12	2.18	0.44
40:k:238:ILE:HG23	40:k:514:TRP:HB3	1.99	0.44
1:2:329:G:H2'	1:2:330:A:C8	2.53	0.44
1:2:373:U:H2'	1:2:374:U:C6	2.52	0.44
1:2:1146:A:H2'	1:2:1147:C:H6	1.81	0.44
1:2:1472:G:C2	1:2:1473:A:C5	3.06	0.44
1:2:1646:A:H2'	1:2:1647:G:H8	1.82	0.44
1:2:1660:G:H2'	1:2:1661:G:C8	2.51	0.44
1:2:1676:A:H2'	1:2:1677:G:O4'	2.18	0.44
10:L:46:LYS:O	10:L:49:ILE:HG22	2.17	0.44
17:a:23:CYS:HB3	17:a:27:SER:N	2.33	0.44
23:K:11:ILE:HD13	23:K:11:ILE:HA	1.81	0.44
24:M:55:LEU:HD21	24:M:81:LYS:HZ3	1.82	0.44
27:R:102:VAL:HB	27:R:106:THR:CG2	2.47	0.44
38:1:7:G:OP1	38:1:14:A:N6	2.37	0.44
39:j:222:LEU:HD21	40:k:324:ASN:HB3	1.98	0.44
1:2:139:C:OP2	6:G:187:LYS:NZ	2.48	0.44
1:2:178:A:H2'	1:2:179:A:O4'	2.18	0.44
1:2:573:G:O6	15:X:65:ASN:ND2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:818:G:C4	1:2:852:G:N2	2.86	0.44
3:B:122:GLU:OE1	3:B:124:ASN:HB2	2.17	0.44
8:I:72:VAL:HG11	8:I:112:TRP:CZ2	2.53	0.44
11:N:102:LEU:HD21	11:N:112:LYS:HA	1.98	0.44
26:Q:29:ILE:HG13	26:Q:65:ILE:HB	1.98	0.44
26:Q:35:PRO:HG2	26:Q:38:LEU:HD23	2.00	0.44
28:S:111:ASP:HA	28:S:114:GLU:HG3	2.00	0.44
29:T:2:PRO:HB2	29:T:3:GLY:H	1.69	0.44
29:T:28:LEU:HD12	29:T:107:SER:HB3	1.98	0.44
39:j:119:PHE:CE2	39:j:165:VAL:HA	2.53	0.44
1:2:26:A:HO2'	1:2:27:U:P	2.40	0.44
1:2:152:G:C6	1:2:161:A:C6	3.06	0.44
1:2:194:G:H2'	1:2:195:G:H5'	2.00	0.44
1:2:253:A:H2'	1:2:254:U:H6	1.83	0.44
1:2:385:G:OP1	8:I:23:LYS:HG2	2.16	0.44
1:2:393:C:H2'	1:2:394:U:C6	2.52	0.44
1:2:779:A:O3'	1:2:781:A:N6	2.50	0.44
1:2:803:A:N3	14:W:105:THR:OG1	2.49	0.44
1:2:860:U:H2'	1:2:861:A:O4'	2.17	0.44
1:2:1050:G:H3'	1:2:1051:U:H4'	1.99	0.44
1:2:1343:A:H2'	1:2:1344:A:C8	2.52	0.44
1:2:1437:C:H2'	1:2:1438:C:H6	1.83	0.44
9:J:123:HIS:CE1	19:e:37:ARG:HB2	2.53	0.44
10:L:35:TYR:CZ	10:L:49:ILE:HD11	2.53	0.44
17:a:10:ARG:HB3	17:a:10:ARG:NH1	2.32	0.44
23:K:3:ILE:HG12	23:K:41:PHE:HB2	1.98	0.44
23:K:10:LYS:HA	23:K:13:GLN:HG3	1.98	0.44
23:K:38:LYS:O	23:K:42:VAL:HG23	2.18	0.44
23:K:59:PHE:CE1	23:K:62:GLN:HA	2.52	0.44
23:K:61:TRP:N	23:K:61:TRP:CD1	2.86	0.44
27:R:41:ILE:HG23	27:R:46:LEU:HD23	1.99	0.44
29:T:113:VAL:HG23	29:T:114:VAL:HG23	2.00	0.44
1:2:23:G:N2	1:2:366:A:O2'	2.50	0.44
1:2:121:U:H1'	5:E:33:ALA:O	2.18	0.44
1:2:846:A:O2'	1:2:847:C:O4'	2.25	0.44
1:2:890:A:H2'	1:2:891:A:C8	2.51	0.44
1:2:1412:U:H5''	27:R:3:ARG:NH2	2.32	0.44
3:B:116:LYS:HB3	3:B:117:TRP:CD1	2.53	0.44
5:E:155:LYS:O	5:E:158:ASP:HB2	2.18	0.44
6:G:1:MET:HE1	6:G:24:VAL:HG21	2.00	0.44
6:G:105:ASP:OD1	6:G:105:ASP:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:25:LYS:HB2	13:V:28:ASP:HB2	1.98	0.44
23:K:16:PHE:HD1	23:K:16:PHE:O	2.00	0.44
28:S:145:ARG:CZ	28:S:145:ARG:HB2	2.47	0.44
36:i:96:ASN:O	36:i:96:ASN:ND2	2.42	0.44
37:3:32:U:H2'	37:3:33:C:C5	2.53	0.44
1:2:405:U:H2'	1:2:406:A:H8	1.82	0.44
1:2:406:A:H2'	1:2:407:C:C6	2.53	0.44
1:2:598:A:H2'	1:2:599:U:C6	2.53	0.44
1:2:692:C:H2'	1:2:693:U:C6	2.52	0.44
1:2:1173:C:OP2	28:S:141:THR:HG21	2.17	0.44
1:2:1337:C:H1'	1:2:1408:A:C5	2.52	0.44
2:A:30:GLN:HE22	2:A:34:GLU:HB2	1.83	0.44
2:A:77:SER:HB2	2:A:86:VAL:HG21	2.00	0.44
21:D:136:VAL:HG22	21:D:186:VAL:HG22	2.00	0.44
23:K:6:GLU:O	23:K:10:LYS:HG3	2.18	0.44
24:M:88:LEU:O	24:M:92:ALA:HB2	2.18	0.44
32:c:52:ASP:C	32:c:53:ILE:HD12	2.42	0.44
35:g:115:ALA:N	35:g:124:ILE:O	2.39	0.44
35:g:243:ALA:O	35:g:244:LYS:HG2	2.17	0.44
39:j:208:ALA:HA	39:j:250:LYS:NZ	2.33	0.44
1:2:472:A:H2'	1:2:473:A:O4'	2.17	0.44
1:2:933:C:C4	1:2:1076:C:H4'	2.52	0.44
1:2:1480:C:H5	1:2:1523:A:H62	1.65	0.44
2:A:56:LYS:HA	2:A:56:LYS:HD2	1.69	0.44
3:B:58:SER:HA	3:B:61:LEU:HD23	1.99	0.44
5:E:136:ILE:HG21	5:E:148:ARG:NH1	2.32	0.44
8:I:64:ASN:OD1	8:I:65:PHE:N	2.51	0.44
10:L:125:VAL:HG22	10:L:137:PHE:HB3	2.00	0.44
11:N:54:LEU:HB3	11:N:60:VAL:HB	1.99	0.44
16:Y:91:LEU:HD13	16:Y:96:LEU:HB2	1.98	0.44
26:Q:63:ILE:HD12	26:Q:92:TYR:CE2	2.40	0.44
27:R:21:TYR:CE2	27:R:61:ILE:HG21	2.53	0.44
37:3:22:U:H2'	37:3:23:A:C4	2.53	0.44
1:2:131:C:H4'	1:2:132:U:H4'	1.99	0.44
1:2:234:G:H2'	1:2:235:A:H8	1.77	0.44
1:2:444:A:N6	1:2:461:G:H1'	2.33	0.44
1:2:592:U:OP1	9:J:40:ARG:HB2	2.18	0.44
1:2:842:U:H2'	1:2:843:A:C8	2.52	0.44
1:2:884:G:H2'	1:2:885:U:C6	2.53	0.44
2:A:198:MET:HE1	27:R:89:SER:HA	1.99	0.44
3:B:195:LYS:HD2	3:B:195:LYS:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:95:LYS:HD2	26:Q:95:LYS:HA	1.82	0.44
35:g:149:THR:OG1	35:g:180:ASP:OD1	2.32	0.44
35:g:258:TRP:O	35:g:259:LEU:HD23	2.18	0.44
1:2:235:A:H2'	1:2:236:C:O4'	2.18	0.43
1:2:337:C:H5''	8:I:10:LYS:HG3	2.00	0.43
1:2:405:U:H2'	1:2:406:A:C8	2.53	0.43
1:2:793:U:H4'	1:2:794:U:OP2	2.18	0.43
1:2:947:G:H2'	1:2:948:C:C6	2.53	0.43
1:2:1795:A:N6	17:a:84:VAL:HG22	2.33	0.43
3:B:32:ILE:HD12	3:B:96:LEU:HD11	2.00	0.43
9:J:101:VAL:HG22	9:J:105:LEU:HD23	2.00	0.43
9:J:134:ILE:HD12	9:J:134:ILE:N	2.33	0.43
12:O:20:PHE:HB3	12:O:27:PHE:HB2	2.00	0.43
21:D:13:ALA:HA	21:D:16:VAL:HG12	2.00	0.43
21:D:64:ARG:O	21:D:67:ASN:HB2	2.17	0.43
22:F:93:GLU:O	22:F:97:ASN:ND2	2.51	0.43
33:d:23:ILE:HD13	33:d:23:ILE:HA	1.81	0.43
39:j:254:VAL:HG13	39:j:258:TYR:HE2	1.82	0.43
40:k:217:LEU:HD23	40:k:247:LEU:HB2	1.99	0.43
1:2:220:A:H2'	1:2:221:A:H8	1.83	0.43
1:2:345:G:OP1	10:L:79:ARG:NH1	2.47	0.43
1:2:589:C:H2'	1:2:590:A:H8	1.82	0.43
1:2:1261:U:H2'	1:2:1262:G:C8	2.54	0.43
5:E:19:MET:SD	5:E:108:ARG:HD2	2.59	0.43
5:E:176:ASP:OD1	5:E:176:ASP:C	2.60	0.43
5:E:241:GLY:O	5:E:244:ILE:HG12	2.18	0.43
12:O:87:GLY:HA3	12:O:120:PRO:HD2	2.00	0.43
24:M:60:THR:C	24:M:62:GLU:H	2.26	0.43
30:U:65:ILE:HD11	33:d:34:TYR:HE2	1.83	0.43
35:g:213:PRO:HD3	35:g:252:PHE:HB3	1.99	0.43
35:g:214:ASP:OD1	35:g:215:GLY:N	2.51	0.43
35:g:243:ALA:O	35:g:268:LYS:NZ	2.52	0.43
40:k:220:GLY:HA2	40:k:262:HIS:CE1	2.53	0.43
1:2:513:G:C2	1:2:514:A:C8	3.07	0.43
1:2:806:A:H2'	1:2:807:U:H6	1.84	0.43
1:2:1059:U:H3'	1:2:1060:U:O2	2.18	0.43
1:2:1070:U:H2'	1:2:1071:C:C6	2.54	0.43
1:2:1198:G:H1	33:d:31:ILE:CD1	2.31	0.43
1:2:1648:U:H2'	1:2:1649:A:H8	1.81	0.43
2:A:38:TYR:OH	27:R:108:GLU:HB2	2.19	0.43
2:A:177:LEU:O	2:A:181:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:ASP:OD1	5:E:122:LYS:NZ	2.35	0.43
5:E:233:ARG:HD2	5:E:233:ARG:HA	1.90	0.43
20:h:1:MET:HE2	20:h:1:MET:HB3	1.93	0.43
27:R:67:ARG:H	27:R:67:ARG:HG2	1.64	0.43
32:c:67:ARG:HG2	37:3:24:U:C5	2.53	0.43
36:i:82:ARG:NH1	36:i:90:ASP:OD1	2.51	0.43
40:k:426:ILE:HD11	40:k:523:LEU:HB3	2.00	0.43
1:2:31:C:OP1	15:X:140:LYS:NZ	2.39	0.43
1:2:1021:C:O2'	1:2:1124:A:N1	2.46	0.43
1:2:1266:G:O2'	1:2:1446:G:O2'	2.25	0.43
1:2:1785:C:H2'	1:2:1786:G:C8	2.53	0.43
2:A:39:LYS:HD2	2:A:39:LYS:HA	1.66	0.43
5:E:11:ARG:HA	5:E:28:ALA:HB2	1.99	0.43
5:E:49:ARG:NE	5:E:50:ASN:OD1	2.37	0.43
7:H:26:ASP:O	7:H:29:ASN:HB2	2.18	0.43
9:J:29:LYS:HD2	19:e:40:TYR:HE1	1.83	0.43
14:W:77:PRO:HB2	14:W:79:PHE:CE1	2.53	0.43
15:X:107:PHE:HB2	15:X:121:ARG:O	2.18	0.43
22:F:72:VAL:HG21	26:Q:47:LYS:HG2	2.01	0.43
29:T:58:ALA:HB1	29:T:108:LEU:HD11	2.01	0.43
31:Z:66:VAL:HG12	31:Z:71:LEU:O	2.18	0.43
1:2:225:A:O2'	1:2:226:U:O4'	2.27	0.43
1:2:867:G:H2'	1:2:868:A:H8	1.83	0.43
1:2:938:A:P	11:N:114:ARG:HH22	2.42	0.43
1:2:953:G:C4	1:2:954:A:C8	3.07	0.43
1:2:1668:G:O2'	1:2:1729:A:N6	2.46	0.43
3:B:48:VAL:CG2	3:B:61:LEU:HD11	2.49	0.43
7:H:62:VAL:HG12	7:H:63:PRO:CD	2.48	0.43
9:J:81:VAL:HG11	9:J:91:LYS:HE3	2.01	0.43
22:F:186:PHE:CD2	22:F:187:ARG:HG2	2.53	0.43
28:S:91:ASP:O	28:S:93:ASN:N	2.48	0.43
40:k:463:MET:HE3	40:k:509:TRP:CG	2.54	0.43
1:2:608:U:O2'	15:X:23:ARG:HD3	2.19	0.43
1:2:871:G:H2'	1:2:872:U:O4'	2.19	0.43
1:2:1171:G:H2'	1:2:1172:C:O4'	2.19	0.43
1:2:1218:A:O2'	23:K:48:SER:HA	2.19	0.43
1:2:1239:U:H2'	1:2:1241:A:OP2	2.18	0.43
1:2:1563:C:H2'	1:2:1564:U:C6	2.53	0.43
7:H:63:PRO:HB2	7:H:65:PRO:CD	2.45	0.43
9:J:128:LEU:HB3	9:J:134:ILE:HD11	2.01	0.43
15:X:107:PHE:CE2	15:X:114:LYS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:138:ILE:HD13	21:D:184:ILE:HG12	2.01	0.43
22:F:83:ARG:HG2	22:F:84:PHE:CD2	2.53	0.43
22:F:158:ARG:HE	22:F:158:ARG:HB3	1.59	0.43
25:P:24:LYS:O	25:P:28:MET:HB3	2.19	0.43
25:P:34:VAL:HG22	25:P:45:PHE:CD2	2.49	0.43
31:Z:71:LEU:HD23	31:Z:76:ALA:HA	1.99	0.43
35:g:35:VAL:HG12	35:g:72:VAL:HG11	2.00	0.43
39:j:118:LYS:HE3	39:j:118:LYS:HB2	1.85	0.43
1:2:345:G:P	10:L:79:ARG:HH12	2.41	0.43
1:2:650:G:O6	1:2:684:A:N6	2.51	0.43
1:2:760:A:C2	1:2:789:U:C5	3.07	0.43
1:2:789:U:C5	1:2:790:A:C8	3.06	0.43
1:2:886:A:H5''	12:O:120:PRO:HB3	2.01	0.43
1:2:998:PSU:OP1	39:j:54:ARG:HD2	2.19	0.43
1:2:1191:C:OP1	1:2:1193:A:H5'	2.19	0.43
1:2:1287:G:OP1	1:2:1622:C:O2'	2.37	0.43
1:2:1373:U:H2'	1:2:1374:C:C6	2.54	0.43
8:I:144:TRP:HA	8:I:147:ARG:HD2	2.00	0.43
12:O:28:VAL:HG11	12:O:67:VAL:HG21	2.00	0.43
27:R:102:VAL:HB	27:R:106:THR:HG23	2.00	0.43
33:d:14:PHE:C	33:d:14:PHE:CD1	2.97	0.43
35:g:71:ASP:HB3	35:g:113:SER:HA	2.00	0.43
36:i:27:ILE:H	36:i:27:ILE:HD12	1.84	0.43
40:k:211:MET:HE2	40:k:211:MET:HB2	1.87	0.43
1:2:15:U:H2'	1:2:16:G:O4'	2.19	0.43
1:2:403:G:H2'	1:2:404:C:C6	2.54	0.43
1:2:582:C:C2	1:2:583:C:C5	3.07	0.43
1:2:1477:A:H5''	29:T:60:SER:HB3	2.01	0.43
1:2:1514:A:O2'	1:2:1515:U:H5'	2.18	0.43
1:2:1716:A:H2'	1:2:1717:A:C8	2.54	0.43
5:E:71:LYS:HB3	5:E:91:THR:HB	2.01	0.43
15:X:55:GLU:OE2	15:X:57:ILE:HG22	2.19	0.43
16:Y:104:SER:OG	16:Y:107:GLN:HG2	2.17	0.43
21:D:218:LEU:HD12	21:D:218:LEU:HA	1.87	0.43
22:F:100:MET:HE2	22:F:106:ASN:O	2.19	0.43
40:k:108:HIS:CD2	40:k:109:VAL:H	2.36	0.43
40:k:150:CYS:HB3	40:k:155:CYS:SG	2.58	0.43
1:2:175:C:N4	1:2:265:A:OP2	2.51	0.43
1:2:305:U:OP1	10:L:105:LYS:HG3	2.18	0.43
1:2:365:A:OP1	1:2:758:U:O2'	2.33	0.43
1:2:583:C:C2	1:2:584:A:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:985:G:H2'	1:2:985:G:N3	2.33	0.43
1:2:1477:A:C2	1:2:1478:G:C8	3.06	0.43
3:B:91:VAL:HG22	3:B:96:LEU:HB3	2.01	0.43
12:O:26:THR:HG21	12:O:97:GLY:HA3	2.01	0.43
15:X:9:LEU:HD23	15:X:9:LEU:HA	1.84	0.43
24:M:21:LEU:HB3	24:M:91:TRP:CH2	2.54	0.43
28:S:116:LEU:HA	28:S:119:ILE:HG22	1.99	0.43
32:c:35:ASP:O	32:c:37:THR:N	2.52	0.43
36:i:27:ILE:HD13	36:i:93:HIS:HD2	1.84	0.43
39:j:251:ILE:HG13	39:j:252:THR:N	2.33	0.43
40:k:242:LYS:HD3	40:k:274:ILE:HG22	2.01	0.43
40:k:471:THR:HB	40:k:487:LEU:HD22	2.01	0.43
1:2:303:U:H2'	1:2:304:C:C6	2.54	0.43
1:2:340:A:H2'	1:2:341:C:C6	2.54	0.43
1:2:870:G:H2'	1:2:871:G:C8	2.54	0.43
1:2:882:C:H2'	1:2:883:A:C8	2.53	0.43
1:2:1713:G:H2'	1:2:1714:C:C6	2.54	0.43
1:2:1791:G:H4'	1:2:1792:A:OP1	2.18	0.43
6:G:49:VAL:O	6:G:113:ILE:HD12	2.19	0.43
10:L:33:ARG:NH2	10:L:53:TYR:O	2.43	0.43
10:L:122:ILE:HG12	10:L:144:SER:HB3	2.01	0.43
17:a:23:CYS:HB2	17:a:74:CYS:HB2	2.01	0.43
22:F:91:ILE:HD11	22:F:139:ILE:HD13	2.01	0.43
29:T:42:GLY:HA2	29:T:84:LYS:HB2	2.00	0.43
32:c:13:ILE:HD12	32:c:13:ILE:HA	1.86	0.43
40:k:230:SER:HB3	40:k:269:PHE:HZ	1.83	0.43
1:2:30:G:H2'	1:2:31:C:H6	1.84	0.42
1:2:760:A:C6	1:2:789:U:O4	2.72	0.42
1:2:811:A:N6	1:2:857:G:H2'	2.34	0.42
1:2:1203:A:H61	33:d:15:GLY:HA3	1.83	0.42
1:2:1403:G:H2'	1:2:1404:A:C8	2.53	0.42
1:2:1568:A:H2'	1:2:1569:C:O4'	2.19	0.42
1:2:1682:U:C2	1:2:1715:G:O6	2.72	0.42
1:2:1711:G:N3	1:2:1711:G:H2'	2.34	0.42
1:2:1768:U:H2'	1:2:1769:U:C6	2.53	0.42
4:C:219:ALA:O	4:C:223:ILE:HG22	2.19	0.42
5:E:45:ILE:HA	5:E:61:VAL:HG11	2.01	0.42
5:E:120:SER:O	5:E:164:LEU:HB3	2.18	0.42
13:V:53:TYR:HE2	13:V:72:LEU:HB3	1.84	0.42
21:D:74:GLU:HA	21:D:79:TYR:HB2	2.01	0.42
29:T:52:GLY:HA2	29:T:55:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:68:ARG:HB2	31:Z:70:LYS:HE2	2.01	0.42
35:g:231:ASN:HB3	35:g:234:HIS:HB2	2.01	0.42
1:2:597:U:O4	1:2:598:A:N6	2.53	0.42
1:2:1679:A:C8	6:G:66:GLY:HA3	2.53	0.42
2:A:89:TYR:HD1	2:A:178:ALA:HB2	1.84	0.42
6:G:2:LYS:O	6:G:108:VAL:HA	2.19	0.42
6:G:37:ASP:HA	6:G:49:VAL:HG23	2.01	0.42
16:Y:57:VAL:HB	16:Y:60:PHE:CE1	2.54	0.42
16:Y:57:VAL:HB	16:Y:60:PHE:HE1	1.84	0.42
24:M:127:LEU:HD23	24:M:127:LEU:HA	1.82	0.42
28:S:116:LEU:O	28:S:119:ILE:HG22	2.19	0.42
35:g:252:PHE:CZ	35:g:259:LEU:HD21	2.55	0.42
36:i:38:ILE:HG12	36:i:47:VAL:HG11	2.01	0.42
38:1:36:U:H2'	38:1:37:T6A:H8	1.84	0.42
1:2:254:U:C2	1:2:255:A:C8	3.08	0.42
1:2:623:G:H2'	1:2:624:C:H6	1.83	0.42
1:2:1059:U:C6	1:2:1060:U:H1'	2.53	0.42
7:H:31:SER:HA	7:H:35:LYS:HE2	2.01	0.42
9:J:39:LYS:HA	9:J:42:ILE:HD12	2.00	0.42
20:h:11:ARG:O	20:h:15:ARG:HG2	2.19	0.42
22:F:221:ARG:NH2	39:j:45:MET:HE3	2.34	0.42
24:M:20:ALA:HB2	24:M:123:GLU:OE2	2.18	0.42
25:P:68:PRO:HD2	25:P:71:GLU:OE2	2.20	0.42
30:U:97:ALA:HB1	30:U:101:LYS:HZ1	1.84	0.42
38:1:28:A:H2'	38:1:29:G:H8	1.84	0.42
40:k:464:VAL:O	40:k:471:THR:OG1	2.36	0.42
1:2:53:G:H2'	1:2:54:C:C6	2.55	0.42
1:2:550:G:OP2	1:2:581:U:H5'	2.19	0.42
1:2:1131:A:H2'	1:2:1132:A:C8	2.49	0.42
1:2:1165:A:H2'	1:2:1166:G:O4'	2.19	0.42
21:D:7:LYS:CG	30:U:27:THR:HG21	2.47	0.42
21:D:80:LYS:O	21:D:83:THR:OG1	2.29	0.42
21:D:114:ALA:HB3	21:D:117:ARG:HB3	2.01	0.42
23:K:25:LYS:HG3	23:K:64:TYR:HE2	1.84	0.42
28:S:25:ASN:HB2	31:Z:40:VAL:HG11	2.01	0.42
29:T:86:ARG:HE	29:T:92:LYS:HG3	1.83	0.42
31:Z:90:LYS:HA	31:Z:91:PRO:HD3	1.88	0.42
32:c:18:ARG:HA	32:c:26:THR:HA	2.01	0.42
35:g:171:ARG:NE	35:g:187:SER:HB2	2.25	0.42
36:i:37:GLN:HE22	36:i:115:ILE:HG21	1.85	0.42
40:k:479:LYS:HG2	40:k:482:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:40:A:H3'	1:2:41:A:H8	1.85	0.42
1:2:62:A:O2'	1:2:267:C:O2'	2.37	0.42
1:2:1353:G:H1'	1:2:1370:G:N2	2.34	0.42
2:A:198:MET:CE	27:R:89:SER:HA	2.49	0.42
4:C:40:TRP:CE2	4:C:72:GLN:HB2	2.54	0.42
10:L:58:CYS:HB3	10:L:62:GLY:N	2.34	0.42
11:N:93:LYS:O	11:N:96:VAL:HG12	2.19	0.42
25:P:18:LYS:HZ2	28:S:90:LYS:HB3	1.83	0.42
25:P:85:ILE:HD11	25:P:116:LEU:HD23	2.01	0.42
35:g:221:ALA:HB1	35:g:247:VAL:CG1	2.49	0.42
36:i:70:TRP:HZ2	37:3:32:U:H1'	1.85	0.42
36:i:96:ASN:C	36:i:96:ASN:ND2	2.74	0.42
39:j:186:ALA:HB2	39:j:268:PRO:HA	2.00	0.42
40:k:106:ILE:HG13	40:k:216:LEU:HA	2.01	0.42
40:k:206:SER:OG	40:k:468:SER:HB2	2.19	0.42
1:2:333:G:O6	8:I:5:ARG:NH2	2.48	0.42
1:2:406:A:H2'	1:2:407:C:H6	1.83	0.42
1:2:899:A:H1'	1:2:914:A:H2	1.84	0.42
1:2:1374:C:H2'	1:2:1375:U:C6	2.54	0.42
1:2:1553:A:OP2	25:P:47:ARG:NE	2.50	0.42
3:B:185:THR:O	3:B:189:ILE:HG12	2.20	0.42
5:E:72:VAL:HB	5:E:77:ARG:HG3	2.00	0.42
5:E:230:GLU:HG3	5:E:231:PRO:HD2	2.02	0.42
8:I:116:HIS:CE1	8:I:147:ARG:HH12	2.37	0.42
9:J:88:GLU:HG2	9:J:91:LYS:HD2	2.01	0.42
9:J:89:ASP:OD1	9:J:89:ASP:N	2.53	0.42
9:J:118:LEU:HB2	9:J:158:PHE:CZ	2.53	0.42
10:L:19:ILE:HG12	10:L:34:TRP:HB2	2.01	0.42
15:X:88:PRO:HD2	15:X:132:LEU:HD23	2.02	0.42
21:D:40:ARG:NH1	30:U:110:PRO:HG3	2.35	0.42
21:D:219:GLU:HB2	21:D:220:PRO:HD3	2.00	0.42
23:K:24:LYS:HB2	23:K:63:TYR:CE1	2.54	0.42
27:R:77:GLU:HG3	27:R:81:LYS:HE2	2.00	0.42
33:d:21:CYS:HB3	33:d:25:GLY:N	2.35	0.42
35:g:171:ARG:HH11	35:g:189:ASN:CG	2.25	0.42
36:i:101:ARG:HG3	36:i:101:ARG:NH1	2.34	0.42
40:k:214:ALA:HB3	40:k:244:VAL:HG13	2.02	0.42
1:2:82:U:H2'	1:2:83:G:O4'	2.18	0.42
1:2:125:U:H4'	5:E:148:ARG:NH2	2.34	0.42
1:2:216:A:H2'	1:2:217:A:C8	2.54	0.42
1:2:345:G:H5''	10:L:79:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:406:A:O2'	1:2:1669:A:N3	2.50	0.42
1:2:444:A:C8	1:2:445:A:C8	3.07	0.42
1:2:510:A:P	9:J:176:ARG:HE	2.43	0.42
1:2:616:U:H6	1:2:616:U:O5'	2.03	0.42
1:2:743:U:OP1	7:H:107:ARG:HA	2.19	0.42
1:2:1226:A:N6	1:2:1255:A:O2'	2.52	0.42
1:2:1251:C:O4'	34:f:131:ALA:HB2	2.20	0.42
1:2:1349:G:O6	1:2:1374:C:N4	2.53	0.42
1:2:1379:U:H1'	1:2:1514:A:N6	2.34	0.42
6:G:103:GLY:H	6:G:106:LEU:HD23	1.84	0.42
7:H:166:LEU:O	7:H:170:GLN:HG3	2.20	0.42
8:I:36:THR:HG21	8:I:174:PRO:HB2	2.01	0.42
12:O:72:LYS:HB2	12:O:72:LYS:HE2	1.78	0.42
22:F:99:LEU:HD23	22:F:99:LEU:HA	1.92	0.42
23:K:11:ILE:HD13	23:K:35:ILE:HG12	2.01	0.42
35:g:21:VAL:HB	35:g:311:GLY:HA3	2.02	0.42
35:g:43:LEU:HD12	35:g:62:TYR:HD2	1.83	0.42
35:g:223:LYS:HD2	35:g:246:GLU:OE1	2.19	0.42
38:1:18:G:H21	38:1:58:1MA:N6	2.17	0.42
40:k:205:LEU:HB2	40:k:465:ASN:ND2	2.34	0.42
1:2:7:G:O6	4:C:210:ARG:NH2	2.53	0.42
1:2:278:G:C6	1:2:280:G:C6	3.07	0.42
1:2:296:U:H2'	1:2:297:C:C6	2.55	0.42
1:2:707:A:N6	1:2:730:G:N1	2.67	0.42
1:2:874:G:O2'	1:2:876:G:OP2	2.27	0.42
1:2:977:A:C4	1:2:978:A:C8	3.07	0.42
1:2:1450:U:H2'	1:2:1451:G:C8	2.53	0.42
1:2:1601:U:H2'	1:2:1602:U:C6	2.55	0.42
3:B:34:ALA:HB3	3:B:41:ARG:HA	2.00	0.42
5:E:173:ILE:HD11	5:E:235:TRP:CE2	2.54	0.42
9:J:78:ARG:HA	9:J:81:VAL:HG22	2.02	0.42
12:O:64:ALA:HB1	12:O:105:LEU:HD23	2.01	0.42
12:O:117:ASP:C	12:O:117:ASP:OD1	2.63	0.42
21:D:105:MET:CE	21:D:184:ILE:HD13	2.44	0.42
23:K:4:PRO:HB2	23:K:7:ASP:OD1	2.20	0.42
27:R:21:TYR:HE2	27:R:61:ILE:HG21	1.83	0.42
29:T:33:TYR:CD1	29:T:33:TYR:C	2.98	0.42
36:i:108:GLU:H	36:i:108:GLU:CD	2.26	0.42
1:2:17:C:C2	1:2:18:C:C5	3.08	0.42
1:2:168:A:C4	1:2:170:A:C8	3.08	0.42
1:2:762:A:OP1	9:J:79:ARG:NH2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1219:C:H2'	1:2:1220:A:C8	2.55	0.42
1:2:1329:G:H2'	1:2:1330:A:O4'	2.20	0.42
1:2:1335:A:H2'	1:2:1336:A:O4'	2.20	0.42
1:2:1470:C:H4'	1:2:1471:U:O5'	2.20	0.42
1:2:1622:C:H2'	1:2:1623:C:C6	2.54	0.42
7:H:37:ASP:OD1	7:H:37:ASP:N	2.52	0.42
10:L:118:GLN:N	10:L:121:ASP:OD2	2.43	0.42
11:N:88:LEU:HD23	11:N:92:ILE:HD11	2.01	0.42
12:O:52:ARG:CZ	22:F:158:ARG:HD2	2.50	0.42
23:K:24:LYS:HB2	23:K:24:LYS:HE2	1.79	0.42
28:S:87:ASN:HD21	28:S:105:LEU:HD13	1.85	0.42
30:U:25:ASN:HA	30:U:90:TYR:HA	2.02	0.42
30:U:69:LYS:HD2	30:U:78:THR:HG22	2.01	0.42
39:j:40:ASP:OD1	39:j:41:ASN:N	2.47	0.42
1:2:631:U:O2'	1:2:1102:U:OP1	2.35	0.42
1:2:700:C:O2'	1:2:701:U:P	2.78	0.42
1:2:878:G:H2'	1:2:879:C:C6	2.55	0.42
1:2:1293:G:C6	1:2:1294:G:N7	2.88	0.42
1:2:1481:A:C6	1:2:1522:A:C6	3.08	0.42
1:2:1739:U:H2'	1:2:1740:U:C6	2.55	0.42
2:A:89:TYR:CD1	2:A:178:ALA:HB2	2.55	0.42
5:E:77:ARG:HD2	5:E:82:PHE:CE1	2.55	0.42
12:O:40:ALA:HB1	12:O:67:VAL:HG12	2.02	0.42
13:V:64:GLU:HG2	18:b:3:LEU:CD2	2.45	0.42
16:Y:6:THR:HG23	16:Y:28:LEU:HB2	2.01	0.42
17:a:46:GLU:O	17:a:50:ILE:HG23	2.20	0.42
22:F:51:GLU:O	22:F:52:ASP:HB3	2.20	0.42
26:Q:7:VAL:HG22	26:Q:22:VAL:CG2	2.49	0.42
35:g:123:ILE:C	35:g:124:ILE:HD13	2.45	0.42
36:i:58:MET:HE3	36:i:58:MET:O	2.19	0.42
39:j:56:ILE:HG23	39:j:56:ILE:O	2.20	0.42
1:2:587:U:OP1	19:e:26:LYS:NZ	2.43	0.41
1:2:608:U:C4	15:X:26:GLU:HG3	2.55	0.41
1:2:720:G:N1	1:2:722:G:O6	2.46	0.41
1:2:802:A:N3	7:H:104:ARG:NH1	2.66	0.41
1:2:1380:A:O2'	1:2:1381:G:H8	2.02	0.41
1:2:1585:A:H2'	1:2:1586:G:H8	1.85	0.41
5:E:75:LYS:HD2	5:E:77:ARG:NH2	2.34	0.41
5:E:159:THR:HG21	5:E:227:VAL:HB	2.02	0.41
6:G:175:ILE:HG22	6:G:178:LEU:HB2	2.02	0.41
7:H:140:VAL:O	14:W:52:TYR:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:96:VAL:HG11	11:N:150:VAL:HG11	2.02	0.41
23:K:80:LEU:HG	23:K:82:LEU:HB2	2.01	0.41
30:U:28:SER:OG	30:U:29:THR:N	2.52	0.41
30:U:62:VAL:HG12	30:U:85:ARG:HG2	2.01	0.41
35:g:224:ASP:OD1	35:g:224:ASP:N	2.53	0.41
39:j:24:VAL:HG13	39:j:34:VAL:HG11	2.00	0.41
40:k:237:GLU:OE2	40:k:275:ALA:N	2.53	0.41
1:2:72:A:H4'	1:2:73:U:O5'	2.20	0.41
1:2:242:G:H2'	1:2:243:A:H8	1.84	0.41
1:2:274:C:H2'	1:2:275:C:O4'	2.20	0.41
1:2:332:A:H8	1:2:332:A:OP1	2.02	0.41
1:2:677:G:H2'	1:2:678:G:C8	2.55	0.41
1:2:1141:A:H2'	1:2:1142:A:O4'	2.20	0.41
1:2:1198:G:H3'	1:2:1198:G:N3	2.35	0.41
3:B:66:VAL:HG23	12:O:33:LEU:HB3	2.02	0.41
6:G:35:GLU:HG3	6:G:49:VAL:HG22	2.02	0.41
7:H:131:PHE:N	7:H:132:PRO:HD2	2.35	0.41
10:L:35:TYR:CE2	10:L:49:ILE:HD11	2.54	0.41
22:F:165:SER:O	22:F:169:ARG:HG3	2.20	0.41
23:K:25:LYS:HD2	23:K:59:PHE:CZ	2.55	0.41
26:Q:41:PRO:C	26:Q:43:ILE:H	2.28	0.41
26:Q:100:GLN:H	26:Q:100:GLN:HG2	1.71	0.41
29:T:60:SER:OG	29:T:80:TYR:OH	2.27	0.41
38:1:70:G:H2'	38:1:71:C:C6	2.55	0.41
39:j:18:ASP:OD1	39:j:73:VAL:HB	2.21	0.41
40:k:310:MET:SD	40:k:310:MET:N	2.93	0.41
40:k:315:LEU:HD22	40:k:342:ILE:HG12	2.01	0.41
1:2:57:G:C2	1:2:91:G:C2	3.08	0.41
1:2:254:U:H2'	1:2:255:A:C8	2.54	0.41
1:2:819:U:H2'	1:2:820:U:H4'	2.02	0.41
1:2:969:A:H2'	1:2:970:A:H5'	2.02	0.41
1:2:1173:C:C2	1:2:1464:G:N2	2.89	0.41
1:2:1480:C:H4'	26:Q:77:GLN:HE21	1.85	0.41
1:2:1565:U:H2'	1:2:1566:C:H1'	2.02	0.41
1:2:1684:C:H2'	1:2:1685:U:O4'	2.20	0.41
3:B:187:LYS:HE3	3:B:187:LYS:HB2	1.50	0.41
4:C:74:ILE:HG13	4:C:138:LYS:O	2.20	0.41
4:C:232:PRO:HA	4:C:235:TRP:CD2	2.54	0.41
5:E:87:MET:HG3	5:E:87:MET:O	2.20	0.41
5:E:205:PHE:HE2	5:E:221:ARG:NH1	2.18	0.41
6:G:142:ARG:O	6:G:146:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:43:PHE:CE1	7:H:60:VAL:HB	2.55	0.41
7:H:147:ASN:OD1	7:H:147:ASN:N	2.51	0.41
26:Q:6:SER:OG	26:Q:23:LYS:HG2	2.20	0.41
26:Q:30:LYS:HE3	26:Q:35:PRO:HD3	2.02	0.41
28:S:132:ARG:HD2	28:S:136:GLN:NE2	2.30	0.41
34:f:83:LYS:HB3	34:f:85:TYR:CE1	2.55	0.41
35:g:176:SER:OG	35:g:186:TRP:NE1	2.42	0.41
35:g:302:SER:HG	35:g:306:GLN:H	1.68	0.41
38:l:27:C:H2'	38:l:28:A:H8	1.84	0.41
40:k:129:LYS:C	40:k:131:GLU:H	2.28	0.41
40:k:384:GLN:HG3	40:k:385:ASN:OD1	2.20	0.41
1:2:78:A:N6	6:G:178:LEU:HD23	2.36	0.41
1:2:219:A:N7	1:2:831:U:H1'	2.36	0.41
1:2:221:A:H2'	1:2:222:U:C6	2.55	0.41
1:2:303:U:C2	1:2:304:C:C5	3.08	0.41
1:2:331:U:OP1	8:I:31:ARG:NH1	2.52	0.41
1:2:432:C:H2'	1:2:433:G:C8	2.54	0.41
1:2:635:A:N1	1:2:860:U:C4	2.88	0.41
1:2:1550:U:H2'	1:2:1551:G:O4'	2.20	0.41
1:2:1679:A:H2'	6:G:65:GLN:NE2	2.35	0.41
2:A:59:LEU:O	2:A:63:ILE:HG13	2.20	0.41
3:B:88:VAL:HG13	3:B:96:LEU:HD13	2.02	0.41
4:C:84:GLU:HG2	4:C:191:LYS:HZ1	1.84	0.41
14:W:71:LYS:HG2	14:W:72:CYS:O	2.20	0.41
22:F:128:ASP:O	22:F:129:GLN:C	2.63	0.41
23:K:25:LYS:HG3	23:K:64:TYR:CE2	2.56	0.41
24:M:81:LYS:HD3	24:M:81:LYS:HA	1.81	0.41
26:Q:92:TYR:HE1	26:Q:96:PHE:HD2	1.68	0.41
26:Q:104:GLU:HA	26:Q:104:GLU:OE2	2.21	0.41
40:k:151:GLN:HE21	40:k:184:LYS:HB2	1.85	0.41
1:2:495:G:H2'	1:2:496:G:C5	2.55	0.41
1:2:511:A:H2'	1:2:512:U:C6	2.56	0.41
1:2:537:A:OP2	9:J:171:ARG:NH2	2.50	0.41
1:2:798:A:H4'	5:E:201:HIS:ND1	2.35	0.41
1:2:817:C:H2'	1:2:818:G:H8	1.84	0.41
1:2:954:A:H2'	1:2:955:C:H6	1.86	0.41
1:2:1124:A:O2'	1:2:1774:A:OP1	2.23	0.41
1:2:1197:G:OP1	1:2:1198:G:H1'	2.21	0.41
1:2:1448:U:H2'	1:2:1449:C:C6	2.55	0.41
1:2:1716:A:H2'	1:2:1717:A:H8	1.85	0.41
12:O:48:VAL:HG21	12:O:59:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:77:ARG:HB3	25:P:102:PHE:CD2	2.55	0.41
36:i:23:LYS:HB3	36:i:23:LYS:HE2	1.73	0.41
40:k:99:ALA:HA	40:k:188:HIS:HD2	1.85	0.41
1:2:180:A:H2'	1:2:181:A:C8	2.56	0.41
1:2:208:U:H2'	1:2:209:A:C8	2.53	0.41
1:2:406:A:H1'	1:2:1669:A:C2	2.56	0.41
1:2:601:U:H2'	1:2:602:U:C6	2.56	0.41
1:2:657:C:O2	1:2:674:A:N6	2.37	0.41
1:2:806:A:H2'	1:2:807:U:C6	2.56	0.41
1:2:866:G:H21	11:N:87:ASP:HB3	1.85	0.41
1:2:977:A:H2'	1:2:978:A:O4'	2.20	0.41
1:2:1539:G:N1	1:2:1567:A:OP2	2.54	0.41
1:2:1564:U:H2'	1:2:1565:U:C6	2.56	0.41
1:2:1601:U:H2'	1:2:1602:U:H6	1.86	0.41
3:B:132:ASP:HB2	3:B:221:PRO:HG3	2.03	0.41
3:B:149:GLN:HG2	3:B:151:LYS:O	2.21	0.41
8:I:23:LYS:HB3	8:I:23:LYS:HE3	1.89	0.41
8:I:70:GLU:HG3	8:I:112:TRP:CH2	2.55	0.41
9:J:64:GLU:OE2	9:J:65:LYS:N	2.50	0.41
12:O:58:TYR:CE2	12:O:62:LEU:HD21	2.55	0.41
13:V:60:ARG:HA	13:V:65:ALA:HB2	2.03	0.41
14:W:24:GLN:OE1	14:W:24:GLN:N	2.54	0.41
16:Y:27:VAL:HG21	16:Y:35:VAL:HG21	2.02	0.41
19:e:56:MET:H	19:e:56:MET:HG2	1.53	0.41
21:D:14:ASP:C	21:D:14:ASP:OD1	2.63	0.41
21:D:72:LEU:HD12	23:K:65:TYR:CD2	2.55	0.41
22:F:126:LEU:HG	31:Z:58:ARG:NH2	2.36	0.41
24:M:17:ILE:HG23	24:M:19:ASP:H	1.86	0.41
25:P:80:LEU:HD23	25:P:80:LEU:HA	1.91	0.41
27:R:116:LYS:HE2	27:R:116:LYS:HB2	1.96	0.41
29:T:103:LYS:HA	29:T:103:LYS:HD3	1.86	0.41
39:j:61:LYS:HA	39:j:61:LYS:HD2	1.90	0.41
40:k:333:LEU:HD23	40:k:333:LEU:HA	1.92	0.41
1:2:10:G:H21	4:C:93:LYS:HA	1.86	0.41
1:2:69:G:C6	1:2:70:C:C4	3.09	0.41
1:2:390:A:O2'	1:2:1728:A:O2'	2.31	0.41
1:2:1036:C:O2	14:W:16:ASN:ND2	2.53	0.41
1:2:1168:G:C2	1:2:1573:7MG:HM71	2.55	0.41
1:2:1201:A:N3	1:2:1201:A:H3'	2.36	0.41
1:2:1450:U:H2'	1:2:1451:G:H8	1.84	0.41
3:B:24:PHE:CE2	12:O:74:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:247:VAL:HG13	4:C:248:TYR:CD1	2.56	0.41
6:G:182:GLN:HE22	6:G:186:ARG:NE	2.19	0.41
8:I:107:THR:N	8:I:108:PRO:HD2	2.36	0.41
9:J:118:LEU:HD23	9:J:118:LEU:H	1.85	0.41
24:M:49:GLU:O	24:M:115:LYS:HG2	2.20	0.41
26:Q:23:LYS:NZ	26:Q:66:ARG:HH12	2.19	0.41
27:R:10:LYS:HG2	27:R:53:TYR:CE2	2.55	0.41
28:S:101:LEU:HD13	28:S:101:LEU:HA	1.84	0.41
29:T:33:TYR:CD1	29:T:37:VAL:HG21	2.54	0.41
1:2:47:A:N1	1:2:385:G:H1'	2.36	0.41
1:2:119:A:H2'	1:2:120:PSU:O4'	2.20	0.41
1:2:160:U:O2'	1:2:161:A:OP2	2.34	0.41
1:2:161:A:OP2	1:2:161:A:H8	2.04	0.41
1:2:210:U:H5''	10:L:20:PHE:CD2	2.56	0.41
1:2:589:C:N4	1:2:590:A:H62	2.19	0.41
1:2:846:A:C5	1:2:847:C:N4	2.89	0.41
1:2:924:G:H2'	1:2:925:A:C8	2.56	0.41
1:2:926:C:O2'	12:O:124:ASP:OD2	2.27	0.41
1:2:1077:C:H2'	1:2:1078:U:C6	2.56	0.41
1:2:1130:A:H2'	1:2:1131:A:O4'	2.20	0.41
1:2:1249:U:H5'	1:2:1250:U:OP2	2.21	0.41
1:2:1296:G:H2'	1:2:1298:G:N7	2.36	0.41
1:2:1447:U:H2'	1:2:1448:U:H6	1.84	0.41
1:2:1773:U:H2'	1:2:1774:A:H8	1.84	0.41
3:B:125:VAL:HG22	3:B:127:VAL:HG13	2.03	0.41
3:B:203:ASP:OD1	3:B:204:ILE:HG13	2.21	0.41
4:C:135:ILE:HD13	4:C:135:ILE:HA	1.92	0.41
6:G:5:ILE:HA	6:G:111:LEU:O	2.20	0.41
7:H:154:LEU:O	7:H:186:PRO:HD2	2.20	0.41
11:N:84:ILE:HD11	11:N:149:LEU:HD22	2.03	0.41
12:O:42:VAL:HG23	12:O:46:MET:HG3	2.03	0.41
21:D:135:GLU:OE2	21:D:137:VAL:HG23	2.21	0.41
24:M:79:LEU:HD23	24:M:81:LYS:HZ1	1.86	0.41
24:M:84:ASP:O	24:M:88:LEU:N	2.44	0.41
26:Q:47:LYS:HE3	26:Q:82:ARG:NE	2.35	0.41
29:T:68:ARG:HA	29:T:68:ARG:HD3	1.97	0.41
35:g:250:LEU:HA	35:g:260:THR:O	2.21	0.41
36:i:41:MET:HE1	36:i:71:MET:O	2.20	0.41
38:1:1:A:N3	38:1:75:C:N4	2.62	0.41
38:1:3:C:H2'	38:1:4:G:H8	1.86	0.41
40:k:142:TYR:CE2	45:k:602:MET:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:66:U:OP1	6:G:136:LYS:NZ	2.51	0.41
1:2:69:G:H2'	1:2:70:C:C6	2.56	0.41
1:2:212:A:H2'	1:2:213:G:O4'	2.21	0.41
1:2:428:G:C2	1:2:429:G:C8	3.09	0.41
1:2:589:C:H2'	1:2:590:A:C8	2.56	0.41
1:2:749:U:H2'	1:2:750:U:C6	2.56	0.41
1:2:778:G:H22	16:Y:8:ARG:HH22	1.68	0.41
1:2:884:G:N2	1:2:927:U:O2	2.54	0.41
1:2:996:G:H1	1:2:1006:5MC:N4	2.19	0.41
1:2:1070:U:P	18:b:17:ARG:HH21	2.44	0.41
1:2:1194:C:OP1	30:U:77:LYS:NZ	2.36	0.41
1:2:1386:A:C6	1:2:1409:A:N7	2.88	0.41
1:2:1499:C:N4	1:2:1500:G:O6	2.54	0.41
1:2:1584:A:OP1	26:Q:134:ALA:N	2.54	0.41
1:2:1607:U:H5''	26:Q:75:VAL:HG22	2.02	0.41
1:2:1613:C:OP2	32:c:47:PRO:HB3	2.21	0.41
1:2:1689:A:N6	1:2:1709:C:C2	2.89	0.41
2:A:80:THR:HA	2:A:83:GLN:OE1	2.21	0.41
5:E:69:HIS:HA	5:E:93:GLU:OE2	2.20	0.41
6:G:20:ASP:CG	6:G:22:HIS:H	2.29	0.41
6:G:137:ARG:HD3	6:G:177:ARG:HD2	2.03	0.41
7:H:62:VAL:HG13	7:H:63:PRO:HD2	1.99	0.41
8:I:41:LYS:H	8:I:61:GLU:CD	2.29	0.41
8:I:157:VAL:HA	8:I:160:GLN:NE2	2.35	0.41
9:J:80:LEU:HD23	9:J:80:LEU:HA	1.81	0.41
15:X:56:LYS:HZ2	15:X:93:LEU:CD1	2.33	0.41
16:Y:7:ILE:HD13	16:Y:40:LEU:HD11	2.03	0.41
16:Y:20:ARG:HD3	16:Y:74:LEU:HD23	2.03	0.41
17:a:70:LYS:HD3	17:a:72:HIS:CE1	2.55	0.41
21:D:40:ARG:HH11	30:U:110:PRO:HG3	1.86	0.41
21:D:72:LEU:O	21:D:76:ARG:N	2.49	0.41
23:K:33:GLU:HB3	23:K:34:GLU:OE2	2.21	0.41
24:M:29:LEU:HD12	24:M:36:ARG:NH2	2.31	0.41
26:Q:87:LYS:HB2	26:Q:87:LYS:HE3	1.81	0.41
29:T:76:LEU:HB3	29:T:101:ASN:ND2	2.32	0.41
32:c:44:VAL:HG11	32:c:48:VAL:HG11	2.03	0.41
34:f:78:LYS:HE2	34:f:78:LYS:HB3	1.85	0.41
35:g:70:GLN:OE1	35:g:86:TRP:NE1	2.54	0.41
35:g:130:LYS:NZ	35:g:149:THR:O	2.40	0.41
36:i:95:TYR:CE2	36:i:103:LEU:HD11	2.56	0.41
38:1:58:1MA:N3	38:1:60:A:H8	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:247:ALA:HA	39:j:250:LYS:HE3	2.01	0.41
40:k:270:ILE:HG23	40:k:273:THR:OG1	2.21	0.41
1:2:127:G:H21	6:G:195:ILE:HD12	1.86	0.41
1:2:183:C:H3'	1:2:184:U:H6	1.86	0.41
1:2:188:C:H2'	1:2:189:C:C6	2.56	0.41
1:2:637:U:O2'	1:2:638:U:P	2.79	0.41
1:2:1009:C:H2'	1:2:1010:G:O4'	2.21	0.41
1:2:1167:U:C2	1:2:1168:G:C8	3.09	0.41
1:2:1343:A:H4'	1:2:1344:A:OP1	2.21	0.41
1:2:1626:U:H2'	1:2:1627:G:C8	2.56	0.41
1:2:1671:G:H2'	1:2:1672:C:H6	1.85	0.41
2:A:8:ASP:OD1	2:A:8:ASP:N	2.54	0.41
2:A:56:LYS:NZ	2:A:158:VAL:HG23	2.36	0.41
2:A:67:ILE:HD11	2:A:120:LEU:HB2	2.03	0.41
6:G:64:LYS:NZ	6:G:81:HIS:HB3	2.36	0.41
6:G:64:LYS:NZ	6:G:82:SER:H	2.18	0.41
7:H:148:LYS:HB2	7:H:148:LYS:HE3	1.87	0.41
9:J:83:ILE:HD13	9:J:83:ILE:HA	1.94	0.41
15:X:33:LEU:HD13	15:X:33:LEU:HA	1.85	0.41
22:F:221:ARG:CZ	39:j:45:MET:HE3	2.51	0.41
25:P:58:LYS:HB2	25:P:58:LYS:HE3	1.94	0.41
30:U:32:LYS:H	30:U:32:LYS:HG2	1.69	0.41
35:g:140:ASP:OD1	35:g:141:CYS:N	2.54	0.41
38:1:28:A:C4	38:1:43:G:N2	2.89	0.41
38:1:47:H2U:O2	38:1:47:H2U:H2'	2.21	0.41
39:j:147:LEU:HD23	39:j:147:LEU:HA	1.95	0.41
40:k:95:ILE:HD11	40:k:187:ARG:HA	2.03	0.41
40:k:318:ILE:HA	40:k:414:GLY:H	1.85	0.41
1:2:249:C:H2'	1:2:250:A:C8	2.51	0.40
1:2:815:G:H2'	1:2:816:A:H8	1.86	0.40
1:2:887:U:H2'	1:2:888:U:C6	2.56	0.40
1:2:917:U:O2'	12:O:18:ARG:NH1	2.53	0.40
1:2:1210:A:H2'	1:2:1211:G:O4'	2.21	0.40
1:2:1414:G:C6	1:2:1415:A:C5	3.09	0.40
1:2:1519:G:N2	1:2:1521:G:O4'	2.54	0.40
2:A:6:THR:O	2:A:191:ARG:NH1	2.54	0.40
2:A:63:ILE:HG12	13:V:36:ILE:HG13	2.03	0.40
2:A:176:LEU:HD23	2:A:176:LEU:HA	1.93	0.40
3:B:181:LEU:O	3:B:185:THR:OG1	2.24	0.40
5:E:68:ARG:NH2	5:E:76:VAL:HG21	2.36	0.40
10:L:30:LYS:O	10:L:31:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:25:TRP:CB	18:b:82:LYS:HD2	2.51	0.40
24:M:34:LEU:HD22	24:M:36:ARG:CZ	2.51	0.40
26:Q:31:VAL:HG12	26:Q:67:VAL:HB	2.03	0.40
31:Z:84:GLU:OE2	31:Z:89:ILE:HG13	2.21	0.40
35:g:119:ASN:OD1	35:g:121:SER:OG	2.28	0.40
35:g:128:ARG:HD3	35:g:151:TRP:CD2	2.56	0.40
38:1:72:U:H2'	38:1:73:A:O4'	2.22	0.40
39:j:35:LYS:HD2	39:j:37:LEU:HD12	2.03	0.40
1:2:242:G:H2'	1:2:243:A:C8	2.56	0.40
1:2:391:G:H5''	1:2:1727:C:O2'	2.20	0.40
1:2:659:G:N3	1:2:659:G:H2'	2.37	0.40
1:2:660:A:O2'	1:2:661:C:OP1	2.34	0.40
1:2:846:A:C6	1:2:847:C:N4	2.89	0.40
1:2:986:G:N2	1:2:1012:A:OP2	2.54	0.40
1:2:1464:G:H2'	1:2:1465:C:C6	2.56	0.40
1:2:1493:C:O2'	1:2:1517:U:O2	2.24	0.40
6:G:14:LYS:HD2	6:G:124:ILE:HD11	2.02	0.40
6:G:72:ARG:HG2	6:G:98:ARG:HA	2.03	0.40
9:J:37:LYS:HG2	9:J:38:ASN:OD1	2.21	0.40
13:V:16:LYS:HG2	13:V:23:ILE:HG22	2.03	0.40
21:D:229:GLU:HA	35:g:171:ARG:CZ	2.51	0.40
22:F:60:LEU:HD11	22:F:169:ARG:NH1	2.36	0.40
22:F:216:LYS:HE3	22:F:216:LYS:HB3	1.87	0.40
26:Q:47:LYS:HD2	26:Q:47:LYS:HA	1.92	0.40
28:S:48:LYS:HG3	28:S:54:LEU:HD21	2.03	0.40
30:U:52:LYS:HB3	30:U:93:LEU:HD22	2.04	0.40
35:g:185:SER:OG	35:g:197:ALA:O	2.31	0.40
38:1:65:G:OP1	38:1:65:G:C8	2.71	0.40
39:j:21:MET:SD	39:j:37:LEU:HB2	2.60	0.40
1:2:9:U:N3	1:2:12:U:OP2	2.38	0.40
1:2:1115:A:H2'	1:2:1116:U:O4'	2.20	0.40
1:2:1230:U:OP1	1:2:1258:U:O2'	2.32	0.40
1:2:1408:A:O2'	1:2:1409:A:O5'	2.39	0.40
1:2:1520:U:O3'	29:T:78:LYS:NZ	2.54	0.40
1:2:1541:A:N6	1:2:1566:C:O2'	2.55	0.40
1:2:1578:C:H2'	1:2:1579:C:C6	2.57	0.40
1:2:1643:G:C2	1:2:1644:C:C5	3.09	0.40
1:2:1752:A:H3'	1:2:1753:A:H5''	2.02	0.40
2:A:133:ILE:HG12	2:A:143:VAL:HG11	2.03	0.40
2:A:193:GLN:HA	2:A:194:PRO:HD3	1.88	0.40
3:B:107:THR:O	3:B:111:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:PRO:HB2	5:E:36:HIS:CD2	2.56	0.40
5:E:100:ARG:HH21	5:E:122:LYS:HA	1.86	0.40
9:J:62:ARG:HB2	9:J:62:ARG:NH1	2.37	0.40
14:W:103:ILE:N	14:W:103:ILE:HD13	2.37	0.40
16:Y:113:ASN:O	16:Y:117:LYS:HG2	2.20	0.40
21:D:48:ILE:HB	21:D:86:LEU:HD23	2.03	0.40
21:D:132:LYS:HB3	21:D:189:MET:HE2	2.03	0.40
22:F:177:LEU:HD22	22:F:200:LEU:HD23	2.03	0.40
26:Q:62:ASN:O	26:Q:63:ILE:HD13	2.21	0.40
26:Q:116:LEU:HD23	26:Q:116:LEU:HA	1.84	0.40
31:Z:42:LEU:HD12	31:Z:43:ASP:N	2.36	0.40
35:g:7:MET:HA	35:g:7:MET:HE3	2.03	0.40
38:l:23:C:H4'	39:j:64:ARG:NH1	2.32	0.40
39:j:116:ALA:O	39:j:120:GLN:N	2.53	0.40
39:j:134:LEU:HD23	39:j:134:LEU:HA	1.92	0.40
1:2:38:C:H5''	9:J:6:ARG:HH21	1.86	0.40
1:2:875:G:H2'	1:2:935:G:N2	2.37	0.40
1:2:903:G:H4'	37:3:25:A:H5'	2.03	0.40
1:2:1481:A:C6	1:2:1522:A:C5	3.09	0.40
2:A:205:ARG:HE	2:A:210:ILE:HD13	1.86	0.40
4:C:95:THR:OG1	4:C:96:ARG:N	2.54	0.40
5:E:181:VAL:HG21	5:E:225:VAL:HG13	2.03	0.40
7:H:154:LEU:HD11	7:H:183:PHE:HD2	1.87	0.40
8:I:107:THR:O	8:I:111:GLN:OE1	2.39	0.40
9:J:32:GLY:HA3	19:e:40:TYR:CG	2.56	0.40
14:W:11:LEU:HD13	14:W:72:CYS:HB3	2.02	0.40
17:a:25:ASN:OD1	17:a:25:ASN:N	2.55	0.40
18:b:67:THR:HG22	18:b:69:GLY:H	1.86	0.40
21:D:11:LEU:HD13	21:D:11:LEU:HA	1.96	0.40
22:F:128:ASP:CG	22:F:129:GLN:H	2.30	0.40
22:F:227:ARG:HB3	32:c:61:ARG:NH2	2.37	0.40
29:T:127:ASN:HA	29:T:130:ARG:NH1	2.37	0.40
32:c:18:ARG:NH1	32:c:23:GLY:O	2.55	0.40
39:j:6:CYS:SG	39:j:124:GLU:HA	2.60	0.40
40:k:316:ILE:HD11	40:k:468:SER:OG	2.21	0.40
40:k:402:VAL:HG11	40:k:406:LEU:HD22	2.03	0.40
1:2:163:A:H2'	1:2:164:G:H8	1.86	0.40
1:2:234:G:C6	1:2:235:A:N6	2.90	0.40
1:2:488:C:H2'	1:2:489:C:C5	2.56	0.40
1:2:494:C:H5''	1:2:495:G:N7	2.35	0.40
1:2:996:G:C6	1:2:997:A:N7	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1368:U:P	29:T:69:LYS:HZ1	2.44	0.40
1:2:1656:G:H2'	1:2:1656:G:N3	2.37	0.40
6:G:145:PHE:HB3	6:G:147:LEU:HD13	2.04	0.40
6:G:163:THR:HG22	6:G:165:GLY:H	1.87	0.40
7:H:64:VAL:N	7:H:65:PRO:HD3	2.36	0.40
8:I:196:ARG:O	8:I:199:ALA:HB3	2.22	0.40
10:L:54:ILE:CG2	10:L:55:ASP:H	2.34	0.40
10:L:84:ILE:HD12	10:L:84:ILE:HA	1.92	0.40
11:N:91:LEU:HD23	11:N:91:LEU:HA	1.89	0.40
12:O:122:PRO:HB2	12:O:124:ASP:O	2.22	0.40
15:X:97:ASP:HB2	15:X:100:ASP:OD2	2.20	0.40
21:D:57:ASP:OD1	21:D:57:ASP:C	2.65	0.40
22:F:121:GLU:O	22:F:125:VAL:HG23	2.21	0.40
26:Q:13:LYS:HD2	26:Q:13:LYS:HA	1.87	0.40
27:R:26:MET:HE1	27:R:58:MET:C	2.46	0.40
29:T:29:GLU:N	29:T:29:GLU:OE1	2.55	0.40
35:g:176:SER:HG	35:g:186:TRP:HE1	1.62	0.40
35:g:269:ILE:HG23	35:g:278:ILE:HG13	2.03	0.40
38:1:64:RIA:O4'	38:1:64:RIA:P	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	217/254 (85%)	194 (89%)	23 (11%)	0	100	100
3	B	221/255 (87%)	204 (92%)	17 (8%)	0	100	100
4	C	218/259 (84%)	207 (95%)	11 (5%)	0	100	100
5	E	258/261 (99%)	237 (92%)	21 (8%)	0	100	100
6	G	228/236 (97%)	218 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	182/190 (96%)	171 (94%)	10 (6%)	1 (0%)	24	52
8	I	184/201 (92%)	169 (92%)	15 (8%)	0	100	100
9	J	180/188 (96%)	169 (94%)	11 (6%)	0	100	100
10	L	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
11	N	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
12	O	127/137 (93%)	115 (91%)	12 (9%)	0	100	100
13	V	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
14	W	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
15	X	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	85 (85%)	15 (15%)	0	100	100
18	b	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
19	e	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	214 (95%)	10 (4%)	1 (0%)	30	58
22	F	204/227 (90%)	188 (92%)	16 (8%)	0	100	100
23	K	94/106 (89%)	84 (89%)	10 (11%)	0	100	100
24	M	113/134 (84%)	101 (89%)	12 (11%)	0	100	100
25	P	115/142 (81%)	108 (94%)	7 (6%)	0	100	100
26	Q	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
27	R	128/136 (94%)	120 (94%)	8 (6%)	0	100	100
28	S	143/146 (98%)	126 (88%)	17 (12%)	0	100	100
29	T	141/144 (98%)	130 (92%)	11 (8%)	0	100	100
30	U	104/117 (89%)	94 (90%)	10 (10%)	0	100	100
31	Z	76/108 (70%)	70 (92%)	6 (8%)	0	100	100
32	c	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
33	d	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
34	f	72/150 (48%)	59 (82%)	13 (18%)	0	100	100
35	g	314/326 (96%)	291 (93%)	23 (7%)	0	100	100
36	i	93/153 (61%)	83 (89%)	10 (11%)	0	100	100
39	j	263/304 (86%)	247 (94%)	15 (6%)	1 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	468/527 (89%)	429 (92%)	39 (8%)	0	100	100
41	l	21/285 (7%)	20 (95%)	1 (5%)	0	100	100
All	All	5691/6582 (86%)	5269 (93%)	419 (7%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	64	VAL
39	j	17	ASP
21	D	220	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	201 (100%)	1 (0%)	81	80
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	222 (100%)	1 (0%)	84	82
6	G	192/200 (96%)	190 (99%)	2 (1%)	68	74
7	H	164/170 (96%)	162 (99%)	2 (1%)	63	72
8	I	147/159 (92%)	146 (99%)	1 (1%)	76	77
9	J	153/158 (97%)	152 (99%)	1 (1%)	76	77
10	L	136/137 (99%)	136 (100%)	0	100	100
11	N	128/128 (100%)	126 (98%)	2 (2%)	55	67
12	O	97/104 (93%)	96 (99%)	1 (1%)	68	74
13	V	73/73 (100%)	72 (99%)	1 (1%)	59	69
14	W	110/111 (99%)	110 (100%)	0	100	100
15	X	119/120 (99%)	119 (100%)	0	100	100
16	Y	108/109 (99%)	107 (99%)	1 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	a	83/100 (83%)	82 (99%)	1 (1%)	63	72
18	b	71/72 (99%)	70 (99%)	1 (1%)	59	69
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	22 (96%)	1 (4%)	26	52
21	D	188/196 (96%)	187 (100%)	1 (0%)	81	80
22	F	174/194 (90%)	173 (99%)	1 (1%)	78	79
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	92 (99%)	1 (1%)	65	73
25	P	99/119 (83%)	98 (99%)	1 (1%)	68	74
26	Q	117/119 (98%)	117 (100%)	0	100	100
27	R	116/124 (94%)	116 (100%)	0	100	100
28	S	127/129 (98%)	127 (100%)	0	100	100
29	T	117/118 (99%)	117 (100%)	0	100	100
30	U	96/107 (90%)	96 (100%)	0	100	100
31	Z	59/88 (67%)	59 (100%)	0	100	100
32	c	55/59 (93%)	55 (100%)	0	100	100
33	d	47/48 (98%)	45 (96%)	2 (4%)	26	52
34	f	60/133 (45%)	60 (100%)	0	100	100
35	g	264/272 (97%)	263 (100%)	1 (0%)	84	82
36	i	80/130 (62%)	77 (96%)	3 (4%)	29	55
39	j	239/274 (87%)	239 (100%)	0	100	100
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	22/246 (9%)	22 (100%)	0	100	100
All	All	4871/5595 (87%)	4845 (100%)	26 (0%)	78	80

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	5	LYS
5	E	118	GLU
6	G	29	ASP
6	G	128	THR
7	H	64	VAL
7	H	160	GLN

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Mol	Chain	Res	Type
8	I	158	ASP
9	J	89	ASP
11	N	105	ASN
11	N	131	THR
12	O	129	LYS
13	V	21	ASN
16	Y	53	ASP
17	a	69	ASN
18	b	3	LEU
20	h	6	ARG
21	D	150	MET
22	F	121	GLU
24	M	74	GLU
25	P	84	ILE
33	d	31	ILE
33	d	34	TYR
35	g	179	MET
36	i	91	VAL
36	i	96	ASN
36	i	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	15	GLN
2	A	23	HIS
2	A	32	HIS
2	A	164	ASN
3	B	40	ASN
3	B	208	GLN
3	B	209	ASN
4	C	115	HIS
4	C	238	GLN
6	G	13	GLN
6	G	197	ASN
8	I	176	GLN
9	J	74	ASN
10	L	16	GLN
10	L	138	ASN
11	N	58	HIS
12	O	29	HIS
15	X	18	HIS

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Mol	Chain	Res	Type
15	X	63	GLN
16	Y	22	GLN
19	e	46	ASN
19	e	51	ASN
21	D	101	GLN
21	D	159	HIS
22	F	36	GLN
22	F	202	ASN
22	F	226	ASN
23	K	29	GLN
24	M	51	GLN
25	P	104	GLN
26	Q	83	GLN
26	Q	100	GLN
27	R	42	GLN
28	S	89	GLN
28	S	136	GLN
29	T	77	ASN
33	d	48	ASN
34	f	132	ASN
34	f	133	HIS
35	g	79	ASN
35	g	231	ASN
35	g	274	ASN
35	g	321	GLN
39	j	103	GLN
40	k	108	HIS
40	k	111	HIS
40	k	151	GLN
40	k	243	HIS
40	k	248	GLN
40	k	425	ASN
41	l	145	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	525 (29%)	32 (1%)
37	3	25/49 (51%)	16 (64%)	0
38	1	72/75 (96%)	26 (36%)	3 (4%)
All	All	1894/1922 (98%)	567 (29%)	35 (1%)

All (567) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	43	A
1	2	47	A
1	2	57	G
1	2	58	U
1	2	59	C
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	78	A
1	2	79	C
1	2	80	A
1	2	81	G
1	2	104	A
1	2	114	C
1	2	115	G
1	2	121	U
1	2	127	G
1	2	129	U
1	2	130	C
1	2	132	U
1	2	133	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	146	A
1	2	152	G
1	2	155	A
1	2	160	U
1	2	161	A

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Mol	Chain	Res	Type
1	2	167	A
1	2	169	U
1	2	173	U
1	2	176	U
1	2	177	U
1	2	178	A
1	2	184	U
1	2	185	C
1	2	187	A
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	216	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	221	A
1	2	224	A
1	2	225	A
1	2	226	U
1	2	227	G
1	2	230	U
1	2	231	U
1	2	232	C
1	2	234	G
1	2	235	A
1	2	237	U
1	2	239	C
1	2	240	U
1	2	248	U
1	2	249	C
1	2	256	A
1	2	259	U
1	2	260	U
1	2	264	A
1	2	271	U
1	2	275	C
1	2	276	U
1	2	278	G
1	2	279	U

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Mol	Chain	Res	Type
1	2	280	G
1	2	289	G
1	2	298	A
1	2	300	A
1	2	301	U
1	2	307	C
1	2	313	C
1	2	315	A
1	2	319	U
1	2	320	C
1	2	321	G
1	2	332	A
1	2	336	G
1	2	337	C
1	2	345	G
1	2	349	U
1	2	358	A
1	2	359	A
1	2	360	C
1	2	382	G
1	2	390	A
1	2	398	A
1	2	399	A
1	2	400	A
1	2	401	C
1	2	404	C
1	2	411	A
1	2	415	A
1	2	416	A
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A
1	2	436	A
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	445	A
1	2	447	C
1	2	454	C

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Mol	Chain	Res	Type
1	2	459	A
1	2	463	A
1	2	467	A
1	2	474	A
1	2	476	A
1	2	482	A
1	2	483	C
1	2	486	G
1	2	487	G
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	493	U
1	2	494	C
1	2	495	G
1	2	496	G
1	2	499	C
1	2	501	U
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	513	G
1	2	514	A
1	2	516	U
1	2	519	A
1	2	527	U
1	2	533	A
1	2	537	A
1	2	540	A
1	2	541	A
1	2	543	A
1	2	558	C
1	2	563	G
1	2	564	C
1	2	565	C
1	2	567	G
1	2	578	A
1	2	584	A
1	2	593	A
1	2	594	G

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Mol	Chain	Res	Type
1	2	597	U
1	2	605	A
1	2	610	U
1	2	618	A
1	2	619	A
1	2	621	A
1	2	622	A
1	2	623	G
1	2	634	A
1	2	638	U
1	2	641	G
1	2	650	G
1	2	651	U
1	2	652	C
1	2	657	C
1	2	659	G
1	2	661	C
1	2	663	U
1	2	664	U
1	2	671	C
1	2	672	G
1	2	675	C
1	2	676	U
1	2	679	U
1	2	680	U
1	2	681	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	688	G
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	701	U
1	2	702	G
1	2	704	C
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	G

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Mol	Chain	Res	Type
1	2	712	U
1	2	714	C
1	2	717	C
1	2	718	U
1	2	721	U
1	2	722	G
1	2	727	C
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	755	A
1	2	765	G
1	2	766	PSU
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	783	C
1	2	786	G
1	2	788	A
1	2	789	U
1	2	792	A
1	2	793	U
1	2	794	U
1	2	809	G
1	2	811	A
1	2	812	U
1	2	813	A
1	2	817	C
1	2	819	U

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Mol	Chain	Res	Type
1	2	820	U
1	2	822	G
1	2	826	C
1	2	828	A
1	2	829	U
1	2	830	U
1	2	832	U
1	2	836	G
1	2	837	G
1	2	839	U
1	2	840	U
1	2	862	A
1	2	863	U
1	2	864	A
1	2	875	G
1	2	876	G
1	2	895	U
1	2	897	A
1	2	903	G
1	2	912	G
1	2	913	G
1	2	914	A
1	2	915	U
1	2	916	U
1	2	917	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	932	A
1	2	934	U
1	2	941	G
1	2	944	U
1	2	950	A
1	2	958	U
1	2	959	U
1	2	965	A
1	2	969	A
1	2	970	A
1	2	972	A
1	2	982	A
1	2	985	G
1	2	986	G

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Mol	Chain	Res	Type
1	2	987	A
1	2	991	A
1	2	995	U
1	2	998	PSU
1	2	1003	U
1	2	1011	U
1	2	1015	C
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1030	U
1	2	1031	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1049	G
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1055	U
1	2	1056	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1075	A
1	2	1081	C
1	2	1082	G
1	2	1085	A
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1095	C
1	2	1096	U
1	2	1099	G
1	2	1108	G
1	2	1112	A
1	2	1113	G
1	2	1137	A
1	2	1149	G

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Mol	Chain	Res	Type
1	2	1150	A
1	2	1155	C
1	2	1157	C
1	2	1158	C
1	2	1163	G
1	2	1166	G
1	2	1184	U
1	2	1185	U
1	2	1189	C
1	2	1190	B8N
1	2	1193	A
1	2	1195	A
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1207	A
1	2	1216	A
1	2	1217	G
1	2	1224	U
1	2	1227	G
1	2	1228	G
1	2	1230	U
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1241	A
1	2	1243	A
1	2	1244	G
1	2	1245	C
1	2	1247	C
1	2	1249	U
1	2	1250	U
1	2	1251	C
1	2	1254	G
1	2	1255	A
1	2	1258	U
1	2	1259	U
1	2	1260	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1275	U

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Mol	Chain	Res	Type
1	2	1283	C
1	2	1284	U
1	2	1292	U
1	2	1296	G
1	2	1298	G
1	2	1306	U
1	2	1313	U
1	2	1314	U
1	2	1315	G
1	2	1317	G
1	2	1320	A
1	2	1321	A
1	2	1324	A
1	2	1332	C
1	2	1336	A
1	2	1337	C
1	2	1338	C
1	2	1339	U
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1347	A
1	2	1353	G
1	2	1355	U
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1366	G
1	2	1370	G
1	2	1380	A
1	2	1386	A
1	2	1388	U
1	2	1389	A
1	2	1396	U
1	2	1397	C
1	2	1400	G
1	2	1401	C
1	2	1408	A
1	2	1409	A
1	2	1410	G
1	2	1411	U

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Mol	Chain	Res	Type
1	2	1413	U
1	2	1425	A
1	2	1426	2MG
1	2	1429	C
1	2	1431	G
1	2	1434	A
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1457	C
1	2	1458	A
1	2	1464	G
1	2	1469	A
1	2	1471	U
1	2	1476	G
1	2	1480	C
1	2	1484	G
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1494	U
1	2	1499	C
1	2	1509	G
1	2	1511	G
1	2	1514	A
1	2	1518	U
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1523	A
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1552	U
1	2	1553	A
1	2	1555	U
1	2	1557	A
1	2	1558	U
1	2	1565	U
1	2	1566	C
1	2	1571	A

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Mol	Chain	Res	Type
1	2	1572	G
1	2	1573	7MG
1	2	1581	A
1	2	1588	G
1	2	1595	A
1	2	1599	G
1	2	1605	G
1	2	1614	G
1	2	1617	C
1	2	1620	G
1	2	1632	C
1	2	1633	A
1	2	1646	A
1	2	1654	U
1	2	1655	U
1	2	1656	G
1	2	1662	C
1	2	1678	G
1	2	1679	A
1	2	1685	U
1	2	1687	A
1	2	1688	G
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U
1	2	1703	C
1	2	1704	C
1	2	1707	C
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1724	G
1	2	1725	G
1	2	1728	A

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Mol	Chain	Res	Type
1	2	1729	A
1	2	1734	G
1	2	1742	A
1	2	1743	G
1	2	1748	A
1	2	1755	G
1	2	1758	G
1	2	1763	A
1	2	1764	A
1	2	1766	G
1	2	1767	U
1	2	1778	G
1	2	1787	G
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1796	U
1	2	1797	U
1	2	1798	A
37	3	16	U
37	3	17	C
37	3	18	U
37	3	20	A
37	3	22	U
37	3	24	U
37	3	25	A
37	3	32	U
37	3	33	C
37	3	34	U
37	3	35	C
37	3	36	U
37	3	37	U
37	3	38	C
37	3	39	U
37	3	40	C
38	1	4	G
38	1	5	C
38	1	6	C
38	1	8	U
38	1	9	1MG

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Mol	Chain	Res	Type
38	1	10	2MG
38	1	13	C
38	1	15	G
38	1	16	H2U
38	1	18	G
38	1	19	G
38	1	20	A
38	1	21	A
38	1	22	G
38	1	26	M2G
38	1	44	A
38	1	46	7MG
38	1	47	H2U
38	1	48	5MC
38	1	49	5MC
38	1	58	1MA
38	1	59	A
38	1	60	A
38	1	70	G
38	1	74	C
38	1	75	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	26	A
1	2	66	U
1	2	74	U
1	2	78	A
1	2	216	A
1	2	217	A
1	2	224	A
1	2	239	C
1	2	277	U
1	2	279	U
1	2	344	U
1	2	423	C
1	2	513	G
1	2	637	U
1	2	649	U
1	2	660	A
1	2	670	G

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Mol	Chain	Res	Type
1	2	695	U
1	2	700	C
1	2	781	A
1	2	793	U
1	2	828	A
1	2	1198	G
1	2	1206	C
1	2	1343	A
1	2	1430	U
1	2	1470	C
1	2	1513	A
1	2	1552	U
1	2	1571	A
1	2	1613	C
1	2	1765	G
38	1	43	G
38	1	47	H2U
38	1	74	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	5MC	1	48	38	19,22,23	3.94	8 (42%)	26,32,35	1.02	2 (7%)
38	7MG	1	46	38	23,26,27	3.62	11 (47%)	27,39,42	2.20	9 (33%)
1	MA6	2	1780	1	23,26,27	1.39	4 (17%)	33,38,41	3.36	12 (36%)
38	H2U	1	47	38	18,21,22	3.24	4 (22%)	19,30,33	1.46	3 (15%)
38	RIA	1	64	38	35,38,39	1.30	4 (11%)	50,57,60	1.82	11 (22%)
1	B8N	2	1190	1	25,29,30	3.36	7 (28%)	28,42,45	1.97	8 (28%)
38	1MG	1	9	38	23,26,27	3.32	7 (30%)	33,39,42	2.32	8 (24%)
38	T6A	1	37	38	31,34,35	1.82	7 (22%)	43,49,52	2.19	14 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2	1006	1	19,22,23	3.69	8 (42%)	26,32,35	1.20	3 (11%)
1	PSU	2	120	1	18,21,22	4.40	7 (38%)	21,30,33	2.03	5 (23%)
1	2MG	2	1426	1,42	23,26,27	2.87	8 (34%)	33,38,41	2.20	10 (30%)
38	M2G	1	26	38	24,27,28	2.69	8 (33%)	33,40,43	1.74	8 (24%)
1	2MG	2	1570	1	23,26,27	2.92	8 (34%)	33,38,41	2.15	10 (30%)
1	PSU	2	766	1	18,21,22	4.36	8 (44%)	21,30,33	2.02	6 (28%)
38	5MC	1	49	38	19,22,23	3.95	8 (42%)	26,32,35	1.04	2 (7%)
1	7MG	2	1573	1,38	23,26,27	3.56	10 (43%)	27,39,42	2.24	9 (33%)
1	5MC	2	1637	1	19,22,23	3.80	8 (42%)	26,32,35	0.98	2 (7%)
38	H2U	1	16	38	18,21,22	3.14	4 (22%)	19,30,33	1.45	4 (21%)
1	PSU	2	1289	1	18,21,22	4.42	7 (38%)	21,30,33	2.01	5 (23%)
1	PSU	2	465	1	18,21,22	4.36	7 (38%)	21,30,33	1.95	5 (23%)
1	PSU	2	998	1	18,21,22	4.39	7 (38%)	21,30,33	2.02	6 (28%)
38	2MG	1	10	38	23,26,27	2.91	8 (34%)	33,38,41	2.22	10 (30%)
38	1MA	1	58	38	21,25,26	3.14	6 (28%)	30,37,40	2.38	8 (26%)

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
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
1	MA6	2	1780	1	-	3/11/29/30	0/3/3/3
38	H2U	1	47	38	-	5/7/38/39	0/2/2/2
38	RIA	1	64	38	-	12/17/51/52	0/4/4/4
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
38	T6A	1	37	38	-	3/23/41/42	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1426	1,42	-	0/9/27/28	0/3/3/3
38	M2G	1	26	38	-	4/11/29/30	0/3/3/3
1	2MG	2	1570	1	-	0/9/27/28	0/3/3/3
1	PSU	2	766	1	-	0/7/25/26	0/2/2/2
38	5MC	1	49	38	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	2	1573	1,38	-	2/7/37/38	0/3/3/3
1	5MC	2	1637	1	-	0/7/25/26	0/2/2/2
38	H2U	1	16	38	-	6/7/38/39	0/2/2/2
1	PSU	2	1289	1	-	0/7/25/26	0/2/2/2
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	PSU	2	998	1	-	4/7/25/26	0/2/2/2
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	1MA	1	58	38	-	2/7/25/26	0/3/3/3

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1289	PSU	C6-C5	11.70	1.48	1.35
1	2	120	PSU	C6-C5	11.55	1.48	1.35
1	2	766	PSU	C6-C5	11.53	1.48	1.35
1	2	465	PSU	C6-C5	11.49	1.48	1.35
1	2	998	PSU	C6-C5	11.46	1.48	1.35
38	1	47	H2U	C2-N1	10.34	1.50	1.35
1	2	1289	PSU	C2-N1	9.92	1.49	1.36
1	2	120	PSU	C2-N1	9.86	1.49	1.36
1	2	998	PSU	C2-N1	9.83	1.49	1.36
38	1	16	H2U	C2-N1	9.80	1.49	1.35
1	2	465	PSU	C2-N1	9.77	1.49	1.36
38	1	58	1MA	C2-N3	9.73	1.48	1.30
1	2	766	PSU	C2-N1	9.62	1.49	1.36
38	1	49	5MC	C6-C5	9.42	1.50	1.34
38	1	48	5MC	C6-C5	9.26	1.49	1.34
1	2	1637	5MC	C6-C5	9.22	1.49	1.34
38	1	9	1MG	C2-N2	9.16	1.50	1.34
1	2	1006	5MC	C6-C5	8.74	1.48	1.34
38	1	46	7MG	C8-N9	8.60	1.51	1.45
1	2	1573	7MG	C8-N9	8.54	1.51	1.45
1	2	1190	B8N	C6-N1	8.38	1.56	1.36
1	2	1190	B8N	C4-N3	-7.78	1.26	1.40
1	2	1570	2MG	C2-N3	7.77	1.46	1.32
1	2	998	PSU	C2-N3	7.77	1.50	1.37
38	1	10	2MG	C2-N3	7.75	1.46	1.32
1	2	120	PSU	C2-N3	7.62	1.50	1.37
1	2	1289	PSU	C2-N3	7.60	1.50	1.37
1	2	766	PSU	C2-N3	7.55	1.49	1.37
1	2	465	PSU	C2-N3	7.51	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1426	2MG	C2-N3	7.49	1.46	1.32
1	2	1190	B8N	C4-C5	7.40	1.64	1.47
38	1	58	1MA	C4-N3	7.18	1.50	1.35
38	1	48	5MC	C5-C4	7.15	1.49	1.44
38	1	46	7MG	C5-N7	7.08	1.44	1.35
38	1	48	5MC	C4-N3	7.04	1.45	1.34
38	1	9	1MG	C2-N3	7.03	1.44	1.33
38	1	49	5MC	C5-C4	6.95	1.49	1.44
38	1	26	M2G	C4-N3	6.87	1.50	1.34
38	1	49	5MC	C4-N3	6.84	1.45	1.34
38	1	10	2MG	C4-N3	6.80	1.49	1.34
1	2	1570	2MG	C4-N3	6.72	1.49	1.34
1	2	1573	7MG	C5-N7	6.72	1.44	1.35
1	2	1006	5MC	C4-N3	6.69	1.44	1.34
38	1	26	M2G	C2-N2	6.61	1.47	1.35
38	1	16	H2U	C2-N3	6.57	1.49	1.38
38	1	47	H2U	C2-N3	6.55	1.49	1.38
1	2	1637	5MC	C5-C4	6.53	1.49	1.44
38	1	9	1MG	C4-N3	6.52	1.49	1.34
1	2	1426	2MG	C4-N3	6.52	1.49	1.34
1	2	1637	5MC	C4-N3	6.51	1.44	1.34
38	1	49	5MC	C2-N3	6.31	1.48	1.36
38	1	48	5MC	C2-N3	6.31	1.48	1.36
1	2	1006	5MC	C2-N3	6.18	1.48	1.36
1	2	1637	5MC	C2-N3	6.10	1.48	1.36
38	1	26	M2G	C2-N3	6.10	1.47	1.32
1	2	1006	5MC	C5-C4	5.98	1.48	1.44
38	1	46	7MG	C2-N3	5.93	1.47	1.33
1	2	1573	7MG	C2-N3	5.90	1.47	1.33
38	1	46	7MG	C4-N3	5.84	1.47	1.34
38	1	10	2MG	C2-N2	5.82	1.45	1.33
1	2	1570	2MG	C2-N2	5.80	1.45	1.33
1	2	1573	7MG	C4-N3	5.71	1.47	1.34
1	2	1426	2MG	C2-N2	5.71	1.45	1.33
1	2	1190	B8N	C2-N1	5.67	1.55	1.39
38	1	9	1MG	C2-N1	5.47	1.47	1.37
1	2	1573	7MG	C4-N9	5.30	1.44	1.37
38	1	46	7MG	C4-N9	5.29	1.44	1.37
1	2	120	PSU	C6-N1	5.26	1.44	1.36
1	2	1289	PSU	C6-N1	5.25	1.44	1.36
1	2	465	PSU	C6-N1	5.23	1.44	1.36
1	2	998	PSU	C6-N1	5.19	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	37	T6A	C10-N6	5.17	1.48	1.37
38	1	37	T6A	C10-N11	5.10	1.49	1.35
1	2	1190	B8N	C6-C5	5.09	1.42	1.35
1	2	766	PSU	C6-N1	5.06	1.44	1.36
38	1	16	H2U	C4-N3	5.04	1.46	1.37
1	2	1573	7MG	C2-N2	5.02	1.45	1.34
38	1	46	7MG	C2-N2	5.01	1.45	1.34
38	1	47	H2U	C4-N3	4.98	1.45	1.37
1	2	1570	2MG	C2-N1	4.93	1.44	1.36
38	1	58	1MA	C2-N1	4.88	1.45	1.35
1	2	1426	2MG	C2-N1	4.86	1.44	1.36
38	1	10	2MG	C2-N1	4.81	1.44	1.36
38	1	49	5MC	C6-N1	4.77	1.46	1.38
38	1	64	RIA	C5-C4	4.75	1.47	1.39
1	2	1637	5MC	C6-N1	4.61	1.45	1.38
38	1	48	5MC	C6-N1	4.59	1.45	1.38
38	1	49	5MC	C2-N1	4.58	1.49	1.40
1	2	1190	B8N	C1'-C5	-4.47	1.40	1.50
38	1	49	5MC	C4-N4	4.46	1.45	1.34
38	1	48	5MC	C4-N4	4.44	1.45	1.34
1	2	1006	5MC	C4-N4	4.42	1.45	1.34
38	1	48	5MC	C2-N1	4.40	1.49	1.40
1	2	1637	5MC	C4-N4	4.38	1.45	1.34
1	2	1006	5MC	C2-N1	4.30	1.49	1.40
1	2	1637	5MC	C2-N1	4.16	1.48	1.40
1	2	1006	5MC	C6-N1	4.08	1.45	1.38
38	1	58	1MA	C5-C6	4.04	1.54	1.43
38	1	46	7MG	C2-N1	3.89	1.47	1.37
1	2	998	PSU	C4-N3	3.84	1.46	1.38
1	2	1780	MA6	C6-N6	3.82	1.47	1.36
1	2	1573	7MG	C2-N1	3.79	1.46	1.37
38	1	9	1MG	O6-C6	-3.75	1.15	1.23
1	2	465	PSU	C4-N3	3.74	1.45	1.38
1	2	766	PSU	C4-N3	3.74	1.45	1.38
1	2	120	PSU	C4-N3	3.73	1.45	1.38
1	2	1289	PSU	C4-N3	3.70	1.45	1.38
38	1	46	7MG	C5-C6	3.67	1.52	1.43
38	1	26	M2G	C2-N1	3.56	1.44	1.36
1	2	1573	7MG	C5-C6	3.55	1.52	1.43
38	1	9	1MG	C5-C6	3.41	1.54	1.45
38	1	46	7MG	C6-N1	3.33	1.45	1.38
38	1	9	1MG	C5-N7	-3.32	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1573	7MG	C6-N1	3.17	1.44	1.38
1	2	1426	2MG	C5-N7	-3.06	1.32	1.39
38	1	58	1MA	C5-N7	-3.06	1.32	1.39
38	1	10	2MG	C5-N7	-2.94	1.33	1.39
1	2	1570	2MG	C5-N7	-2.92	1.33	1.39
1	2	1780	MA6	C5-C4	-2.89	1.33	1.39
1	2	1637	5MC	O2-C2	-2.80	1.18	1.23
1	2	1006	5MC	O2-C2	-2.80	1.18	1.23
38	1	26	M2G	C5-N7	-2.78	1.33	1.39
38	1	49	5MC	O2-C2	-2.70	1.18	1.23
38	1	48	5MC	O2-C2	-2.70	1.18	1.23
38	1	64	RIA	C5-C6	2.69	1.48	1.41
38	1	26	M2G	C6-N1	2.68	1.43	1.38
38	1	37	T6A	C5-N7	-2.66	1.34	1.39
38	1	26	M2G	C5-C6	2.62	1.54	1.44
1	2	1426	2MG	O6-C6	-2.61	1.18	1.23
1	2	1573	7MG	O6-C6	-2.60	1.18	1.23
1	2	1289	PSU	O4-C4	-2.57	1.18	1.23
1	2	120	PSU	O4-C4	-2.54	1.18	1.23
1	2	766	PSU	O4-C4	-2.53	1.18	1.23
38	1	10	2MG	C5-C6	2.52	1.53	1.44
1	2	998	PSU	O4-C4	-2.52	1.18	1.23
38	1	47	H2U	O2-C2	-2.50	1.18	1.23
38	1	16	H2U	O2-C2	-2.50	1.18	1.23
1	2	1570	2MG	C5-C6	2.50	1.53	1.44
1	2	465	PSU	O4-C4	-2.49	1.18	1.23
38	1	46	7MG	O6-C6	-2.48	1.18	1.23
38	1	10	2MG	O6-C6	-2.47	1.18	1.23
1	2	1570	2MG	O6-C6	-2.47	1.18	1.23
1	2	1426	2MG	C5-C6	2.44	1.53	1.44
38	1	37	T6A	ODA-C13	2.40	1.29	1.22
1	2	1780	MA6	C5-N7	-2.39	1.34	1.39
38	1	26	M2G	O6-C6	-2.37	1.19	1.23
38	1	10	2MG	C6-N1	2.32	1.43	1.38
1	2	1570	2MG	C6-N1	2.31	1.43	1.38
38	1	64	RIA	C5-N7	-2.30	1.34	1.39
1	2	766	PSU	O4'-C1'	-2.29	1.40	1.43
38	1	64	RIA	C8-N7	2.28	1.36	1.31
1	2	1426	2MG	C6-N1	2.27	1.43	1.38
1	2	766	PSU	O2-C2	-2.26	1.18	1.23
38	1	37	T6A	C5-C4	-2.26	1.35	1.39
38	1	37	T6A	C6-N6	2.23	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	120	PSU	O2-C2	-2.20	1.18	1.23
1	2	465	PSU	O2-C2	-2.19	1.18	1.23
38	1	37	T6A	C2-N1	2.18	1.37	1.33
1	2	1289	PSU	O2-C2	-2.16	1.18	1.23
1	2	998	PSU	O2-C2	-2.14	1.18	1.23
1	2	1780	MA6	C8-N9	-2.12	1.33	1.37
38	1	58	1MA	CM1-N1	-2.11	1.42	1.46
1	2	1190	B8N	O2-C2	-2.07	1.18	1.22
38	1	46	7MG	C5-C4	2.06	1.44	1.37

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-12.57	101.53	116.86
1	2	1780	MA6	C5-C6-N6	8.30	138.47	125.33
38	1	10	2MG	C2-N3-C4	6.81	120.52	112.00
38	1	58	1MA	C1'-N9-C8	-6.68	107.76	126.73
38	1	9	1MG	C1'-N9-C4	-6.56	107.12	126.49
1	2	1426	2MG	C2-N3-C4	6.49	120.11	112.00
1	2	1570	2MG	C2-N3-C4	6.43	120.04	112.00
38	1	64	RIA	C5-C4-N3	-6.33	118.00	126.72
38	1	9	1MG	C1'-N9-C8	6.09	144.03	126.73
38	1	37	T6A	N3-C2-N1	-5.82	119.77	128.58
38	1	10	2MG	C5-C4-N3	-5.75	119.23	128.39
38	1	58	1MA	C1'-N9-C4	5.72	143.39	126.49
1	2	1780	MA6	N1-C2-N3	-5.57	120.15	128.58
38	1	26	M2G	C5-C4-N3	-5.45	119.71	128.39
1	2	1426	2MG	C5-C4-N3	-5.38	119.82	128.39
1	2	1570	2MG	C5-C4-N3	-5.32	119.93	128.39
38	1	9	1MG	C5-C4-N3	-5.22	120.08	128.39
38	1	64	RIA	N3-C4-N9	5.11	135.85	127.17
1	2	1190	B8N	C5-C4-N3	5.10	125.42	116.15
1	2	1573	7MG	C5-C6-N1	5.09	119.90	110.94
38	1	46	7MG	C5-C6-N1	5.03	119.80	110.94
38	1	58	1MA	N1-C2-N3	-5.00	120.05	126.00
1	2	120	PSU	C4-N3-C2	-4.89	119.63	126.37
38	1	58	1MA	C5-C4-N3	-4.84	120.14	127.27
1	2	1289	PSU	C4-N3-C2	-4.84	119.70	126.37
1	2	1780	MA6	C5-C4-N3	-4.83	120.06	126.72
1	2	998	PSU	C4-N3-C2	-4.77	119.81	126.37
1	2	1573	7MG	C2-N3-C4	4.75	120.49	112.30
38	1	37	T6A	C12-N11-C10	4.74	129.88	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	465	PSU	C4-N3-C2	-4.72	119.87	126.37
38	1	46	7MG	C2-N3-C4	4.68	120.37	112.30
38	1	37	T6A	C5-C4-N3	-4.68	120.28	126.72
1	2	766	PSU	C4-N3-C2	-4.68	119.93	126.37
1	2	766	PSU	N1-C2-N3	4.51	119.93	115.17
1	2	120	PSU	N1-C2-N3	4.48	119.89	115.17
1	2	1573	7MG	C5-C4-N3	-4.45	119.78	128.13
1	2	465	PSU	N1-C2-N3	4.40	119.81	115.17
1	2	1289	PSU	N1-C2-N3	4.40	119.81	115.17
1	2	998	PSU	N1-C2-N3	4.38	119.79	115.17
1	2	1190	B8N	C4-N3-C2	-4.33	120.29	125.62
1	2	1426	2MG	C2-N1-C6	-4.29	119.36	124.55
1	2	1780	MA6	N9-C8-N7	-4.28	107.87	113.94
38	1	37	T6A	N6-C10-N11	4.23	119.58	113.77
38	1	46	7MG	C5-C4-N3	-4.23	120.20	128.13
38	1	37	T6A	N9-C8-N7	-4.20	107.97	113.94
38	1	26	M2G	C2-N3-C4	4.17	120.23	112.51
38	1	10	2MG	C2-N1-C6	-4.16	119.52	124.55
1	2	1570	2MG	C2-N1-C6	-4.11	119.59	124.55
38	1	37	T6A	C4-C5-C6	4.04	120.14	116.78
1	2	1780	MA6	C4-C5-C6	3.90	119.95	115.91
1	2	1190	B8N	C1'-C5-C4	3.87	123.49	117.61
38	1	46	7MG	C4-C5-N7	3.82	109.89	105.38
38	1	58	1MA	C2-N3-C4	3.80	119.97	112.53
1	2	1573	7MG	C4-C5-N7	3.78	109.84	105.38
38	1	64	RIA	C2-N3-C4	3.77	121.03	111.83
1	2	1006	5MC	C5-C6-N1	-3.71	119.29	123.31
38	1	10	2MG	N9-C4-N3	3.61	133.18	125.95
38	1	9	1MG	C2-N3-C4	3.61	120.09	111.98
1	2	1190	B8N	N3-C2-N1	3.48	120.97	116.72
1	2	766	PSU	C6-N1-C2	-3.43	119.51	122.69
1	2	1426	2MG	N1-C2-N2	3.42	120.05	116.56
38	1	16	H2U	N3-C2-N1	3.38	120.05	116.65
38	1	9	1MG	N9-C4-N3	3.38	132.71	125.95
38	1	47	H2U	N3-C2-N1	3.37	120.03	116.65
1	2	1780	MA6	C2-N1-C6	3.34	120.00	111.83
38	1	9	1MG	N9-C8-N7	-3.34	107.21	113.40
1	2	1570	2MG	N9-C4-N3	3.33	132.62	125.95
1	2	998	PSU	C6-N1-C2	-3.32	119.61	122.69
1	2	1573	7MG	C5-C4-N9	3.32	110.59	106.33
1	2	1780	MA6	C2-N3-C4	3.28	119.85	111.83
38	1	26	M2G	N9-C4-N3	3.27	132.49	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	120	PSU	C6-C5-C4	3.26	120.38	118.17
38	1	64	RIA	C4-C5-N7	-3.26	106.86	110.58
38	1	37	T6A	C2-N3-C4	3.25	119.78	111.83
1	2	998	PSU	C6-C5-C4	3.25	120.37	118.17
38	1	58	1MA	N9-C8-N7	-3.24	107.40	113.40
1	2	465	PSU	C6-N1-C2	-3.23	119.70	122.69
38	1	10	2MG	N1-C2-N2	3.21	119.84	116.56
38	1	37	T6A	O10-C10-N6	-3.21	117.94	123.64
1	2	1289	PSU	C6-N1-C2	-3.20	119.72	122.69
1	2	120	PSU	C6-N1-C2	-3.17	119.75	122.69
38	1	48	5MC	C5-C6-N1	-3.16	119.88	123.31
38	1	47	H2U	C5-C6-N1	3.15	121.05	111.52
38	1	46	7MG	C5-C4-N9	3.14	110.35	106.33
1	2	1426	2MG	N9-C4-N3	3.14	132.22	125.95
1	2	766	PSU	C6-C5-C4	3.09	120.26	118.17
1	2	1289	PSU	C6-C5-C4	3.06	120.24	118.17
1	2	1573	7MG	C2-N1-C6	-2.98	119.70	125.11
38	1	64	RIA	N3-C2-N1	-2.98	124.07	128.58
1	2	1780	MA6	N3-C4-N9	2.95	132.18	127.17
38	1	16	H2U	C5-C6-N1	2.87	120.21	111.52
1	2	1780	MA6	C5-N7-C8	2.85	107.92	103.45
1	2	1573	7MG	N9-C4-N3	2.85	129.63	125.46
38	1	16	H2U	C5-C4-N3	2.84	119.71	116.69
38	1	37	T6A	C5-N7-C8	2.84	107.92	103.45
1	2	1570	2MG	N9-C8-N7	-2.84	108.14	113.40
38	1	9	1MG	C5-C6-N1	2.84	120.26	115.02
38	1	46	7MG	O6-C6-C5	-2.83	120.66	127.62
1	2	1573	7MG	O6-C6-C5	-2.83	120.67	127.62
1	2	766	PSU	O2-C2-N1	-2.82	119.88	122.79
38	1	49	5MC	C5-C6-N1	-2.81	120.26	123.31
38	1	47	H2U	C5-C4-N3	2.81	119.68	116.69
1	2	465	PSU	C6-C5-C4	2.81	120.07	118.17
1	2	1570	2MG	N1-C2-N2	2.79	119.41	116.56
38	1	46	7MG	C2-N1-C6	-2.79	120.05	125.11
1	2	1190	B8N	O4-C4-N3	-2.77	115.49	119.99
1	2	998	PSU	O2-C2-N1	-2.77	119.94	122.79
38	1	64	RIA	C1'-O2A-C2A	-2.73	111.51	117.98
38	1	46	7MG	N9-C4-N3	2.72	129.45	125.46
1	2	1426	2MG	N9-C8-N7	-2.68	108.44	113.40
38	1	37	T6A	N3-C4-N9	2.67	131.71	127.17
38	1	10	2MG	C5-C6-N1	2.66	120.02	113.25
1	2	1570	2MG	C5-C6-N1	2.65	120.01	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	26	M2G	N9-C8-N7	-2.64	108.50	113.40
38	1	26	M2G	C5-C6-N1	2.64	119.98	113.25
1	2	120	PSU	O2-C2-N1	-2.63	120.07	122.79
1	2	1426	2MG	C5-C6-N1	2.62	119.93	113.25
38	1	10	2MG	N9-C8-N7	-2.62	108.55	113.40
38	1	64	RIA	C2'-C3'-C4'	2.62	107.66	102.61
1	2	1637	5MC	C5-C6-N1	-2.62	120.47	123.31
1	2	465	PSU	O2-C2-N1	-2.61	120.09	122.79
38	1	16	H2U	O2-C2-N1	-2.55	120.03	123.10
1	2	1570	2MG	O6-C6-C5	-2.54	119.83	126.53
38	1	58	1MA	N9-C4-N3	2.50	132.61	126.90
38	1	26	M2G	O6-C6-C5	-2.50	119.94	126.53
1	2	1426	2MG	O6-C6-C5	-2.50	119.94	126.53
1	2	1573	7MG	N9-C8-N7	2.48	106.89	103.37
1	2	1780	MA6	C4-N9-C8	2.46	108.32	105.74
38	1	10	2MG	O6-C6-C5	-2.45	120.06	126.53
38	1	64	RIA	C5-N7-C8	2.43	107.27	103.45
38	1	64	RIA	C4-N9-C8	2.42	108.28	105.74
38	1	64	RIA	O3'-C3'-C4'	-2.39	104.21	111.08
38	1	9	1MG	C8-N7-C5	2.38	108.50	104.26
1	2	1289	PSU	O2-C2-N1	-2.38	120.33	122.79
38	1	46	7MG	N9-C8-N7	2.35	106.70	103.37
1	2	1190	B8N	C31-N3-C4	2.28	120.41	117.18
38	1	58	1MA	C8-N7-C5	2.27	108.30	104.26
1	2	1006	5MC	CM5-C5-C6	-2.23	119.83	122.85
38	1	37	T6A	C4-C5-N7	-2.21	108.06	110.58
38	1	37	T6A	C4-N9-C8	2.19	108.04	105.74
1	2	1190	B8N	O4'-C1'-C2'	2.18	108.17	105.15
1	2	998	PSU	O4'-C1'-C2'	2.14	108.12	105.15
1	2	1780	MA6	C4-C5-N7	-2.14	108.13	110.58
1	2	766	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	2	1426	2MG	CM2-N2-C2	-2.13	119.07	123.65
38	1	64	RIA	C6-C5-N7	2.13	136.19	132.09
38	1	26	M2G	C1'-N9-C8	-2.12	120.71	126.73
38	1	48	5MC	CM5-C5-C6	-2.12	119.99	122.85
38	1	10	2MG	N1-C2-N3	-2.11	120.12	123.68
1	2	1006	5MC	C5-C4-N3	-2.09	119.61	121.75
38	1	37	T6A	N6-C6-N1	2.09	122.95	117.54
1	2	1570	2MG	N1-C2-N3	-2.09	120.16	123.68
38	1	49	5MC	O2-C2-N3	-2.08	119.06	122.33
1	2	1637	5MC	C5-C4-N3	-2.05	119.65	121.75
38	1	37	T6A	C5-C4-N9	2.02	108.02	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1190	B8N	O4-C4-C5	-2.02	119.09	122.58
38	1	10	2MG	C8-N7-C5	2.02	107.85	104.26
1	2	1426	2MG	C1'-N9-C4	-2.02	120.53	126.49
1	2	1570	2MG	C8-N7-C5	2.01	107.84	104.26
38	1	26	M2G	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1190	B8N	C31-C32-C33-N34
1	2	1780	MA6	O4'-C4'-C5'-O5'
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	16	H2U	C4'-C5'-O5'-P
38	1	26	M2G	O4'-C4'-C5'-O5'
38	1	37	T6A	C14-C12-N11-C10
38	1	47	H2U	O4'-C4'-C5'-O5'
38	1	47	H2U	C3'-C4'-C5'-O5'
38	1	48	5MC	C4'-C5'-O5'-P
38	1	49	5MC	O4'-C4'-C5'-O5'
38	1	58	1MA	O4'-C4'-C5'-O5'
38	1	64	RIA	C4A-C5A-O5A-P
38	1	64	RIA	C2'-C1'-O2A-C2A
38	1	64	RIA	C5'-O5'-P'-O2X
38	1	64	RIA	C5'-O5'-P'-O3X
1	2	1573	7MG	C3'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	10	2MG	O4'-C4'-C5'-O5'
38	1	26	M2G	C3'-C4'-C5'-O5'
38	1	48	5MC	O4'-C4'-C5'-O5'
38	1	48	5MC	C3'-C4'-C5'-O5'
38	1	58	1MA	C3'-C4'-C5'-O5'
38	1	64	RIA	O1'-C4'-C5'-O5'
1	2	998	PSU	O4'-C4'-C5'-O5'
1	2	1573	7MG	O4'-C4'-C5'-O5'
38	1	64	RIA	C3'-C4'-C5'-O5'
1	2	1780	MA6	C3'-C4'-C5'-O5'
38	1	49	5MC	C3'-C4'-C5'-O5'
38	1	16	H2U	C2'-C1'-N1-C6
38	1	37	T6A	C14-C12-C13-ODA
1	2	1190	B8N	O4'-C4'-C5'-O5'
38	1	10	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
38	1	64	RIA	O1'-C1'-O2A-C2A
38	1	64	RIA	C5'-O5'-P'-O1X
38	1	64	RIA	C3A-C4A-C5A-O5A
38	1	37	T6A	C14-C12-C13-ODB
1	2	998	PSU	C3'-C4'-C5'-O5'
38	1	64	RIA	O4'-C4A-C5A-O5A
38	1	16	H2U	C3'-C4'-C5'-O5'
38	1	16	H2U	C2'-C1'-N1-C2
38	1	47	H2U	C2'-C1'-N1-C2
38	1	47	H2U	C2'-C1'-N1-C6
38	1	47	H2U	C4'-C5'-O5'-P
1	2	998	PSU	O4'-C1'-C5-C4
38	1	64	RIA	C2A-C1A-N9-C4
38	1	64	RIA	C2A-C1A-N9-C8
1	2	1190	B8N	N34-C33-C34-O36
38	1	16	H2U	O4'-C1'-N1-C2
38	1	46	7MG	C4'-C5'-O5'-P
1	2	1190	B8N	C3'-C4'-C5'-O5'
1	2	1780	MA6	C4'-C5'-O5'-P
1	2	998	PSU	C4'-C5'-O5'-P
38	1	26	M2G	C4'-C5'-O5'-P
38	1	26	M2G	C2'-C1'-N9-C4
38	1	16	H2U	O4'-C1'-N1-C6
1	2	1190	B8N	N34-C33-C34-O35

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	47	H2U	2	0
38	1	64	RIA	6	0
38	1	37	T6A	2	0
1	2	1006	5MC	2	0
1	2	120	PSU	1	0
1	2	1570	2MG	1	0
1	2	1573	7MG	2	0
1	2	1637	5MC	2	0
38	1	16	H2U	1	0
1	2	1289	PSU	1	0
1	2	998	PSU	1	0
38	1	58	1MA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 118 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
44	GCP	k	601	-	32,34,34	3.17	12 (37%)	49,54,54	1.64	9 (18%)
45	MET	k	602	-	6,7,8	0.47	0	2,7,9	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GCP	k	601	-	-	2/19/38/38	0/3/3/3
45	MET	k	602	-	-	0/5/6/8	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	O4'-C1'	8.68	1.62	1.42
44	k	601	GCP	C2'-C1'	-7.25	1.30	1.53
44	k	601	GCP	O4'-C4'	-6.19	1.31	1.45
44	k	601	GCP	PB-O3A	6.13	1.65	1.58
44	k	601	GCP	PA-O3A	5.30	1.65	1.59
44	k	601	GCP	C2-N2	4.85	1.45	1.34
44	k	601	GCP	C6-N1	-3.22	1.32	1.38
44	k	601	GCP	O2'-C2'	2.82	1.49	1.43
44	k	601	GCP	O3'-C3'	-2.75	1.36	1.43
44	k	601	GCP	O6-C6	-2.57	1.18	1.23
44	k	601	GCP	C5-N7	-2.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	PB-O2B	-2.03	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	GCP	C5-C4-N3	-5.21	120.10	128.39
44	k	601	GCP	C2-N3-C4	4.50	120.05	112.30
44	k	601	GCP	N9-C8-N7	-2.97	107.90	113.40
44	k	601	GCP	N9-C4-N3	2.95	131.86	125.95
44	k	601	GCP	C2-N1-C6	-2.79	120.06	125.11
44	k	601	GCP	C5-C6-N1	2.64	119.98	113.25
44	k	601	GCP	PB-O3A-PA	-2.61	123.87	132.37
44	k	601	GCP	O6-C6-C5	-2.39	120.22	126.53
44	k	601	GCP	C8-N7-C5	2.16	108.10	104.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

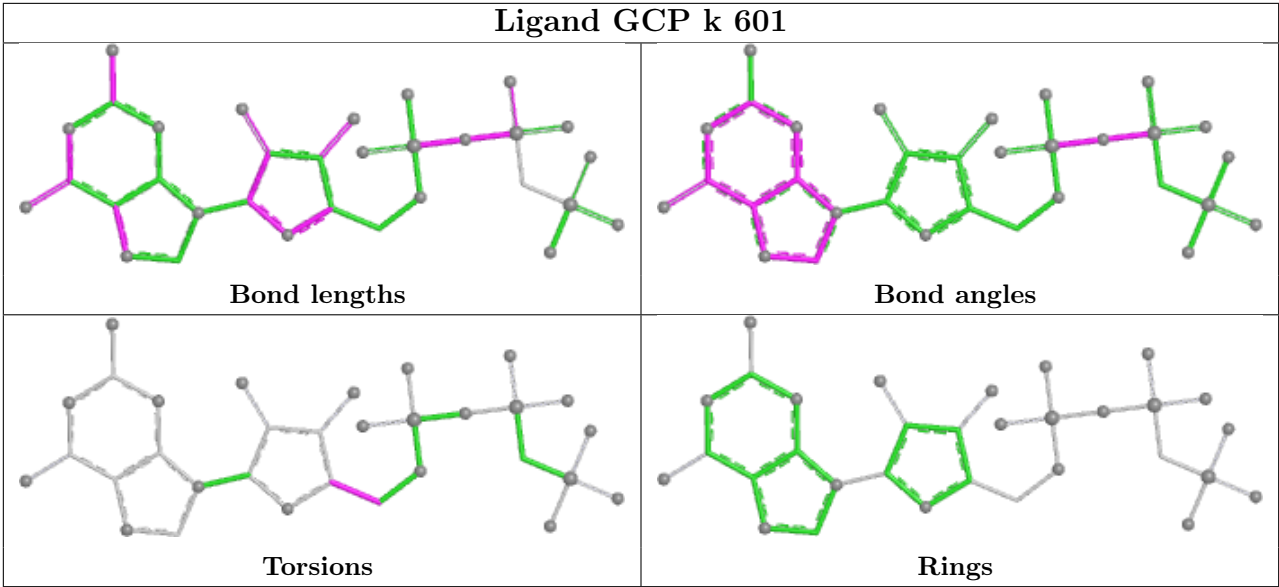
Mol	Chain	Res	Type	Atoms
44	k	601	GCP	O4'-C4'-C5'-O5'
44	k	601	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	k	601	GCP	1	0
45	k	602	MET	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3'	65:G	P	8.93
1	1	63:G	O3'	64:RIA	P	4.61
1	1	16:H2U	O3'	18:G	P	3.39

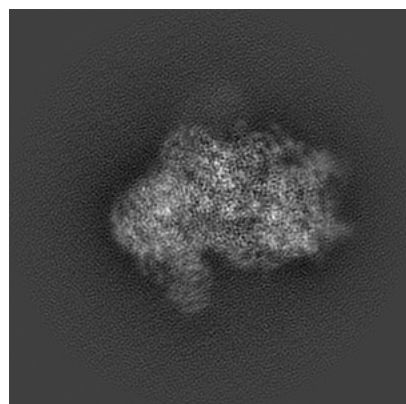
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19541. These allow visual inspection of the internal detail of the map and identification of artifacts.

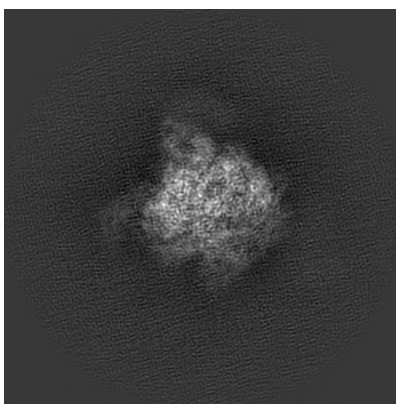
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

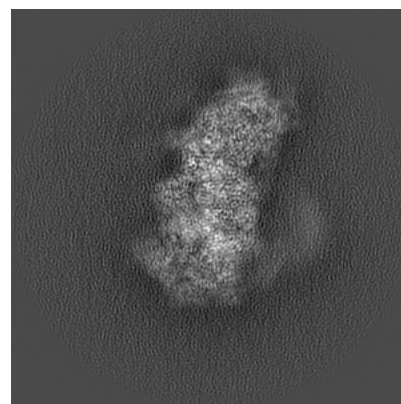
6.1.1 Primary map



X

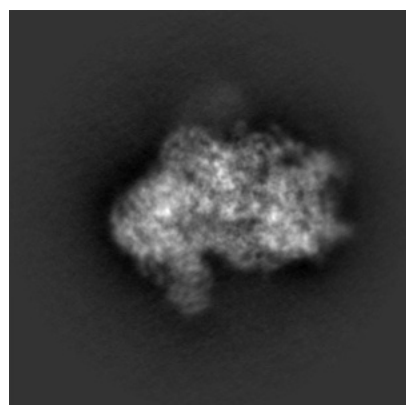


Y

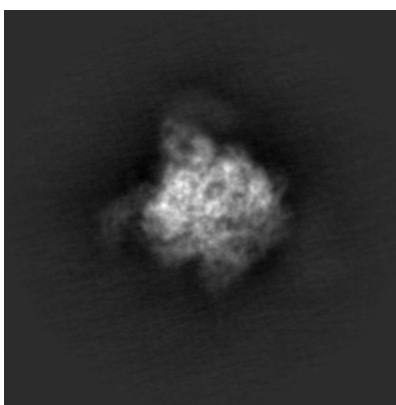


Z

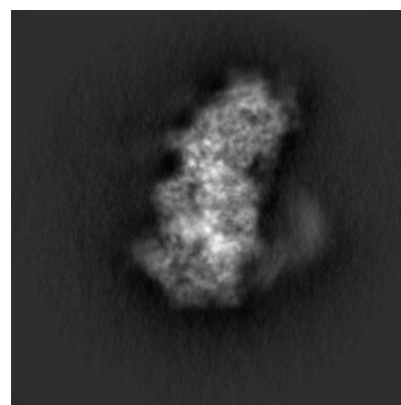
6.1.2 Raw map



X



Y

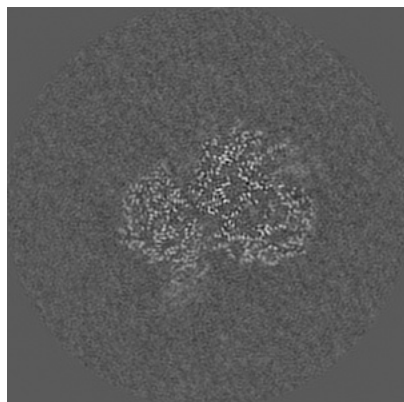


Z

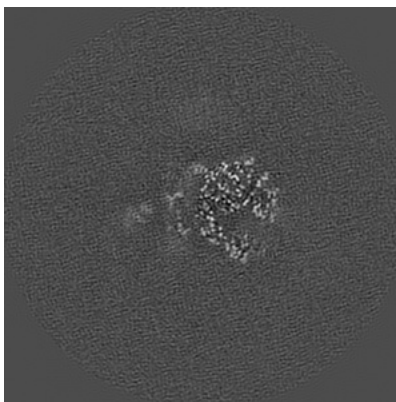
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

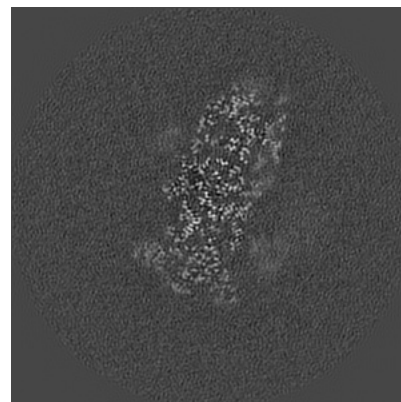
6.2.1 Primary map



X Index: 150

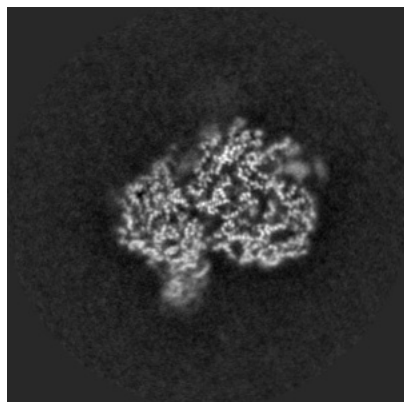


Y Index: 150

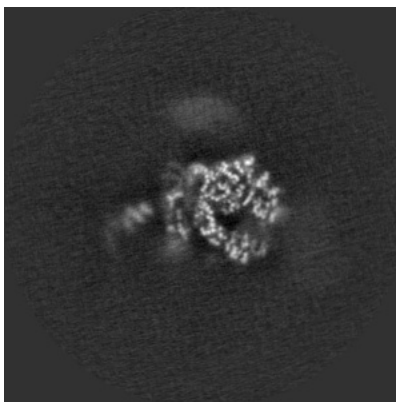


Z Index: 150

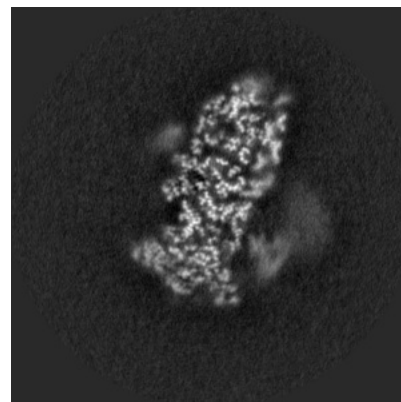
6.2.2 Raw map



X Index: 150



Y Index: 150

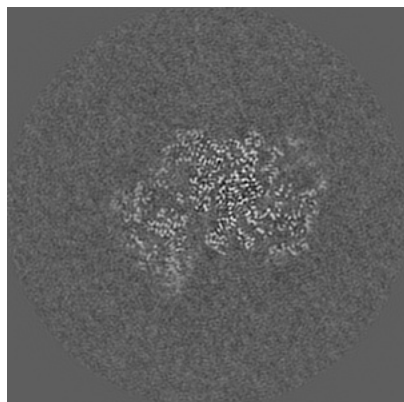


Z Index: 150

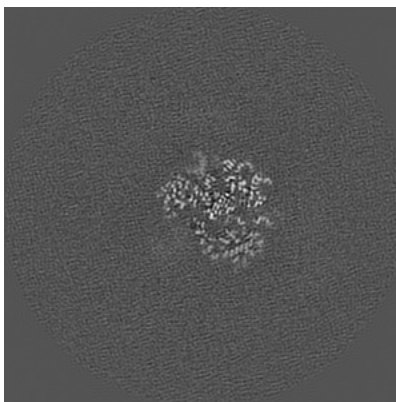
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

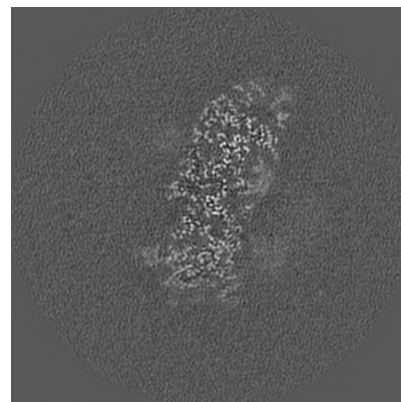
6.3.1 Primary map



X Index: 157

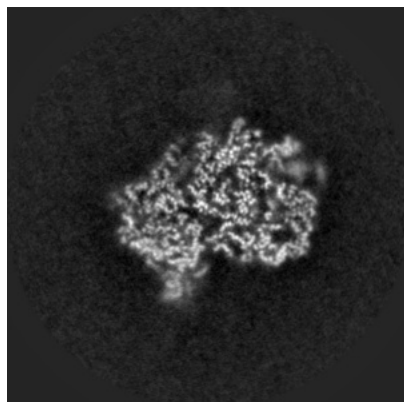


Y Index: 161

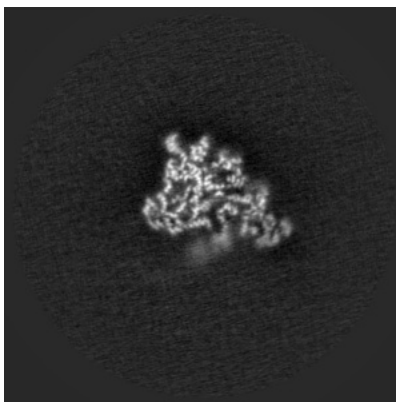


Z Index: 147

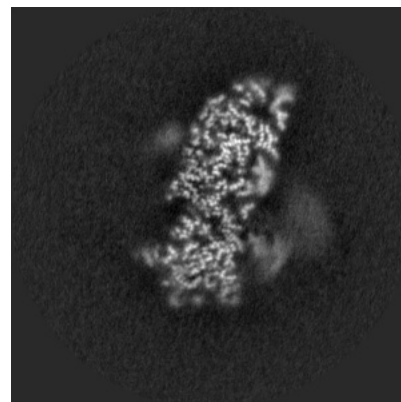
6.3.2 Raw map



X Index: 152



Y Index: 198

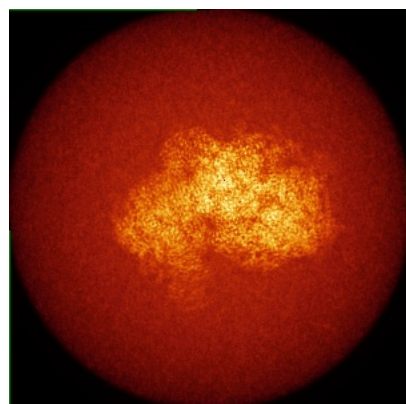


Z Index: 146

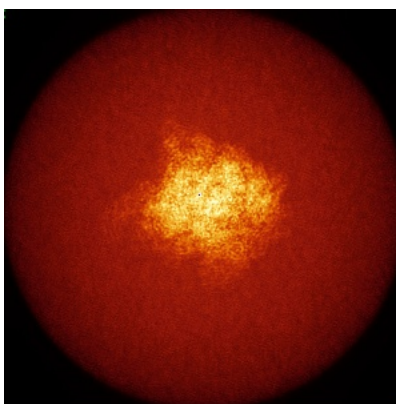
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

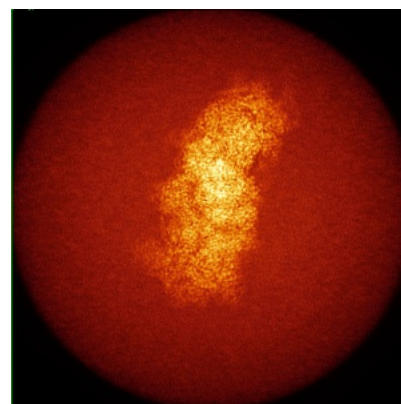
6.4.1 Primary map



X

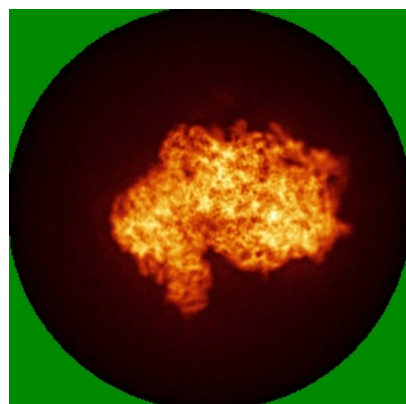


Y

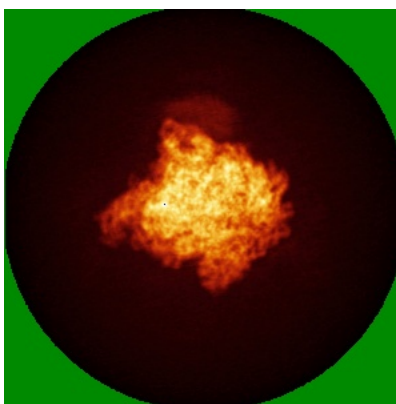


Z

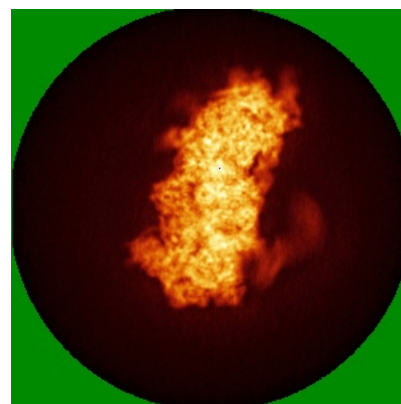
6.4.2 Raw map



X



Y

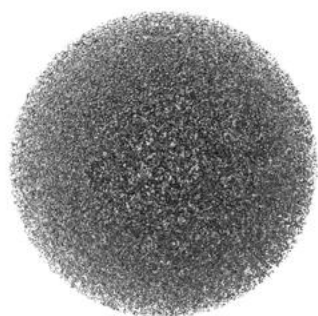


Z

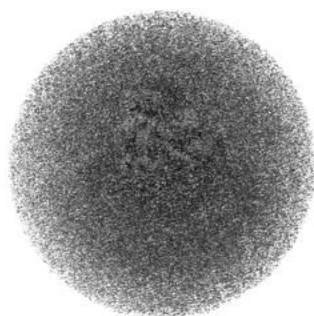
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

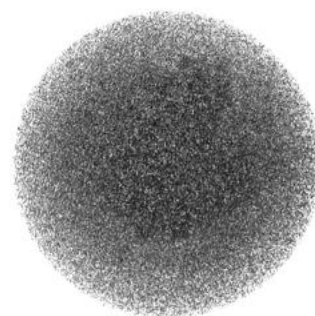
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

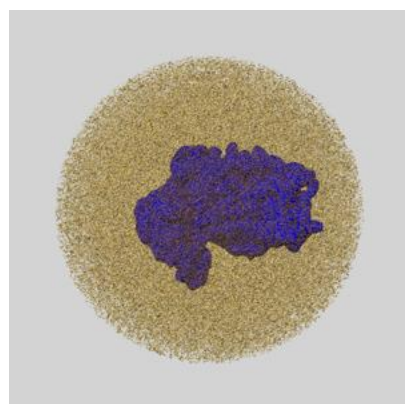
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

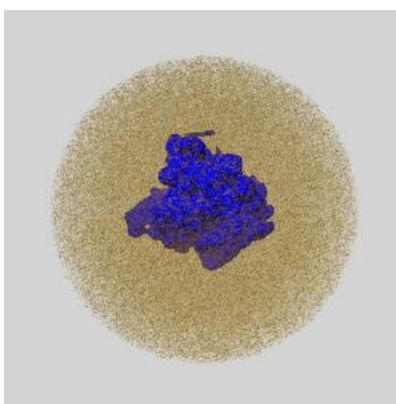
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

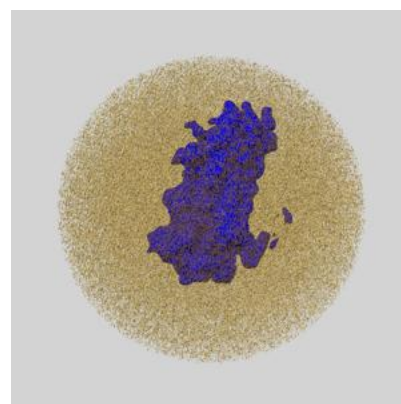
6.6.1 emd_19541_msk_1.map [i](#)



X



Y

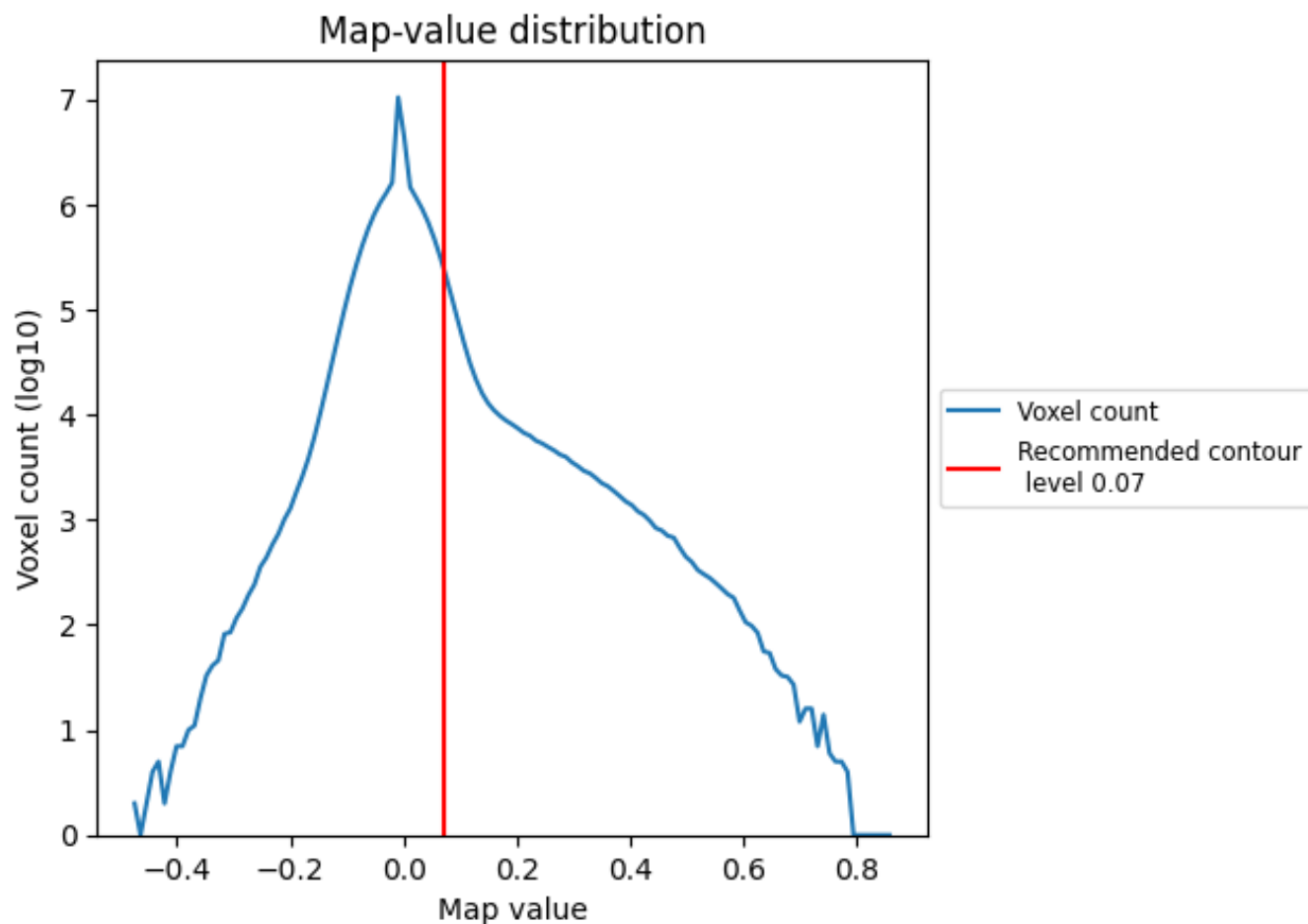


Z

7 Map analysis [i](#)

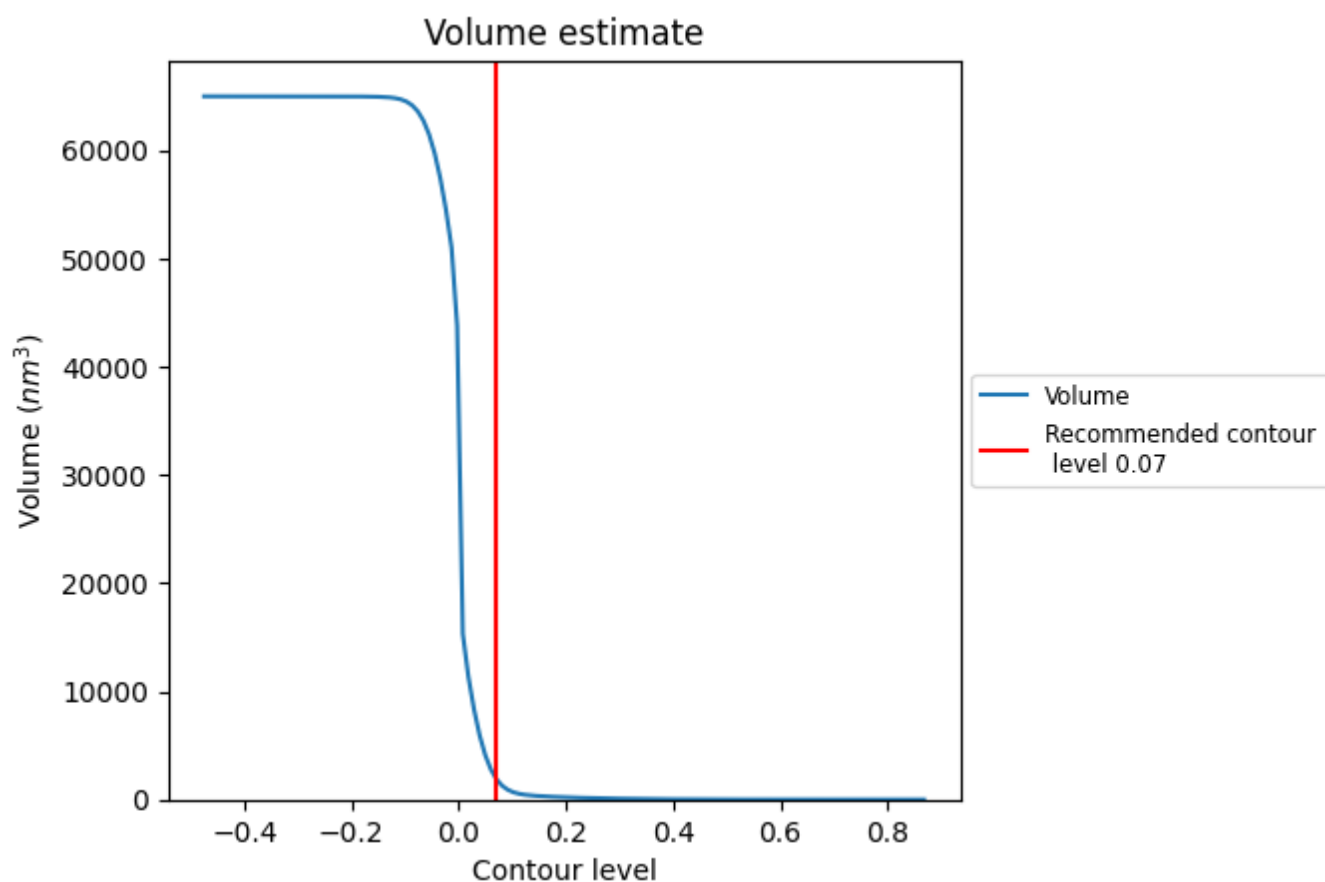
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

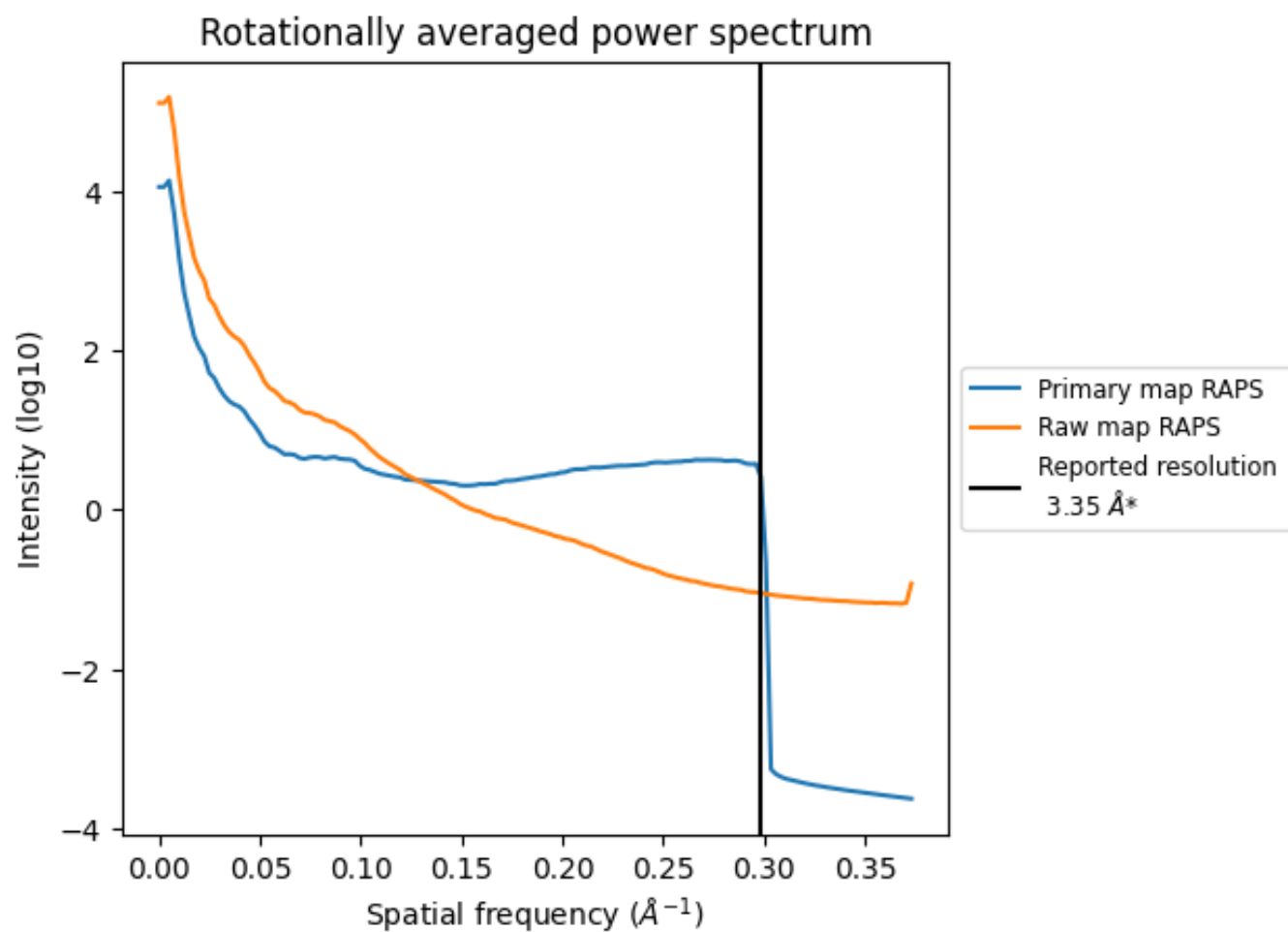
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1921 nm³; this corresponds to an approximate mass of 1736 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

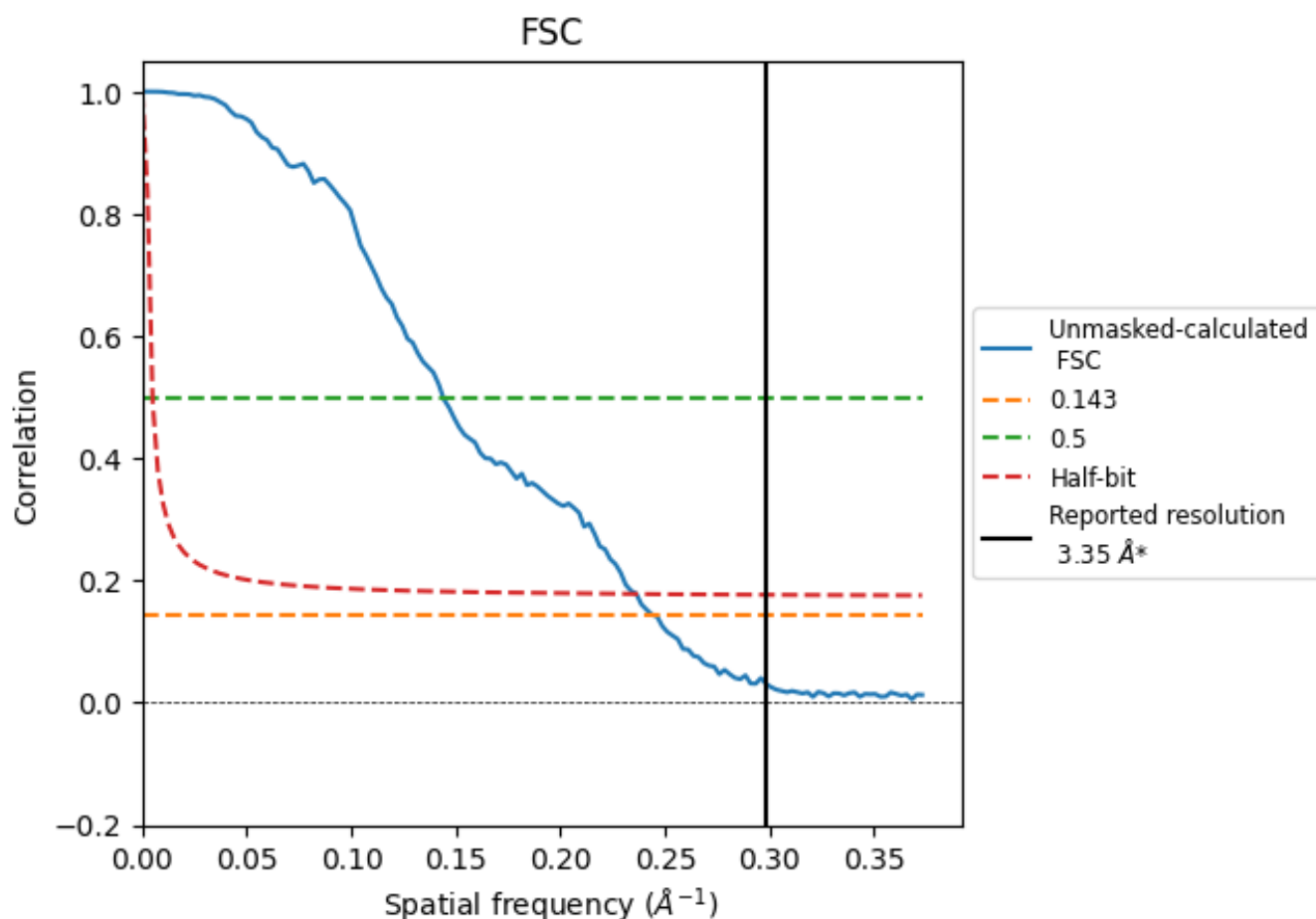


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

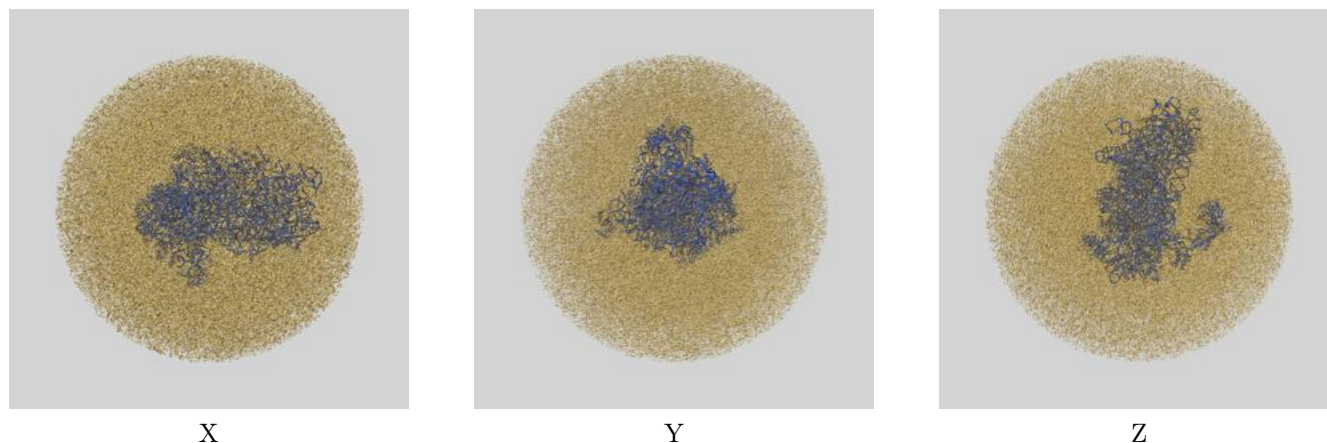
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	6.95	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

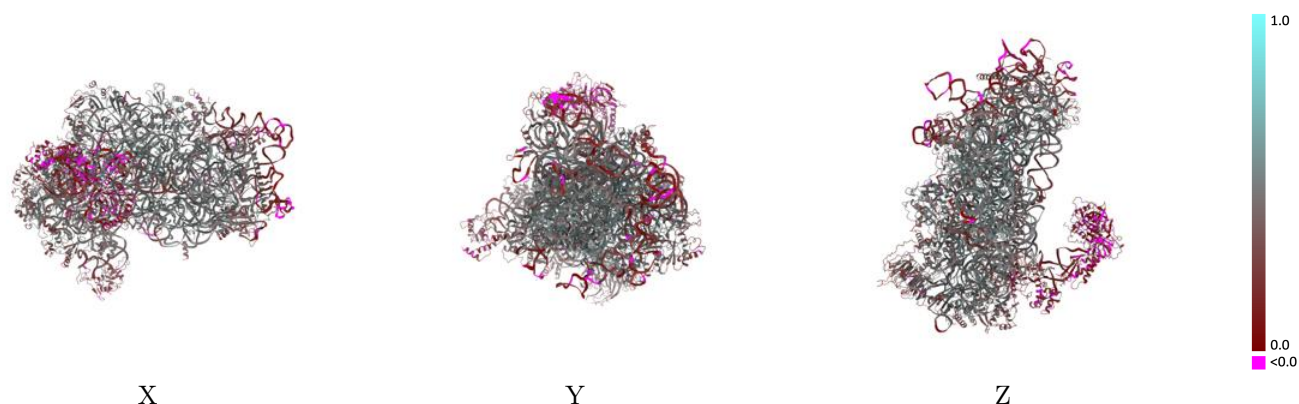
This section contains information regarding the fit between EMDB map EMD-19541 and PDB model 8RW1. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



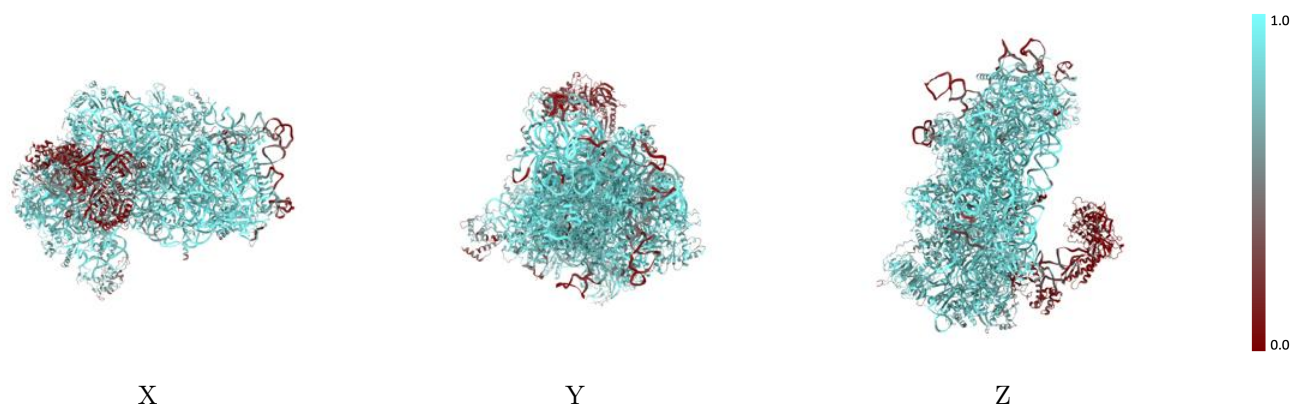
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



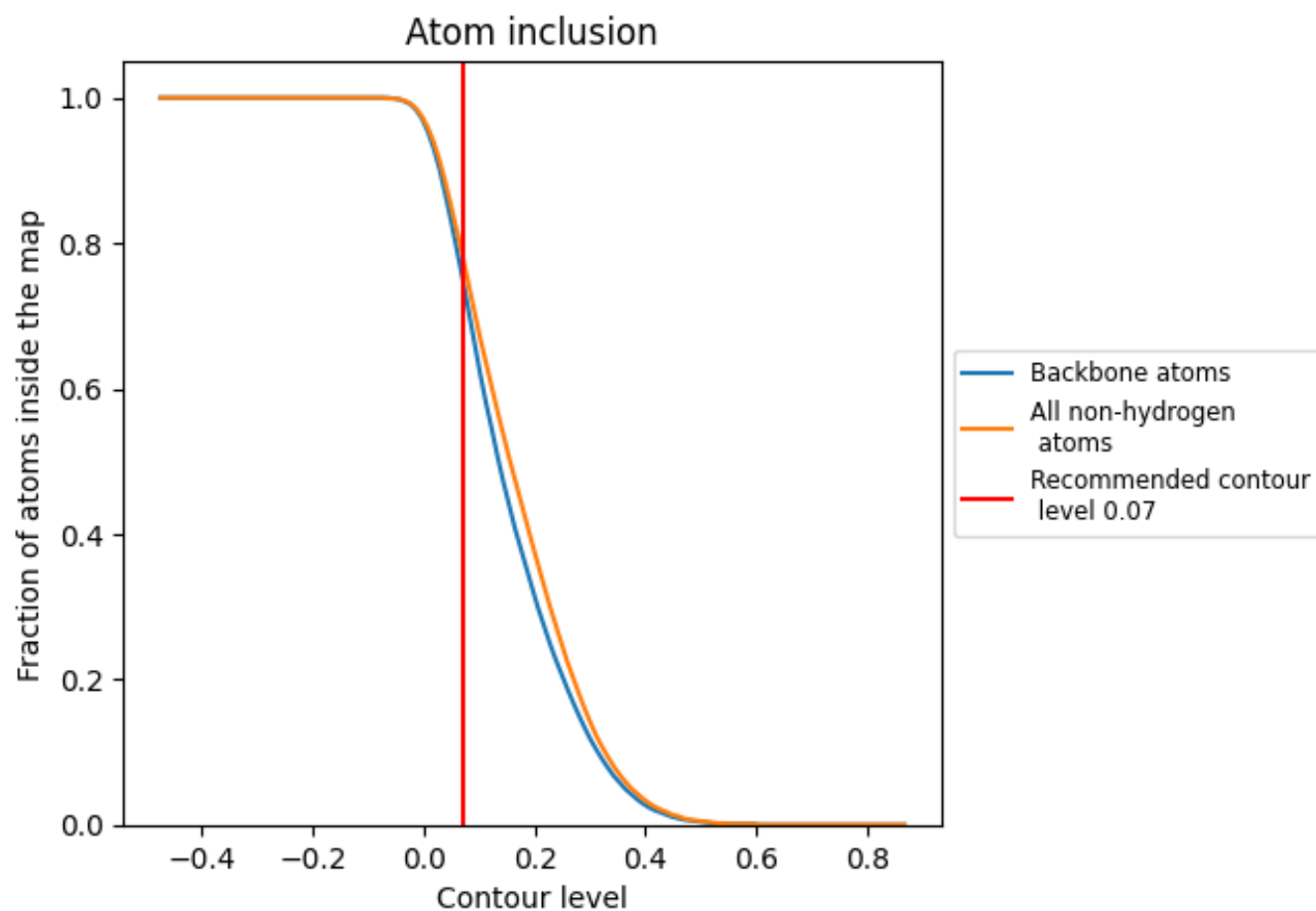
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.3990
1	 0.5110	 0.2620
2	 0.8800	 0.4190
3	 0.4730	 0.3100
A	 0.8730	 0.4670
B	 0.8280	 0.4290
C	 0.8950	 0.5070
D	 0.8060	 0.4210
E	 0.8840	 0.4810
F	 0.8060	 0.4480
G	 0.8040	 0.3770
H	 0.7650	 0.3900
I	 0.8460	 0.4440
J	 0.8740	 0.4790
K	 0.7980	 0.3890
L	 0.8270	 0.4520
M	 0.4560	 0.1800
N	 0.9050	 0.4800
O	 0.8750	 0.4640
P	 0.7980	 0.3770
Q	 0.8660	 0.4700
R	 0.7930	 0.4210
S	 0.7950	 0.3860
T	 0.8810	 0.4480
U	 0.7510	 0.3700
V	 0.8740	 0.4850
W	 0.9090	 0.5240
X	 0.8770	 0.4960
Y	 0.8620	 0.4480
Z	 0.6060	 0.2950
a	 0.8780	 0.4880
b	 0.8610	 0.4540
c	 0.8330	 0.4560
d	 0.9050	 0.5020
e	 0.7400	 0.4180



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Chain	Atom inclusion	Q-score
f	 0.6110	 0.2380
g	 0.7820	 0.3660
h	 0.4760	 0.3520
i	 0.3520	 0.3090
j	 0.1900	 0.1660
k	 0.0920	 0.1200
l	 0.0590	 0.1150