



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 3JAP / pdb_00003jap
EMDB ID : EMD-3048
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 4.90 Å(reported)
Based on initial models : 3CW2, 4U1E, 4U1D, 3J81, 4U1C, 2D74

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:

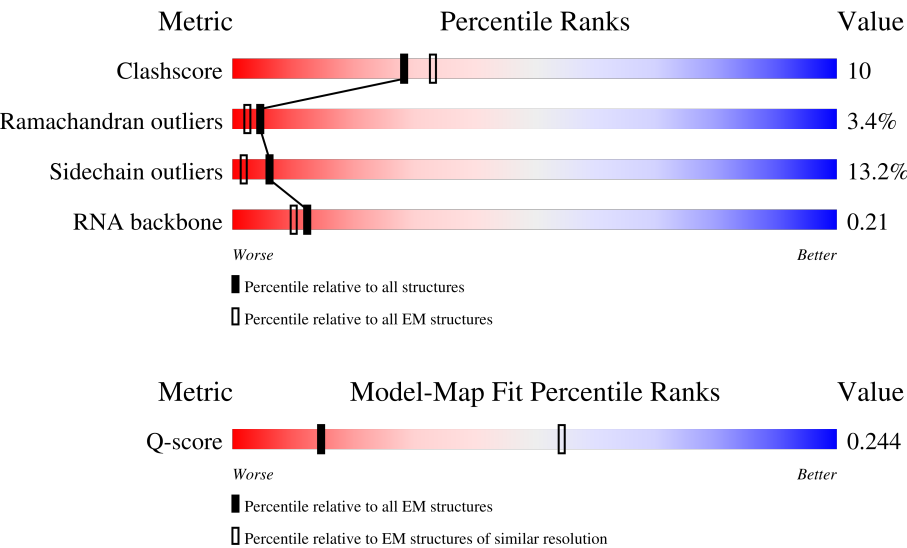
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.90 Å.

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



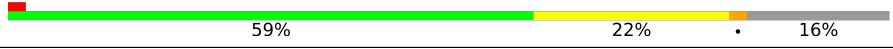
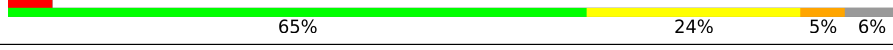
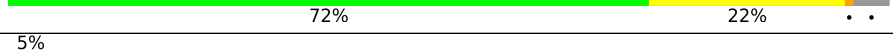
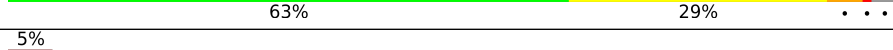
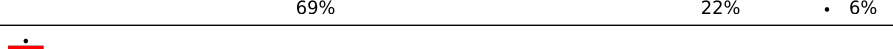
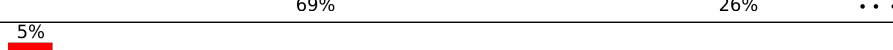
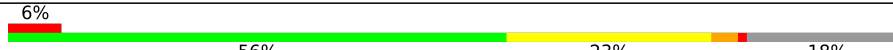
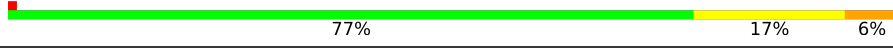
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1274 (4.40 - 5.40)

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	1	75	28% 29% 40% 29% .
2	2	1781	6% 25% 50% 24% .
3	3	25	20% 52% 44% .

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Mol	Chain	Length	Quality of chain
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	

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Mol	Chain	Length	Quality of chain
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	588	
44	p	652	
45	q	347	
46	r	31	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 98333 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Met-tRNAi (U31:A39 variant).

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

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

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

- Molecule 3 is a RNA chain called mRNA.

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

- Molecule 4 is a protein called uS2.

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

- Molecule 5 is a protein called eS1.

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

- Molecule 6 is a protein called uS5.

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

- Molecule 7 is a protein called uS3.

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

- Molecule 8 is a protein called eS4.

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

- Molecule 9 is a protein called uS7.

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

- Molecule 10 is a protein called eS6.

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

- Molecule 11 is a protein called eS7.

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

- Molecule 12 is a protein called eS8.

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

- Molecule 13 is a protein called uS4.

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

- Molecule 14 is a protein called eS10.

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

- Molecule 15 is a protein called uS17.

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

- Molecule 16 is a protein called eS12.

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

- Molecule 17 is a protein called uS15.

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

- Molecule 18 is a protein called uS11.

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

- Molecule 19 is a protein called uS19.

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

- Molecule 20 is a protein called uS9.

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

- Molecule 21 is a protein called eS17.

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

- Molecule 22 is a protein called uS13.

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

- Molecule 23 is a protein called eS19.

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

- Molecule 24 is a protein called uS10.

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

- Molecule 25 is a protein called eS21.

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

- Molecule 26 is a protein called uS8.

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

- Molecule 27 is a protein called uS12.

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

- Molecule 28 is a protein called eS24.

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

- Molecule 29 is a protein called eS25.

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

- Molecule 30 is a protein called eS26.

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

- Molecule 31 is a protein called eS27.

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

- Molecule 32 is a protein called eS28.

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

- Molecule 33 is a protein called uS14.

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

- Molecule 34 is a protein called eS30.

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

- Molecule 35 is a protein called eS31.

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

- Molecule 36 is a protein called RACK1.

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

- Molecule 37 is a protein called eL41.

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

- Molecule 38 is a protein called eIF1A.

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

- Molecule 39 is a protein called eIF2 alpha.

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

- Molecule 40 is a protein called eIF2 gamma.

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

- Molecule 41 is a protein called eIF2 beta.

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

- Molecule 42 is a protein called eIF1.

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

- Molecule 43 is a protein called eIF3a.

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

- Molecule 44 is a protein called eIF3c.

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

- Molecule 45 is a protein called eIF3i.

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

- Molecule 46 is a protein called eIF3b.

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

- Molecule 47 is a protein called eIF3g.

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

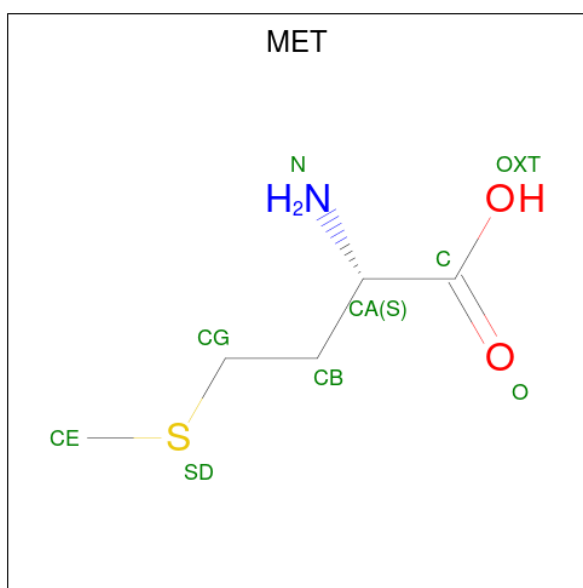
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

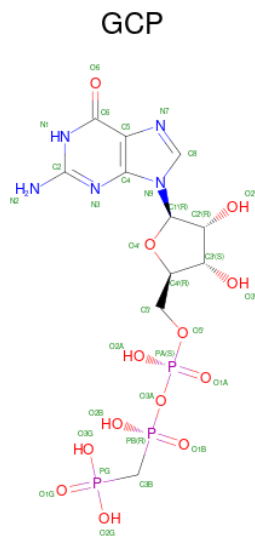
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



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

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

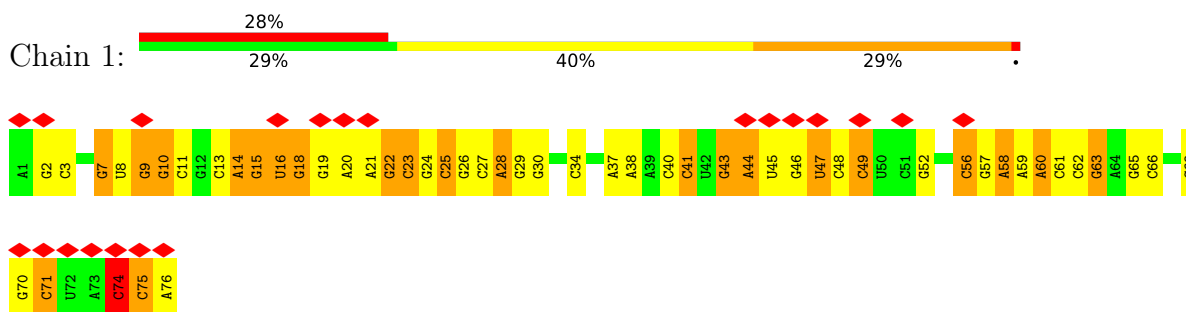


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

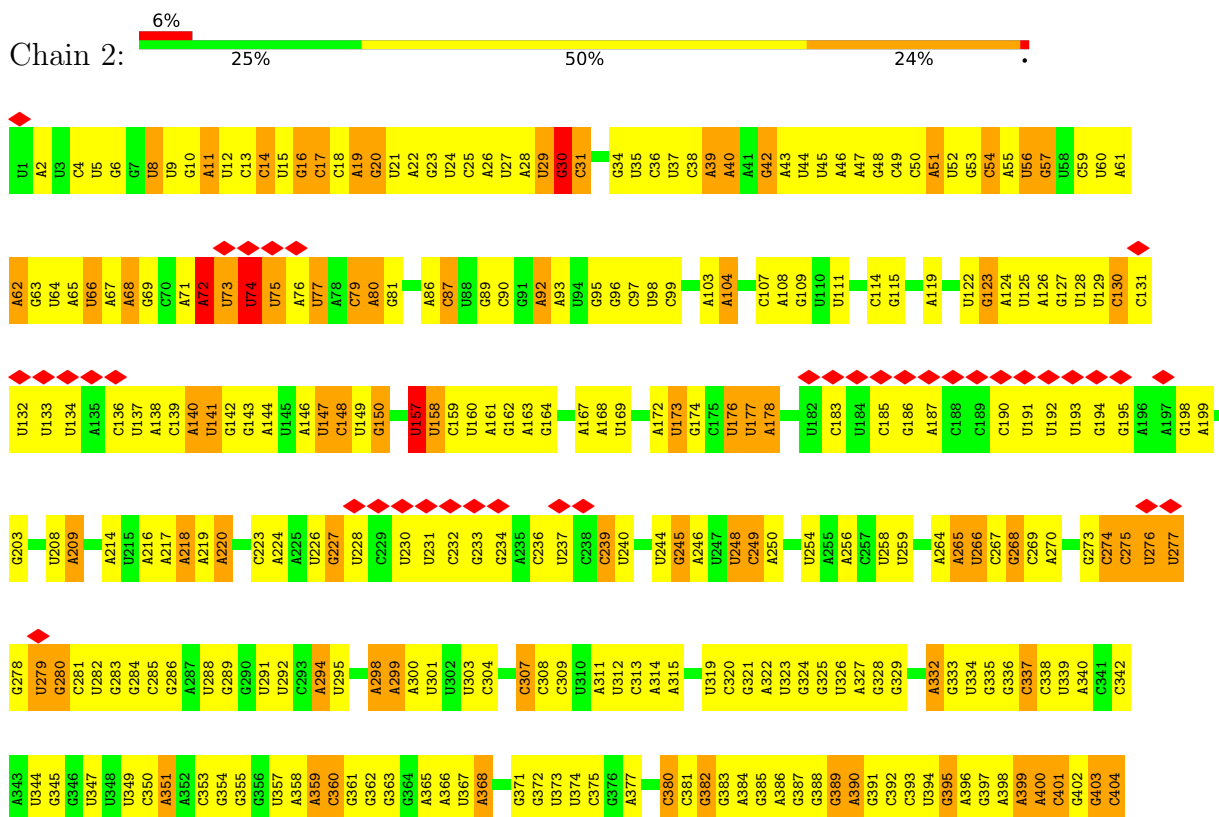
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

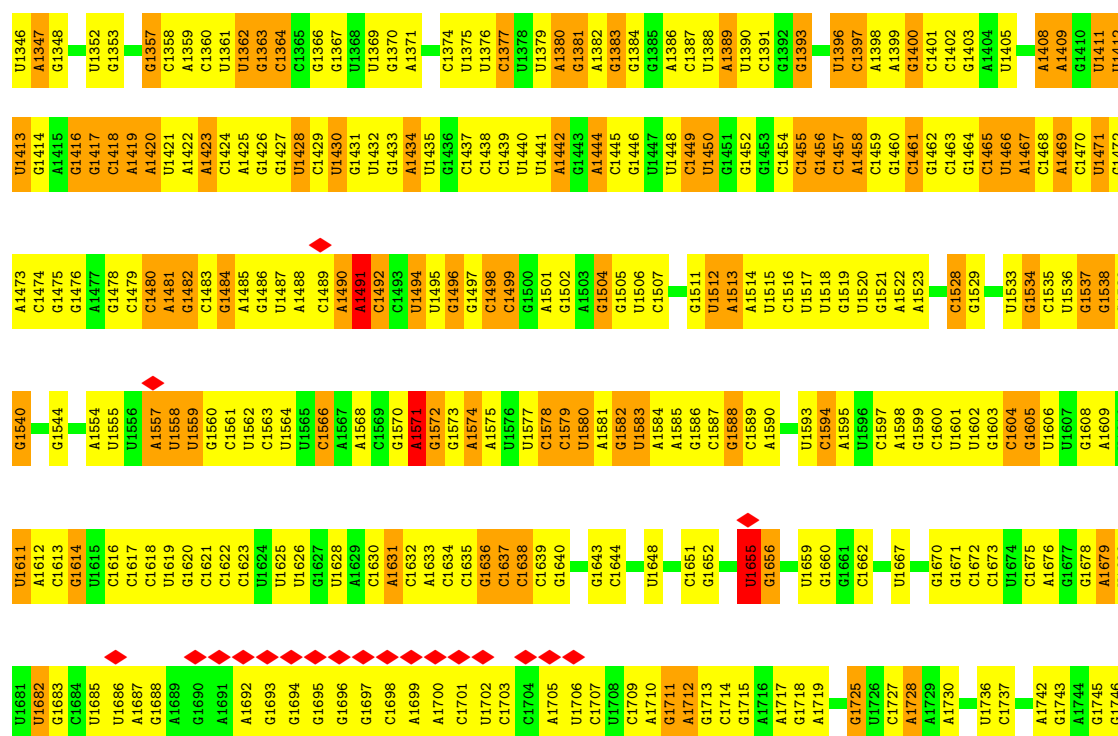
• Molecule 1: Met-tRNAi (U31:A39 variant)



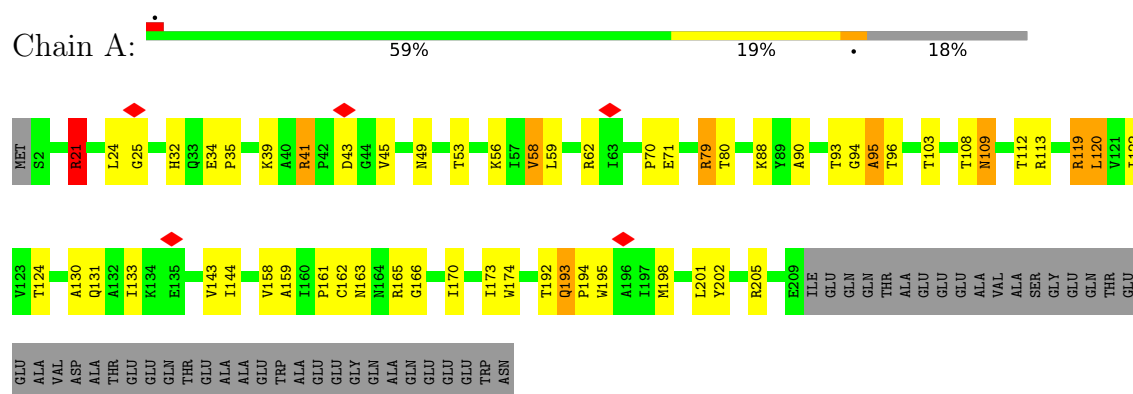
• Molecule 2: 18S rRNA



U1281	U1282	C1283	U1284	U1285	A1286	G1287	U1288	U1289	G1290	G1291	U1292	G1293	G1294	A1295	G1296	U1297	G1298	A1299	U1300	U1301	U1302	G1303	U1304	C1305	U1306	G1307	C1308	U1309	U1310	A1311	A1312	U1313	U1314	G1315	C1316	G1317	A1318	U1319	A1320	C1321	C1322	G1323	A1324	A1328	C1332	U1333	U1334	A1335	U1336	C1337	C1338	U1339	A1340	A1343	A1344	A1345																																																																																																																																																																				
G1214	C1215	A1216	G1217	A1218	C1221	A1222	A1223	A1224	A1225	A1226	G1227	G1228	A1229	U1230	U1231	G1232	A1243	G1244	C1245	C1247	U1250	C1251	U1252	U1253	A1254	U1255	U1256	U1257	U1258	U1259	G1260	U1261	G1262	G1263	G1266	G1267	U1268	A1269	U1270	A1271	U1272	C1273	U1274	U1275	G1276	G1277	C1278	G1279	G1280																																																																																																																																																																											
G1153	G1154	C1155	A1156	C1157	A1158	A1159	C1160	A1161	A1162	G1163	G1164	A1165	G1166	U1167	G1168	G1169	A1170	G1171	C1172	C1173	U1174	G1175	G1176	G1177	G1178	C1179	A1182	A1183	U1184	U1185	U1186	G1187	A1188	C1189	U1190	C1191	A1192	A1193	C1194	A1195	C1196	G1197	G1198	G1199	G1200	A1201	A1202	A1203	C1204	A1205	C1206	A1207	C1208	C1209	A1210	G1211	G1212	U1213																																																																																																																																																																		
U1088	C1089	A1090	A1091	A1092	G1093	U1094	C1095	U1096	U1097	U1098	G1099	G1100	G1101	U1102	U1103	G1106	G1107	G1108	U1109	G1110	G1111	A1112	G1113	U1114	A1115	G1116	G1117	G1118	U1119	C1120	A1123	A1124	G1125	G1126	C1127	U1128	G1129	A1132	G1133	U1134	U1135	A1136	A1137	A1138	G1139	G1140	A1141	A1142	U1143	U1144	G1145	A1146	C1149	A1150																																																																																																																																																																						
A1025	A1026	C1027	U1030	G1031	C1032	G1033	G1034	A1038	G1039	G1040	G1041	A1042	U1043	C1044	G1045	G1046	G1047	U1048	G1049	G1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	G1063	C1065	C1066	C1067	A1068	C1069	U1070	C1071	G1072	G1073	C1074	A1075	C1076	U1077	U1078	U1079	A1080	C1081	G1082	A1083	G1084	A1085	A1086	A1087																																																																																																																																																																						
U958	U959	A962	A965	A966	U967	C968	A969	G970	G971	C974	G975	A976	A977	A978	U981	A982	G983	G984	G985	G986	A987	A991	A992	G993	A994	U995	G996	A997	C999	U1000	U1003	A1004	C1005	C1006	G1007	U1008	C1009	U1010	U1011	A1012	G1013	U1014	C1015	U1016	U1017	A1018	A1019	G1021	A1022	U1023	A1085	A1024																																																																																																																																																																								
G922	G923	U924	U925	U926	C927	A928	U929	U930	U931	U932	G933	U934	U935	C936	G937	U938	U939	C941	U942	G943	G944	G945	A946	C947	C948	C951	G952	U953	A954	U955	U956	A957	U958	U959	A960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087																																																										
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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	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038</																																							

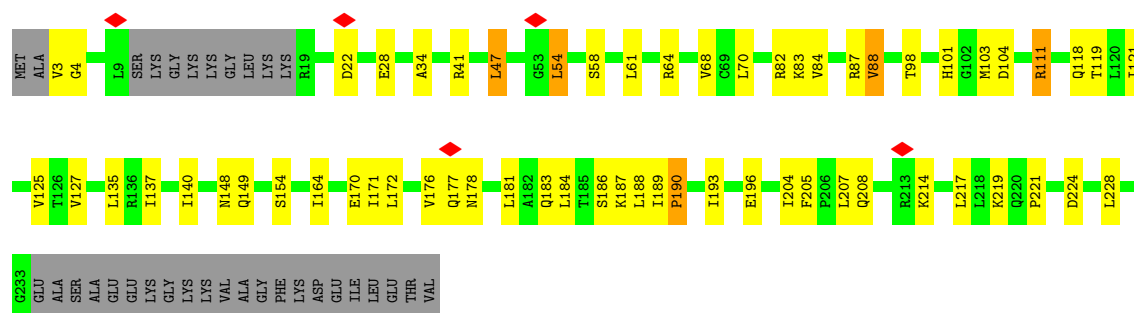


• Molecule 4: uS2

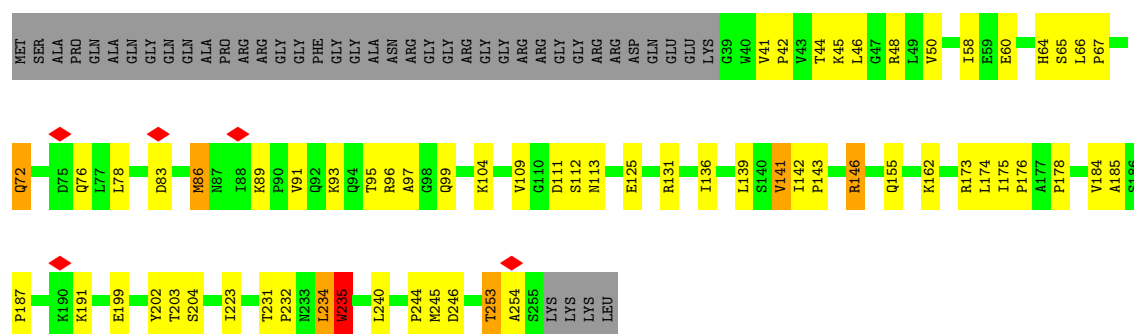


• Molecule 5: eS1

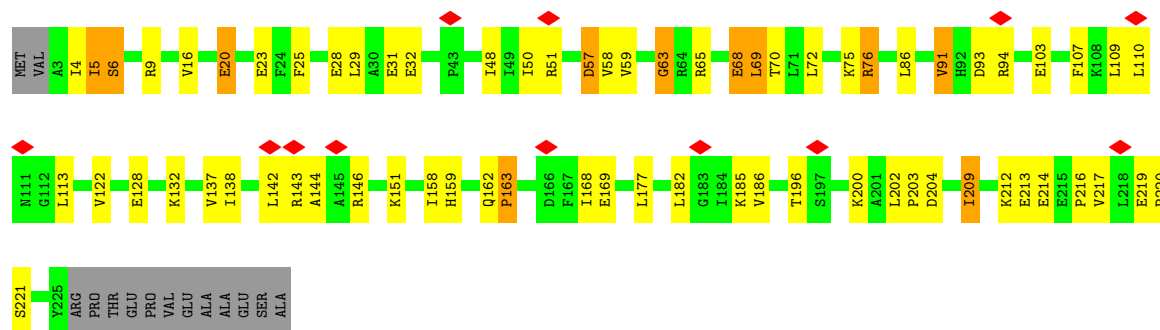




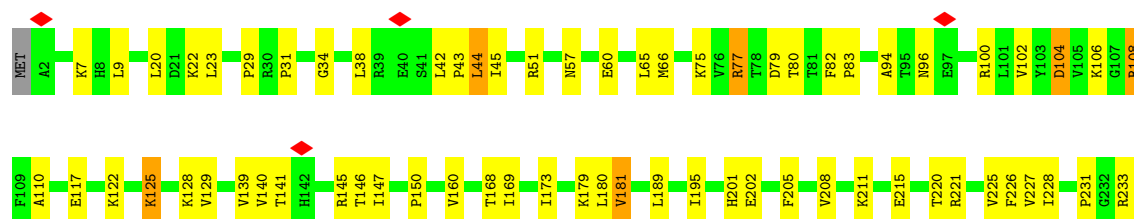
• Molecule 6: uS5

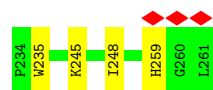


• Molecule 7: uS3

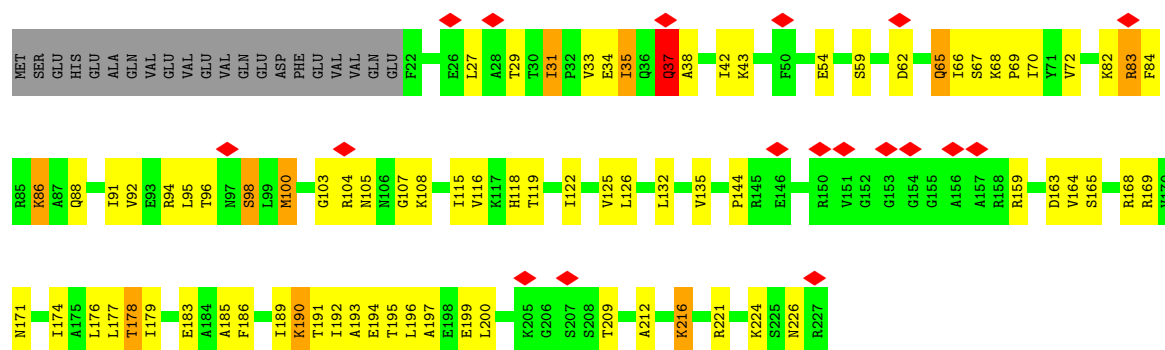


• Molecule 8: eS4

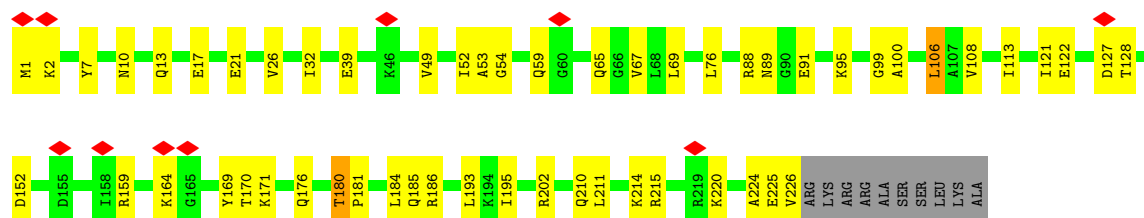




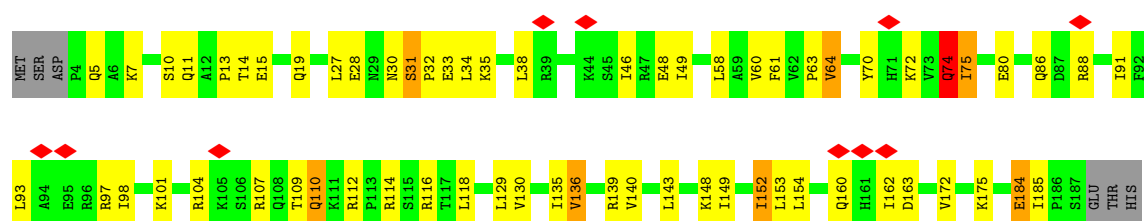
• Molecule 9: uS7



• Molecule 10: eS6



• Molecule 11: eS7

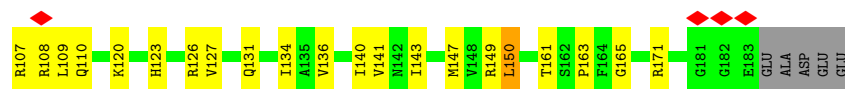
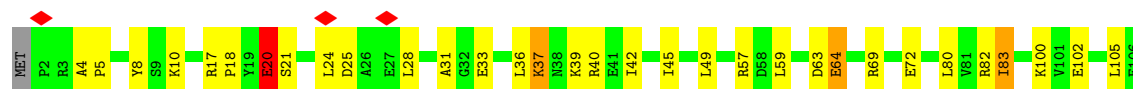


• Molecule 12: eS8

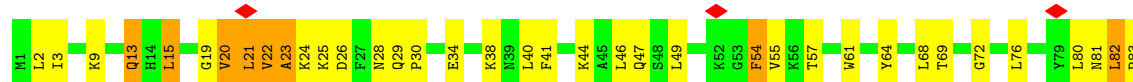




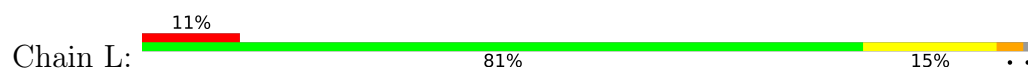
• Molecule 13: uS4



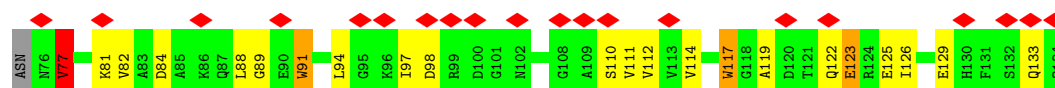
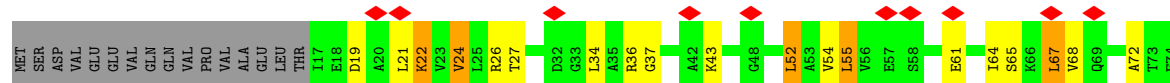
• Molecule 14: eS10



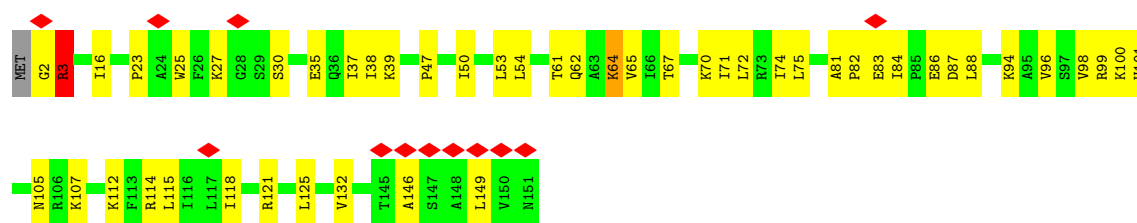
• Molecule 15: uS17



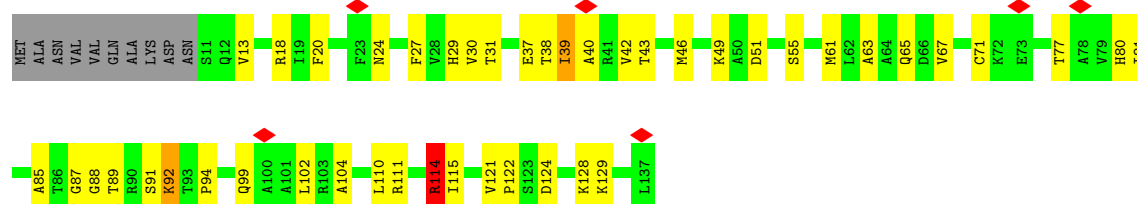
• Molecule 16: eS12



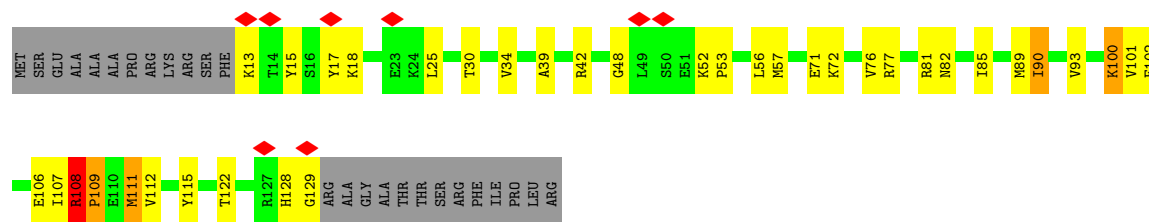
• Molecule 17: uS15



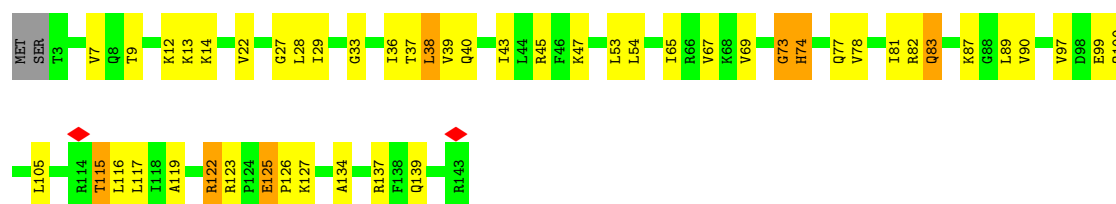
• Molecule 18: uS11



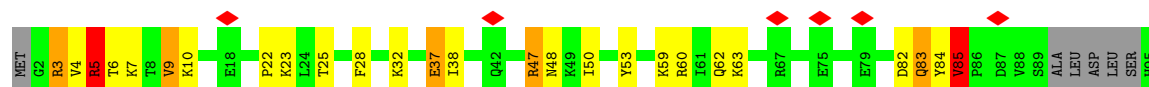
• Molecule 19: uS19

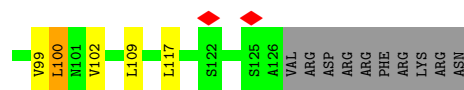


• Molecule 20: uS9

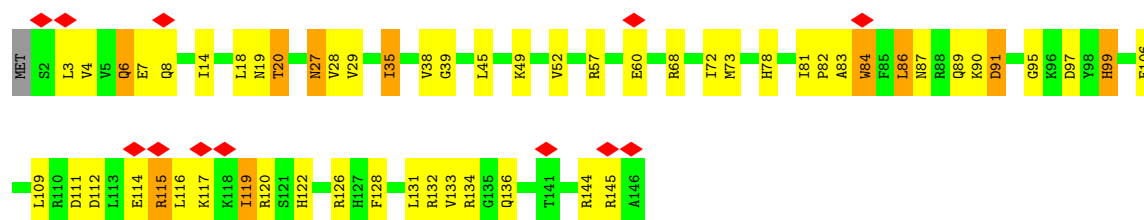


• Molecule 21: eS17

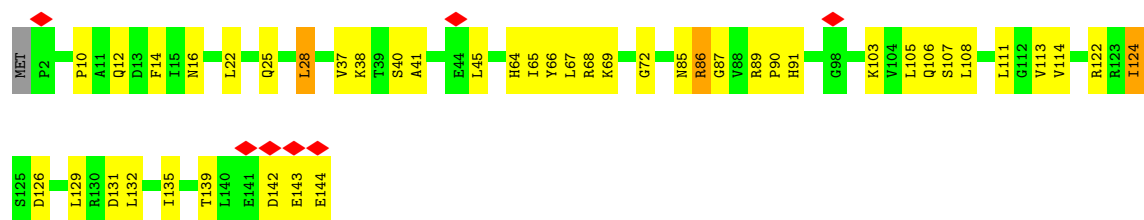




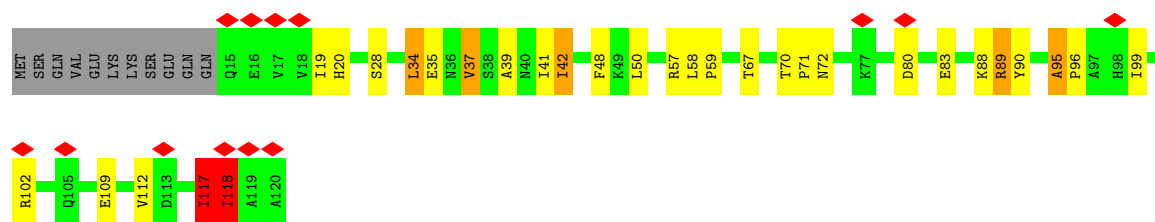
• Molecule 22: uS13



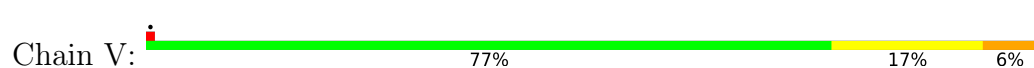
• Molecule 23: eS19



• Molecule 24: uS10

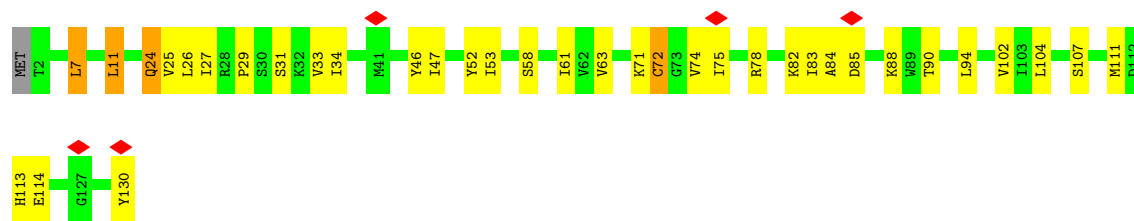


• Molecule 25: eS21

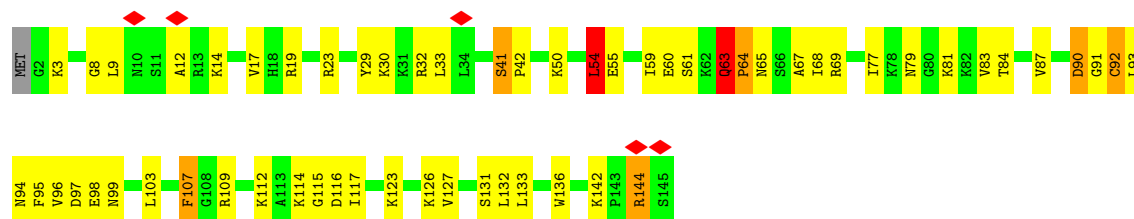


• Molecule 26: uS8

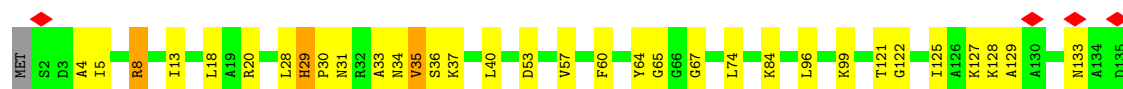
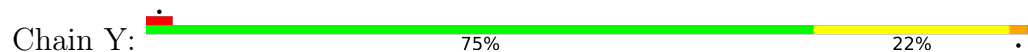




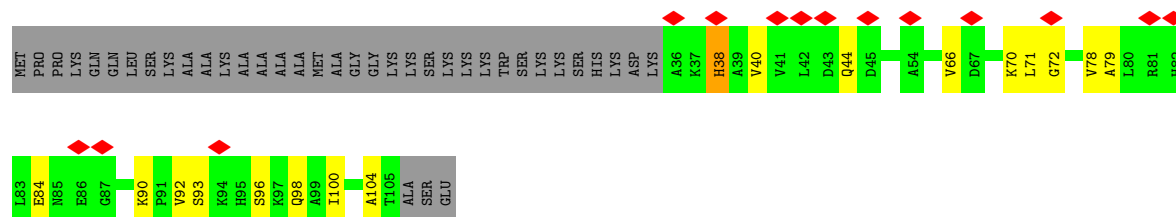
• Molecule 27: uS12



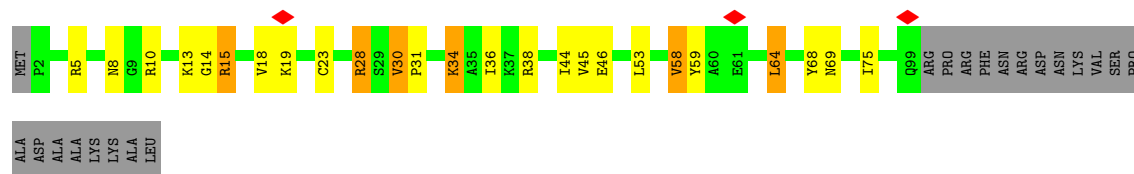
• Molecule 28: eS24



• Molecule 29: eS25

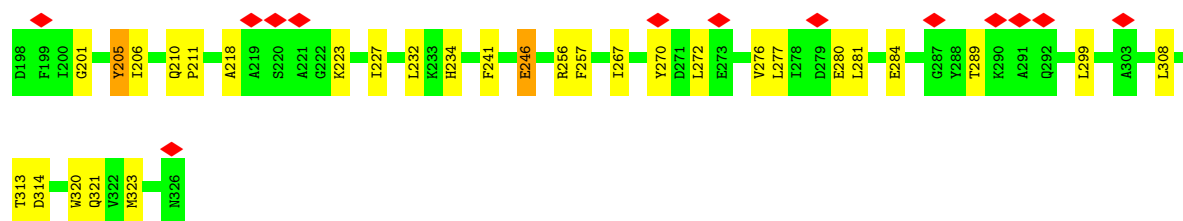


• Molecule 30: eS26

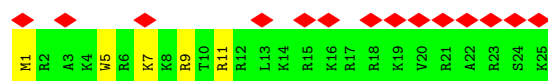
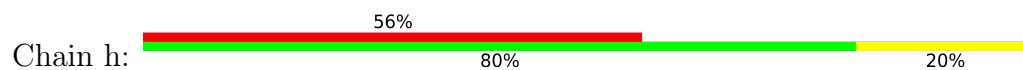


• Molecule 31: eS27

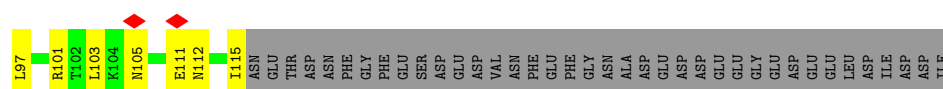




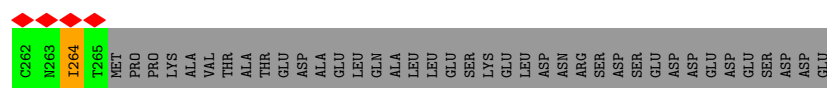
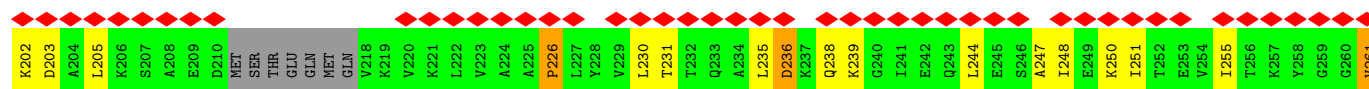
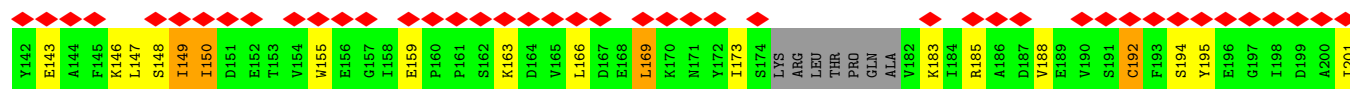
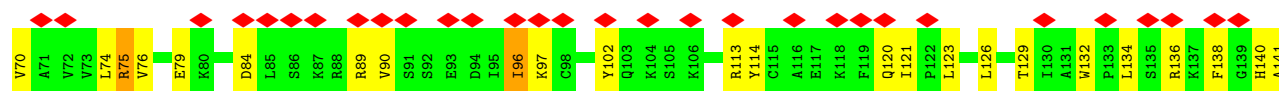
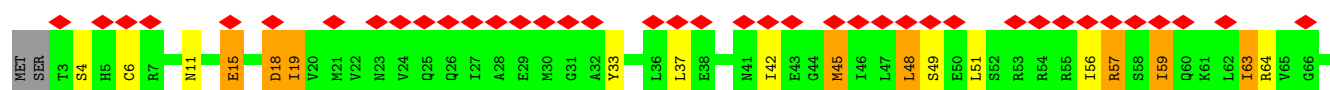
• Molecule 37: eL41



• Molecule 38: eIF1A

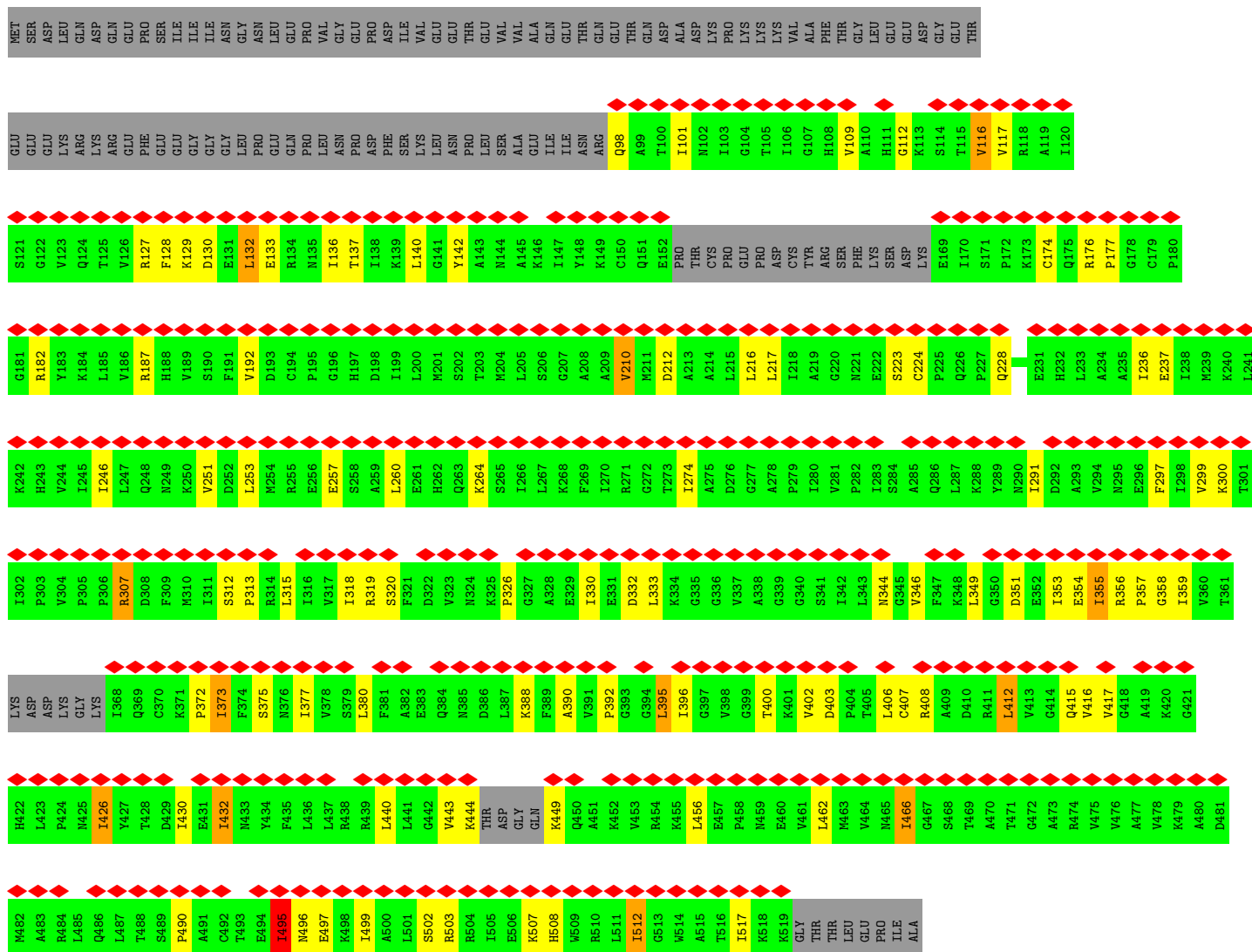


• Molecule 39: eIF2 alpha

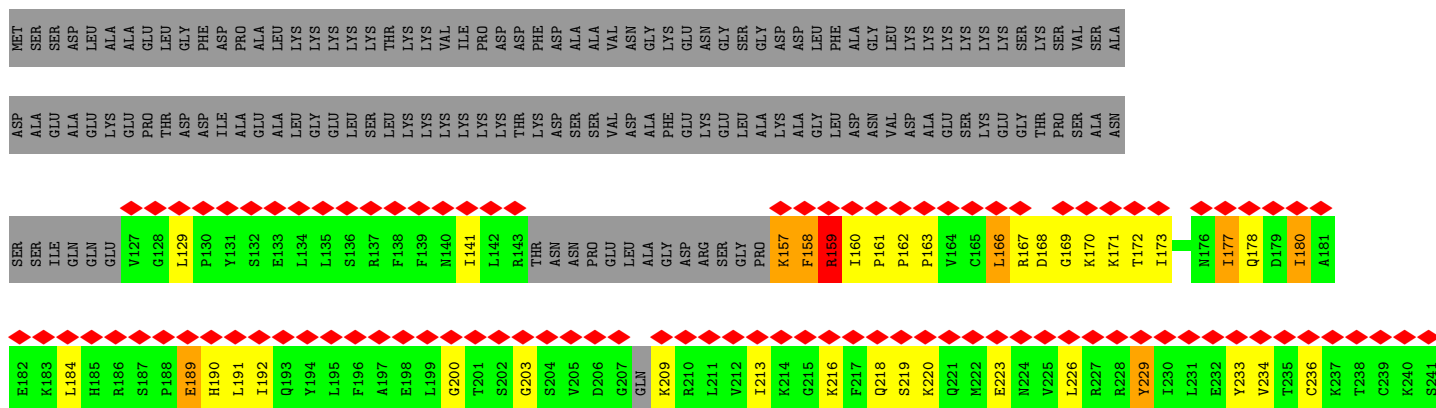
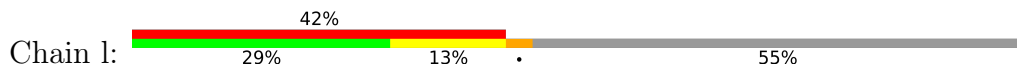


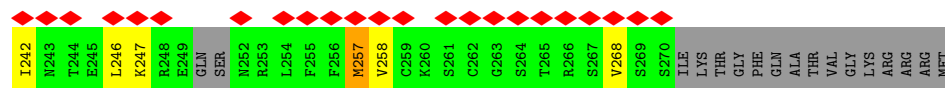
• Molecule 40: eIF2 gamma

Chain k:

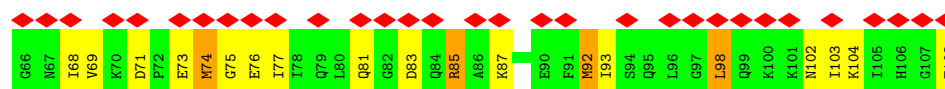
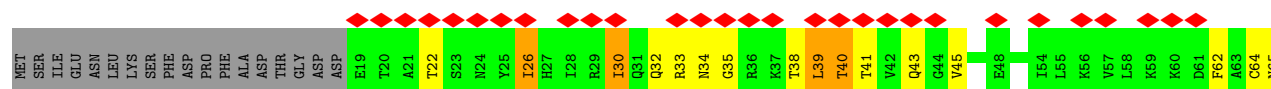


Chain 1:

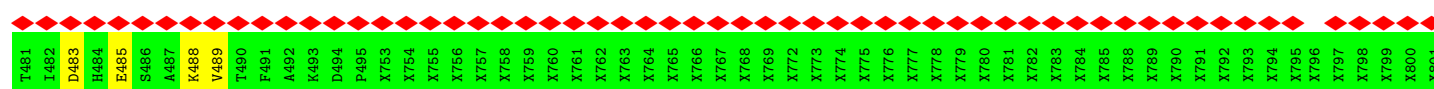
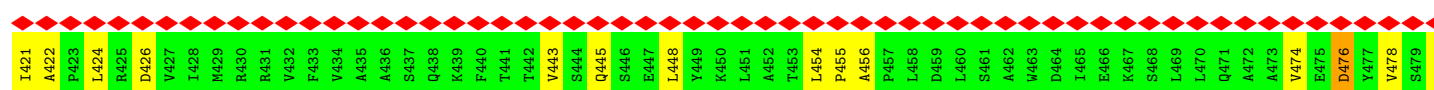
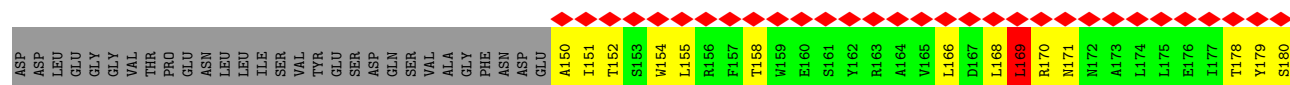
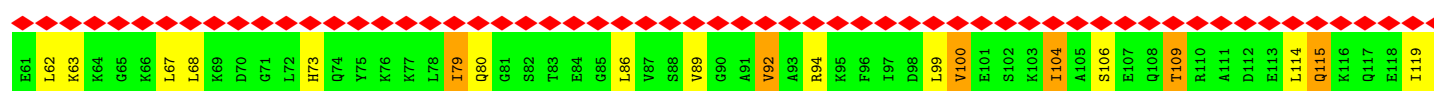
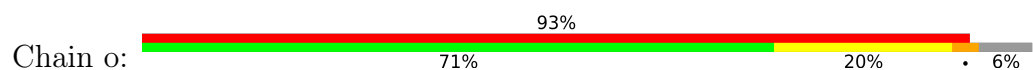


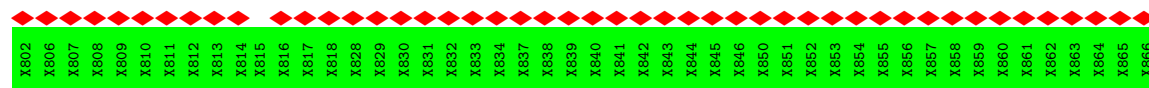


• Molecule 42: eIF1

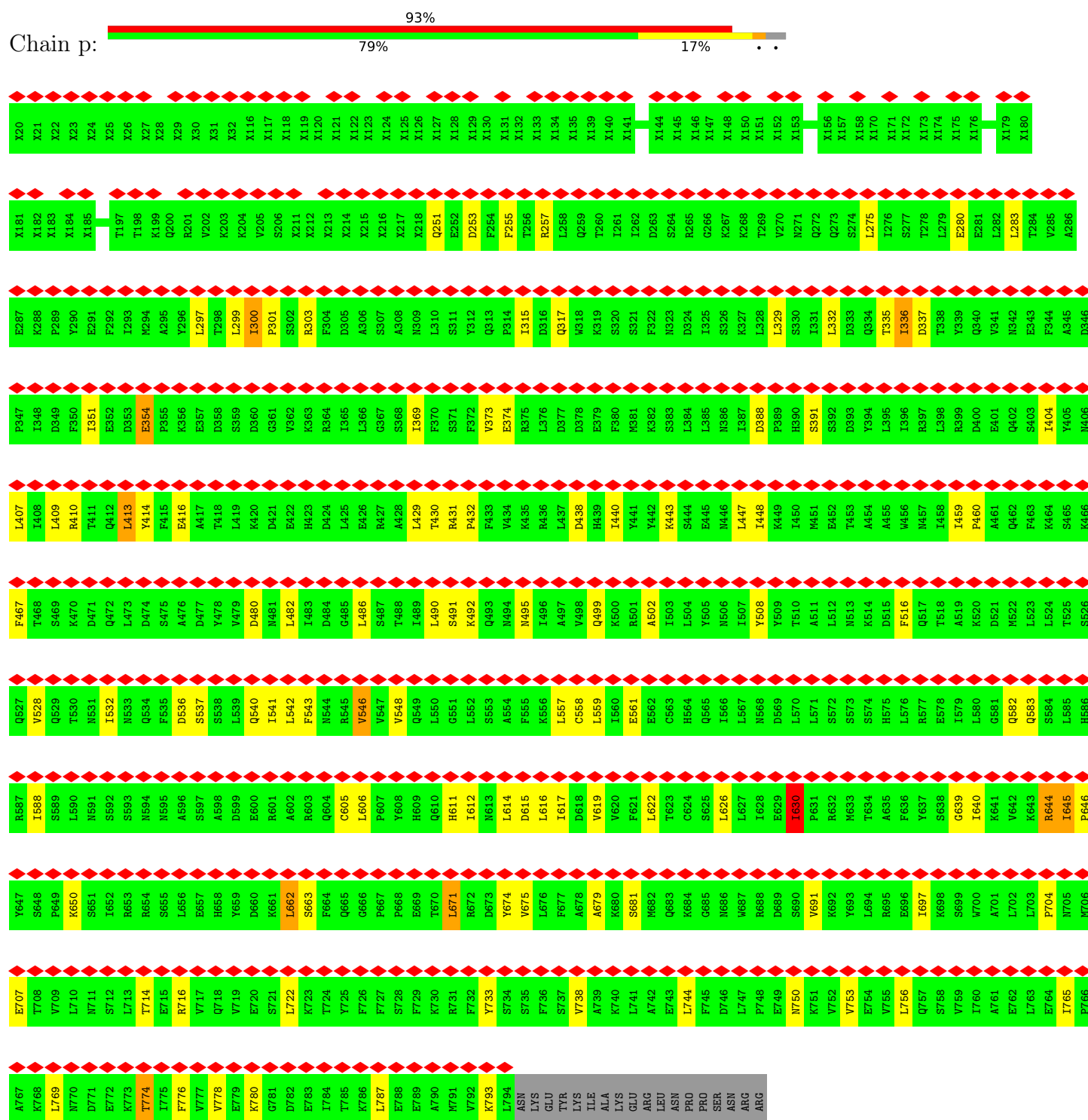


• Molecule 43: eIF3a

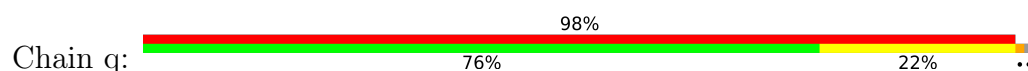




• Molecule 44: eIF3c

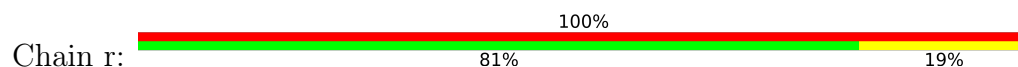


• Molecule 45: eIF3i



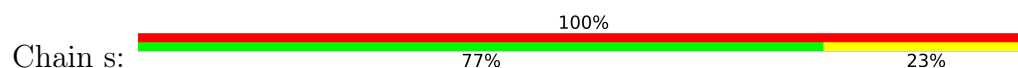
I301	S302	P303	Q304	G305	T306	S307	Y308	A309	S310	G311	G312	E313	D314	G315	F316	I317	R318	L319	H320	H321	F322	E323	K324	S325	Y326	F327	D328	F329	K330	Y331	D332	V333	E334	K335	A336	A337	E338	A339	K340	E341	H342	MET	GLN	GLU	ALA	ASN													
N241	T242	A243	V244	T245	T246	P247	L248	K249	E250	F251	I252	I253	L254	G255	G256	G257	Q258	E259	A260	K261	D262	V263	T264	T265	T266	S267	A268	N269	E270	G271	K272	F273	E274	A275	R276	F277	Y278	H279	K280	S281	F282	E283	E284	E285	I286	G287	R288	V289	Q290	G291	H292	F293	G294	P295	L296	H297	T298	V299	A300
D181	V182	S183	N184	M185	Y186	E187	Y188	V189	D190	S191	I192	D193	L194	H195	E196	K197	S198	I199	S200	D201	H202	Q203	F204	S205	P206	D207	L208	T209	V210	F211	T212	T213	S214	S215	R216	D217	T218	N219	S220	F221	L222	V223	D224	V225	S226	T227	L228	Q229	V230	L231	K232	K233	Y234	E235	T236	D237	C238	P239	L240
S121	T122	M123	T124	Y125	E126	I127	E128	R129	D130	S131	A132	T133	H134	E135	L136	T137	K138	V139	S140	E141	D142	P143	T144	H145	K146	I147	T148	H149	H150	E151	G152	L153	D154	A155	A156	T157	V158	A159	G160	W161	S162	T163	K164	G165	K166	Y167	T168	I169	A170	G171	H172	K173	D174	G175	K176	I177	S178	K179	Y180
D61	C62	F63	T64	K65	Y66	C67	C68	T69	G70	S71	A72	D73	Y74	S75	I76	K77	L78	W79	D80	V81	S82	N83	G84	Q85	C86	W87	A88	T89	W90	K91	S92	P93	V94	P95	V96	K97	R98	V99	E100	F101	S102	P103	C104	G105	N106	Y107	F108	L109	A110	T111	L112	D113	N114	V115	M116	K117	N118	P119	G120

● Molecule 46: eIF3b



L704	H705	Q706	R707	E708	L709	L710	K711	W712	W713	T714	E715	Y716	R717	E718	K719	I720	G721	Q722	E723	H724	E725	K726	S727	M728	S729	F730	K731	I732	F733	D734
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● Molecule 47: eIF3g



V45	H46	K47	S48	V49	A50	E51	R52	K53	N54	W55	H56	K57	Y58	G59	S60	E61	K62	G63	S64	P65	A66	G67	P68	S69	A70	V71	T72	A73	R74	L75	G76	E77	E78	V79	E80	L81	R82	L83	S84	R85	N86	W87	K88	Q89	A90	E91	E92	E93	R94	I95	Q96
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21401	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, GCP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.41	0/1797	0.78	5/2799 (0.2%)
2	2	0.40	0/42269	0.80	37/65862 (0.1%)
3	3	0.41	0/317	0.81	0/489
4	A	0.55	0/1666	1.11	0/2279
5	B	0.53	0/1793	1.01	2/2414 (0.1%)
6	C	0.50	0/1659	1.08	3/2252 (0.1%)
7	D	0.54	0/1769	1.07	1/2378 (0.0%)
8	E	0.49	0/2122	0.96	0/2861
9	F	0.56	0/1628	1.14	2/2198 (0.1%)
10	G	0.54	0/1835	1.00	0/2451
11	H	0.58	0/1507	1.08	2/2028 (0.1%)
12	I	0.49	0/1515	1.04	0/2029
13	J	0.50	0/1495	1.10	0/2001
14	K	0.57	0/831	1.14	0/1123
15	L	0.55	0/1276	0.91	0/1718
16	M	0.66	0/891	1.11	0/1201
17	N	0.51	0/1210	1.17	0/1628
18	O	0.54	0/953	1.02	0/1279
19	P	0.57	0/946	1.16	2/1273 (0.2%)
20	Q	0.56	0/1125	1.08	2/1510 (0.1%)
21	R	0.59	0/969	1.14	3/1299 (0.2%)
22	S	0.56	0/1212	1.10	0/1629
23	T	0.50	0/1129	1.14	0/1520
24	U	0.59	0/857	1.10	2/1158 (0.2%)
25	V	0.47	0/696	0.94	0/938
26	W	0.48	0/1039	1.07	1/1399 (0.1%)
27	X	0.49	0/1137	1.04	1/1516 (0.1%)
28	Y	0.49	0/1075	1.08	2/1433 (0.1%)
29	Z	0.60	0/567	1.03	0/762
30	a	0.54	0/791	0.95	0/1059
31	b	0.51	0/619	0.94	1/837 (0.1%)
32	c	0.57	0/489	0.84	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.47	0/457	0.86	0/607
34	e	0.53	0/440	1.03	0/586
35	f	0.67	0/559	1.06	0/747
36	g	0.54	0/2521	0.87	3/3431 (0.1%)
37	h	0.40	0/234	1.11	0/300
38	i	0.51	0/894	0.95	1/1188 (0.1%)
39	j	0.63	0/2034	1.12	6/2737 (0.2%)
40	k	0.71	0/3079	1.03	3/4157 (0.1%)
41	l	0.64	0/1051	1.05	2/1402 (0.1%)
42	m	0.56	0/724	1.13	4/968 (0.4%)
43	o	0.61	0/3796	1.22	9/5128 (0.2%)
44	p	0.63	1/4602 (0.0%)	1.17	4/6226 (0.1%)
45	q	0.69	0/2757	0.99	6/3733 (0.2%)
46	r	0.52	0/282	1.14	1/373 (0.3%)
47	s	0.62	0/426	0.97	0/571
All	All	0.51	1/103040 (0.0%)	0.95	105/148132 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	p	630	ILE	CA-CB	5.80	1.57	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1157	C	C4'-C3'-O3'	10.34	124.91	109.40
2	2	685	A	C2'-C3'-O3'	9.06	127.30	113.70
2	2	279	U	C2'-C3'-O3'	8.80	122.71	109.50
2	2	1430	U	C2'-C3'-O3'	8.38	122.07	109.50
2	2	1080	A	C4'-C3'-O3'	8.24	121.76	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	538	G	C2'-C3'-O3'	7.99	121.48	109.50
2	2	277	U	C2'-C3'-O3'	7.92	121.39	109.50
24	U	95	ALA	CA-C-N	7.66	129.41	119.84
24	U	95	ALA	C-N-CA	7.66	129.41	119.84
41	l	258	VAL	N-CA-C	7.50	117.97	108.82
19	P	111	MET	N-CA-C	-7.41	104.49	113.97
45	q	267	SER	N-CA-C	7.38	119.97	111.11
2	2	1030	U	C4'-C3'-O3'	7.26	120.29	109.40
1	1	47	U	C2'-C3'-O3'	7.00	120.00	109.50
2	2	239	C	C2'-C3'-O3'	7.00	120.00	109.50
2	2	721	U	C4'-C3'-O3'	6.97	119.86	109.40
2	2	828	A	C2'-C3'-O3'	6.87	119.80	109.50
2	2	564	C	C2'-C3'-O3'	6.82	119.72	109.50
43	o	391	ILE	N-CA-C	6.75	116.76	110.42
43	o	397	VAL	N-CA-C	6.74	117.24	110.23
45	q	238	CYS	CA-C-N	6.74	128.26	119.84
45	q	238	CYS	C-N-CA	6.74	128.26	119.84
43	o	62	LEU	N-CA-C	6.64	118.41	111.03
39	j	194	SER	N-CA-C	6.61	117.20	108.07
43	o	353	ARG	N-CA-C	-6.41	103.12	111.71
2	2	1411	U	C2'-C3'-O3'	6.40	119.10	109.50
2	2	1455	C	C4'-C3'-O3'	6.33	118.90	109.40
2	2	1491	A	C4'-C3'-O3'	6.31	122.47	113.00
2	2	157	U	C4'-C3'-O3'	6.31	118.86	109.40
2	2	524	A	C1'-C2'-O2'	-6.24	102.44	111.80
28	Y	29	HIS	CA-C-N	6.21	127.61	119.84
28	Y	29	HIS	C-N-CA	6.21	127.61	119.84
2	2	74	U	C4'-C3'-O3'	6.18	118.67	109.40
2	2	1655	U	C4'-C3'-O3'	6.18	118.67	109.40
1	1	74	C	C2'-C3'-O3'	6.16	118.75	109.50
43	o	169	LEU	N-CA-C	6.15	120.04	112.54
2	2	1491	A	C2'-C3'-O3'	6.12	122.88	113.70
2	2	66	U	C4'-C3'-O3'	6.10	118.55	109.40
44	p	662	LEU	N-CA-C	6.07	118.13	110.24
2	2	72	A	C4'-C3'-O3'	6.06	118.48	109.40
40	k	356	ARG	N-CA-C	6.05	123.19	109.81
39	j	159	GLU	N-CA-C	5.99	117.44	109.83
44	p	300	ILE	O-C-N	5.95	124.30	120.07
2	2	1534	G	C4'-C3'-O3'	5.95	118.33	109.40
1	1	7	G	C2'-C3'-O3'	5.95	118.42	109.50
2	2	700	C	C2'-C3'-O3'	5.92	122.59	113.70
41	l	203	GLY	N-CA-C	5.89	118.52	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	q	271	GLY	N-CA-C	-5.88	106.63	115.32
9	F	105	ASN	N-CA-C	5.84	118.41	110.06
21	R	100	LEU	N-CA-C	5.80	118.68	110.50
2	2	1110	G	C1'-C2'-O2'	-5.79	103.11	111.80
45	q	46	GLY	N-CA-C	5.78	119.43	110.88
20	Q	125	GLU	CA-C-N	5.74	127.02	119.84
20	Q	125	GLU	C-N-CA	5.74	127.02	119.84
40	k	430	ILE	N-CA-C	5.71	116.70	108.48
43	o	456	ALA	N-CA-C	5.69	121.36	113.45
46	r	732	ILE	N-CA-C	5.68	115.73	108.12
2	2	466	G	C4'-C3'-O3'	5.68	121.52	113.00
45	q	65	LYS	N-CA-C	-5.61	108.22	114.62
36	g	197	ALA	N-CA-C	5.61	118.40	110.50
44	p	630	ILE	O-C-N	5.60	124.01	120.42
42	m	45	VAL	CA-C-N	5.58	126.81	119.84
42	m	45	VAL	C-N-CA	5.58	126.81	119.84
11	H	75	ILE	N-CA-C	5.57	116.02	110.23
2	2	1571	A	C4'-C3'-O3'	5.55	117.72	109.40
43	o	92	VAL	N-CA-CB	5.54	118.08	110.54
39	j	150	ILE	N-CA-CB	5.54	117.03	110.55
2	2	922	A	C4'-C3'-O3'	-5.53	104.71	113.00
5	B	205	PHE	CA-C-N	5.52	126.74	119.84
5	B	205	PHE	C-N-CA	5.52	126.74	119.84
31	b	31	HIS	N-CA-C	5.52	115.40	108.45
2	2	1320	A	C4'-C3'-O3'	5.51	117.66	109.40
6	C	231	THR	CA-C-N	5.49	126.70	119.84
6	C	231	THR	C-N-CA	5.49	126.70	119.84
2	2	1206	C	C4'-C3'-O3'	5.45	117.57	109.40
39	j	45	MET	N-CA-C	5.41	117.72	108.90
43	o	100	VAL	N-CA-CB	5.38	117.85	110.54
44	p	546	VAL	N-CA-CB	5.35	116.81	110.55
36	g	38	SER	N-CA-C	5.35	115.19	108.45
38	i	34	GLU	N-CA-C	5.34	116.76	109.18
2	2	30	G	C4'-C3'-O3'	-5.28	105.08	113.00
43	o	422	ALA	O-C-N	5.23	124.52	120.38
9	F	103	GLY	N-CA-C	5.23	120.23	113.27
21	R	53	TYR	CB-CA-C	5.22	120.69	110.67
40	k	223	SER	N-CA-C	5.19	117.23	110.43
1	1	7	G	C4'-C3'-O3'	5.19	117.18	109.40
1	1	58	A	C2'-C3'-O3'	5.17	117.26	109.50
42	m	30	ILE	N-CA-C	5.17	111.74	106.21
2	2	130	C	C4'-C3'-O3'	5.15	117.12	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	97	ARG	N-CA-C	5.13	116.69	111.14
39	j	192	CYS	N-CA-C	5.12	116.90	110.24
26	W	111	MET	N-CA-C	5.12	114.90	108.45
27	X	33	LEU	N-CA-C	5.12	116.71	111.03
42	m	76	GLU	N-CA-C	-5.10	95.81	107.48
2	2	351	A	C2'-C3'-O3'	5.09	117.14	109.50
39	j	149	ILE	N-CA-CB	5.08	117.45	110.54
2	2	299	A	C4'-C3'-O3'	-5.07	105.39	113.00
7	D	76	ARG	N-CA-C	5.07	116.65	111.03
2	2	695	U	C2'-C3'-O3'	5.06	117.09	109.50
2	2	564	C	C4'-C3'-O3'	5.06	116.98	109.40
2	2	542	C	C2'-C3'-O3'	5.05	117.07	109.50
6	C	141	VAL	N-CA-C	5.03	119.81	109.34
19	P	15	TYR	N-CA-C	5.03	116.49	107.80
36	g	20	TRP	N-CA-C	5.02	117.62	110.24
21	R	85	VAL	N-CA-C	5.01	119.69	108.88

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts [\(i\)](#)

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	1	1607	0	815	53	0
2	2	37797	0	19016	892	0
3	3	287	0	149	2	0
4	A	1626	0	1633	21	0
5	B	1769	0	1829	16	0
6	C	1629	0	1710	28	0
7	D	1744	0	1826	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	2078	0	2157	24	0
9	F	1609	0	1679	34	0
10	G	1812	0	1911	25	0
11	H	1483	0	1579	18	0
12	I	1489	0	1504	20	0
13	J	1471	0	1554	18	0
14	K	809	0	810	18	0
15	L	1248	0	1311	10	0
16	M	885	0	917	20	0
17	N	1187	0	1251	19	0
18	O	942	0	979	19	0
19	P	927	0	971	18	0
20	Q	1105	0	1170	21	0
21	R	959	0	1006	19	0
22	S	1193	0	1217	25	0
23	T	1110	0	1124	18	0
24	U	845	0	913	13	0
25	V	687	0	682	9	0
26	W	1021	0	1056	15	0
27	X	1119	0	1198	27	0
28	Y	1061	0	1111	11	0
29	Z	558	0	585	7	0
30	a	779	0	831	11	0
31	b	609	0	630	10	0
32	c	487	0	528	5	0
33	d	446	0	436	4	0
34	e	433	0	470	3	0
35	f	546	0	557	8	0
36	g	2466	0	2406	36	0
37	h	233	0	284	4	0
38	i	884	0	891	13	0
39	j	2006	0	2066	32	0
40	k	3034	0	3195	48	0
41	l	1036	0	1079	22	0
42	m	716	0	742	15	0
43	o	4189	0	3874	64	0
44	p	4899	0	4599	46	0
45	q	2693	0	2609	36	0
46	r	277	0	273	2	0
47	s	418	0	411	5	0
48	2	80	0	0	0	0
48	k	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	a	1	0	0	0	0
49	b	1	0	0	0	0
49	f	1	0	0	0	0
49	l	1	0	0	1	0
50	k	8	0	8	0	0
51	k	32	0	14	1	0
All	All	98333	0	79566	1670	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 10.

All (1670) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:567:G:H22	2:2:573:G:N2	1.34	1.24
2:2:567:G:N2	2:2:573:G:H22	1.36	1.23
36:g:20:TRP:HB3	36:g:313:THR:HA	1.19	1.08
2:2:480:A:N1	2:2:506:U:O4	1.89	1.05
2:2:1292:U:O4	2:2:1321:A:N1	1.89	1.05
44:p:626:LEU:HD11	44:p:679:ALA:HB2	1.35	1.05
1:1:18:G:H1'	1:1:58:A:N1	1.71	1.04
44:p:645:ILE:H	44:p:646:PRO:HD3	1.24	1.03
2:2:991:A:N1	2:2:1011:U:O4	1.92	1.02
2:2:299:A:H2'	2:2:300:A:C8	1.94	1.01
1:1:14:A:H3'	1:1:15:G:C5'	1.91	1.01
2:2:1396:U:H3'	2:2:1397:C:H5'	1.41	1.01
1:1:14:A:C2'	1:1:15:G:H5''	1.91	1.00
43:o:257:TYR:HB2	43:o:289:VAL:HG11	1.41	1.00
1:1:18:G:H1'	1:1:58:A:C2	1.97	1.00
2:2:420:A:H2	2:2:421:G:H8	1.07	0.97
41:l:158:PHE:O	41:l:160:ILE:N	1.96	0.97
1:1:14:A:C3'	1:1:15:G:H5''	1.93	0.97
2:2:991:A:N6	2:2:1011:U:H3	1.65	0.94
2:2:763:G:H1	2:2:772:G:H1	1.14	0.94
2:2:420:A:H2	2:2:421:G:C8	1.85	0.94
2:2:1266:G:H1	2:2:1440:U:H3	1.14	0.94
2:2:420:A:C2	2:2:421:G:H8	1.87	0.93
2:2:1583:U:C4	2:2:1609:A:N1	2.36	0.93
19:P:111:MET:HE2	22:S:119:ILE:HG12	1.51	0.92
2:2:157:U:H4'	2:2:158:U:OP1	1.69	0.92
43:o:166:LEU:HB3	43:o:209:HIS:HE1	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:15:G:H2'	1:1:16:U:O4'	1.72	0.90
2:2:1292:U:C4	2:2:1321:A:N1	2.40	0.88
1:1:14:A:C3'	1:1:15:G:C5'	2.48	0.88
2:2:40:A:H62	2:2:466:G:H21	1.21	0.88
2:2:1402:C:H2'	2:2:1403:G:H8	1.39	0.88
2:2:1583:U:O4	2:2:1609:A:N1	2.06	0.88
2:2:480:A:N1	2:2:506:U:C4	2.41	0.87
2:2:1670:G:H2'	2:2:1671:G:C8	2.10	0.87
2:2:645:U:H3	2:2:688:G:H1	1.23	0.86
2:2:1289:U:H2'	2:2:1290:G:C8	2.10	0.86
2:2:991:A:H61	2:2:1011:U:H3	0.90	0.86
2:2:1402:C:H2'	2:2:1403:G:C8	2.11	0.86
41:l:236:CYS:SG	49:l:301:ZN:ZN	1.63	0.86
43:o:195:ARG:HB3	43:o:198:GLU:HB2	1.57	0.85
8:E:106:LYS:HB3	8:E:108:ARG:HE	1.43	0.84
1:1:14:A:O2'	1:1:15:G:H5''	1.79	0.83
2:2:763:G:H22	2:2:772:G:H22	1.27	0.83
2:2:1292:U:O4	2:2:1321:A:C6	2.32	0.82
43:o:244:VAL:HG22	43:o:259:SER:HB3	1.60	0.82
2:2:1774:A:H2'	2:2:1775:G:C8	2.14	0.81
2:2:709:C:H2'	2:2:710:U:H4'	1.62	0.81
36:g:90:LEU:HB2	36:g:104:PHE:HB2	1.63	0.81
40:k:499:ILE:HD11	40:k:517:ILE:HG13	1.63	0.80
2:2:20:G:H4'	2:2:570:G:N7	1.96	0.80
2:2:394:U:H3'	2:2:395:G:H8	1.46	0.80
2:2:1391:C:H42	2:2:1403:G:H1	1.30	0.80
15:L:54:ILE:HG23	15:L:55:ASP:H	1.48	0.78
19:P:30:THR:O	19:P:34:VAL:HG23	1.84	0.78
43:o:180:SER:HB2	43:o:235:ARG:HG3	1.63	0.78
2:2:1085:A:H2'	2:2:1086:A:C8	2.19	0.78
2:2:1332:C:H42	2:2:1416:G:H1	1.31	0.78
36:g:20:TRP:CB	36:g:313:THR:HA	2.09	0.78
40:k:112:GLY:HA3	51:k:603:GCP:H8	1.66	0.78
6:C:50:VAL:HG12	6:C:76:GLN:HE21	1.49	0.77
1:1:37:A:H2'	1:1:38:A:C8	2.19	0.76
6:C:111:ASP:CG	6:C:112:SER:H	1.94	0.76
2:2:1108:G:H1	2:2:1135:U:H3	1.29	0.76
2:2:97:C:H2'	2:2:98:U:C6	2.21	0.75
2:2:732:G:H1'	2:2:734:A:H61	1.51	0.75
1:1:74:C:H4'	1:1:75:C:O5'	1.86	0.75
44:p:645:ILE:N	44:p:646:PRO:HD3	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1583:U:H2'	2:2:1583:U:O2	1.86	0.75
36:g:20:TRP:HB3	36:g:313:THR:CA	2.11	0.74
2:2:1559:U:H2'	2:2:1560:G:H8	1.53	0.74
2:2:1292:U:O4	2:2:1321:A:C2	2.41	0.74
2:2:420:A:C2	2:2:421:G:C8	2.70	0.74
2:2:591:G:H2'	2:2:592:U:O4'	1.86	0.74
1:1:28:A:H2'	1:1:29:G:C8	2.23	0.74
2:2:1017:U:O2	2:2:1017:U:H2'	1.86	0.74
41:l:158:PHE:C	41:l:160:ILE:H	1.94	0.74
9:F:118:HIS:O	9:F:122:ILE:HG12	1.89	0.73
2:2:419:A:H3'	2:2:420:A:H8	1.53	0.73
2:2:925:A:H4'	2:2:1015:C:H4'	1.70	0.73
5:B:149:GLN:HE22	5:B:154:SER:HB3	1.54	0.73
2:2:480:A:C6	2:2:506:U:O4	2.42	0.73
2:2:17:C:H2'	2:2:18:C:C6	2.24	0.72
2:2:771:A:H3'	2:2:772:G:H8	1.54	0.72
43:o:183:VAL:HG11	43:o:239:GLN:HB2	1.70	0.72
19:P:108:ARG:HB2	19:P:109:PRO:HD3	1.72	0.72
6:C:142:ILE:HG13	6:C:143:PRO:HD2	1.72	0.71
2:2:1157:C:N4	2:2:1162:A:H61	1.86	0.71
2:2:360:C:C2	2:2:383:G:N2	2.58	0.71
2:2:452:U:O2	2:2:452:U:H2'	1.89	0.71
2:2:1768:U:H2'	2:2:1769:U:C6	2.24	0.71
5:B:186:SER:O	5:B:190:PRO:HD3	1.89	0.71
2:2:642:G:N2	2:2:692:C:C2	2.59	0.71
25:V:1:MET:HA	25:V:10:GLU:HB2	1.71	0.71
2:2:15:U:H2'	2:2:16:G:O4'	1.89	0.70
2:2:1671:G:H2'	2:2:1672:C:C6	2.26	0.70
2:2:1670:G:H2'	2:2:1671:G:H8	1.57	0.70
2:2:1290:G:H1	2:2:1323:G:H22	1.38	0.70
2:2:1044:C:H42	2:2:1072:G:H1	1.39	0.70
7:D:6:SER:HB2	7:D:9:ARG:HB2	1.73	0.70
2:2:804:U:O2	2:2:804:U:H2'	1.92	0.70
2:2:39:A:H2	2:2:466:G:H22	1.37	0.70
45:q:9:HIS:HD2	45:q:317:ILE:HD11	1.56	0.70
2:2:952:G:H2'	2:2:953:G:C8	2.27	0.70
39:j:248:ILE:HG12	39:j:264:ILE:HG21	1.74	0.70
43:o:183:VAL:CG1	43:o:239:GLN:HB2	2.21	0.70
2:2:946:U:HO2'	2:2:947:G:H8	1.39	0.70
26:W:11:LEU:HD12	26:W:74:VAL:HG23	1.74	0.70
1:1:14:A:H3'	1:1:15:G:H5'	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:166:LEU:HB3	12:I:184:ILE:HD11	1.73	0.69
2:2:1413:U:O2	2:2:1413:U:H2'	1.92	0.69
43:o:445:GLN:HG2	43:o:489:VAL:HG23	1.75	0.69
2:2:567:G:H1	2:2:573:G:H1	0.84	0.69
2:2:399:A:C6	12:I:26:LYS:HG3	2.27	0.69
2:2:1221:C:H2'	2:2:1222:A:C8	2.27	0.69
2:2:1320:A:H2	4:A:131:GLN:NE2	1.90	0.69
44:p:583:GLN:HG3	44:p:605:CYS:HB3	1.75	0.69
2:2:394:U:H3'	2:2:395:G:C8	2.28	0.69
2:2:1449:C:H5'	33:d:10:HIS:HB3	1.75	0.69
39:j:201:ILE:HG22	40:k:330:ILE:HG21	1.73	0.69
44:p:614:LEU:HA	44:p:617:ILE:HD12	1.75	0.69
2:2:51:A:H61	2:2:439:U:H3	1.38	0.68
2:2:1176:C:H4'	2:2:1188:A:H61	1.56	0.68
2:2:419:A:H3'	2:2:420:A:C8	2.28	0.68
2:2:1198:G:H4'	2:2:1199:G:O5'	1.93	0.68
13:J:31:ALA:HA	13:J:36:LEU:HD12	1.76	0.68
18:O:81:ILE:HB	18:O:115:ILE:HG22	1.76	0.68
7:D:137:VAL:HB	7:D:185:LYS:HB2	1.73	0.68
2:2:1206:C:H42	2:2:1454:C:H41	1.40	0.68
40:k:116:VAL:HG21	40:k:217:LEU:HD21	1.75	0.68
2:2:30:G:H4'	27:X:131:SER:HB2	1.75	0.68
43:o:386:GLU:O	43:o:390:ILE:HG12	1.94	0.68
44:p:615:ASP:O	44:p:619:VAL:HG23	1.93	0.68
27:X:60:GLU:HG2	38:i:60:HIS:CE1	2.28	0.67
2:2:993:G:C6	2:2:1009:C:N4	2.62	0.67
2:2:1774:A:H2'	2:2:1775:G:H8	1.57	0.67
41:l:189:GLU:HA	41:l:192:ILE:HD12	1.76	0.67
1:1:9:G:H21	1:1:43:G:H3'	1.57	0.67
2:2:703:G:N2	2:2:736:C:C2	2.62	0.67
2:2:399:A:H4'	2:2:400:A:H5''	1.77	0.67
2:2:1217:G:N2	2:2:1442:A:OP2	2.27	0.67
2:2:1380:A:H2'	2:2:1381:G:C8	2.30	0.67
2:2:1207:A:H2'	2:2:1207:A:N3	2.09	0.67
2:2:894:G:H1	2:2:916:U:H3	1.43	0.66
4:A:70:PRO:HB2	4:A:94:GLY:HA3	1.77	0.66
9:F:159:ARG:HH21	39:j:48:LEU:HB2	1.61	0.66
1:1:26:G:C2	1:1:27:C:N3	2.63	0.66
2:2:1157:C:H4'	2:2:1158:C:OP1	1.95	0.66
31:b:49:HIS:CE1	31:b:70:LYS:HE2	2.30	0.66
2:2:1221:C:H2'	2:2:1222:A:H8	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:29:U:O2	2:2:29:U:H2'	1.96	0.66
2:2:337:C:H5''	12:I:10:LYS:HG3	1.77	0.66
2:2:1198:G:H2'	2:2:1198:G:N3	2.11	0.66
2:2:771:A:H3'	2:2:772:G:C8	2.31	0.66
2:2:1344:A:H2'	2:2:1347:A:N6	2.10	0.66
41:l:247:LYS:H	41:l:257:MET:HB3	1.60	0.66
2:2:459:A:H3'	2:2:460:G:H8	1.61	0.66
2:2:984:G:H1	2:2:1015:C:H5	1.44	0.66
2:2:999:C:H2'	2:2:1000:A:H3'	1.78	0.66
2:2:1293:G:H21	2:2:1320:A:H8	1.44	0.66
2:2:1492:C:H42	2:2:1511:G:H1	1.44	0.66
20:Q:22:VAL:HG12	20:Q:65:ILE:HG12	1.78	0.66
36:g:48:LEU:HA	36:g:56:GLY:HA2	1.76	0.66
1:1:26:G:C6	1:1:27:C:N4	2.64	0.65
2:2:992:A:H3'	2:2:993:G:H5''	1.79	0.65
2:2:147:U:H5''	2:2:148:C:H5	1.61	0.65
2:2:867:G:H1	2:2:959:U:H3	1.43	0.65
2:2:1285:U:H2'	2:2:1286:A:O4'	1.96	0.65
27:X:63:GLN:C	27:X:65:ASN:H	2.05	0.65
39:j:147:LEU:O	39:j:150:ILE:HG13	1.96	0.65
44:p:645:ILE:H	44:p:646:PRO:CD	2.05	0.65
2:2:1115:A:H62	2:2:1129:G:H21	1.44	0.65
13:J:64:GLU:HA	13:J:69:ARG:HD2	1.79	0.65
44:p:644:ARG:HD2	44:p:646:PRO:HD2	1.78	0.65
2:2:1775:G:H1	2:2:1782:C:H42	1.45	0.65
35:f:109:ASP:HB2	35:f:113:LYS:HB3	1.78	0.65
2:2:1161:C:N3	2:2:1614:G:C2	2.65	0.65
2:2:1564:U:H5'	22:S:39:GLY:HA3	1.78	0.65
2:2:480:A:C2	2:2:506:U:O4	2.49	0.64
2:2:922:A:H2'	2:2:923:A:C8	2.32	0.64
45:q:330:LYS:HB2	45:q:335:LYS:HG3	1.79	0.64
2:2:444:A:H8	2:2:524:A:H5''	1.63	0.64
2:2:873:C:H2'	2:2:874:G:C8	2.31	0.64
36:g:211:PRO:HA	36:g:218:ALA:HA	1.80	0.64
2:2:763:G:O6	2:2:772:G:O6	2.14	0.64
2:2:1583:U:O4	2:2:1609:A:C6	2.51	0.64
2:2:597:U:O2	2:2:597:U:H2'	1.97	0.64
2:2:763:G:H22	2:2:772:G:N2	1.93	0.64
2:2:803:A:C4	2:2:804:U:H6	2.15	0.64
41:l:178:GLN:HB2	41:l:209:LYS:HA	1.80	0.64
2:2:443:C:H1'	2:2:444:A:C2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1437:C:H2'	2:2:1438:C:C6	2.33	0.64
8:E:31:PRO:HG3	8:E:43:PRO:HG3	1.78	0.64
43:o:240:ARG:O	43:o:244:VAL:HG23	1.98	0.64
44:p:738:VAL:HG12	44:p:774:THR:HB	1.79	0.64
2:2:930:C:H3'	2:2:931:U:H5''	1.79	0.64
7:D:58:VAL:O	7:D:65:ARG:HB3	1.97	0.64
7:D:69:LEU:HA	7:D:72:LEU:HD12	1.79	0.64
2:2:410:C:O2	2:2:410:C:H2'	1.98	0.64
2:2:1050:G:N2	2:2:1067:C:C2	2.66	0.64
39:j:75:ARG:HB2	39:j:84:ASP:HB2	1.79	0.64
44:p:255:PHE:HB3	44:p:354:GLU:HB3	1.80	0.64
2:2:991:A:N1	2:2:1011:U:C4	2.66	0.63
2:2:1292:U:C4	2:2:1321:A:C2	2.86	0.63
2:2:601:U:H5''	27:X:32:ARG:HH21	1.63	0.63
1:1:28:A:H2'	1:1:29:G:H8	1.61	0.63
2:2:1159:A:H2'	2:2:1160:C:C6	2.33	0.63
2:2:1380:A:H2'	2:2:1381:G:H8	1.63	0.63
2:2:1601:U:H2'	2:2:1602:U:C6	2.33	0.63
41:l:161:PRO:HB2	41:l:180:ILE:HG13	1.79	0.63
2:2:267:C:H3'	10:G:186:ARG:HH22	1.63	0.63
24:U:39:ALA:O	24:U:42:ILE:HG22	1.98	0.63
45:q:179:LYS:HB2	45:q:228:LEU:HD11	1.81	0.63
2:2:1540:G:C5'	23:T:87:GLY:HA3	2.29	0.63
2:2:107:C:H2'	2:2:108:A:C8	2.33	0.63
2:2:566:A:C6	2:2:567:G:H1'	2.34	0.63
2:2:823:G:C6	2:2:848:C:N3	2.66	0.63
45:q:214:SER:HB3	45:q:243:ALA:HB2	1.80	0.63
2:2:409:A:H3'	2:2:410:C:C6	2.34	0.63
27:X:63:GLN:HB3	27:X:64:PRO:CD	2.29	0.63
2:2:55:A:H3'	2:2:402:G:H1	1.64	0.62
2:2:1267:G:H1	2:2:1439:C:H42	1.45	0.62
43:o:60:VAL:HG21	43:o:99:LEU:HB3	1.79	0.62
2:2:530:C:H3'	2:2:531:U:H5''	1.80	0.62
2:2:1043:U:C2	2:2:1044:C:H5	2.17	0.62
2:2:1408:A:O2'	2:2:1409:A:C8	2.52	0.62
10:G:2:LYS:HG3	10:G:17:GLU:HG3	1.80	0.62
2:2:480:A:H61	2:2:506:U:H3	1.47	0.62
2:2:826:C:H2'	2:2:827:U:C6	2.34	0.62
2:2:1073:G:C6	2:2:1074:C:N4	2.68	0.62
10:G:67:VAL:HB	10:G:99:GLY:HA2	1.82	0.62
30:a:23:CYS:HB3	30:a:28:ARG:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:703:G:C2	2:2:736:C:N3	2.68	0.62
2:2:1772:G:H2'	2:2:1773:U:O4'	1.99	0.62
22:S:68:ARG:O	22:S:72:ILE:HG12	1.99	0.62
22:S:86:LEU:HD23	22:S:86:LEU:H	1.64	0.62
2:2:588:C:HO2'	2:2:589:C:H6	1.46	0.62
2:2:1475:G:H1	2:2:1528:C:H42	1.46	0.62
4:A:130:ALA:HA	4:A:133:ILE:HD12	1.82	0.62
7:D:48:ILE:HB	7:D:86:LEU:HD23	1.82	0.62
16:M:34:LEU:HD13	16:M:36:ARG:HH21	1.64	0.62
2:2:1132:A:O2'	2:2:1133:C:O4'	2.18	0.61
2:2:1439:C:H2'	2:2:1440:U:H6	1.63	0.61
40:k:426:ILE:HG22	40:k:490:PRO:HB2	1.82	0.61
23:T:126:ASP:HA	23:T:129:LEU:HD12	1.82	0.61
36:g:257:PHE:HB3	36:g:272:LEU:HB3	1.82	0.61
27:X:144:ARG:HG3	47:s:96:GLN:HA	1.82	0.61
1:1:25:C:H2'	1:1:26:G:C8	2.35	0.61
2:2:360:C:N3	2:2:383:G:C2	2.69	0.61
5:B:87:ARG:HB3	5:B:101:HIS:HB2	1.82	0.61
2:2:107:C:H5''	2:2:382:G:O2'	2.00	0.61
2:2:274:C:N4	2:2:275:C:N4	2.49	0.61
36:g:308:LEU:HB2	36:g:320:TRP:HB2	1.81	0.61
2:2:29:U:O2	2:2:30:G:N7	2.32	0.61
2:2:491:A:H2'	2:2:491:A:N3	2.15	0.61
38:i:41:MET:HA	38:i:47:VAL:HG23	1.81	0.61
1:1:2:G:H1'	40:k:326:PRO:HB2	1.83	0.61
2:2:1788:A:C2	2:2:1789:A:C6	2.89	0.61
5:B:111:ARG:HG2	30:a:68:TYR:HB2	1.82	0.61
12:I:57:ALA:HB2	12:I:178:GLY:HA2	1.83	0.61
16:M:129:GLU:HA	16:M:133:GLN:HB2	1.83	0.61
2:2:1083:A:H2'	2:2:1084:G:O4'	2.01	0.61
2:2:1294:G:H2'	2:2:1295:A:H5'	1.82	0.61
23:T:67:LEU:HB3	23:T:68:ARG:HD2	1.83	0.61
27:X:99:ASN:ND2	45:q:269:ASN:HB2	2.15	0.61
2:2:1559:U:H2'	2:2:1560:G:C8	2.36	0.60
2:2:1540:G:H5''	23:T:87:GLY:HA3	1.83	0.60
2:2:1639:C:H2'	2:2:1640:G:C8	2.36	0.60
44:p:542:LEU:O	44:p:546:VAL:HG13	2.01	0.60
2:2:363:G:N2	2:2:380:C:C2	2.68	0.60
2:2:1338:C:H42	2:2:1383:G:H1	1.49	0.60
43:o:184:LYS:HG2	43:o:242:GLN:HE22	1.65	0.60
45:q:90:TRP:HD1	45:q:141:GLU:HA	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1295:A:H2'	2:2:1296:G:O4'	2.02	0.60
2:2:599:U:O2	2:2:599:U:H2'	2.00	0.60
2:2:779:A:H1'	2:2:781:A:H62	1.67	0.60
2:2:952:G:H2'	2:2:953:G:H8	1.65	0.60
41:l:166:LEU:HB3	41:l:173:ILE:HG23	1.83	0.60
45:q:78:LEU:HB3	45:q:88:ALA:HB3	1.82	0.60
10:G:32:ILE:HG23	10:G:53:ALA:HA	1.84	0.60
13:J:141:VAL:HG12	13:J:143:ILE:H	1.67	0.60
40:k:358:GLY:HA2	40:k:372:PRO:HA	1.84	0.60
41:l:159:ARG:HD2	41:l:242:ILE:HA	1.83	0.60
44:p:645:ILE:N	44:p:646:PRO:CD	2.63	0.60
44:p:508:TYR:HD2	44:p:546:VAL:HG12	1.67	0.60
18:O:61:MET:HG3	18:O:104:ALA:HB2	1.83	0.59
1:1:3:C:H42	1:1:70:G:H1	1.48	0.59
2:2:403:G:N2	2:2:404:C:C2	2.69	0.59
39:j:205:LEU:HG	40:k:330:ILE:HB	1.84	0.59
40:k:346:VAL:HG22	40:k:392:PRO:HD3	1.84	0.59
1:1:25:C:H2'	1:1:26:G:H8	1.65	0.59
2:2:760:A:C2	2:2:761:G:H1'	2.38	0.59
44:p:440:ILE:HG23	44:p:448:ILE:HG21	1.84	0.59
2:2:815:G:H2'	2:2:816:A:H8	1.66	0.59
8:E:45:ILE:HG13	8:E:80:THR:HB	1.83	0.59
2:2:732:G:H1'	2:2:734:A:N6	2.16	0.59
27:X:50:LYS:HB3	27:X:77:ILE:HD12	1.85	0.59
1:1:18:G:C1'	1:1:58:A:C2	2.81	0.59
14:K:3:ILE:HG12	14:K:41:PHE:HB2	1.83	0.59
16:M:19:ASP:HA	16:M:22:LYS:HE3	1.84	0.59
31:b:56:CYS:HB2	31:b:63:LEU:HD21	1.85	0.59
2:2:393:C:H2'	2:2:394:U:O4'	2.03	0.59
2:2:1462:G:C6	2:2:1463:C:N4	2.71	0.59
12:I:83:TYR:HD2	12:I:101:ILE:HD13	1.68	0.59
39:j:146:LYS:O	39:j:149:ILE:HG13	2.02	0.59
2:2:866:G:OP1	17:N:3:ARG:HA	2.01	0.59
16:M:88:LEU:HA	16:M:91:TRP:HD1	1.67	0.59
37:h:5:TRP:HA	37:h:5:TRP:CE3	2.38	0.59
2:2:79:C:H3'	2:2:80:A:H8	1.68	0.58
2:2:1043:U:O2	2:2:1043:U:H3'	2.03	0.58
2:2:1157:C:H42	2:2:1162:A:H61	1.50	0.58
44:p:543:PHE:O	44:p:546:VAL:HG22	2.03	0.58
2:2:16:G:H21	2:2:1137:A:H62	1.51	0.58
2:2:476:A:H2'	2:2:477:A:H8	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1133:C:H2'	2:2:1134:U:O4'	2.03	0.58
2:2:1651:C:H2'	2:2:1652:G:O4'	2.03	0.58
12:I:85:PRO:HB3	15:L:12:ALA:HB2	1.85	0.58
44:p:537:SER:O	44:p:541:ILE:HG12	2.02	0.58
2:2:444:A:C8	2:2:524:A:H5''	2.39	0.58
2:2:597:U:O2	2:2:597:U:C2'	2.51	0.58
2:2:865:G:H5''	17:N:2:GLY:HA2	1.84	0.58
16:M:52:LEU:HB3	16:M:114:VAL:HB	1.85	0.58
2:2:291:U:H2'	2:2:292:U:C6	2.38	0.58
2:2:1229:A:H2'	2:2:1230:U:O4'	2.03	0.58
2:2:590:A:H2'	2:2:591:G:C8	2.39	0.58
2:2:1499:C:H42	2:2:1504:G:H1	1.52	0.58
2:2:1620:G:N2	2:2:1621:C:C2	2.70	0.58
11:H:140:VAL:HB	26:W:52:TYR:HB3	1.85	0.58
39:j:226:PRO:HG3	40:k:408:ARG:HD2	1.85	0.58
2:2:1047:G:H1	2:2:1069:C:H42	1.50	0.58
2:2:1215:C:C2	2:2:1446:G:N2	2.71	0.58
2:2:550:G:H1	2:2:572:C:H42	1.52	0.58
2:2:1332:C:N4	2:2:1416:G:H1	1.99	0.58
16:M:24:VAL:HG21	16:M:52:LEU:HG	1.86	0.58
2:2:42:G:H1	2:2:432:C:H42	1.52	0.58
43:o:303:TRP:HA	43:o:303:TRP:CE3	2.39	0.58
45:q:90:TRP:CD1	45:q:141:GLU:HA	2.39	0.58
2:2:923:A:H2'	2:2:924:G:C8	2.39	0.58
2:2:309:C:H42	2:2:355:G:H1	1.52	0.57
2:2:817:C:H42	2:2:852:G:H1	1.52	0.57
2:2:887:U:H2'	2:2:888:U:C6	2.38	0.57
38:i:55:ASN:HB3	38:i:57:ARG:HE	1.69	0.57
40:k:313:PRO:HA	40:k:344:ASN:O	2.03	0.57
44:p:626:LEU:HD13	44:p:675:VAL:HG12	1.84	0.57
2:2:108:A:H2'	2:2:109:G:C8	2.38	0.57
2:2:448:C:N4	2:2:456:G:O6	2.37	0.57
8:E:34:GLY:HA3	8:E:83:PRO:HG2	1.84	0.57
16:M:88:LEU:HA	16:M:91:TRP:CD1	2.39	0.57
1:1:14:A:C2'	1:1:15:G:C5'	2.75	0.57
2:2:619:A:H2'	2:2:620:A:C8	2.39	0.57
2:2:698:U:H2'	2:2:699:U:C6	2.39	0.57
2:2:1396:U:H3'	2:2:1397:C:C5'	2.27	0.57
2:2:1472:G:H2'	2:2:1473:A:C8	2.40	0.57
2:2:1782:C:H2'	2:2:1783:U:C6	2.39	0.57
12:I:167:TYR:HB3	12:I:185:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:11:ARG:HB2	36:g:55:PHE:HE1	1.68	0.57
41:l:233:TYR:HA	41:l:268:VAL:HG13	1.86	0.57
2:2:360:C:H2'	2:2:361:G:H8	1.69	0.57
36:g:267:ILE:HB	36:g:281:LEU:HB2	1.86	0.57
1:1:49:C:H42	1:1:65:G:H1	1.52	0.57
2:2:208:U:H2'	2:2:209:A:O4'	2.05	0.57
2:2:245:G:H2'	2:2:246:A:C8	2.39	0.57
2:2:813:A:H61	2:2:856:U:H3	1.52	0.57
2:2:107:C:H2'	2:2:108:A:H8	1.68	0.57
2:2:1038:A:H4'	25:V:62:ARG:HH12	1.70	0.57
22:S:84:TRP:H	22:S:84:TRP:CD1	2.22	0.57
26:W:102:VAL:HB	26:W:113:HIS:HB3	1.85	0.57
27:X:67:ALA:HB3	27:X:69:ARG:HE	1.69	0.57
2:2:545:C:H42	2:2:591:G:H1	1.53	0.57
2:2:1651:C:H42	2:2:1745:G:H1	1.51	0.57
2:2:598:A:H2'	2:2:599:U:H6	1.69	0.57
2:2:617:U:H3'	2:2:618:A:H5''	1.86	0.57
21:R:28:PHE:O	21:R:32:LYS:HB2	2.05	0.57
2:2:57:G:H1	2:2:90:C:H42	1.53	0.57
2:2:1603:G:N2	2:2:1604:C:C2	2.72	0.57
26:W:27:ILE:HB	26:W:61:ILE:HB	1.87	0.57
1:1:18:G:H4'	1:1:60:A:C2	2.40	0.56
2:2:823:G:N1	2:2:848:C:C2	2.73	0.56
2:2:1062:U:H3'	2:2:1063:G:H8	1.69	0.56
2:2:363:G:C2	2:2:380:C:C2	2.93	0.56
12:I:107:THR:N	12:I:108:PRO:HD2	2.19	0.56
40:k:320:SER:HB3	40:k:412:LEU:H	1.68	0.56
2:2:548:G:H1	2:2:588:C:H5	1.53	0.56
2:2:992:A:H3'	2:2:993:G:C5'	2.35	0.56
2:2:1074:C:O2'	30:a:14:GLY:HA3	2.06	0.56
2:2:1097:U:H1'	26:W:71:LYS:HD2	1.85	0.56
1:1:2:G:H1	1:1:71:C:H42	1.53	0.56
2:2:423:C:O2	2:2:427:A:N6	2.38	0.56
2:2:780:A:H8	28:Y:8:ARG:HB3	1.70	0.56
1:1:10:G:C6	1:1:11:C:N4	2.73	0.56
2:2:266:U:H2'	2:2:267:C:H6	1.71	0.56
2:2:524:A:H2'	2:2:525:A:C8	2.41	0.56
42:m:30:ILE:HD12	42:m:108:PHE:H	1.69	0.56
2:2:1344:A:H2'	2:2:1347:A:H62	1.71	0.56
2:2:267:C:H5''	10:G:186:ARG:HH12	1.70	0.56
2:2:634:A:H2'	2:2:635:A:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:702:G:H1	2:2:736:C:H42	1.54	0.56
2:2:1140:G:H2'	2:2:1141:A:C8	2.41	0.56
2:2:1482:G:H21	2:2:1604:C:H1'	1.69	0.56
24:U:57:ARG:HG3	24:U:89:ARG:HG2	1.87	0.56
25:V:39:VAL:HA	25:V:45:ALA:HA	1.87	0.56
2:2:1174:U:O2	2:2:1174:U:H2'	2.06	0.56
2:2:1232:G:H1	2:2:1251:C:H42	1.54	0.56
28:Y:37:LYS:HA	28:Y:40:LEU:HD12	1.86	0.56
45:q:121:SER:HB3	45:q:148:ILE:HD13	1.88	0.56
15:L:99:ARG:HD3	27:X:8:GLY:O	2.05	0.56
40:k:307:ARG:HG2	40:k:392:PRO:HB2	1.87	0.56
2:2:412:U:H2'	2:2:412:U:O2	2.05	0.56
2:2:1155:C:H42	2:2:1620:G:H1	1.53	0.56
2:2:1158:C:H5'	2:2:1159:A:H5''	1.86	0.56
2:2:558:C:O2	2:2:558:C:H2'	2.05	0.55
2:2:566:A:H3'	2:2:567:G:H5''	1.88	0.55
2:2:1043:U:C2	2:2:1044:C:C5	2.94	0.55
6:C:136:ILE:HA	6:C:139:LEU:HD12	1.87	0.55
25:V:71:ARG:HD3	31:b:4:VAL:HG21	1.88	0.55
43:o:100:VAL:HB	43:o:158:THR:HG22	1.88	0.55
2:2:337:C:H2'	2:2:338:C:C6	2.41	0.55
2:2:1161:C:C2	2:2:1614:G:N2	2.75	0.55
6:C:175:ILE:HB	6:C:202:TYR:HB2	1.87	0.55
12:I:168:ALA:HB2	12:I:184:ILE:HD12	1.89	0.55
2:2:40:A:N6	2:2:466:G:H21	1.99	0.55
2:2:395:G:H22	2:2:397:G:H3'	1.71	0.55
2:2:638:U:H5	11:H:101:LYS:H	1.54	0.55
11:H:30:ASN:HB2	11:H:34:LEU:HB2	1.89	0.55
45:q:275:ALA:H	45:q:289:VAL:HB	1.72	0.55
2:2:1226:A:H5'	2:2:1228:G:O4'	2.06	0.55
9:F:86:LYS:HD3	9:F:94:ARG:HH12	1.72	0.55
10:G:211:LEU:O	10:G:214:LYS:HG2	2.06	0.55
38:i:61:ILE:HA	38:i:91:VAL:HG12	1.88	0.55
1:1:2:G:C6	1:1:3:C:N4	2.74	0.55
6:C:184:VAL:HB	6:C:202:TYR:HA	1.88	0.55
2:2:1671:G:C2	2:2:1672:C:C2	2.95	0.55
40:k:140:LEU:HD12	40:k:319:ARG:HH21	1.70	0.55
13:J:39:LYS:HA	13:J:42:ILE:HD12	1.88	0.55
2:2:1174:U:O2	2:2:1174:U:C2'	2.55	0.55
1:1:10:G:N2	1:1:11:C:C2	2.75	0.55
2:2:30:G:H2'	2:2:31:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1320:A:H4'	2:2:1321:A:OP1	2.06	0.55
2:2:1380:A:P	24:U:59:PRO:HA	2.46	0.55
43:o:59:GLY:HA3	43:o:68:LEU:HD11	1.88	0.55
43:o:166:LEU:HB3	43:o:209:HIS:CE1	2.27	0.55
43:o:257:TYR:HB2	43:o:289:VAL:CG1	2.26	0.55
2:2:703:G:C2	2:2:736:C:C2	2.95	0.54
2:2:865:G:H2'	2:2:866:G:C8	2.41	0.54
27:X:103:LEU:HB3	27:X:126:LYS:HB2	1.90	0.54
2:2:440:A:H2'	2:2:441:C:C6	2.42	0.54
2:2:617:U:H3'	2:2:618:A:C5'	2.38	0.54
36:g:171:ARG:HA	36:g:189:ASN:HA	1.89	0.54
42:m:92:MET:HE2	42:m:98:LEU:HD13	1.88	0.54
46:r:724:MET:HB3	46:r:730:PHE:HB3	1.90	0.54
2:2:273:G:C6	2:2:274:C:N4	2.76	0.54
2:2:1267:G:H1	2:2:1439:C:N4	2.05	0.54
2:2:1464:G:N2	2:2:1465:C:C2	2.75	0.54
2:2:1711:G:H3'	2:2:1712:A:C8	2.42	0.54
36:g:223:LYS:HA	36:g:246:GLU:HG2	1.88	0.54
2:2:823:G:C2	2:2:848:C:O2	2.61	0.54
2:2:835:U:H2'	2:2:836:G:O4'	2.07	0.54
2:2:1052:G:H1	2:2:1065:C:H42	1.56	0.54
2:2:1557:A:H1'	22:S:134:ARG:HB3	1.90	0.54
6:C:48:ARG:HE	6:C:254:ALA:H	1.55	0.54
2:2:843:A:H2'	2:2:844:G:C8	2.43	0.54
8:E:179:LYS:HA	8:E:231:PRO:HD3	1.88	0.54
2:2:1671:G:C6	2:2:1672:C:N4	2.76	0.54
13:J:140:ILE:HD13	28:Y:65:GLY:HA3	1.88	0.54
18:O:30:VAL:HG12	18:O:39:ILE:HB	1.90	0.54
28:Y:8:ARG:HH22	28:Y:28:LEU:HD13	1.73	0.54
36:g:112:LEU:HD22	36:g:153:THR:HA	1.90	0.54
44:p:528:VAL:HB	44:p:532:ILE:HD11	1.90	0.54
2:2:223:C:H2'	2:2:224:A:C8	2.43	0.54
2:2:804:U:O2	2:2:804:U:C2'	2.55	0.54
2:2:1306:U:H3'	2:2:1307:G:H8	1.72	0.54
2:2:1315:G:N2	2:2:1316:C:C2	2.76	0.54
43:o:294:GLY:HA3	43:o:348:HIS:HE1	1.72	0.54
2:2:8:U:H3	2:2:1138:A:N6	2.04	0.54
2:2:993:G:C2	2:2:1009:C:N3	2.76	0.54
6:C:72:GLN:NE2	6:C:72:GLN:H	2.06	0.54
6:C:234:LEU:HD11	25:V:14:PRO:HD2	1.90	0.54
7:D:32:GLU:HG3	7:D:57:ASP:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:290:PHE:HB3	43:o:299:HIS:HB2	1.89	0.54
44:p:482:LEU:O	44:p:486:LEU:HG	2.08	0.54
7:D:209:ILE:HG22	21:R:38:ILE:HG23	1.90	0.54
43:o:94:ARG:HG3	43:o:178:THR:HG23	1.90	0.54
2:2:1466:U:H2'	2:2:1467:A:O4'	2.08	0.53
40:k:503:ARG:HD3	40:k:512:ILE:HG21	1.89	0.53
2:2:163:A:H2'	2:2:164:G:C8	2.43	0.53
2:2:473:A:N6	2:2:593:A:OP1	2.41	0.53
2:2:617:U:O4	2:2:1086:A:N6	2.40	0.53
2:2:1338:C:C2	2:2:1384:G:C2	2.96	0.53
2:2:1775:G:H1	2:2:1782:C:N4	2.05	0.53
38:i:33:GLN:HA	38:i:80:SER:HA	1.90	0.53
44:p:626:LEU:CD1	44:p:679:ALA:HB2	2.24	0.53
2:2:613:C:H42	2:2:1106:G:H1	1.56	0.53
2:2:1480:C:O2	2:2:1480:C:O4'	2.26	0.53
18:O:80:HIS:CD2	18:O:114:ARG:HB2	2.43	0.53
28:Y:18:LEU:HB2	28:Y:20:ARG:HG2	1.90	0.53
42:m:43:GLN:HG2	42:m:75:GLY:HA2	1.90	0.53
43:o:180:SER:CB	43:o:235:ARG:HG3	2.34	0.53
2:2:829:U:H2'	2:2:830:U:O4'	2.09	0.53
2:2:1062:U:H3'	2:2:1063:G:C8	2.44	0.53
4:A:53:THR:HG22	4:A:161:PRO:HG2	1.89	0.53
2:2:28:A:N1	2:2:596:G:O6	2.41	0.53
2:2:1003:U:H2'	2:2:1003:U:O2	2.09	0.53
2:2:1399:A:P	21:R:60:ARG:HH12	2.31	0.53
2:2:1588:G:N2	2:2:1589:C:C2	2.77	0.53
37:h:5:TRP:HA	37:h:5:TRP:HE3	1.72	0.53
2:2:1086:A:H2'	2:2:1087:A:C8	2.44	0.53
2:2:1270:G:N2	2:2:1438:C:C2	2.77	0.53
4:A:56:LYS:HZ2	4:A:159:ALA:H	1.56	0.53
26:W:85:ASP:HA	26:W:88:LYS:HE3	1.90	0.53
2:2:12:U:H2'	2:2:13:C:C6	2.44	0.53
2:2:405:U:H2'	2:2:406:A:C8	2.43	0.53
2:2:1258:U:N3	2:2:1259:U:H5	2.06	0.53
45:q:333:VAL:HG21	46:r:706:GLN:HB3	1.89	0.53
1:1:2:G:C2	1:1:3:C:N3	2.77	0.53
2:2:403:G:N1	2:2:404:C:C4	2.76	0.53
2:2:421:G:H3'	2:2:422:G:C8	2.43	0.53
2:2:763:G:N2	2:2:772:G:H22	2.02	0.53
39:j:236:ASP:C	39:j:238:GLN:H	2.17	0.53
2:2:1120:C:H42	2:2:1125:G:H1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1258:U:H2'	2:2:1259:U:H5'	1.90	0.53
4:A:21:ARG:HD2	4:A:24:LEU:HD13	1.91	0.53
1:1:10:G:C2	1:1:11:C:C4	2.98	0.52
2:2:30:G:C6	2:2:31:C:N4	2.77	0.52
2:2:387:G:N3	2:2:387:G:H2'	2.23	0.52
2:2:599:U:O2	2:2:599:U:C2'	2.57	0.52
2:2:803:A:C4	2:2:804:U:C6	2.97	0.52
2:2:865:G:H2'	2:2:866:G:H8	1.74	0.52
2:2:914:A:H5''	2:2:914:A:H8	1.74	0.52
2:2:1044:C:N4	2:2:1072:G:H1	2.06	0.52
2:2:1161:C:N4	2:2:1614:G:C6	2.77	0.52
4:A:35:PRO:HG3	25:V:87:ARG:HH21	1.74	0.52
1:1:37:A:H1'	42:m:35:GLY:H	1.74	0.52
2:2:925:A:H3'	2:2:926:C:H6	1.73	0.52
2:2:1512:U:O2	2:2:1512:U:O4'	2.26	0.52
2:2:409:A:H3'	2:2:410:C:H6	1.75	0.52
2:2:1727:C:H2'	2:2:1728:A:O4'	2.09	0.52
11:H:31:SER:HB2	11:H:32:PRO:HD3	1.92	0.52
12:I:154:GLU:HB3	12:I:157:VAL:HG23	1.91	0.52
20:Q:115:THR:HB	20:Q:119:ALA:HA	1.91	0.52
41:l:226:LEU:HA	41:l:229:TYR:CD2	2.43	0.52
2:2:488:C:H2'	2:2:489:C:H5	1.73	0.52
2:2:567:G:N2	2:2:568:C:C2	2.77	0.52
2:2:1240:G:H5'	19:P:77:ARG:HB2	1.91	0.52
2:2:1781:C:H2'	2:2:1782:C:C6	2.44	0.52
4:A:124:THR:HG22	4:A:174:TRP:HE1	1.74	0.52
9:F:27:LEU:HB2	9:F:31:ILE:HD11	1.91	0.52
23:T:14:PHE:HA	23:T:139:THR:HG21	1.90	0.52
44:p:495:ASN:O	44:p:499:GLN:HG3	2.10	0.52
45:q:72:ALA:HA	45:q:95:PRO:HB3	1.91	0.52
2:2:711:G:H1	2:2:727:C:H42	1.56	0.52
2:2:1363:G:N2	2:2:1364:C:C2	2.78	0.52
2:2:1595:A:H5'	33:d:19:ARG:HH21	1.75	0.52
9:F:98:SER:HB3	9:F:178:THR:HG21	1.91	0.52
22:S:91:ASP:HB3	22:S:95:GLY:H	1.75	0.52
2:2:18:C:H4'	2:2:1136:A:H61	1.73	0.52
2:2:173:U:H3'	2:2:174:G:H8	1.73	0.52
27:X:107:PHE:HA	27:X:123:LYS:HD2	1.90	0.52
29:Z:66:VAL:HG22	29:Z:72:GLY:HA2	1.90	0.52
29:Z:90:LYS:HE2	29:Z:104:ALA:HA	1.91	0.52
43:o:183:VAL:O	43:o:187:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:18:TYR:HE2	45:q:39:SER:HB3	1.75	0.52
2:2:1203:A:H2'	2:2:1204:C:C6	2.44	0.52
2:2:1215:C:N3	2:2:1446:G:C2	2.78	0.52
2:2:1290:G:H22	2:2:1323:G:N2	2.08	0.52
2:2:1585:A:H2'	2:2:1586:G:H8	1.75	0.52
5:B:47:LEU:HD23	18:O:37:GLU:HG2	1.91	0.52
12:I:107:THR:HG22	12:I:110:ARG:HH21	1.75	0.52
20:Q:127:LYS:HA	20:Q:134:ALA:HA	1.89	0.52
39:j:48:LEU:HA	39:j:51:LEU:HD13	1.91	0.52
2:2:548:G:H2'	2:2:549:A:O4'	2.09	0.52
2:2:1206:C:H42	2:2:1454:C:N4	2.06	0.52
2:2:1583:U:H3	2:2:1609:A:H61	1.56	0.52
21:R:4:VAL:C	21:R:5:ARG:HE	2.17	0.52
39:j:140:HIS:CG	39:j:141:ALA:H	2.28	0.52
40:k:216:LEU:HD23	40:k:246:ILE:HG12	1.92	0.52
13:J:105:LEU:HA	13:J:108:ARG:HD3	1.91	0.52
2:2:40:A:H62	2:2:466:G:N2	2.01	0.52
2:2:1298:G:H2'	2:2:1299:A:C8	2.45	0.52
2:2:1423:A:H1'	6:C:97:ALA:HB1	1.92	0.52
2:2:1560:G:N2	2:2:1561:C:C2	2.78	0.52
2:2:1586:G:H1	2:2:1606:U:H3	1.58	0.52
11:H:109:THR:O	11:H:110:GLN:HG2	2.10	0.52
40:k:109:VAL:HG23	40:k:136:ILE:HG21	1.92	0.52
2:2:421:G:N3	2:2:421:G:H2'	2.24	0.51
2:2:530:C:H3'	2:2:531:U:C5'	2.40	0.51
5:B:137:ILE:HD12	5:B:172:LEU:HD22	1.92	0.51
17:N:62:GLN:HB2	17:N:65:VAL:HB	1.92	0.51
21:R:84:TYR:O	21:R:85:VAL:HB	2.10	0.51
42:m:33:ARG:H	42:m:38:THR:HA	1.74	0.51
2:2:28:A:H2'	2:2:29:U:O4'	2.09	0.51
2:2:1073:G:C2	2:2:1074:C:C4	2.99	0.51
2:2:1469:A:H62	2:2:1536:U:H3	1.56	0.51
2:2:74:U:H4'	2:2:75:U:OP1	2.09	0.51
2:2:1171:G:H2'	2:2:1172:C:O4'	2.09	0.51
2:2:1245:C:O2	2:2:1245:C:O4'	2.27	0.51
2:2:1446:G:N3	2:2:1446:G:H2'	2.25	0.51
2:2:1468:C:H4'	2:2:1538:G:H21	1.74	0.51
28:Y:53:ASP:HB3	28:Y:96:LEU:HD21	1.91	0.51
40:k:98:GLN:HE22	40:k:396:ILE:HD11	1.75	0.51
1:1:9:G:N2	1:1:43:G:H3'	2.24	0.51
2:2:838:U:H2'	2:2:839:U:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1126:G:N2	2:2:1127:C:C2	2.79	0.51
2:2:1377:C:O2	2:2:1377:C:H2'	2.08	0.51
2:2:1578:C:H2'	2:2:1579:C:C6	2.46	0.51
43:o:31:LEU:HB3	43:o:55:PHE:HB2	1.92	0.51
44:p:626:LEU:HA	44:p:630:ILE:HD13	1.92	0.51
2:2:1603:G:N1	2:2:1604:C:C4	2.78	0.51
4:A:49:ASN:HA	21:R:109:LEU:HD11	1.91	0.51
13:J:110:GLN:HE22	13:J:126:ARG:HB2	1.75	0.51
27:X:63:GLN:HB3	27:X:64:PRO:HD2	1.92	0.51
44:p:691:VAL:HG21	44:p:714:THR:HG23	1.92	0.51
45:q:254:LEU:HD12	45:q:278:TYR:CE2	2.45	0.51
2:2:52:U:H2'	2:2:53:G:H8	1.76	0.51
2:2:360:C:H2'	2:2:361:G:C8	2.46	0.51
2:2:1154:G:N2	2:2:1622:C:C2	2.77	0.51
2:2:1484:G:H3'	2:2:1485:A:H8	1.75	0.51
43:o:45:PRO:HB3	43:o:79:ILE:HG12	1.93	0.51
43:o:303:TRP:HA	43:o:303:TRP:HE3	1.73	0.51
44:p:753:VAL:HG13	44:p:769:LEU:HD21	1.92	0.51
2:2:481:U:H3	2:2:504:A:H61	1.57	0.51
2:2:762:A:H2'	2:2:762:A:N3	2.24	0.51
2:2:1058:C:O4'	2:2:1058:C:O2	2.27	0.51
2:2:1362:U:H5''	2:2:1363:G:H8	1.74	0.51
2:2:1432:U:O2	2:2:1432:U:H2'	2.10	0.51
6:C:232:PRO:HA	6:C:235:TRP:CD2	2.46	0.51
9:F:82:LYS:HG2	9:F:83:ARG:H	1.75	0.51
29:Z:93:SER:HB3	29:Z:100:ILE:HD12	1.91	0.51
2:2:452:U:O2	2:2:452:U:C2'	2.55	0.51
2:2:1400:G:H4'	21:R:4:VAL:HG13	1.92	0.51
2:2:1417:G:C6	2:2:1418:C:N4	2.79	0.51
4:A:58:VAL:O	4:A:62:ARG:HG3	2.11	0.51
2:2:360:C:C2	2:2:383:G:C2	2.99	0.51
2:2:429:G:N2	2:2:430:C:C2	2.79	0.51
2:2:455:A:H2'	2:2:456:G:O4'	2.11	0.51
9:F:190:LYS:HD2	9:F:195:THR:HG22	1.93	0.51
14:K:82:LEU:HD12	14:K:86:ILE:HG21	1.92	0.51
16:M:37:GLY:O	16:M:111:VAL:HB	2.11	0.51
39:j:183:LYS:HB3	39:j:231:THR:HB	1.92	0.51
41:l:223:GLU:HA	41:l:226:LEU:HD12	1.92	0.51
45:q:328:ASP:O	45:q:330:LYS:HG3	2.11	0.51
2:2:140:A:H2	2:2:265:A:H4'	1.76	0.51
2:2:778:G:H2'	2:2:779:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:5:ILE:HG21	7:D:9:ARG:HH11	1.75	0.51
18:O:80:HIS:HD2	18:O:114:ARG:HB2	1.74	0.51
33:d:36:LEU:HD22	33:d:38:ILE:HD11	1.93	0.51
39:j:148:SER:HG	39:j:155:TRP:CD1	2.29	0.51
44:p:413:LEU:HD13	44:p:459:ILE:HG21	1.92	0.51
16:M:117:TRP:CE3	16:M:117:TRP:HA	2.46	0.50
21:R:3:ARG:H	21:R:3:ARG:NE	2.09	0.50
22:S:3:LEU:H	29:Z:78:VAL:HG11	1.76	0.50
36:g:172:ILE:HB	36:g:188:LEU:HB3	1.92	0.50
40:k:456:LEU:HD23	40:k:503:ARG:HD2	1.92	0.50
43:o:191:LEU:HB2	43:o:246:VAL:HG22	1.93	0.50
2:2:815:G:H2'	2:2:816:A:C8	2.46	0.50
2:2:1143:U:H2'	2:2:1144:U:C6	2.46	0.50
2:2:1413:U:O2	2:2:1413:U:C2'	2.59	0.50
2:2:1497:G:C2	2:2:1507:C:O2	2.64	0.50
2:2:218:A:H2'	2:2:219:A:H8	1.76	0.50
2:2:1176:C:H42	2:2:1460:G:H1	1.58	0.50
5:B:176:VAL:C	5:B:178:ASN:H	2.19	0.50
13:J:37:LYS:HA	34:e:33:ARG:HB3	1.92	0.50
36:g:68:ILE:HB	36:g:86:TRP:CD1	2.47	0.50
45:q:16:VAL:HB	45:q:25:LEU:HD11	1.93	0.50
2:2:8:U:N3	2:2:1138:A:N6	2.59	0.50
2:2:21:U:H4'	13:J:18:PRO:HG3	1.93	0.50
2:2:1043:U:O2	2:2:1043:U:C2'	2.60	0.50
2:2:1149:G:H2'	2:2:1766:G:N3	2.27	0.50
2:2:1185:U:H2'	2:2:1186:U:O4'	2.12	0.50
11:H:58:LEU:HD21	11:H:88:ARG:HH11	1.77	0.50
44:p:332:LEU:HB3	44:p:414:TYR:CZ	2.47	0.50
2:2:163:A:H2'	2:2:164:G:H8	1.75	0.50
2:2:249:C:H2'	2:2:250:A:H8	1.75	0.50
2:2:1452:G:H4'	19:P:81:ARG:HH21	1.77	0.50
2:2:1679:A:C8	10:G:65:GLN:HG3	2.47	0.50
8:E:125:LYS:HB2	8:E:226:PHE:CE2	2.47	0.50
21:R:37:GLU:HG3	36:g:151:TRP:HH2	1.76	0.50
41:l:177:ILE:HD11	41:l:191:LEU:HD22	1.94	0.50
42:m:64:CYS:HA	42:m:81:GLN:HB2	1.93	0.50
43:o:454:LEU:HB3	43:o:455:PRO:HD2	1.93	0.50
2:2:564:C:N4	2:2:576:G:C6	2.80	0.50
2:2:1417:G:C2	2:2:1418:C:N3	2.79	0.50
2:2:1432:U:O4	2:2:1434:A:N7	2.45	0.50
15:L:84:ILE:HB	15:L:111:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:257:TYR:CB	43:o:289:VAL:HG11	2.28	0.50
44:p:622:LEU:HB3	44:p:675:VAL:HG11	1.92	0.50
2:2:605:A:C8	2:2:607:U:H2'	2.45	0.50
2:2:1042:A:C4	2:2:1043:U:H6	2.29	0.50
2:2:1594:C:O2	2:2:1594:C:O4'	2.27	0.50
9:F:65:GLN:HE22	9:F:68:LYS:HB2	1.77	0.50
2:2:39:A:N3	2:2:39:A:H2'	2.26	0.50
2:2:786:G:H2'	2:2:786:G:N3	2.27	0.50
6:C:86:MET:HE1	6:C:191:LYS:HD2	1.93	0.50
12:I:44:HIS:HB2	12:I:56:ARG:HB2	1.93	0.50
16:M:67:LEU:HD13	35:f:103:LEU:HD23	1.93	0.50
31:b:54:VAL:HG23	31:b:63:LEU:HB2	1.94	0.50
40:k:320:SER:HB3	40:k:412:LEU:HB2	1.94	0.50
40:k:320:SER:HB2	40:k:407:CYS:HA	1.94	0.50
43:o:169:LEU:HD23	43:o:179:TYR:HA	1.93	0.50
43:o:287:VAL:HG21	43:o:303:TRP:CE3	2.46	0.50
1:1:37:A:H1'	42:m:34:ASN:HA	1.94	0.50
2:2:1343:A:H4'	2:2:1344:A:OP1	2.12	0.50
2:2:1462:G:C2	2:2:1463:C:N3	2.79	0.50
2:2:1659:U:H2'	2:2:1660:G:C8	2.47	0.50
13:J:82:ARG:HH21	13:J:149:ARG:HD3	1.77	0.50
2:2:840:U:O2	2:2:840:U:H2'	2.11	0.49
2:2:1117:G:H3'	2:2:1118:G:H8	1.77	0.49
22:S:57:ARG:HB2	22:S:60:GLU:HB2	1.94	0.49
40:k:237:GLU:HB3	40:k:274:ILE:HD12	1.94	0.49
43:o:367:LEU:HD22	43:o:388:TYR:CE1	2.47	0.49
2:2:531:U:H2'	2:2:532:U:O4'	2.12	0.49
2:2:859:U:O4'	11:H:114:ARG:HD2	2.12	0.49
2:2:884:G:H2'	2:2:885:U:C6	2.47	0.49
2:2:1192:A:H1'	2:2:1281:U:H4'	1.94	0.49
2:2:1195:A:H4'	2:2:1196:C:H5''	1.94	0.49
2:2:1768:U:H2'	2:2:1769:U:H6	1.74	0.49
9:F:144:PRO:HD3	9:F:216:LYS:HE3	1.93	0.49
16:M:68:VAL:HG21	16:M:111:VAL:HG21	1.93	0.49
40:k:349:LEU:HD12	40:k:388:LYS:HA	1.93	0.49
43:o:191:LEU:HB2	43:o:246:VAL:HG13	1.94	0.49
1:1:23:C:H2'	1:1:24:G:C8	2.46	0.49
2:2:50:C:H2'	2:2:423:C:H41	1.77	0.49
2:2:266:U:H2'	2:2:267:C:C6	2.47	0.49
2:2:395:G:N2	2:2:397:G:H3'	2.26	0.49
2:2:930:C:H3'	2:2:931:U:C5'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1389:A:H61	2:2:1405:U:H3	1.60	0.49
2:2:1756:U:H2'	2:2:1757:C:C6	2.48	0.49
13:J:17:ARG:HB3	13:J:20:GLU:HG3	1.93	0.49
17:N:94:LYS:O	17:N:98:VAL:HG23	2.11	0.49
20:Q:87:LYS:HA	20:Q:90:VAL:HG22	1.94	0.49
35:f:139:CYS:HB2	35:f:146:PHE:HB3	1.94	0.49
38:i:79:VAL:HG22	38:i:91:VAL:HG23	1.94	0.49
2:2:71:A:H3'	2:2:72:A:H5''	1.93	0.49
2:2:570:G:P	2:2:570:G:H21	2.35	0.49
2:2:805:A:C2	2:2:806:A:C5	3.00	0.49
2:2:1539:G:H21	2:2:1568:A:H62	1.58	0.49
2:2:1671:G:C6	2:2:1672:C:C4	3.01	0.49
8:E:94:ALA:C	8:E:96:ASN:H	2.20	0.49
14:K:80:LEU:HB3	14:K:82:LEU:HD23	1.94	0.49
2:2:1073:G:C2	2:2:1074:C:N3	2.81	0.49
2:2:1600:C:H2'	2:2:1601:U:C6	2.46	0.49
2:2:1602:U:H2'	2:2:1603:G:H8	1.77	0.49
33:d:10:HIS:HB2	33:d:11:PRO:HD2	1.95	0.49
2:2:14:C:H42	2:2:1139:G:H1	1.60	0.49
2:2:419:A:C3'	2:2:420:A:H8	2.24	0.49
2:2:1165:A:N1	2:2:1577:U:O4	2.45	0.49
2:2:1558:U:O2	2:2:1558:U:O4'	2.30	0.49
2:2:1583:U:O2	2:2:1583:U:C2'	2.56	0.49
2:2:1714:C:H2'	2:2:1715:G:O4'	2.13	0.49
2:2:1736:U:H2'	2:2:1737:C:C6	2.48	0.49
14:K:80:LEU:O	14:K:81:ASN:HB3	2.12	0.49
43:o:80:GLN:HB2	43:o:223:ASN:OD1	2.13	0.49
44:p:490:LEU:HD23	44:p:502:ALA:HB2	1.93	0.49
2:2:176:U:H3'	2:2:177:U:H2'	1.94	0.49
2:2:248:U:H3'	2:2:249:C:H5'	1.94	0.49
2:2:698:U:H1'	11:H:107:ARG:HG2	1.94	0.49
2:2:1075:A:H2'	2:2:1076:C:O4'	2.13	0.49
14:K:15:LEU:HD22	14:K:68:LEU:HD11	1.95	0.49
36:g:88:LYS:HA	36:g:110:ASP:HA	1.94	0.49
2:2:56:U:O2	2:2:56:U:O4'	2.31	0.49
2:2:365:A:H2'	2:2:366:A:C8	2.48	0.49
2:2:387:G:C8	2:2:422:G:N2	2.80	0.49
2:2:737:A:HO2'	2:2:738:G:H8	1.59	0.49
2:2:1162:A:H2'	2:2:1163:G:O4'	2.12	0.49
2:2:1454:C:O2	2:2:1454:C:O4'	2.28	0.49
43:o:260:ILE:HG23	43:o:282:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:671:LEU:HA	44:p:674:TYR:HD2	1.77	0.49
45:q:34:ALA:HB3	45:q:48:LEU:HB2	1.95	0.49
12:I:42:ARG:HE	12:I:59:ARG:HD2	1.78	0.49
27:X:91:GLY:O	27:X:93:LEU:N	2.46	0.49
28:Y:34:ASN:CG	28:Y:35:VAL:H	2.20	0.49
40:k:187:ARG:HH21	40:k:299:VAL:HG13	1.78	0.49
40:k:444:LYS:HB2	40:k:449:LYS:HB2	1.95	0.49
43:o:329:PHE:HB3	43:o:384:LEU:HD12	1.95	0.49
2:2:162:G:H2'	2:2:163:A:H8	1.78	0.49
2:2:642:G:C2	2:2:692:C:N3	2.81	0.49
2:2:1170:A:H2'	2:2:1171:G:C8	2.48	0.49
18:O:85:ALA:HB2	18:O:94:PRO:HA	1.94	0.49
44:p:671:LEU:O	44:p:675:VAL:HG23	2.13	0.49
2:2:162:G:H2'	2:2:163:A:C8	2.48	0.48
2:2:1393:G:O6	2:2:1401:C:N4	2.45	0.48
2:2:1486:G:H3'	2:2:1513:A:H61	1.78	0.48
5:B:135:LEU:HD23	5:B:217:LEU:HA	1.93	0.48
11:H:63:PRO:O	11:H:64:VAL:HB	2.13	0.48
21:R:9:VAL:HG22	21:R:50:ILE:HG13	1.95	0.48
2:2:886:A:C5	2:2:887:U:C5	3.01	0.48
2:2:1161:C:C2	2:2:1614:G:C2	3.01	0.48
2:2:1243:A:H2'	2:2:1243:A:N3	2.28	0.48
2:2:1788:A:H2'	2:2:1789:A:C8	2.48	0.48
7:D:107:PHE:O	7:D:110:LEU:HG	2.13	0.48
26:W:11:LEU:HD13	26:W:72:CYS:HB3	1.94	0.48
40:k:390:ALA:HB1	40:k:396:ILE:HD13	1.95	0.48
43:o:106:SER:O	43:o:109:THR:HG22	2.12	0.48
44:p:443:LYS:HD3	44:p:447:LEU:HD23	1.94	0.48
2:2:273:G:H1	2:2:281:C:H42	1.60	0.48
2:2:325:G:H2'	2:2:326:U:C6	2.49	0.48
2:2:844:G:H2'	2:2:845:G:O4'	2.13	0.48
2:2:946:U:O2'	2:2:947:G:H8	1.93	0.48
2:2:1381:G:H2'	2:2:1382:A:C8	2.48	0.48
2:2:1786:G:H2'	2:2:1787:G:O4'	2.13	0.48
7:D:142:LEU:C	7:D:144:ALA:H	2.19	0.48
11:H:28:GLU:HB3	11:H:35:LYS:HE3	1.94	0.48
24:U:58:LEU:HD21	24:U:90:TYR:HD1	1.78	0.48
1:1:13:C:H42	1:1:22:G:H1	1.61	0.48
2:2:644:C:H2'	2:2:645:U:O4'	2.14	0.48
2:2:701:U:H2'	2:2:702:G:O4'	2.13	0.48
2:2:1085:A:H2'	2:2:1086:A:H8	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1091:A:N3	2:2:1091:A:H2'	2.28	0.48
2:2:1231:U:H2'	2:2:1232:G:H8	1.78	0.48
2:2:1502:G:H4'	23:T:41:ALA:HB2	1.93	0.48
2:2:1605:G:H2'	2:2:1606:U:C6	2.48	0.48
2:2:1671:G:C5	2:2:1672:C:C4	3.01	0.48
2:2:1679:A:H5'	2:2:1680:U:C6	2.48	0.48
9:F:135:VAL:HA	9:F:200:LEU:HD21	1.95	0.48
22:S:115:ARG:O	22:S:119:ILE:HG13	2.14	0.48
38:i:38:ILE:HD12	38:i:75:ASP:HB3	1.94	0.48
2:2:488:C:H2'	2:2:489:C:C5	2.48	0.48
2:2:1068:A:H2'	2:2:1069:C:O4'	2.13	0.48
2:2:1106:G:H2'	2:2:1107:G:N3	2.28	0.48
2:2:1156:A:O2'	2:2:1158:C:OP1	2.30	0.48
2:2:1464:G:C6	2:2:1465:C:N4	2.81	0.48
6:C:89:LYS:HG3	6:C:104:LYS:HB3	1.95	0.48
26:W:53:ILE:HD11	31:b:8:LEU:HD23	1.96	0.48
2:2:298:A:H2'	2:2:299:A:H5'	1.96	0.48
2:2:639:U:H2'	2:2:640:G:O4'	2.14	0.48
2:2:867:G:H22	2:2:959:U:H3	1.61	0.48
2:2:1277:G:C2	2:2:1278:C:C2	3.02	0.48
2:2:1287:G:H8	2:2:1287:G:O5'	1.97	0.48
2:2:1651:C:N4	2:2:1745:G:H1	2.11	0.48
6:C:178:PRO:HG3	13:J:57:ARG:HE	1.78	0.48
23:T:86:ARG:HH11	23:T:89:ARG:HB3	1.78	0.48
30:a:44:ILE:HG23	30:a:45:VAL:HG23	1.95	0.48
2:2:392:C:H5''	2:2:399:A:C2	2.49	0.48
2:2:566:A:H3'	2:2:567:G:C5'	2.43	0.48
2:2:1050:G:C2	2:2:1067:C:C2	3.01	0.48
2:2:1292:U:H2'	4:A:109:ASN:HD21	1.78	0.48
2:2:1357:G:H1	2:2:1364:C:H42	1.59	0.48
5:B:58:SER:HA	5:B:61:LEU:HD12	1.94	0.48
40:k:357:PRO:HD3	40:k:416:VAL:HG22	1.95	0.48
2:2:141:U:H2'	2:2:142:G:H8	1.79	0.48
2:2:871:G:H1'	31:b:68:GLY:HA2	1.94	0.48
2:2:1252:U:H5''	16:M:43:LYS:HZ1	1.77	0.48
2:2:1771:C:C2	2:2:1787:G:N2	2.81	0.48
38:i:39:THR:H	38:i:49:ALA:HA	1.79	0.48
2:2:410:C:H2'	2:2:411:A:O4'	2.14	0.48
2:2:444:A:H61	2:2:460:G:N2	2.12	0.48
2:2:1746:G:H2'	2:2:1747:A:C8	2.49	0.48
14:K:13:GLN:HA	14:K:80:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:112:ASP:O	22:S:116:LEU:HG	2.13	0.48
23:T:105:LEU:HA	23:T:108:LEU:HD12	1.95	0.48
43:o:180:SER:O	43:o:184:LYS:HG3	2.13	0.48
2:2:1504:G:H2'	2:2:1505:G:O4'	2.14	0.48
16:M:89:GLY:HA2	16:M:94:LEU:HD13	1.96	0.48
44:p:329:LEU:HD13	44:p:410:ARG:HD3	1.93	0.48
2:2:323:U:H2'	2:2:324:G:C8	2.48	0.47
2:2:940:A:C2	2:2:975:G:H5'	2.49	0.47
2:2:1204:C:H5''	2:2:1205:U:C5	2.49	0.47
2:2:1794:C:O2	30:a:5:ARG:HG2	2.14	0.47
10:G:32:ILE:HD12	10:G:100:ALA:HA	1.95	0.47
15:L:14:GLN:HB3	15:L:54:ILE:HG12	1.96	0.47
1:1:3:C:N4	1:1:70:G:H1	2.12	0.47
1:1:74:C:H4'	1:1:75:C:C5'	2.45	0.47
2:2:642:G:C2	2:2:692:C:C2	3.02	0.47
2:2:877:G:H2'	2:2:878:G:C8	2.49	0.47
2:2:1209:C:H2'	2:2:1210:A:H8	1.79	0.47
23:T:113:VAL:HG23	23:T:114:VAL:HG23	1.95	0.47
39:j:4:SER:HB3	39:j:113:ARG:NH1	2.29	0.47
40:k:355:ILE:HG12	40:k:417:VAL:HG22	1.95	0.47
44:p:300:ILE:N	44:p:301:PRO:HD2	2.29	0.47
2:2:453:U:C2	8:E:66:MET:HG3	2.49	0.47
2:2:642:G:N1	2:2:692:C:C4	2.83	0.47
2:2:877:G:H1	2:2:949:C:H42	1.62	0.47
22:S:49:LYS:HG3	22:S:81:ILE:HD11	1.95	0.47
28:Y:129:ALA:O	28:Y:133:ASN:HB2	2.14	0.47
44:p:640:ILE:HG13	44:p:765:ILE:HG12	1.96	0.47
1:1:10:G:C2	1:1:11:C:N3	2.82	0.47
2:2:444:A:H1'	2:2:524:A:H5''	1.95	0.47
2:2:646:G:H2'	2:2:647:G:O4'	2.14	0.47
2:2:1389:A:H4'	21:R:28:PHE:HE2	1.78	0.47
2:2:1571:A:H4'	2:2:1572:G:O5'	2.14	0.47
2:2:1586:G:C2	2:2:1587:C:C2	3.02	0.47
7:D:72:LEU:HA	14:K:20:VAL:HG21	1.96	0.47
36:g:115:ALA:HB3	36:g:124:ILE:HG23	1.95	0.47
39:j:236:ASP:HB2	39:j:239:LYS:HG3	1.96	0.47
40:k:357:PRO:HB2	40:k:415:GLN:HE21	1.79	0.47
43:o:403:GLN:O	43:o:407:LEU:HB3	2.13	0.47
2:2:832:U:H5'	2:2:833:G:H5''	1.96	0.47
2:2:1014:U:H3'	2:2:1015:C:H5'	1.96	0.47
2:2:1137:A:H2'	2:2:1138:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:2:LYS:HE2	47:s:78:GLU:HB2	1.97	0.47
2:2:597:U:C2	2:2:598:A:C8	3.02	0.47
2:2:805:A:H2	2:2:806:A:C5	2.33	0.47
2:2:862:A:H2'	2:2:864:A:C8	2.50	0.47
2:2:1182:A:C8	19:P:100:LYS:HD2	2.50	0.47
2:2:1458:A:H1'	41:l:169:GLY:HA2	1.96	0.47
2:2:1497:G:C6	2:2:1507:C:N3	2.82	0.47
2:2:1631:A:C8	2:2:1631:A:H5''	2.49	0.47
2:2:1639:C:H4'	37:h:1:MET:HB2	1.96	0.47
16:M:21:LEU:O	16:M:24:VAL:HG22	2.15	0.47
39:j:132:TRP:O	39:j:136:ARG:HB3	2.15	0.47
42:m:40:THR:HG23	42:m:83:ASP:HA	1.95	0.47
2:2:142:G:H2'	2:2:143:G:C8	2.50	0.47
2:2:520:A:H2'	2:2:521:U:O4'	2.15	0.47
2:2:1127:C:H2'	2:2:1128:U:O4'	2.15	0.47
2:2:1628:U:C2	2:2:1630:C:N4	2.83	0.47
5:B:88:VAL:HG22	5:B:98:THR:HG22	1.97	0.47
5:B:187:LYS:O	5:B:190:PRO:HD2	2.14	0.47
8:E:128:LYS:HB2	8:E:140:VAL:HB	1.96	0.47
11:H:49:ILE:HG23	11:H:175:LYS:HG3	1.96	0.47
13:J:21:SER:HA	13:J:24:LEU:HD12	1.97	0.47
13:J:59:LEU:HD21	13:J:72:GLU:HB2	1.97	0.47
16:M:123:GLU:HA	16:M:126:ILE:HD12	1.96	0.47
22:S:117:LYS:HE2	22:S:128:PHE:HB2	1.97	0.47
26:W:24:GLN:HA	26:W:63:VAL:O	2.15	0.47
31:b:50:ALA:O	31:b:51:GLN:HB2	2.15	0.47
32:c:12:VAL:HG22	32:c:52:ASP:H	1.80	0.47
36:g:160:LYS:HZ2	36:g:171:ARG:HG2	1.80	0.47
1:1:29:G:H1	1:1:41:C:H42	1.62	0.47
2:2:223:C:H2'	2:2:224:A:H8	1.80	0.47
2:2:323:U:H2'	2:2:324:G:H8	1.80	0.47
2:2:325:G:C2	2:2:342:C:O2	2.68	0.47
24:U:117:ILE:HG22	24:U:118:ILE:HG13	1.97	0.47
31:b:20:LYS:O	31:b:21:LEU:HB2	2.15	0.47
36:g:65:HIS:CE1	36:g:91:ARG:HD2	2.50	0.47
36:g:133:ARG:HG2	36:g:144:VAL:HG13	1.97	0.47
2:2:373:U:H2'	2:2:374:U:C6	2.50	0.47
2:2:417:G:H8	10:G:59:GLN:NE2	2.13	0.47
2:2:1116:U:H2'	2:2:1117:G:O4'	2.15	0.47
2:2:1711:G:H2'	2:2:1711:G:N3	2.29	0.47
6:C:111:ASP:CG	6:C:112:SER:N	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:129:VAL:HG22	8:E:139:VAL:HG23	1.97	0.47
9:F:37:GLN:HB3	9:F:38:ALA:H	1.54	0.47
2:2:394:U:O2	2:2:394:U:H2'	2.14	0.47
2:2:601:U:H2'	2:2:602:U:C6	2.50	0.47
2:2:702:G:H1	2:2:736:C:N4	2.13	0.47
2:2:730:G:H2'	2:2:730:G:N3	2.30	0.47
2:2:1240:G:OP2	19:P:77:ARG:HD3	2.15	0.47
2:2:1482:G:C6	2:2:1483:C:N4	2.83	0.47
4:A:79:ARG:HB2	4:A:79:ARG:HH11	1.79	0.47
16:M:64:ILE:HG22	35:f:103:LEU:HD22	1.96	0.47
18:O:63:ALA:O	18:O:67:VAL:HG23	2.15	0.47
21:R:37:GLU:HG3	36:g:151:TRP:CH2	2.50	0.47
45:q:179:LYS:HB3	45:q:189:VAL:HB	1.96	0.47
1:1:9:G:N2	1:1:43:G:H5''	2.30	0.46
2:2:97:C:O2	2:2:424:A:O2'	2.33	0.46
2:2:391:G:H5'	2:2:1727:C:O2'	2.15	0.46
2:2:810:A:C2	2:2:857:G:H1'	2.50	0.46
2:2:976:A:H2'	2:2:977:A:O4'	2.14	0.46
2:2:1317:G:H2'	2:2:1318:A:C8	2.51	0.46
2:2:1475:G:H1	2:2:1528:C:N4	2.13	0.46
26:W:46:TYR:CZ	26:W:130:TYR:HA	2.50	0.46
35:f:83:LYS:HD3	38:i:23:LYS:HD2	1.97	0.46
40:k:297:PHE:HA	40:k:300:LYS:HB2	1.96	0.46
43:o:247:SER:HB3	43:o:256:ALA:HB2	1.97	0.46
45:q:156:ALA:HA	45:q:172:HIS:HA	1.97	0.46
1:1:9:G:H1'	1:1:44:A:C8	2.50	0.46
2:2:328:G:H2'	2:2:329:G:H8	1.79	0.46
2:2:334:U:H2'	2:2:335:G:C8	2.50	0.46
2:2:409:A:H3'	2:2:410:C:C5	2.50	0.46
2:2:410:C:O2	2:2:410:C:C2'	2.63	0.46
2:2:1043:U:O2	2:2:1043:U:C3'	2.63	0.46
2:2:1540:G:C6	2:2:1566:C:N3	2.83	0.46
2:2:1611:U:OP1	9:F:171:ASN:HB3	2.15	0.46
2:2:1798:A:H2'	2:2:1798:A:N3	2.30	0.46
20:Q:117:LEU:HD23	20:Q:117:LEU:H	1.79	0.46
36:g:117:ASP:HB2	36:g:122:LYS:H	1.79	0.46
2:2:778:G:H5'	2:2:780:A:H2	1.79	0.46
2:2:825:U:H2'	2:2:826:C:H4'	1.97	0.46
2:2:1464:G:C2	2:2:1465:C:C4	3.04	0.46
2:2:1617:C:H2'	2:2:1618:C:H6	1.79	0.46
39:j:4:SER:HB3	39:j:113:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:338:C:H2'	2:2:339:U:C6	2.50	0.46
2:2:339:U:H2'	2:2:340:A:H8	1.81	0.46
2:2:390:A:H2'	2:2:391:G:O4'	2.16	0.46
2:2:984:G:H22	2:2:1015:C:H5	1.64	0.46
2:2:1263:G:H8	2:2:1263:G:O5'	1.99	0.46
19:P:77:ARG:HB3	19:P:102:PHE:HE2	1.80	0.46
23:T:105:LEU:HD22	23:T:122:ARG:HD3	1.96	0.46
42:m:32:GLN:HG2	42:m:38:THR:HG22	1.98	0.46
2:2:28:A:N3	2:2:29:U:H1'	2.30	0.46
2:2:50:C:O2	2:2:429:G:C2	2.69	0.46
2:2:365:A:H2'	2:2:366:A:H8	1.80	0.46
2:2:1017:U:O2	2:2:1017:U:C2'	2.58	0.46
2:2:1343:A:H2'	2:2:1344:A:C8	2.50	0.46
2:2:1619:U:H2'	2:2:1620:G:H8	1.81	0.46
9:F:185:ALA:CB	9:F:192:ILE:HG12	2.45	0.46
11:H:154:LEU:HB2	11:H:185:ILE:HG13	1.97	0.46
17:N:87:ASP:OD1	17:N:87:ASP:N	2.49	0.46
24:U:48:PHE:HB3	24:U:50:LEU:HG	1.98	0.46
44:p:431:ARG:HD3	44:p:431:ARG:HA	1.73	0.46
2:2:444:A:H8	2:2:524:A:C5'	2.25	0.46
2:2:609:G:H8	2:2:612:G:H21	1.63	0.46
2:2:1457:C:H5'	22:S:131:LEU:HD21	1.98	0.46
2:2:1464:G:N1	2:2:1465:C:C4	2.84	0.46
2:2:1673:C:C2	2:2:1725:G:N2	2.84	0.46
4:A:41:ARG:HB2	4:A:45:VAL:O	2.15	0.46
6:C:46:LEU:O	6:C:50:VAL:HG23	2.15	0.46
13:J:163:PRO:C	13:J:165:GLY:H	2.23	0.46
23:T:66:TYR:HA	23:T:124:ILE:HG12	1.96	0.46
2:2:52:U:H2'	2:2:53:G:C8	2.50	0.46
2:2:119:A:H1'	2:2:396:A:C4	2.51	0.46
2:2:925:A:H3'	2:2:926:C:C6	2.50	0.46
2:2:1031:G:C2	2:2:1032:C:C2	3.04	0.46
2:2:1073:G:N2	2:2:1074:C:C2	2.83	0.46
2:2:1288:U:H2'	2:2:1289:U:C6	2.51	0.46
2:2:1412:U:O4'	2:2:1412:U:O2	2.33	0.46
4:A:193:GLN:HA	4:A:194:PRO:HD3	1.78	0.46
9:F:43:LYS:HE2	20:Q:54:LEU:HD23	1.97	0.46
39:j:123:LEU:O	39:j:126:LEU:HG	2.16	0.46
1:1:62:C:H2'	1:1:63:G:H8	1.81	0.46
2:2:220:A:H61	2:2:839:U:H3	1.64	0.46
28:Y:122:GLY:HA2	28:Y:125:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:294:A:C2	2:2:295:U:C2	3.04	0.46
2:2:599:U:H2'	2:2:600:A:C8	2.51	0.46
2:2:994:A:H61	2:2:1007:G:H1	1.64	0.46
2:2:1162:A:N1	2:2:1580:U:O4	2.49	0.46
2:2:1206:C:N4	2:2:1454:C:H41	2.08	0.46
2:2:1306:U:H3'	2:2:1307:G:C8	2.50	0.46
2:2:1315:G:OP2	21:R:7:LYS:HB2	2.16	0.46
2:2:1333:U:H2'	2:2:1334:U:O4'	2.16	0.46
2:2:1499:C:C2	2:2:1505:G:N2	2.84	0.46
2:2:1620:G:N1	2:2:1621:C:C4	2.84	0.46
2:2:1637:C:H42	2:2:1761:A:H61	1.64	0.46
6:C:95:THR:HG22	6:C:96:ARG:H	1.80	0.46
10:G:7:TYR:HD1	10:G:113:ILE:HG23	1.81	0.46
23:T:22:LEU:HD22	23:T:28:LEU:HD23	1.98	0.46
1:1:56:C:H2'	1:1:57:G:O4'	2.16	0.46
2:2:842:U:H2'	2:2:843:A:C8	2.50	0.46
2:2:944:U:H2'	2:2:945:U:C6	2.51	0.46
2:2:1269:G:C2	2:2:1439:C:C2	3.03	0.46
2:2:1577:U:H2'	2:2:1578:C:C6	2.51	0.46
2:2:1588:G:N1	2:2:1589:C:C4	2.83	0.46
18:O:24:ASN:HA	18:O:55:SER:HB3	1.98	0.46
19:P:77:ARG:HB3	19:P:102:PHE:CE2	2.51	0.46
19:P:111:MET:SD	22:S:119:ILE:HG21	2.56	0.46
20:Q:38:LEU:HD21	23:T:10:PRO:HA	1.97	0.46
27:X:87:VAL:HG13	27:X:132:LEU:HD11	1.98	0.46
39:j:15:GLU:HG3	39:j:18:ASP:HB3	1.98	0.46
47:s:70:ALA:HA	47:s:74:ARG:HH12	1.81	0.46
2:2:541:A:H3'	2:2:542:C:H3'	1.98	0.45
2:2:797:C:H2'	2:2:798:A:C8	2.50	0.45
2:2:1038:A:O2'	2:2:1039:G:C8	2.70	0.45
2:2:1338:C:N4	2:2:1383:G:H1	2.11	0.45
2:2:1659:U:H2'	2:2:1660:G:H8	1.81	0.45
5:B:176:VAL:HG12	5:B:177:GLN:H	1.80	0.45
40:k:312:SER:HA	40:k:313:PRO:HD3	1.84	0.45
1:1:11:C:H42	1:1:24:G:H1	1.63	0.45
2:2:541:A:H2	2:2:543:A:H1'	1.80	0.45
2:2:993:G:N1	2:2:1009:C:C4	2.84	0.45
14:K:83:PRO:HG2	14:K:86:ILE:HD13	1.98	0.45
22:S:35:ILE:HD12	22:S:38:VAL:HG21	1.98	0.45
36:g:86:TRP:HA	36:g:110:ASP:HB2	1.98	0.45
40:k:174:CYS:HB2	40:k:182:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:375:SER:HB2	40:k:400:THR:HB	1.98	0.45
43:o:89:VAL:O	43:o:92:VAL:HG22	2.16	0.45
45:q:6:LEU:HD21	45:q:319:LEU:HD22	1.98	0.45
2:2:178:A:H61	10:G:202:ARG:NH2	2.15	0.45
2:2:1204:C:H5''	2:2:1205:U:H5	1.81	0.45
2:2:1284:U:O2	2:2:1284:U:O4'	2.34	0.45
2:2:1393:G:N2	2:2:1402:C:C2	2.85	0.45
2:2:1484:G:H3'	2:2:1485:A:C8	2.51	0.45
17:N:114:ARG:O	17:N:118:ILE:HG12	2.15	0.45
19:P:128:HIS:HA	41:l:168:ASP:HB3	1.98	0.45
2:2:332:A:C6	2:2:333:G:C6	3.04	0.45
2:2:967:U:C4	2:2:968:C:C4	3.04	0.45
2:2:1288:U:H2'	2:2:1289:U:H6	1.81	0.45
2:2:1334:U:H2'	2:2:1335:A:H8	1.81	0.45
2:2:1496:G:H5''	23:T:72:GLY:HA3	1.99	0.45
8:E:104:ASP:HB3	8:E:110:ALA:HB2	1.98	0.45
9:F:119:THR:HG21	9:F:196:LEU:HD22	1.97	0.45
24:U:34:LEU:O	24:U:37:VAL:HG12	2.16	0.45
45:q:63:PHE:HD2	45:q:129:ARG:HH12	1.64	0.45
45:q:150:HIS:HB3	45:q:153:LEU:HD12	1.98	0.45
2:2:28:A:C2	2:2:29:U:H1'	2.52	0.45
2:2:970:A:H3'	2:2:971:G:H8	1.82	0.45
2:2:1178:G:C2	2:2:1179:C:C2	3.04	0.45
2:2:1179:C:H42	2:2:1456:G:H1	1.64	0.45
10:G:10:ASN:HB3	10:G:128:THR:HA	1.99	0.45
21:R:59:LYS:O	21:R:62:GLN:HB2	2.17	0.45
41:l:218:GLN:C	41:l:220:LYS:H	2.24	0.45
2:2:48:G:C2	2:2:49:C:C2	3.05	0.45
2:2:92:A:H5'	2:2:93:A:H5''	1.99	0.45
2:2:547:G:H1	2:2:589:C:H42	1.63	0.45
2:2:1100:G:H8	2:2:1100:G:H5''	1.81	0.45
4:A:90:ALA:HA	4:A:95:ALA:HB3	1.98	0.45
6:C:146:ARG:HH11	6:C:146:ARG:HB2	1.82	0.45
20:Q:78:VAL:HA	20:Q:81:ILE:HD12	1.99	0.45
36:g:227:ILE:HB	36:g:241:PHE:HB2	1.98	0.45
40:k:351:ASP:HB2	40:k:377:ILE:HD12	1.98	0.45
1:1:74:C:C4	40:k:128:PHE:HB2	2.52	0.45
2:2:22:A:H2'	2:2:23:G:O4'	2.17	0.45
2:2:389:G:O2'	2:2:390:A:O4'	2.34	0.45
2:2:564:C:C2	2:2:576:G:C2	3.04	0.45
2:2:878:G:C6	2:2:879:C:N4	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:121:ILE:HD13	5:B:164:ILE:HG21	1.99	0.45
9:F:176:LEU:HB3	9:F:212:ALA:HB1	1.99	0.45
22:S:89:GLN:C	22:S:91:ASP:H	2.24	0.45
40:k:315:LEU:HB3	40:k:417:VAL:HB	1.99	0.45
41:l:184:LEU:HD22	41:l:234:VAL:HG11	1.98	0.45
2:2:442:C:C2	2:2:461:G:C2	3.04	0.45
2:2:1153:G:H2'	2:2:1154:G:O4'	2.16	0.45
4:A:120:LEU:HD11	4:A:144:ILE:HD12	1.99	0.45
16:M:54:VAL:HB	16:M:112:VAL:HB	1.98	0.45
2:2:362:G:C2	2:2:381:C:C2	3.05	0.45
2:2:1171:G:C6	2:2:1172:C:C4	3.05	0.45
2:2:1270:G:H2'	2:2:1271:U:C6	2.51	0.45
2:2:1467:A:H4'	2:2:1539:G:H4'	1.97	0.45
2:2:1643:G:C6	2:2:1644:C:N4	2.84	0.45
2:2:1673:C:C2	2:2:1725:G:C2	3.05	0.45
15:L:3:THR:HA	15:L:82:ARG:HH21	1.80	0.45
20:Q:69:VAL:HG21	20:Q:81:ILE:HG12	1.99	0.45
43:o:260:ILE:HD11	43:o:285:ASN:HB3	1.99	0.45
2:2:550:G:H1	2:2:572:C:N4	2.14	0.45
2:2:803:A:C8	26:W:107:SER:HA	2.51	0.45
2:2:1171:G:H1	2:2:1465:C:H42	1.63	0.45
2:2:1462:G:N2	2:2:1463:C:C2	2.85	0.45
2:2:1588:G:H1	2:2:1604:C:H42	1.65	0.45
8:E:100:ARG:HH22	8:E:122:LYS:HA	1.82	0.45
18:O:31:THR:HG22	18:O:38:THR:HA	1.99	0.45
42:m:92:MET:HG2	42:m:93:ILE:N	2.31	0.45
2:2:340:A:H4'	12:I:87:ASN:ND2	2.32	0.44
2:2:477:A:H2	2:2:509:G:H22	1.65	0.44
2:2:564:C:N3	2:2:576:G:C2	2.85	0.44
2:2:1268:U:O2	2:2:1268:U:O4'	2.34	0.44
2:2:1586:G:C6	2:2:1587:C:C4	3.06	0.44
2:2:1789:A:H5'	30:a:8:ASN:HB3	1.99	0.44
7:D:65:ARG:HA	7:D:68:GLU:HG3	1.99	0.44
9:F:115:ILE:HG23	9:F:193:ALA:HB2	1.99	0.44
18:O:89:THR:HB	18:O:128:LYS:HG3	1.99	0.44
23:T:38:LYS:C	23:T:40:SER:H	2.25	0.44
39:j:169:LEU:O	39:j:173:ILE:HG13	2.18	0.44
41:l:157:LYS:HA	41:l:159:ARG:HG3	1.99	0.44
43:o:222:ASN:O	43:o:223:ASN:HB2	2.17	0.44
43:o:244:VAL:HG12	43:o:285:ASN:HD22	1.82	0.44
2:2:30:G:C2	2:2:31:C:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1300:U:H2'	2:2:1301:U:O4'	2.17	0.44
2:2:1367:G:H5''	23:T:69:LYS:HD3	1.99	0.44
2:2:1655:U:H4'	2:2:1656:G:O5'	2.17	0.44
7:D:59:VAL:HG13	7:D:63:GLY:HA2	2.00	0.44
13:J:80:LEU:O	13:J:83:ILE:HG22	2.17	0.44
14:K:21:LEU:HG	14:K:46:LEU:HD21	2.00	0.44
36:g:218:ALA:HB2	36:g:232:LEU:HD11	1.99	0.44
38:i:65:LEU:HG	38:i:69:VAL:HB	2.00	0.44
2:2:385:G:H2'	2:2:386:A:C8	2.53	0.44
2:2:480:A:N6	2:2:506:U:H3	2.15	0.44
2:2:1075:A:C2	2:2:1076:C:C2	3.05	0.44
2:2:1145:G:H3'	2:2:1146:A:H8	1.81	0.44
2:2:1272:G:N7	2:2:1428:U:H3'	2.32	0.44
2:2:1462:G:C2	2:2:1463:C:C4	3.05	0.44
2:2:1494:U:H2'	2:2:1495:U:H6	1.83	0.44
2:2:1497:G:C2	2:2:1507:C:C2	3.05	0.44
10:G:88:ARG:HB2	10:G:91:GLU:HB2	1.99	0.44
14:K:69:THR:HG23	14:K:72:GLY:H	1.82	0.44
17:N:71:ILE:HA	17:N:74:ILE:HD12	1.98	0.44
27:X:63:GLN:C	27:X:65:ASN:N	2.70	0.44
39:j:19:ILE:HD13	39:j:19:ILE:H	1.82	0.44
2:2:6:G:H1	2:2:18:C:H42	1.64	0.44
2:2:14:C:C2	2:2:1140:G:C2	3.06	0.44
2:2:1175:G:C5	2:2:1462:G:C6	3.05	0.44
2:2:1363:G:C6	2:2:1364:C:N4	2.86	0.44
2:2:1605:G:H2'	2:2:1606:U:H6	1.82	0.44
2:2:1606:U:O3'	20:Q:73:GLY:HA3	2.17	0.44
2:2:1620:G:C6	2:2:1621:C:N4	2.86	0.44
7:D:137:VAL:HG22	7:D:151:LYS:HG2	2.00	0.44
9:F:100:MET:HG3	9:F:107:GLY:O	2.18	0.44
25:V:37:ALA:HA	25:V:50:TYR:HB3	1.99	0.44
2:2:268:G:C2	2:2:269:C:C2	3.06	0.44
2:2:429:G:N1	2:2:430:C:C4	2.85	0.44
2:2:1286:A:N6	2:2:1328:A:O4'	2.51	0.44
2:2:1367:G:H5''	23:T:69:LYS:HB3	2.00	0.44
2:2:1437:C:H2'	2:2:1438:C:H6	1.81	0.44
2:2:1441:U:H4'	2:2:1444:A:H1'	1.99	0.44
2:2:1679:A:H2	2:2:1718:G:H21	1.65	0.44
7:D:25:PHE:CE2	7:D:50:ILE:HG12	2.52	0.44
17:N:25:TRP:HB2	31:b:82:LYS:HZ3	1.82	0.44
17:N:35:GLU:HA	17:N:38:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:77:GLN:O	20:Q:81:ILE:HG13	2.17	0.44
1:1:10:G:N1	1:1:11:C:C4	2.86	0.44
2:2:602:U:H2'	2:2:603:A:C8	2.53	0.44
2:2:930:C:H5''	2:2:931:U:H5'	2.00	0.44
2:2:1045:G:H2'	2:2:1046:G:O4'	2.17	0.44
20:Q:29:ILE:HB	20:Q:36:ILE:HD12	1.99	0.44
26:W:90:THR:HG23	26:W:94:LEU:HD12	2.00	0.44
2:2:77:U:H5	10:G:159:ARG:HD2	1.82	0.44
2:2:567:G:N1	2:2:568:C:C4	2.85	0.44
2:2:1123:A:H2'	2:2:1124:A:C8	2.53	0.44
2:2:1154:G:C6	2:2:1155:C:C4	3.06	0.44
2:2:1208:C:O5'	2:2:1208:C:H6	2.01	0.44
8:E:173:ILE:HD11	8:E:235:TRP:CE2	2.53	0.44
44:p:776:PHE:HB3	44:p:778:VAL:HG23	1.99	0.44
1:1:30:G:C2	1:1:41:C:C2	3.05	0.44
2:2:10:G:C6	2:2:1631:A:C2	3.06	0.44
2:2:283:G:O6	10:G:185:GLN:HG3	2.18	0.44
2:2:374:U:H2'	2:2:375:C:C6	2.52	0.44
2:2:450:A:H2'	2:2:452:U:C6	2.52	0.44
2:2:877:G:H2'	2:2:878:G:H8	1.82	0.44
2:2:1136:A:O3'	2:2:1137:A:H4'	2.18	0.44
2:2:1171:G:C2	2:2:1172:C:C2	3.06	0.44
2:2:1279:C:C2	2:2:1427:G:C2	3.06	0.44
6:C:173:ARG:HB3	6:C:204:SER:HB2	2.00	0.44
14:K:54:PHE:HA	14:K:72:GLY:HA3	1.99	0.44
14:K:82:LEU:HD13	14:K:83:PRO:HD2	2.00	0.44
36:g:126:ALA:HB2	36:g:132:ILE:HG23	1.99	0.44
2:2:403:G:C2	2:2:404:C:C2	3.04	0.44
2:2:1482:G:C2	2:2:1483:C:N3	2.86	0.44
5:B:3:VAL:HB	39:j:89:ARG:HD2	1.99	0.44
27:X:61:SER:HB2	27:X:116:ASP:HB2	2.00	0.44
30:a:30:VAL:HG22	30:a:31:PRO:HD2	2.00	0.44
36:g:267:ILE:HG23	36:g:299:LEU:HD11	2.00	0.44
39:j:134:LEU:HD12	39:j:141:ALA:HA	2.00	0.44
1:1:22:G:N2	1:1:23:C:C2	2.86	0.43
2:2:1038:A:O2'	2:2:1039:G:H8	2.01	0.43
2:2:1155:C:N4	2:2:1620:G:H1	2.16	0.43
2:2:1583:U:O4	2:2:1609:A:C2	2.69	0.43
2:2:1670:G:C2	2:2:1671:G:C5	3.05	0.43
11:H:70:TYR:O	11:H:74:GLN:N	2.49	0.43
14:K:22:VAL:HB	14:K:23:ALA:H	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:64:LYS:HG3	17:N:70:LYS:HD2	1.99	0.43
21:R:32:LYS:HD3	21:R:47:ARG:HD3	1.99	0.43
24:U:28:SER:HB2	24:U:112:VAL:HG23	1.99	0.43
27:X:109:ARG:HB3	27:X:112:LYS:HB2	2.00	0.43
36:g:111:VAL:HA	36:g:127:SER:HA	2.00	0.43
39:j:201:ILE:HG22	40:k:330:ILE:CG2	2.43	0.43
44:p:491:SER:HA	44:p:499:GLN:HG2	2.00	0.43
1:1:65:G:N2	1:1:66:C:C2	2.86	0.43
2:2:1015:C:O2	2:2:1015:C:O4'	2.35	0.43
2:2:1141:A:H2'	2:2:1142:A:C8	2.52	0.43
2:2:1192:A:N3	2:2:1192:A:H2'	2.33	0.43
2:2:1236:G:H1	2:2:1247:C:H42	1.65	0.43
2:2:1492:C:N4	2:2:1511:G:H1	2.12	0.43
10:G:1:MET:HE1	10:G:106:LEU:H	1.83	0.43
12:I:148:ALA:C	12:I:150:GLU:H	2.26	0.43
17:N:101:HIS:CE1	17:N:105:ASN:HD21	2.36	0.43
20:Q:125:GLU:HA	20:Q:126:PRO:HD2	1.81	0.43
27:X:42:PRO:HA	27:X:81:LYS:HD2	2.00	0.43
2:2:275:C:H1'	2:2:276:U:C5	2.53	0.43
2:2:280:G:C2	2:2:281:C:C2	3.07	0.43
2:2:935:G:C2	2:2:936:C:C2	3.07	0.43
2:2:1136:A:H1'	2:2:1137:A:H1'	2.01	0.43
2:2:1175:G:C2	2:2:1176:C:C2	3.07	0.43
2:2:1482:G:N2	2:2:1483:C:C2	2.87	0.43
2:2:1537:G:H3'	2:2:1538:G:H5'	2.00	0.43
6:C:174:LEU:HD23	6:C:203:THR:HG22	2.00	0.43
9:F:190:LYS:HB3	9:F:195:THR:HG22	2.00	0.43
22:S:126:ARG:HD3	22:S:133:VAL:HA	2.00	0.43
43:o:287:VAL:HG13	43:o:299:HIS:CE1	2.53	0.43
45:q:326:TYR:O	45:q:329:PHE:HB2	2.18	0.43
1:1:13:C:H4'	42:m:73:GLU:HG2	2.00	0.43
2:2:18:C:H4'	2:2:1136:A:N6	2.34	0.43
2:2:176:U:H2'	2:2:177:U:C6	2.53	0.43
2:2:512:U:O2	2:2:512:U:O4'	2.33	0.43
2:2:573:G:C2	2:2:574:C:C2	3.07	0.43
2:2:846:A:O5'	2:2:846:A:H8	2.01	0.43
2:2:1126:G:N1	2:2:1127:C:C4	2.87	0.43
2:2:1261:U:H2'	2:2:1262:G:C8	2.53	0.43
5:B:34:ALA:HB3	5:B:41:ARG:HA	2.01	0.43
7:D:51:ARG:HB3	7:D:91:VAL:HG22	1.99	0.43
9:F:119:THR:HG23	9:F:197:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:99:ILE:HA	24:U:102:ARG:HD2	1.99	0.43
27:X:23:ARG:HB3	27:X:29:TYR:CE2	2.53	0.43
44:p:429:LEU:HD23	44:p:432:PRO:HG2	2.00	0.43
2:2:57:G:H1	2:2:90:C:N4	2.17	0.43
2:2:339:U:H2'	2:2:340:A:C8	2.53	0.43
2:2:1497:G:C2	2:2:1498:C:C2	3.06	0.43
4:A:119:ARG:HE	6:C:245:MET:HE3	1.84	0.43
8:E:20:LEU:HD11	8:E:29:PRO:HD3	2.00	0.43
8:E:44:LEU:HD12	8:E:82:PHE:HB3	2.00	0.43
41:l:190:HIS:HE1	41:l:233:TYR:CD2	2.37	0.43
45:q:309:ALA:HB2	45:q:319:LEU:HD12	2.01	0.43
2:2:89:G:H2'	2:2:90:C:O4'	2.19	0.43
2:2:460:G:H2'	2:2:461:G:O4'	2.19	0.43
2:2:598:A:H2'	2:2:598:A:N3	2.34	0.43
2:2:1031:G:C6	2:2:1032:C:C4	3.07	0.43
2:2:1157:C:C5	2:2:1580:U:C5	3.07	0.43
2:2:1179:C:N4	2:2:1456:G:H1	2.16	0.43
2:2:1637:C:H2'	2:2:1638:C:O4'	2.19	0.43
6:C:64:HIS:CD2	6:C:244:PRO:HD3	2.52	0.43
8:E:140:VAL:HG22	8:E:146:THR:HG22	1.99	0.43
11:H:61:PHE:HA	11:H:93:LEU:O	2.18	0.43
16:M:72:ALA:O	16:M:77:VAL:HA	2.18	0.43
18:O:87:GLY:HA2	18:O:92:LYS:HA	2.01	0.43
25:V:55:LEU:HB3	25:V:59:ILE:HD11	2.01	0.43
41:l:162:PRO:HA	41:l:163:PRO:HD3	1.91	0.43
2:2:18:C:H2'	2:2:19:A:H8	1.84	0.43
2:2:1418:C:H3'	2:2:1419:A:H8	1.83	0.43
10:G:180:THR:HG22	10:G:181:PRO:HD2	2.01	0.43
15:L:67:ARG:NH2	15:L:129:ARG:HA	2.34	0.43
27:X:107:PHE:HE1	27:X:114:LYS:HZ3	1.66	0.43
45:q:275:ALA:HB2	45:q:296:LEU:HD22	2.00	0.43
2:2:30:G:N2	2:2:31:C:C2	2.87	0.43
2:2:48:G:C6	2:2:49:C:C4	3.06	0.43
2:2:89:G:C6	2:2:90:C:C4	3.06	0.43
2:2:481:U:H3	2:2:504:A:N6	2.16	0.43
2:2:1033:C:C2	2:2:1101:G:C2	3.06	0.43
2:2:1154:G:C2	2:2:1622:C:C2	3.07	0.43
2:2:1178:G:H2'	2:2:1179:C:C6	2.54	0.43
2:2:1295:A:C6	2:2:1296:G:C5	3.07	0.43
2:2:1560:G:N1	2:2:1561:C:C4	2.86	0.43
2:2:1673:C:N3	2:2:1725:G:C2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:20:PHE:HD2	18:O:27:PHE:HB2	1.84	0.43
35:f:121:CYS:HA	35:f:122:PRO:HD3	1.87	0.43
36:g:270:TYR:HA	36:g:277:LEU:HA	2.01	0.43
39:j:188:VAL:HG22	39:j:264:ILE:HG23	2.01	0.43
43:o:474:VAL:C	43:o:476:ASP:H	2.26	0.43
43:o:483:ASP:HB2	43:o:488:LYS:HB2	2.01	0.43
2:2:30:G:C2	2:2:31:C:N3	2.87	0.43
2:2:168:A:H5''	10:G:176:GLN:HG2	1.99	0.43
2:2:326:U:H2'	2:2:327:A:C8	2.54	0.43
2:2:546:U:H2'	2:2:547:G:C8	2.54	0.43
2:2:687:C:H6	2:2:687:C:H5''	1.84	0.43
2:2:1014:U:C3'	2:2:1015:C:H5'	2.49	0.43
5:B:103:MET:HE2	5:B:188:LEU:HD11	1.99	0.43
8:E:45:ILE:CG1	8:E:80:THR:HB	2.49	0.43
8:E:211:LYS:HG2	8:E:215:GLU:HA	2.00	0.43
9:F:185:ALA:HB2	9:F:192:ILE:HG12	1.99	0.43
10:G:32:ILE:HG12	10:G:54:GLY:H	1.84	0.43
20:Q:12:LYS:H	20:Q:83:GLN:HE22	1.65	0.43
24:U:70:THR:HA	24:U:71:PRO:HD3	1.92	0.43
38:i:63:GLY:O	38:i:65:LEU:N	2.51	0.43
39:j:192:CYS:HA	39:j:261:VAL:H	1.82	0.43
2:2:380:C:O2'	2:2:755:A:N1	2.52	0.43
2:2:589:C:H5'	34:e:56:MET:HE2	2.01	0.43
2:2:685:A:H2'	2:2:686:C:C6	2.53	0.43
2:2:1153:G:N2	2:2:1623:C:C2	2.87	0.43
2:2:1460:G:C2	2:2:1461:C:C2	3.06	0.43
2:2:1497:G:C6	2:2:1498:C:C4	3.07	0.43
18:O:30:VAL:HG11	18:O:71:CYS:SG	2.58	0.43
32:c:9:LEU:HD12	32:c:33:LEU:HD21	2.01	0.43
39:j:149:ILE:HG21	39:j:173:ILE:HG21	2.01	0.43
44:p:280:GLU:HA	44:p:283:LEU:HD12	2.00	0.43
45:q:79:TRP:HB3	45:q:86:CYS:HA	2.00	0.43
2:2:150:G:H21	10:G:13:GLN:HE22	1.66	0.42
2:2:446:U:OP2	8:E:57:ASN:HB2	2.18	0.42
2:2:620:A:H8	2:2:620:A:O5'	2.02	0.42
2:2:623:G:C2	2:2:624:C:C2	3.07	0.42
2:2:1651:C:C2	2:2:1746:G:C2	3.07	0.42
6:C:162:LYS:HE2	6:C:175:ILE:HG12	2.01	0.42
14:K:15:LEU:O	14:K:19:GLY:N	2.43	0.42
26:W:82:LYS:O	26:W:84:ALA:N	2.52	0.42
1:1:9:G:H22	1:1:43:G:H5''	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:68:A:P	10:G:171:LYS:HZ3	2.42	0.42
2:2:425:G:N2	2:2:426:C:C2	2.87	0.42
2:2:1145:G:H3'	2:2:1146:A:C8	2.55	0.42
2:2:1154:G:C2	2:2:1622:C:N3	2.86	0.42
2:2:1437:C:C2	2:2:1438:C:C5	3.08	0.42
2:2:1490:A:O2'	2:2:1491:A:C8	2.71	0.42
2:2:1620:G:C2	2:2:1621:C:C2	3.07	0.42
8:E:181:VAL:HG23	8:E:227:VAL:HA	2.00	0.42
9:F:92:VAL:O	9:F:96:THR:HG23	2.18	0.42
19:P:90:ILE:HG23	19:P:108:ARG:HA	2.00	0.42
21:R:9:VAL:CG2	21:R:50:ILE:HG13	2.48	0.42
30:a:15:ARG:HG2	30:a:18:VAL:HG22	2.00	0.42
30:a:23:CYS:HB3	30:a:28:ARG:N	2.32	0.42
2:2:328:G:H2'	2:2:329:G:C8	2.54	0.42
2:2:700:C:H2'	2:2:701:U:C6	2.54	0.42
2:2:1012:A:H3'	2:2:1013:G:H8	1.84	0.42
2:2:1717:A:H2'	2:2:1718:G:O4'	2.18	0.42
7:D:202:LEU:HA	7:D:203:PRO:HD3	1.93	0.42
9:F:168:ARG:HD3	32:c:46:GLY:HA3	2.01	0.42
17:N:47:PRO:HA	17:N:50:ILE:HD12	2.00	0.42
2:2:367:U:H3'	2:2:368:A:C8	2.54	0.42
2:2:725:U:O5'	2:2:725:U:H6	2.03	0.42
2:2:945:U:O2'	2:2:946:U:H5'	2.20	0.42
2:2:977:A:N6	2:2:1023:U:H3	2.16	0.42
2:2:1222:A:N1	2:2:1259:U:O4	2.53	0.42
1:1:38:A:O2'	2:2:1000:A:O5'	2.35	0.42
2:2:16:G:C6	2:2:17:C:N3	2.87	0.42
2:2:594:G:H2'	2:2:595:C:O4'	2.19	0.42
2:2:775:G:C6	2:2:785:C:N4	2.88	0.42
2:2:1257:U:O2	2:2:1257:U:O4'	2.38	0.42
2:2:1315:G:N1	2:2:1316:C:C4	2.87	0.42
2:2:1481:A:H61	2:2:1589:C:H1'	1.84	0.42
2:2:1499:C:C2	2:2:1505:G:C2	3.07	0.42
6:C:66:LEU:HA	6:C:67:PRO:HD3	1.86	0.42
14:K:28:ASN:H	14:K:40:LEU:HD21	1.85	0.42
15:L:133:LYS:HG2	15:L:134:THR:HG23	2.01	0.42
39:j:96:ILE:H	39:j:96:ILE:HG13	1.51	0.42
40:k:176:ARG:HB2	40:k:177:PRO:HD3	2.00	0.42
40:k:495:ILE:HB	40:k:496:ASN:H	1.65	0.42
43:o:171:ASN:HD21	43:o:212:ALA:HB1	1.83	0.42
43:o:206:LEU:HB3	43:o:236:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:947:G:C2	2:2:948:C:C2	3.08	0.42
2:2:1419:A:H5'	7:D:159:HIS:HB3	2.01	0.42
2:2:1517:U:H2'	2:2:1518:U:C6	2.54	0.42
2:2:1602:U:H2'	2:2:1603:G:C8	2.54	0.42
11:H:135:ILE:HG23	11:H:152:ILE:HG23	2.01	0.42
16:M:27:THR:HG21	16:M:119:ALA:H	1.84	0.42
22:S:119:ILE:HG13	22:S:119:ILE:H	1.76	0.42
28:Y:57:VAL:HB	28:Y:60:PHE:CE1	2.55	0.42
39:j:247:ALA:HA	39:j:250:LYS:HE3	2.01	0.42
2:2:61:A:H2'	2:2:62:A:C8	2.55	0.42
2:2:244:U:H2'	2:2:245:G:H3'	2.02	0.42
2:2:703:G:H3'	2:2:704:C:H3'	2.01	0.42
2:2:1016:U:O2	2:2:1016:U:H2'	2.19	0.42
4:A:41:ARG:HB2	4:A:41:ARG:HH11	1.85	0.42
9:F:165:SER:OG	9:F:168:ARG:HB3	2.19	0.42
19:P:107:ILE:HG23	19:P:111:MET:HB2	2.01	0.42
19:P:129:GLY:HA3	41:l:173:ILE:HG21	2.01	0.42
22:S:6:GLN:CD	22:S:6:GLN:H	2.28	0.42
36:g:151:TRP:O	36:g:178:GLY:HA3	2.18	0.42
40:k:355:ILE:HD12	40:k:373:ILE:HB	2.02	0.42
2:2:299:A:H2'	2:2:300:A:H8	1.71	0.42
2:2:392:C:H42	2:2:404:C:H42	1.68	0.42
2:2:550:G:H5'	2:2:580:U:O2	2.20	0.42
2:2:974:C:O2	2:2:974:C:H2'	2.19	0.42
2:2:1251:C:O2'	35:f:140:GLY:HA3	2.19	0.42
11:H:46:ILE:HG12	11:H:60:VAL:HG12	2.02	0.42
11:H:49:ILE:HG21	11:H:172:VAL:HA	2.00	0.42
17:N:146:ALA:HA	17:N:149:LEU:HD12	2.02	0.42
22:S:4:VAL:HG23	29:Z:79:ALA:HA	2.02	0.42
27:X:54:LEU:HA	45:q:266:THR:HB	2.02	0.42
40:k:432:ILE:HD11	40:k:499:ILE:HD13	2.01	0.42
40:k:466:ILE:HG12	40:k:499:ILE:HG12	2.01	0.42
43:o:115:GLN:O	43:o:119:ILE:HG12	2.20	0.42
43:o:203:ALA:HA	43:o:240:ARG:HH22	1.85	0.42
45:q:147:ILE:HD11	45:q:186:TYR:HB3	2.02	0.42
2:2:532:U:H4'	28:Y:33:ALA:HB2	2.02	0.42
2:2:568:C:H2'	2:2:569:A:H5'	2.01	0.42
2:2:588:C:O2'	2:2:589:C:H6	2.01	0.42
2:2:760:A:H3'	2:2:761:G:H8	1.85	0.42
2:2:1322:C:H2'	2:2:1323:G:C8	2.55	0.42
2:2:1389:A:C8	2:2:1389:A:H5''	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1462:G:H2'	2:2:1463:C:C6	2.54	0.42
2:2:1589:C:H42	2:2:1603:G:H1	1.67	0.42
6:C:41:VAL:HA	6:C:42:PRO:HD3	1.89	0.42
10:G:225:GLU:HB3	10:G:226:VAL:H	1.67	0.42
26:W:113:HIS:CG	26:W:114:GLU:N	2.88	0.42
43:o:104:ILE:HD13	43:o:104:ILE:HA	1.93	0.42
2:2:335:G:O6	12:I:5:ARG:HB3	2.19	0.42
2:2:547:G:H2'	2:2:548:G:O4'	2.20	0.42
2:2:556:G:C2	2:2:558:C:C2	3.07	0.42
2:2:958:U:O2	2:2:958:U:O4'	2.36	0.42
2:2:981:U:H5'	2:2:982:A:OP2	2.20	0.42
2:2:1222:A:H2'	2:2:1223:A:O4'	2.20	0.42
7:D:162:GLN:N	7:D:163:PRO:HD2	2.35	0.42
8:E:42:LEU:HA	8:E:43:PRO:HD3	1.89	0.42
9:F:144:PRO:HD2	9:F:169:ARG:CG	2.50	0.42
14:K:24:LYS:C	14:K:26:ASP:H	2.28	0.42
24:U:58:LEU:HB2	24:U:88:LYS:HB2	2.02	0.42
39:j:59:ILE:HG12	39:j:63:ILE:HD13	2.02	0.42
43:o:152:THR:HA	43:o:155:LEU:HD12	2.01	0.42
2:2:77:U:C5	10:G:159:ARG:HD2	2.55	0.41
2:2:585:G:C2	2:2:586:C:C2	3.08	0.41
2:2:610:U:H2'	2:2:611:U:O4'	2.20	0.41
2:2:633:G:N3	2:2:633:G:H2'	2.35	0.41
2:2:1212:G:C2	2:2:1449:C:C2	3.08	0.41
2:2:1643:G:C2	2:2:1644:C:N3	2.88	0.41
9:F:179:ILE:O	9:F:183:GLU:HG2	2.20	0.41
12:I:65:PHE:HA	12:I:182:GLY:O	2.20	0.41
23:T:89:ARG:HA	23:T:90:PRO:HD3	1.82	0.41
40:k:260:LEU:O	40:k:264:LYS:HG2	2.20	0.41
44:p:716:ARG:HA	44:p:716:ARG:HD2	1.83	0.41
2:2:42:G:H1	2:2:432:C:N4	2.18	0.41
2:2:89:G:C2	2:2:90:C:C2	3.08	0.41
2:2:249:C:H2'	2:2:250:A:C8	2.53	0.41
2:2:280:G:C6	2:2:281:C:C4	3.08	0.41
2:2:327:A:H2'	2:2:328:G:C8	2.55	0.41
2:2:416:A:H1'	2:2:417:G:C2	2.55	0.41
2:2:651:U:H3'	2:2:652:C:C6	2.56	0.41
2:2:1016:U:O2	2:2:1016:U:C2'	2.68	0.41
2:2:1168:G:H21	2:2:1574:A:H62	1.67	0.41
2:2:1560:G:C2	2:2:1561:C:C2	3.09	0.41
2:2:1588:G:C2	2:2:1589:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:185:ALA:HA	6:C:203:THR:OG1	2.21	0.41
16:M:55:LEU:HD12	16:M:65:SER:HB2	2.02	0.41
22:S:87:ASN:HB2	22:S:99:HIS:CD2	2.54	0.41
27:X:99:ASN:ND2	45:q:266:THR:OG1	2.53	0.41
27:X:142:LYS:HG2	27:X:144:ARG:H	1.86	0.41
40:k:101:ILE:HG13	40:k:212:ASP:HB2	2.02	0.41
40:k:132:LEU:HD13	40:k:137:THR:HA	2.02	0.41
2:2:53:G:C2	2:2:54:C:C2	3.07	0.41
2:2:122:U:H2'	2:2:123:G:O4'	2.20	0.41
2:2:598:A:N3	2:2:599:U:C6	2.88	0.41
2:2:812:U:H4'	15:L:156:PHE:HA	2.01	0.41
2:2:944:U:H2'	2:2:945:U:H6	1.84	0.41
2:2:1154:G:C2	2:2:1155:C:C2	3.09	0.41
2:2:1191:C:H3'	2:2:1192:A:H5''	2.01	0.41
2:2:1672:C:H2'	2:2:1673:C:C6	2.56	0.41
15:L:66:ILE:HD13	15:L:128:CYS:HB3	2.02	0.41
19:P:115:TYR:N	19:P:115:TYR:CD1	2.88	0.41
29:Z:96:SER:O	29:Z:98:GLN:N	2.45	0.41
35:f:94:LYS:HB3	35:f:95:HIS:H	1.72	0.41
39:j:37:LEU:HB3	39:j:102:TYR:HE1	1.85	0.41
40:k:116:VAL:HG21	40:k:217:LEU:CD2	2.47	0.41
42:m:39:LEU:HD22	42:m:41:THR:HG23	2.02	0.41
2:2:11:A:H2'	2:2:12:U:H5'	2.02	0.41
2:2:1073:G:N1	2:2:1074:C:C4	2.88	0.41
2:2:1416:G:H5''	2:2:1416:G:C8	2.55	0.41
2:2:1505:G:C6	2:2:1506:U:C2	3.08	0.41
2:2:1558:U:H3'	2:2:1559:U:C6	2.55	0.41
2:2:1682:U:H2'	2:2:1683:G:H8	1.85	0.41
2:2:1712:A:H2'	2:2:1713:G:C8	2.55	0.41
8:E:160:VAL:HG11	8:E:169:ILE:HG12	2.02	0.41
9:F:29:THR:HG21	20:Q:29:ILE:H	1.86	0.41
9:F:96:THR:HG22	9:F:116:VAL:HG21	2.02	0.41
22:S:27:ASN:O	22:S:29:VAL:N	2.53	0.41
36:g:81:ALA:HB3	36:g:93:TRP:HB2	2.02	0.41
36:g:196:GLU:HB3	36:g:197:ALA:H	1.70	0.41
37:h:7:LYS:HE2	37:h:11:ARG:HE	1.84	0.41
38:i:82:ARG:HH11	38:i:82:ARG:HB2	1.85	0.41
43:o:206:LEU:HG	43:o:239:GLN:NE2	2.35	0.41
43:o:263:VAL:HG12	43:o:267:MET:HE2	2.00	0.41
45:q:308:TYR:HB3	45:q:322:PHE:HE2	1.86	0.41
2:2:50:C:N4	2:2:428:G:H1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:353:C:H2'	2:2:354:G:O4'	2.19	0.41
2:2:1153:G:C2	2:2:1623:C:C2	3.09	0.41
2:2:1400:G:C2	2:2:1401:C:C2	3.08	0.41
2:2:1449:C:O2'	2:2:1450:U:H5'	2.20	0.41
2:2:1617:C:H2'	2:2:1618:C:C6	2.55	0.41
9:F:84:PHE:HZ	32:c:47:PRO:HB2	1.86	0.41
10:G:89:ASN:C	10:G:91:GLU:H	2.29	0.41
13:J:4:ALA:HA	13:J:5:PRO:HD3	1.95	0.41
21:R:83:GLN:HB2	21:R:84:TYR:H	1.68	0.41
42:m:69:VAL:HB	42:m:77:ILE:HB	2.02	0.41
43:o:288:LYS:HD3	43:o:288:LYS:HA	1.92	0.41
43:o:330:LEU:HG	43:o:384:LEU:HD11	2.02	0.41
44:p:369:ILE:O	44:p:373:VAL:HG23	2.20	0.41
2:2:38:C:C2	2:2:39:A:C8	3.09	0.41
2:2:71:A:C3'	2:2:72:A:H5''	2.51	0.41
2:2:429:G:C2	2:2:430:C:C2	3.08	0.41
2:2:1379:U:O3'	24:U:59:PRO:HA	2.21	0.41
2:2:1675:C:H2'	2:2:1676:A:O4'	2.20	0.41
10:G:181:PRO:HA	10:G:184:LEU:HD12	2.03	0.41
17:N:37:ILE:HG12	17:N:54:LEU:HD11	2.02	0.41
21:R:22:PRO:O	21:R:23:LYS:HB2	2.20	0.41
41:l:170:LYS:HA	41:l:216:LYS:HG3	2.02	0.41
42:m:26:ILE:HD13	42:m:102:ASN:HB3	2.02	0.41
2:2:72:A:H4'	2:2:73:U:OP1	2.20	0.41
2:2:1088:U:H2'	2:2:1089:C:C6	2.56	0.41
2:2:1577:U:H2'	2:2:1578:C:H6	1.85	0.41
2:2:1620:G:C2	2:2:1621:C:C4	3.09	0.41
7:D:20:GLU:HG3	14:K:61:TRP:CG	2.55	0.41
7:D:138:ILE:HG23	7:D:182:LEU:HD21	2.02	0.41
8:E:122:LYS:HD2	8:E:145:ARG:HH21	1.84	0.41
12:I:107:THR:N	12:I:108:PRO:CD	2.83	0.41
20:Q:29:ILE:HG22	20:Q:65:ILE:HD12	2.01	0.41
25:V:71:ARG:HD2	31:b:4:VAL:HG11	2.01	0.41
43:o:183:VAL:HG13	43:o:239:GLN:HB2	2.00	0.41
44:p:299:LEU:O	44:p:303:ARG:HG3	2.20	0.41
45:q:56:TRP:NE1	45:q:72:ALA:HB2	2.36	0.41
2:2:49:C:H2'	2:2:50:C:O4'	2.21	0.41
2:2:878:G:C2	2:2:879:C:C2	3.08	0.41
2:2:940:A:H2	2:2:975:G:H5'	1.85	0.41
2:2:1420:A:H2'	2:2:1421:U:C6	2.56	0.41
2:2:1422:A:H2'	2:2:1423:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:3:A:H3'	3:3:3:A:N3	2.36	0.41
6:C:45:LYS:HE3	6:C:253:THR:HG23	2.03	0.41
17:N:30:SER:HB2	17:N:67:THR:HG22	2.01	0.41
20:Q:29:ILE:HD12	20:Q:36:ILE:HB	2.01	0.41
39:j:202:LYS:HG3	40:k:333:LEU:HD12	2.02	0.41
43:o:39:ARG:HA	43:o:42:TRP:HD1	1.85	0.41
43:o:206:LEU:HD13	43:o:206:LEU:HA	1.81	0.41
1:1:58:A:O5'	1:1:58:A:H8	2.03	0.41
2:2:16:G:C5	2:2:17:C:C4	3.09	0.41
2:2:303:U:H2'	2:2:304:C:C6	2.56	0.41
2:2:392:C:N4	2:2:404:C:H42	2.18	0.41
2:2:400:A:O2'	2:2:401:C:H4'	2.21	0.41
2:2:476:A:H2'	2:2:477:A:C8	2.53	0.41
2:2:564:C:H4'	2:2:565:C:O5'	2.21	0.41
2:2:595:C:H2'	2:2:596:G:O4'	2.21	0.41
2:2:1005:C:H3'	2:2:1006:C:H6	1.86	0.41
2:2:1012:A:H3'	2:2:1013:G:C8	2.56	0.41
2:2:1040:G:OP1	4:A:32:HIS:HB2	2.21	0.41
2:2:1157:C:C5	2:2:1580:U:H5	2.39	0.41
2:2:1562:U:H2'	2:2:1563:C:O4'	2.21	0.41
2:2:1787:G:H2'	2:2:1788:A:H8	1.86	0.41
3:3:14:U:H6	3:3:14:U:O5'	2.04	0.41
4:A:162:CYS:SG	4:A:163:ASN:N	2.93	0.41
7:D:209:ILE:HB	21:R:38:ILE:O	2.21	0.41
9:F:84:PHE:CZ	32:c:47:PRO:HB2	2.55	0.41
11:H:153:LEU:HD23	11:H:184:GLU:HB3	2.02	0.41
17:N:23:PRO:HG3	17:N:61:THR:HG21	2.03	0.41
19:P:17:TYR:CD1	19:P:18:LYS:HB2	2.55	0.41
19:P:52:LYS:HB2	19:P:53:PRO:HD3	2.02	0.41
22:S:35:ILE:H	22:S:35:ILE:HG13	1.65	0.41
27:X:41:SER:HA	27:X:42:PRO:HD3	1.89	0.41
27:X:90:ASP:CG	27:X:136:TRP:HE1	2.29	0.41
27:X:92:CYS:HA	27:X:95:PHE:CD2	2.55	0.41
36:g:39:ARG:HA	36:g:68:ILE:HG23	2.02	0.41
38:i:27:ILE:H	38:i:27:ILE:HG13	1.68	0.41
43:o:247:SER:HA	43:o:252:LEU:HD12	2.03	0.41
44:p:582:GLN:HE22	44:p:612:ILE:HB	1.86	0.41
45:q:1:MET:HG2	47:s:81:LEU:HB2	2.02	0.41
2:2:309:C:N4	2:2:355:G:H1	2.16	0.41
2:2:354:G:H2'	2:2:355:G:H8	1.86	0.41
2:2:556:G:H1	2:2:586:C:H42	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:897:A:H4'	18:O:46:MET:HE3	2.02	0.41
2:2:947:G:C6	2:2:948:C:C4	3.09	0.41
2:2:1033:C:C2	2:2:1101:G:N2	2.89	0.41
2:2:1244:G:H22	2:2:1247:C:H5	1.69	0.41
2:2:1363:G:H2'	2:2:1363:G:N3	2.36	0.41
2:2:1471:U:OP1	9:F:192:ILE:HG13	2.21	0.41
2:2:1482:G:C2	2:2:1483:C:C2	3.09	0.41
2:2:1582:G:C8	20:Q:122:ARG:HB3	2.56	0.41
2:2:1603:G:C2	2:2:1604:C:C2	3.09	0.41
2:2:1625:U:H2'	2:2:1626:U:O4'	2.21	0.41
2:2:1636:G:C6	2:2:1637:C:N3	2.89	0.41
9:F:68:LYS:HA	9:F:69:PRO:HD3	1.89	0.41
14:K:30:PRO:HA	14:K:38:LYS:HG3	2.03	0.41
43:o:150:ALA:HB2	44:p:391:SER:HA	2.03	0.41
44:p:697:ILE:H	44:p:697:ILE:HG13	1.71	0.41
2:2:514:A:H62	2:2:536:G:H21	1.69	0.40
2:2:1009:C:N4	2:2:1010:G:C6	2.89	0.40
2:2:1400:G:C6	2:2:1401:C:C4	3.09	0.40
2:2:1482:G:O2'	2:2:1483:C:H5''	2.21	0.40
9:F:125:VAL:HG21	29:Z:92:VAL:HG21	2.03	0.40
13:J:123:HIS:HB3	34:e:33:ARG:HH22	1.86	0.40
18:O:27:PHE:HA	18:O:43:THR:HG22	2.03	0.40
20:Q:36:ILE:C	20:Q:38:LEU:H	2.28	0.40
22:S:18:LEU:C	22:S:20:THR:H	2.29	0.40
36:g:20:TRP:CD1	36:g:20:TRP:H	2.39	0.40
40:k:142:TYR:CE1	40:k:395:LEU:HB3	2.56	0.40
2:2:86:A:H2'	2:2:87:C:C6	2.56	0.40
2:2:96:G:C2	2:2:97:C:C2	3.09	0.40
2:2:104:A:N6	2:2:307:C:O4'	2.55	0.40
2:2:425:G:C2	2:2:426:C:C2	3.09	0.40
2:2:630:G:C5	2:2:631:U:C4	3.09	0.40
18:O:111:ARG:HD3	30:a:58:VAL:HG22	2.02	0.40
19:P:39:ALA:HA	19:P:42:ARG:HD3	2.02	0.40
24:U:20:HIS:HB2	24:U:95:ALA:O	2.21	0.40
43:o:264:PHE:CZ	43:o:356:ASN:N	2.90	0.40
45:q:259:GLU:HG2	45:q:260:ALA:H	1.86	0.40
2:2:284:G:C2	2:2:285:C:C2	3.09	0.40
2:2:325:G:C2	2:2:342:C:C2	3.10	0.40
2:2:337:C:H2'	2:2:338:C:H6	1.84	0.40
2:2:977:A:H2'	2:2:978:A:O4'	2.21	0.40
2:2:1022:A:H5''	2:2:1126:G:H4'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1050:G:N1	2:2:1067:C:C4	2.90	0.40
2:2:1115:A:H62	2:2:1129:G:N2	2.17	0.40
2:2:1154:G:N1	2:2:1155:C:C2	2.88	0.40
2:2:1621:C:H2'	2:2:1622:C:C6	2.57	0.40
7:D:29:LEU:HB3	7:D:32:GLU:HB2	2.04	0.40
17:N:37:ILE:HG23	17:N:50:ILE:HG21	2.02	0.40
17:N:81:ALA:HA	17:N:82:PRO:HD3	1.95	0.40
17:N:98:VAL:HG11	17:N:115:LEU:HB2	2.03	0.40
18:O:88:GLY:HA2	18:O:122:PRO:HG3	2.04	0.40
26:W:7:LEU:HA	26:W:34:ILE:HG12	2.04	0.40
43:o:334:SER:O	43:o:335:THR:C	2.64	0.40
45:q:222:LEU:HB2	45:q:234:TYR:HE2	1.86	0.40
2:2:50:C:H42	2:2:428:G:H1	1.69	0.40
2:2:96:G:C6	2:2:97:C:C4	3.10	0.40
2:2:337:C:C5'	12:I:10:LYS:HG3	2.49	0.40
2:2:357:U:H2'	2:2:359:A:H8	1.86	0.40
2:2:1005:C:H5''	2:2:1006:C:H5	1.85	0.40
2:2:1291:G:H2'	2:2:1292:U:O4'	2.21	0.40
2:2:1464:G:C2	2:2:1465:C:N3	2.89	0.40
2:2:1474:C:H2'	2:2:1475:G:H8	1.86	0.40
2:2:1604:C:C6	2:2:1604:C:H5''	2.56	0.40
6:C:175:ILE:HA	6:C:176:PRO:HD3	1.96	0.40
8:E:125:LYS:O	8:E:141:THR:HA	2.22	0.40
9:F:35:ILE:HG23	20:Q:53:LEU:HD21	2.03	0.40
18:O:13:VAL:HB	18:O:77:THR:H	1.86	0.40
20:Q:99:GLU:HB3	36:g:58:PRO:HB2	2.03	0.40
44:p:516:PHE:HB3	44:p:557:LEU:HD11	2.02	0.40
2:2:98:U:H2'	2:2:99:C:C6	2.57	0.40
2:2:227:G:O6	2:2:236:C:N3	2.55	0.40
2:2:347:U:H4'	12:I:14:THR:HG22	2.03	0.40
2:2:551:G:C2	2:2:572:C:C2	3.10	0.40
2:2:776:G:C2	2:2:777:C:C2	3.10	0.40
2:2:888:U:O2	2:2:987:A:H4'	2.21	0.40
2:2:941:G:C2	2:2:942:C:C2	3.09	0.40
2:2:1178:G:C6	2:2:1179:C:C4	3.10	0.40
2:2:1315:G:C2	2:2:1316:C:C2	3.10	0.40
2:2:1586:G:H22	2:2:1606:U:H3	1.70	0.40
2:2:1619:U:H2'	2:2:1620:G:C8	2.57	0.40
4:A:25:GLY:HA3	4:A:163:ASN:CG	2.46	0.40
7:D:50:ILE:HD11	7:D:86:LEU:HD22	2.03	0.40
30:a:10:ARG:HG2	30:a:34:LYS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:30:ILE:HG12	42:m:85:ARG:NH1	2.36	0.40
43:o:200:LYS:HA	43:o:258:ARG:HH12	1.87	0.40
45:q:1:MET:HG3	47:s:79:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	206/254 (81%)	170 (82%)	27 (13%)	9 (4%)	2	17
5	B	218/255 (86%)	185 (85%)	25 (12%)	8 (4%)	2	19
6	C	215/259 (83%)	186 (86%)	22 (10%)	7 (3%)	3	20
7	D	221/237 (93%)	196 (89%)	16 (7%)	9 (4%)	2	17
8	E	258/261 (99%)	225 (87%)	28 (11%)	5 (2%)	6	31
9	F	204/227 (90%)	169 (83%)	28 (14%)	7 (3%)	3	20
10	G	224/236 (95%)	197 (88%)	23 (10%)	4 (2%)	6	33
11	H	182/190 (96%)	157 (86%)	15 (8%)	10 (6%)	1	15
12	I	184/201 (92%)	160 (87%)	15 (8%)	9 (5%)	1	16
13	J	180/188 (96%)	154 (86%)	19 (11%)	7 (4%)	2	18
14	K	94/106 (89%)	81 (86%)	7 (7%)	6 (6%)	1	13
15	L	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	16
16	M	113/134 (84%)	85 (75%)	21 (19%)	7 (6%)	1	13
17	N	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	18	55
18	O	125/137 (91%)	102 (82%)	16 (13%)	7 (6%)	1	14
19	P	115/142 (81%)	96 (84%)	13 (11%)	6 (5%)	1	15
20	Q	139/143 (97%)	108 (78%)	20 (14%)	11 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	R	116/136 (85%)	101 (87%)	13 (11%)	2 (2%)	7	35
22	S	143/146 (98%)	111 (78%)	21 (15%)	11 (8%)	1	10
23	T	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
24	U	104/117 (89%)	84 (81%)	16 (15%)	4 (4%)	2	19
25	V	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	16
26	W	127/130 (98%)	112 (88%)	10 (8%)	5 (4%)	2	18
27	X	142/145 (98%)	117 (82%)	14 (10%)	11 (8%)	1	10
28	Y	132/135 (98%)	118 (89%)	7 (5%)	7 (5%)	1	15
29	Z	68/108 (63%)	50 (74%)	17 (25%)	1 (2%)	8	38
30	a	96/119 (81%)	81 (84%)	11 (12%)	4 (4%)	2	17
31	b	79/82 (96%)	61 (77%)	15 (19%)	3 (4%)	2	19
32	c	60/67 (90%)	51 (85%)	6 (10%)	3 (5%)	1	16
33	d	51/56 (91%)	33 (65%)	15 (29%)	3 (6%)	1	13
34	e	52/63 (82%)	45 (86%)	6 (12%)	1 (2%)	6	31
35	f	67/150 (45%)	48 (72%)	9 (13%)	10 (15%)	0	3
36	g	312/326 (96%)	257 (82%)	45 (14%)	10 (3%)	3	21
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	92 (84%)	14 (13%)	3 (3%)	4	24
39	j	243/304 (80%)	205 (84%)	32 (13%)	6 (2%)	4	26
40	k	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	8	38
41	l	120/285 (42%)	100 (83%)	16 (13%)	4 (3%)	3	20
42	m	88/108 (82%)	76 (86%)	10 (11%)	2 (2%)	5	28
43	o	451/588 (77%)	417 (92%)	31 (7%)	3 (1%)	18	55
44	p	554/652 (85%)	497 (90%)	45 (8%)	12 (2%)	5	28
45	q	340/347 (98%)	302 (89%)	33 (10%)	5 (2%)	8	38
46	r	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
47	s	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
All	All	7149/8360 (86%)	6131 (86%)	778 (11%)	240 (3%)	4	20

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	95	ALA

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Mol	Chain	Res	Type
4	A	166	GLY
6	C	141	VAL
6	C	235	TRP
7	D	216	PRO
7	D	220	PRO
8	E	245	LYS
10	G	69	LEU
11	H	14	THR
11	H	31	SER
11	H	64	VAL
11	H	74	GLN
12	I	22	ARG
12	I	147	ARG
15	L	105	LYS
20	Q	97	VAL
21	R	85	VAL
22	S	19	ASN
22	S	27	ASN
22	S	28	VAL
22	S	82	PRO
22	S	91	ASP
24	U	96	PRO
26	W	83	ILE
27	X	12	ALA
27	X	64	PRO
27	X	90	ASP
27	X	92	CYS
28	Y	30	PRO
34	e	47	VAL
35	f	94	LYS
39	j	48	LEU
40	k	129	LYS
43	o	63	LYS
44	p	460	PRO
44	p	558	CYS
4	A	21	ARG
5	B	148	ASN
5	B	214	LYS
5	B	221	PRO
5	B	224	ASP
6	C	253	THR
7	D	221	SER

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Mol	Chain	Res	Type
9	F	66	ILE
10	G	122	GLU
11	H	10	SER
11	H	136	VAL
11	H	163	ASP
12	I	40	THR
12	I	52	ASN
12	I	153	ILE
13	J	136	VAL
14	K	22	VAL
14	K	54	PHE
14	K	64	TYR
15	L	7	VAL
16	M	82	VAL
16	M	84	ASP
16	M	110	SER
17	N	3	ARG
18	O	124	ASP
20	Q	39	VAL
20	Q	40	GLN
20	Q	122	ARG
22	S	7	GLU
22	S	83	ALA
22	S	145	ARG
25	V	12	TYR
25	V	45	ALA
26	W	78	ARG
27	X	115	GLY
28	Y	4	ALA
30	a	13	LYS
30	a	59	TYR
33	d	23	ILE
35	f	100	LEU
35	f	102	VAL
36	g	130	LYS
39	j	57	ARG
40	k	495	ILE
40	k	507	LYS
41	l	200	GLY
45	q	329	PHE
4	A	39	LYS
4	A	109	ASN

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Mol	Chain	Res	Type
5	B	54	LEU
5	B	190	PRO
5	B	207	LEU
6	C	187	PRO
7	D	163	PRO
8	E	205	PHE
9	F	37	GLN
9	F	59	SER
9	F	190	LYS
12	I	120	SER
13	J	20	GLU
13	J	134	ILE
13	J	150	LEU
14	K	23	ALA
15	L	4	GLU
15	L	30	LYS
15	L	55	ASP
16	M	98	ASP
18	O	18	ARG
18	O	40	ALA
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
19	P	108	ARG
19	P	109	PRO
20	Q	14	LYS
20	Q	27	GLY
20	Q	115	THR
20	Q	116	LEU
21	R	5	ARG
22	S	8	GLN
25	V	9	VAL
26	W	29	PRO
26	W	58	SER
27	X	3	LYS
27	X	41	SER
27	X	54	LEU
27	X	97	ASP
28	Y	36	SER
31	b	21	LEU
35	f	111	GLU
35	f	122	PRO

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Mol	Chain	Res	Type
35	f	140	GLY
35	f	143	HIS
36	g	106	GLY
36	g	120	SER
36	g	201	GLY
36	g	205	TYR
38	i	17	ASN
38	i	64	LYS
39	j	49	SER
39	j	64	ARG
39	j	138	PHE
40	k	127	ARG
40	k	497	GLU
41	l	159	ARG
42	m	85	ARG
44	p	492	LYS
44	p	536	ASP
44	p	639	GLY
45	q	291	GLY
6	C	44	THR
6	C	65	SER
6	C	155	GLN
7	D	143	ARG
8	E	77	ARG
8	E	150	PRO
8	E	195	ILE
9	F	65	GLN
9	F	67	SER
11	H	13	PRO
11	H	110	GLN
12	I	148	ALA
13	J	120	LYS
13	J	171	ARG
14	K	25	LYS
16	M	81	LYS
18	O	42	VAL
19	P	90	ILE
24	U	89	ARG
25	V	10	GLU
26	W	72	CYS
29	Z	38	HIS
32	c	35	ASP

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Mol	Chain	Res	Type
32	c	49	ARG
33	d	34	TYR
35	f	110	ASP
36	g	31	PRO
36	g	50	GLU
41	l	129	LEU
41	l	219	SER
42	m	74	MET
43	o	394	ASN
44	p	337	ASP
44	p	650	LYS
44	p	774	THR
45	q	162	SER
4	A	103	THR
4	A	158	VAL
4	A	195	TRP
4	A	202	TYR
5	B	4	GLY
7	D	196	THR
11	H	98	ILE
12	I	149	ALA
13	J	147	MET
16	M	77	VAL
18	O	91	SER
19	P	100	LYS
20	Q	74	HIS
22	S	14	ILE
22	S	90	LYS
28	Y	31	ASN
28	Y	64	TYR
30	a	36	ILE
31	b	62	VAL
35	f	90	LYS
35	f	98	VAL
36	g	15	GLU
38	i	16	LYS
39	j	226	PRO
43	o	335	THR
44	p	351	ILE
44	p	645	ILE
44	p	704	PRO
7	D	63	GLY

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Mol	Chain	Res	Type
7	D	219	GLU
9	F	100	MET
10	G	152	ASP
10	G	224	ALA
12	I	59	ARG
15	L	3	THR
16	M	122	GLN
28	Y	67	GLY
20	Q	33	GLY
24	U	118	ILE
30	a	64	LEU
19	P	48	GLY
24	U	117	ILE
27	X	63	GLN
27	X	96	VAL
45	q	50	GLY
45	q	239	PRO
15	L	54	ILE
31	b	10	PRO
32	c	24	GLY
33	d	29	GLY
36	g	159	PRO
7	D	217	VAL
14	K	82	LEU
20	Q	73	GLY
36	g	64	GLY
40	k	210	VAL
44	p	336	ILE
28	Y	5	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	174/211 (82%)	147 (84%)	27 (16%)	2 13
5	B	198/228 (87%)	168 (85%)	30 (15%)	3 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	176/203 (87%)	156 (89%)	20 (11%)	5	19
7	D	185/196 (94%)	150 (81%)	35 (19%)	1	9
8	E	223/224 (100%)	191 (86%)	32 (14%)	3	14
9	F	174/194 (90%)	140 (80%)	34 (20%)	1	8
10	G	192/200 (96%)	172 (90%)	20 (10%)	7	22
11	H	164/170 (96%)	134 (82%)	30 (18%)	2	10
12	I	147/159 (92%)	131 (89%)	16 (11%)	6	21
13	J	153/158 (97%)	132 (86%)	21 (14%)	3	15
14	K	88/96 (92%)	73 (83%)	15 (17%)	2	11
15	L	136/137 (99%)	126 (93%)	10 (7%)	13	34
16	M	93/109 (85%)	80 (86%)	13 (14%)	3	15
17	N	127/128 (99%)	107 (84%)	20 (16%)	2	13
18	O	96/104 (92%)	85 (88%)	11 (12%)	5	19
19	P	100/119 (84%)	85 (85%)	15 (15%)	3	13
20	Q	117/119 (98%)	98 (84%)	19 (16%)	2	12
21	R	109/124 (88%)	93 (85%)	16 (15%)	3	14
22	S	128/129 (99%)	106 (83%)	22 (17%)	2	11
23	T	117/118 (99%)	95 (81%)	22 (19%)	1	9
24	U	96/107 (90%)	83 (86%)	13 (14%)	4	15
25	V	73/73 (100%)	64 (88%)	9 (12%)	4	18
26	W	110/111 (99%)	100 (91%)	10 (9%)	9	28
27	X	119/120 (99%)	100 (84%)	19 (16%)	2	12
28	Y	108/109 (99%)	99 (92%)	9 (8%)	10	30
29	Z	60/88 (68%)	54 (90%)	6 (10%)	7	24
30	a	83/100 (83%)	71 (86%)	12 (14%)	3	14
31	b	71/72 (99%)	66 (93%)	5 (7%)	14	36
32	c	54/59 (92%)	47 (87%)	7 (13%)	4	16
33	d	46/48 (96%)	37 (80%)	9 (20%)	1	8
34	e	47/55 (86%)	39 (83%)	8 (17%)	2	11
35	f	57/133 (43%)	49 (86%)	8 (14%)	3	15
36	g	265/272 (97%)	235 (89%)	30 (11%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	h	23/23 (100%)	22 (96%)	1 (4%)	26	48
38	i	93/130 (72%)	74 (80%)	19 (20%)	1	7
39	j	224/274 (82%)	185 (83%)	39 (17%)	2	11
40	k	332/449 (74%)	294 (89%)	38 (11%)	5	19
41	l	119/246 (48%)	105 (88%)	14 (12%)	5	19
42	m	77/96 (80%)	63 (82%)	14 (18%)	2	10
43	o	411/444 (93%)	357 (87%)	54 (13%)	4	16
44	p	507/536 (95%)	463 (91%)	44 (9%)	9	29
45	q	297/301 (99%)	279 (94%)	18 (6%)	17	39
46	r	30/30 (100%)	28 (93%)	2 (7%)	15	37
47	s	43/43 (100%)	37 (86%)	6 (14%)	3	15
All	All	6242/7045 (89%)	5420 (87%)	822 (13%)	6	16

All (822) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	ARG
4	A	34	GLU
4	A	41	ARG
4	A	43	ASP
4	A	58	VAL
4	A	59	LEU
4	A	71	GLU
4	A	79	ARG
4	A	80	THR
4	A	88	LYS
4	A	93	THR
4	A	96	THR
4	A	108	THR
4	A	112	THR
4	A	113	ARG
4	A	119	ARG
4	A	120	LEU
4	A	122	ILE
4	A	143	VAL
4	A	165	ARG
4	A	170	ILE
4	A	173	ILE

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Mol	Chain	Res	Type
4	A	192	THR
4	A	193	GLN
4	A	198	MET
4	A	201	LEU
4	A	205	ARG
5	B	22	ASP
5	B	28	GLU
5	B	47	LEU
5	B	54	LEU
5	B	64	ARG
5	B	68	VAL
5	B	70	LEU
5	B	82	ARG
5	B	83	LYS
5	B	84	VAL
5	B	88	VAL
5	B	104	ASP
5	B	111	ARG
5	B	118	GLN
5	B	119	THR
5	B	125	VAL
5	B	127	VAL
5	B	140	ILE
5	B	170	GLU
5	B	171	ILE
5	B	181	LEU
5	B	183	GLN
5	B	184	LEU
5	B	189	ILE
5	B	193	ILE
5	B	196	GLU
5	B	204	ILE
5	B	208	GLN
5	B	219	LYS
5	B	228	LEU
6	C	58	ILE
6	C	60	GLU
6	C	72	GLN
6	C	78	LEU
6	C	83	ASP
6	C	86	MET
6	C	91	VAL

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Mol	Chain	Res	Type
6	C	93	LYS
6	C	99	GLN
6	C	109	VAL
6	C	113	ASN
6	C	125	GLU
6	C	131	ARG
6	C	146	ARG
6	C	199	GLU
6	C	223	ILE
6	C	234	LEU
6	C	235	TRP
6	C	240	LEU
6	C	246	ASP
7	D	4	ILE
7	D	5	ILE
7	D	6	SER
7	D	16	VAL
7	D	20	GLU
7	D	23	GLU
7	D	28	GLU
7	D	31	GLU
7	D	57	ASP
7	D	68	GLU
7	D	69	LEU
7	D	70	THR
7	D	75	LYS
7	D	76	ARG
7	D	91	VAL
7	D	93	ASP
7	D	94	ARG
7	D	103	GLU
7	D	109	LEU
7	D	113	LEU
7	D	122	VAL
7	D	128	GLU
7	D	132	LYS
7	D	146	ARG
7	D	158	ILE
7	D	168	ILE
7	D	169	GLU
7	D	177	LEU
7	D	186	VAL

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Mol	Chain	Res	Type
7	D	200	LYS
7	D	204	ASP
7	D	209	ILE
7	D	212	LYS
7	D	213	GLU
7	D	214	GLU
8	E	7	LYS
8	E	9	LEU
8	E	22	LYS
8	E	23	LEU
8	E	38	LEU
8	E	44	LEU
8	E	51	ARG
8	E	60	GLU
8	E	65	LEU
8	E	75	LYS
8	E	77	ARG
8	E	79	ASP
8	E	102	VAL
8	E	104	ASP
8	E	108	ARG
8	E	117	GLU
8	E	125	LYS
8	E	147	ILE
8	E	168	THR
8	E	180	LEU
8	E	181	VAL
8	E	189	LEU
8	E	201	HIS
8	E	202	GLU
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	228	ILE
8	E	233	ARG
8	E	248	ILE
8	E	259	HIS
9	F	31	ILE
9	F	33	VAL
9	F	34	GLU
9	F	35	ILE

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Mol	Chain	Res	Type
9	F	37	GLN
9	F	42	ILE
9	F	54	GLU
9	F	62	ASP
9	F	70	ILE
9	F	72	VAL
9	F	83	ARG
9	F	86	LYS
9	F	88	GLN
9	F	91	ILE
9	F	95	LEU
9	F	98	SER
9	F	104	ARG
9	F	108	LYS
9	F	126	LEU
9	F	132	LEU
9	F	163	ASP
9	F	164	VAL
9	F	174	ILE
9	F	177	LEU
9	F	178	THR
9	F	186	PHE
9	F	189	ILE
9	F	194	GLU
9	F	199	GLU
9	F	209	THR
9	F	216	LYS
9	F	221	ARG
9	F	224	LYS
9	F	226	ASN
10	G	21	GLU
10	G	26	VAL
10	G	39	GLU
10	G	49	VAL
10	G	52	ILE
10	G	76	LEU
10	G	95	LYS
10	G	106	LEU
10	G	108	VAL
10	G	121	ILE
10	G	127	ASP
10	G	164	LYS

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Mol	Chain	Res	Type
10	G	169	TYR
10	G	170	THR
10	G	180	THR
10	G	193	LEU
10	G	195	ILE
10	G	210	GLN
10	G	215	ARG
10	G	220	LYS
11	H	5	GLN
11	H	7	LYS
11	H	11	GLN
11	H	15	GLU
11	H	19	GLN
11	H	27	LEU
11	H	33	GLU
11	H	38	LEU
11	H	48	GLU
11	H	72	LYS
11	H	74	GLN
11	H	75	ILE
11	H	80	GLU
11	H	86	GLN
11	H	91	ILE
11	H	104	ARG
11	H	112	ARG
11	H	116	ARG
11	H	118	LEU
11	H	129	LEU
11	H	130	VAL
11	H	136	VAL
11	H	139	ARG
11	H	143	LEU
11	H	148	LYS
11	H	149	ILE
11	H	152	ILE
11	H	160	GLN
11	H	162	ILE
11	H	184	GLU
12	I	20	GLN
12	I	26	LYS
12	I	29	LEU
12	I	43	ILE

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Mol	Chain	Res	Type
12	I	47	ARG
12	I	53	GLN
12	I	70	GLU
12	I	72	VAL
12	I	78	ILE
12	I	96	LEU
12	I	104	ILE
12	I	119	GLN
12	I	140	THR
12	I	153	ILE
12	I	190	LEU
12	I	201	LYS
13	J	8	TYR
13	J	10	LYS
13	J	20	GLU
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU
13	J	37	LYS
13	J	40	ARG
13	J	45	ILE
13	J	49	LEU
13	J	63	ASP
13	J	64	GLU
13	J	83	ILE
13	J	100	LYS
13	J	102	GLU
13	J	107	ARG
13	J	109	LEU
13	J	127	VAL
13	J	131	GLN
13	J	150	LEU
13	J	161	THR
14	K	2	LEU
14	K	9	LYS
14	K	13	GLN
14	K	15	LEU
14	K	20	VAL
14	K	21	LEU
14	K	29	GLN
14	K	34	GLU
14	K	44	LYS

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Mol	Chain	Res	Type
14	K	47	GLN
14	K	49	LEU
14	K	55	VAL
14	K	57	THR
14	K	76	LEU
14	K	85	HIS
15	L	5	LEU
15	L	10	GLU
15	L	32	LYS
15	L	36	LYS
15	L	63	LEU
15	L	80	MET
15	L	84	ILE
15	L	99	ARG
15	L	118	GLN
15	L	124	THR
16	M	22	LYS
16	M	24	VAL
16	M	26	ARG
16	M	52	LEU
16	M	55	LEU
16	M	61	GLU
16	M	67	LEU
16	M	77	VAL
16	M	91	TRP
16	M	97	ILE
16	M	117	TRP
16	M	123	GLU
16	M	125	GLU
17	N	3	ARG
17	N	16	ILE
17	N	27	LYS
17	N	39	LYS
17	N	53	LEU
17	N	64	LYS
17	N	72	LEU
17	N	75	LEU
17	N	83	GLU
17	N	84	ILE
17	N	86	GLU
17	N	88	LEU
17	N	96	VAL

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Mol	Chain	Res	Type
17	N	99	ARG
17	N	100	LYS
17	N	107	LYS
17	N	112	LYS
17	N	121	ARG
17	N	125	LEU
17	N	132	VAL
18	O	29	HIS
18	O	39	ILE
18	O	49	LYS
18	O	65	GLN
18	O	92	LYS
18	O	99	GLN
18	O	102	LEU
18	O	110	LEU
18	O	114	ARG
18	O	121	VAL
18	O	129	LYS
19	P	13	LYS
19	P	25	LEU
19	P	56	LEU
19	P	57	MET
19	P	71	GLU
19	P	72	LYS
19	P	76	VAL
19	P	82	ASN
19	P	85	ILE
19	P	93	VAL
19	P	101	VAL
19	P	106	GLU
19	P	108	ARG
19	P	112	VAL
19	P	122	THR
20	Q	7	VAL
20	Q	9	THR
20	Q	13	LYS
20	Q	28	LEU
20	Q	37	THR
20	Q	38	LEU
20	Q	43	ILE
20	Q	45	ARG
20	Q	47	LYS

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Mol	Chain	Res	Type
20	Q	67	VAL
20	Q	74	HIS
20	Q	82	ARG
20	Q	83	GLN
20	Q	89	LEU
20	Q	100	GLN
20	Q	105	LEU
20	Q	123	ARG
20	Q	137	ARG
20	Q	139	GLN
21	R	3	ARG
21	R	5	ARG
21	R	6	THR
21	R	9	VAL
21	R	10	LYS
21	R	25	THR
21	R	37	GLU
21	R	47	ARG
21	R	48	ASN
21	R	63	LYS
21	R	82	ASP
21	R	83	GLN
21	R	99	VAL
21	R	100	LEU
21	R	102	VAL
21	R	117	LEU
22	S	6	GLN
22	S	20	THR
22	S	35	ILE
22	S	45	LEU
22	S	52	VAL
22	S	73	MET
22	S	78	HIS
22	S	84	TRP
22	S	86	LEU
22	S	97	ASP
22	S	99	HIS
22	S	106	GLU
22	S	109	LEU
22	S	111	ASP
22	S	114	GLU
22	S	115	ARG

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Mol	Chain	Res	Type
22	S	119	ILE
22	S	120	ARG
22	S	122	HIS
22	S	132	ARG
22	S	136	GLN
22	S	144	ARG
23	T	12	GLN
23	T	16	ASN
23	T	25	GLN
23	T	28	LEU
23	T	37	VAL
23	T	45	LEU
23	T	64	HIS
23	T	65	ILE
23	T	85	ASN
23	T	86	ARG
23	T	91	HIS
23	T	103	LYS
23	T	106	GLN
23	T	107	SER
23	T	111	LEU
23	T	124	ILE
23	T	131	ASP
23	T	132	LEU
23	T	135	ILE
23	T	142	ASP
23	T	143	GLU
23	T	144	GLU
24	U	19	ILE
24	U	34	LEU
24	U	35	GLU
24	U	37	VAL
24	U	41	ILE
24	U	42	ILE
24	U	67	THR
24	U	72	ASN
24	U	80	ASP
24	U	83	GLU
24	U	109	GLU
24	U	117	ILE
24	U	118	ILE
25	V	1	MET

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Mol	Chain	Res	Type
25	V	8	LEU
25	V	9	VAL
25	V	12	TYR
25	V	16	LYS
25	V	21	ASN
25	V	44	ARG
25	V	69	LEU
25	V	80	LYS
26	W	7	LEU
26	W	11	LEU
26	W	24	GLN
26	W	25	VAL
26	W	26	LEU
26	W	31	SER
26	W	33	VAL
26	W	47	ILE
26	W	75	ILE
26	W	104	LEU
27	X	9	LEU
27	X	14	LYS
27	X	17	VAL
27	X	19	ARG
27	X	30	LYS
27	X	54	LEU
27	X	55	GLU
27	X	59	ILE
27	X	68	ILE
27	X	79	ASN
27	X	83	VAL
27	X	84	THR
27	X	94	ASN
27	X	98	GLU
27	X	107	PHE
27	X	117	ILE
27	X	127	VAL
27	X	133	LEU
27	X	144	ARG
28	Y	8	ARG
28	Y	13	ILE
28	Y	35	VAL
28	Y	74	LEU
28	Y	84	LYS

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Mol	Chain	Res	Type
28	Y	99	LYS
28	Y	121	THR
28	Y	127	LYS
28	Y	128	LYS
29	Z	38	HIS
29	Z	40	VAL
29	Z	44	GLN
29	Z	70	LYS
29	Z	71	LEU
29	Z	84	GLU
30	a	15	ARG
30	a	19	LYS
30	a	28	ARG
30	a	30	VAL
30	a	34	LYS
30	a	38	ARG
30	a	46	GLU
30	a	53	LEU
30	a	58	VAL
30	a	64	LEU
30	a	69	ASN
30	a	75	ILE
31	b	3	LEU
31	b	4	VAL
31	b	24	LEU
31	b	67	THR
31	b	70	LYS
32	c	9	LEU
32	c	14	LYS
32	c	31	GLU
32	c	43	ASN
32	c	49	ARG
32	c	54	LEU
32	c	62	GLU
33	d	4	GLU
33	d	6	VAL
33	d	20	GLN
33	d	22	ARG
33	d	23	ILE
33	d	30	LEU
33	d	31	ILE
33	d	34	TYR

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Mol	Chain	Res	Type
33	d	38	ILE
34	e	18	THR
34	e	22	GLU
34	e	24	GLN
34	e	31	LYS
34	e	33	ARG
34	e	38	LEU
34	e	39	LEU
34	e	54	ARG
35	f	91	ILE
35	f	92	ARG
35	f	100	LEU
35	f	108	VAL
35	f	117	LEU
35	f	119	LYS
35	f	129	PHE
35	f	138	TYR
36	g	6	ILE
36	g	8	LEU
36	g	11	ARG
36	g	13	THR
36	g	15	GLU
36	g	20	TRP
36	g	33	LEU
36	g	39	ARG
36	g	43	LEU
36	g	67	HIS
36	g	70	GLN
36	g	116	ILE
36	g	124	ILE
36	g	129	ASP
36	g	146	LEU
36	g	152	VAL
36	g	188	LEU
36	g	205	TYR
36	g	206	ILE
36	g	210	GLN
36	g	234	HIS
36	g	246	GLU
36	g	256	ARG
36	g	276	VAL
36	g	280	GLU

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Mol	Chain	Res	Type
36	g	284	GLU
36	g	289	THR
36	g	314	ASP
36	g	321	GLN
36	g	323	MET
37	h	9	ARG
38	i	18	ASP
38	i	26	LEU
38	i	27	ILE
38	i	34	GLU
38	i	41	MET
38	i	58	MET
38	i	61	ILE
38	i	62	ARG
38	i	65	LEU
38	i	69	VAL
38	i	82	ARG
38	i	91	VAL
38	i	97	LEU
38	i	101	ARG
38	i	103	LEU
38	i	105	ASN
38	i	111	GLU
38	i	112	ASN
38	i	115	ILE
39	j	6	CYS
39	j	11	ASN
39	j	15	GLU
39	j	18	ASP
39	j	19	ILE
39	j	33	TYR
39	j	42	ILE
39	j	45	MET
39	j	56	ILE
39	j	57	ARG
39	j	59	ILE
39	j	63	ILE
39	j	70	VAL
39	j	74	LEU
39	j	75	ARG
39	j	76	VAL
39	j	79	GLU

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Mol	Chain	Res	Type
39	j	90	VAL
39	j	96	ILE
39	j	97	LYS
39	j	114	TYR
39	j	120	GLN
39	j	121	ILE
39	j	129	THR
39	j	143	GLU
39	j	163	LYS
39	j	166	LEU
39	j	169	LEU
39	j	185	ARG
39	j	195	TYR
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	236	ASP
39	j	244	LEU
39	j	251	ILE
39	j	255	ILE
39	j	261	VAL
39	j	264	ILE
40	k	116	VAL
40	k	117	VAL
40	k	130	ASP
40	k	132	LEU
40	k	133	GLU
40	k	192	VAL
40	k	210	VAL
40	k	224	CYS
40	k	228	GLN
40	k	236	ILE
40	k	251	VAL
40	k	253	LEU
40	k	257	GLU
40	k	291	ILE
40	k	307	ARG
40	k	318	ILE
40	k	332	ASP
40	k	353	ILE
40	k	354	GLU
40	k	355	ILE

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Mol	Chain	Res	Type
40	k	359	ILE
40	k	373	ILE
40	k	380	LEU
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	406	LEU
40	k	412	LEU
40	k	426	ILE
40	k	432	ILE
40	k	440	LEU
40	k	443	VAL
40	k	462	LEU
40	k	466	ILE
40	k	495	ILE
40	k	502	SER
40	k	508	HIS
40	k	512	ILE
41	l	141	ILE
41	l	157	LYS
41	l	159	ARG
41	l	166	LEU
41	l	167	ARG
41	l	171	LYS
41	l	172	THR
41	l	177	ILE
41	l	180	ILE
41	l	189	GLU
41	l	213	ILE
41	l	229	TYR
41	l	246	LEU
41	l	257	MET
42	m	22	THR
42	m	26	ILE
42	m	39	LEU
42	m	40	THR
42	m	62	PHE
42	m	65	ASN
42	m	68	ILE
42	m	71	ASP
42	m	74	MET
42	m	87	LYS

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Mol	Chain	Res	Type
42	m	92	MET
42	m	98	LEU
42	m	103	ILE
42	m	104	LYS
43	o	9	GLU
43	o	17	GLU
43	o	39	ARG
43	o	67	LEU
43	o	73	HIS
43	o	79	ILE
43	o	86	LEU
43	o	104	ILE
43	o	109	THR
43	o	114	LEU
43	o	115	GLN
43	o	120	ASP
43	o	151	ILE
43	o	154	TRP
43	o	168	LEU
43	o	169	LEU
43	o	170	ARG
43	o	183	VAL
43	o	186	THR
43	o	188	HIS
43	o	190	CYS
43	o	211	ASP
43	o	219	LYS
43	o	223	ASN
43	o	235	ARG
43	o	246	VAL
43	o	248	VAL
43	o	260	ILE
43	o	265	HIS
43	o	268	LYS
43	o	278	THR
43	o	279	LEU
43	o	282	TYR
43	o	284	GLU
43	o	298	LEU
43	o	303	TRP
43	o	329	PHE
43	o	351	MET

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Mol	Chain	Res	Type
43	o	354	LEU
43	o	365	GLU
43	o	387	LEU
43	o	397	VAL
43	o	407	LEU
43	o	415	THR
43	o	420	TYR
43	o	421	ILE
43	o	424	LEU
43	o	426	ASP
43	o	443	VAL
43	o	448	LEU
43	o	476	ASP
43	o	478	VAL
43	o	480	ILE
43	o	485	GLU
44	p	251	GLN
44	p	253	ASP
44	p	257	ARG
44	p	275	LEU
44	p	297	LEU
44	p	315	ILE
44	p	317	GLN
44	p	335	THR
44	p	336	ILE
44	p	354	GLU
44	p	374	GLU
44	p	388	ASP
44	p	404	ILE
44	p	407	LEU
44	p	409	LEU
44	p	413	LEU
44	p	416	GLU
44	p	430	THR
44	p	438	ASP
44	p	467	PHE
44	p	480	ASP
44	p	540	GLN
44	p	548	VAL
44	p	559	LEU
44	p	561	GLU
44	p	588	ILE

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Mol	Chain	Res	Type
44	p	606	LEU
44	p	611	HIS
44	p	616	LEU
44	p	630	ILE
44	p	644	ARG
44	p	662	LEU
44	p	663	SER
44	p	671	LEU
44	p	681	SER
44	p	707	GLU
44	p	722	LEU
44	p	733	TYR
44	p	744	LEU
44	p	750	ASN
44	p	756	LEU
44	p	780	LYS
44	p	787	LEU
44	p	793	LYS
45	q	7	THR
45	q	40	LEU
45	q	47	THR
45	q	49	ASP
45	q	79	TRP
45	q	100	GLU
45	q	135	GLU
45	q	138	LYS
45	q	157	THR
45	q	193	ASP
45	q	201	ASP
45	q	212	ILE
45	q	216	ARG
45	q	223	VAL
45	q	264	THR
45	q	308	TYR
45	q	317	ILE
45	q	329	PHE
46	r	704	LEU
46	r	725	GLU
47	s	58	TYR
47	s	61	GLU
47	s	83	LEU
47	s	85	ARG

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Mol	Chain	Res	Type
47	s	86	ASN
47	s	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	46	ASN
4	A	83	GLN
4	A	109	ASN
4	A	131	GLN
4	A	140	ASN
5	B	95	ASN
5	B	118	GLN
5	B	146	GLN
5	B	148	ASN
5	B	149	GLN
5	B	183	GLN
5	B	194	ASN
6	C	64	HIS
6	C	72	GLN
6	C	76	GLN
6	C	87	ASN
6	C	92	GLN
6	C	194	GLN
6	C	225	ASN
6	C	238	GLN
7	D	67	ASN
7	D	101	GLN
8	E	17	HIS
8	E	67	GLN
8	E	69	HIS
8	E	153	ASN
8	E	188	ASN
8	E	216	ASN
9	F	39	GLN
9	F	40	GLN
9	F	65	GLN
9	F	105	ASN
9	F	141	ASN
9	F	172	GLN
9	F	188	ASN
10	G	10	ASN

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Mol	Chain	Res	Type
10	G	13	GLN
10	G	65	GLN
10	G	139	ASN
10	G	182	GLN
11	H	19	GLN
11	H	22	GLN
11	H	71	HIS
11	H	110	GLN
11	H	170	GLN
11	H	174	ASN
11	H	180	GLN
12	I	9	HIS
12	I	35	ASN
12	I	53	GLN
12	I	64	ASN
13	J	110	GLN
14	K	14	HIS
14	K	28	ASN
15	L	8	GLN
15	L	14	GLN
15	L	22	ASN
15	L	98	ASN
15	L	104	HIS
15	L	110	HIS
15	L	118	GLN
17	N	36	GLN
17	N	49	GLN
17	N	58	HIS
17	N	62	GLN
17	N	69	ASN
17	N	78	ASN
17	N	105	ASN
18	O	24	ASN
18	O	80	HIS
20	Q	8	GLN
20	Q	83	GLN
20	Q	139	GLN
21	R	95	HIS
22	S	13	HIS
22	S	19	ASN
22	S	21	ASN
22	S	25	ASN

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Mol	Chain	Res	Type
22	S	71	GLN
22	S	78	HIS
22	S	99	HIS
23	T	17	ASN
23	T	70	GLN
24	U	72	ASN
24	U	105	GLN
25	V	21	ASN
25	V	33	GLN
25	V	38	GLN
25	V	70	ASN
26	W	24	GLN
26	W	92	ASN
26	W	98	GLN
27	X	22	ASN
27	X	48	HIS
27	X	79	ASN
27	X	94	ASN
27	X	99	ASN
28	Y	106	GLN
28	Y	107	GLN
28	Y	110	GLN
28	Y	113	ASN
29	Z	98	GLN
30	a	43	ASN
30	a	80	HIS
33	d	10	HIS
33	d	41	GLN
35	f	132	ASN
36	g	18	ASN
36	g	65	HIS
36	g	94	ASN
36	g	231	ASN
36	g	321	GLN
38	i	37	GLN
38	i	44	ASN
38	i	60	HIS
38	i	85	GLN
38	i	106	GLN
39	j	41	ASN
40	k	98	GLN
40	k	111	HIS

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Mol	Chain	Res	Type
40	k	144	ASN
40	k	226	GLN
40	k	415	GLN
40	k	433	ASN
40	k	496	ASN
40	k	508	HIS
41	l	140	ASN
41	l	190	HIS
42	m	43	GLN
42	m	65	ASN
42	m	79	GLN
42	m	81	GLN
42	m	84	GLN
43	o	29	GLN
43	o	32	HIS
43	o	80	GLN
43	o	171	ASN
43	o	172	ASN
43	o	209	HIS
43	o	242	GLN
43	o	254	HIS
43	o	281	ASN
43	o	299	HIS
43	o	313	ASN
43	o	348	HIS
43	o	402	GLN
44	p	272	GLN
44	p	457	ASN
44	p	591	ASN
44	p	683	GLN
45	q	9	HIS
45	q	83	ASN
45	q	106	ASN
45	q	195	HIS
45	q	269	ASN
45	q	297	ASN
45	q	304	GLN

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	33 (44%)	7 (9%)
2	2	1778/1781 (99%)	894 (50%)	146 (8%)
3	3	13/25 (52%)	11 (84%)	1 (7%)
All	All	1865/1881 (99%)	938 (50%)	154 (8%)

All (938) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	G
1	1	10	G
1	1	14	A
1	1	15	G
1	1	16	U
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	25	C
1	1	28	A
1	1	34	C
1	1	40	C
1	1	41	C
1	1	44	A
1	1	45	U
1	1	46	G
1	1	48	C
1	1	49	C
1	1	52	G
1	1	56	C
1	1	59	A
1	1	60	A
1	1	61	C
1	1	63	G
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
1	1	76	A

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Mol	Chain	Res	Type
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	9	U
2	2	11	A
2	2	14	C
2	2	16	G
2	2	17	C
2	2	19	A
2	2	20	G
2	2	24	U
2	2	25	C
2	2	26	A
2	2	27	U
2	2	29	U
2	2	30	G
2	2	31	C
2	2	34	G
2	2	35	U
2	2	36	C
2	2	37	U
2	2	39	A
2	2	40	A
2	2	42	G
2	2	43	A
2	2	44	U
2	2	45	U
2	2	47	A
2	2	51	A
2	2	54	C
2	2	56	U
2	2	57	G
2	2	59	C
2	2	60	U
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G

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Mol	Chain	Res	Type
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	81	G
2	2	87	C
2	2	92	A
2	2	95	G
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	123	G
2	2	124	A
2	2	125	U
2	2	126	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	141	U
2	2	144	A
2	2	146	A
2	2	147	U
2	2	148	C
2	2	149	U
2	2	150	G
2	2	157	U
2	2	158	U
2	2	159	C

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Mol	Chain	Res	Type
2	2	160	U
2	2	161	A
2	2	167	A
2	2	169	U
2	2	172	A
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	183	C
2	2	185	C
2	2	186	G
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	193	U
2	2	194	G
2	2	195	G
2	2	198	G
2	2	199	A
2	2	203	G
2	2	209	A
2	2	214	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	226	U
2	2	227	G
2	2	228	U
2	2	230	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	237	U
2	2	239	C
2	2	240	U
2	2	245	G
2	2	248	U
2	2	249	C
2	2	254	U

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Mol	Chain	Res	Type
2	2	256	A
2	2	259	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	268	G
2	2	270	A
2	2	274	C
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	288	U
2	2	289	G
2	2	294	A
2	2	298	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	319	U
2	2	320	C
2	2	321	G
2	2	322	A
2	2	332	A
2	2	336	G
2	2	337	C
2	2	344	U
2	2	345	G
2	2	349	U
2	2	350	C
2	2	351	A
2	2	358	A
2	2	359	A

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Mol	Chain	Res	Type
2	2	360	C
2	2	368	A
2	2	371	G
2	2	372	G
2	2	377	A
2	2	380	C
2	2	382	G
2	2	384	A
2	2	388	G
2	2	389	G
2	2	390	A
2	2	395	G
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	403	G
2	2	404	C
2	2	406	A
2	2	409	A
2	2	411	A
2	2	412	U
2	2	413	C
2	2	415	A
2	2	416	A
2	2	417	G
2	2	418	G
2	2	420	A
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	426	C
2	2	433	G
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	447	C
2	2	448	C
2	2	451	A

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Mol	Chain	Res	Type
2	2	452	U
2	2	454	C
2	2	455	A
2	2	456	G
2	2	457	G
2	2	458	G
2	2	459	A
2	2	461	G
2	2	467	A
2	2	468	C
2	2	473	A
2	2	474	A
2	2	475	U
2	2	479	G
2	2	480	A
2	2	482	A
2	2	483	C
2	2	487	G
2	2	488	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	497	G
2	2	499	C
2	2	500	U
2	2	501	U
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	511	A
2	2	512	U
2	2	513	G
2	2	515	G
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A

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Mol	Chain	Res	Type
2	2	521	U
2	2	522	G
2	2	523	U
2	2	525	A
2	2	527	U
2	2	530	C
2	2	531	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	550	G
2	2	553	C
2	2	554	A
2	2	555	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	559	U
2	2	560	G
2	2	564	C
2	2	565	C
2	2	566	A
2	2	567	G
2	2	568	C
2	2	569	A
2	2	570	G
2	2	571	C
2	2	573	G
2	2	574	C
2	2	576	G
2	2	577	U
2	2	578	A

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Mol	Chain	Res	Type
2	2	579	A
2	2	580	U
2	2	581	U
2	2	584	A
2	2	586	C
2	2	589	C
2	2	590	A
2	2	593	A
2	2	594	G
2	2	597	U
2	2	599	U
2	2	600	A
2	2	601	U
2	2	605	A
2	2	610	U
2	2	612	G
2	2	613	C
2	2	614	A
2	2	615	G
2	2	616	U
2	2	617	U
2	2	618	A
2	2	619	A
2	2	620	A
2	2	621	A
2	2	622	A
2	2	624	C
2	2	634	A
2	2	638	U
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	681	U

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Mol	Chain	Res	Type
2	2	684	A
2	2	685	A
2	2	686	C
2	2	687	C
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	700	C
2	2	701	U
2	2	702	G
2	2	703	G
2	2	704	C
2	2	705	U
2	2	706	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	713	A
2	2	714	C
2	2	715	U
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	723	G
2	2	725	U
2	2	727	C
2	2	729	G
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	735	C
2	2	736	C
2	2	737	A
2	2	738	G
2	2	741	C
2	2	742	U

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Mol	Chain	Res	Type
2	2	743	U
2	2	744	U
2	2	745	U
2	2	753	A
2	2	755	A
2	2	762	A
2	2	763	G
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	774	A
2	2	775	G
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	783	C
2	2	784	U
2	2	785	C
2	2	788	A
2	2	790	A
2	2	793	U
2	2	794	U
2	2	796	G
2	2	803	A
2	2	805	A
2	2	806	A
2	2	809	G
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U

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Mol	Chain	Res	Type
2	2	828	A
2	2	829	U
2	2	832	U
2	2	834	U
2	2	836	G
2	2	837	G
2	2	839	U
2	2	840	U
2	2	841	C
2	2	845	G
2	2	847	C
2	2	851	C
2	2	854	A
2	2	855	A
2	2	856	U
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	864	A
2	2	872	U
2	2	875	G
2	2	883	A
2	2	885	U
2	2	886	A
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	904	A
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	919	U
2	2	920	U
2	2	925	A

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Mol	Chain	Res	Type
2	2	927	U
2	2	930	C
2	2	931	U
2	2	932	A
2	2	934	U
2	2	936	C
2	2	938	A
2	2	939	A
2	2	941	G
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	957	U
2	2	958	U
2	2	959	U
2	2	962	A
2	2	965	A
2	2	970	A
2	2	978	A
2	2	981	U
2	2	982	A
2	2	983	G
2	2	986	G
2	2	987	A
2	2	991	A
2	2	992	A
2	2	993	G
2	2	994	A
2	2	995	U
2	2	996	G
2	2	998	U
2	2	999	C
2	2	1000	A
2	2	1003	U
2	2	1004	A
2	2	1007	G
2	2	1008	U
2	2	1009	C
2	2	1010	G
2	2	1011	U

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Mol	Chain	Res	Type
2	2	1012	A
2	2	1013	G
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1022	A
2	2	1023	U
2	2	1024	A
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1039	G
2	2	1041	G
2	2	1042	A
2	2	1043	U
2	2	1046	G
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1064	A
2	2	1065	C
2	2	1066	C
2	2	1069	C
2	2	1070	U
2	2	1075	A
2	2	1076	C
2	2	1077	C

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Mol	Chain	Res	Type
2	2	1079	U
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1086	A
2	2	1089	C
2	2	1090	A
2	2	1091	A
2	2	1092	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1098	U
2	2	1099	G
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1107	G
2	2	1108	G
2	2	1110	G
2	2	1111	G
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1117	G
2	2	1118	G
2	2	1123	A
2	2	1125	G
2	2	1133	C
2	2	1135	U
2	2	1136	A
2	2	1137	A
2	2	1138	A
2	2	1145	G
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1157	C
2	2	1158	C
2	2	1161	C

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Mol	Chain	Res	Type
2	2	1162	A
2	2	1163	G
2	2	1164	G
2	2	1166	G
2	2	1168	G
2	2	1169	G
2	2	1172	C
2	2	1174	U
2	2	1175	G
2	2	1176	C
2	2	1184	U
2	2	1185	U
2	2	1186	U
2	2	1188	A
2	2	1189	C
2	2	1190	U
2	2	1191	C
2	2	1192	A
2	2	1193	A
2	2	1195	A
2	2	1196	C
2	2	1197	G
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1218	A
2	2	1224	U
2	2	1225	A
2	2	1226	A
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1237	A
2	2	1240	G

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Mol	Chain	Res	Type
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1247	C
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1260	G
2	2	1268	U
2	2	1272	G
2	2	1273	C
2	2	1275	U
2	2	1282	U
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1286	A
2	2	1287	G
2	2	1292	U
2	2	1294	G
2	2	1295	A
2	2	1296	G
2	2	1298	G
2	2	1300	U
2	2	1303	G
2	2	1305	C
2	2	1306	U
2	2	1309	U
2	2	1311	A
2	2	1312	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1332	C

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Mol	Chain	Res	Type
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1340	A
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1346	U
2	2	1347	A
2	2	1348	G
2	2	1352	U
2	2	1353	G
2	2	1357	G
2	2	1358	C
2	2	1359	A
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1374	C
2	2	1375	U
2	2	1376	U
2	2	1377	C
2	2	1380	A
2	2	1381	G
2	2	1383	G
2	2	1386	A
2	2	1387	C
2	2	1388	U
2	2	1389	A
2	2	1390	U
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1408	A

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Mol	Chain	Res	Type
2	2	1409	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1417	G
2	2	1418	C
2	2	1419	A
2	2	1420	A
2	2	1423	A
2	2	1424	C
2	2	1425	A
2	2	1426	G
2	2	1428	U
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1433	G
2	2	1434	A
2	2	1435	U
2	2	1442	A
2	2	1444	A
2	2	1448	U
2	2	1449	C
2	2	1450	U
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A
2	2	1459	C
2	2	1461	C
2	2	1465	C
2	2	1466	U
2	2	1467	A
2	2	1469	A
2	2	1470	C
2	2	1471	U
2	2	1476	G
2	2	1478	G
2	2	1479	C
2	2	1480	C

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Mol	Chain	Res	Type
2	2	1481	A
2	2	1482	G
2	2	1484	G
2	2	1487	U
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1496	G
2	2	1498	C
2	2	1499	C
2	2	1501	A
2	2	1504	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1528	C
2	2	1529	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1537	G
2	2	1538	G
2	2	1540	G
2	2	1544	G
2	2	1554	A
2	2	1555	U
2	2	1557	A
2	2	1558	U
2	2	1559	U
2	2	1566	C
2	2	1570	G
2	2	1571	A

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Mol	Chain	Res	Type
2	2	1572	G
2	2	1573	G
2	2	1574	A
2	2	1575	A
2	2	1578	C
2	2	1579	C
2	2	1580	U
2	2	1581	A
2	2	1582	G
2	2	1583	U
2	2	1584	A
2	2	1588	G
2	2	1590	A
2	2	1593	U
2	2	1594	C
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1605	G
2	2	1608	G
2	2	1611	U
2	2	1612	A
2	2	1613	C
2	2	1614	G
2	2	1616	C
2	2	1631	A
2	2	1632	C
2	2	1633	A
2	2	1634	C
2	2	1635	C
2	2	1636	G
2	2	1637	C
2	2	1638	C
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1667	U
2	2	1678	G
2	2	1679	A
2	2	1682	U

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Mol	Chain	Res	Type
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1719	A
2	2	1725	G
2	2	1728	A
2	2	1730	A
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U
2	2	1753	A
2	2	1754	A
2	2	1758	G
2	2	1763	A
2	2	1764	A
2	2	1765	G
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1778	G
2	2	1779	A

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

All (154) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	43	G
1	1	44	A
1	1	47	U
1	1	48	C
1	1	59	A
1	1	74	C
2	2	42	G
2	2	46	A
2	2	66	U
2	2	68	A
2	2	72	A
2	2	73	U
2	2	74	U
2	2	103	A

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Mol	Chain	Res	Type
2	2	115	G
2	2	126	A
2	2	129	U
2	2	130	C
2	2	131	C
2	2	133	U
2	2	134	U
2	2	140	A
2	2	157	U
2	2	177	U
2	2	186	G
2	2	190	C
2	2	193	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	248	U
2	2	258	U
2	2	265	A
2	2	277	U
2	2	278	G
2	2	279	U
2	2	294	A
2	2	312	U
2	2	320	C
2	2	321	G
2	2	344	U
2	2	349	U
2	2	368	A
2	2	388	G
2	2	389	G
2	2	403	G
2	2	451	A
2	2	473	A
2	2	497	G
2	2	517	A
2	2	538	G
2	2	540	A
2	2	542	C
2	2	554	A
2	2	564	C
2	2	570	G

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Mol	Chain	Res	Type
2	2	588	C
2	2	589	C
2	2	593	A
2	2	600	A
2	2	617	U
2	2	620	A
2	2	654	G
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	704	C
2	2	721	U
2	2	736	C
2	2	781	A
2	2	793	U
2	2	810	A
2	2	811	A
2	2	826	C
2	2	828	A
2	2	854	A
2	2	855	A
2	2	860	U
2	2	896	C
2	2	907	U
2	2	938	A
2	2	946	U
2	2	956	G
2	2	986	G
2	2	995	U
2	2	998	U
2	2	1010	G
2	2	1030	U
2	2	1038	A
2	2	1056	U
2	2	1080	A
2	2	1089	C
2	2	1092	A
2	2	1095	C
2	2	1096	U
2	2	1099	G
2	2	1107	G

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Mol	Chain	Res	Type
2	2	1110	G
2	2	1117	G
2	2	1136	A
2	2	1157	C
2	2	1188	A
2	2	1192	A
2	2	1194	C
2	2	1195	A
2	2	1196	C
2	2	1198	G
2	2	1202	A
2	2	1206	C
2	2	1225	A
2	2	1226	A
2	2	1283	C
2	2	1314	U
2	2	1315	G
2	2	1320	A
2	2	1343	A
2	2	1345	A
2	2	1360	C
2	2	1363	G
2	2	1375	U
2	2	1389	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1416	G
2	2	1419	A
2	2	1423	A
2	2	1425	A
2	2	1430	U
2	2	1445	C
2	2	1455	C
2	2	1457	C
2	2	1465	C
2	2	1479	C
2	2	1481	A
2	2	1482	G
2	2	1489	C
2	2	1491	A
2	2	1533	U

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

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	GCP	k	603	48	32,34,34	1.81	7 (21%)	49,54,54	1.82	7 (14%)
50	MET	k	601	-	6,7,8	0.45	0	2,7,9	0.12	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
51	GCP	k	603	48	-	2/19/38/38	0/3/3/3
50	MET	k	601	-	-	1/5/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.61	1.61	1.50
51	k	603	GCP	C5-C4	3.50	1.48	1.38
51	k	603	GCP	PB-O3A	3.13	1.61	1.58
51	k	603	GCP	PG-O2G	2.91	1.61	1.55
51	k	603	GCP	PG-O3G	-2.86	1.48	1.55
51	k	603	GCP	PA-O3A	2.13	1.61	1.59
51	k	603	GCP	PB-O2B	2.00	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C5-C4-N3	-6.40	118.20	128.39
51	k	603	GCP	C2-N3-C4	5.40	121.60	112.30
51	k	603	GCP	N9-C4-N3	4.68	135.30	125.95
51	k	603	GCP	C6-C5-N7	3.31	136.31	130.29
51	k	603	GCP	PB-O3A-PA	-3.30	121.61	132.37
51	k	603	GCP	C4-C5-N7	-2.64	106.49	110.67
51	k	603	GCP	O6-C6-C5	-2.07	121.06	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

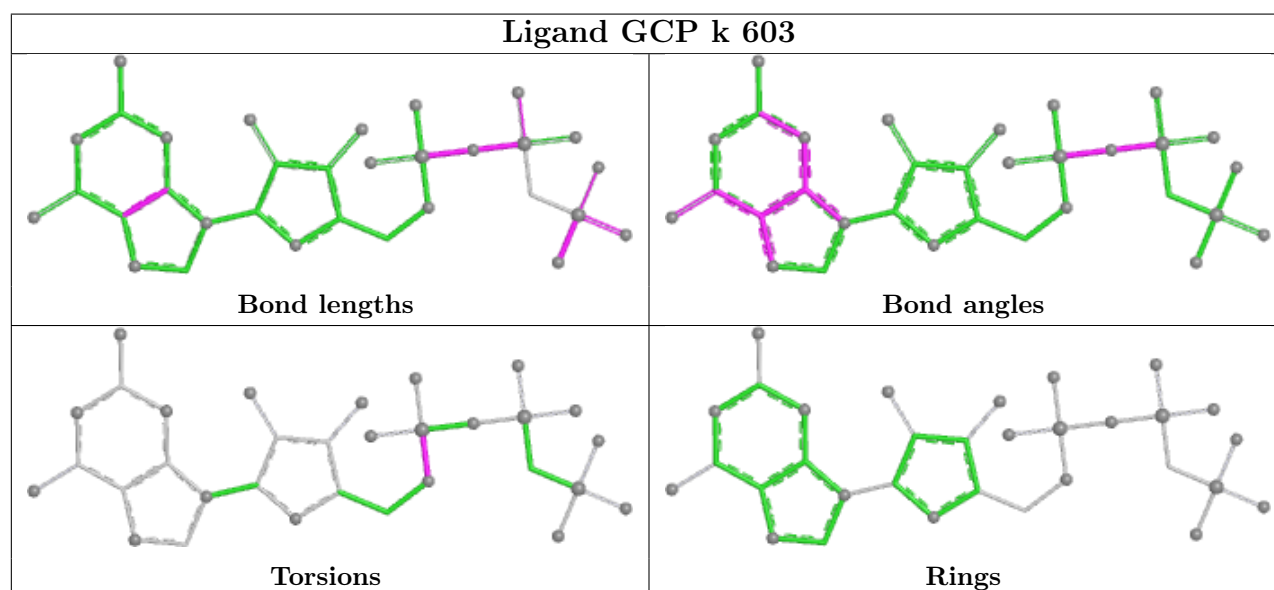
Mol	Chain	Res	Type	Atoms
51	k	603	GCP	C5'-O5'-PA-O3A
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	k	603	GCP	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	o	7
44	p	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	495:PRO	C	753:UNK	N	221.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	218:UNK	C	251:GLN	N	63.04
1	p	32:UNK	C	116:UNK	N	42.95
1	p	185:UNK	C	193:ARG	N	15.92
1	o	818:UNK	C	828:UNK	N	14.63
1	p	158:UNK	C	170:UNK	N	13.31
1	o	846:UNK	C	850:UNK	N	8.27
1	o	769:UNK	C	772:UNK	N	6.84
1	p	135:UNK	C	139:UNK	N	5.98
1	o	802:UNK	C	806:UNK	N	4.31
1	o	834:UNK	C	837:UNK	N	4.08
1	o	785:UNK	C	788:UNK	N	3.70
1	p	206:SER	C	211:UNK	N	3.67
1	p	148:UNK	C	150:UNK	N	3.24

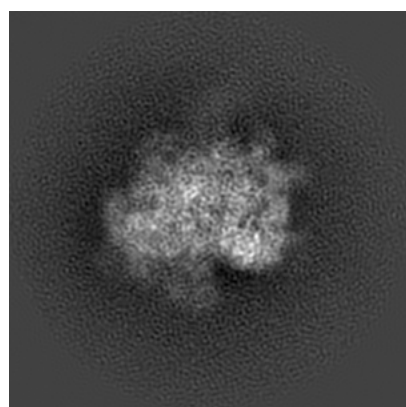
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3048. These allow visual inspection of the internal detail of the map and identification of artifacts.

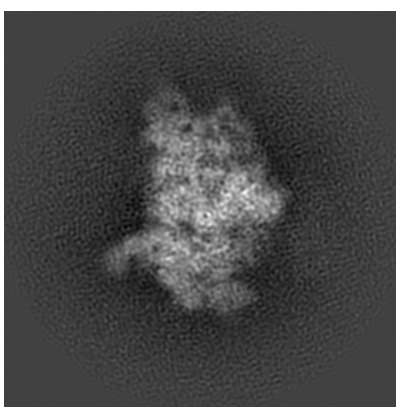
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

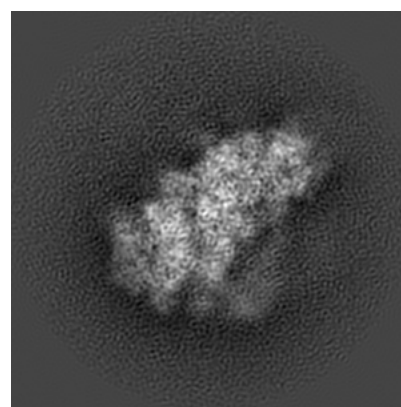
6.1.1 Primary map



X



Y

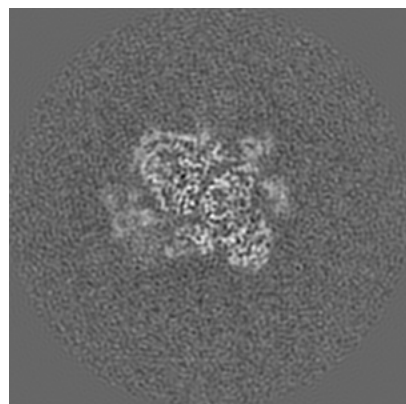


Z

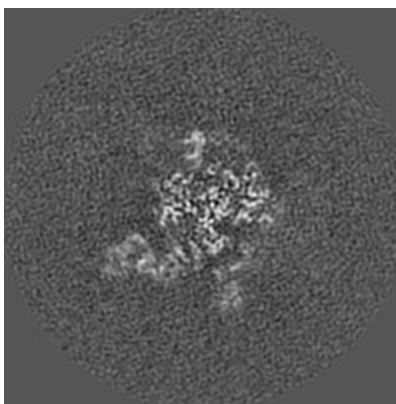
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

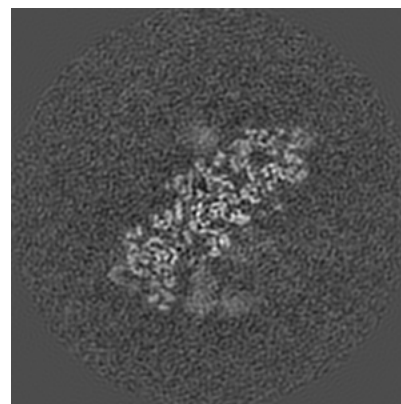
6.2.1 Primary map



X Index: 150



Y Index: 150

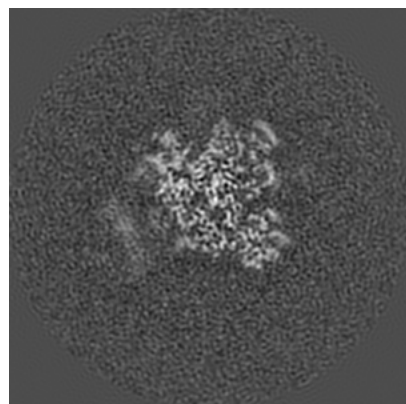


Z Index: 150

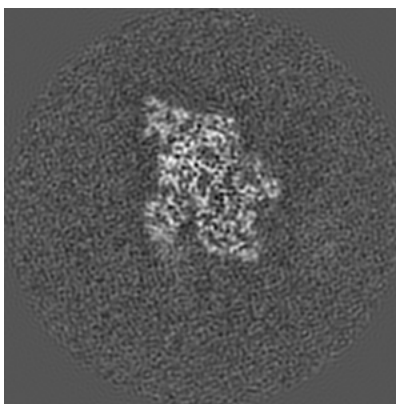
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

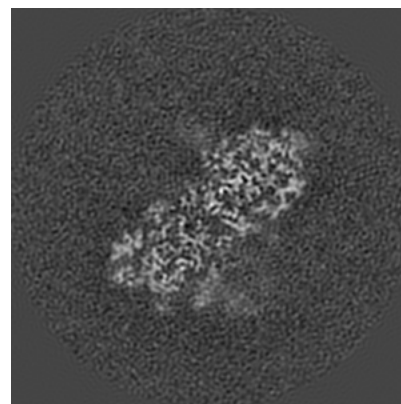
6.3.1 Primary map



X Index: 161



Y Index: 171

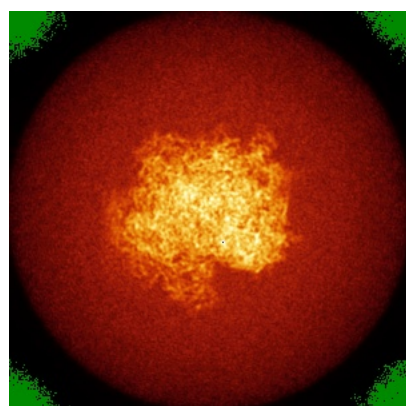


Z Index: 143

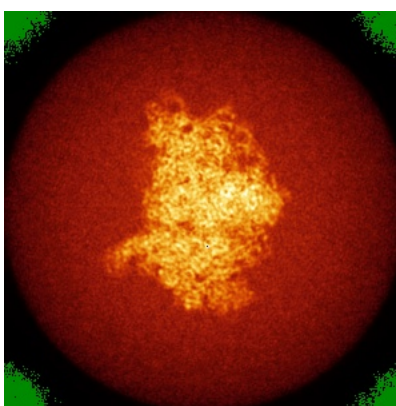
The images above show the largest variance slices of the map in three orthogonal directions.

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

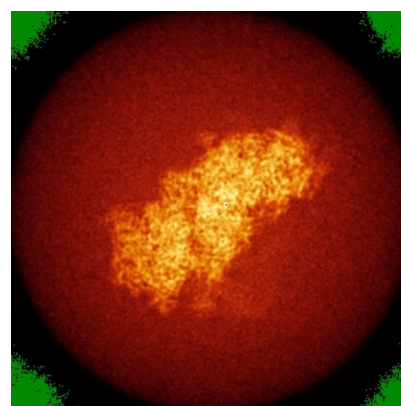
6.4.1 Primary map



X



Y

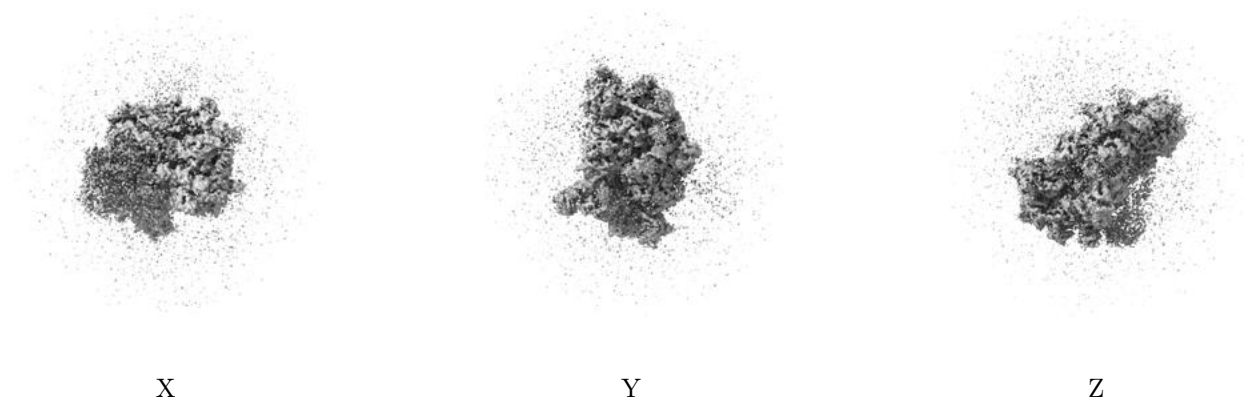


Z

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



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.

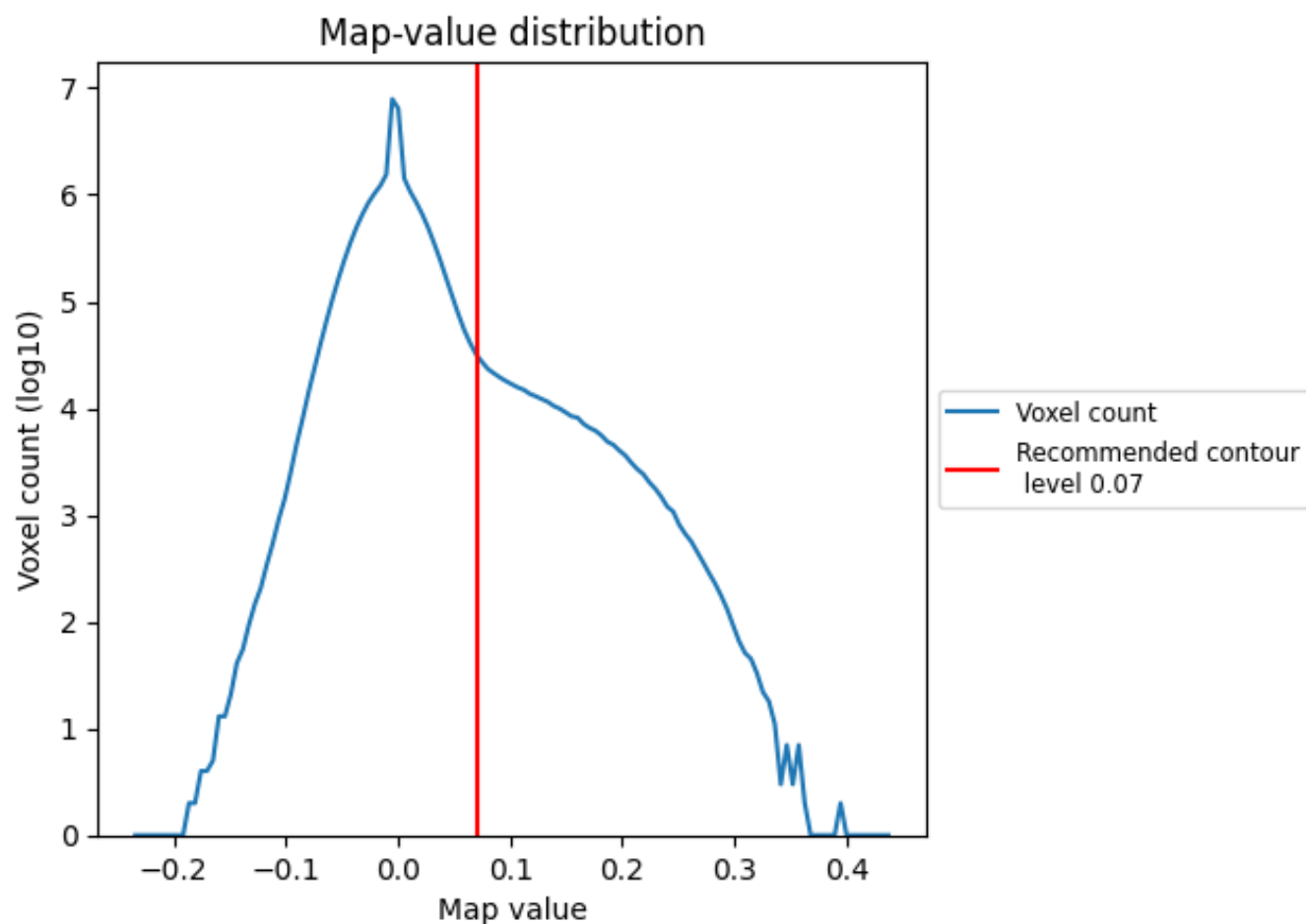
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

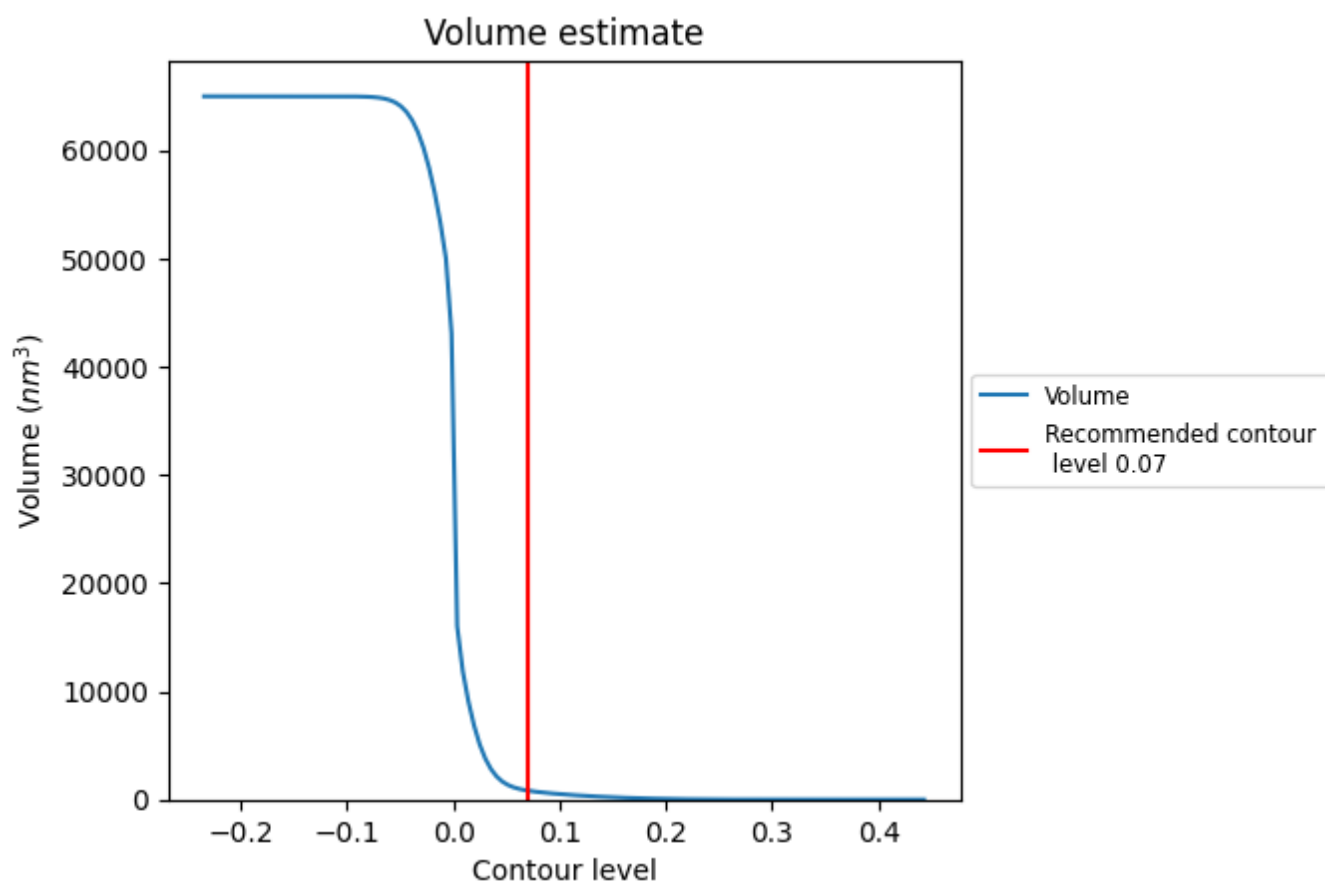
This section contains the results of statistical analysis of the map.

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.

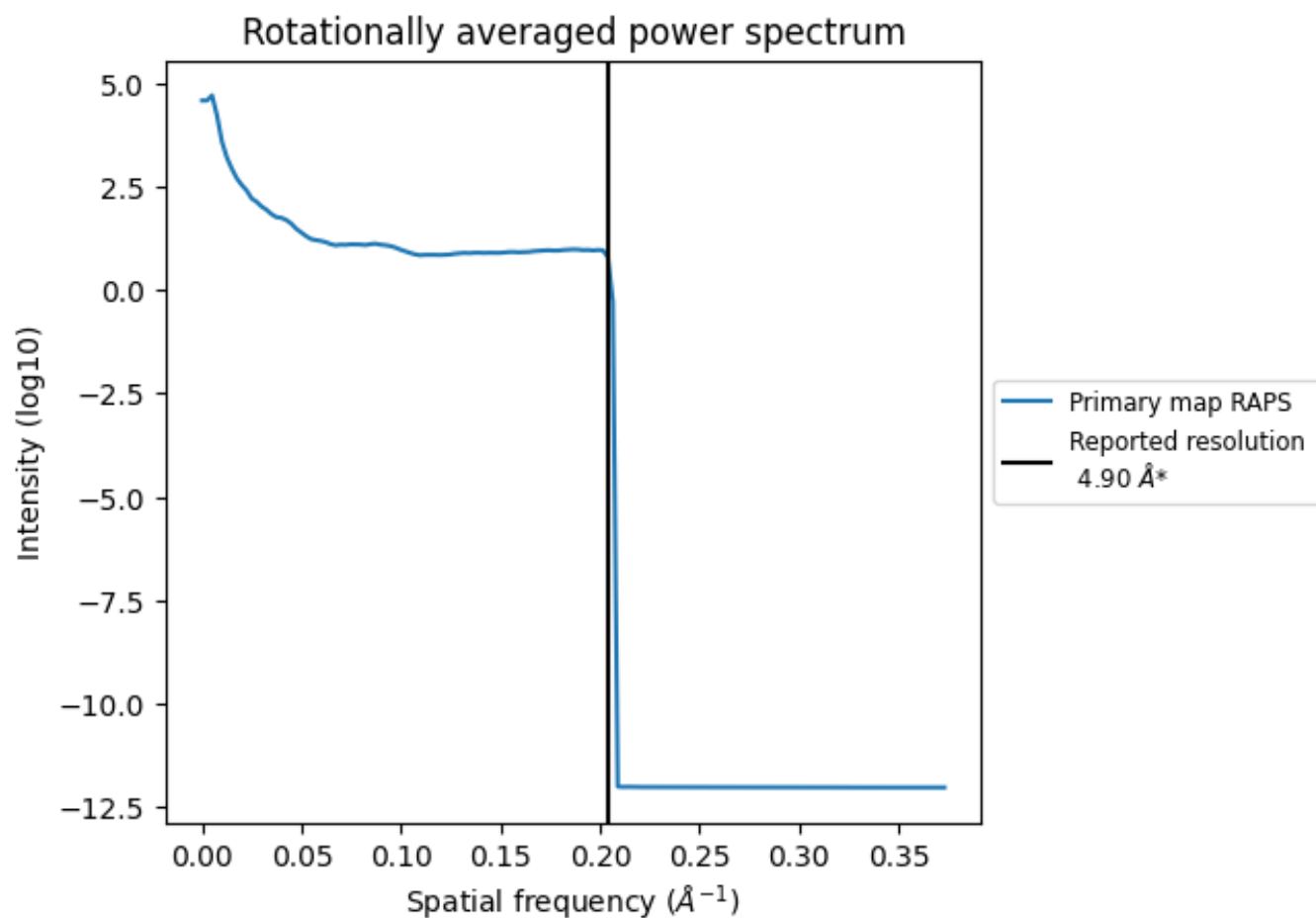
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; this corresponds to an approximate mass of 750 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 ⓘ

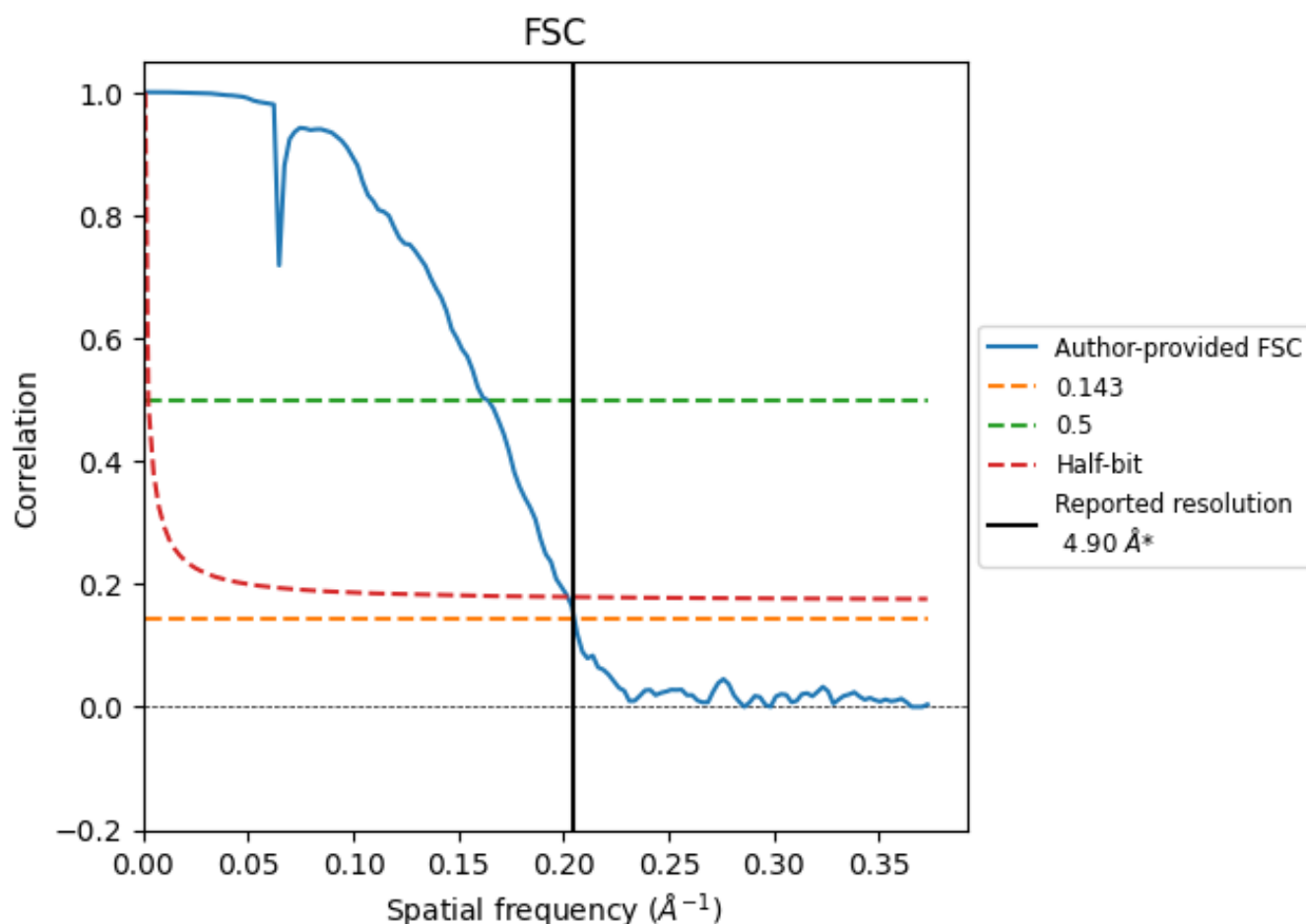


*Reported resolution corresponds to spatial frequency of 0.204 $\text{\AA}^{-1}$

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

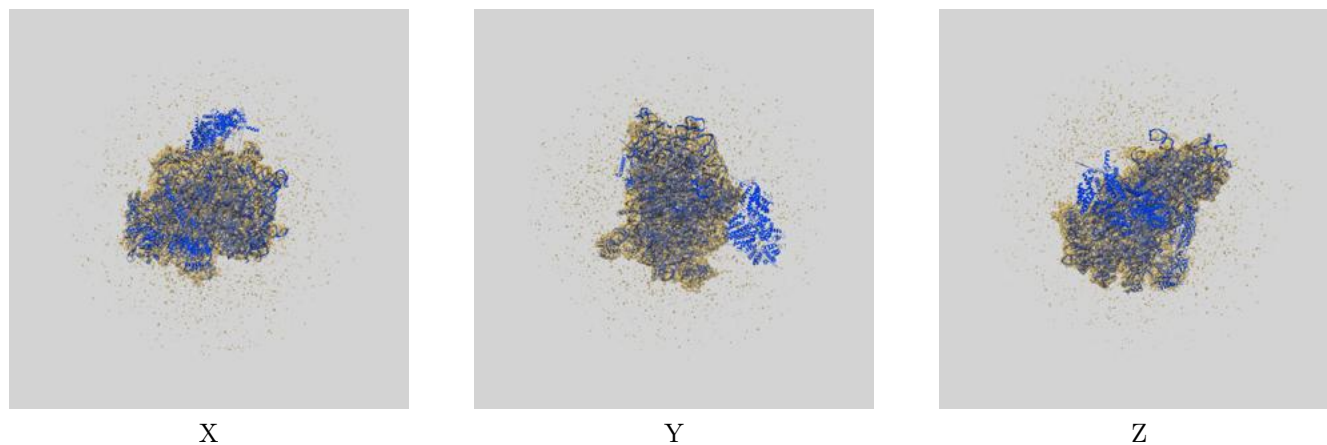
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.88	6.12	4.95
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

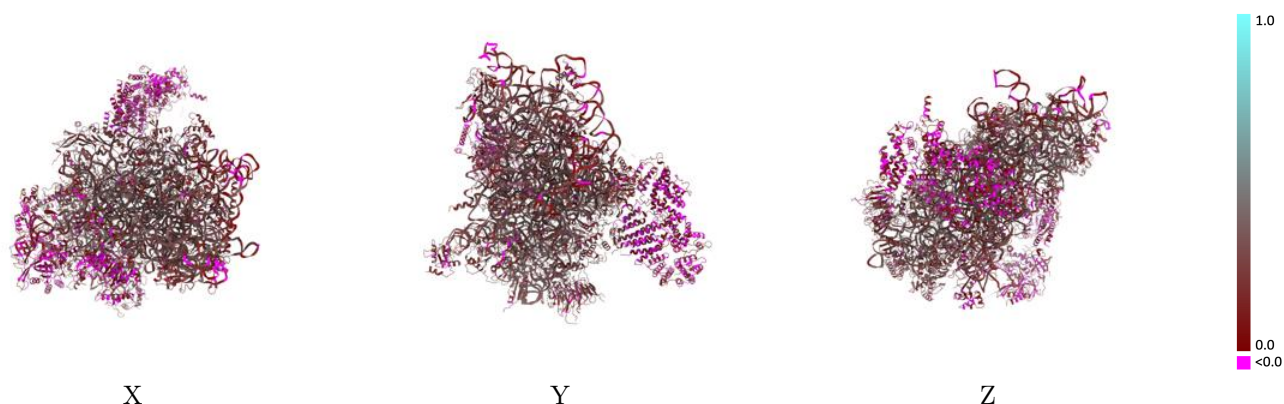
This section contains information regarding the fit between EMDB map EMD-3048 and PDB model 3JAP. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



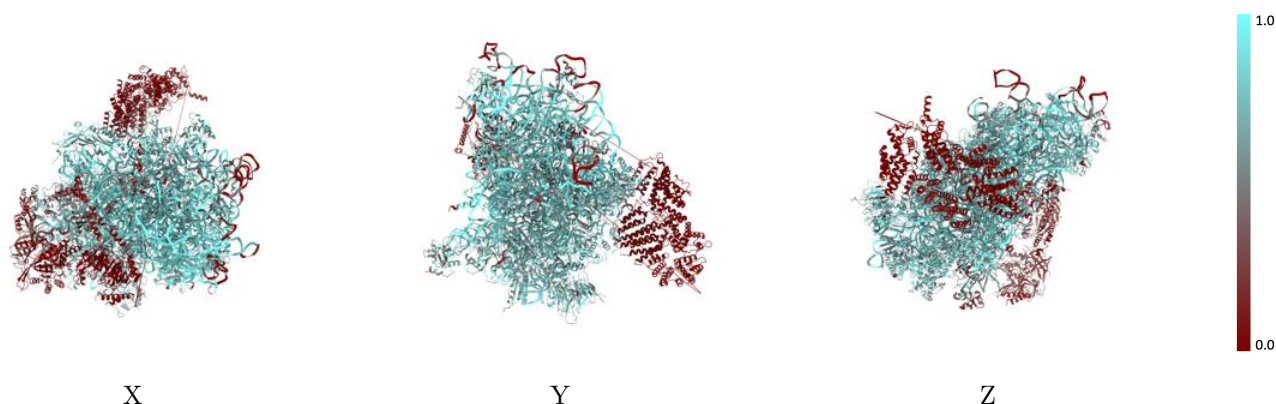
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



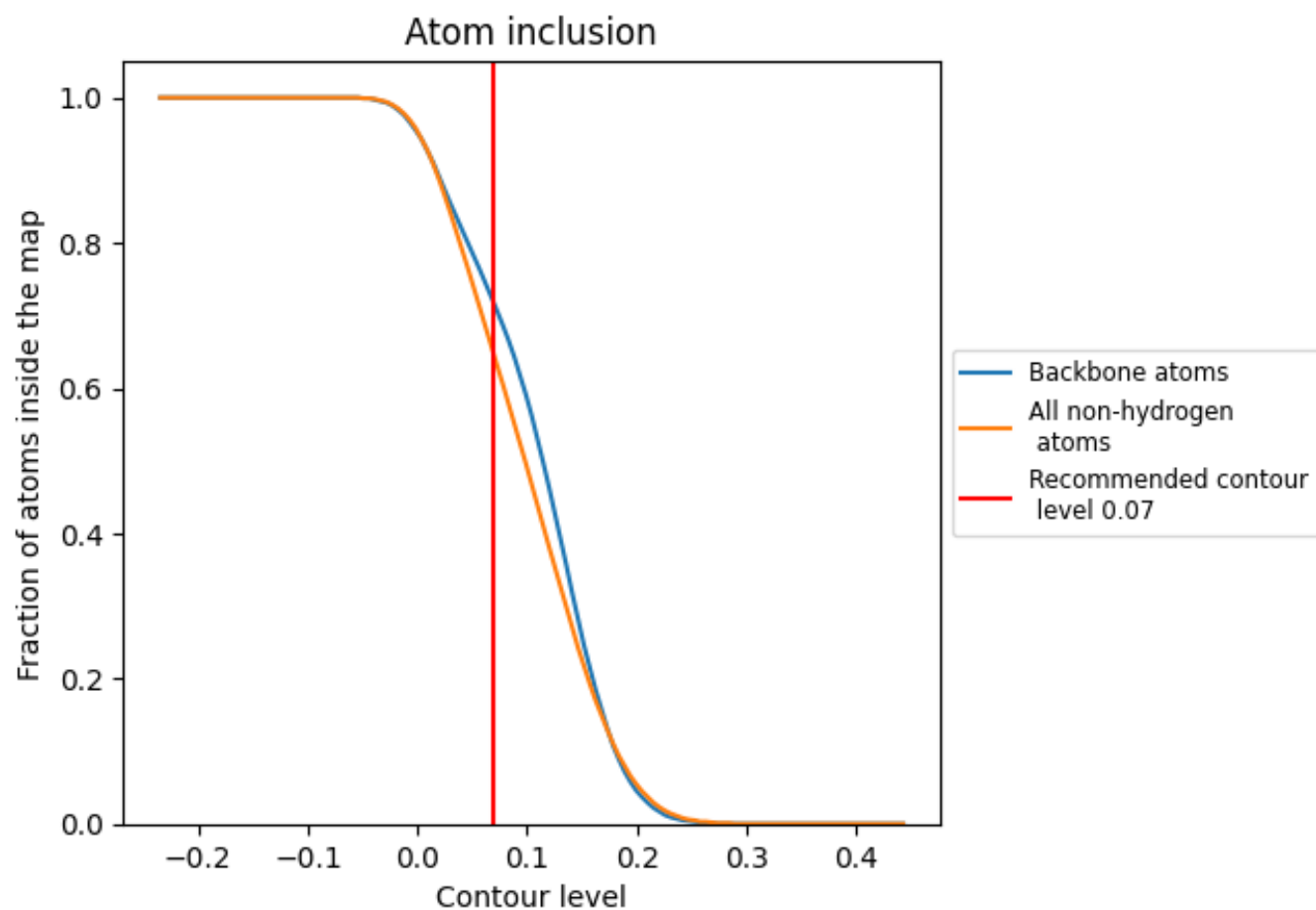
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 64% 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	 0.6440	 0.2440
1	 0.5980	 0.1680
2	 0.8680	 0.2900
3	 0.5500	 0.2110
A	 0.7510	 0.2890
B	 0.7500	 0.2810
C	 0.7190	 0.3090
D	 0.6810	 0.2810
E	 0.7300	 0.2980
F	 0.6790	 0.2580
G	 0.7150	 0.2460
H	 0.6710	 0.2540
I	 0.7160	 0.2620
J	 0.7290	 0.2960
K	 0.7120	 0.2710
L	 0.6860	 0.2970
M	 0.5650	 0.2000
N	 0.7280	 0.2870
O	 0.7510	 0.2800
P	 0.7200	 0.2620
Q	 0.7090	 0.2650
R	 0.7170	 0.2850
S	 0.6780	 0.2640
T	 0.7290	 0.2560
U	 0.6470	 0.2680
V	 0.7320	 0.3010
W	 0.7130	 0.2930
X	 0.7190	 0.3190
Y	 0.7650	 0.2910
Z	 0.6190	 0.2420
a	 0.7430	 0.3170
b	 0.7180	 0.2800
c	 0.6940	 0.2950
d	 0.7590	 0.3010
e	 0.7160	 0.3180



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Chain	Atom inclusion	Q-score
f	 0.6550	 0.2270
g	 0.7090	 0.2410
h	 0.3730	 0.2170
i	 0.6400	 0.2810
j	 0.3060	 0.1650
k	 0.1170	 0.1100
l	 0.1040	 0.1240
m	 0.2760	 0.2020
o	 0.0130	 0.0720
p	 0.0310	 0.0920
q	 0.0260	 0.0530
r	 0.0180	 0.0550
s	 0.0030	 0.0760