



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 10:58 AM JST

PDB ID : 6LQS  
EMDB ID : EMD-0952  
Title : Cryo-EM structure of 90S small subunit preribosomes in transition states (State D)  
Authors : Du, Y.; Ye, K.  
Deposited on : 2020-01-14  
Resolution : 3.80 Å (reported)  
Based on initial model : 6LQP

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

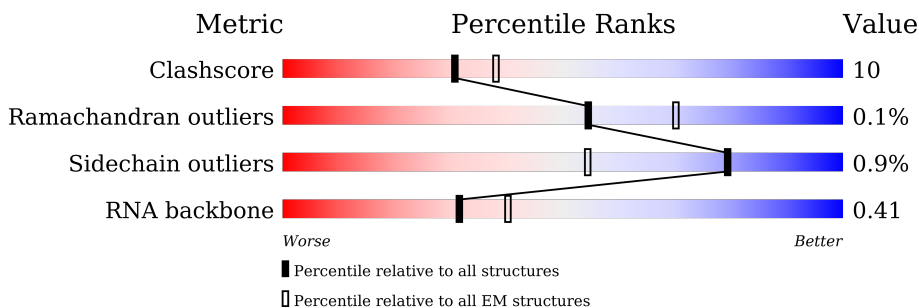
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	3A	333	
2	5A	700	
3	SA	1809	
4	SC	255	
5	SF	261	
6	SG	225	
7	SH	236	

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Mol	Chain	Length	Quality of chain
8	SI	190	
9	SJ	200	
10	SK	197	
11	SM	156	
12	SO	151	
13	SP	137	
14	SR	143	
15	SX	130	
16	SY	145	
17	SZ	135	
18	Sc	82	
19	Sd	67	
20	3B	327	
20	3C	327	
21	3D	504	
22	3E	511	
23	3F	573	
24	3G	126	
24	3H	126	
25	A4	776	
26	A5	643	
27	A8	713	
28	A9	575	
29	AE	1769	
30	AF	513	

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Mol	Chain	Length	Quality of chain
31	AG	896	
32	B1	900	
33	B2	943	
34	B3	817	
35	B8	594	
36	BE	939	
37	B6	440	
38	5B	214	
39	5C	554	
40	5D	250	
41	5E	593	
42	5F	183	
43	5G	290	
44	5H	610	
45	5I	489	
46	5J	217	
47	5K	189	
48	RD	1729	
49	RE	1237	
50	RF	297	
51	RG	252	
51	RH	252	
52	RJ	1183	
53	RK	367	
54	RN	810	

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Mol	Chain	Length	Quality of chain
55	RO	552	95% 78% 17% 5%
56	RP	2493	81% 6% 13%
57	RQ	899	22% 75%
58	RS	480	51% 36% 16% 48%
59	RT	326	6% 40% 12% 48%
60	RW	206	56% 71% 27%
61	X1	347	22% 77%
62	X2	694	20% 80%
63	R5	305	98% 68% 30%
64	R1	246	99% 70% 28%
65	R3	394	86% 61% 25% 14%
66	R6	223	100% 66% 34%
67	R2	265	100% 71% 29%
68	M3	250	86% 61% 24% 14%
69	R0	240	99% 72% 26%
70	r4	359	82% 81% 18%
71	C4	292	76% 55% 21% 24%
72	R4	1001	95% 61% 33% 5%
73	r6	733	14% 86%
74	R7	184	46% 34% 12% 54%
75	M4	1073	81% 51% 30% 19%
76	M6	186	22% 18% 78%

## 2 Entry composition

There are 79 unique types of molecules in this entry. The entry contains 238320 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 U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3A	234	4962	2220	863	1645	234	0	0

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	152	3260	1455	593	1060	152	0	0

- Molecule 3 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	1249	26609	11894	4706	8760	1249	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SC	232	1848	1168	339	337	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SF	250	1930	1232	354	341	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SG	213	1669	1045	307	314	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SH	182	1457	917	273	266	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SI	164	1310	847	222	241		0	0

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SJ	140	1104	689	211	202	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SK	171	1388	879	268	240	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SM	137	1113	715	212	183	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SO	134	1087	698	202	186	1	0	0

- Molecule 13 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SP	118	868	536	164	165	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 15 is a protein called 40S ribosomal protein S22-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SX	127	Total	C	N	O	S	0	0
			1003	640	183	177	3		

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SY	106	Total	C	N	O	S	0	0
			807	515	148	142	2		

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	SZ	123	Total	C	N	O	0	0
			986	626	188	172		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Sc	80	Total	C	N	O	S	0	0
			603	377	109	112	5		

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 20 is a protein called rRNA 2'-O-methyltransferase fibrillar.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
20	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 21 is a protein called Nucleolar protein 56.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	3D	378	Total	C	N	O	S	0	0
			2974	1886	511	568	9		

- Molecule 22 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3E	432	Total	C	N	O	S	0	0
			3041	1895	545	592	9		

- Molecule 23 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3F	437	Total	C	N	O	S	0	0
			3498	2227	609	652	10		

- Molecule 24 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
24	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A4	664	Total	C	N	O	S	0	0
			5243	3320	912	990	21		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A5	511	Total	C	N	O	S	0	0
			3953	2507	682	751	13		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A8	548	Total	C	N	O	S	0	0
			3307	2054	608	642	3		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	A9	128	939	594	173	170	2	0	0

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AE	1534	9956	6243	1771	1923	19	0	0

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AF	479	3807	2395	685	715	12	0	0

- Molecule 31 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AG	826	6570	4181	1111	1259	19	0	0

- Molecule 32 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	B1	806	6427	4104	1099	1205	19	0	0

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	B2	825	6502	4156	1096	1223	27	0	0

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	B3	757	5919	3769	993	1130	27	0	0

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	B8	477	3764	2387	662	705	10	0	0

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BE	823	6475	4107	1119	1228	21	0	0

- Molecule 37 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	B6	374	2800	1782	501	505	12	0	0

- Molecule 38 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	5B	60	495	310	101	84	0	0

- Molecule 39 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	5C	458	3612	2276	636	689	11	0	0

- Molecule 40 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	5D	204	1733	1082	340	306	5	0	0

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	5E	193	1564	970	280	310	4	0	0

- Molecule 42 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 43 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5G	216	Total	C	N	O	S	0	0
			1732	1093	321	312	6		

- Molecule 44 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	5H	74	Total	C	N	O	0	0
			596	373	122	101		

- Molecule 45 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5I	460	Total	C	N	O	S	0	0
			3756	2349	685	706	16		

- Molecule 46 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5J	134	Total	C	N	O	S	0	0
			1127	712	205	207	3		

- Molecule 47 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5K	166	Total	C	N	O	S	0	0
			1323	849	238	226	10		

- Molecule 48 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	RD	316	Total	C	N	O	S	0	0
			2413	1541	415	452	5		

- Molecule 49 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	RE	1090	8805	5720	1452	1609	24	0	0

- Molecule 50 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	RF	241	1963	1253	335	367	8	0	0

- Molecule 51 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	RG	216	1701	1079	296	315	11	0	0
51	RH	230	1799	1142	313	333	11	0	0

- Molecule 52 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	RJ	731	5935	3812	1051	1046	26	0	0

- Molecule 53 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	RK	360	2781	1781	473	516	11	0	0

- Molecule 54 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	RN	553	4088	2590	731	758	9	0	0

- Molecule 55 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	RO	525	3766	2412	646	696	12	0	0

- Molecule 56 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	RP	2180	12716	7827	2389	2484	16	0	0

- Molecule 57 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	RQ	226	1655	1026	314	313	2	0	0

- Molecule 58 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	RS	251	2051	1340	349	359	3	0	0

- Molecule 59 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	RT	171	1357	864	249	240	4	0	0

- Molecule 60 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	RW	150	747	447	150	150	0	0

- Molecule 61 is a protein called Unassigned helices 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	X1	80	400	240	80	80	0	0

- Molecule 62 is a protein called Unassigned helices 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	X2	141	705	423	141	141	0	0

- Molecule 63 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	R5	299	2304	1444	393	451	16	0	0

- Molecule 64 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	R1	244	1886	1177	335	366	8	0	0

- Molecule 65 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	R3	339	2588	1640	441	497	10	1	0

- Molecule 66 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	R6	223	1696	1067	285	334	10	0	0

- Molecule 67 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	R2	265	2030	1296	334	395	5	0	0

- Molecule 68 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	M3	215	1639	1024	273	332	10	0	0

- Molecule 69 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	R0	237	1792	1143	295	344	10	0	0

- Molecule 70 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	r4	293	2236	1393	403	428	12	0	0

- Molecule 71 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	C4	222	1653	1034	287	325	7	0	0

- Molecule 72 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	R4	948	7430	4693	1308	1394	35	0	0

- Molecule 73 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	r6	104	802	496	144	157	5	0	0

- Molecule 74 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	R7	85	681	428	117	132	4	0	0

- Molecule 75 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	M4	874	6814	4354	1166	1254	40	0	0

- Molecule 76 is a protein called M-phase phosphoprotein 6 homolog.

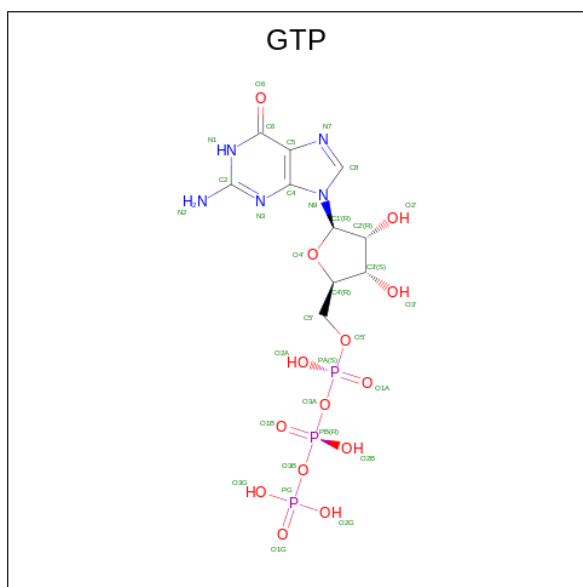
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	M6	40	275	170	51	54	0	0

- Molecule 77 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		AltConf
77	Sc	1	Total	Zn	0
			1	1	
77	5K	1	Total	Zn	0
			1	1	

- Molecule 78 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

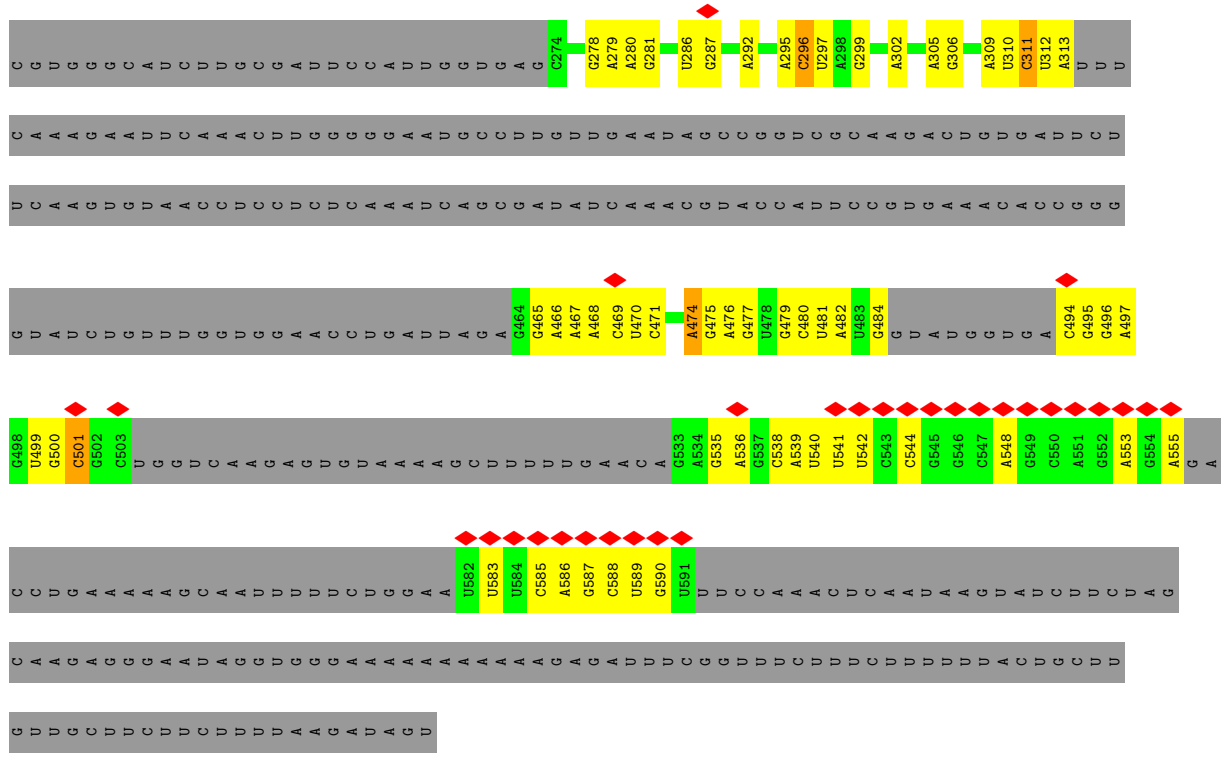


Mol	Chain	Residues	Atoms					AltConf
78	RJ	1	Total	C	N	O	P	0
			32	10	5	14	3	

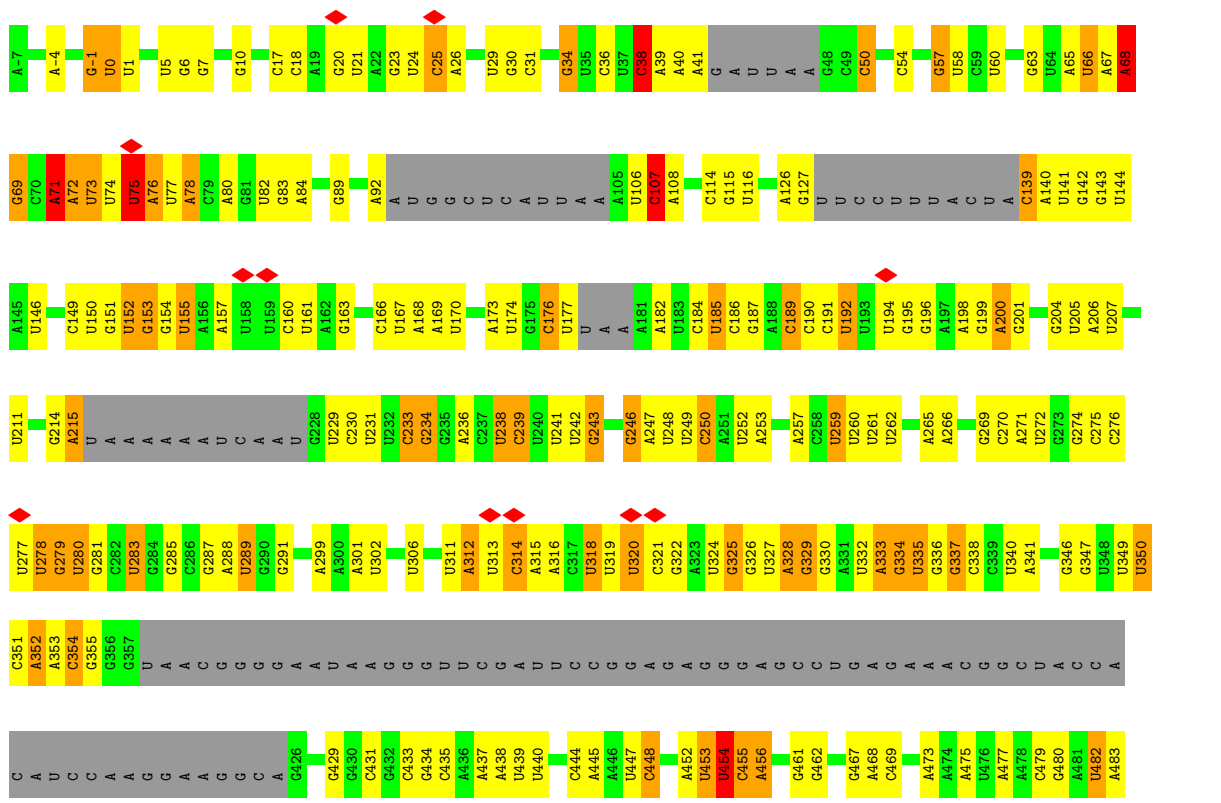
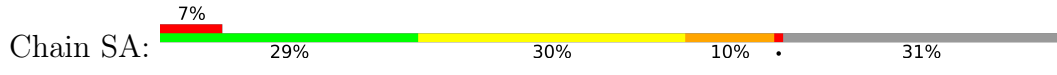
- Molecule 79 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	RJ	1	Total	Mg	0
			1	1	

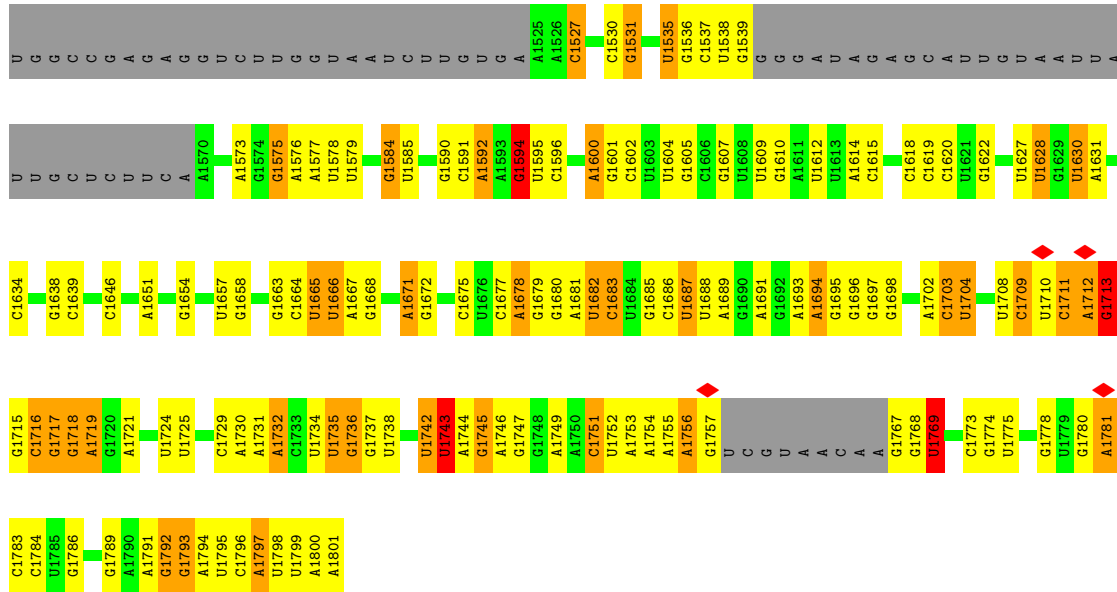




• Molecule 3: 18S pre-rRNA

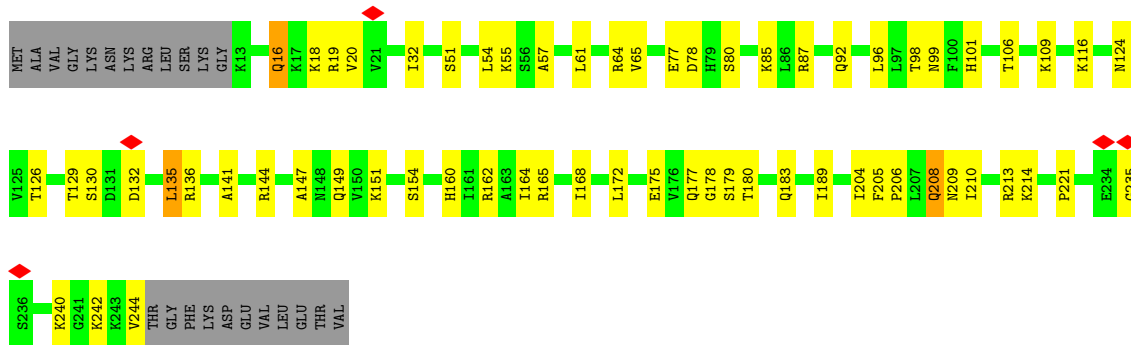






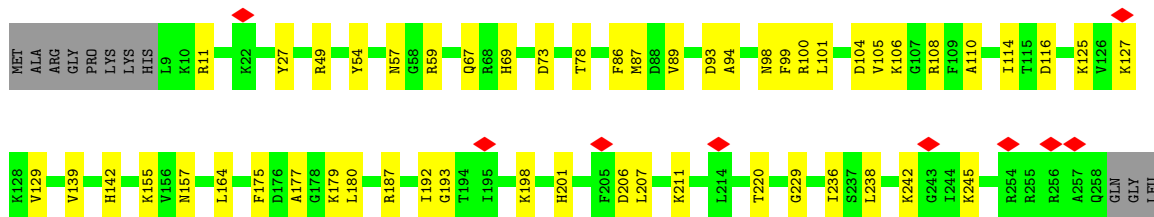
• Molecule 4: 40S ribosomal protein S1-A

Chain SC:



• Molecule 5: 40S ribosomal protein S4-A

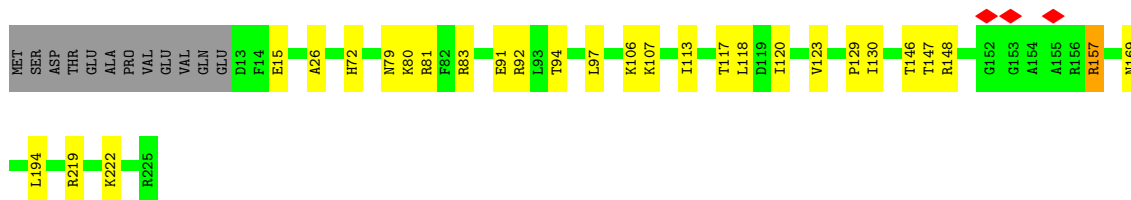
Chain SF:



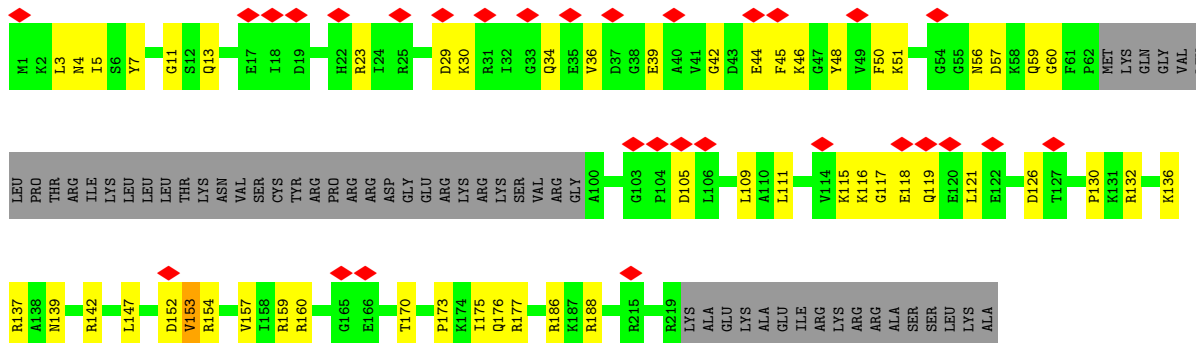
• Molecule 6: 40S ribosomal protein S5

Chain SG:

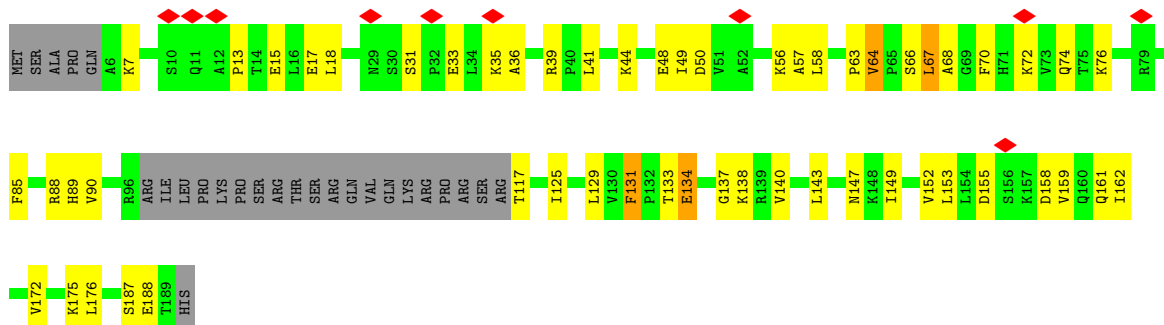




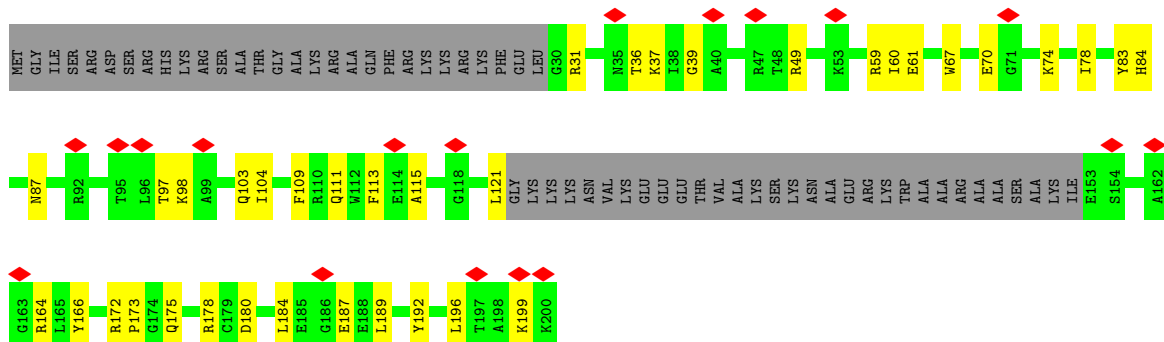
• Molecule 7: 40S ribosomal protein S6-A



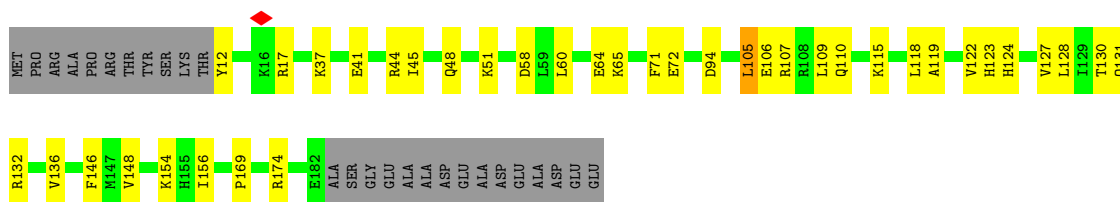
• Molecule 8: 40S ribosomal protein S7-A



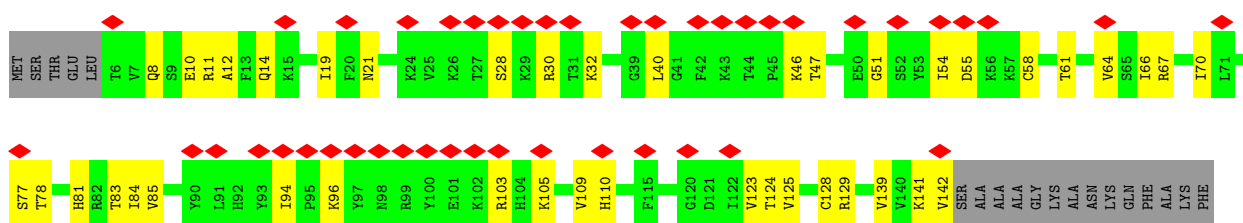
• Molecule 9: 40S ribosomal protein S8-A



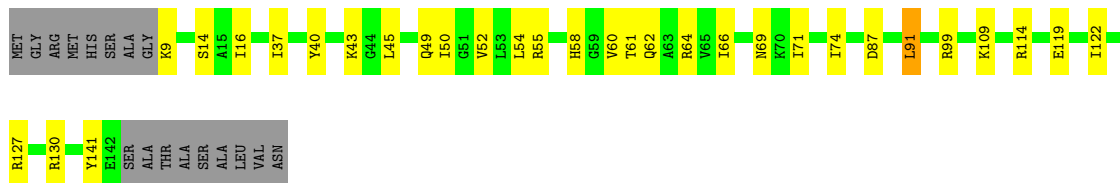
• Molecule 10: 40S ribosomal protein S9-A



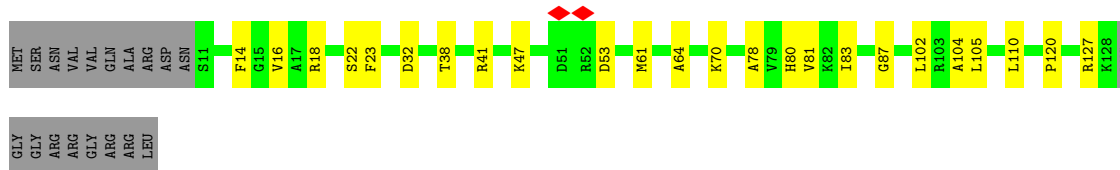
• Molecule 11: 40S ribosomal protein S11-A



• Molecule 12: 40S ribosomal protein S13



• Molecule 13: 40S ribosomal protein S14-A



• Molecule 14: 40S ribosomal protein S16-A

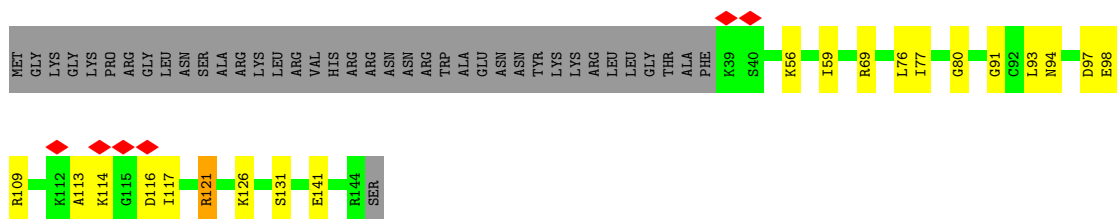


SER  
TYR  
ARG

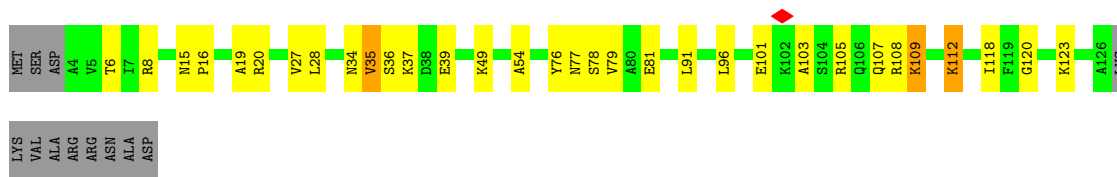
- Molecule 15: 40S ribosomal protein S22-B



- Molecule 16: 40S ribosomal protein S23-A



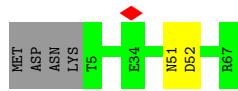
- Molecule 17: 40S ribosomal protein S24-A



- Molecule 18: 40S ribosomal protein S27-A



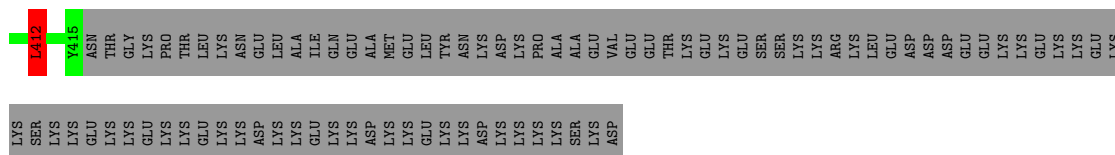
- Molecule 19: 40S ribosomal protein S28-A



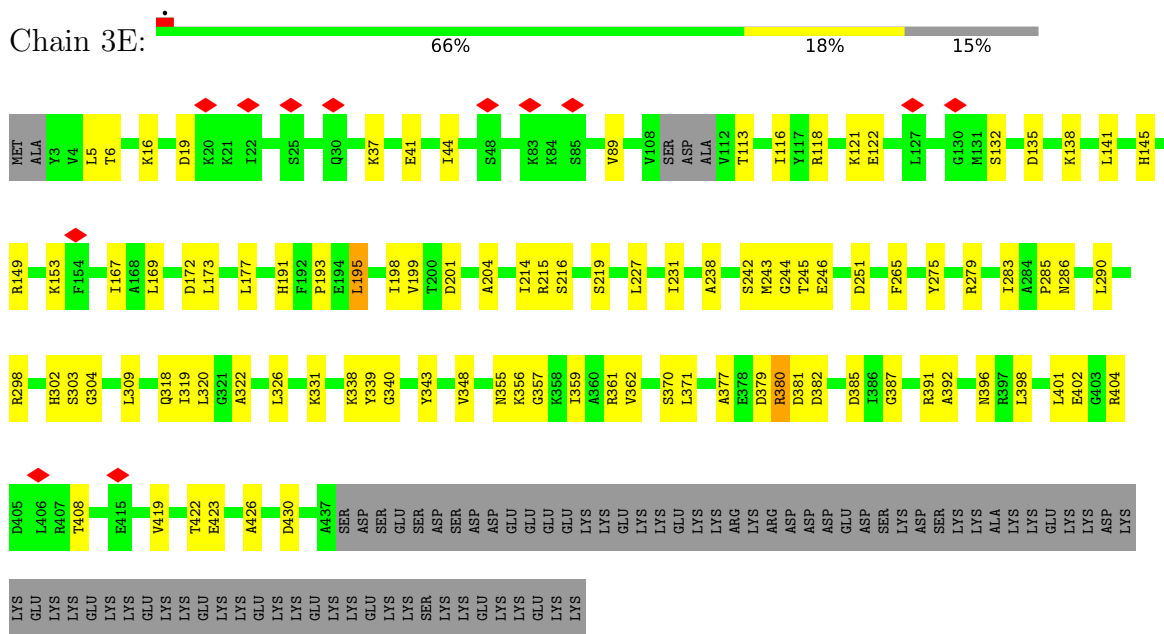
- Molecule 20: rRNA 2'-O-methyltransferase fibrillar



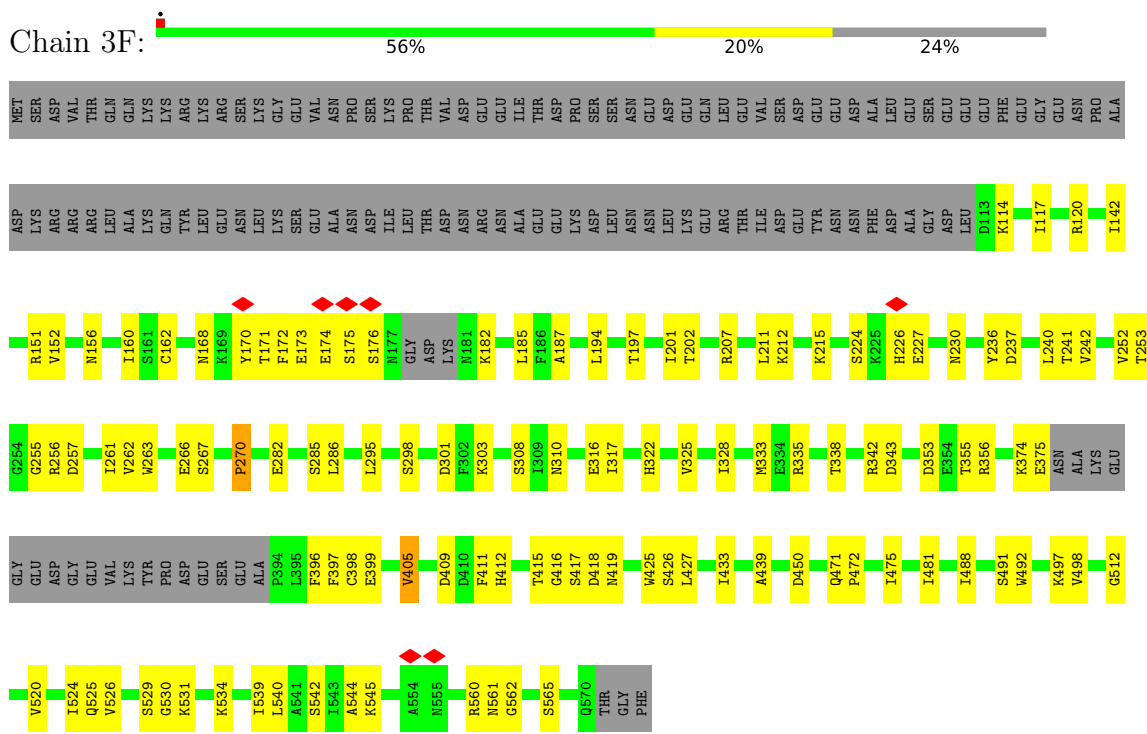




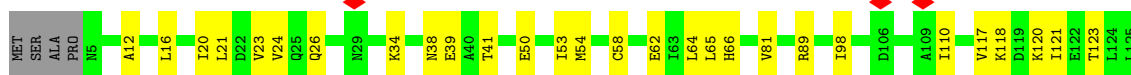
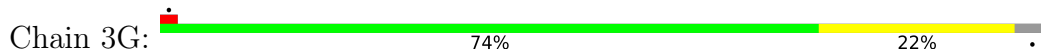
• Molecule 22: Nucleolar protein 58



• Molecule 23: Ribosomal RNA-processing protein 9



• Molecule 24: 13 kDa ribonucleoprotein-associated protein



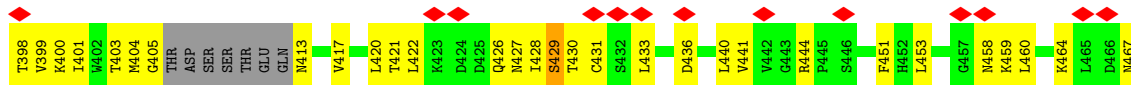
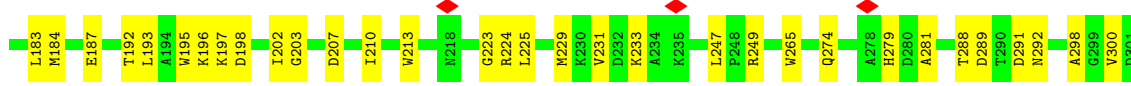
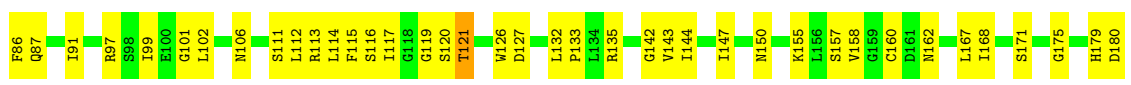
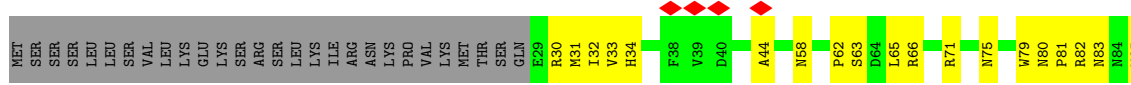
ILE

- Molecule 24: 13 kDa ribonucleoprotein-associated protein



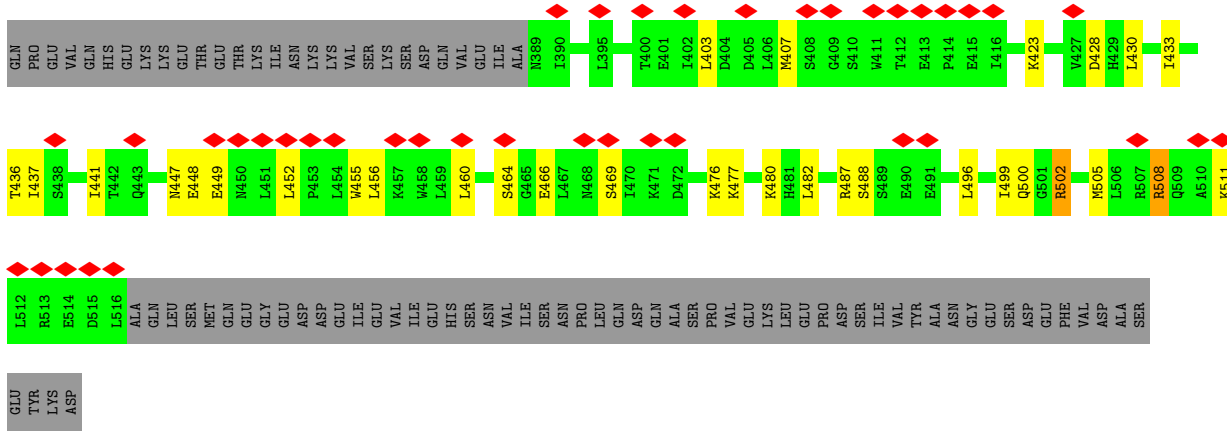
ILE

- Molecule 25: U3 small nucleolar RNA-associated protein 4

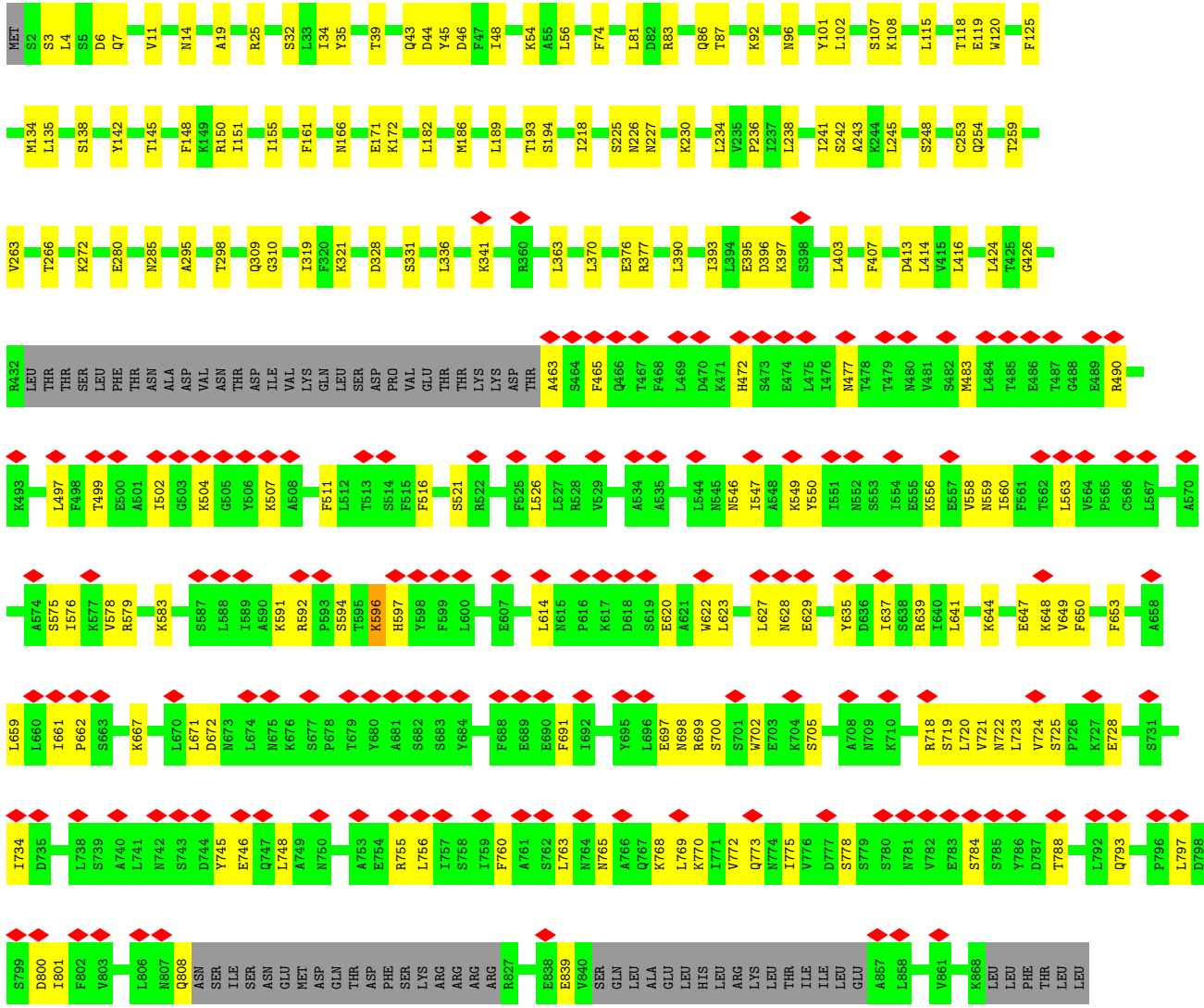
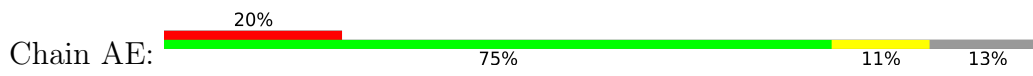


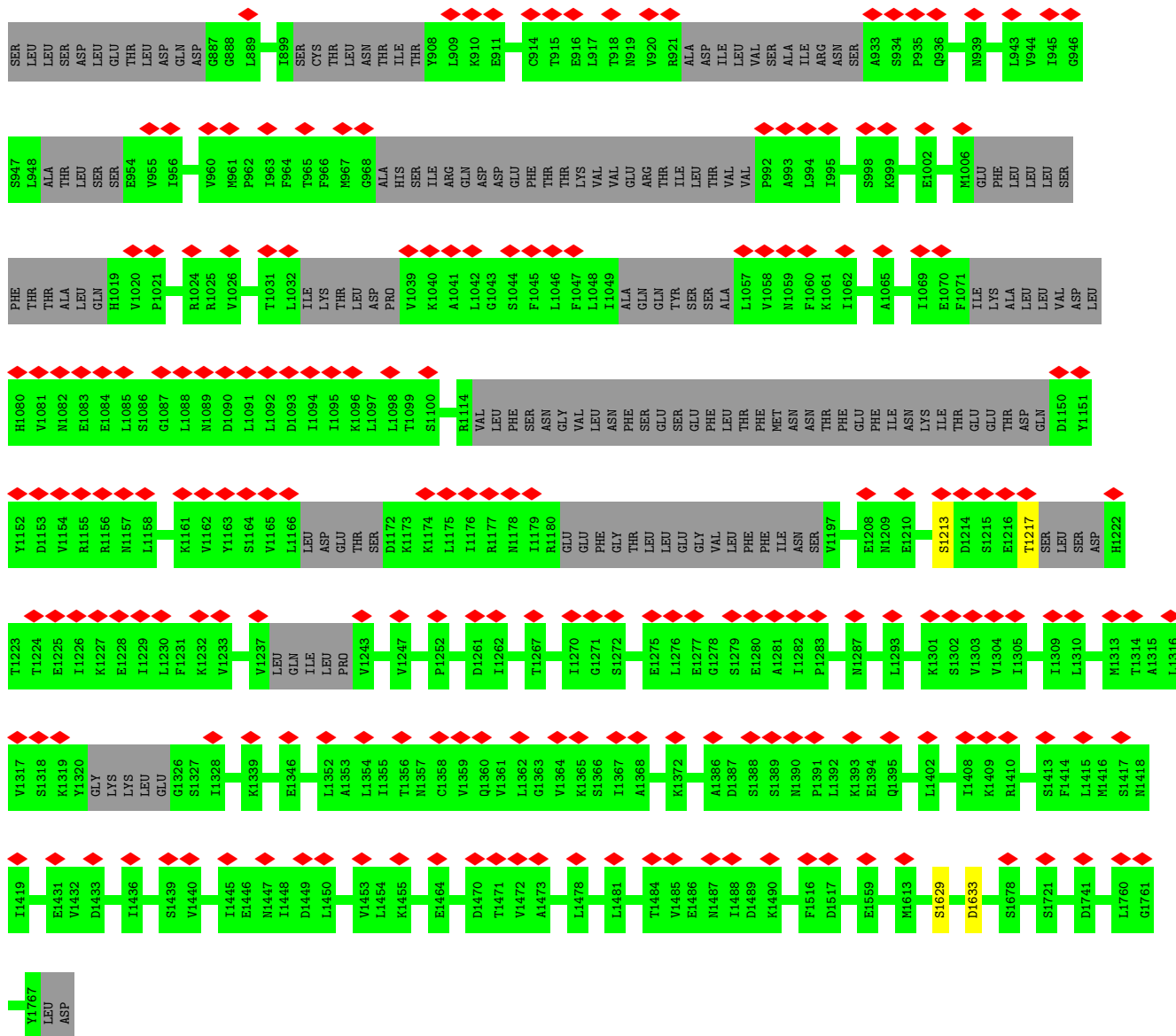




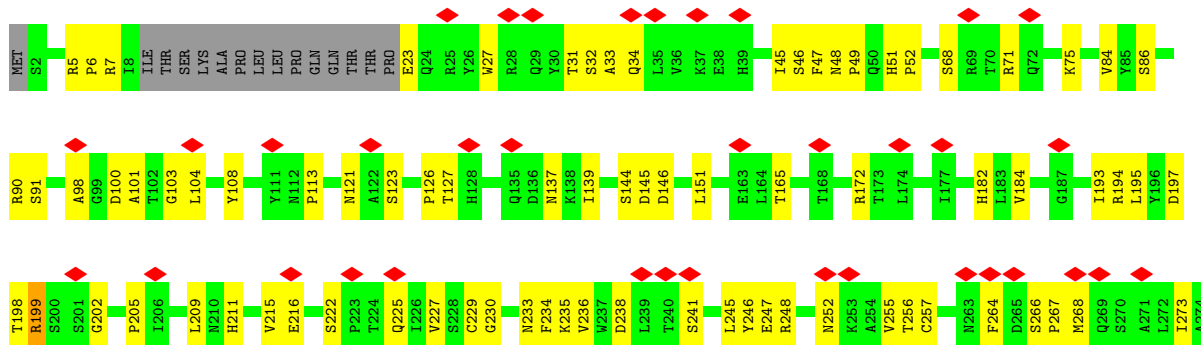


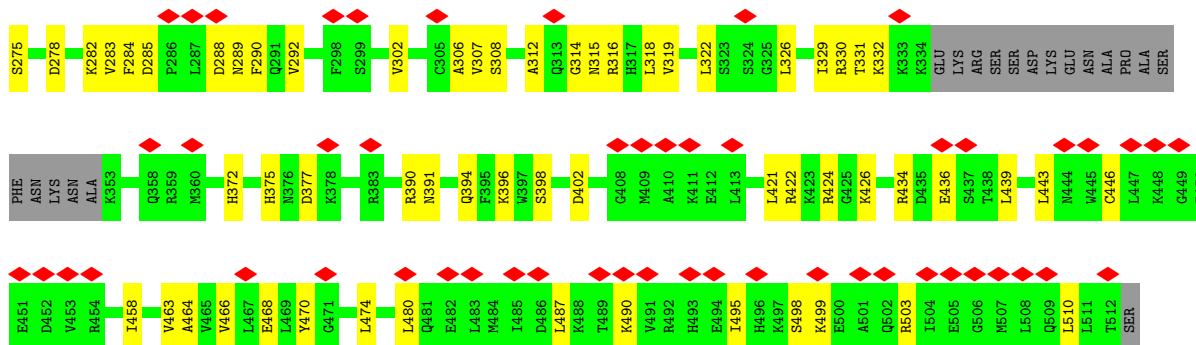
• Molecule 29: U3 small nucleolar RNA-associated protein 10



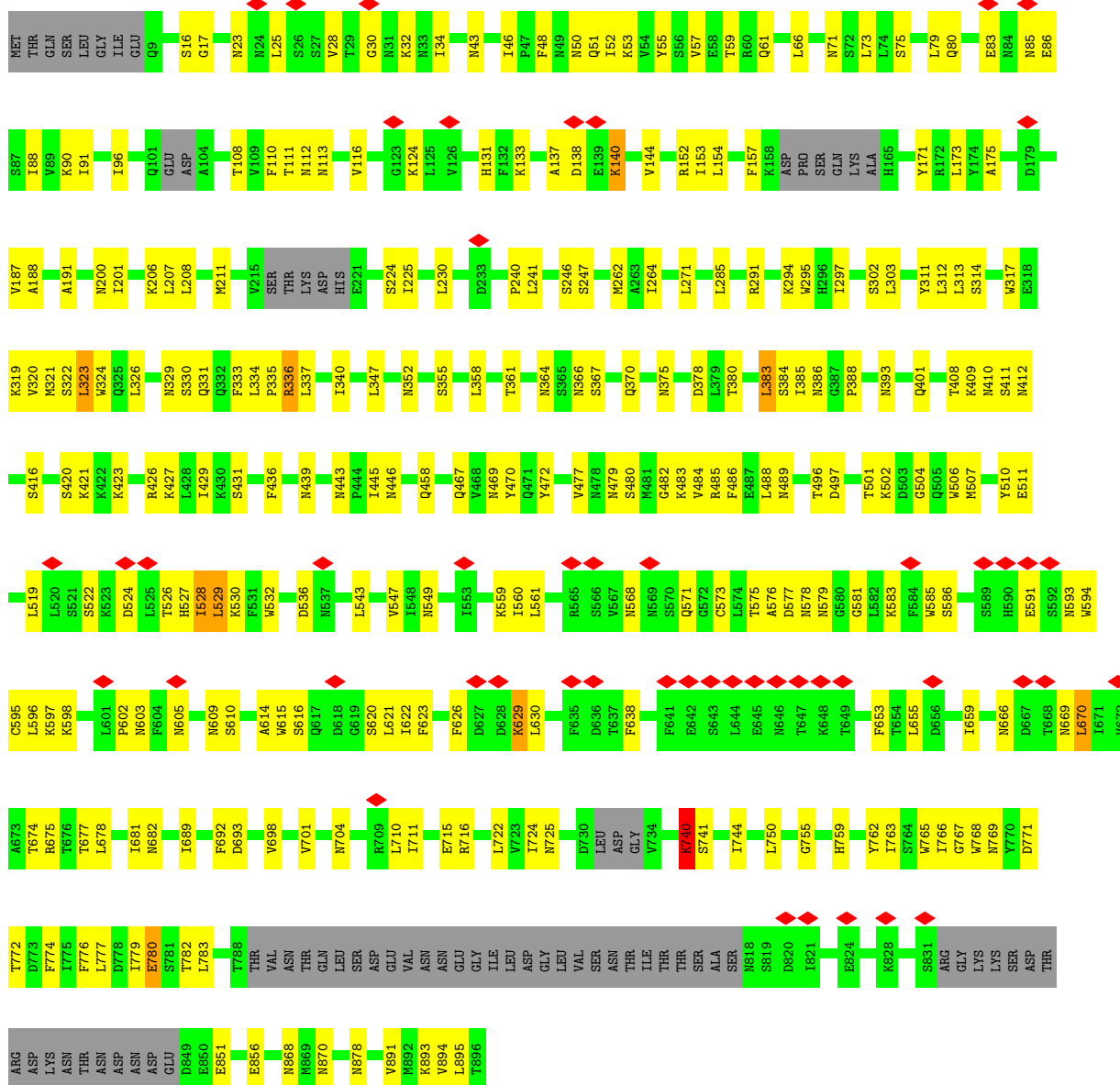


• Molecule 30: U3 small nucleolar RNA-associated protein 15





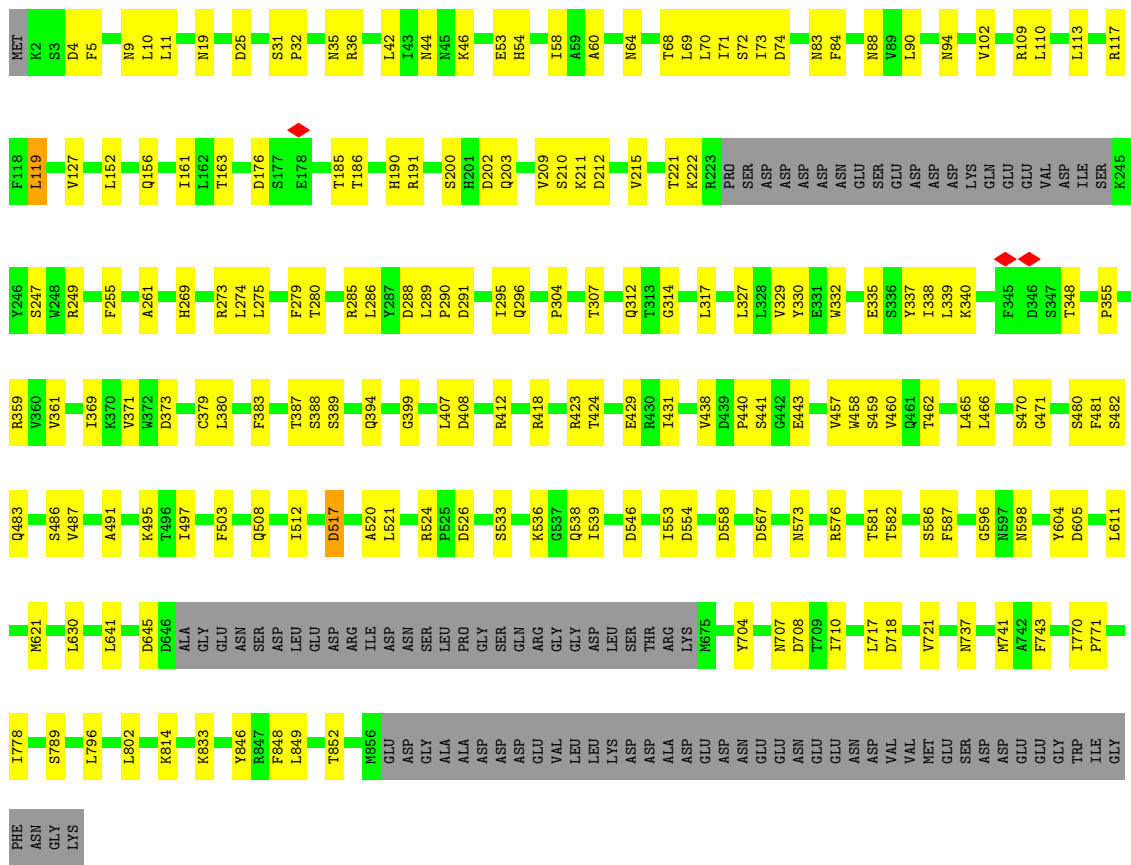
• Molecule 31: NET1-associated nuclear protein 1





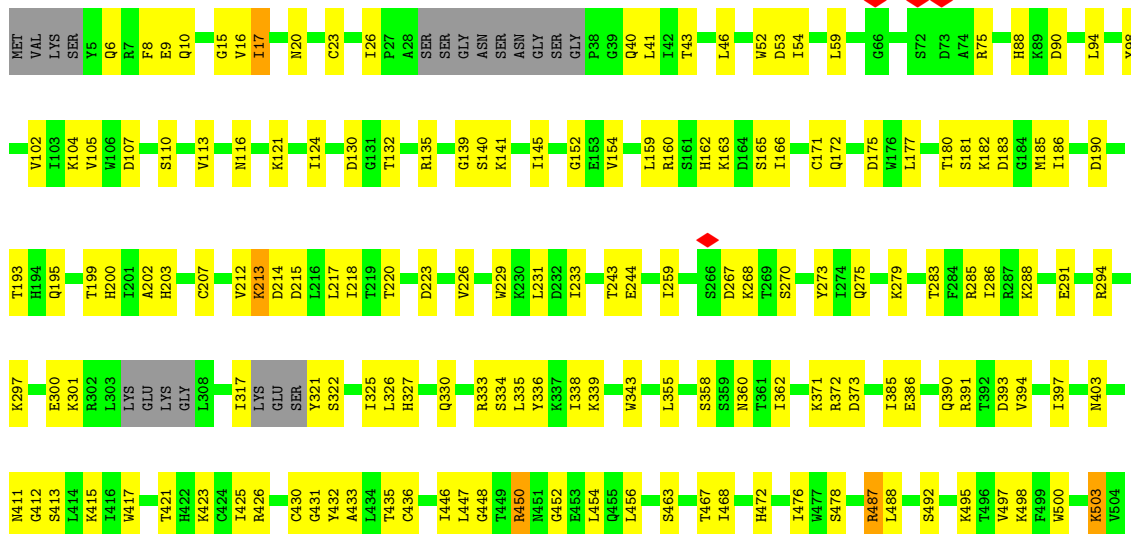
• Molecule 32: Periodic tryptophan protein 2

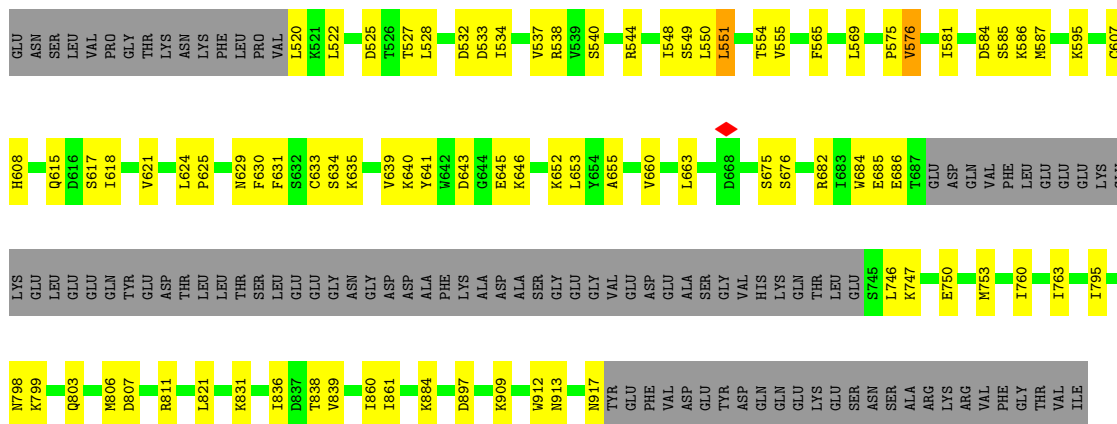
Chain B1:  69% 21% 10%



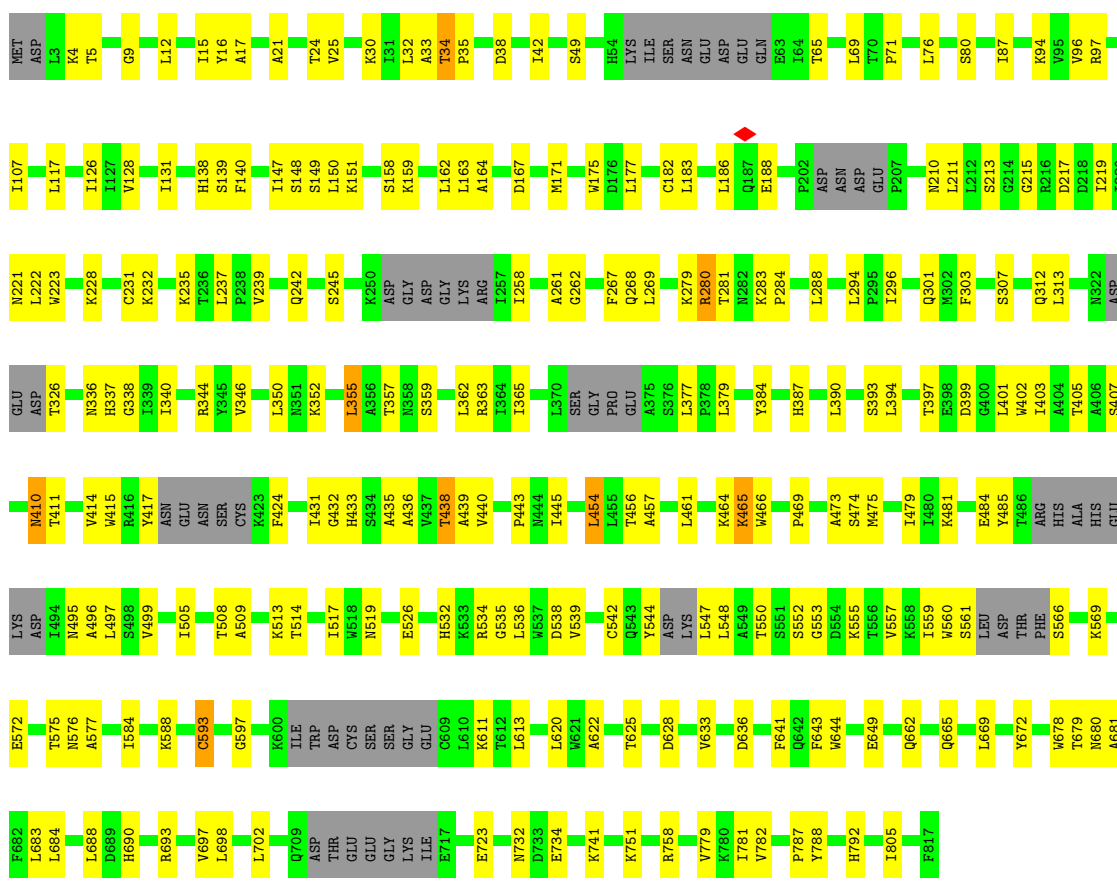
• Molecule 33: U3 small nucleolar RNA-associated protein 12

Chain B2:  62% 25% 13%

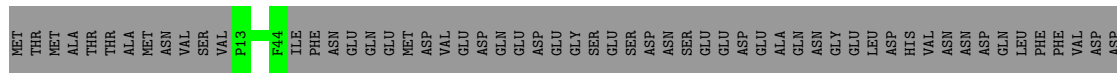


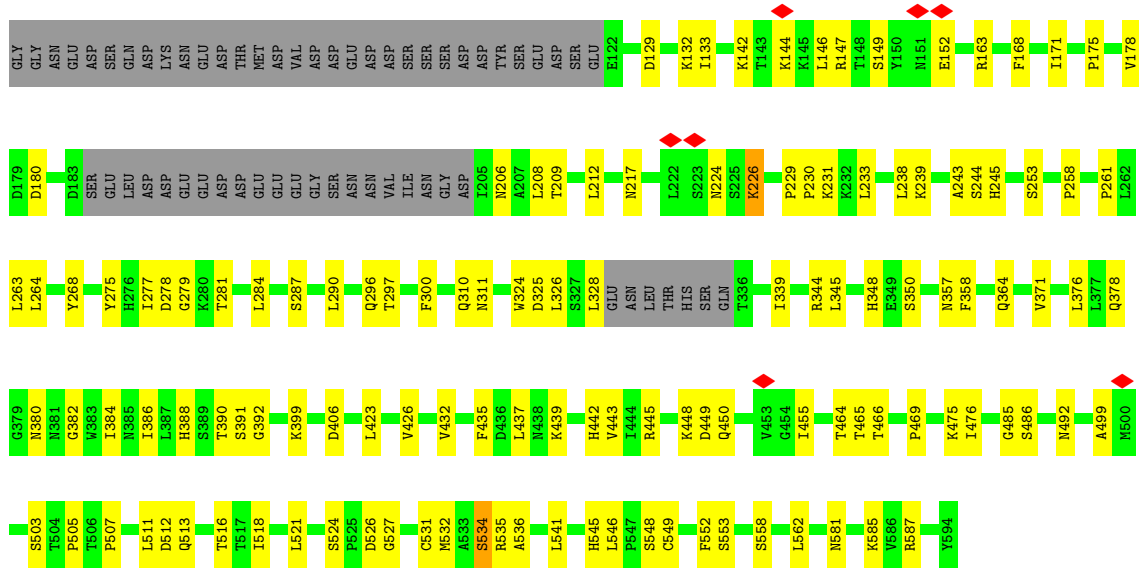


• Molecule 34: U3 small nucleolar RNA-associated protein 13

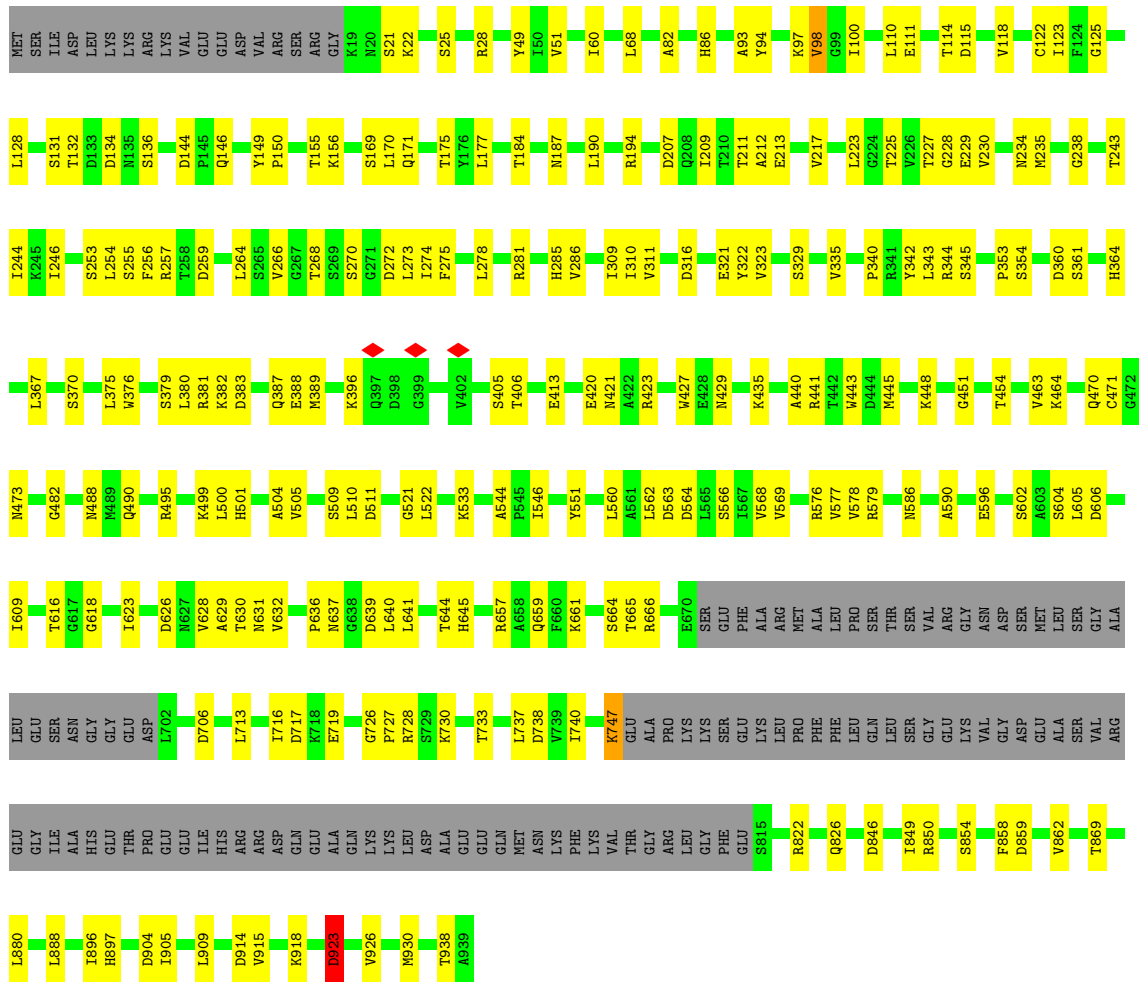


• Molecule 35: U3 small nucleolar RNA-associated protein 18

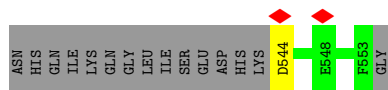




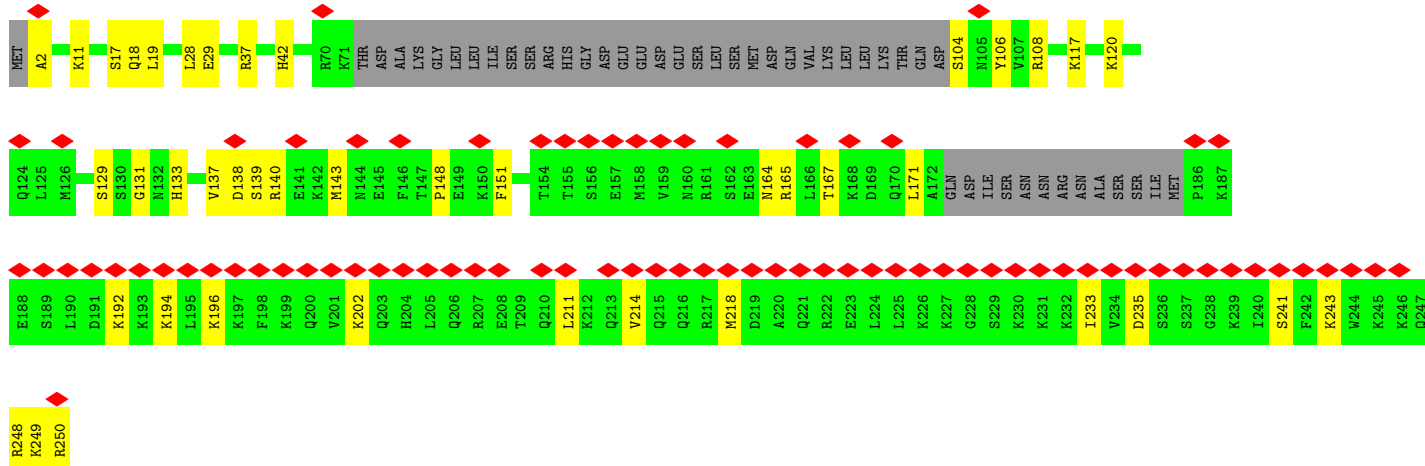
● Molecule 36: U3 small nucleolar RNA-associated protein 21



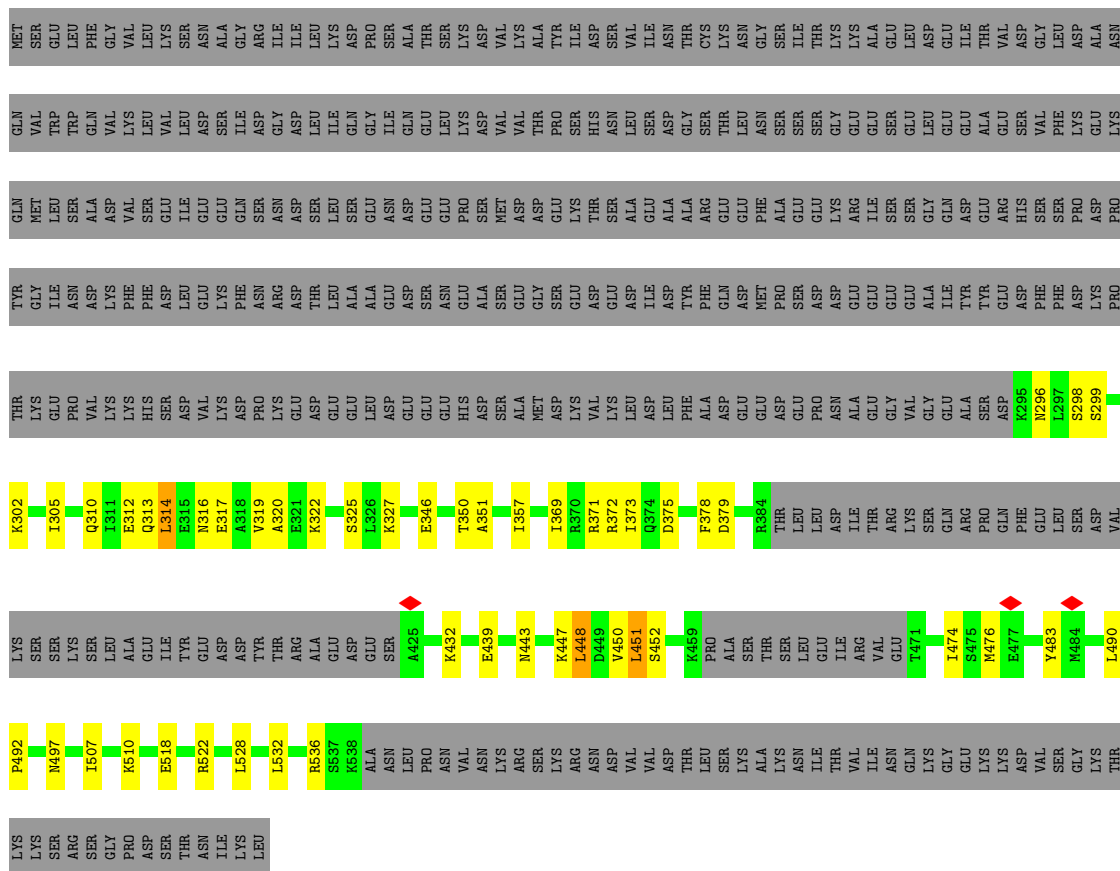




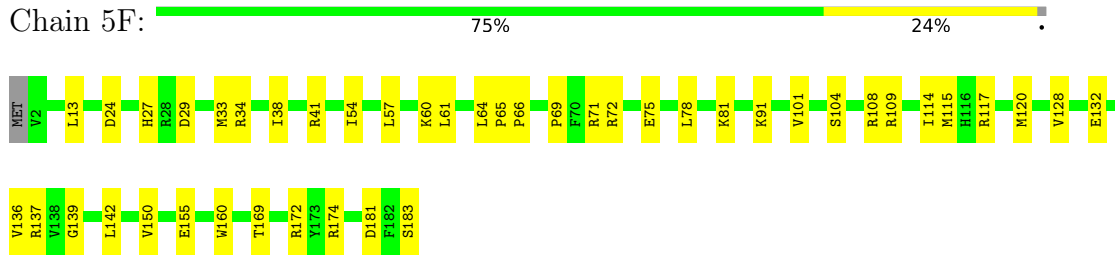
• Molecule 40: U3 small nucleolar RNA-associated protein 11



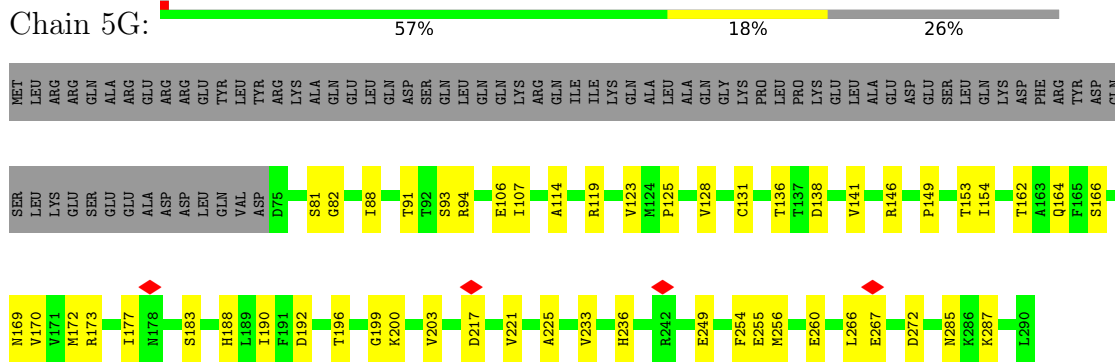
• Molecule 41: U3 small nucleolar RNA-associated protein MPP10



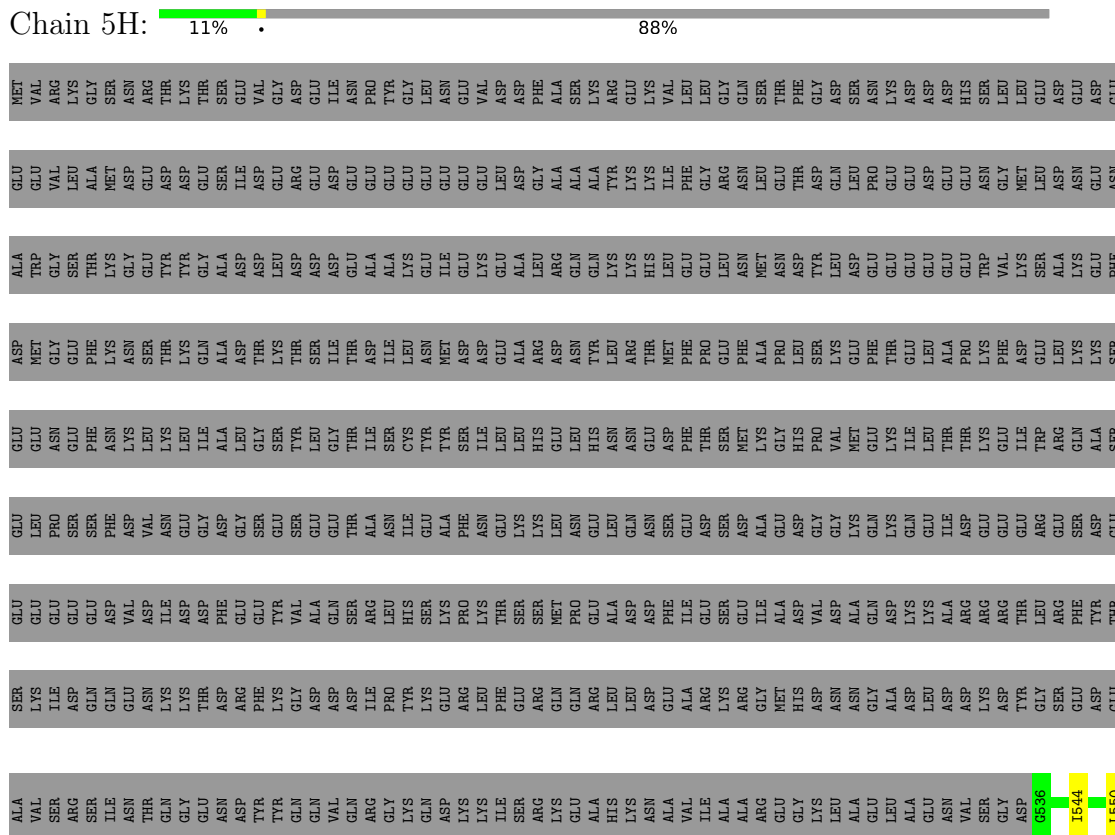
• Molecule 42: U3 small nucleolar ribonucleoprotein protein IMP3



• Molecule 43: U3 small nucleolar ribonucleoprotein protein IMP4

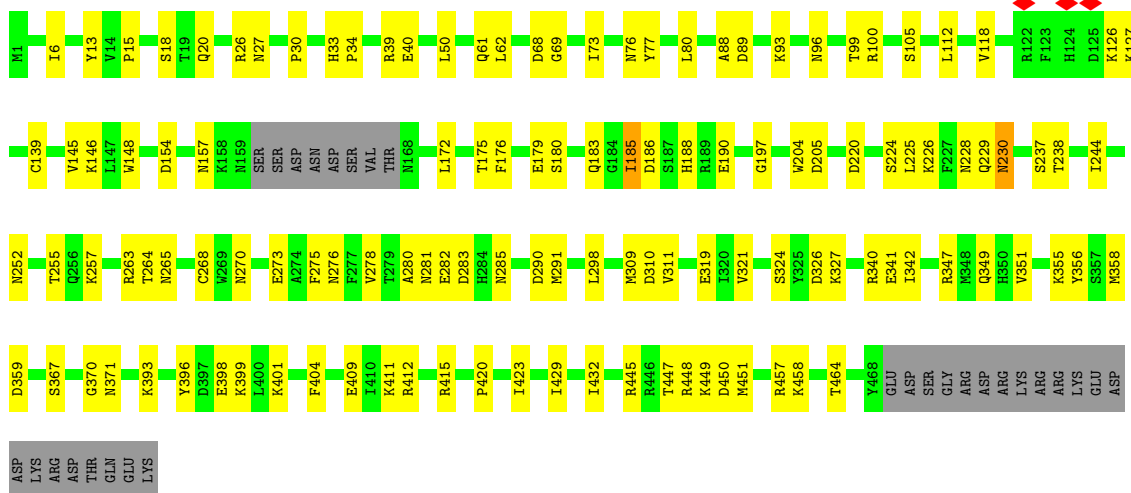


• Molecule 44: Something about silencing protein 10

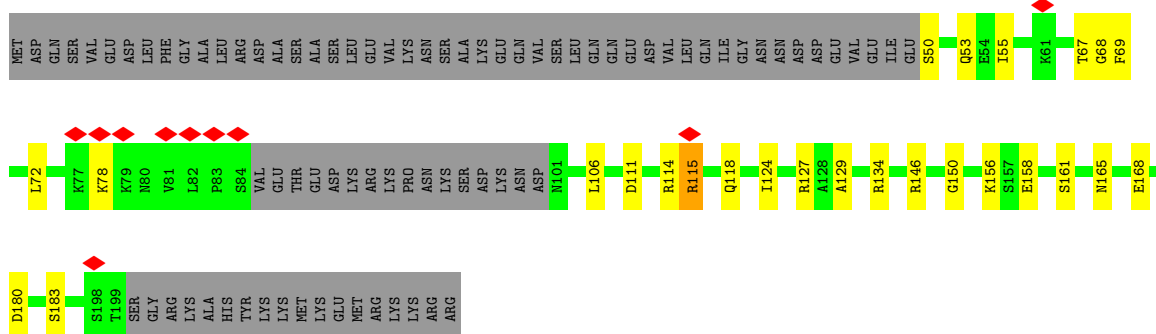




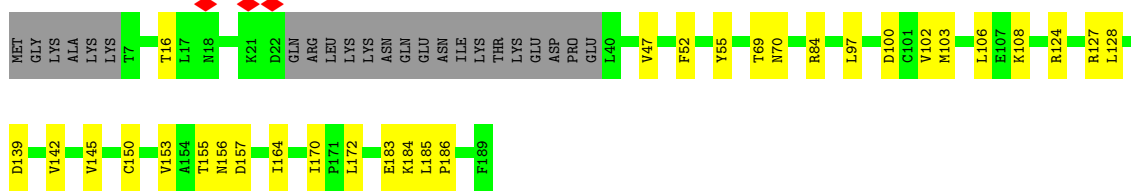
• Molecule 45: Protein SOF1



• Molecule 46: rRNA-processing protein FCF2



• Molecule 47: rRNA-processing protein FCF1

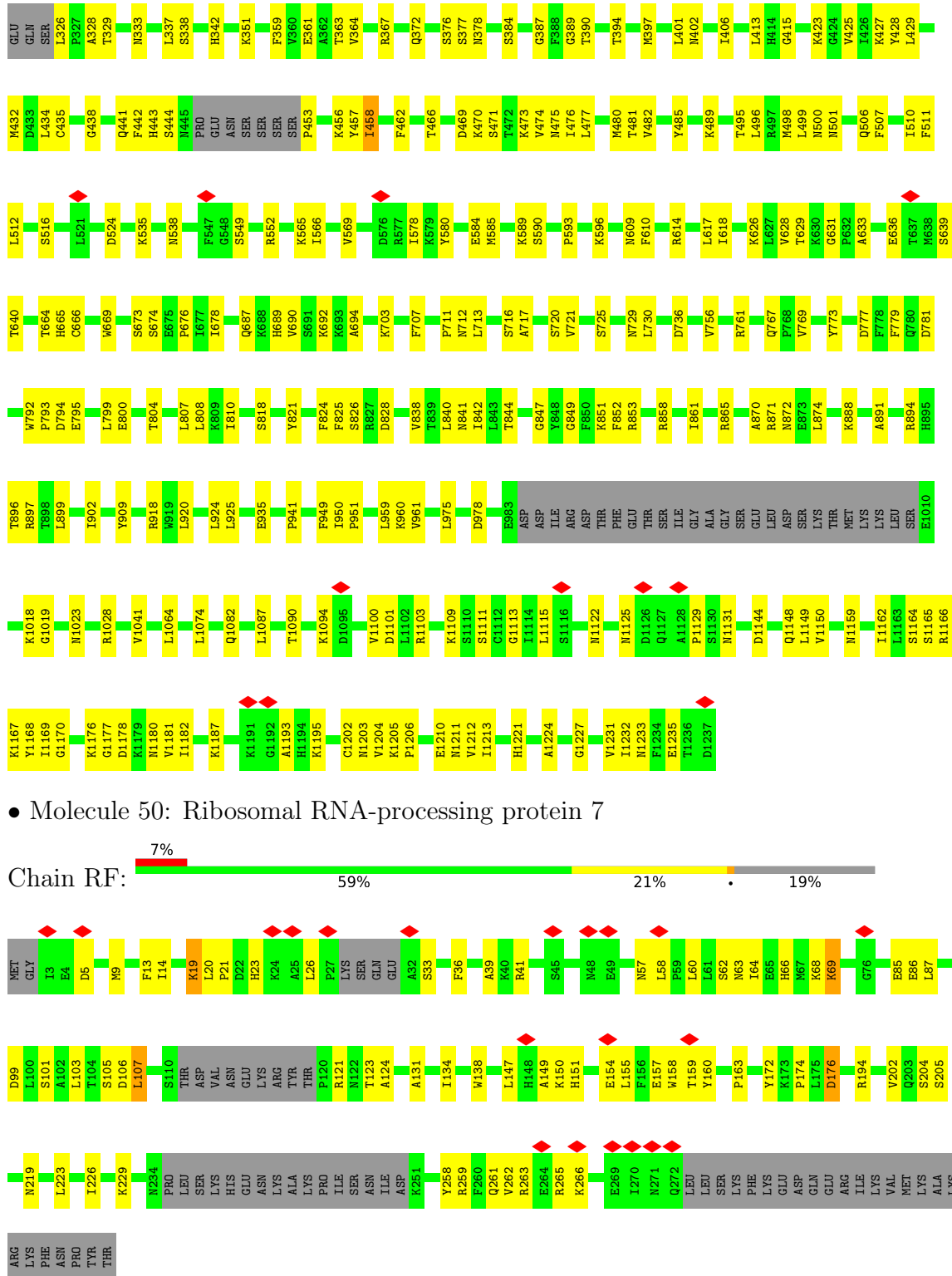


• Molecule 48: rRNA biogenesis protein RRP5

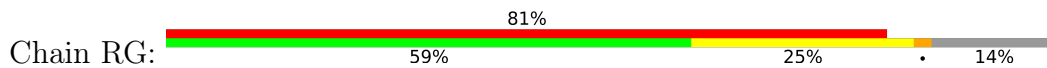


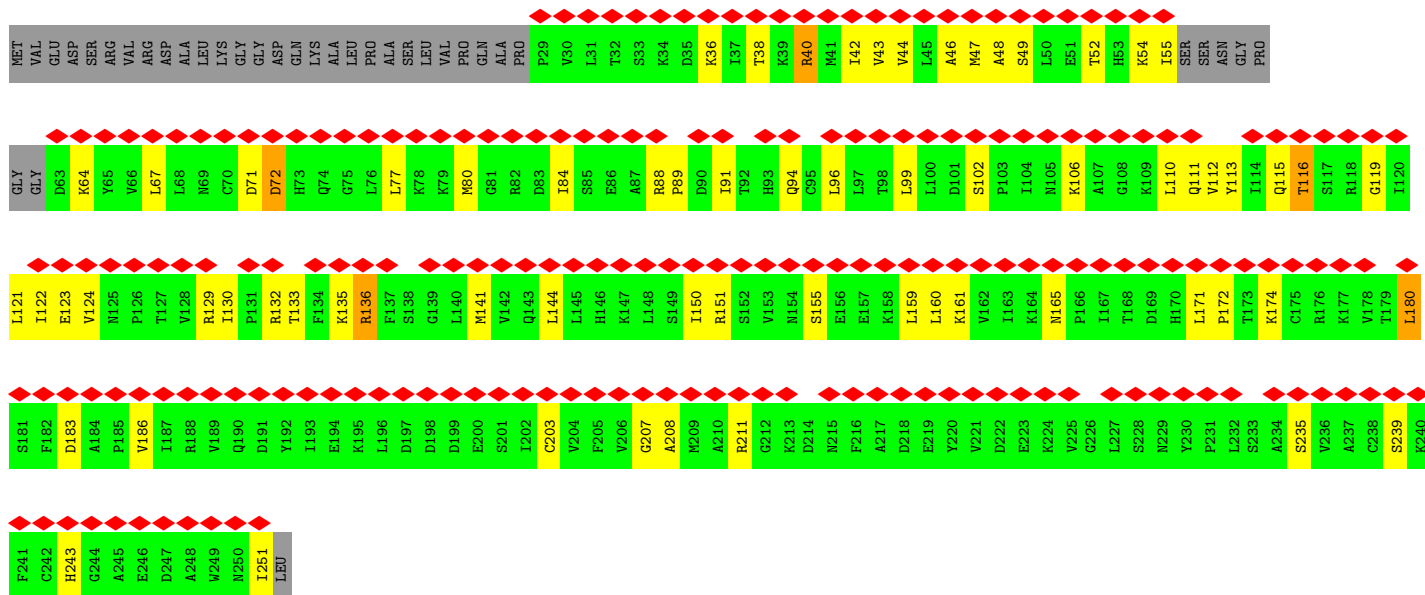




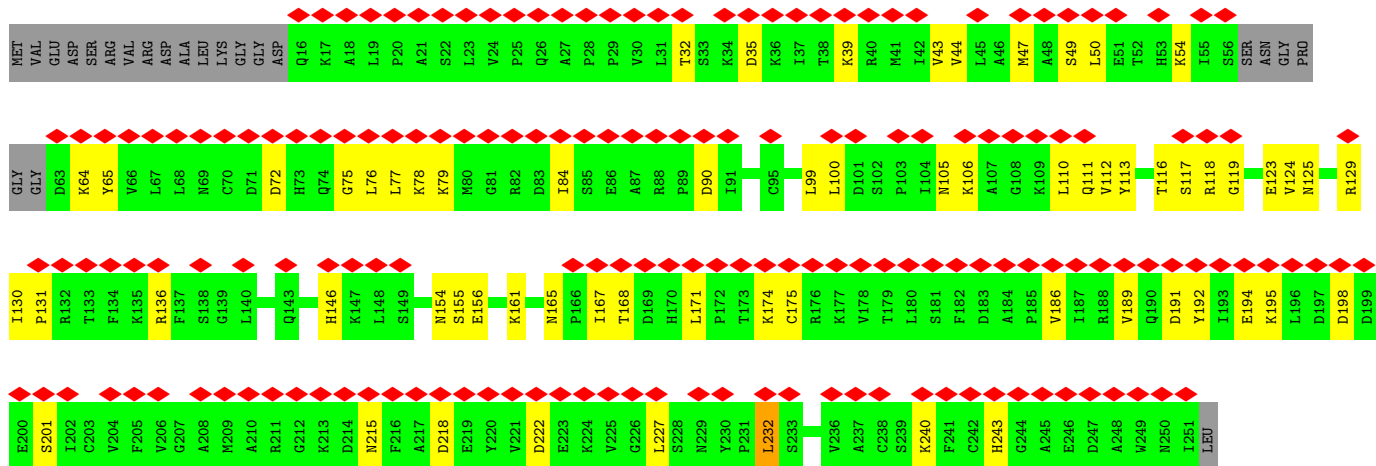


• Molecule 51: Ribosomal RNA small subunit methyltransferase NEP1

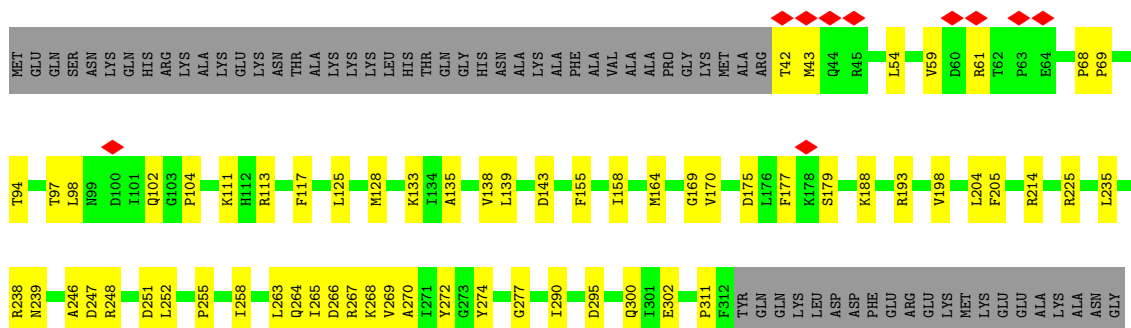


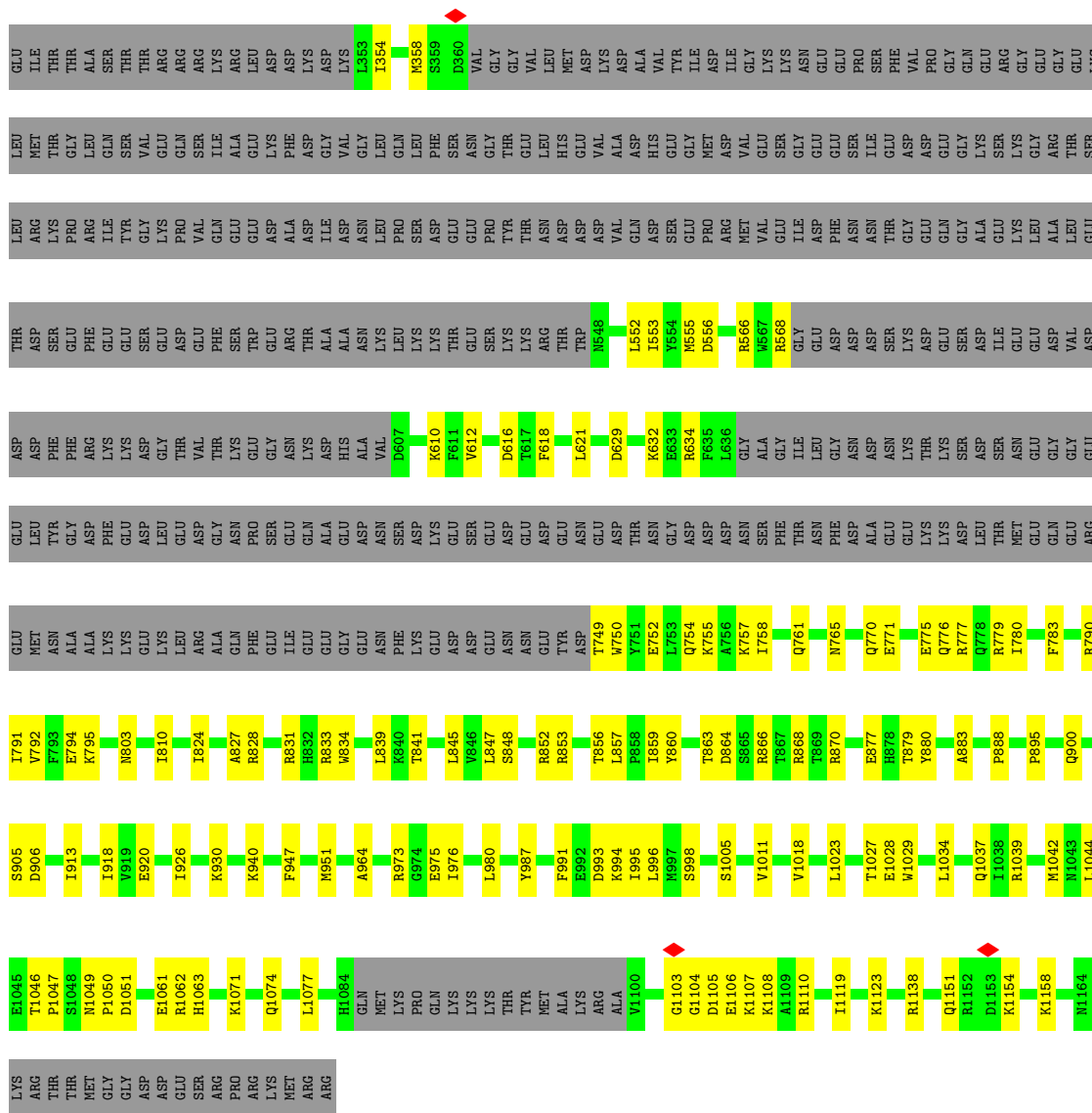


• Molecule 51: Ribosomal RNA small subunit methyltransferase NEP1

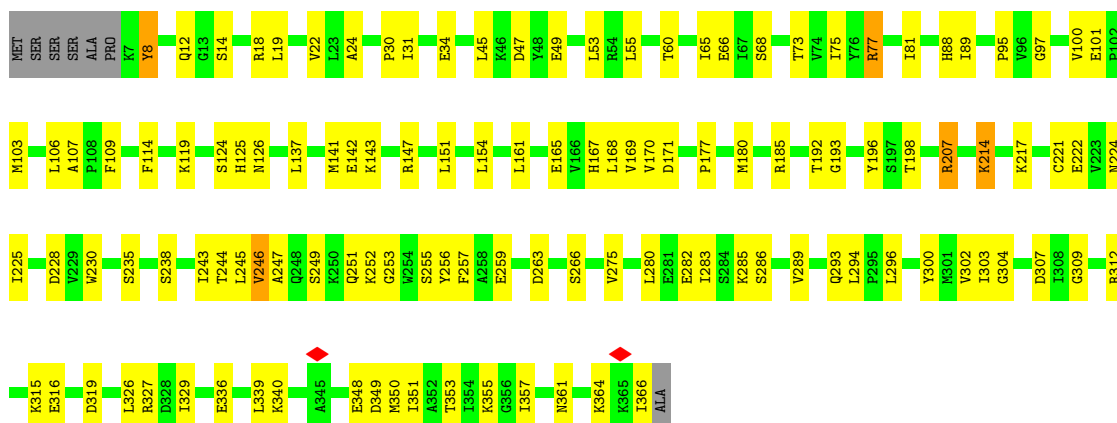


• Molecule 52: Ribosome biogenesis protein BMS1

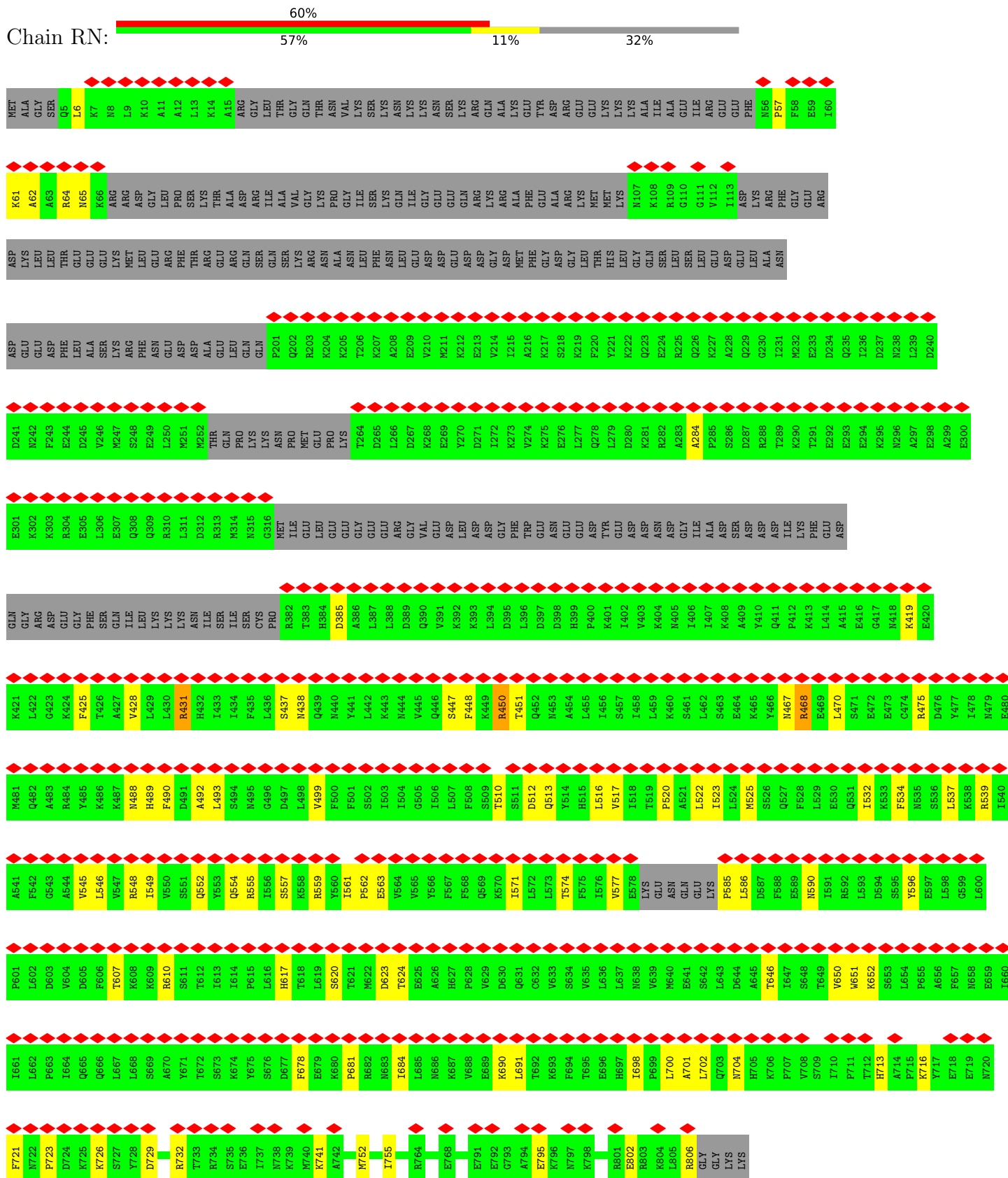




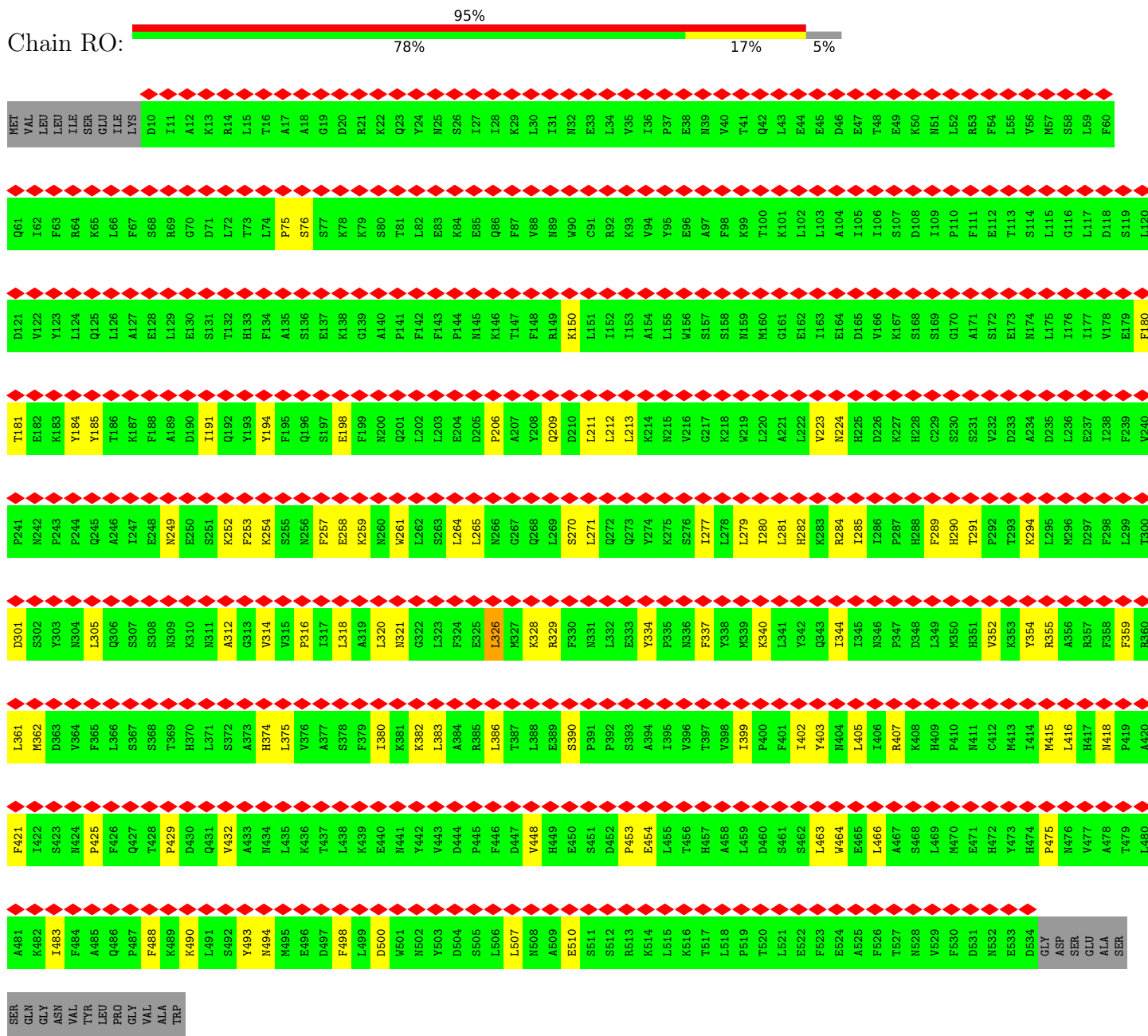
● Molecule 53: RNA 3'-terminal phosphate cyclase-like protein



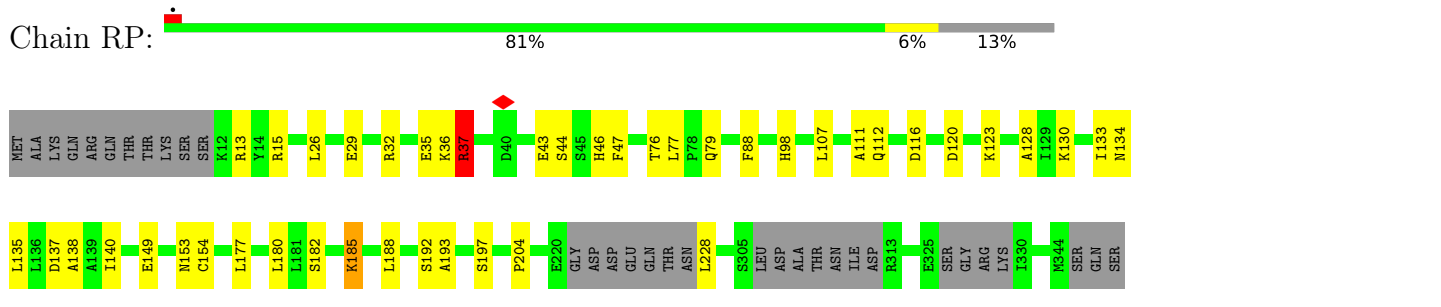
• Molecule 54: Nucleolar complex protein 14



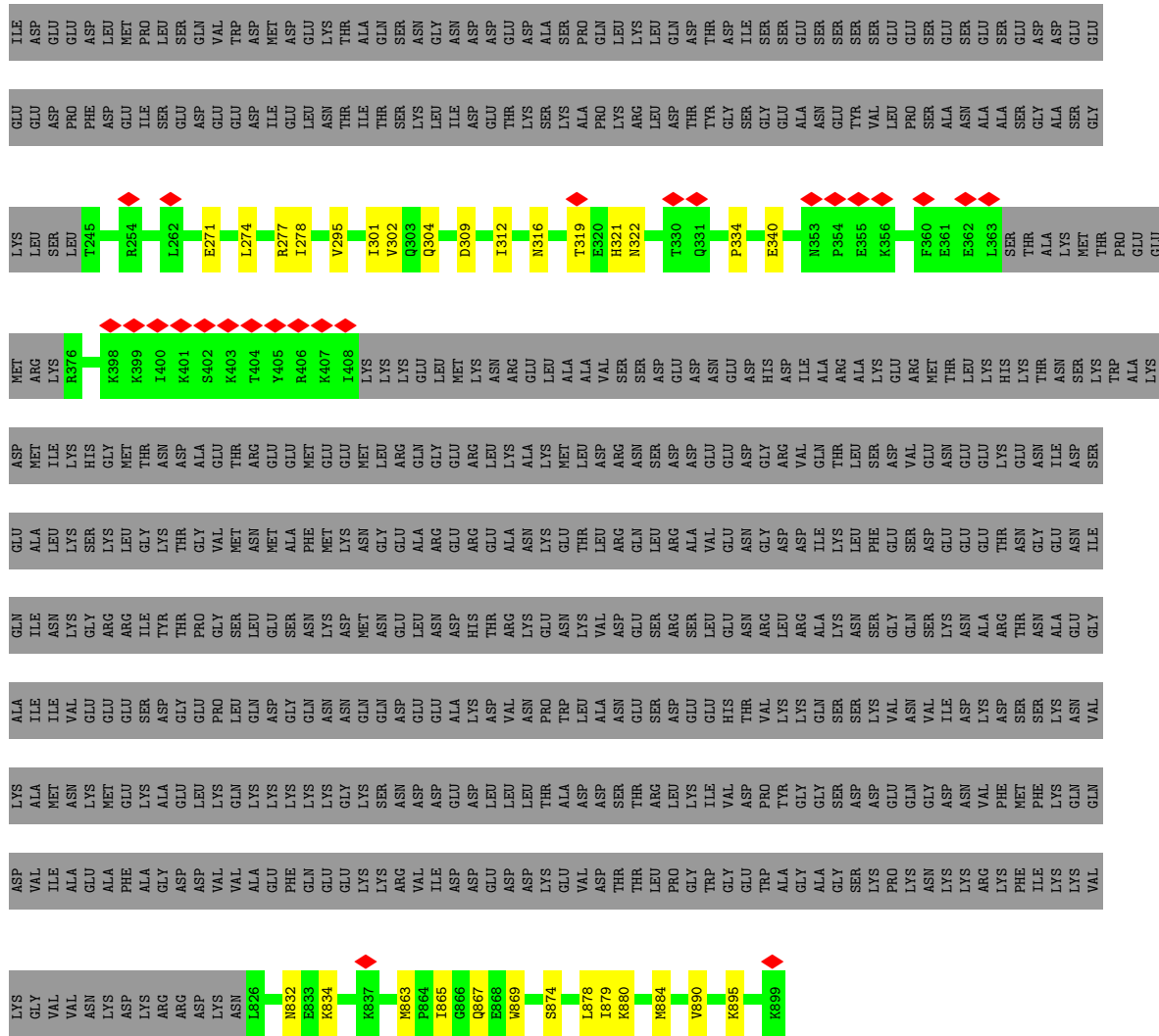
• Molecule 55: Nucleolar complex protein 4



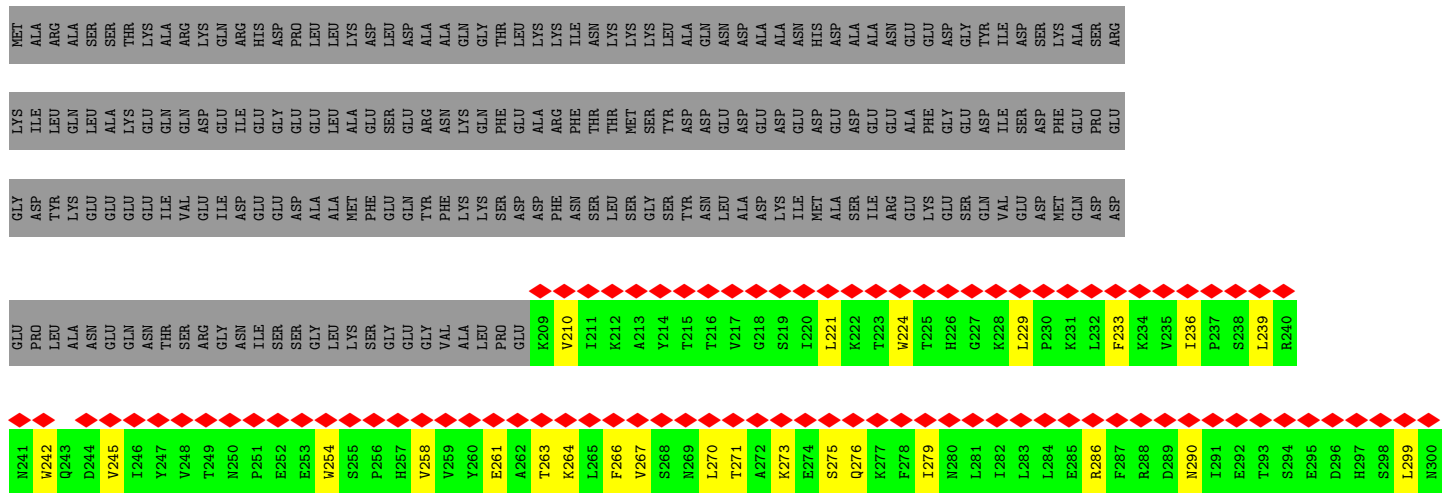
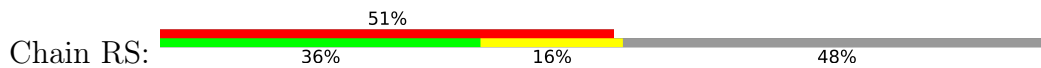
• Molecule 56: U3 small nucleolar RNA-associated protein 20



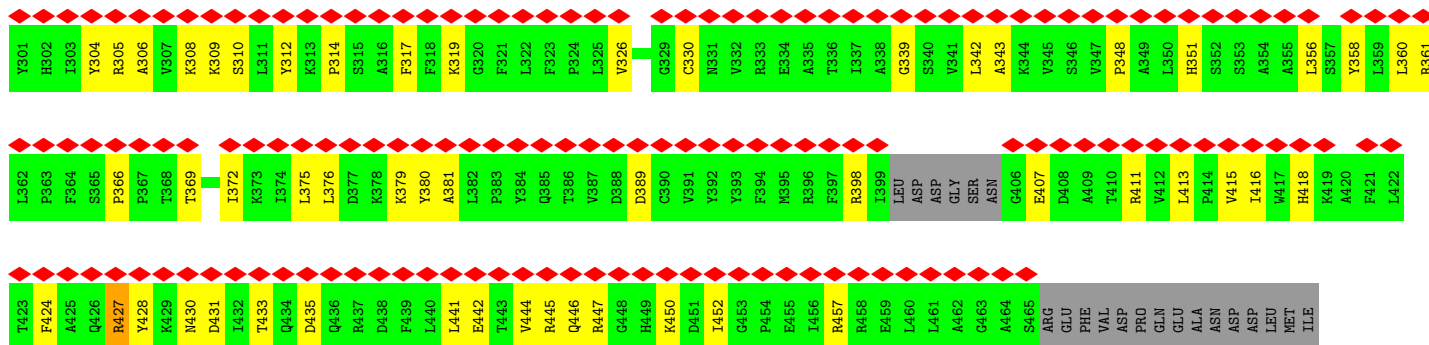




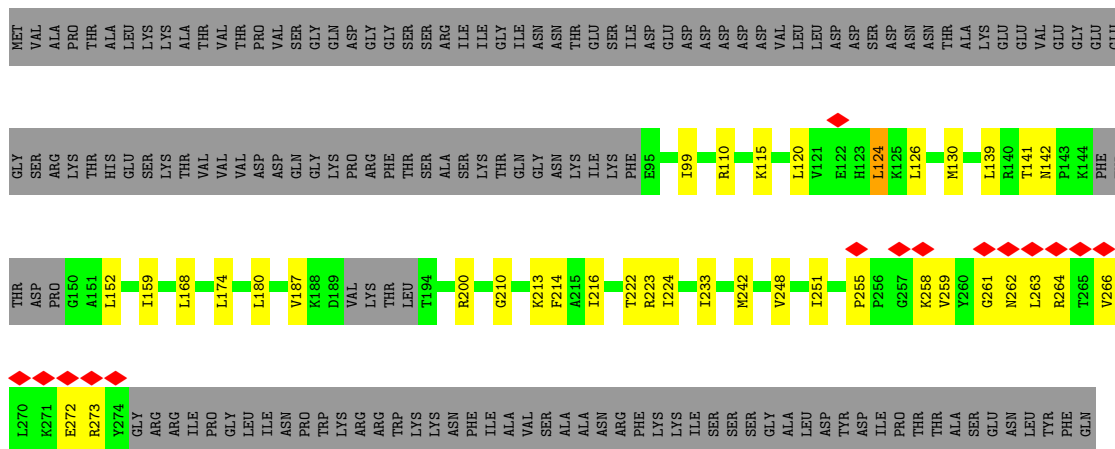
● Molecule 58: Essential nuclear protein 1



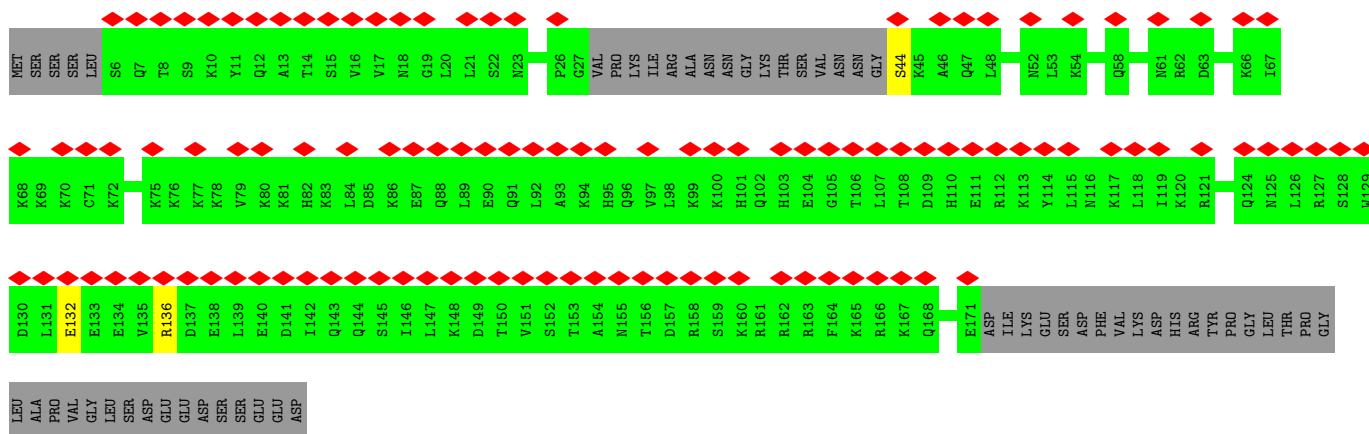
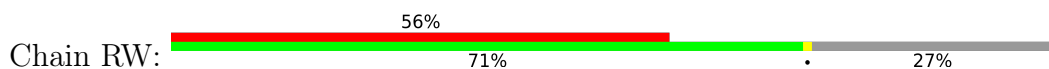




• Molecule 59: Pno1

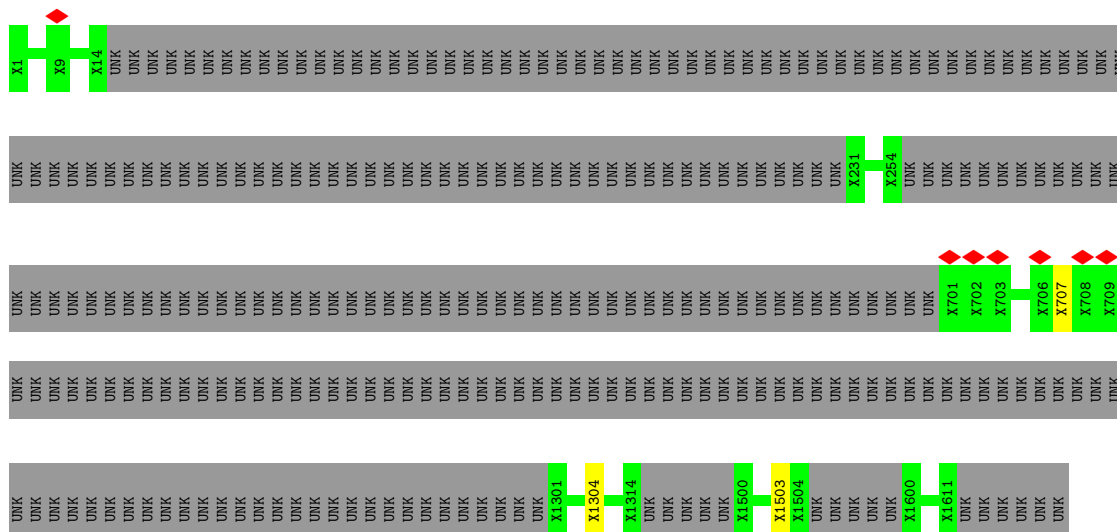


• Molecule 60: Regulator of rDNA transcription protein 14

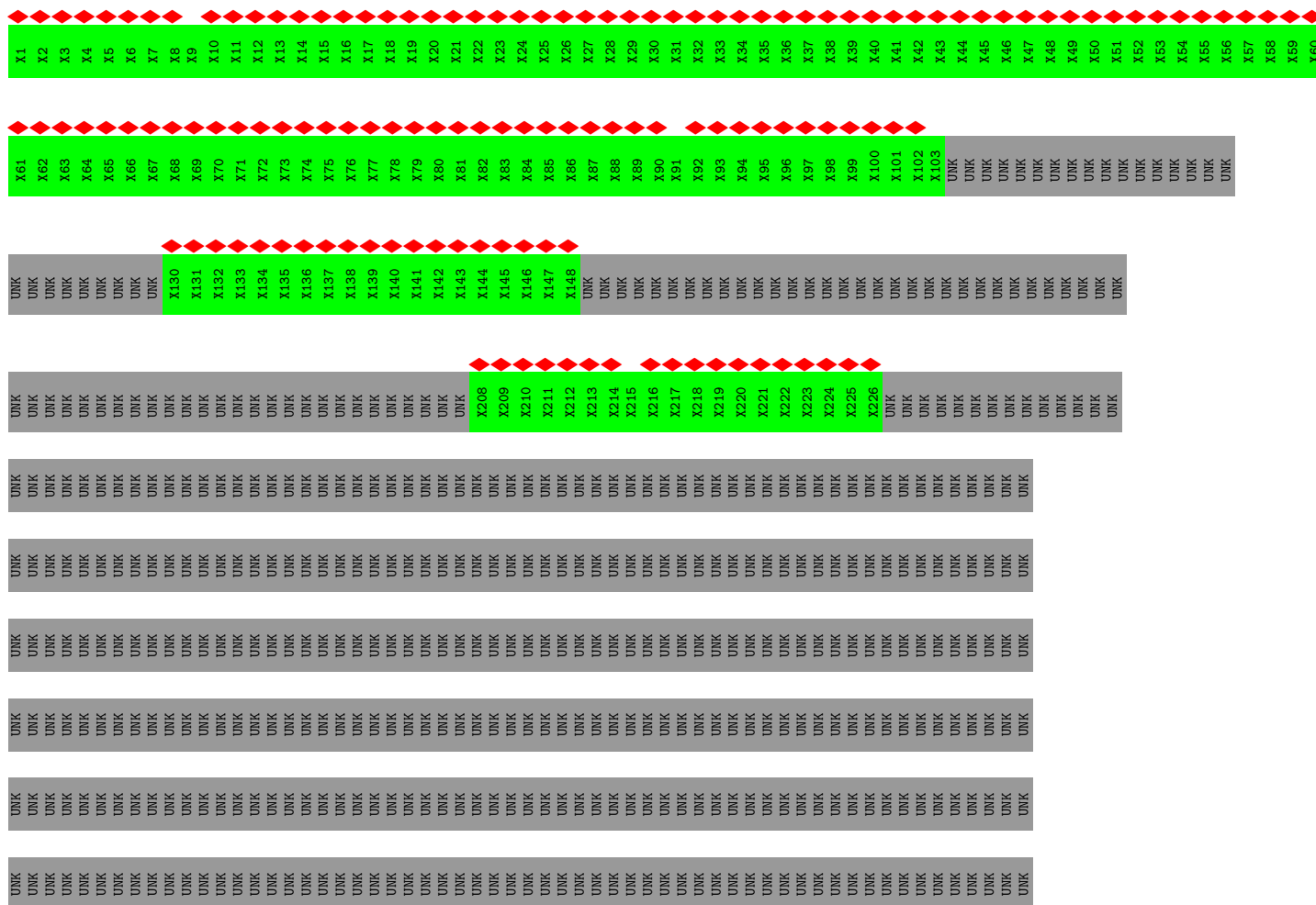


• Molecule 61: Unassigned helices 1

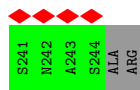




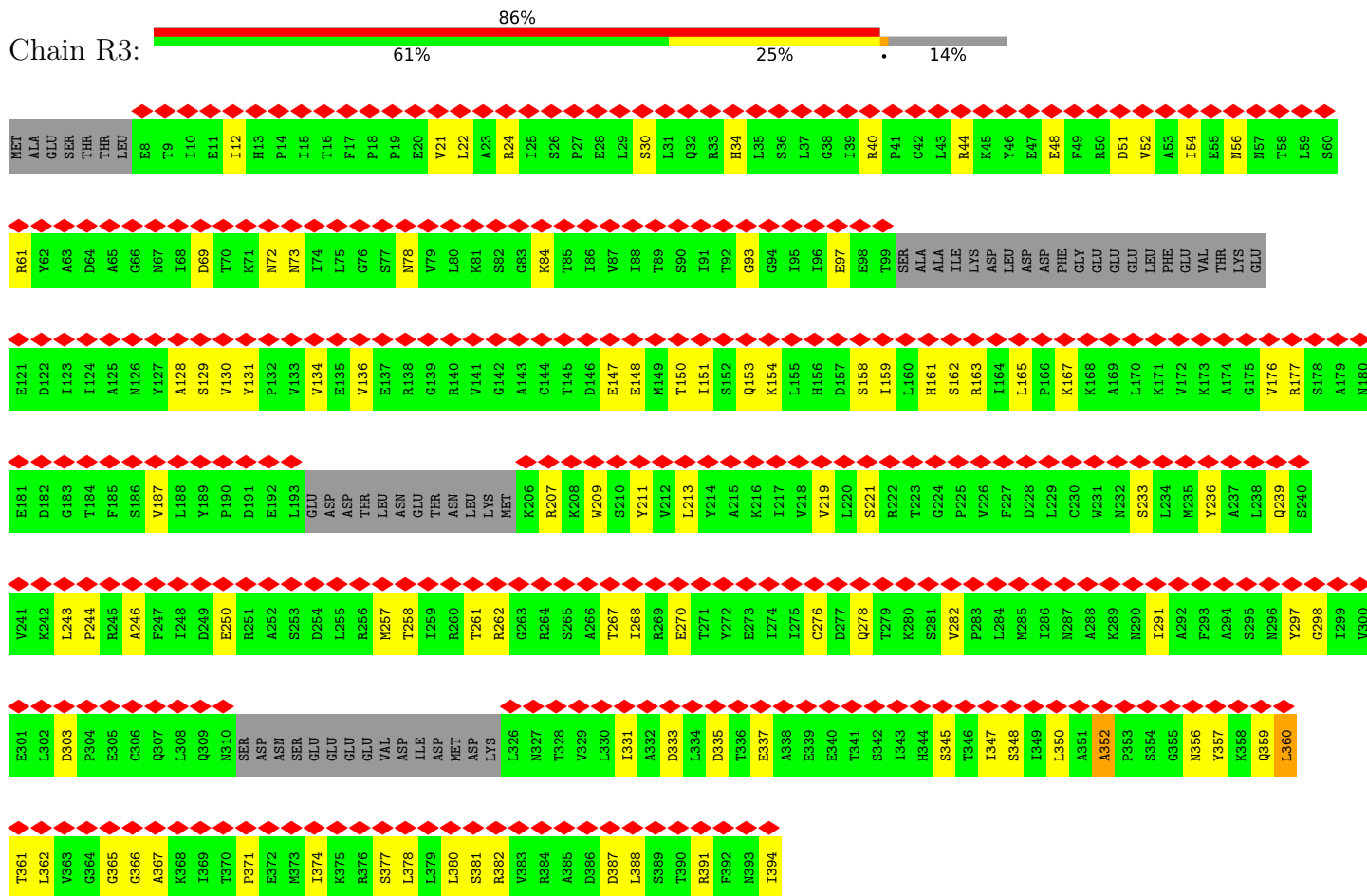
• Molecule 62: Unassigned helices 2



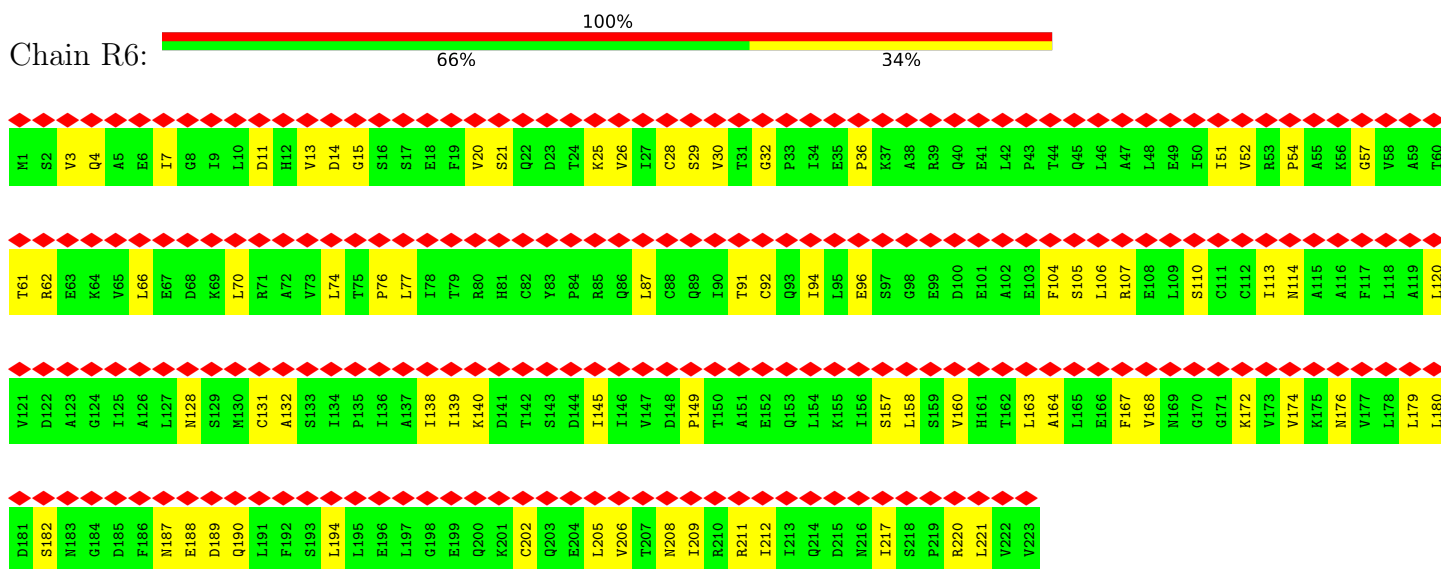




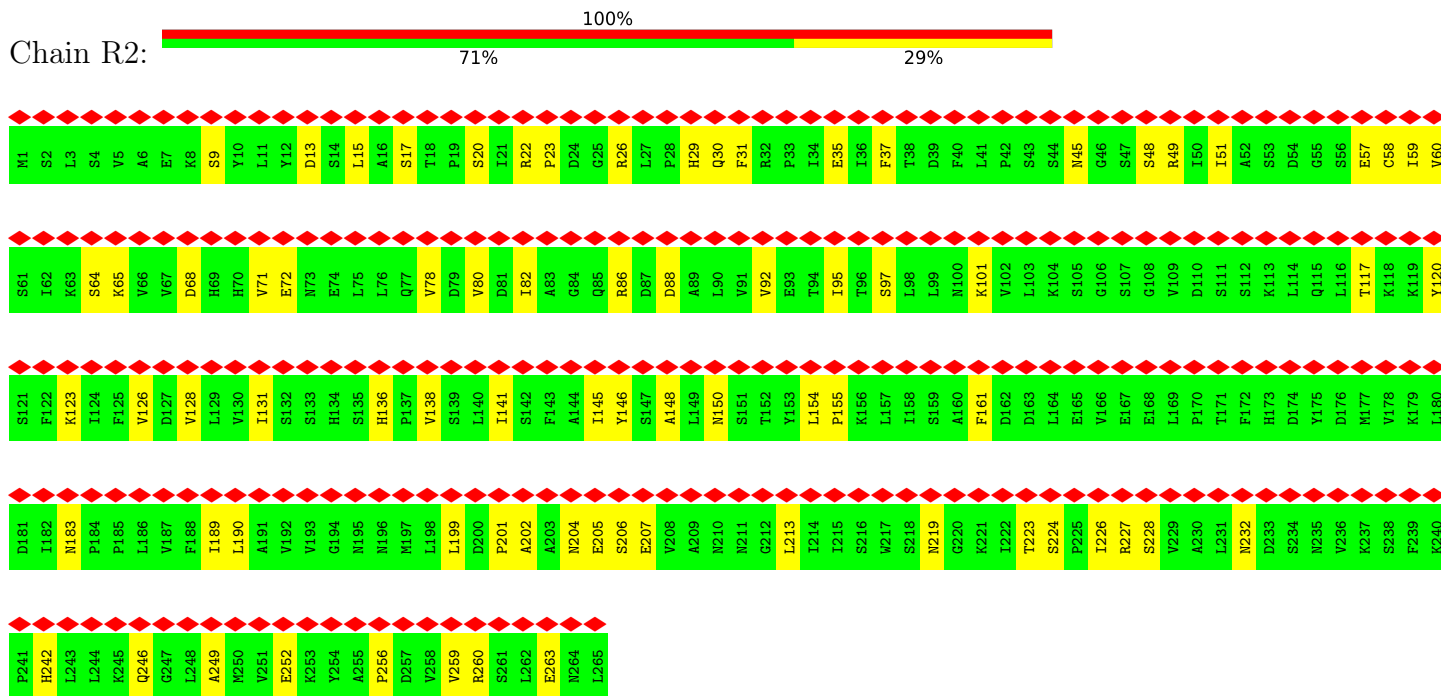
• Molecule 65: Exosome complex component RRP43



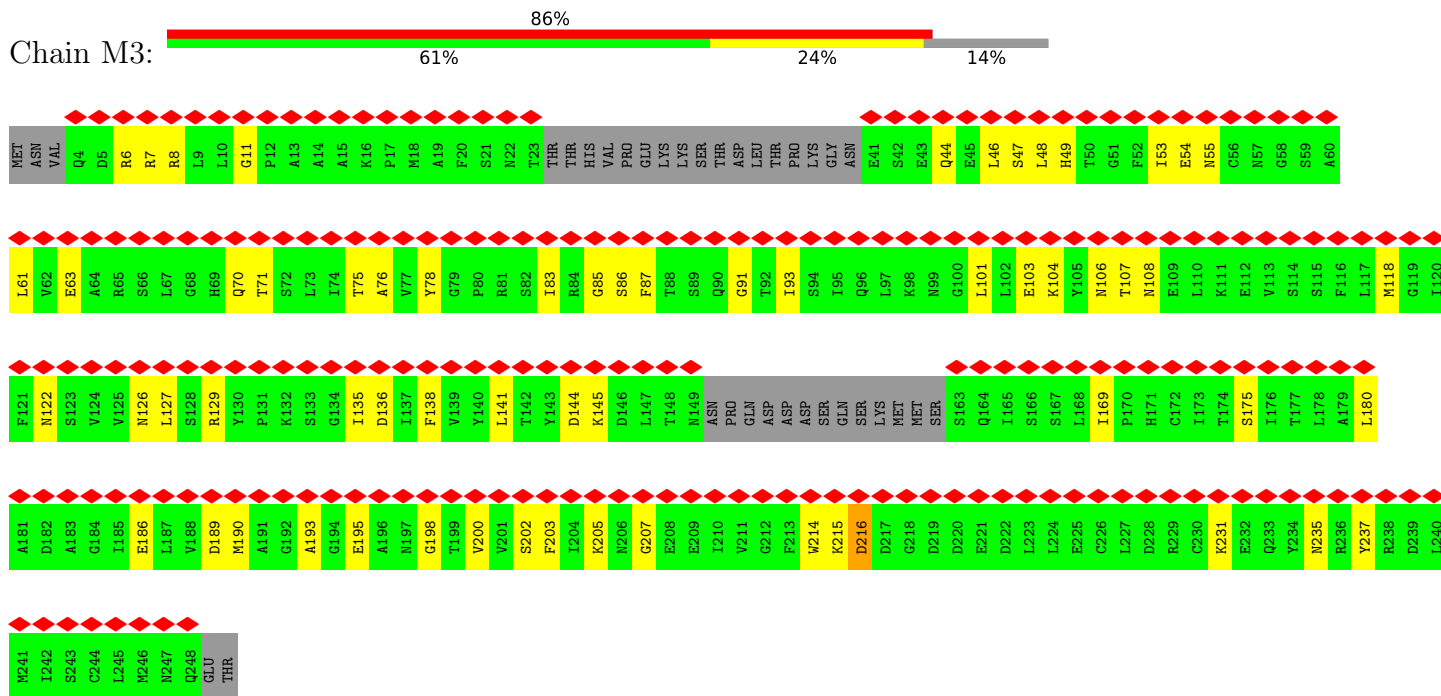
• Molecule 66: Exosome complex component RRP46



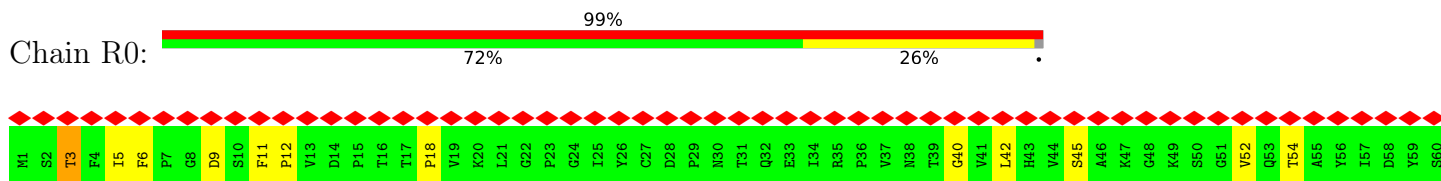
• Molecule 67: Exosome complex component RRP42



• Molecule 68: Exosome complex component MTR3

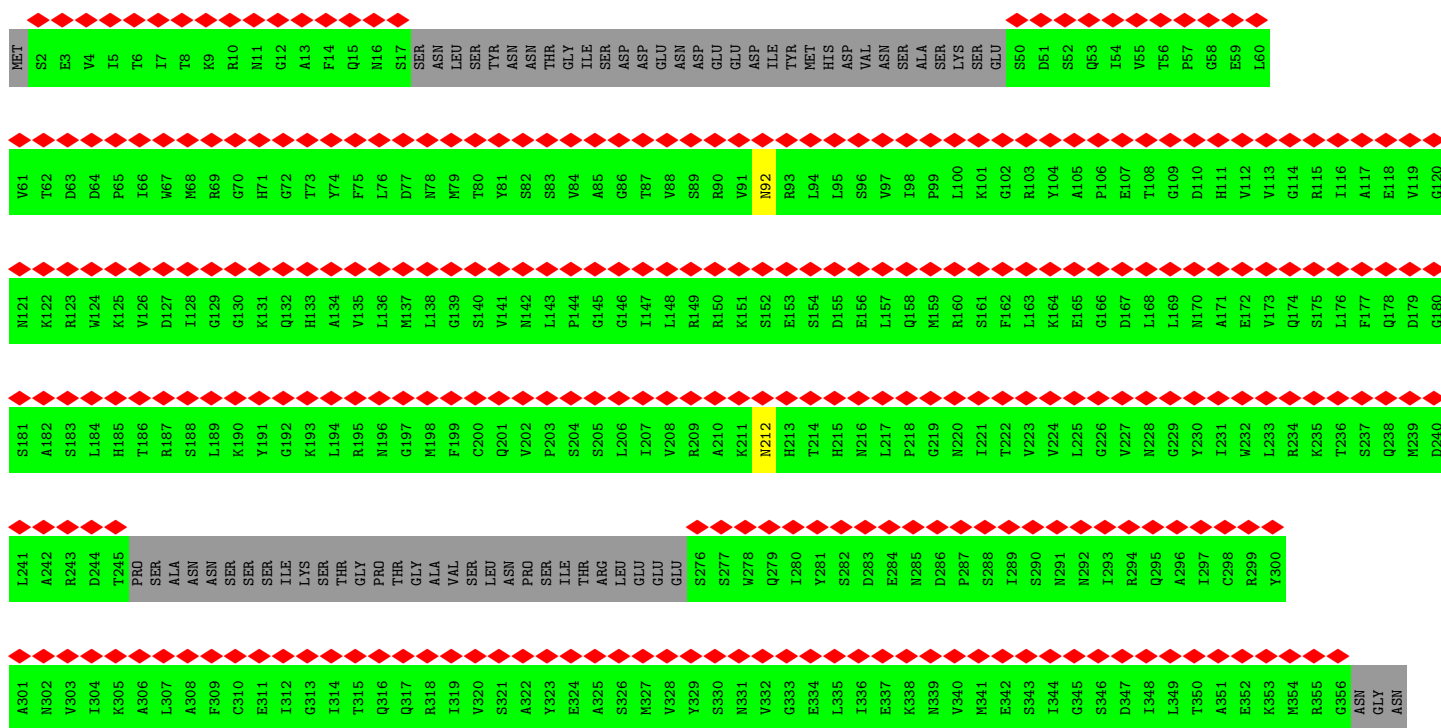
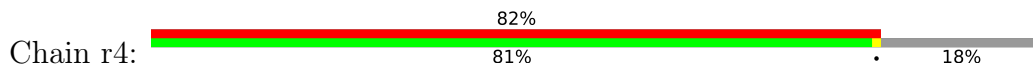


• Molecule 69: Exosome complex component RRP40

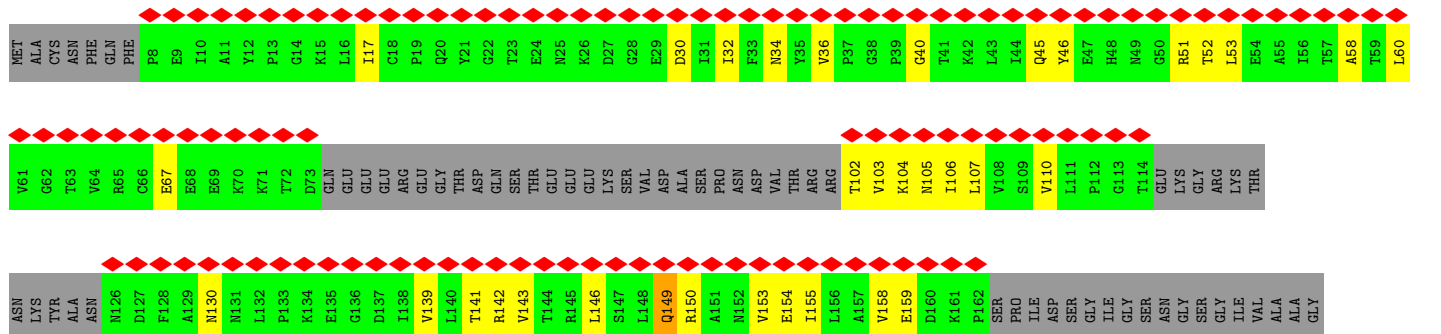
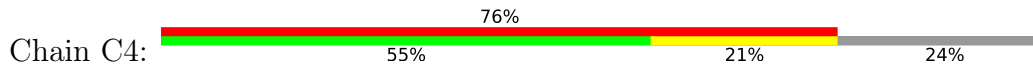




• Molecule 70: Exosome complex component RRP4



• Molecule 71: Exosome complex component CSL4



GLY	T241	ALA	A186	T187	F188	S189	V190	S191	Q192	A193	S194	S195	D196	L197	E198	E199	T200	F201	R202	G203	I204	I205	R206	S207	Q208	D209	V210	R211	S212	T213	D214	R215	D216	R217	V218	K219	V220	I221	E222	C223	F224	K225	P226	G227	D228	I229	V230	R231	A232	Q233	V234	L235	S236	L237	D238	G240
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T242	N243	Y244	L245	T246	A248	R249	N250	D251	L252	G253	V255	F256	A257	R258	A259	N261	G262	A263	G264	G265	L266	M267	Y268	A269	T270	D271	V272	Q273	M274	M275	T276	S277	P278	V279	T280	G281	C282	T283	E284	K285	R286	K287	C288	A289	K290	P291	PHE
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• Molecule 72: Exosome complex exonuclease DIS3



MET	R9	R10	K11	R12	L13	A14	D15	G16	L17	S18	V19	T20	Q21	K22	V23	F24	V25	R26	S27	R28	N29	G30	G31	A32	T33	K34	I35	V36	R37	E38	H39	Y40	L41	R42	D44	I45	P46	C47	L48	S49	R50	S51	C52	K54	C55	P56	Q57	I58	V59	L60
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P61	D62	A63	Q64	N65	E66	L67	P68	R69	F70	I71	L72	S73	D74	S75	P76	L77	E78	L79	S80	A81	P82	I83	G84	R85	H86	Y87	V88	V89	L90	D91	T92	N93	V94	V95	L96	Q97	A98	I99	D100	L101	L102	E103	N104	P105	M106	C107	F108	F109	D110	S111	I112	V113	P114	Q115	I116	V117	L118	D119	E120
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V121	R122	M123	K124	S125	Y126	P127	V128	Y129	T130	R131	L132	R133	T134	L135	C136	R137	D138	S139	D140	H141	K142	K143	R144	F145	I146	V147	F148	H149	N150	E151	F152	S153	E154	H155	T156	F157	V158	E159	R160	L161	P162	M163	E164	T165	I166	M167	D168	R169	N170	D171	R172	A173	I174	R175	K176	T177	C178	Q179	W180
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Y181	S182	E183	H184	L185	K186	P187	Y188	D189	I190	M191	V192	V193	L194	V195	T196	D197	R198	R199	L200	N201	H202	E203	A204	A205	G206	G207	L208	E208	V209	E210	S211	N212	I213	I214	T215	K216	S217	L218	V219	Q220	Y221	I222	E223	L224	L225	G226	N227	A228	D229	D230	I231	R232	D233	S234	I235	P236	Q237	MET	ASP	SER
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PHE	T249	F250	S251	D252	F253	T254	F255	P256	Y258	Y259	S260	A262	R263	V264	G266	G267	L268	K269	N270	G271	V272	Y274	Q275	I276	G277	N277	L278	Q279	L280	S281	E282	Y283	N284	F285	L286	E287	G288	S289	V290	S291	L292	P293	R294	F295	S296	K297	P298	V299	L300
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I301	V302	G303	Q304	K305	N306	L307	N308	R309	A310	F311	N312	G313	D314	Q315	V316	I317	V318	E319	L320	L321	Q322	S323	K324	E325	V326	K327	A328	SER	ILE	VAL	LEU	ASP	SER	GLU	HIS	PHE	ASP	VAL	ASN	ASP	ASN	PRO	ASP	ILE	GLU	ALA	GLY	ASP	ASP	ASP	ASN	ASN	GLU	SER	SER	SER
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ASN	THR	THR	V364	I365	S366	D367	K368	Q369	R370	R371	L372	L373	A374	K375	D376	A377	M378	I379	A380	Q381	R382	S383	K384	K385	I386	Q387	K447	R448	I449	V450	V451	S452	F453	Y454	I455	S456	W456	P457	R458	S399	W400	R401	Q402	Y403	Y404	G405	Q406	L407	A408	P409	S410	S411	V412	D413	P414	Q415	S416	S417	S418	T419	Q420
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M421	V422	F423	W424	L425	L426	M427	D428	K429	C430	L431	P432	K433	V434	R435	L436	R437	T438	R439	R440	A441	A442	E443	L444	L445	D446	K447	R448	I449	V450	V451	S452	F453	Y454	I455	S456	W456	P457	R458	S399	W400	R401	Q402	Y403	Y404	G405	Q406	L407	A408	P409	S410	S411	V412	D413	P414	Q415	S416	S417	S418	T419	Q420
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T481	F482	A483	L484	L485	L486	E487	H488	D489	V490	E491	Y492	R493	P494	F495	S496	K497	K498	V499	L500	E501	C502	L503	P504	A505	E506	G507	H508	D509	W510	K511	A512	P513	T514	A515	L516	D517	D518	P519	E520	A521	S522	S523	K524	D525	P526	L527	L528	T529	K530	R531	K532	D533	L534	R535	L536	D537	L538	I539	C540
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S541	I542	D543	P544	P545	G546	C547	V548	D549	I550	D551	D552	A553	L554	H555	A556	K557	K558	L559	P560	N561	G562	M563	W564	E565	V566	G567	V568	H569	I570	A571	D572	V573	T574	H575	F576	V577	D578	P579	G580	T581	A582	L583	D584	A585	E586	G587	S588	A589	R590	G591	T592	S593	V594	F595	L596	V597	D598	K599	R600
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I601	D602	M603	L604	P605	M606	L607	L608	G609	T610	D611	L612	C613	S614	L615	K616	Y617	Y618	V619	D620	R621	F622	A623	F624	S625	V626	I627	W628	E629	L630	D631	D632	S633	A634	M635	I636	V637	M638	V639	N640	F641	M642	K643	S644	V645	I646	R647	S648	R649	E650	A651	F652	S653	Y654	E655	Q656	A657	L658	L659	R660
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E301	ASN	F302	GLN	A303	ILE	E304	GLY	K305	ASP	I306	PRO	C307	ASN	K308	THR	I309	THR	H310	ASP	S311	SER	Q312	GLY	P313	LYS	C314	GLY	H315	GLN	I316	TYR	V317	LYS	Y318	GLY	T319	GLY	N320	ALA	F321	LYS	P322	ASP	P323	ALA	T324	ALA	P325	LYS	G392	ASP	L326	ASP	Q327	LYS	I394	LYS	Y395	LYS	K396	LYS	L330	ASP	F331	ASP	P332	LYS	A333	M400	H334	I401	G335	LYS	D336	ASP	G337	K403	I338	K404	Y339	K405	L340	Y406	V341	N407	P408	P409	V342	LYS	D343	I410	E344	V411	K345	F412	S346	S413	T347	F414	F348	S415	R349	K416	E350	R417	E351	R418	F352	C419	F353	LYS	K355	A356	M357	A358	S359	I360
S361	ASN	L422	L483	L424	L485	M425	M426	S427	K428	L429	D430	F431	M432	S433	D434	D435	E436	K437	F438	E439	A439	L440	T441	K442	I443	F444	N445	N446	A447	I448	A449	L450	L451	P452	E453	L454	D455	R456	E457	L458	P459	Q460	I461	K462	H463	I464	L465	F412	S413	T347	F414	F348	S415	R349	K416	E350	R417	E351	R418	F352	C419	F353	LYS	K355	A356	M357	A358	S359	I360																																																
P481	I482	L483	K484	E485	V486	I487	E488	I489	L490	F491	Q492	S493	G494	F495	L496	K497	V498	L499	F500	A501	T502	E503	T504	F505	S506	I507	G508	L509	N510	M511	P512	A513	K514	T515	V516	V517	F518	T519	S520	R521	V522	K523	M524	D525	G526	Q527	Q528	F529	R530	M531	V532	S533	G534	H475	H476	S477	G478	L479	L480																																																										
S541	G542	R543	A544	G545	R546	R547	G548	L549	D550	F551	R552	G553	I554	V555	I556	M557	M558	I559	D560	E561	K562	M563	E564	P565	Q566	V567	A568	K569	G570	M571	V572	K573	G574	Q575	A576	D577	L579	D580	S581	F583	H584	L585	G586	Y887	N588	M589	L591	N592	L593	M594	R595	V596	E597	G598	I599	S600																																																													
P601	F602	F603	M604	L605	E606	H607	S608	F609	F610	Q611	F612	G613	Q614	V615	I616	S617	V618	P619	V620	M621	E622	K623	LYS	LEU	ALA	GLU	GLU	LYS	LYS	ASP	PHE	ASP	GLY	ILE	VAL	GLU	VAL	GLU	ASP	GLU	GLU	ASN	VAL	GLU	LYS	ILE	GLU	LYS	GLN	ALA	ILE	LYS	GLY	TYR	ARG	GLU	ASP	VAL																																																											
ARG	GLN	VAL	VAL	THR	H666	P667	A668	N669	A670	L671	S672	F673	L674	Q675	F676	G677	R678	L679	V680	E681	I682	V684	N685	G686	K687	D688	N689	V690	G691	M692	G693	A694	V695	V696	D697	F698	A699	K700	R701	I702	N703	K704	R705	N706	P707	S708	A709	V710	Y711	T712	D713	H714	E715	S716	Y717	I718	V719	N720																																																											
V721	V722	V723	N724	T725	M726	Y727	I728	D729	S730	P731	V732	N733	L734	L735	K736	P737	F738	N739	P740	T741	L742	P743	E744	G745	I746	R747	F748	A749	E750	E751	G752	E753	K754	S755	I756	C757	A758	V759	I760	P761	I762	T763	L764	D765	S766	I767	K768	S769	I770	G771	N772	L773	R774	L775	Y776	N777	K778	D780																																																											
I781	R782	A783	S784	G785	Q786	K787	E788	T789	V790	G791	K792	S793	L794	R795	E796	V797	N798	R799	R800	F801	D802	G803	G804	I805	P806	V807	L808	D809	P810	M811	K812	M813	H814	K815	I816	GLU	ASP	GLU	ASP	PHE	LEU	LYS	LEU	MET	LYS	LYS	ILE	ASP	VAL	LEU	ASN	THR	LYS	GLU	C895	T896	P897	M898	D899	I900																																																									
THR	ASN	SER	MET	ARG	LEU	GLU	GLU	LEU	TYR	GLY	LYS	TYR	ASP	HIS	ASP	LEU	HIS	GLU	ASP	K863	K864	Q865	L866	K867	K868	K869	I870	S871	E872	S873	A874	A875	V876	I877	R878	L879	D880	D881	L882	R883	R884	R885	K886	R887	V888	L889	R890	R891	L892	G893	F894	C895	T896	P897	M898	D899	I900																																																												
I901	E902	L903	K904	G905	R906	V907	E908	C909	E910	I911	S912	S913	G914	D915	E916	L917	L918	L919	T920	E921	I922	I923	F924	N925	G926	N927	F928	N929	E930	L931	K932	F933	R934	Q935	E936	A937	A938	L939	L940	S941	C942	F943	A944	F945	C1005	A1006	G1007	A1008	T1009	F1010	E951	A952	P953	R954	L955	K956	P957	E958	L959	A960																																																									
E961	P962	L963	K964	A965	M966	R967	E968	I969	A970	A971	K972	I973	A974	K975	I976	M977	K978	D979	S980	K981	I982	E983	V984	V985	I986	K987	D988	Y989	E990	E991	S992	F993	R994	H995	E996	L997	M998	E999	V1000	V1001	Y1002	E1003	V1004	C1005	A1006	G1007	A1008	T1009	F1010	E951	A952	P953	R954	L955	K956	P957	E958	L959	A960																																																										
E1021	G1022	S1023	L1024	I1025	R1026	M1027	F1028	R1029	A1030	R1031	L1032	E1033	L1034	V1035	K1036	E1037	L1038	V1039	D1040	V1041	A1042	M1043	T1044	I1045	G1046	M1047	S1048	L1049	L1050	K1051	E1052	K1053	M1054	E1055	A1056	V1057	L1058	K1059	L1060	I1061	H1062	R1063	D1064	I1065	V1066	S1067	A1068	G1069	L1070	L1071	TYR	LEU																																																																	

• Molecule 76: M-phase phosphoprotein 6 homolog



M1	S2	A3	M4	N5	G6	V7	T8	G9	K10	L11	SER	SER	ARG	ARG	VAL	MET	ASN	ASN	PHE	PHE	LYS	PHE	GLY	GLY	THR	ASP	ASP	GLU	GLU	SER	SER	ASN	SER	ASN	PRO	PRO	ILE	ILE	GLU	GLN	LYS	GLY	LYS	LEU	PHE	GLY	LEU	ASP	SER	ALA											
TRP	ASP	LEU	ASN	SER	TYR	LYS	ASP	ASP	LEU	LYS	LYS	ILE	SER	GLY	GLY	LYS	LYS	LYS	VAL	VAL	ARG	ARG	TYR	LYS	LYS	ARG	P90	N91	L92	I93	I94	S95	N96	V97	G98	Y99	S100	E101	L102	R103	K104	P105	E106	G107	V108	I109	S110	G111	R112	K113	T114	F115	G116	D117	N118	SER	ASP				
ASP	SER	GLY	ASN	SER	LYS	ARG	LYS	PHE	ASP	GLU	GLY	GLN	ASN	GLU	GLU	GLU	LYS	ARG	ASP	VAL	ALA	LYS	ASP	VAL	LYS	GLU	PHE	THR	THR	GLY	SER	GLN	ASP	ASP	GLY	GLU	GLU	ASP	GLU	TYR	ASP	LEU	ASP	LYS	LEU	PHE	LYS	ASP	SER	ILE	LYS	LYS	LYS	THR	ASN	HIS	ASN	GLY	LYS	ASN	LYS
ASN	ARG	ASN	SER	LYS	LYS																																																								

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	597.632, 597.632, 597.632	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, ZN

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	3A	0.66	0/5532	1.21	32/8585 (0.4%)
2	5A	0.52	0/3643	1.20	23/5663 (0.4%)
3	SA	0.65	0/29737	1.18	205/46285 (0.4%)
4	SC	0.46	0/1874	0.71	3/2512 (0.1%)
5	SF	0.41	0/1969	0.70	3/2661 (0.1%)
6	SG	0.44	0/1690	0.63	0/2285
7	SH	0.31	0/1477	0.58	1/1977 (0.1%)
8	SI	0.41	0/1330	0.71	1/1792 (0.1%)
9	SJ	0.31	0/1124	0.61	0/1510
10	SK	0.51	0/1410	0.66	2/1888 (0.1%)
11	SM	0.31	0/1139	0.57	0/1535
12	SO	0.44	0/1109	0.64	0/1495
13	SP	0.42	0/879	0.63	0/1186
14	SR	0.53	0/990	0.69	1/1335 (0.1%)
15	SX	0.49	0/1020	0.66	0/1371
16	SY	0.42	0/819	0.60	0/1093
17	SZ	0.52	0/1000	0.65	0/1334
18	Sc	0.45	0/613	0.73	1/828 (0.1%)
19	Sd	0.49	0/499	0.71	1/670 (0.1%)
20	3B	0.56	0/1901	0.66	1/2567 (0.0%)
20	3C	0.36	0/1796	0.63	1/2424 (0.0%)
21	3D	0.45	0/3020	0.66	4/4066 (0.1%)
22	3E	0.38	0/3072	0.61	2/4169 (0.0%)
23	3F	0.50	0/3569	0.67	0/4806
24	3G	0.40	0/928	0.72	0/1262
24	3H	0.53	0/928	0.68	1/1262 (0.1%)
25	A4	0.36	0/5338	0.64	1/7230 (0.0%)
26	A5	0.45	0/4021	0.63	1/5462 (0.0%)
27	A8	0.27	0/3328	0.60	0/4565
28	A9	0.27	0/951	0.68	2/1287 (0.2%)
29	AE	0.34	0/10050	0.54	1/13739 (0.0%)
30	AF	0.32	0/3885	0.61	2/5261 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	AG	0.34	0/6699	0.64	5/9077 (0.1%)
32	B1	0.56	0/6570	0.67	1/8892 (0.0%)
33	B2	0.42	0/6628	0.67	1/8954 (0.0%)
34	B3	0.37	0/6014	0.71	4/8137 (0.0%)
35	B8	0.43	0/3848	0.65	2/5218 (0.0%)
36	BE	0.55	0/6606	0.66	1/8935 (0.0%)
37	B6	0.45	0/2849	0.56	0/3853
38	5B	0.26	0/499	0.62	0/659
39	5C	0.53	0/3690	0.65	0/4991
40	5D	0.33	0/1757	0.57	0/2320
41	5E	0.40	0/1580	0.67	2/2115 (0.1%)
42	5F	0.50	0/1559	0.66	1/2097 (0.0%)
43	5G	0.51	0/1768	0.66	0/2392
44	5H	0.45	0/601	0.63	1/789 (0.1%)
45	5I	0.64	0/3835	0.67	2/5162 (0.0%)
46	5J	0.35	0/1147	0.57	0/1531
47	5K	0.51	0/1346	0.63	0/1812
48	RD	0.31	0/2454	0.59	0/3310
49	RE	0.37	0/9015	0.63	7/12195 (0.1%)
50	RF	0.37	0/2004	0.64	2/2697 (0.1%)
51	RG	0.29	0/1727	0.63	1/2329 (0.0%)
51	RH	0.28	0/1828	0.61	0/2470
52	RJ	0.45	0/6067	0.62	2/8170 (0.0%)
53	RK	0.41	0/2832	0.63	0/3825
54	RN	0.30	0/4146	0.58	0/5604
55	RO	0.29	0/3849	0.60	1/5261 (0.0%)
56	RP	0.31	0/12777	0.51	4/17558 (0.0%)
57	RQ	0.44	0/1682	0.60	0/2286
58	RS	0.34	0/2104	0.70	2/2854 (0.1%)
59	RT	0.33	0/1379	0.62	0/1853
60	RW	0.23	0/745	0.38	0/1038
63	R5	0.57	0/2340	0.64	1/3161 (0.0%)
64	R1	0.54	0/1910	0.68	0/2579
65	R3	0.50	0/2628	0.69	2/3569 (0.1%)
66	R6	0.54	0/1714	0.70	0/2328
67	R2	0.51	0/2069	0.69	0/2817
68	M3	0.53	0/1661	0.65	0/2243
69	R0	0.55	0/1828	0.69	0/2486
70	r4	0.52	0/2269	0.66	0/3066
71	C4	0.48	0/1676	0.66	0/2277
72	R4	0.42	0/7575	0.61	3/10290 (0.0%)
73	r6	0.47	0/810	0.58	0/1091
74	R7	0.39	0/686	0.57	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	M4	0.50	0/6945	0.67	3/9400 (0.0%)
76	M6	0.43	0/277	0.66	0/371
All	All	0.47	0/244634	0.76	337/339083 (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
4	SC	0	4
7	SH	0	1
8	SI	0	4
12	SO	0	1
18	Sc	0	2
19	Sd	0	1
20	3C	0	1
23	3F	0	1
26	A5	0	1
27	A8	0	6
29	AE	0	1
30	AF	0	1
31	AG	0	5
32	B1	0	1
33	B2	0	2
34	B3	0	5
38	5B	0	1
41	5E	0	1
45	5I	0	3
49	RE	0	3
50	RF	0	3
51	RH	0	1
52	RJ	0	1
53	RK	0	1
55	RO	0	4
56	RP	0	11
57	RQ	0	2
59	RT	0	1
64	R1	0	1
65	R3	0	3
66	R6	0	1
67	R2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	M3	0	2
70	r4	0	1
71	C4	0	1
72	R4	0	1
75	M4	0	3
All	All	0	83

There are no bond length outliers.

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	27	U	C2-N1-C1'	11.58	131.59	117.70
1	3A	27	U	N1-C2-O2	11.42	130.79	122.80
1	3A	27	U	N3-C2-O2	-10.83	114.62	122.20
3	SA	453	U	N3-C2-O2	-10.59	114.79	122.20
3	SA	453	U	N1-C2-O2	9.83	129.68	122.80
3	SA	287	G	O4'-C1'-N9	9.66	115.92	108.20
3	SA	453	U	C2-N1-C1'	9.57	129.19	117.70
3	SA	73	U	N3-C2-O2	-9.43	115.60	122.20
3	SA	1743	U	N1-C2-O2	9.02	129.12	122.80
3	SA	73	U	N1-C2-O2	8.87	129.01	122.80
3	SA	1743	U	C2-N1-C1'	8.62	128.04	117.70
3	SA	1729	C	N3-C2-O2	-8.22	116.14	121.90
31	AG	383	LEU	CA-CB-CG	8.21	134.18	115.30
3	SA	507	U	C2-N1-C1'	8.16	127.49	117.70
1	3A	27	U	C6-N1-C1'	-7.96	110.06	121.20
3	SA	484	C	C5-C6-N1	7.93	124.97	121.00
3	SA	1053	G	C8-N9-C4	-7.88	103.25	106.40
3	SA	1743	U	N3-C2-O2	-7.85	116.70	122.20
26	A5	25	ASP	CB-CG-OD1	7.82	125.34	118.30
3	SA	1717	G	C4-N9-C1'	7.77	136.60	126.50
3	SA	1174	C	N1-C2-O2	7.76	123.56	118.90
3	SA	800	U	N3-C2-O2	-7.72	116.79	122.20
1	3A	75	C	C5-C6-N1	7.72	124.86	121.00
3	SA	1769	U	N1-C2-O2	7.71	128.20	122.80
3	SA	190	C	N3-C2-O2	-7.70	116.51	121.90
21	3D	184	LEU	CA-CB-CG	7.67	132.95	115.30
3	SA	229	U	N1-C2-O2	7.56	128.09	122.80
3	SA	1441	C	N3-C2-O2	-7.54	116.62	121.90
3	SA	279	G	N3-C4-N9	-7.53	121.48	126.00
3	SA	107	C	C6-N1-C2	-7.51	117.30	120.30
3	SA	767	U	C2-N1-C1'	7.46	126.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1769	U	N3-C2-O2	-7.43	117.00	122.20
3	SA	767	U	N3-C2-O2	-7.40	117.02	122.20
3	SA	767	U	N1-C2-O2	7.34	127.94	122.80
3	SA	1174	C	C2-N1-C1'	7.32	126.86	118.80
3	SA	482	U	N3-C2-O2	-7.32	117.08	122.20
3	SA	107	C	N1-C2-O2	7.27	123.26	118.90
3	SA	73	U	C6-N1-C2	-7.21	116.68	121.00
1	3A	75	C	C6-N1-C2	-7.14	117.44	120.30
2	5A	311	C	P-O3'-C3'	7.13	128.26	119.70
3	SA	484	C	C6-N1-C2	-7.13	117.45	120.30
3	SA	1066	C	N3-C2-O2	-7.13	116.91	121.90
58	RS	239	LEU	CA-CB-CG	7.11	131.66	115.30
3	SA	73	U	C5-C6-N1	7.11	126.25	122.70
3	SA	1053	G	O5'-P-OP1	-7.09	99.31	105.70
42	5F	13	LEU	CA-CB-CG	7.08	131.58	115.30
3	SA	1784	C	N3-C2-O2	-7.07	116.95	121.90
1	3A	269	C	N1-C2-O2	7.05	123.13	118.90
3	SA	962	C	N3-C2-O2	-7.05	116.97	121.90
1	3A	43	C	C6-N1-C2	-7.02	117.49	120.30
3	SA	800	U	N1-C2-O2	7.01	127.71	122.80
3	SA	502	U	N3-C2-O2	-7.00	117.30	122.20
3	SA	507	U	C6-N1-C1'	-6.97	111.45	121.20
21	3D	181	LEU	CA-CB-CG	6.94	131.27	115.30
3	SA	229	U	N3-C2-O2	-6.93	117.35	122.20
3	SA	864	U	N3-C2-O2	-6.92	117.36	122.20
3	SA	1441	C	N1-C2-O2	6.92	123.05	118.90
3	SA	230	C	N1-C2-O2	6.88	123.03	118.90
3	SA	189	C	N1-C2-O2	6.88	123.03	118.90
1	3A	99	U	C5-C6-N1	6.87	126.13	122.70
3	SA	73	U	C2-N1-C1'	6.86	125.93	117.70
3	SA	579	A	P-O3'-C3'	6.86	127.93	119.70
3	SA	873	U	N1-C2-O2	6.81	127.56	122.80
3	SA	1174	C	C6-N1-C2	-6.79	117.58	120.30
3	SA	1742	U	N1-C2-O2	6.76	127.53	122.80
21	3D	292	LEU	CA-CB-CG	6.72	130.75	115.30
3	SA	1713	G	C4-N9-C1'	6.71	135.22	126.50
3	SA	107	C	N3-C2-O2	-6.66	117.24	121.90
3	SA	489	C	C6-N1-C2	-6.64	117.64	120.30
3	SA	653	C	N1-C2-O2	6.59	122.86	118.90
3	SA	507	U	N1-C2-O2	6.59	127.41	122.80
3	SA	1174	C	N3-C2-O2	-6.58	117.29	121.90
3	SA	1743	U	C6-N1-C1'	-6.57	112.00	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	502	U	N1-C2-O2	6.56	127.39	122.80
3	SA	1709	C	N3-C2-O2	-6.55	117.31	121.90
49	RE	730	LEU	CA-CB-CG	6.54	130.35	115.30
34	B3	401	LEU	CA-CB-CG	6.54	130.34	115.30
3	SA	1717	G	N3-C4-C5	-6.50	125.35	128.60
3	SA	1717	G	C8-N9-C1'	-6.48	118.58	127.00
3	SA	686	C	C2-N1-C1'	6.47	125.92	118.80
3	SA	633	U	N3-C2-O2	-6.46	117.67	122.20
28	A9	452	LEU	CA-CB-CG	6.39	130.00	115.30
20	3B	306	LEU	CA-CB-CG	6.39	129.99	115.30
3	SA	1709	C	N1-C2-O2	6.38	122.73	118.90
31	AG	529	LEU	CA-CB-CG	6.38	129.97	115.30
3	SA	489	C	C5-C6-N1	6.34	124.17	121.00
3	SA	454	U	C6-N1-C2	-6.33	117.20	121.00
3	SA	36	C	N1-C2-O2	6.32	122.69	118.90
3	SA	519	C	N1-C2-O2	6.31	122.69	118.90
3	SA	1687	U	N1-C2-O2	6.29	127.20	122.80
3	SA	542	A	P-O3'-C3'	6.25	127.20	119.70
28	A9	430	LEU	CA-CB-CG	6.25	129.66	115.30
3	SA	777	C	N1-C2-O2	6.23	122.64	118.90
3	SA	1646	C	N1-C2-O2	6.23	122.64	118.90
2	5A	83	U	N1-C2-O2	6.20	127.14	122.80
3	SA	1717	G	N3-C4-N9	6.19	129.72	126.00
3	SA	189	C	C2-N1-C1'	6.18	125.60	118.80
3	SA	1729	C	N1-C2-O2	6.14	122.58	118.90
1	3A	313	A	C2-N3-C4	6.13	113.67	110.60
2	5A	64	U	N3-C2-O2	-6.13	117.91	122.20
3	SA	873	U	N3-C2-O2	-6.12	117.91	122.20
3	SA	484	C	C2-N1-C1'	6.12	125.53	118.80
56	RP	1887	LEU	CA-CB-CG	6.09	129.30	115.30
58	RS	342	LEU	CA-CB-CG	6.08	129.28	115.30
3	SA	1053	G	OP1-P-OP2	6.06	128.69	119.60
3	SA	1742	U	N3-C2-O2	-6.05	117.96	122.20
31	AG	670	LEU	CA-CB-CG	6.05	129.21	115.30
7	SH	29	ASP	CB-CG-OD1	6.05	123.74	118.30
2	5A	501	C	N1-C2-O2	6.04	122.53	118.90
3	SA	1687	U	N3-C2-O2	-6.04	117.97	122.20
3	SA	1620	C	N1-C2-O2	6.04	122.52	118.90
75	M4	940	LEU	CA-CB-CG	-6.04	101.41	115.30
3	SA	50	C	C2-N1-C1'	6.02	125.42	118.80
3	SA	637	C	P-O3'-C3'	6.01	126.91	119.70
3	SA	648	G	N3-C4-N9	6.00	129.60	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B3	162	LEU	CA-CB-CG	6.00	129.09	115.30
3	SA	637	C	OP1-P-O3'	5.99	118.38	105.20
1	3A	248	G	P-O3'-C3'	5.97	126.86	119.70
2	5A	65	U	C5-C6-N1	5.96	125.68	122.70
3	SA	230	C	C5-C6-N1	5.96	123.98	121.00
3	SA	149	C	C2-N1-C1'	5.96	125.35	118.80
1	3A	269	C	C2-N1-C1'	5.96	125.35	118.80
3	SA	536	C	C5-C6-N1	5.95	123.97	121.00
1	3A	294	U	C2-N1-C1'	5.95	124.84	117.70
3	SA	75	U	C2-N1-C1'	5.95	124.84	117.70
2	5A	4	C	C5-C6-N1	5.94	123.97	121.00
3	SA	0	U	P-O3'-C3'	5.93	126.82	119.70
3	SA	280	U	P-O3'-C3'	5.91	126.80	119.70
14	SR	116	LEU	CA-CB-CG	5.91	128.90	115.30
3	SA	230	C	C6-N1-C2	-5.91	117.94	120.30
3	SA	453	U	C6-N1-C1'	-5.90	112.94	121.20
3	SA	1070	C	C6-N1-C2	-5.90	117.94	120.30
45	5I	62	LEU	CA-CB-CG	5.90	128.87	115.30
35	B8	328	LEU	CA-CB-CG	5.89	128.86	115.30
3	SA	487	G	N3-C4-N9	5.89	129.53	126.00
4	SC	172	LEU	CA-CB-CG	5.88	128.83	115.30
3	SA	686	C	C5-C6-N1	5.88	123.94	121.00
19	Sd	52	ASP	CB-CG-OD1	5.88	123.59	118.30
1	3A	42	U	C5-C6-N1	5.87	125.64	122.70
2	5A	84	G	N3-C4-N9	5.86	129.52	126.00
3	SA	490	C	C6-N1-C2	-5.85	117.96	120.30
49	RE	213	LEU	CA-CB-CG	5.85	128.75	115.30
3	SA	777	C	C2-N1-C1'	5.84	125.23	118.80
1	3A	269	C	N3-C2-O2	-5.84	117.81	121.90
3	SA	36	C	N3-C2-O2	-5.84	117.81	121.90
3	SA	1769	U	C2-N1-C1'	5.82	124.68	117.70
20	3C	306	LEU	CA-CB-CG	5.82	128.69	115.30
3	SA	1066	C	N1-C2-O2	5.81	122.39	118.90
1	3A	162	U	N1-C2-O2	5.80	126.86	122.80
3	SA	279	G	C6-C5-N7	5.79	133.88	130.40
41	5E	314	LEU	CA-CB-CG	5.79	128.62	115.30
3	SA	107	C	C2-N1-C1'	5.78	125.16	118.80
3	SA	278	U	P-O3'-C3'	5.78	126.63	119.70
3	SA	75	U	N1-C2-O2	5.77	126.84	122.80
3	SA	656	G	O4'-C1'-N9	5.77	112.81	108.20
3	SA	139	C	P-O3'-C3'	5.75	126.60	119.70
2	5A	64	U	N1-C2-O2	5.75	126.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	RE	268	LEU	CA-CB-CG	5.75	128.52	115.30
1	3A	147	C	N1-C2-O2	5.75	122.35	118.90
3	SA	1594	G	P-O3'-C3'	5.74	126.58	119.70
25	A4	390	LEU	CA-CB-CG	5.73	128.48	115.30
3	SA	1053	G	N9-C4-C5	5.73	107.69	105.40
1	3A	44	U	C5-C6-N1	5.72	125.56	122.70
2	5A	494	C	C2-N1-C1'	5.72	125.09	118.80
1	3A	248	G	O4'-C1'-N9	5.69	112.75	108.20
1	3A	162	U	N3-C2-O2	-5.68	118.23	122.20
3	SA	536	C	C6-N1-C2	-5.67	118.03	120.30
3	SA	786	C	C5-C6-N1	5.67	123.83	121.00
31	AG	670	LEU	CB-CG-CD1	-5.65	101.39	111.00
3	SA	800	U	C2-N1-C1'	5.65	124.47	117.70
5	SF	193	GLY	N-CA-C	5.64	127.21	113.10
2	5A	61	U	C2-N1-C1'	5.63	124.46	117.70
56	RP	1876	LEU	CA-CB-CG	-5.63	102.34	115.30
52	RJ	252	LEU	CA-CB-CG	5.63	128.25	115.30
3	SA	781	U	P-O3'-C3'	5.63	126.45	119.70
49	RE	240	LEU	CA-CB-CG	5.62	128.24	115.30
3	SA	773	C	P-O3'-C3'	5.62	126.44	119.70
3	SA	1055	U	N1-C2-O2	5.62	126.73	122.80
3	SA	283	U	C2-N1-C1'	5.62	124.44	117.70
3	SA	965	U	C2-N1-C1'	5.61	124.44	117.70
45	5I	310	ASP	CB-CG-OD1	5.61	123.35	118.30
10	SK	118	LEU	CA-CB-CG	5.60	128.18	115.30
3	SA	243	G	N3-C4-N9	-5.59	122.64	126.00
56	RP	1987	LEU	CA-CB-CG	5.59	128.15	115.30
3	SA	279	G	N9-C4-C5	5.58	107.63	105.40
3	SA	1646	C	N3-C2-O2	-5.57	118.00	121.90
36	BE	923	ASP	CB-CG-OD1	5.56	123.31	118.30
3	SA	827	C	C2-N1-C1'	5.56	124.92	118.80
3	SA	289	U	N3-C2-O2	-5.56	118.31	122.20
3	SA	873	U	C2-N1-C1'	5.55	124.36	117.70
49	RE	959	LEU	CA-CB-CG	5.54	128.05	115.30
3	SA	1784	C	N1-C2-O2	5.54	122.23	118.90
2	5A	84	G	C4-N9-C1'	5.53	133.69	126.50
2	5A	494	C	C6-N1-C2	-5.53	118.09	120.30
3	SA	71	A	O4'-C1'-N9	5.53	112.62	108.20
1	3A	62	C	C5-C6-N1	5.51	123.76	121.00
3	SA	274	G	C4-N9-C1'	5.51	133.66	126.50
65	R3	360	LEU	CB-CG-CD2	-5.49	101.66	111.00
3	SA	1620	C	N3-C2-O2	-5.49	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	530	C	N1-C2-O2	5.49	122.19	118.90
3	SA	786	C	C6-N1-C2	-5.48	118.11	120.30
24	3H	22	ASP	CB-CG-OD1	5.48	123.23	118.30
3	SA	653	C	N3-C2-O2	-5.48	118.06	121.90
3	SA	1141	G	N3-C4-N9	5.47	129.28	126.00
31	AG	323	LEU	CA-CB-CG	5.47	127.89	115.30
3	SA	1713	G	C8-N9-C1'	-5.47	119.89	127.00
3	SA	230	C	C2-N1-C1'	5.46	124.80	118.80
34	B3	454	LEU	CA-CB-CG	5.45	127.83	115.30
3	SA	1713	G	N3-C4-N9	5.43	129.26	126.00
33	B2	551	LEU	CA-CB-CG	5.43	127.78	115.30
3	SA	454	U	C5-C6-N1	5.42	125.41	122.70
8	SI	67	LEU	CA-CB-CG	5.41	127.74	115.30
56	RP	107	LEU	CB-CG-CD2	-5.41	101.81	111.00
3	SA	484	C	P-O3'-C3'	5.40	126.19	119.70
3	SA	1174	C	C5-C6-N1	5.40	123.70	121.00
2	5A	499	U	N3-C2-O2	-5.40	118.42	122.20
3	SA	864	U	N1-C2-O2	5.40	126.58	122.80
2	5A	83	U	C2-N1-C1'	5.39	124.17	117.70
3	SA	802	G	N1-C2-N2	-5.38	111.36	116.20
3	SA	211	U	C2-N1-C1'	5.38	124.15	117.70
1	3A	97	C	C5-C6-N1	5.37	123.69	121.00
3	SA	1268	G	N3-C4-N9	5.37	129.22	126.00
3	SA	1778	G	N3-C4-N9	-5.37	122.78	126.00
30	AF	326	LEU	CA-CB-CG	5.37	127.66	115.30
3	SA	185	U	N1-C2-O2	5.37	126.56	122.80
3	SA	1055	U	N3-C2-O2	-5.37	118.44	122.20
4	SC	147	ALA	C-N-CA	5.36	135.10	121.70
2	5A	57	C	C5-C6-N1	5.35	123.68	121.00
49	RE	1149	LEU	CA-CB-CG	5.35	127.60	115.30
3	SA	1064	G	C4-N9-C1'	5.34	133.44	126.50
3	SA	54	C	C6-N1-C2	-5.34	118.17	120.30
3	SA	1476	C	C2-N1-C1'	5.33	124.67	118.80
41	5E	448	LEU	CA-CB-CG	5.33	127.56	115.30
3	SA	279	G	C5-C6-O6	5.32	131.79	128.60
3	SA	211	U	N1-C2-O2	5.32	126.52	122.80
3	SA	506	A	C2-N3-C4	5.32	113.26	110.60
3	SA	230	C	N3-C2-O2	-5.31	118.18	121.90
3	SA	149	C	N1-C2-O2	5.30	122.08	118.90
29	AE	234	LEU	CA-CB-CG	5.30	127.48	115.30
49	RE	730	LEU	CB-CG-CD2	-5.29	102.01	111.00
34	B3	355	LEU	CA-CB-CG	5.28	127.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	250	C	C6-N1-C2	-5.28	118.19	120.30
2	5A	57	C	C2-N1-C1'	5.28	124.61	118.80
1	3A	107	C	OP1-P-O3'	5.27	116.80	105.20
2	5A	7	A	O5'-P-OP1	-5.27	100.96	105.70
3	SA	302	U	N3-C2-O2	-5.27	118.51	122.20
3	SA	453	U	C6-N1-C2	-5.27	117.84	121.00
22	3E	195	LEU	CA-CB-CG	5.27	127.42	115.30
3	SA	536	C	N1-C2-O2	5.26	122.06	118.90
3	SA	502	U	C2-N1-C1'	5.26	124.02	117.70
1	3A	27	U	C5-C6-N1	5.26	125.33	122.70
2	5A	4	C	C6-N1-C2	-5.26	118.20	120.30
55	RO	326	LEU	CA-CB-CG	5.26	127.39	115.30
1	3A	164	C	N1-C2-O2	5.25	122.05	118.90
3	SA	279	G	C8-N9-C1'	5.25	133.83	127.00
3	SA	531	C	N1-C2-O2	5.25	122.05	118.90
3	SA	340	U	C5-C6-N1	5.24	125.32	122.70
63	R5	229	LEU	CA-CB-CG	-5.24	103.25	115.30
3	SA	1476	C	C5-C6-N1	5.23	123.61	121.00
3	SA	658	C	C6-N1-C1'	5.23	127.07	120.80
3	SA	1609	U	N3-C2-O2	-5.22	118.55	122.20
50	RF	60	LEU	CA-CB-CG	5.22	127.31	115.30
72	R4	551	ASP	CB-CG-OD2	5.22	123.00	118.30
3	SA	921	U	C2-N1-C1'	5.21	123.96	117.70
3	SA	50	C	N1-C2-O2	5.21	122.03	118.90
5	SF	11	ARG	C-N-CA	5.21	134.73	121.70
3	SA	190	C	C6-N1-C2	-5.21	118.22	120.30
21	3D	412	LEU	CA-CB-CG	5.21	127.28	115.30
3	SA	283	U	N1-C2-O2	5.20	126.44	122.80
3	SA	1675	C	N1-C2-O2	5.20	122.02	118.90
10	SK	105	LEU	CA-CB-CG	5.20	127.26	115.30
3	SA	767	U	C6-N1-C1'	-5.20	113.93	121.20
3	SA	176	C	C6-N1-C1'	5.19	127.03	120.80
1	3A	243	U	C2-N1-C1'	5.19	123.93	117.70
1	3A	243	U	N1-C2-O2	5.19	126.43	122.80
22	3E	371	LEU	CA-CB-CG	5.19	127.24	115.30
3	SA	1527	C	C5-C6-N1	5.19	123.59	121.00
3	SA	324	U	N3-C2-O2	-5.18	118.57	122.20
1	3A	243	U	N3-C2-O2	-5.18	118.57	122.20
1	3A	46	U	N1-C2-O2	5.18	126.43	122.80
5	SF	101	LEU	CA-CB-CG	5.18	127.21	115.30
3	SA	107	C	C5-C6-N1	5.17	123.59	121.00
4	SC	54	LEU	CA-CB-CG	5.17	127.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	RF	147	LEU	CA-CB-CG	5.17	127.20	115.30
3	SA	279	G	C4-N9-C1'	-5.16	119.79	126.50
3	SA	306	U	N1-C2-O2	5.16	126.41	122.80
2	5A	588	C	C2-N1-C1'	5.16	124.47	118.80
3	SA	487	G	C2-N3-C4	5.16	114.48	111.90
51	RG	180	LEU	CA-CB-CG	5.15	127.15	115.30
72	R4	171	ASP	CB-CG-OD2	5.15	122.94	118.30
3	SA	1620	C	C6-N1-C2	-5.15	118.24	120.30
3	SA	276	C	C2-N1-C1'	-5.14	113.15	118.80
3	SA	802	G	N3-C2-N2	5.14	123.50	119.90
2	5A	538	C	N1-C2-O2	5.14	121.98	118.90
18	Sc	3	LEU	CA-CB-CG	5.14	127.11	115.30
3	SA	813	U	C2-N1-C1'	5.13	123.86	117.70
3	SA	335	U	N3-C2-O2	-5.13	118.61	122.20
3	SA	38	C	C6-N1-C2	-5.13	118.25	120.30
3	SA	75	U	N3-C2-O2	-5.13	118.61	122.20
3	SA	283	U	N3-C2-O2	-5.12	118.62	122.20
3	SA	685	A	P-O3'-C3'	5.12	125.84	119.70
35	B8	290	LEU	CA-CB-CG	5.12	127.07	115.30
1	3A	306	G	C4-N9-C1'	5.12	133.15	126.50
3	SA	579	A	OP2-P-O3'	5.11	116.44	105.20
3	SA	68	A	P-O3'-C3'	5.11	125.83	119.70
3	SA	658	C	C2-N1-C1'	-5.11	113.18	118.80
3	SA	1612	U	N3-C2-O2	-5.11	118.63	122.20
3	SA	1703	C	C6-N1-C2	-5.10	118.26	120.30
30	AF	421	LEU	CA-CB-CG	5.10	127.03	115.30
72	R4	786	LEU	CA-CB-CG	5.09	127.01	115.30
65	R3	303	ASP	CB-CG-OD1	5.09	122.88	118.30
3	SA	1742	U	C5-C6-N1	5.09	125.24	122.70
3	SA	519	C	N3-C2-O2	-5.08	118.34	121.90
3	SA	1440	C	N1-C2-O2	5.08	121.95	118.90
2	5A	84	G	C8-N9-C1'	-5.08	120.40	127.00
3	SA	50	C	C5-C6-N1	5.07	123.54	121.00
3	SA	629	U	C5-C6-N1	5.07	125.24	122.70
3	SA	1612	U	N1-C2-O2	5.07	126.35	122.80
3	SA	454	U	N3-C2-O2	-5.05	118.66	122.20
3	SA	827	C	N1-C2-O2	5.05	121.93	118.90
75	M4	919	LEU	CB-CG-CD2	-5.05	102.41	111.00
3	SA	192	U	C2-N1-C1'	5.05	123.76	117.70
3	SA	633	U	N1-C2-O2	5.05	126.34	122.80
3	SA	748	U	N1-C2-O2	5.05	126.34	122.80
3	SA	1742	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	M4	440	LEU	CA-CB-CG	5.05	126.92	115.30
52	RJ	845	LEU	CA-CB-CG	5.05	126.92	115.30
32	B1	327	LEU	CA-CB-CG	5.05	126.91	115.30
1	3A	243	U	C5-C6-N1	5.04	125.22	122.70
3	SA	632	U	N3-C2-O2	-5.04	118.67	122.20
44	5H	576	LEU	CA-CB-CG	5.04	126.89	115.30
2	5A	65	U	N1-C2-O2	5.04	126.32	122.80
3	SA	777	C	C6-N1-C2	-5.04	118.29	120.30
1	3A	107	C	P-O3'-C3'	5.03	125.74	119.70
3	SA	1585	U	N3-C2-O2	-5.03	118.68	122.20
3	SA	431	C	C6-N1-C2	-5.02	118.29	120.30
2	5A	589	U	C5-C6-N1	5.01	125.21	122.70

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	3C	246	GLN	Peptide
23	3F	173	GLU	Peptide
38	5B	191	PRO	Peptide
41	5E	483	TYR	Peptide
45	5I	185	ILE	Peptide
45	5I	230	ASN	Peptide
45	5I	283	ASP	Peptide
26	A5	166	ALA	Peptide
27	A8	257	SER	Peptide
27	A8	266	ILE	Peptide
27	A8	435	ASP	Peptide
27	A8	529	HIS	Peptide
27	A8	537	THR	Peptide
27	A8	677	ASN	Peptide
29	AE	596	LYS	Peptide
30	AF	289	ASN	Peptide
31	AG	140	LYS	Peptide
31	AG	386	ASN	Peptide
31	AG	502	LYS	Peptide
31	AG	740	LYS	Peptide
31	AG	780	GLU	Peptide
32	B1	348	THR	Peptide
33	B2	212	VAL	Peptide
33	B2	213	LYS	Peptide
34	B3	34	THR	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
34	B3	410	ASN	Peptide
34	B3	445	ILE	Peptide
34	B3	473	ALA	Peptide
34	B3	593	CYS	Peptide
71	C4	149	GLN	Peptide
68	M3	141	LEU	Peptide
68	M3	216	ASP	Peptide
75	M4	541	SER	Peptide
75	M4	573	LYS	Peptide
75	M4	874	GLN	Peptide
64	R1	166	TYR	Peptide
67	R2	136	HIS	Peptide
65	R3	335	ASP	Peptide
65	R3	352	ALA	Peptide
65	R3	54	ILE	Peptide
72	R4	504	PRO	Peptide
66	R6	188	GLU	Peptide
49	RE	1028	ARG	Peptide
49	RE	1168	TYR	Peptide
49	RE	458	ILE	Peptide
50	RF	107	LEU	Peptide
50	RF	155	LEU	Peptide
50	RF	157	GLU	Peptide
51	RH	232	LEU	Peptide
52	RJ	783	PHE	Peptide
53	RK	259	GLU	Peptide
55	RO	270	SER	Peptide
55	RO	390	SER	Peptide
55	RO	493	TYR	Peptide
55	RO	76	SER	Peptide
56	RP	1003	ILE	Peptide
56	RP	1005	ASN	Peptide
56	RP	13	ARG	Peptide
56	RP	1707	HIS	Peptide
56	RP	1804	SER	Peptide
56	RP	1848	VAL	Peptide
56	RP	185	LYS	Peptide
56	RP	1907	ASN	Peptide
56	RP	1996	GLN	Peptide
56	RP	36	LYS	Peptide
56	RP	903	THR	Peptide
57	RQ	271	GLU	Peptide

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Mol	Chain	Res	Type	Group
57	RQ	312	ILE	Peptide
59	RT	124	LEU	Peptide
4	SC	135	LEU	Peptide
4	SC	16	GLN	Peptide
4	SC	177	GLN	Peptide
4	SC	208	GLN	Peptide
7	SH	152	ASP	Peptide
8	SI	131	PHE	Peptide
8	SI	134	GLU	Peptide
8	SI	31	SER	Peptide
8	SI	64	VAL	Peptide
12	SO	58	HIS	Peptide
18	Sc	49	HIS	Peptide
18	Sc	74	SER	Peptide
19	Sd	51	ASN	Peptide
70	r4	92	ASN	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	3A	4962	0	2519	58	0
2	5A	3260	0	1643	34	0
3	SA	26609	0	13415	315	0
4	SC	1848	0	1940	41	0
5	SF	1930	0	1950	30	0
6	SG	1669	0	1724	21	0
7	SH	1457	0	1504	39	0
8	SI	1310	0	1374	36	0
9	SJ	1104	0	1107	28	0
10	SK	1388	0	1467	28	0
11	SM	1113	0	1181	29	0
12	SO	1087	0	1152	26	0
13	SP	868	0	894	18	0
14	SR	973	0	1029	19	0
15	SX	1003	0	1040	24	0
16	SY	807	0	865	16	0
17	SZ	986	0	1042	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Sc	603	0	621	0	0
19	Sd	497	0	535	0	0
20	3B	1865	0	1910	46	0
20	3C	1763	0	1805	48	0
21	3D	2974	0	3001	53	0
22	3E	3041	0	2831	68	0
23	3F	3498	0	3515	80	0
24	3G	916	0	964	17	0
24	3H	916	0	964	23	0
25	A4	5243	0	5216	195	0
26	A5	3953	0	3894	86	0
27	A8	3307	0	2316	45	0
28	A9	939	0	898	25	0
29	AE	9956	0	7969	130	0
30	AF	3807	0	3791	89	0
31	AG	6570	0	6473	189	0
32	B1	6427	0	6329	127	0
33	B2	6502	0	6493	156	0
34	B3	5919	0	6007	146	0
35	B8	3764	0	3757	84	0
36	BE	6475	0	6453	156	0
37	B6	2800	0	2517	43	0
38	5B	495	0	561	10	0
39	5C	3612	0	3578	66	0
40	5D	1733	0	1815	36	0
41	5E	1564	0	1592	41	0
42	5F	1530	0	1572	30	0
43	5G	1732	0	1744	37	0
44	5H	596	0	661	8	0
45	5I	3756	0	3708	86	0
46	5J	1127	0	1150	17	0
47	5K	1323	0	1401	20	0
48	RD	2413	0	2264	29	0
49	RE	8805	0	8911	192	0
50	RF	1963	0	1942	42	0
51	RG	1701	0	1767	49	0
51	RH	1799	0	1872	46	0
52	RJ	5935	0	6100	130	0
53	RK	2781	0	2878	79	0
54	RN	4088	0	3798	62	0
55	RO	3766	0	3269	63	0
56	RP	12716	0	8235	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RQ	1655	0	1461	22	0
58	RS	2051	0	2096	46	0
59	RT	1357	0	1426	23	0
60	RW	747	0	312	2	0
61	X1	400	0	99	3	0
62	X2	705	0	151	0	0
63	R5	2304	0	2265	61	0
64	R1	1886	0	1904	51	0
65	R3	2588	0	2607	70	0
66	R6	1696	0	1744	46	0
67	R2	2030	0	2047	51	0
68	M3	1639	0	1592	42	0
69	R0	1792	0	1747	41	0
70	r4	2236	0	2215	0	0
71	C4	1653	0	1616	41	0
72	R4	7430	0	7346	218	0
73	r6	802	0	776	0	0
74	R7	681	0	707	13	0
75	M4	6814	0	6792	224	0
76	M6	275	0	254	6	0
77	5K	1	0	0	0	0
77	Sc	1	0	0	0	0
78	RJ	32	0	12	0	0
79	RJ	1	0	0	0	0
All	All	238320	0	212092	4259	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 (4259) 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)
25:A4:741:LEU:HD11	25:A4:744:VAL:CG2	1.48	1.42
25:A4:740:PRO:O	25:A4:756:GLU:HG2	1.44	1.16
25:A4:741:LEU:HD11	25:A4:744:VAL:HG21	1.16	1.13
25:A4:741:LEU:HD21	25:A4:744:VAL:HG23	1.39	1.04
25:A4:741:LEU:CD1	25:A4:744:VAL:CG2	2.39	1.00
3:SA:1170:G:H1	3:SA:1469:A:N6	1.62	0.97
3:SA:656:G:H1	3:SA:678:A:H2	1.00	0.96
3:SA:142:G:N1	3:SA:173:A:C2	2.33	0.96
58:RS:275:SER:O	58:RS:279:ILE:HB	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:656:G:N1	3:SA:678:A:C2	2.34	0.94
3:SA:902:G:H21	3:SA:907:A:H62	1.01	0.93
26:A5:519:LEU:O	26:A5:523:LEU:HB2	1.69	0.93
27:A8:264:SER:O	27:A8:267:ILE:HA	1.68	0.92
3:SA:69:G:H1	3:SA:82:U:H3	1.12	0.91
3:SA:1697:G:H1	3:SA:1704:U:H3	0.98	0.90
51:RH:44:VAL:HA	51:RH:113:TYR:O	1.72	0.89
3:SA:142:G:H1	3:SA:173:A:H2	0.92	0.89
3:SA:1688:U:H3	3:SA:1713:G:H1	0.89	0.88
3:SA:1170:G:H1	3:SA:1469:A:H61	0.90	0.87
36:BE:360:ASP:O	36:BE:636:PRO:HG2	1.73	0.87
1:3A:12:U:H3	3:SA:1112:G:H1	0.89	0.87
3:SA:142:G:N1	3:SA:173:A:H2	1.68	0.87
25:A4:739:LYS:HB2	25:A4:740:PRO:HD3	1.54	0.86
53:RK:114:PHE:O	53:RK:169:VAL:HA	1.75	0.86
3:SA:902:G:N2	3:SA:907:A:H62	1.75	0.84
55:RO:301:ASP:O	55:RO:305:LEU:HB2	1.79	0.83
25:A4:739:LYS:HE2	25:A4:739:LYS:HA	1.60	0.82
25:A4:740:PRO:O	25:A4:756:GLU:CG	2.26	0.82
46:5J:114:ARG:O	46:5J:118:GLN:HB3	1.79	0.82
3:SA:656:G:N1	3:SA:678:A:H2	1.74	0.82
29:AE:3:SER:O	29:AE:7:GLN:HB2	1.79	0.82
51:RG:42:ILE:O	51:RG:203:CYS:HA	1.78	0.81
25:A4:741:LEU:CD2	25:A4:744:VAL:HG23	2.09	0.81
12:SO:40:TYR:HB3	12:SO:45:LEU:HD12	1.62	0.81
75:M4:524:TRP:CH2	75:M4:734:LEU:HD11	2.16	0.81
33:B2:322:SER:O	33:B2:326:LEU:HB2	1.78	0.81
3:SA:902:G:H21	3:SA:907:A:N6	1.78	0.81
23:3F:263:TRP:HZ3	23:3F:270:PRO:HD3	1.45	0.81
75:M4:80:VAL:HG12	75:M4:81:LEU:N	1.96	0.81
25:A4:741:LEU:HD11	25:A4:744:VAL:HG22	1.61	0.80
37:B6:319:TYR:O	37:B6:323:PHE:HB2	1.81	0.80
55:RO:209:GLN:O	55:RO:213:LEU:HB2	1.80	0.80
35:B8:311:ASN:HA	35:B8:324:TRP:O	1.80	0.79
28:A9:460:LEU:O	28:A9:464:SER:HB3	1.80	0.79
23:3F:263:TRP:CZ3	23:3F:270:PRO:HG3	2.18	0.79
49:RE:442:PHE:O	49:RE:469:ASP:HA	1.82	0.78
39:5C:116:ILE:H	39:5C:380:ASN:HD21	1.30	0.78
75:M4:80:VAL:HG12	75:M4:81:LEU:H	1.47	0.78
25:A4:741:LEU:CD1	25:A4:744:VAL:HG21	2.07	0.78
58:RS:271:THR:O	58:RS:275:SER:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A4:739:LYS:HE2	25:A4:739:LYS:CA	2.15	0.76
33:B2:386:GLU:HA	33:B2:391:ARG:HH22	1.50	0.76
36:BE:361:SER:HA	36:BE:636:PRO:CB	2.15	0.76
30:AF:86:SER:O	30:AF:98:ALA:HA	1.85	0.76
29:AE:309:GLN:HG2	35:B8:224:ASN:HD22	1.51	0.76
66:R6:25:LYS:H	66:R6:96:GLU:HB3	1.50	0.76
43:5G:131:CYS:HG	43:5G:136:THR:HG1	1.34	0.75
35:B8:435:PHE:HB3	35:B8:443:VAL:HA	1.69	0.74
75:M4:524:TRP:HH2	75:M4:734:LEU:CD1	2.00	0.74
66:R6:138:ILE:HG12	66:R6:145:ILE:HG12	1.68	0.74
1:3A:67:G:H1	2:5A:286:U:H3	1.35	0.74
3:SA:311:U:H3	3:SA:355:G:H1	1.33	0.74
53:RK:103:MET:O	53:RK:107:ALA:HB2	1.88	0.74
69:R0:3:THR:HG23	69:R0:42:LEU:HB3	1.70	0.74
72:R4:732:LEU:HD23	72:R4:735:ASN:HD22	1.53	0.74
39:5C:257:SER:HG	39:5C:259:TRP:HE1	1.34	0.73
49:RE:438:GLY:HA2	49:RE:458:ILE:O	1.88	0.73
55:RO:340:LYS:O	55:RO:344:ILE:HB	1.88	0.72
64:R1:30:ASN:HD22	64:R1:239:ARG:HH12	1.37	0.72
35:B8:357:ASN:HB2	35:B8:378:GLN:HG2	1.71	0.72
3:SA:174:U:H3	3:SA:266:A:H62	1.38	0.72
75:M4:80:VAL:CG1	75:M4:81:LEU:H	2.02	0.72
52:RJ:1034:LEU:H	52:RJ:1037:GLN:HE21	1.37	0.71
75:M4:939:LEU:HD11	75:M4:966:MET:HG2	1.71	0.71
39:5C:265:GLU:OE1	57:RQ:834:LYS:HD2	1.89	0.71
25:A4:741:LEU:HD11	25:A4:744:VAL:HG23	1.66	0.71
32:B1:71:ILE:HD11	32:B1:102:VAL:HG21	1.73	0.70
68:M3:75:THR:HG21	68:M3:175:SER:OG	1.91	0.70
30:AF:222:SER:HB2	30:AF:225:GLN:H	1.57	0.70
16:SY:97:ASP:HB3	52:RJ:828:ARG:HH22	1.57	0.70
52:RJ:235:LEU:O	52:RJ:239:ASN:HB2	1.92	0.70
71:C4:34:ASN:HB3	71:C4:105:ASN:HA	1.74	0.70
3:SA:1051:G:H21	45:5I:447:THR:HG21	1.57	0.69
31:AG:585:TRP:HB3	31:AG:594:TRP:HE1	1.57	0.69
25:A4:739:LYS:HB2	25:A4:740:PRO:CD	2.22	0.69
36:BE:209:ILE:HA	36:BE:225:THR:HA	1.73	0.69
75:M4:611:GLN:HE22	75:M4:876:VAL:HG22	1.57	0.69
23:3F:263:TRP:HZ3	23:3F:270:PRO:CD	2.05	0.69
69:R0:69:ASN:HA	69:R0:122:ARG:HH11	1.58	0.68
23:3F:426:SER:HB3	23:3F:433:ILE:HD11	1.74	0.68
40:5D:167:THR:O	40:5D:171:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RD:1612:LEU:HD21	48:RD:1616:ASN:HB2	1.76	0.68
33:B2:10:GLN:HE22	33:B2:682:ARG:HB2	1.59	0.68
25:A4:353:GLU:HA	25:A4:766:GLN:HE22	1.59	0.68
34:B3:561:SER:HG	34:B3:566:SER:N	1.92	0.68
8:SI:58:LEU:HB2	8:SI:90:VAL:HG12	1.76	0.68
64:R1:52:LEU:HB2	64:R1:125:GLU:HB2	1.76	0.68
25:A4:741:LEU:HD21	25:A4:744:VAL:CG2	2.21	0.68
34:B3:496:ALA:O	34:B3:508:THR:HA	1.94	0.68
10:SK:127:VAL:HG22	10:SK:131:GLN:HE22	1.60	0.67
21:3D:254:ASN:HA	21:3D:257:ILE:HG22	1.75	0.67
3:SA:656:G:O6	3:SA:678:A:N1	2.27	0.67
22:3E:286:ASN:HD22	22:3E:387:GLY:H	1.40	0.67
24:3G:53:ILE:HD11	24:3G:81:VAL:HG13	1.75	0.67
3:SA:68:A:H5'	7:SH:160:ARG:HH22	1.60	0.67
23:3F:545:LYS:HG2	23:3F:561:ASN:HD21	1.60	0.67
26:A5:8:SER:HB2	26:A5:17:LEU:HD11	1.76	0.67
3:SA:1167:G:H1	3:SA:1578:U:H3	1.42	0.67
72:R4:83:ILE:O	72:R4:191:ASN:ND2	2.27	0.67
75:M4:1025:ILE:HA	75:M4:1028:PHE:HB2	1.76	0.67
17:SZ:20:ARG:HA	17:SZ:76:TYR:HB3	1.77	0.66
35:B8:455:ILE:HA	35:B8:486:SER:HA	1.78	0.66
67:R2:35:GLU:HB2	67:R2:51:ILE:HB	1.77	0.66
75:M4:475:HIS:HE1	75:M4:504:THR:HB	1.60	0.66
1:3A:250:C:H41	23:3F:560:ARG:HH12	1.42	0.66
58:RS:339:GLY:O	58:RS:343:ALA:HB2	1.96	0.66
72:R4:857:GLN:HE21	72:R4:871:HIS:HB3	1.60	0.66
56:RP:137:ASP:HA	56:RP:140:ILE:HD12	1.76	0.66
49:RE:584:GLU:O	49:RE:614:ARG:HB2	1.95	0.66
56:RP:2045:GLN:O	56:RP:2049:GLU:HB2	1.96	0.66
31:AG:682:ASN:HB2	31:AG:689:ILE:HD11	1.78	0.66
31:AG:715:GLU:HG3	31:AG:716:ARG:HG2	1.77	0.66
29:AE:248:SER:HG	29:AE:253:CYS:HG	1.43	0.66
34:B3:461:LEU:HB3	34:B3:484:GLU:HB3	1.78	0.66
45:5I:76:ASN:HA	45:5I:118:VAL:HG21	1.77	0.65
33:B2:217:LEU:HB3	33:B2:229:TRP:HB2	1.77	0.65
22:3E:6:THR:O	22:3E:16:LYS:HA	1.96	0.65
29:AE:644:LYS:H	29:AE:647:GLU:HG2	1.61	0.65
34:B3:548:LEU:O	34:B3:559:ILE:HA	1.96	0.65
3:SA:349:U:H4'	3:SA:353:A:H1'	1.78	0.65
33:B2:160:ARG:HH21	41:5E:522:ARG:HD2	1.62	0.65
34:B3:513:LYS:H	34:B3:535:GLY:HA2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:498:MET:O	49:RE:506:GLN:NE2	2.28	0.65
51:RG:55:ILE:O	51:RG:64:LYS:HB2	1.96	0.65
51:RG:150:ILE:HG23	51:RG:159:LEU:HB2	1.78	0.65
53:RK:114:PHE:HB2	53:RK:170:VAL:HG22	1.78	0.65
25:A4:614:TRP:O	25:A4:618:ASN:HB2	1.97	0.65
72:R4:868:SER:HB3	72:R4:871:HIS:HD2	1.61	0.65
3:SA:1663:G:H1	3:SA:1738:U:H3	1.42	0.65
22:3E:149:ARG:O	22:3E:153:LYS:HB2	1.97	0.65
31:AG:741:SER:HB2	31:AG:759:HIS:HB3	1.77	0.65
49:RE:179:LYS:HB2	49:RE:210:PRO:HG2	1.79	0.65
3:SA:763:G:H21	3:SA:774:A:H62	1.44	0.65
24:3G:54:MET:HB3	24:3G:64:LEU:HD21	1.79	0.65
46:5J:111:ASP:O	46:5J:115:ARG:NH2	2.30	0.65
50:RF:5:ASP:HA	50:RF:149:ALA:HB1	1.79	0.64
3:SA:656:G:C6	3:SA:678:A:N1	2.66	0.64
20:3C:94:ALA:HB3	20:3C:166:PRO:HG3	1.78	0.64
36:BE:504:ALA:HB3	36:BE:522:LEU:HD12	1.78	0.64
49:RE:1101:ASP:HB2	49:RE:1233:ASN:HB3	1.80	0.64
65:R3:297:TYR:HB2	65:R3:347:ILE:HB	1.78	0.64
25:A4:453:LEU:HB3	25:A4:460:LEU:HD22	1.78	0.64
3:SA:142:G:O6	3:SA:173:A:N1	2.31	0.64
34:B3:665:GLN:HE22	34:B3:688:LEU:HD21	1.62	0.64
35:B8:386:ILE:HD13	35:B8:437:LEU:HD12	1.79	0.64
75:M4:524:TRP:CH2	75:M4:734:LEU:CD1	2.79	0.64
49:RE:441:GLN:HE21	49:RE:456:LYS:HB2	1.61	0.64
31:AG:507:MET:HB2	31:AG:532:TRP:HB2	1.80	0.64
33:B2:338:ILE:HB	33:B2:355:LEU:HD11	1.78	0.64
3:SA:1213:G:H1	3:SA:1450:U:H3	1.46	0.64
3:SA:1688:U:O2	3:SA:1713:G:N2	2.28	0.64
22:3E:169:LEU:O	22:3E:173:LEU:HB2	1.98	0.64
23:3F:171:THR:OG1	23:3F:172:PHE:N	2.31	0.64
31:AG:320:VAL:HG12	31:AG:335:PRO:HA	1.79	0.64
59:RT:126:LEU:HB3	59:RT:139:LEU:HD12	1.80	0.64
65:R3:56:ASN:HD22	65:R3:394:ILE:HG13	1.63	0.64
3:SA:573:C:O2'	52:RJ:870:ARG:NH2	2.30	0.64
13:SP:87:GLY:HA3	13:SP:120:PRO:HD2	1.79	0.64
55:RO:253:PHE:O	55:RO:257:PHE:HB2	1.97	0.64
34:B3:443:PRO:HA	34:B3:499:VAL:HG11	1.79	0.63
64:R1:69:LYS:HB2	64:R1:114:LEU:HB3	1.80	0.63
25:A4:117:ILE:HD11	25:A4:147:ILE:HG12	1.79	0.63
49:RE:149:VAL:HA	49:RE:152:PHE:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:450:VAL:HB	72:R4:469:ARG:H	1.62	0.63
24:3H:33:LEU:HD11	24:3H:100:ALA:HB1	1.81	0.63
75:M4:260:ILE:HA	75:M4:290:VAL:HB	1.80	0.63
75:M4:401:ILE:HG23	75:M4:406:TYR:HB2	1.80	0.63
45:5I:148:TRP:HE1	45:5I:172:LEU:HD13	1.62	0.63
49:RE:1170:GLY:HA3	49:RE:1177:GLY:HA2	1.81	0.63
51:RG:44:VAL:HG12	51:RG:113:TYR:HB2	1.80	0.63
75:M4:480:LEU:H	75:M4:483:LEU:HD12	1.62	0.63
3:SA:205:U:H2'	3:SA:206:A:H8	1.64	0.63
35:B8:511:LEU:HB2	35:B8:513:GLN:HE22	1.64	0.63
58:RS:221:LEU:HD23	58:RS:224:TRP:HE1	1.64	0.63
5:SF:177:ALA:HA	5:SF:198:LYS:HE2	1.80	0.63
35:B8:521:LEU:HA	35:B8:531:CYS:O	1.99	0.63
36:BE:268:THR:HG22	36:BE:270:SER:H	1.64	0.63
51:RH:116:THR:HG22	51:RH:118:ARG:H	1.64	0.63
31:AG:581:GLY:HA2	31:AG:602:PRO:HD2	1.80	0.63
54:RN:554:GLN:HE22	54:RN:561:ILE:HG22	1.64	0.63
72:R4:142:HIS:O	72:R4:144:ARG:NH2	2.31	0.63
23:3F:211:LEU:HB3	23:3F:212:LYS:HD2	1.81	0.63
30:AF:84:VAL:HA	30:AF:100:ASP:HA	1.80	0.63
29:AE:241:ILE:O	29:AE:245:LEU:HB2	1.99	0.63
65:R3:352:ALA:HB3	65:R3:356:ASN:HB2	1.81	0.63
9:SJ:109:PHE:O	9:SJ:113:PHE:HB2	1.99	0.62
63:R5:237:VAL:HG23	63:R5:248:VAL:HG22	1.80	0.62
67:R2:15:LEU:HD11	67:R2:23:PRO:HD3	1.80	0.62
72:R4:274:TYR:HE1	72:R4:294:ARG:HD2	1.63	0.62
3:SA:1175:U:H3	3:SA:1464:G:H22	1.46	0.62
13:SP:16:VAL:HA	13:SP:80:HIS:O	1.97	0.62
75:M4:139:ARG:NH1	75:M4:159:SER:OG	2.32	0.62
33:B2:268:LYS:HG2	33:B2:288:LYS:HG2	1.81	0.62
56:RP:1724:ASN:HD22	56:RP:1748:ASN:HB2	1.64	0.62
75:M4:139:ARG:NH1	75:M4:155:ASP:O	2.28	0.62
30:AF:273:ILE:HD11	30:AF:306:ALA:HA	1.81	0.62
65:R3:176:VAL:HB	65:R3:250:GLU:HA	1.82	0.62
65:R3:177:ARG:HA	65:R3:187:VAL:HA	1.82	0.62
71:C4:270:THR:H	71:C4:275:MET:HA	1.64	0.62
75:M4:80:VAL:HB	75:M4:125:LEU:HB2	1.81	0.62
23:3F:230:ASN:ND2	23:3F:236:TYR:OH	2.32	0.62
23:3F:405:VAL:HG13	23:3F:415:THR:HG22	1.82	0.62
71:C4:143:VAL:HA	71:C4:153:VAL:HG12	1.80	0.62
72:R4:104:ASN:ND2	72:R4:107:CYS:SG	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3D:4:ILE:H	21:3D:23:GLN:HE22	1.48	0.62
29:AE:671:LEU:HD11	29:AE:723:LEU:HD11	1.80	0.62
30:AF:45:ILE:HD11	30:AF:306:ALA:HB3	1.81	0.62
50:RF:202:VAL:HG22	50:RF:223:LEU:HD12	1.81	0.62
52:RJ:1071:LYS:HA	52:RJ:1074:GLN:HG2	1.81	0.62
52:RJ:1103:GLY:HA2	52:RJ:1107:LYS:HD3	1.82	0.62
65:R3:61:ARG:NH1	65:R3:69:ASP:O	2.33	0.62
75:M4:1042:ALA:HB2	75:M4:1050:LEU:HD23	1.82	0.62
8:SI:57:ALA:HA	8:SI:89:HIS:O	1.99	0.62
36:BE:28:ARG:NH2	36:BE:383:ASP:OD2	2.32	0.62
71:C4:154:GLU:HA	71:C4:202:ARG:HA	1.82	0.62
4:SC:144:ARG:HB2	4:SC:208:GLN:H	1.65	0.62
8:SI:125:ILE:O	8:SI:129:LEU:HB2	2.00	0.62
30:AF:6:PRO:HD2	31:AG:480:SER:HB3	1.82	0.62
58:RS:424:PHE:O	58:RS:428:TYR:HB2	2.00	0.62
65:R3:163:ARG:NH1	66:R6:158:LEU:O	2.33	0.62
33:B2:452:GLY:HA3	33:B2:472:HIS:H	1.65	0.62
3:SA:475:A:H5'	10:SK:130:THR:HG21	1.80	0.61
3:SA:487:G:H1	52:RJ:1119:ILE:HG23	1.64	0.61
20:3B:171:LEU:HB3	20:3B:240:VAL:HG12	1.81	0.61
29:AE:756:LEU:O	29:AE:760:PHE:HB2	2.00	0.61
31:AG:320:VAL:HA	31:AG:334:LEU:O	2.00	0.61
34:B3:669:LEU:HD13	34:B3:684:LEU:HB3	1.81	0.61
35:B8:585:LYS:HE3	35:B8:587:ARG:HH21	1.63	0.61
43:5G:188:HIS:HB2	43:5G:221:VAL:HG12	1.82	0.61
7:SH:56:ASN:HB3	7:SH:60:GLY:HA2	1.83	0.61
21:3D:160:ARG:HG3	21:3D:165:PHE:HB3	1.81	0.61
25:A4:656:ARG:HB3	25:A4:733:PHE:HB3	1.82	0.61
49:RE:307:LYS:HA	49:RE:312:ARG:HG3	1.83	0.61
51:RG:38:THR:O	51:RG:40:ARG:NH1	2.33	0.61
52:RJ:616:ASP:N	52:RJ:616:ASP:OD1	2.31	0.61
56:RP:1761:ILE:HG22	56:RP:1763:LEU:H	1.63	0.61
63:R5:34:ARG:NH1	63:R5:51:MET:O	2.33	0.61
72:R4:663:ASP:OD1	72:R4:675:ARG:NH1	2.33	0.61
1:3A:206:C:N3	1:3A:243:U:O4	2.33	0.61
20:3B:261:LEU:O	21:3D:129:ARG:NH1	2.33	0.61
20:3C:172:TYR:HH	20:3C:180:SER:HG	1.48	0.61
25:A4:398:THR:HG23	25:A4:421:THR:HG22	1.83	0.61
42:5F:115:MET:HG3	42:5F:120:MET:HB3	1.83	0.61
55:RO:181:THR:HA	55:RO:185:TYR:HB3	1.82	0.61
59:RT:110:ARG:NH1	59:RT:130:MET:SD	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3F:398:CYS:SG	23:3F:399:GLU:N	2.72	0.61
35:B8:450:GLN:NE2	35:B8:505:PRO:O	2.33	0.61
36:BE:361:SER:HA	36:BE:636:PRO:CG	2.30	0.61
49:RE:1122:ASN:HA	49:RE:1125:ASN:HB2	1.82	0.61
50:RF:176:ASP:N	50:RF:176:ASP:OD1	2.33	0.61
69:R0:155:ILE:HD11	69:R0:193:LYS:HB3	1.83	0.61
3:SA:748:U:H3	3:SA:801:G:H1	1.46	0.61
3:SA:886:U:H2'	3:SA:887:A:H8	1.65	0.61
3:SA:1731:A:OP2	3:SA:1732:A:N6	2.32	0.61
31:AG:583:LYS:HD3	31:AG:596:LEU:HD13	1.82	0.61
32:B1:581:THR:HG22	32:B1:596:GLY:HA2	1.83	0.61
36:BE:321:GLU:OE1	36:BE:344:ARG:NH1	2.34	0.61
69:R0:124:CYS:SG	69:R0:125:THR:N	2.74	0.61
72:R4:112:ILE:HG12	72:R4:146:ILE:HD11	1.83	0.61
72:R4:182:SER:O	72:R4:186:LYS:N	2.34	0.61
75:M4:288:ARG:NH1	75:M4:312:GLN:OE1	2.34	0.61
75:M4:448:ILE:HG22	75:M4:456:ARG:HG2	1.81	0.61
24:3G:23:VAL:HG11	24:3G:117:VAL:HG21	1.81	0.61
25:A4:279:HIS:HD2	25:A4:281:ALA:H	1.47	0.61
25:A4:589:ASN:HD21	25:A4:632:ASN:HA	1.66	0.61
31:AG:701:VAL:HG11	31:AG:724:ILE:HG21	1.82	0.61
55:RO:494:ASN:O	55:RO:498:PHE:HB2	2.01	0.61
72:R4:198:ASP:HB3	72:R4:201:ASN:HB2	1.83	0.61
33:B2:175:ASP:N	33:B2:175:ASP:OD1	2.33	0.61
34:B3:403:ILE:O	34:B3:414:VAL:HA	2.00	0.61
39:5C:265:GLU:OE2	57:RQ:832:ASN:ND2	2.33	0.61
49:RE:713:LEU:HB2	49:RE:716:SER:HB3	1.83	0.61
50:RF:258:TYR:HB2	50:RF:261:GLN:HG3	1.83	0.61
53:RK:60:THR:HG22	53:RK:81:ILE:HG22	1.81	0.61
7:SH:44:GLU:O	7:SH:119:GLN:NE2	2.34	0.61
14:SR:122:ARG:NH1	14:SR:123:ARG:O	2.34	0.61
25:A4:642:ASN:HB3	25:A4:645:ARG:HB2	1.83	0.61
33:B2:9:GLU:O	33:B2:684:TRP:HA	2.01	0.61
33:B2:537:VAL:HG12	33:B2:548:ILE:HG22	1.83	0.61
59:RT:259:VAL:HA	59:RT:262:ASN:HD22	1.64	0.61
25:A4:565:ARG:HH11	29:AE:628:ASN:HB3	1.65	0.61
29:AE:14:ASN:HB3	39:5C:101:ASN:HD21	1.66	0.61
33:B2:760:ILE:HG13	33:B2:831:LYS:HB2	1.83	0.61
36:BE:727:PRO:HG2	36:BE:730:LYS:HG3	1.83	0.61
53:RK:282:GLU:O	53:RK:286:SER:HB3	2.01	0.61
63:R5:24:ARG:O	69:R0:209:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:R5:250:LYS:HB3	64:R1:199:LEU:HB3	1.83	0.61
72:R4:171:ASP:OD2	72:R4:201:ASN:ND2	2.33	0.61
75:M4:614:ASN:ND2	75:M4:873:SER:O	2.33	0.61
8:SI:172:VAL:O	8:SI:176:LEU:HB2	2.01	0.60
21:3D:65:ASN:ND2	21:3D:75:SER:OG	2.34	0.60
3:SA:647:G:H1	3:SA:687:G:H22	1.48	0.60
23:3F:201:ILE:HG12	23:3F:540:LEU:HD11	1.82	0.60
25:A4:656:ARG:NH1	25:A4:731:HIS:O	2.33	0.60
27:A8:590:PHE:O	27:A8:592:ARG:NH1	2.34	0.60
31:AG:630:LEU:HB3	31:AG:653:PHE:HB2	1.82	0.60
66:R6:131:CYS:SG	66:R6:132:ALA:N	2.74	0.60
67:R2:227:ARG:NH2	68:M3:215:LYS:O	2.30	0.60
68:M3:78:TYR:HB2	68:M3:136:ASP:HB2	1.83	0.60
17:SZ:77:ASN:N	17:SZ:77:ASN:OD1	2.33	0.60
20:3B:238:ASP:HB3	20:3B:262:LYS:HD3	1.83	0.60
30:AF:248:ARG:NH1	30:AF:290:PHE:O	2.35	0.60
39:5C:226:SER:HB3	39:5C:228:LEU:HD13	1.83	0.60
48:RD:1518:ILE:HG12	48:RD:1552:LYS:HG2	1.82	0.60
69:R0:185:GLU:HG2	76:M6:114:THR:HG22	1.83	0.60
1:3A:321:C:OP2	40:5D:120:LYS:NZ	2.33	0.60
3:SA:895:G:H22	3:SA:917:U:H3	1.48	0.60
30:AF:499:LYS:HB3	30:AF:503:ARG:HH21	1.67	0.60
31:AG:439:ASN:ND2	31:AG:496:THR:O	2.34	0.60
37:B6:148:ILE:HG22	46:5J:67:THR:HG22	1.82	0.60
45:5I:273:GLU:HA	57:RQ:302:VAL:HG21	1.83	0.60
34:B3:261:ALA:HB3	34:B3:268:GLN:HB2	1.83	0.60
65:R3:128:ALA:HB2	65:R3:167:LYS:HE3	1.83	0.60
4:SC:19:ARG:HG3	4:SC:20:VAL:HG12	1.84	0.60
15:SX:14:ILE:HG22	15:SX:25:VAL:HG21	1.84	0.60
23:3F:328:ILE:HG13	23:3F:338:THR:HG22	1.83	0.60
23:3F:417:SER:OG	23:3F:418:ASP:N	2.34	0.60
49:RE:466:THR:HG22	49:RE:475:ASN:HD21	1.65	0.60
65:R3:84:LYS:HD2	68:M3:54:GLU:HG3	1.84	0.60
75:M4:197:TYR:HB3	75:M4:236:VAL:HG22	1.84	0.60
3:SA:959:U:H5 <sup>7</sup>	12:SO:14:SER:HB2	1.83	0.60
3:SA:1691:A:N6	3:SA:1711:C:O2 <sup>7</sup>	2.34	0.60
20:3C:253:ILE:HD12	20:3C:269:ILE:HG12	1.83	0.60
32:B1:423:ARG:NH2	32:B1:460:VAL:O	2.35	0.60
33:B2:607:CYS:SG	33:B2:608:HIS:N	2.75	0.60
43:5G:128:VAL:HG11	43:5G:267:GLU:HB2	1.83	0.60
56:RP:111:ALA:HB2	56:RP:154:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:R5:202:ASN:ND2	63:R5:205:ASP:O	2.35	0.60
65:R3:207:ARG:NH1	65:R3:270:GLU:O	2.35	0.60
71:C4:276:THR:HA	71:C4:283:THR:HA	1.83	0.60
3:SA:789:A:N6	10:SK:72:GLU:OE2	2.34	0.60
12:SO:16:ILE:O	15:SX:57:ARG:NH2	2.34	0.60
22:3E:5:LEU:O	22:3E:89:VAL:HA	2.00	0.60
25:A4:741:LEU:C	25:A4:741:LEU:HD23	2.21	0.60
37:B6:26:LYS:HA	37:B6:29:VAL:HG12	1.83	0.60
51:RH:75:GLY:HA2	51:RH:78:LYS:HE3	1.82	0.60
64:R1:47:ASN:ND2	64:R1:133:GLY:O	2.32	0.60
67:R2:260:ARG:HA	67:R2:263:GLU:HB3	1.84	0.60
3:SA:327:U:H1'	11:SM:10:GLU:HG2	1.84	0.60
20:3C:225:ARG:NH1	20:3C:248:ASP:OD2	2.35	0.60
31:AG:598:LYS:HD2	31:AG:638:PHE:HB2	1.84	0.60
45:5I:61:GLN:OE1	45:5I:371:ASN:ND2	2.35	0.60
53:RK:141:MET:HG2	53:RK:300:TYR:HE2	1.67	0.60
63:R5:82:GLU:OE2	68:M3:6:ARG:NH1	2.34	0.60
63:R5:92:GLU:HB2	63:R5:95:ASN:HB2	1.84	0.60
64:R1:53:VAL:HG22	64:R1:124:ILE:HG12	1.84	0.60
3:SA:259:U:H1'	9:SJ:178:ARG:HH12	1.65	0.60
3:SA:1162:C:OP1	6:SG:148:ARG:NH2	2.35	0.60
31:AG:510:TYR:HB2	31:AG:529:LEU:HG	1.84	0.60
65:R3:78:ASN:ND2	65:R3:233:SER:O	2.32	0.60
74:R7:90:ALA:HA	74:R7:93:TYR:HB3	1.84	0.60
23:3F:263:TRP:CZ3	23:3F:270:PRO:CD	2.84	0.59
36:BE:309:ILE:HG22	36:BE:323:VAL:HG23	1.83	0.59
55:RO:320:LEU:HD22	55:RO:361:LEU:HD13	1.84	0.59
63:R5:239:LEU:HG	63:R5:245:VAL:HA	1.84	0.59
65:R3:246:ALA:HA	65:R3:276:CYS:HA	1.84	0.59
75:M4:80:VAL:CG1	75:M4:81:LEU:N	2.59	0.59
75:M4:92:GLU:HB3	75:M4:112:LYS:HB3	1.84	0.59
21:3D:293:CYS:HA	21:3D:309:GLU:HG2	1.85	0.59
26:A5:116:GLN:OE1	26:A5:118:TRP:NE1	2.36	0.59
31:AG:610:SER:HB3	31:AG:704:ASN:HB2	1.84	0.59
31:AG:766:ILE:HD11	31:AG:774:PHE:HB3	1.84	0.59
51:RG:111:GLN:NE2	51:RG:124:VAL:O	2.35	0.59
51:RH:32:THR:OG1	51:RH:125:ASN:ND2	2.35	0.59
3:SA:115:G:H5'	11:SM:129:ARG:HH11	1.67	0.59
31:AG:30:GLY:HA3	31:AG:200:ASN:HA	1.84	0.59
33:B2:629:ASN:HD22	33:B2:643:ASP:HA	1.66	0.59
67:R2:226:ILE:HD12	68:M3:215:LYS:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3B:228:GLN:NE2	21:3D:101:SER:O	2.35	0.59
33:B2:362:ILE:HG12	33:B2:385:ILE:HB	1.85	0.59
36:BE:118:VAL:HA	36:BE:132:THR:HA	1.85	0.59
53:RK:24:ALA:HB2	53:RK:31:ILE:HD12	1.84	0.59
63:R5:209:ASN:O	64:R1:195:LYS:NZ	2.32	0.59
3:SA:551:G:N7	40:5D:2:ALA:N	2.50	0.59
32:B1:524:ARG:NH1	32:B1:526:ASP:OD2	2.36	0.59
49:RE:312:ARG:HH11	49:RE:314:CYS:H	1.50	0.59
49:RE:1148:GLN:NE2	50:RF:172:TYR:OH	2.35	0.59
51:RH:54:LYS:HA	51:RH:65:TYR:HA	1.85	0.59
54:RN:802:GLU:O	54:RN:806:ARG:NH1	2.35	0.59
58:RS:413:LEU:HB3	58:RS:447:ARG:HH12	1.67	0.59
59:RT:99:ILE:HD13	59:RT:159:ILE:HD11	1.84	0.59
68:M3:7:ARG:HG3	68:M3:8:ARG:HG3	1.84	0.59
68:M3:200:VAL:HB	68:M3:214:TRP:HB3	1.84	0.59
72:R4:857:GLN:NE2	72:R4:871:HIS:O	2.35	0.59
33:B2:203:HIS:NE2	33:B2:220:THR:O	2.36	0.59
33:B2:317:ILE:O	33:B2:321:TYR:N	2.36	0.59
34:B3:38:ASP:N	34:B3:38:ASP:OD1	2.35	0.59
45:5I:319:GLU:OE2	45:5I:340:ARG:NH1	2.35	0.59
56:RP:2066:ASP:O	56:RP:2069:GLN:NE2	2.34	0.59
63:R5:28:ARG:NH2	63:R5:32:GLN:O	2.34	0.59
29:AE:477:ASN:HB3	29:AE:490:ARG:HD3	1.84	0.59
29:AE:724:VAL:H	29:AE:755:ARG:HH21	1.49	0.59
31:AG:43:ASN:HA	31:AG:55:TYR:O	2.01	0.59
33:B2:446:ILE:HG21	33:B2:488:LEU:HD11	1.85	0.59
46:5J:106:LEU:O	46:5J:146:ARG:NH1	2.35	0.59
55:RO:289:PHE:HB3	55:RO:329:ARG:HH12	1.67	0.59
59:RT:268:SER:O	59:RT:272:GLU:HB2	2.03	0.59
72:R4:368:LYS:HA	72:R4:371:ARG:HH21	1.67	0.59
72:R4:713:ASN:HA	72:R4:906:VAL:HA	1.85	0.59
75:M4:524:TRP:HH2	75:M4:734:LEU:HD11	1.59	0.59
4:SC:16:GLN:HB2	34:B3:390:LEU:HD21	1.84	0.59
13:SP:16:VAL:HG12	13:SP:80:HIS:HB2	1.84	0.59
21:3D:267:ASP:HB3	22:3E:275:TYR:HE1	1.68	0.59
29:AE:698:ASN:O	29:AE:702:TRP:HB3	2.03	0.59
31:AG:445:ILE:HG12	31:AG:504:GLY:HA3	1.85	0.59
32:B1:389:SER:HB3	32:B1:407:LEU:HD13	1.85	0.59
34:B3:702:LEU:HD21	34:B3:758:ARG:HD3	1.84	0.59
36:BE:747:LYS:H	41:5E:474:ILE:HD12	1.67	0.59
50:RF:23:HIS:HB3	50:RF:26:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:R3:61:ARG:NH2	65:R3:72:ASN:O	2.36	0.59
67:R2:80:VAL:HA	67:R2:128:VAL:HB	1.84	0.59
1:3A:76:U:O2'	31:AG:868:ASN:ND2	2.36	0.59
7:SH:23:ARG:HD3	7:SH:42:GLY:HA2	1.84	0.59
11:SM:125:VAL:HG12	11:SM:139:VAL:HA	1.85	0.59
22:3E:283:ILE:O	22:3E:380:ARG:NH2	2.36	0.59
26:A5:457:LEU:HG	26:A5:483:ARG:HH22	1.67	0.59
30:AF:245:LEU:HD12	30:AF:246:TYR:HB2	1.85	0.59
33:B2:430:CYS:SG	33:B2:431:GLY:N	2.76	0.59
42:5F:69:PRO:HA	42:5F:72:ARG:HG2	1.84	0.59
49:RE:629:THR:HG22	49:RE:669:TRP:HE1	1.67	0.59
53:RK:89:ILE:HA	53:RK:119:LYS:HB2	1.85	0.59
75:M4:970:ALA:HA	75:M4:973:ILE:HD12	1.84	0.59
3:SA:868:G:H1	3:SA:960:U:H3	1.49	0.59
15:SX:44:HIS:NE2	15:SX:112:ASP:OD2	2.36	0.59
25:A4:649:TRP:NE1	25:A4:744:VAL:O	2.35	0.59
26:A5:123:SER:O	26:A5:141:ARG:NH2	2.35	0.59
32:B1:440:PRO:HG3	32:B1:483:GLN:HA	1.85	0.59
36:BE:98:VAL:HG23	36:BE:110:LEU:HB2	1.84	0.59
49:RE:243:LEU:HD22	49:RE:248:LEU:HD21	1.84	0.59
53:RK:339:LEU:HD12	53:RK:350:MET:HB3	1.83	0.59
66:R6:62:ARG:NH2	66:R6:104:PHE:O	2.36	0.59
3:SA:532:U:OP1	10:SK:132:ARG:NH2	2.36	0.58
12:SO:40:TYR:CB	12:SO:45:LEU:HD12	2.31	0.58
20:3C:277:ASP:OD1	25:A4:162:ASN:ND2	2.36	0.58
31:AG:86:GLU:OE1	31:AG:113:ASN:ND2	2.35	0.58
34:B3:288:LEU:HB3	34:B3:307:SER:HB3	1.85	0.58
34:B3:355:LEU:HB3	34:B3:363:ARG:O	2.03	0.58
49:RE:363:THR:HG21	49:RE:394:THR:HG22	1.83	0.58
51:RH:175:CYS:HA	51:RH:201:SER:O	2.03	0.58
69:R0:3:THR:HG23	69:R0:3:THR:O	2.03	0.58
3:SA:1215:C:H42	3:SA:1449:U:H3	1.50	0.58
14:SR:50:GLU:OE2	14:SR:82:ARG:NH1	2.36	0.58
23:3F:263:TRP:CZ3	23:3F:270:PRO:CG	2.86	0.58
25:A4:426:GLN:H	25:A4:444:ARG:HH11	1.49	0.58
25:A4:444:ARG:NH2	38:5B:186:ASP:OD1	2.36	0.58
26:A5:281:ILE:HG12	26:A5:328:VAL:HB	1.84	0.58
26:A5:355:ASN:OD1	31:AG:479:ASN:ND2	2.36	0.58
29:AE:765:ASN:HA	29:AE:768:LYS:HG2	1.85	0.58
31:AG:526:THR:HG22	31:AG:549:ASN:HD21	1.66	0.58
75:M4:436:GLU:O	75:M4:440:LEU:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:151:G:N3	7:SH:13:GLN:NE2	2.51	0.58
3:SA:1627:U:H5''	3:SA:1628:U:H5'	1.85	0.58
25:A4:741:LEU:CD1	25:A4:744:VAL:HG23	2.29	0.58
31:AG:467:GLN:NE2	31:AG:469:ASN:O	2.36	0.58
3:SA:862:A:OP2	12:SO:64:ARG:NH2	2.37	0.58
3:SA:1775:U:O2	3:SA:1786:G:N2	2.35	0.58
11:SM:103:ARG:HH21	11:SM:105:LYS:HD3	1.69	0.58
22:3E:348:VAL:HG12	22:3E:359:ILE:HG23	1.85	0.58
26:A5:20:VAL:HG22	26:A5:29:VAL:HG22	1.84	0.58
34:B3:269:LEU:HB2	34:B3:279:LYS:HB2	1.86	0.58
15:SX:87:GLU:OE2	15:SX:117:ARG:NH2	2.37	0.58
16:SY:141:GLU:HB2	52:RJ:833:ARG:HH12	1.68	0.58
30:AF:216:GLU:N	30:AF:229:CYS:O	2.34	0.58
31:AG:527:HIS:O	31:AG:549:ASN:ND2	2.37	0.58
33:B2:26:ILE:HB	33:B2:40:GLN:HB2	1.85	0.58
49:RE:828:ASP:OD2	49:RE:888:LYS:NZ	2.37	0.58
52:RJ:1018:VAL:O	52:RJ:1029:TRP:NE1	2.36	0.58
53:RK:251:GLN:HE21	53:RK:252:LYS:HE3	1.68	0.58
75:M4:225:ASP:HB3	75:M4:226:ILE:HD12	1.85	0.58
75:M4:325:PRO:O	75:M4:553:GLY:N	2.35	0.58
5:SF:106:LYS:HD2	5:SF:108:ARG:HE	1.69	0.58
7:SH:36:VAL:HB	7:SH:50:PHE:HB2	1.86	0.58
26:A5:463:ARG:HA	26:A5:466:ARG:HE	1.69	0.58
29:AE:336:LEU:O	29:AE:341:LYS:NZ	2.36	0.58
29:AE:659:LEU:HD21	29:AE:691:PHE:HA	1.85	0.58
34:B3:231:CYS:SG	34:B3:232:LYS:N	2.76	0.58
52:RJ:553:ILE:HG21	53:RK:326:LEU:HD23	1.86	0.58
75:M4:742:LEU:HD12	75:M4:746:ILE:HG21	1.86	0.58
20:3B:90:PRO:HD3	46:5J:106:LEU:HD12	1.85	0.58
20:3C:91:HIS:ND1	40:5D:164:ASN:OD1	2.37	0.58
22:3E:339:TYR:HB3	22:3E:343:TYR:HB2	1.84	0.58
26:A5:472:LEU:HD12	26:A5:476:LEU:HD21	1.86	0.58
29:AE:556:LYS:HG3	29:AE:558:VAL:H	1.69	0.58
34:B3:294:LEU:HB2	34:B3:303:PHE:HB2	1.84	0.58
49:RE:1205:LYS:O	49:RE:1212:VAL:HA	2.04	0.58
64:R1:95:ARG:HA	64:R1:98:LEU:HD12	1.86	0.58
26:A5:168:HIS:H	26:A5:191:VAL:HG23	1.69	0.58
31:AG:88:ILE:HA	31:AG:111:THR:HA	1.85	0.58
33:B2:94:LEU:O	33:B2:105:VAL:HA	2.04	0.58
48:RD:1659:VAL:HG21	48:RD:1678:ILE:HD11	1.86	0.58
49:RE:429:LEU:O	49:RE:489:LYS:NZ	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:RK:68:SER:HB2	53:RK:73:THR:HG22	1.86	0.58
55:RO:280:ILE:HB	55:RO:284:ARG:HB2	1.85	0.58
68:M3:44:GLN:OE1	68:M3:237:TYR:OH	2.22	0.58
68:M3:47:SER:HG	68:M3:49:HIS:HE2	1.45	0.58
72:R4:858:LEU:HD12	72:R4:861:ALA:HB3	1.85	0.58
75:M4:132:THR:O	75:M4:163:ARG:NH1	2.35	0.58
75:M4:492:GLN:NE2	75:M4:510:ASN:O	2.37	0.58
3:SA:57:G:OP1	17:SZ:112:LYS:NZ	2.37	0.58
20:3B:277:ASP:N	20:3B:277:ASP:OD1	2.37	0.58
30:AF:256:THR:N	30:AF:275:SER:O	2.37	0.58
49:RE:496:LEU:O	49:RE:500:ASN:ND2	2.37	0.58
49:RE:1205:LYS:HB2	49:RE:1213:ILE:O	2.03	0.58
63:R5:210:ILE:HG22	63:R5:211:LYS:HG2	1.86	0.58
66:R6:52:VAL:HG22	66:R6:92:CYS:HB2	1.86	0.58
67:R2:22:ARG:HD2	67:R2:26:ARG:HB2	1.86	0.58
3:SA:886:U:OP1	4:SC:214:LYS:NZ	2.37	0.58
8:SI:56:LYS:HB2	8:SI:88:ARG:HD3	1.86	0.58
27:A8:305:VAL:HA	27:A8:311:VAL:HA	1.86	0.58
33:B2:20:ASN:HA	33:B2:339:LYS:HD3	1.86	0.58
34:B3:559:ILE:HB	34:B3:569:LYS:HB2	1.85	0.58
35:B8:180:ASP:OD2	36:BE:281:ARG:NH2	2.36	0.58
49:RE:975:LEU:HD22	49:RE:1041:VAL:HG12	1.83	0.58
66:R6:7:ILE:O	66:R6:220:ARG:NH2	2.35	0.58
66:R6:107:ARG:NH2	66:R6:149:PRO:O	2.37	0.58
20:3B:165:ALA:HB3	20:3B:168:LYS:HG2	1.86	0.57
22:3E:199:VAL:HG11	22:3E:227:LEU:HD22	1.85	0.57
25:A4:312:ASN:HA	25:A4:315:GLN:HE21	1.68	0.57
33:B2:390:GLN:O	33:B2:411:ASN:ND2	2.37	0.57
49:RE:793:PRO:HG2	49:RE:799:LEU:HA	1.85	0.57
72:R4:83:ILE:HD11	72:R4:224:LEU:HD13	1.86	0.57
1:3A:321:C:OP1	40:5D:117:LYS:NZ	2.38	0.57
22:3E:430:ASP:HA	36:BE:125:GLY:HA2	1.86	0.57
29:AE:641:LEU:O	29:AE:644:LYS:NZ	2.37	0.57
29:AE:718:ARG:HA	29:AE:721:VAL:HG12	1.87	0.57
30:AF:466:VAL:O	30:AF:470:TYR:HB2	2.04	0.57
34:B3:267:PHE:H	34:B3:281:THR:HG22	1.69	0.57
51:RG:239:SER:O	51:RG:243:HIS:ND1	2.29	0.57
63:R5:262:MET:O	63:R5:266:HIS:ND1	2.33	0.57
72:R4:444:LEU:HA	72:R4:447:LYS:HD2	1.85	0.57
72:R4:617:PRO:HA	72:R4:648:SER:HB3	1.86	0.57
2:5A:86:C:O2'	30:AF:5:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:332:U:OP1	9:SJ:31:ARG:NE	2.37	0.57
26:A5:55:ASP:N	26:A5:55:ASP:OD1	2.37	0.57
27:A8:536:ARG:NH1	27:A8:537:THR:OG1	2.37	0.57
31:AG:321:MET:HB3	31:AG:334:LEU:HB3	1.86	0.57
32:B1:119:LEU:HD22	32:B1:163:THR:HG21	1.85	0.57
37:B6:38:ASP:OD2	37:B6:42:ARG:NH1	2.36	0.57
39:5C:183:GLU:OE2	42:5F:41:ARG:NH2	2.37	0.57
41:5E:351:ALA:HA	43:5G:285:ASN:HB3	1.86	0.57
56:RP:1948:SER:O	56:RP:1985:ARG:NH2	2.37	0.57
64:R1:13:ARG:HD3	64:R1:171:LEU:HD22	1.86	0.57
75:M4:502:THR:OG1	75:M4:503:GLU:N	2.38	0.57
3:SA:318:U:O2	3:SA:346:G:O6	2.23	0.57
16:SY:121:ARG:NH2	54:RN:795:GLU:OE2	2.38	0.57
20:3B:125:VAL:HG12	46:5J:150:GLY:HA3	1.86	0.57
20:3B:253:ILE:HD13	20:3B:269:ILE:HD12	1.85	0.57
30:AF:283:VAL:H	30:AF:292:VAL:HG23	1.69	0.57
33:B2:448:GLY:HA3	33:B2:476:ILE:HD11	1.86	0.57
34:B3:30:LYS:HA	34:B3:42:ILE:O	2.04	0.57
34:B3:337:HIS:HD2	34:B3:363:ARG:HE	1.51	0.57
39:5C:114:TYR:HA	39:5C:128:THR:O	2.04	0.57
39:5C:415:GLU:OE2	45:5I:33:HIS:ND1	2.34	0.57
56:RP:182:SER:HG	56:RP:228:LEU:N	2.03	0.57
71:C4:158:VAL:O	71:C4:189:SER:N	2.37	0.57
75:M4:201:ILE:HG22	75:M4:203:ALA:H	1.69	0.57
75:M4:1009:THR:HG22	75:M4:1011:THR:H	1.69	0.57
3:SA:5:U:O2	3:SA:7:G:N2	2.37	0.57
3:SA:901:G:H3'	3:SA:902:G:H8	1.70	0.57
10:SK:58:ASP:N	10:SK:58:ASP:OD1	2.36	0.57
20:3B:244:VAL:O	20:3B:249:GLN:NE2	2.37	0.57
23:3F:333:MET:SD	23:3F:335:ARG:NH1	2.76	0.57
26:A5:547:LEU:HD11	30:AF:487:LEU:HD21	1.87	0.57
47:5K:145:VAL:HG11	47:5K:170:ILE:HD13	1.87	0.57
49:RE:792:TRP:HE3	49:RE:793:PRO:HD2	1.69	0.57
50:RF:262:VAL:HA	50:RF:265:ARG:HG2	1.86	0.57
51:RH:168:THR:HA	51:RH:171:LEU:HG	1.84	0.57
65:R3:371:PRO:HA	65:R3:374:ILE:HD12	1.87	0.57
72:R4:566:VAL:HB	72:R4:628:TRP:HB2	1.86	0.57
20:3B:306:LEU:HD11	20:3B:313:HIS:HB2	1.86	0.57
21:3D:14:GLY:HA3	21:3D:55:PRO:HA	1.87	0.57
49:RE:218:ASP:HA	49:RE:223:ARG:HH12	1.70	0.57
57:RQ:316:ASN:HD21	57:RQ:895:LYS:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:RS:398:ARG:NH1	58:RS:446:GLN:OE1	2.38	0.57
71:C4:228:ASP:OD2	71:C4:286:ARG:NH1	2.38	0.57
75:M4:747:ARG:NH1	75:M4:750:GLU:OE1	2.37	0.57
22:3E:303:SER:HB2	22:3E:309:LEU:HB3	1.87	0.57
26:A5:552:ASN:HA	26:A5:555:LYS:HB2	1.86	0.57
29:AE:424:LEU:HG	29:AE:426:GLY:H	1.69	0.57
30:AF:33:ALA:HA	30:AF:329:ILE:O	2.05	0.57
33:B2:17:ILE:HG12	33:B2:360:ASN:HB2	1.87	0.57
34:B3:15:ILE:HG21	34:B3:379:LEU:HD11	1.87	0.57
35:B8:311:ASN:ND2	35:B8:325:ASP:OD1	2.38	0.57
39:5C:356:GLY:O	39:5C:364:ARG:NH1	2.37	0.57
41:5E:302:LYS:HA	41:5E:305:ILE:HG12	1.87	0.57
54:RN:467:ASN:HD22	54:RN:470:LEU:HD11	1.70	0.57
75:M4:351:GLU:O	75:M4:355:LYS:N	2.34	0.57
2:5A:480:C:O2	37:B6:46:ARG:NH2	2.38	0.57
3:SA:953:G:H2 <sup>?</sup>	3:SA:954:G:H8	1.69	0.57
8:SI:147:ASN:ND2	45:5I:180:SER:OG	2.37	0.57
26:A5:284:LYS:NZ	26:A5:330:ILE:O	2.37	0.57
29:AE:413:ASP:HA	29:AE:416:LEU:HB2	1.86	0.57
31:AG:616:SER:HB3	31:AG:621:LEU:HG	1.87	0.57
33:B2:259:ILE:HA	33:B2:273:TYR:O	2.04	0.57
37:B6:175:ASN:OD1	37:B6:175:ASN:N	2.37	0.57
53:RK:89:ILE:HG22	53:RK:119:LYS:HG3	1.86	0.57
54:RN:554:GLN:HA	54:RN:557:SER:HB2	1.87	0.57
68:M3:103:GLU:HG3	68:M3:144:ASP:HB3	1.85	0.57
1:3A:168:C:OP1	23:3F:182:LYS:NZ	2.38	0.57
20:3C:171:LEU:HB2	20:3C:237:VAL:HG11	1.87	0.57
22:3E:355:ASN:ND2	22:3E:402:GLU:OE2	2.38	0.57
32:B1:520:ALA:HB3	32:B1:533:SER:HB3	1.87	0.57
36:BE:429:ASN:HD22	36:BE:445:MET:HB3	1.69	0.57
48:RD:1674:LEU:HA	48:RD:1677:ARG:HG2	1.87	0.57
53:RK:361:ASN:O	53:RK:364:LYS:NZ	2.37	0.57
66:R6:26:VAL:HG22	66:R6:94:ILE:HA	1.87	0.57
72:R4:881:CYS:O	72:R4:885:ASN:ND2	2.38	0.57
72:R4:985:SER:HA	72:R4:997:GLU:H	1.70	0.57
3:SA:67:A:N6	3:SA:83:G:O2 <sup>?</sup>	2.37	0.57
3:SA:207:U:O2	9:SJ:178:ARG:NH1	2.38	0.57
8:SI:187:SER:OG	8:SI:188:GLU:N	2.38	0.57
23:3F:475:ILE:HA	23:3F:491:SER:HB3	1.87	0.57
25:A4:497:ILE:HD11	25:A4:555:LEU:HD12	1.86	0.57
25:A4:621:ASN:ND2	25:A4:663:PHE:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A8:563:LEU:HA	27:A8:566:LEU:HB2	1.87	0.57
40:5D:37:ARG:NH2	52:RJ:994:LYS:O	2.38	0.57
49:RE:202:SER:OG	49:RE:203:ILE:N	2.37	0.57
49:RE:756:VAL:O	49:RE:761:ARG:NH2	2.37	0.57
49:RE:1166:ARG:HG3	49:RE:1181:VAL:HG22	1.87	0.57
50:RF:85:GLU:HG2	50:RF:86:GLU:HG3	1.87	0.57
51:RH:50:LEU:O	51:RH:118:ARG:NH1	2.38	0.57
52:RJ:169:GLY:O	52:RJ:204:LEU:HA	2.05	0.57
53:RK:161:LEU:HB2	53:RK:238:SER:HB2	1.86	0.57
72:R4:558:LYS:HA	72:R4:564:TRP:HA	1.85	0.57
75:M4:588:ASN:ND2	75:M4:912:SER:OG	2.38	0.57
3:SA:283:U:H5'	7:SH:188:ARG:HD3	1.87	0.56
25:A4:75:ASN:HA	25:A4:91:ILE:O	2.05	0.56
32:B1:209:VAL:HG22	32:B1:215:VAL:HG22	1.87	0.56
32:B1:558:ASP:N	32:B1:558:ASP:OD1	2.37	0.56
33:B2:897:ASP:OD2	34:B3:758:ARG:NH1	2.38	0.56
51:RG:44:VAL:HA	51:RG:113:TYR:O	2.05	0.56
65:R3:24:ARG:NH2	71:C4:193:ALA:O	2.38	0.56
67:R2:37:PHE:HB2	67:R2:49:ARG:HB3	1.87	0.56
67:R2:259:VAL:O	67:R2:263:GLU:N	2.32	0.56
72:R4:492:TYR:HA	72:R4:601:ILE:HG21	1.87	0.56
72:R4:692:GLY:HA2	72:R4:784:LYS:HB2	1.86	0.56
75:M4:285:ASP:OD1	75:M4:310:HIS:ND1	2.34	0.56
75:M4:524:TRP:HH2	75:M4:734:LEU:HD13	1.70	0.56
1:3A:95:A:H61	1:3A:321:C:H42	1.52	0.56
25:A4:739:LYS:HE2	25:A4:739:LYS:N	2.20	0.56
31:AG:59:THR:O	31:AG:61:GLN:NE2	2.38	0.56
32:B1:737:ASN:O	32:B1:741:MET:HB2	2.04	0.56
48:RD:1583:SER:HA	48:RD:1586:VAL:HG22	1.86	0.56
49:RE:1162:ILE:HG23	49:RE:1187:LYS:HZ1	1.70	0.56
68:M3:86:SER:OG	68:M3:87:PHE:N	2.37	0.56
75:M4:344:GLU:OE2	75:M4:552:ARG:NH1	2.37	0.56
1:3A:329:C:H2'	1:3A:330:A:H8	1.70	0.56
3:SA:447:U:O2'	5:SF:27:TYR:O	2.23	0.56
5:SF:100:ARG:HH11	5:SF:236:ILE:HG23	1.70	0.56
27:A8:28:TYR:HA	27:A8:356:THR:HA	1.87	0.56
33:B2:655:ALA:O	33:B2:682:ARG:NH1	2.39	0.56
48:RD:1607:ASN:HD22	48:RD:1610:LYS:HZ3	1.53	0.56
49:RE:423:LYS:HG2	49:RE:427:LYS:HE2	1.86	0.56
50:RF:14:ILE:HB	50:RF:39:ALA:HB3	1.87	0.56
52:RJ:864:ASP:OD2	52:RJ:868:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:R2:58:CYS:SG	67:R2:59:ILE:N	2.79	0.56
69:R0:122:ARG:NH1	69:R0:123:VAL:O	2.38	0.56
72:R4:484:LEU:O	72:R4:488:HIS:ND1	2.38	0.56
75:M4:441:THR:OG1	75:M4:469:ARG:NH1	2.37	0.56
11:SM:128:CYS:SG	11:SM:129:ARG:N	2.79	0.56
22:3E:430:ASP:OD2	35:B8:142:LYS:NZ	2.39	0.56
29:AE:218:ILE:HG22	29:AE:263:VAL:HG11	1.87	0.56
33:B2:795:ILE:O	33:B2:798:ASN:ND2	2.39	0.56
49:RE:377:SER:HB3	49:RE:389:GLY:HA3	1.86	0.56
68:M3:76:ALA:HB3	68:M3:138:PHE:HB2	1.88	0.56
69:R0:73:ILE:O	69:R0:191:ASN:ND2	2.38	0.56
72:R4:537:LYS:O	72:R4:649:ARG:NH2	2.38	0.56
72:R4:852:VAL:HA	72:R4:855:HIS:HD2	1.70	0.56
75:M4:926:GLY:O	75:M4:929:ASN:ND2	2.37	0.56
3:SA:1170:G:N2	3:SA:1469:A:N1	2.51	0.56
23:3F:162:CYS:HA	23:3F:187:ALA:HA	1.88	0.56
31:AG:75:SER:HB2	31:AG:79:LEU:HG	1.88	0.56
57:RQ:874:SER:O	57:RQ:878:LEU:HB2	2.06	0.56
72:R4:139:SER:HB3	72:R4:144:ARG:HA	1.88	0.56
3:SA:564:G:O6	40:5D:42:HIS:NE2	2.39	0.56
25:A4:488:ILE:O	25:A4:495:VAL:HA	2.06	0.56
27:A8:596:LYS:HE2	27:A8:643:ASP:HB3	1.87	0.56
32:B1:379:CYS:SG	32:B1:380:LEU:N	2.78	0.56
33:B2:171:CYS:SG	33:B2:172:GLN:N	2.79	0.56
34:B3:9:GLY:HA2	34:B3:644:TRP:HA	1.87	0.56
52:RJ:831:ARG:NH1	52:RJ:877:GLU:O	2.38	0.56
54:RN:448:PHE:HA	54:RN:451:THR:HG22	1.87	0.56
56:RP:1798:LEU:HD12	56:RP:1801:ASN:HD22	1.70	0.56
58:RS:221:LEU:HA	58:RS:224:TRP:HD1	1.70	0.56
68:M3:93:ILE:HA	68:M3:135:ILE:HB	1.87	0.56
72:R4:401:ARG:NH1	72:R4:402:GLN:O	2.38	0.56
72:R4:538:LEU:HA	72:R4:649:ARG:HH21	1.71	0.56
75:M4:810:PRO:O	75:M4:816:ILE:N	2.38	0.56
2:5A:20:C:H2'	2:5A:21:A:H8	1.70	0.56
3:SA:505:A:OP1	3:SA:585:A:N6	2.39	0.56
25:A4:579:ARG:NH2	25:A4:612:THR:OG1	2.39	0.56
26:A5:253:LEU:HB2	26:A5:291:ILE:HD11	1.87	0.56
31:AG:154:LEU:HD11	31:AG:171:TYR:HB3	1.87	0.56
34:B3:42:ILE:HG22	34:B3:49:SER:HA	1.88	0.56
39:5C:378:VAL:HG12	39:5C:394:HIS:HB3	1.88	0.56
50:RF:101:SER:O	50:RF:105:SER:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RJ:300:GLN:HE21	52:RJ:792:VAL:HG21	1.70	0.56
64:R1:131:GLN:HG3	64:R1:135:ILE:HD13	1.86	0.56
72:R4:867:LEU:O	72:R4:872:ARG:NH2	2.38	0.56
75:M4:194:ARG:HB2	75:M4:256:VAL:HG22	1.87	0.56
26:A5:299:ASP:HA	26:A5:319:TRP:HE3	1.70	0.56
28:A9:433:ILE:HA	28:A9:436:THR:HG22	1.88	0.56
40:5D:29:GLU:OE2	40:5D:37:ARG:NH1	2.39	0.56
43:5G:93:SER:O	43:5G:119:ARG:NH2	2.38	0.56
52:RJ:135:ALA:O	52:RJ:238:ARG:NH1	2.39	0.56
69:R0:5:ILE:N	69:R0:40:GLY:O	2.38	0.56
72:R4:316:VAL:HG12	72:R4:395:ILE:HG23	1.87	0.56
75:M4:325:PRO:HD2	75:M4:552:ARG:HA	1.88	0.56
3:SA:1688:U:O4	3:SA:1713:G:O6	2.23	0.56
10:SK:94:ASP:N	10:SK:94:ASP:OD1	2.37	0.56
10:SK:169:PRO:O	10:SK:174:ARG:NH2	2.39	0.56
20:3C:142:ARG:NH1	20:3C:186:ASP:OD2	2.39	0.56
26:A5:210:ARG:NH1	36:BE:563:ASP:OD2	2.37	0.56
32:B1:152:LEU:HD11	32:B1:161:ILE:HD11	1.88	0.56
32:B1:789:SER:O	36:BE:728:ARG:NH2	2.39	0.56
33:B2:162:HIS:O	41:5E:522:ARG:NH2	2.39	0.56
47:5K:103:MET:SD	47:5K:127:ARG:NH1	2.79	0.56
64:R1:162:SER:HA	64:R1:186:THR:HA	1.87	0.56
72:R4:115:GLN:HB2	72:R4:149:HIS:HA	1.87	0.56
75:M4:422:LEU:HD23	75:M4:425:LYS:HD2	1.88	0.56
3:SA:246:G:N2	11:SM:66:ILE:O	2.38	0.56
3:SA:576:G:H4'	41:5E:327:LYS:HE2	1.87	0.56
3:SA:857:U:OP2	50:RF:259:ARG:NH2	2.39	0.56
25:A4:479:LYS:NZ	25:A4:535:GLU:OE1	2.39	0.56
26:A5:2:ASP:HB3	35:B8:281:THR:HG21	1.88	0.56
29:AE:35:TYR:O	29:AE:150:ARG:NH1	2.39	0.56
29:AE:171:GLU:OE2	29:AE:172:LYS:NZ	2.39	0.56
36:BE:733:THR:O	36:BE:737:LEU:HB3	2.06	0.56
41:5E:312:GLU:O	41:5E:316:ASN:ND2	2.38	0.56
49:RE:804:THR:HG22	49:RE:838:VAL:HG22	1.87	0.56
55:RO:224:ASN:HB3	55:RO:280:ILE:HD13	1.87	0.56
65:R3:69:ASP:OD2	68:M3:145:LYS:NZ	2.39	0.56
11:SM:47:THR:O	11:SM:51:GLY:HA3	2.06	0.55
20:3C:92:ARG:NH1	20:3C:160:ASP:O	2.39	0.55
30:AF:48:ASN:ND2	30:AF:51:HIS:O	2.39	0.55
49:RE:118:GLN:HA	49:RE:121:VAL:HG12	1.88	0.55
51:RG:72:ASP:N	51:RG:72:ASP:OD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:RK:109:PHE:HA	53:RK:361:ASN:HD22	1.70	0.55
63:R5:50:LYS:HG3	63:R5:55:LYS:HG2	1.88	0.55
67:R2:190:LEU:HB2	67:R2:213:LEU:HB2	1.88	0.55
75:M4:695:VAL:HA	75:M4:721:VAL:HG22	1.87	0.55
3:SA:65:A:H2	3:SA:84:A:H62	1.54	0.55
21:3D:254:ASN:O	21:3D:258:SER:HB3	2.07	0.55
36:BE:738:ASP:N	36:BE:738:ASP:OD1	2.38	0.55
52:RJ:263:LEU:O	52:RJ:264:GLN:NE2	2.40	0.55
53:RK:340:LYS:HB2	53:RK:351:ILE:HB	1.89	0.55
72:R4:160:ARG:NH1	72:R4:164:GLU:O	2.40	0.55
72:R4:630:LEU:HD13	72:R4:634:ALA:HA	1.88	0.55
3:SA:1472:C:N4	3:SA:1535:U:OP2	2.39	0.55
3:SA:1576:A:H5''	51:RH:165:ASN:HB2	1.89	0.55
22:3E:359:ILE:HA	22:3E:362:VAL:HG12	1.89	0.55
56:RP:149:GLU:O	56:RP:153:ASN:HB2	2.07	0.55
72:R4:181:TYR:HB3	72:R4:192:VAL:HG11	1.88	0.55
75:M4:531:TRP:NE1	75:M4:561:GLU:OE2	2.37	0.55
7:SH:3:LEU:HA	7:SH:109:LEU:O	2.06	0.55
10:SK:60:LEU:HD22	56:RP:1848:VAL:HG11	1.89	0.55
22:3E:385:ASP:N	22:3E:385:ASP:OD1	2.39	0.55
25:A4:119:GLY:HA3	38:5B:194:LYS:HG3	1.89	0.55
25:A4:491:CYS:O	25:A4:530:ARG:NH2	2.39	0.55
26:A5:85:ILE:HB	26:A5:99:PHE:HB2	1.88	0.55
26:A5:366:GLY:O	31:AG:583:LYS:NZ	2.39	0.55
26:A5:548:ASP:O	26:A5:552:ASN:ND2	2.40	0.55
35:B8:448:LYS:NZ	35:B8:449:ASP:O	2.37	0.55
42:5F:33:MET:HB2	42:5F:38:ILE:HB	1.88	0.55
56:RP:1721:ILE:HA	56:RP:1748:ASN:HD21	1.72	0.55
65:R3:136:VAL:HA	65:R3:219:VAL:HB	1.89	0.55
65:R3:158:SER:O	65:R3:162:SER:N	2.39	0.55
72:R4:100:ASP:OD1	72:R4:131:ARG:NH2	2.34	0.55
75:M4:863:MET:O	75:M4:867:LYS:N	2.37	0.55
20:3C:199:PHE:HB2	20:3C:223:ASP:HA	1.87	0.55
21:3D:174:ILE:HD13	21:3D:296:MET:HG2	1.89	0.55
34:B3:94:LYS:HB2	59:RT:273:ARG:HH21	1.71	0.55
34:B3:466:TRP:HA	34:B3:479:ILE:HG12	1.88	0.55
34:B3:732:ASN:ND2	34:B3:734:GLU:OE2	2.40	0.55
40:5D:148:PRO:HD2	40:5D:151:PHE:HB2	1.87	0.55
43:5G:123:VAL:HG12	43:5G:125:PRO:HD2	1.87	0.55
52:RJ:255:PRO:HA	52:RJ:258:ILE:HG22	1.88	0.55
66:R6:110:SER:O	66:R6:114:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:R0:84:TYR:N	69:R0:97:LEU:O	2.36	0.55
72:R4:520:GLU:O	72:R4:524:LYS:N	2.39	0.55
75:M4:684:VAL:HA	75:M4:766:SER:HA	1.89	0.55
27:A8:671:ARG:NH1	28:A9:447:ASN:O	2.39	0.55
29:AE:637:ILE:O	29:AE:641:LEU:HB2	2.07	0.55
30:AF:184:VAL:O	30:AF:195:LEU:HA	2.07	0.55
31:AG:510:TYR:HE1	31:AG:527:HIS:HB3	1.72	0.55
49:RE:228:ARG:HG3	49:RE:296:ILE:HD11	1.88	0.55
52:RJ:133:LYS:O	52:RJ:238:ARG:NH2	2.40	0.55
63:R5:107:ILE:O	63:R5:111:SER:N	2.37	0.55
63:R5:235:LEU:HD13	63:R5:250:LYS:HB2	1.87	0.55
72:R4:900:GLU:O	72:R4:904:GLY:N	2.35	0.55
72:R4:921:VAL:HA	72:R4:926:ILE:HG22	1.88	0.55
34:B3:303:PHE:HA	34:B3:312:GLN:O	2.06	0.55
46:5J:124:ILE:HA	46:5J:127:ARG:HG3	1.88	0.55
63:R5:164:LYS:O	63:R5:185:VAL:N	2.35	0.55
4:SC:144:ARG:HB3	4:SC:206:PRO:HB2	1.89	0.55
9:SJ:78:ILE:HA	9:SJ:104:ILE:HG23	1.89	0.55
12:SO:71:ILE:HA	12:SO:74:ILE:HG12	1.89	0.55
23:3F:263:TRP:CH2	23:3F:270:PRO:HG3	2.42	0.55
24:3G:118:LYS:HA	24:3G:121:ILE:HD12	1.88	0.55
25:A4:274:GLN:HE22	25:A4:320:TRP:H	1.53	0.55
25:A4:583:VAL:HA	25:A4:592:TYR:O	2.05	0.55
25:A4:740:PRO:C	25:A4:756:GLU:HG2	2.24	0.55
41:5E:314:LEU:HA	41:5E:317:GLU:HB2	1.88	0.55
53:RK:18:ARG:NH2	53:RK:101:GLU:OE1	2.39	0.55
55:RO:383:LEU:HD12	55:RO:386:LEU:HD23	1.89	0.55
65:R3:159:ILE:O	65:R3:162:SER:OG	2.25	0.55
68:M3:49:HIS:HD2	68:M3:61:LEU:HD12	1.72	0.55
72:R4:753:ARG:HD3	72:R4:839:TYR:HE2	1.72	0.55
75:M4:465:LEU:O	75:M4:469:ARG:N	2.39	0.55
75:M4:794:LEU:O	75:M4:798:ASN:N	2.35	0.55
3:SA:215:A:N6	3:SA:242:U:OP2	2.39	0.55
3:SA:1663:G:N2	3:SA:1738:U:O2	2.29	0.55
3:SA:1671:A:N6	3:SA:1730:A:O2'	2.40	0.55
13:SP:64:ALA:HB1	13:SP:105:LEU:HG	1.89	0.55
14:SR:99:GLU:HB3	36:BE:490:GLN:HE22	1.72	0.55
23:3F:471:GLN:HG3	24:3H:83:SER:HB2	1.88	0.55
29:AE:186:MET:N	29:AE:186:MET:SD	2.80	0.55
31:AG:561:LEU:O	31:AG:573:CYS:HA	2.07	0.55
36:BE:846:ASP:OD2	36:BE:850:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B6:41:HIS:O	37:B6:45:SER:HB3	2.07	0.55
43:5G:88:ILE:O	43:5G:114:ALA:HA	2.07	0.55
43:5G:91:THR:O	43:5G:141:VAL:HA	2.06	0.55
52:RJ:634:ARG:NH2	53:RK:256:TYR:OH	2.40	0.55
66:R6:208:ASN:OD1	66:R6:211:ARG:NH2	2.37	0.55
67:R2:227:ARG:NH1	68:M3:216:ASP:OD1	2.39	0.55
68:M3:129:ARG:NH1	68:M3:186:GLU:OE2	2.40	0.55
72:R4:493:ARG:O	72:R4:590:ARG:NH2	2.33	0.55
75:M4:398:VAL:O	75:M4:402:TRP:N	2.34	0.55
75:M4:419:CYS:O	75:M4:423:ALA:N	2.37	0.55
2:5A:85:G:H21	2:5A:86:C:H41	1.55	0.55
3:SA:269:G:OP2	7:SH:186:ARG:NH2	2.37	0.55
6:SG:117:THR:HG21	6:SG:194:LEU:HD23	1.89	0.55
25:A4:111:SER:OG	25:A4:113:ARG:NH1	2.40	0.55
27:A8:657:ASN:HA	27:A8:660:LEU:HD12	1.88	0.55
27:A8:671:ARG:NH1	28:A9:449:GLU:O	2.40	0.55
31:AG:388:PRO:HA	31:AG:458:GLN:HE22	1.72	0.55
33:B2:454:LEU:O	33:B2:467:THR:HA	2.07	0.55
49:RE:142:GLU:O	49:RE:144:LYS:NZ	2.40	0.55
53:RK:53:LEU:HD23	53:RK:65:ILE:HG21	1.89	0.55
54:RN:61:LYS:NZ	54:RN:62:ALA:O	2.39	0.55
71:C4:159:GLU:HA	71:C4:188:PHE:HA	1.89	0.55
72:R4:328:ALA:HA	72:R4:386:ILE:HA	1.89	0.55
3:SA:142:G:C6	3:SA:173:A:N1	2.74	0.54
11:SM:21:ASN:OD1	11:SM:30:ARG:NH2	2.40	0.54
26:A5:242:ASP:OD1	26:A5:242:ASP:N	2.34	0.54
32:B1:412:ARG:NH1	32:B1:424:THR:OG1	2.40	0.54
49:RE:376:SER:OG	49:RE:378:ASN:ND2	2.40	0.54
50:RF:226:ILE:HA	50:RF:229:LYS:HG2	1.89	0.54
65:R3:367:ALA:O	66:R6:176:ASN:ND2	2.40	0.54
72:R4:531:ARG:NH1	72:R4:644:SER:O	2.40	0.54
72:R4:752:LEU:HD13	72:R4:821:SER:HB3	1.89	0.54
75:M4:540:MET:O	75:M4:543:ARG:NH2	2.40	0.54
75:M4:890:ARG:NH2	75:M4:899:ASP:OD1	2.39	0.54
3:SA:1219:A:N6	3:SA:1264:G:H21	2.05	0.54
3:SA:1634:C:OP1	32:B1:418:ARG:NH1	2.41	0.54
12:SO:99:ARG:NH2	12:SO:119:GLU:OE2	2.40	0.54
23:3F:303:LYS:HD3	23:3F:317:ILE:HD11	1.89	0.54
29:AE:556:LYS:O	29:AE:592:ARG:NH2	2.39	0.54
30:AF:233:ASN:ND2	30:AF:247:GLU:OE1	2.40	0.54
34:B3:454:LEU:O	34:B3:465:LYS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5C:354:CYS:SG	39:5C:355:PHE:N	2.78	0.54
48:RD:1633:ASP:OD2	48:RD:1636:ARG:NH1	2.40	0.54
68:M3:126:ASN:ND2	68:M3:186:GLU:OE1	2.40	0.54
69:R0:97:LEU:HD13	69:R0:134:ILE:HG13	1.88	0.54
72:R4:767:ASN:HA	72:R4:770:LEU:HB2	1.88	0.54
3:SA:1194:A:N6	51:RG:129:ARG:O	2.40	0.54
21:3D:335:ILE:HD12	21:3D:338:ALA:HB3	1.89	0.54
25:A4:116:SER:HB3	25:A4:126:TRP:HE1	1.72	0.54
29:AE:499:THR:HA	29:AE:502:ILE:HG23	1.90	0.54
30:AF:314:GLY:O	30:AF:332:LYS:NZ	2.40	0.54
35:B8:217:ASN:OD1	35:B8:217:ASN:N	2.41	0.54
37:B6:290:LYS:HD2	37:B6:294:ALA:HA	1.87	0.54
45:5I:228:ASN:ND2	45:5I:230:ASN:O	2.41	0.54
52:RJ:246:ALA:HB3	52:RJ:810:ILE:HG13	1.89	0.54
67:R2:78:VAL:HA	67:R2:126:VAL:HB	1.89	0.54
71:C4:142:ARG:NH2	71:C4:154:GLU:OE2	2.40	0.54
75:M4:666:HIS:HB3	75:M4:669:ASN:HB2	1.88	0.54
3:SA:152:U:O2	7:SH:4:ASN:ND2	2.41	0.54
3:SA:826:U:O2'	3:SA:827:C:O2	2.22	0.54
3:SA:916:U:O4	13:SP:41:ARG:NH2	2.40	0.54
7:SH:50:PHE:HB3	7:SH:111:LEU:HD22	1.90	0.54
16:SY:76:LEU:O	16:SY:80:GLY:CA	2.55	0.54
20:3C:301:LEU:HD11	20:3C:319:ARG:HG2	1.87	0.54
25:A4:397:SER:H	25:A4:428:ILE:HB	1.71	0.54
31:AG:319:LYS:HG3	31:AG:482:GLY:HA2	1.90	0.54
34:B3:242:GLN:HE21	34:B3:245:SER:HB2	1.73	0.54
36:BE:209:ILE:HG22	36:BE:225:THR:HG22	1.90	0.54
36:BE:511:ASP:OD1	36:BE:551:TYR:OH	2.24	0.54
55:RO:316:PRO:O	55:RO:320:LEU:HB2	2.06	0.54
68:M3:47:SER:HB3	68:M3:63:GLU:HB2	1.90	0.54
72:R4:10:ARG:HG3	72:R4:20:THR:HB	1.89	0.54
75:M4:86:GLU:HA	75:M4:120:ARG:HA	1.90	0.54
75:M4:293:SER:OG	75:M4:294:ALA:N	2.39	0.54
3:SA:454:U:OP1	3:SA:455:C:N4	2.41	0.54
3:SA:1192:C:O2'	3:SA:1194:A:N6	2.40	0.54
3:SA:1665:U:O2	3:SA:1736:G:O6	2.25	0.54
5:SF:73:ASP:HB2	5:SF:164:LEU:HD11	1.89	0.54
8:SI:50:ASP:HA	8:SI:56:LYS:HA	1.89	0.54
20:3B:238:ASP:OD1	20:3B:238:ASP:N	2.40	0.54
22:3E:251:ASP:N	22:3E:251:ASP:OD1	2.39	0.54
26:A5:162:GLN:HA	26:A5:173:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AF:227:VAL:HG12	30:AF:236:VAL:HG12	1.89	0.54
32:B1:708:ASP:OD1	32:B1:708:ASP:N	2.40	0.54
33:B2:334:SER:OG	33:B2:335:LEU:N	2.40	0.54
33:B2:540:SER:HB2	33:B2:544:ARG:H	1.72	0.54
33:B2:565:PHE:O	53:RK:207:ARG:NH2	2.36	0.54
49:RE:443:HIS:HB3	49:RE:470:LYS:HB2	1.88	0.54
54:RN:729:ASP:O	54:RN:732:ARG:NH2	2.39	0.54
56:RP:1797:LEU:HD13	56:RP:1877:ARG:HB3	1.90	0.54
64:R1:67:THR:HG22	64:R1:119:ARG:HE	1.73	0.54
65:R3:153:GLN:NE2	66:R6:61:THR:OG1	2.40	0.54
3:SA:319:U:H5'	3:SA:320:U:H5''	1.88	0.54
8:SI:155:ASP:N	8:SI:155:ASP:OD1	2.36	0.54
25:A4:433:LEU:HD13	25:A4:440:LEU:HB2	1.90	0.54
26:A5:10:TYR:OH	26:A5:302:ASN:ND2	2.40	0.54
29:AE:396:ASP:OD1	29:AE:396:ASP:N	2.41	0.54
29:AE:650:PHE:HA	29:AE:653:PHE:HB3	1.89	0.54
31:AG:370:GLN:HE22	31:AG:384:SER:HB2	1.72	0.54
33:B2:500:TRP:HB3	33:B2:522:LEU:HD12	1.90	0.54
34:B3:182:CYS:SG	34:B3:183:LEU:N	2.80	0.54
34:B3:336:ASN:O	34:B3:363:ARG:NH2	2.40	0.54
34:B3:411:THR:HG22	34:B3:431:ILE:HA	1.89	0.54
36:BE:342:TYR:OH	36:BE:345:SER:OG	2.24	0.54
38:5B:163:LEU:HB3	38:5B:167:ARG:HH21	1.72	0.54
39:5C:265:GLU:OE2	57:RQ:832:ASN:CG	2.46	0.54
40:5D:138:ASP:OD1	40:5D:138:ASP:N	2.38	0.54
49:RE:1193:ALA:HA	49:RE:1212:VAL:O	2.07	0.54
56:RP:1735:SER:OG	56:RP:1736:GLU:N	2.39	0.54
67:R2:117:THR:OG1	67:R2:120:TYR:N	2.38	0.54
69:R0:63:ARG:HA	69:R0:89:GLN:HE22	1.72	0.54
71:C4:36:VAL:HB	71:C4:107:LEU:HA	1.88	0.54
72:R4:411:SER:HB2	72:R4:422:VAL:HA	1.89	0.54
75:M4:921:GLU:O	75:M4:925:ASN:N	2.40	0.54
3:SA:71:A:H8	3:SA:72:A:H5''	1.72	0.54
7:SH:45:PHE:HA	7:SH:119:GLN:HG2	1.89	0.54
22:3E:392:ALA:O	22:3E:396:ASN:ND2	2.40	0.54
26:A5:255:ILE:HG23	26:A5:277:LYS:HB2	1.89	0.54
29:AE:734:ILE:HD11	29:AE:770:LYS:HG2	1.89	0.54
32:B1:279:PHE:HE2	32:B1:285:ARG:HG3	1.73	0.54
33:B2:98:TYR:HD2	33:B2:102:VAL:HG13	1.73	0.54
36:BE:82:ALA:O	36:BE:93:ALA:HB3	2.08	0.54
41:5E:316:ASN:O	41:5E:320:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:160:VAL:HG21	49:RE:230:VAL:HG12	1.90	0.54
49:RE:313:ASN:HB2	49:RE:328:ALA:HA	1.89	0.54
49:RE:1195:LYS:HA	49:RE:1210:GLU:O	2.08	0.54
50:RF:69:LYS:NZ	50:RF:159:THR:OG1	2.39	0.54
51:RG:42:ILE:HA	51:RG:111:GLN:O	2.08	0.54
56:RP:1873:LEU:HG	56:RP:1910:VAL:HG22	1.89	0.54
65:R3:61:ARG:NH1	65:R3:278:GLN:OE1	2.41	0.54
65:R3:243:LEU:N	65:R3:282:VAL:O	2.37	0.54
66:R6:66:LEU:HD11	66:R6:105:SER:HB2	1.89	0.54
67:R2:22:ARG:HH12	67:R2:199:LEU:H	1.53	0.54
67:R2:202:ALA:O	67:R2:206:SER:N	2.35	0.54
74:R7:44:ARG:NH1	74:R7:44:ARG:O	2.40	0.54
8:SI:15:GLU:HA	8:SI:18:LEU:HD12	1.89	0.54
9:SJ:113:PHE:HE2	9:SJ:121:LEU:HB3	1.72	0.54
25:A4:739:LYS:CA	25:A4:739:LYS:CE	2.85	0.54
26:A5:484:LEU:HB3	26:A5:502:VAL:HG22	1.90	0.54
33:B2:803:GLN:NE2	33:B2:807:ASP:OD1	2.40	0.54
36:BE:49:TYR:OH	36:BE:86:HIS:O	2.26	0.54
36:BE:375:LEU:HD22	36:BE:389:MET:HG3	1.90	0.54
52:RJ:270:ALA:HA	52:RJ:791:ILE:O	2.08	0.54
52:RJ:993:ASP:N	52:RJ:993:ASP:OD1	2.39	0.54
63:R5:29:SER:HB3	63:R5:32:GLN:HB2	1.90	0.54
69:R0:129:GLU:HG3	71:C4:225:LYS:HE3	1.90	0.54
1:3A:325:C:O2'	40:5D:108:ARG:NH1	2.40	0.54
4:SC:19:ARG:HH11	34:B3:338:GLY:HA3	1.73	0.54
6:SG:91:GLU:HA	6:SG:94:THR:HG22	1.90	0.54
11:SM:8:GLN:NE2	11:SM:12:ALA:O	2.41	0.54
20:3C:264:GLN:OE1	20:3C:319:ARG:NH2	2.40	0.54
25:A4:329:HIS:ND1	25:A4:353:GLU:OE2	2.37	0.54
29:AE:395:GLU:OE2	29:AE:397:LYS:NZ	2.38	0.54
29:AE:667:LYS:O	29:AE:671:LEU:HB2	2.08	0.54
31:AG:302:SER:O	31:AG:314:SER:HA	2.08	0.54
32:B1:497:ILE:HG23	32:B1:512:ILE:HB	1.89	0.54
33:B2:181:SER:OG	33:B2:183:ASP:OD1	2.23	0.54
34:B3:213:SER:OG	34:B3:221:ASN:ND2	2.39	0.54
48:RD:1530:GLU:HA	48:RD:1533:LEU:HB2	1.90	0.54
56:RP:1692:TYR:HA	56:RP:1743:LYS:HD2	1.90	0.54
64:R1:5:GLU:OE2	72:R4:122:ARG:NH2	2.41	0.54
72:R4:109:PHE:HA	72:R4:143:LYS:HG3	1.89	0.54
3:SA:141:U:O2'	3:SA:266:A:N3	2.36	0.54
3:SA:1483:A:HO2'	3:SA:1607:G:HO2'	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SH:159:ARG:NH1	7:SH:170:THR:OG1	2.40	0.54
14:SR:59:LYS:HD3	14:SR:105:LEU:HD21	1.89	0.54
20:3B:104:ASP:OD1	20:3B:104:ASP:N	2.39	0.54
21:3D:117:ASP:OD1	45:5I:157:ASN:ND2	2.41	0.54
30:AF:5:ARG:O	30:AF:7:ARG:NH1	2.40	0.54
32:B1:247:SER:O	32:B1:249:ARG:NH1	2.41	0.54
35:B8:524:SER:OG	35:B8:527:GLY:N	2.38	0.54
35:B8:581:ASN:HD21	35:B8:585:LYS:HG3	1.73	0.54
66:R6:139:ILE:HA	66:R6:157:SER:HA	1.90	0.54
67:R2:242:HIS:O	67:R2:246:GLN:N	2.41	0.54
72:R4:109:PHE:O	72:R4:144:ARG:N	2.35	0.54
3:SA:816:G:OP1	3:SA:858:G:N2	2.40	0.53
8:SI:158:ASP:OD2	8:SI:161:GLN:NE2	2.40	0.53
14:SR:99:GLU:HG2	14:SR:102:LYS:HE3	1.90	0.53
20:3C:96:VAL:HG21	20:3C:155:ILE:HG21	1.89	0.53
25:A4:99:ILE:HD11	25:A4:102:LEU:HB3	1.90	0.53
27:A8:587:LEU:HB2	31:AG:605:ASN:HB2	1.89	0.53
27:A8:663:ASP:OD1	28:A9:500:GLN:NE2	2.41	0.53
32:B1:25:ASP:OD1	32:B1:25:ASP:N	2.40	0.53
33:B2:426:ARG:NH1	33:B2:463:SER:OG	2.40	0.53
35:B8:445:ARG:HH11	35:B8:503:SER:H	1.57	0.53
36:BE:310:ILE:O	36:BE:321:GLU:HA	2.08	0.53
42:5F:136:VAL:HA	42:5F:160:TRP:HA	1.90	0.53
52:RJ:59:VAL:O	52:RJ:239:ASN:ND2	2.40	0.53
55:RO:180:PHE:HA	55:RO:184:TYR:HB2	1.89	0.53
65:R3:40:ARG:N	65:R3:44:ARG:O	2.40	0.53
66:R6:106:LEU:HD22	66:R6:160:VAL:HB	1.90	0.53
69:R0:63:ARG:NH1	69:R0:92:SER:OG	2.40	0.53
71:C4:30:ASP:O	71:C4:102:THR:OG1	2.25	0.53
71:C4:146:LEU:HD11	71:C4:225:LYS:HA	1.90	0.53
1:3A:2:U:O4	3:SA:1123:C:N3	2.40	0.53
23:3F:257:ASP:OD1	23:3F:257:ASP:N	2.36	0.53
25:A4:213:TRP:HA	25:A4:225:LEU:HA	1.90	0.53
25:A4:573:VAL:HG22	25:A4:584:VAL:HG23	1.90	0.53
29:AE:4:LEU:HD13	39:5C:108:LEU:HD11	1.90	0.53
29:AE:161:PHE:HD1	29:AE:182:LEU:HD11	1.73	0.53
31:AG:322:SER:OG	31:AG:331:GLN:NE2	2.39	0.53
33:B2:639:VAL:HG23	33:B2:653:LEU:HB2	1.90	0.53
43:5G:272:ASP:N	43:5G:272:ASP:OD1	2.41	0.53
52:RJ:841:THR:HG22	52:RJ:860:TYR:H	1.73	0.53
56:RP:1877:ARG:HA	56:RP:1880:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:R1:137:GLY:O	64:R1:141:ASN:ND2	2.41	0.53
65:R3:129:SER:OG	65:R3:130:VAL:N	2.39	0.53
69:R0:45:SER:OG	69:R0:54:THR:N	2.39	0.53
72:R4:45:ILE:HG13	72:R4:153:SER:HA	1.89	0.53
72:R4:508:HIS:ND1	72:R4:611:ASP:OD2	2.41	0.53
75:M4:196:ILE:HB	75:M4:259:VAL:HG13	1.91	0.53
2:5A:295:A:N7	36:BE:381:ARG:NH1	2.55	0.53
22:3E:290:LEU:O	22:3E:391:ARG:NH2	2.41	0.53
23:3F:194:LEU:HD21	23:3F:237:ASP:HA	1.90	0.53
31:AG:573:CYS:O	31:AG:585:TRP:HB2	2.08	0.53
36:BE:209:ILE:HD12	36:BE:223:LEU:HD12	1.90	0.53
37:B6:63:VAL:HG13	37:B6:88:ILE:HD11	1.89	0.53
43:5G:164:GLN:NE2	43:5G:260:GLU:OE1	2.41	0.53
54:RN:571:ILE:HA	54:RN:574:THR:HG22	1.90	0.53
58:RS:326:VAL:HG13	58:RS:330:CYS:HB3	1.90	0.53
63:R5:168:THR:HB	63:R5:175:ILE:HB	1.90	0.53
72:R4:219:VAL:HA	72:R4:222:ILE:HB	1.91	0.53
72:R4:237:GLN:NE2	72:R4:465:GLY:O	2.42	0.53
1:3A:255:U:O4	24:3H:84:ARG:NH1	2.42	0.53
16:SY:141:GLU:OE1	52:RJ:833:ARG:NH2	2.41	0.53
17:SZ:54:ALA:HB2	17:SZ:79:VAL:HG12	1.90	0.53
21:3D:258:SER:OG	21:3D:259:MET:N	2.42	0.53
32:B1:645:ASP:OD1	32:B1:645:ASP:N	2.39	0.53
34:B3:223:TRP:HA	34:B3:232:LYS:HA	1.89	0.53
34:B3:505:ILE:HB	34:B3:517:ILE:HG22	1.90	0.53
34:B3:584:ILE:HG13	34:B3:588:LYS:HG3	1.91	0.53
36:BE:666:ARG:NH1	36:BE:706:ASP:OD2	2.41	0.53
45:5I:448:ARG:NH1	45:5I:451:MET:SD	2.81	0.53
72:R4:17:LEU:HD11	72:R4:42:ARG:HA	1.91	0.53
1:3A:197:U:OP2	23:3F:207:ARG:NH1	2.42	0.53
3:SA:629:U:OP1	12:SO:127:ARG:NH2	2.34	0.53
3:SA:1781:A:O2'	3:SA:1783:C:N4	2.39	0.53
25:A4:565:ARG:HG3	29:AE:629:GLU:HG2	1.89	0.53
30:AF:285:ASP:N	30:AF:285:ASP:OD1	2.41	0.53
33:B2:291:GLU:HA	33:B2:294:ARG:HG2	1.90	0.53
49:RE:807:LEU:HA	49:RE:810:ILE:HG22	1.91	0.53
56:RP:1876:LEU:HD13	56:RP:1914:THR:HG22	1.90	0.53
69:R0:204:THR:O	69:R0:208:TYR:N	2.41	0.53
71:C4:46:TYR:N	71:C4:53:LEU:O	2.42	0.53
72:R4:217:SER:H	72:R4:220:GLN:HB3	1.74	0.53
72:R4:557:LYS:HB2	72:R4:565:GLU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1192:C:OP1	51:RG:132:ARG:NH1	2.40	0.53
5:SF:93:ASP:N	5:SF:93:ASP:OD1	2.40	0.53
14:SR:94:GLN:HG3	14:SR:102:LYS:HE2	1.90	0.53
20:3C:163:PHE:HZ	20:3C:319:ARG:HD2	1.72	0.53
24:3G:20:ILE:HA	24:3G:23:VAL:HG12	1.91	0.53
26:A5:79:GLY:HA3	26:A5:107:ILE:HD11	1.89	0.53
33:B2:534:ILE:HD13	33:B2:548:ILE:HB	1.90	0.53
34:B3:107:ILE:HD11	34:B3:147:ILE:HG23	1.90	0.53
35:B8:512:ASP:O	40:5D:248:ARG:NH1	2.41	0.53
36:BE:144:ASP:C	36:BE:146:GLN:H	2.12	0.53
36:BE:364:HIS:HB2	36:BE:381:ARG:HH21	1.72	0.53
36:BE:440:ALA:HB2	36:BE:463:VAL:HG21	1.89	0.53
37:B6:82:SER:OG	37:B6:83:LEU:N	2.42	0.53
39:5C:284:ARG:NH1	39:5C:408:GLU:OE2	2.41	0.53
49:RE:707:PHE:O	49:RE:918:ARG:NH1	2.41	0.53
49:RE:1103:ARG:HB2	49:RE:1232:ILE:HD12	1.91	0.53
56:RP:1741:LYS:NZ	56:RP:1743:LYS:O	2.37	0.53
66:R6:54:PRO:HA	66:R6:94:ILE:HD12	1.91	0.53
72:R4:440:ARG:NH1	72:R4:443:GLU:OE2	2.41	0.53
72:R4:678:LEU:HA	72:R4:681:SER:HB3	1.91	0.53
75:M4:328:HIS:HA	75:M4:555:VAL:HB	1.90	0.53
2:5A:535:G:H5'	37:B6:127:LYS:HE3	1.89	0.53
3:SA:493:U:H4'	52:RJ:1138:ARG:HH12	1.73	0.53
11:SM:94:ILE:HG12	11:SM:96:LYS:H	1.74	0.53
15:SX:89:TRP:O	15:SX:93:LEU:HB3	2.09	0.53
30:AF:71:ARG:HD3	30:AF:331:THR:HG21	1.91	0.53
31:AG:409:LYS:HG2	31:AG:489:ASN:HD22	1.74	0.53
34:B3:410:ASN:ND2	34:B3:433:HIS:O	2.42	0.53
42:5F:66:PRO:O	42:5F:72:ARG:NH2	2.42	0.53
53:RK:12:GLN:NE2	53:RK:34:GLU:OE1	2.32	0.53
72:R4:97:GLN:OE1	72:R4:197:ASN:ND2	2.42	0.53
72:R4:542:ILE:HD13	72:R4:723:THR:HB	1.90	0.53
3:SA:106:U:H3'	3:SA:107:C:H4'	1.91	0.53
3:SA:200:A:O2'	56:RP:1061:CYS:O	2.26	0.53
3:SA:906:A:H3'	3:SA:907:A:H8	1.74	0.53
4:SC:98:THR:OG1	4:SC:99:ASN:N	2.42	0.53
20:3C:277:ASP:OD2	20:3C:288:ARG:NH2	2.41	0.53
23:3F:531:LYS:HE2	23:3F:534:LYS:HB2	1.91	0.53
26:A5:447:SER:OG	26:A5:448:ASN:N	2.42	0.53
30:AF:101:ALA:HA	30:AF:126:PRO:HB3	1.91	0.53
31:AG:393:ASN:HB2	31:AG:436:PHE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BE:609:ILE:HG23	36:BE:623:ILE:HB	1.90	0.53
3:SA:760:A:H2'	3:SA:761:G:H8	1.73	0.53
3:SA:805:U:OP1	15:SX:32:LYS:NZ	2.41	0.53
5:SF:98:ASN:ND2	5:SF:114:ILE:O	2.39	0.53
20:3B:271:ILE:O	20:3B:313:HIS:HA	2.09	0.53
21:3D:83:ASP:OD2	37:B6:173:ARG:NH2	2.41	0.53
29:AE:54:LYS:NZ	46:5J:78:LYS:O	2.42	0.53
31:AG:519:LEU:HB3	31:AG:522:SER:HB3	1.91	0.53
33:B2:175:ASP:O	33:B2:190:ASP:HA	2.09	0.53
33:B2:640:LYS:HE2	33:B2:652:LYS:HE2	1.90	0.53
38:5B:163:LEU:HD12	38:5B:167:ARG:HE	1.74	0.53
49:RE:406:ILE:HG13	49:RE:457:TYR:HB3	1.91	0.53
52:RJ:125:LEU:HA	52:RJ:128:MET:HB3	1.91	0.53
56:RP:2143:LYS:O	56:RP:2147:ALA:HB2	2.09	0.53
67:R2:183:ASN:HD21	67:R2:219:ASN:HA	1.74	0.53
75:M4:205:SER:O	75:M4:209:TYR:N	2.34	0.53
16:SY:91:GLY:O	16:SY:94:ASN:ND2	2.42	0.53
23:3F:152:VAL:HG12	23:3F:562:GLY:HA2	1.89	0.53
24:3G:120:LYS:NZ	25:A4:187:GLU:OE1	2.42	0.53
30:AF:319:VAL:HG12	30:AF:329:ILE:HG12	1.90	0.53
30:AF:443:LEU:HG	30:AF:480:LEU:HD21	1.90	0.53
31:AG:16:SER:HB2	31:AG:783:LEU:HB2	1.91	0.53
32:B1:394:GLN:HE21	32:B1:438:VAL:HG12	1.74	0.53
33:B2:124:ILE:HA	33:B2:140:SER:HA	1.91	0.53
34:B3:65:THR:HA	34:B3:80:SER:HB2	1.91	0.53
35:B8:348:HIS:HD2	35:B8:350:SER:H	1.56	0.53
35:B8:545:HIS:HD2	35:B8:548:SER:HB3	1.73	0.53
43:5G:88:ILE:HG12	43:5G:138:ASP:HB2	1.90	0.53
45:5I:448:ARG:HD2	45:5I:451:MET:HG3	1.91	0.53
48:RD:1510:GLU:HA	48:RD:1513:LYS:HE3	1.89	0.53
49:RE:824:PHE:HB2	50:RF:174:PRO:HB3	1.91	0.53
52:RJ:749:THR:OG1	52:RJ:750:TRP:N	2.42	0.53
55:RO:403:TYR:OH	55:RO:490:LYS:O	2.26	0.53
56:RP:116:ASP:N	56:RP:116:ASP:OD1	2.39	0.53
58:RS:299:LEU:HD13	58:RS:304:TYR:HB2	1.90	0.53
75:M4:251:GLU:OE1	75:M4:254:ARG:NE	2.36	0.53
1:3A:93:U:O4	22:3E:298:ARG:NH1	2.40	0.52
23:3F:175:SER:OG	23:3F:176:SER:N	2.40	0.52
23:3F:439:ALA:O	23:3F:497:LYS:NZ	2.37	0.52
25:A4:399:VAL:HG12	25:A4:420:LEU:HB2	1.91	0.52
34:B3:352:LYS:HA	34:B3:365:ILE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5C:334:ARG:HB2	39:5C:337:HIS:HB2	1.91	0.52
56:RP:2070:TYR:O	56:RP:2076:ARG:NE	2.42	0.52
63:R5:250:LYS:NZ	64:R1:197:SER:O	2.36	0.52
67:R2:82:ILE:HD12	67:R2:92:VAL:HG22	1.91	0.52
72:R4:317:ILE:HB	72:R4:394:TYR:HB3	1.91	0.52
72:R4:378:MET:HB3	72:R4:382:ARG:HH12	1.74	0.52
75:M4:265:HIS:ND1	75:M4:293:SER:OG	2.36	0.52
75:M4:399:LYS:O	75:M4:403:LYS:N	2.38	0.52
75:M4:925:ASN:O	75:M4:927:ASN:ND2	2.43	0.52
4:SC:78:ASP:OD1	4:SC:78:ASP:N	2.43	0.52
24:3G:62:GLU:HA	24:3G:65:LEU:HG	1.90	0.52
25:A4:773:LYS:NZ	25:A4:774:LEU:O	2.42	0.52
30:AF:463:VAL:HA	30:AF:466:VAL:HG12	1.91	0.52
33:B2:193:THR:O	33:B2:195:GLN:NE2	2.43	0.52
34:B3:24:THR:HG21	34:B3:69:LEU:HA	1.91	0.52
34:B3:96:VAL:O	34:B3:97:ARG:NH1	2.42	0.52
34:B3:779:VAL:HA	34:B3:782:VAL:HG12	1.91	0.52
36:BE:413:GLU:O	36:BE:435:LYS:N	2.43	0.52
40:5D:233:ILE:HD13	40:5D:243:LYS:HB3	1.89	0.52
49:RE:151:SER:HA	49:RE:154:LYS:HE2	1.91	0.52
53:RK:47:ASP:OD1	53:RK:47:ASP:N	2.39	0.52
59:RT:187:VAL:HG13	59:RT:251:ILE:HD12	1.90	0.52
68:M3:91:GLY:H	68:M3:127:LEU:HB3	1.73	0.52
72:R4:572:ASP:HB3	72:R4:622:PHE:HB3	1.92	0.52
3:SA:1594:G:HO2'	3:SA:1600:A:H61	1.54	0.52
10:SK:106:GLU:OE2	10:SK:115:LYS:NZ	2.42	0.52
10:SK:119:ALA:O	10:SK:124:HIS:ND1	2.32	0.52
23:3F:114:LYS:HA	23:3F:117:ILE:HD12	1.89	0.52
23:3F:286:LEU:HB3	23:3F:295:LEU:HD11	1.91	0.52
23:3F:409:ASP:OD1	23:3F:412:HIS:N	2.41	0.52
29:AE:370:LEU:HD13	29:AE:407:PHE:HZ	1.74	0.52
36:BE:361:SER:HA	36:BE:636:PRO:HG2	1.90	0.52
39:5C:451:SER:OG	39:5C:452:VAL:N	2.42	0.52
49:RE:673:SER:N	49:RE:717:ALA:O	2.43	0.52
52:RJ:555:MET:O	53:RK:327:ARG:NH2	2.42	0.52
52:RJ:1105:ASP:HA	52:RJ:1108:LYS:HG2	1.91	0.52
53:RK:214:LYS:HA	53:RK:217:LYS:HE3	1.91	0.52
72:R4:318:VAL:HG12	72:R4:392:VAL:HG12	1.90	0.52
72:R4:406:GLN:O	72:R4:425:ILE:N	2.42	0.52
13:SP:14:PHE:HA	13:SP:78:ALA:O	2.09	0.52
20:3B:228:GLN:O	20:3B:231:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3B:239:CYS:SG	20:3B:240:VAL:N	2.83	0.52
23:3F:241:THR:HG21	23:3F:285:SER:HA	1.91	0.52
34:B3:217:ASP:OD1	34:B3:217:ASP:N	2.42	0.52
35:B8:378:GLN:HA	35:B8:384:ILE:HG22	1.91	0.52
36:BE:859:ASP:OD1	36:BE:859:ASP:N	2.41	0.52
42:5F:104:SER:OG	42:5F:108:ARG:NH1	2.43	0.52
49:RE:511:PHE:HB2	49:RE:512:LEU:HD22	1.91	0.52
52:RJ:158:ILE:HG13	52:RJ:913:ILE:HD11	1.90	0.52
72:R4:422:VAL:O	72:R4:436:ILE:N	2.39	0.52
75:M4:587:TYR:HA	75:M4:590:ILE:HD12	1.92	0.52
1:3A:328:A:H3'	40:5D:249:LYS:HD3	1.90	0.52
3:SA:871:G:H2'	3:SA:872:G:C8	2.44	0.52
5:SF:238:LEU:HD12	5:SF:242:LYS:HG3	1.92	0.52
8:SI:70:PHE:O	8:SI:74:GLN:NE2	2.42	0.52
14:SR:100:GLN:HB3	36:BE:488:ASN:HD21	1.74	0.52
23:3F:224:SER:O	23:3F:226:HIS:ND1	2.32	0.52
24:3H:58:CYS:HA	24:3H:84:ARG:HD3	1.90	0.52
39:5C:64:ASP:OD1	39:5C:64:ASP:N	2.42	0.52
41:5E:371:ARG:NH1	41:5E:375:ASP:OD2	2.39	0.52
45:5I:270:ASN:ND2	45:5I:273:GLU:OE1	2.42	0.52
49:RE:316:ARG:NH1	49:RE:549:SER:OG	2.42	0.52
56:RP:2010:HIS:NE2	56:RP:2049:GLU:O	2.39	0.52
64:R1:23:ARG:N	64:R1:173:ASP:OD2	2.40	0.52
67:R2:45:ASN:OD1	67:R2:64:SER:N	2.43	0.52
67:R2:95:ILE:HG12	67:R2:138:VAL:CG2	2.39	0.52
72:R4:652:PHE:HZ	72:R4:660:ARG:HH11	1.58	0.52
3:SA:25:C:N4	10:SK:12:TYR:OH	2.43	0.52
14:SR:100:GLN:HE21	14:SR:104:GLU:HG3	1.74	0.52
25:A4:477:LEU:H	25:A4:489:CYS:HB3	1.73	0.52
34:B3:17:ALA:HB3	34:B3:35:PRO:HA	1.92	0.52
36:BE:904:ASP:N	36:BE:904:ASP:OD1	2.39	0.52
37:B6:85:ASP:N	37:B6:85:ASP:OD1	2.40	0.52
49:RE:589:LYS:O	49:RE:609:ASN:ND2	2.41	0.52
51:RH:49:SER:HA	51:RH:116:THR:HG23	1.92	0.52
55:RO:211:LEU:HD12	55:RO:212:LEU:HG	1.92	0.52
63:R5:207:GLU:O	63:R5:211:LYS:N	2.39	0.52
65:R3:258:THR:HG22	65:R3:267:THR:HG22	1.91	0.52
72:R4:284:ASN:ND2	72:R4:287:GLU:OE1	2.43	0.52
3:SA:41:A:N6	3:SA:467:G:C2	2.78	0.52
3:SA:479:C:O2	3:SA:510:G:N2	2.42	0.52
23:3F:539:ILE:O	23:3F:565:SER:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A4:493:ASP:HB3	25:A4:513:LEU:HD11	1.92	0.52
26:A5:536:LEU:O	26:A5:540:LEU:N	2.36	0.52
32:B1:19:ASN:HA	32:B1:307:THR:HG21	1.92	0.52
32:B1:58:ILE:HA	32:B1:74:ASP:HA	1.91	0.52
36:BE:225:THR:OG1	36:BE:227:THR:O	2.28	0.52
49:RE:215:GLU:OE2	49:RE:223:ARG:NH1	2.42	0.52
49:RE:720:SER:OG	49:RE:721:VAL:N	2.41	0.52
49:RE:844:THR:O	49:RE:847:GLY:N	2.37	0.52
52:RJ:803:ASN:ND2	52:RJ:1023:LEU:O	2.43	0.52
52:RJ:905:SER:N	52:RJ:1028:GLU:OE2	2.43	0.52
3:SA:563:U:OP2	43:5G:287:LYS:NZ	2.38	0.52
3:SA:754:A:O4'	5:SF:187:ARG:NH2	2.43	0.52
9:SJ:180:ASP:N	9:SJ:180:ASP:OD1	2.43	0.52
14:SR:64:ASP:N	14:SR:64:ASP:OD1	2.43	0.52
20:3B:219:PRO:O	21:3D:159:SER:OG	2.28	0.52
21:3D:26:ASP:HB2	45:5I:80:LEU:HD23	1.91	0.52
21:3D:212:ASP:O	21:3D:216:PHE:HB2	2.09	0.52
30:AF:90:ARG:NH1	30:AF:137:ASN:O	2.42	0.52
33:B2:8:PHE:HA	33:B2:685:GLU:O	2.10	0.52
33:B2:633:CYS:HB3	33:B2:663:LEU:HD22	1.92	0.52
45:5I:226:LYS:HD3	45:5I:268:CYS:HA	1.91	0.52
48:RD:1466:ARG:HH12	48:RD:1470:GLY:HA3	1.73	0.52
48:RD:1525:ASN:HD22	48:RD:1556:ILE:HG12	1.73	0.52
49:RE:676:PRO:HB2	49:RE:678:ILE:HG22	1.92	0.52
51:RG:46:ALA:HA	51:RG:115:GLN:HG3	1.91	0.52
51:RH:167:ILE:HG22	51:RH:171:LEU:HD23	1.91	0.52
53:RK:249:SER:O	53:RK:253:GLY:N	2.43	0.52
56:RP:2032:SER:O	56:RP:2036:ARG:NE	2.39	0.52
63:R5:74:GLU:HG2	63:R5:121:GLU:HG2	1.90	0.52
72:R4:695:ASN:O	72:R4:806:ARG:NH2	2.43	0.52
72:R4:940:ARG:O	72:R4:944:LEU:N	2.42	0.52
75:M4:327:GLN:NE2	75:M4:344:GLU:OE2	2.34	0.52
5:SF:175:PHE:HA	5:SF:179:LYS:HD2	1.91	0.52
14:SR:58:ASP:OD1	14:SR:58:ASP:N	2.40	0.52
20:3C:263:ASP:OD1	22:3E:118:ARG:NH2	2.42	0.52
21:3D:181:LEU:HA	21:3D:184:LEU:HG	1.91	0.52
25:A4:62:PRO:HG2	25:A4:65:LEU:HD21	1.92	0.52
26:A5:537:LEU:HD21	30:AF:498:SER:HB2	1.90	0.52
26:A5:545:ALA:HB3	27:A8:677:ASN:HD21	1.75	0.52
30:AF:194:ARG:HG3	30:AF:205:PRO:HG3	1.92	0.52
31:AG:324:TRP:HA	31:AG:330:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B3:438:THR:HG21	34:B3:495:ASN:HA	1.91	0.52
47:5K:69:THR:HG22	47:5K:106:LEU:HB2	1.91	0.52
49:RE:495:THR:O	49:RE:499:LEU:HB2	2.09	0.52
51:RG:48:ALA:HB3	51:RG:116:THR:HA	1.92	0.52
55:RO:418:ASN:HD22	55:RO:421:PHE:HB2	1.74	0.52
65:R3:158:SER:HA	65:R3:161:HIS:HB2	1.90	0.52
72:R4:596:LEU:HD22	72:R4:898:SER:HB2	1.91	0.52
75:M4:771:GLY:HA2	75:M4:807:VAL:HA	1.91	0.52
3:SA:939:A:OP1	12:SO:114:ARG:NH2	2.42	0.52
21:3D:102:ASP:OD2	21:3D:105:LEU:N	2.39	0.52
22:3E:145:HIS:O	22:3E:149:ARG:NE	2.35	0.52
25:A4:360:SER:HG	25:A4:363:SER:HG	1.55	0.52
27:A8:500:PRO:O	27:A8:504:ASN:ND2	2.43	0.52
29:AE:769:LEU:O	29:AE:773:GLN:NE2	2.43	0.52
31:AG:133:LYS:NZ	31:AG:137:ALA:O	2.36	0.52
31:AG:246:SER:OG	31:AG:247:SER:N	2.43	0.52
32:B1:586:SER:OG	32:B1:587:PHE:N	2.42	0.52
33:B2:397:ILE:HD12	33:B2:675:SER:HB3	1.92	0.52
34:B3:171:MET:HA	34:B3:186:LEU:O	2.08	0.52
34:B3:788:TYR:O	34:B3:792:HIS:ND1	2.43	0.52
36:BE:268:THR:HB	36:BE:272:ASP:HB2	1.92	0.52
39:5C:194:ARG:NE	39:5C:210:GLU:OE2	2.43	0.52
45:5I:96:ASN:ND2	45:5I:99:THR:OG1	2.43	0.52
52:RJ:251:ASP:HB2	52:RJ:267:ARG:HH21	1.73	0.52
52:RJ:1039:ARG:HH11	52:RJ:1046:THR:HG22	1.75	0.52
63:R5:198:PHE:HE1	63:R5:221:ILE:HG12	1.75	0.52
67:R2:60:VAL:HG11	67:R2:145:ILE:HG12	1.92	0.52
67:R2:183:ASN:ND2	67:R2:219:ASN:OD1	2.43	0.52
72:R4:41:LEU:HD13	72:R4:154:GLU:HA	1.92	0.52
3:SA:34:G:N1	3:SA:475:A:C6	2.78	0.51
3:SA:152:U:N3	3:SA:163:G:N7	2.58	0.51
3:SA:522:U:H5 <sup>''</sup>	17:SZ:37:LYS:HE3	1.92	0.51
10:SK:136:VAL:HG12	10:SK:156:ILE:HG12	1.91	0.51
25:A4:739:LYS:N	25:A4:739:LYS:CE	2.73	0.51
28:A9:437:ILE:HD12	28:A9:456:LEU:HD13	1.92	0.51
29:AE:671:LEU:HD23	29:AE:719:SER:HB2	1.92	0.51
32:B1:718:ASP:N	32:B1:718:ASP:OD1	2.43	0.51
33:B2:285:ARG:NH2	33:B2:371:LYS:O	2.42	0.51
45:5I:220:ASP:N	45:5I:220:ASP:OD1	2.44	0.51
50:RF:9:MET:HB2	50:RF:13:PHE:HB2	1.93	0.51
68:M3:101:LEU:O	68:M3:104:LYS:NZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:R0:203:ASN:O	69:R0:207:CYS:N	2.40	0.51
72:R4:222:ILE:HG21	72:R4:235:ILE:HD11	1.92	0.51
1:3A:264:C:O2	1:3A:307:G:N2	2.39	0.51
3:SA:1192:C:O2	51:RG:136:ARG:NH2	2.42	0.51
5:SF:207:LEU:HD22	5:SF:220:THR:H	1.75	0.51
21:3D:171:ASP:OD1	21:3D:171:ASP:N	2.40	0.51
24:3G:38:ASN:N	24:3G:38:ASN:OD1	2.39	0.51
24:3H:43:THR:OG1	24:3H:48:ILE:O	2.29	0.51
25:A4:80:ASN:HD21	25:A4:82:ARG:HH11	1.58	0.51
25:A4:405:GLY:O	25:A4:413:ASN:N	2.43	0.51
28:A9:428:ASP:OD1	28:A9:428:ASP:N	2.43	0.51
31:AG:211:MET:HG2	31:AG:225:ILE:HG12	1.92	0.51
33:B2:166:ILE:HA	33:B2:181:SER:HA	1.91	0.51
34:B3:557:VAL:HB	34:B3:572:GLU:HB2	1.92	0.51
36:BE:228:GLY:O	36:BE:246:ILE:HB	2.11	0.51
36:BE:275:PHE:HE2	36:BE:340:PRO:HG3	1.75	0.51
37:B6:166:ASN:O	37:B6:170:ASN:ND2	2.42	0.51
43:5G:154:ILE:O	43:5G:162:THR:HA	2.10	0.51
45:5I:445:ARG:NH2	45:5I:451:MET:O	2.43	0.51
53:RK:66:GLU:H	53:RK:75:ILE:HG22	1.76	0.51
56:RP:46:HIS:O	56:RP:112:GLN:NE2	2.43	0.51
66:R6:140:LYS:HA	66:R6:158:LEU:HB2	1.91	0.51
69:R0:232:LYS:O	69:R0:236:THR:N	2.43	0.51
75:M4:864:LYS:O	75:M4:868:ARG:N	2.38	0.51
75:M4:966:MET:HA	75:M4:969:ILE:HD12	1.92	0.51
7:SH:30:LYS:HD3	7:SH:34:GLN:HB2	1.93	0.51
29:AE:465:PHE:H	29:AE:507:LYS:HE3	1.74	0.51
33:B2:285:ARG:HB3	33:B2:327:HIS:HB3	1.91	0.51
36:BE:144:ASP:HB3	36:BE:146:GLN:HG3	1.91	0.51
36:BE:316:ASP:OD1	36:BE:316:ASP:N	2.34	0.51
36:BE:630:THR:N	36:BE:644:THR:O	2.43	0.51
51:RG:43:VAL:HB	51:RG:112:VAL:HG22	1.92	0.51
56:RP:1809:GLU:HA	56:RP:1812:LEU:HB2	1.92	0.51
65:R3:211:TYR:OH	65:R3:244:PRO:O	2.28	0.51
72:R4:636:ILE:HD11	72:R4:733:LEU:HD11	1.92	0.51
75:M4:938:ALA:HB1	75:M4:998:MET:HB3	1.92	0.51
3:SA:805:U:O3'	15:SX:78:ARG:NH2	2.42	0.51
7:SH:46:LYS:HG2	7:SH:119:GLN:HB2	1.93	0.51
25:A4:62:PRO:O	25:A4:82:ARG:NH2	2.43	0.51
29:AE:328:ASP:OD1	29:AE:328:ASP:N	2.43	0.51
31:AG:366:ASN:OD1	31:AG:366:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AG:769:ASN:ND2	31:AG:771:ASP:OD1	2.43	0.51
33:B2:909:LYS:O	33:B2:913:ASN:ND2	2.44	0.51
34:B3:139:SER:OG	34:B3:140:PHE:N	2.44	0.51
34:B3:188:GLU:OE2	34:B3:221:ASN:ND2	2.43	0.51
34:B3:787:PRO:HB2	41:5E:492:PRO:HG3	1.92	0.51
36:BE:122:CYS:SG	36:BE:123:ILE:N	2.83	0.51
48:RD:1466:ARG:NH1	48:RD:1466:ARG:O	2.40	0.51
51:RG:133:THR:HB	51:RG:136:ARG:HE	1.74	0.51
53:RK:22:VAL:HG23	53:RK:106:LEU:HD12	1.91	0.51
67:R2:117:THR:HA	67:R2:161:PHE:HB2	1.92	0.51
72:R4:412:VAL:HG11	72:R4:445:LEU:HD22	1.90	0.51
75:M4:489:ILE:O	75:M4:493:GLU:N	2.40	0.51
3:SA:326:G:O6	3:SA:337:G:O6	2.29	0.51
3:SA:500:C:H4'	3:SA:501:U:H3'	1.93	0.51
25:A4:63:SER:O	25:A4:82:ARG:NH1	2.43	0.51
25:A4:142:GLY:HA3	25:A4:160:CYS:HB3	1.92	0.51
25:A4:210:ILE:HG23	25:A4:229:MET:HB2	1.92	0.51
25:A4:249:ARG:NH2	25:A4:309:GLN:OE1	2.44	0.51
26:A5:504:TRP:HA	26:A5:507:ILE:HD12	1.92	0.51
31:AG:511:GLU:HG2	31:AG:528:ILE:HG23	1.92	0.51
33:B2:621:VAL:HA	33:B2:631:PHE:O	2.11	0.51
36:BE:562:LEU:HD12	36:BE:566:SER:HB2	1.91	0.51
45:5I:183:GLN:N	45:5I:197:GLY:O	2.34	0.51
51:RH:215:ASN:ND2	51:RH:218:ASP:OD2	2.43	0.51
65:R3:134:VAL:HG11	65:R3:151:ILE:HB	1.92	0.51
67:R2:71:VAL:HG23	67:R2:72:GLU:HG2	1.92	0.51
69:R0:168:PHE:HB3	76:M6:103:ARG:HH21	1.75	0.51
72:R4:173:ALA:O	72:R4:177:THR:N	2.43	0.51
75:M4:680:VAL:HG12	75:M4:770:ILE:HG23	1.93	0.51
3:SA:521:A:N3	17:SZ:34:ASN:ND2	2.57	0.51
3:SA:557:G:N2	3:SA:571:G:O2'	2.43	0.51
20:3C:171:LEU:HB3	20:3C:240:VAL:HG12	1.92	0.51
25:A4:102:LEU:HD12	25:A4:114:LEU:HD12	1.92	0.51
29:AE:46:ASP:OD1	29:AE:46:ASP:N	2.44	0.51
29:AE:243:ALA:HB2	35:B8:208:LEU:HD23	1.91	0.51
29:AE:793:GLN:NE2	29:AE:839:GLU:O	2.43	0.51
30:AF:84:VAL:HG12	30:AF:100:ASP:HB3	1.92	0.51
32:B1:361:VAL:HG22	32:B1:371:VAL:HG22	1.91	0.51
33:B2:104:LYS:HD2	33:B2:113:VAL:HG21	1.92	0.51
39:5C:193:ALA:O	39:5C:194:ARG:NH1	2.40	0.51
41:5E:372:ARG:HH11	41:5E:378:PHE:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RG:111:GLN:HE22	51:RG:124:VAL:HG23	1.75	0.51
52:RJ:1042:MET:HG3	52:RJ:1044:LEU:HD13	1.90	0.51
52:RJ:1049:ASN:ND2	52:RJ:1051:ASP:OD1	2.43	0.51
7:SH:46:LYS:NZ	7:SH:118:GLU:OE1	2.43	0.51
15:SX:84:GLY:O	15:SX:88:LYS:NZ	2.44	0.51
23:3F:151:ARG:HD2	23:3F:560:ARG:HE	1.74	0.51
25:A4:291:ASP:OD1	25:A4:291:ASP:N	2.39	0.51
25:A4:363:SER:HB2	25:A4:366:ASN:HB3	1.93	0.51
29:AE:702:TRP:HE1	29:AE:705:SER:H	1.58	0.51
33:B2:165:SER:O	33:B2:182:LYS:N	2.44	0.51
35:B8:426:VAL:HG12	35:B8:432:VAL:HG12	1.93	0.51
45:5I:450:ASP:OD1	45:5I:450:ASP:N	2.44	0.51
54:RN:545:VAL:HA	54:RN:548:ARG:HG2	1.92	0.51
65:R3:12:ILE:HG21	71:C4:268:TYR:HB3	1.93	0.51
69:R0:137:PHE:HE1	69:R0:143:ARG:HA	1.76	0.51
72:R4:561:ASN:ND2	72:R4:629:GLU:OE2	2.41	0.51
4:SC:77:GLU:O	4:SC:80:SER:OG	2.29	0.51
20:3B:170:VAL:HB	20:3B:194:VAL:HG22	1.93	0.51
23:3F:343:ASP:OD1	23:3F:343:ASP:N	2.43	0.51
25:A4:302:ARG:NH2	25:A4:330:GLY:O	2.44	0.51
29:AE:34:ILE:HG12	29:AE:119:GLU:HG3	1.92	0.51
29:AE:83:ARG:NH1	29:AE:125:PHE:O	2.43	0.51
29:AE:724:VAL:HB	29:AE:755:ARG:HE	1.76	0.51
33:B2:180:THR:OG1	33:B2:207:CYS:SG	2.63	0.51
45:5I:324:SER:OG	45:5I:326:ASP:OD1	2.22	0.51
46:5J:158:GLU:OE2	46:5J:161:SER:OG	2.28	0.51
49:RE:139:PRO:HD2	49:RE:238:HIS:HE1	1.75	0.51
49:RE:565:LYS:HZ1	49:RE:689:HIS:HB3	1.76	0.51
49:RE:1019:GLY:O	49:RE:1023:ASN:ND2	2.44	0.51
50:RF:101:SER:O	50:RF:105:SER:HB2	2.11	0.51
51:RH:232:LEU:HD11	51:RH:240:LYS:HZ2	1.76	0.51
63:R5:40:PHE:HA	63:R5:47:VAL:HA	1.92	0.51
65:R3:130:VAL:HG12	65:R3:213:LEU:HB2	1.91	0.51
65:R3:236:TYR:OH	65:R3:388:LEU:O	2.26	0.51
66:R6:167:PHE:HE1	66:R6:174:VAL:HG22	1.76	0.51
67:R2:97:SER:HB2	68:M3:108:ASN:HB3	1.93	0.51
72:R4:99:ILE:HD12	72:R4:102:LEU:HD12	1.93	0.51
5:SF:180:LEU:N	5:SF:229:GLY:O	2.44	0.51
25:A4:395:SER:HB2	25:A4:398:THR:HB	1.93	0.51
31:AG:173:LEU:HB2	31:AG:191:ALA:HB3	1.92	0.51
31:AG:677:THR:OG1	31:AG:678:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B1:42:LEU:HD23	32:B1:338:ILE:HG21	1.93	0.51
34:B3:5:THR:HB	34:B3:611:LYS:HG2	1.93	0.51
34:B3:440:VAL:HG12	34:B3:456:THR:HG22	1.93	0.51
36:BE:726:GLY:O	36:BE:728:ARG:NH1	2.44	0.51
45:5I:154:ASP:N	45:5I:154:ASP:OD1	2.40	0.51
48:RD:1695:TRP:HD1	48:RD:1696:LEU:HD22	1.74	0.51
49:RE:139:PRO:HD2	49:RE:238:HIS:CE1	2.46	0.51
49:RE:236:THR:HG21	49:RE:256:TYR:HE1	1.75	0.51
49:RE:773:TYR:OH	49:RE:1131:ASN:O	2.29	0.51
52:RJ:266:ASP:HB3	52:RJ:795:LYS:HA	1.92	0.51
52:RJ:754:GLN:HA	52:RJ:757:LYS:HD2	1.92	0.51
54:RN:678:PHE:HB3	54:RN:681:PRO:HD2	1.93	0.51
64:R1:61:LEU:HB2	64:R1:64:GLN:HG2	1.93	0.51
64:R1:164:GLY:HA2	64:R1:184:THR:HA	1.93	0.51
72:R4:423:PHE:HB3	72:R4:433:LYS:HB2	1.92	0.51
75:M4:353:PHE:O	75:M4:357:MET:N	2.42	0.51
2:5A:2:U:H2'	2:5A:3:G:H8	1.76	0.51
3:SA:1697:G:O6	3:SA:1704:U:O4	2.29	0.51
25:A4:207:ASP:O	25:A4:233:LYS:NZ	2.44	0.51
25:A4:394:TRP:HB3	25:A4:399:VAL:HG23	1.93	0.51
25:A4:582:VAL:O	25:A4:593:GLU:HA	2.11	0.51
26:A5:56:SER:O	26:A5:59:LYS:NZ	2.44	0.51
31:AG:96:ILE:HG12	31:AG:108:THR:HG21	1.93	0.51
34:B3:280:ARG:NH1	34:B3:281:THR:O	2.44	0.51
39:5C:322:VAL:HA	39:5C:331:ALA:O	2.11	0.51
49:RE:257:SER:OG	49:RE:269:ARG:NH1	2.44	0.51
51:RH:43:VAL:HG21	51:RH:99:LEU:HD13	1.92	0.51
63:R5:34:ARG:NE	63:R5:222:ASP:OD2	2.41	0.51
64:R1:136:MET:HB3	64:R1:186:THR:HG21	1.92	0.51
72:R4:289:SER:HB3	72:R4:300:LEU:HD23	1.93	0.51
72:R4:911:GLU:OE1	72:R4:982:GLN:NE2	2.41	0.51
3:SA:1461:C:OP2	54:RN:726:LYS:NZ	2.45	0.50
10:SK:110:GLN:HE21	10:SK:122:VAL:HG12	1.75	0.50
15:SX:6:VAL:HG22	15:SX:34:ILE:HD11	1.93	0.50
25:A4:741:LEU:HD23	25:A4:743:PHE:N	2.25	0.50
27:A8:664:LYS:NZ	28:A9:448:GLU:OE2	2.35	0.50
31:AG:225:ILE:HG13	31:AG:241:LEU:HD22	1.92	0.50
31:AG:659:ILE:HA	31:AG:674:THR:HA	1.93	0.50
33:B2:140:SER:OG	33:B2:141:LYS:N	2.44	0.50
33:B2:497:VAL:HG13	33:B2:528:LEU:HB2	1.92	0.50
34:B3:279:LYS:NZ	34:B3:326:THR:OG1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B3:544:TYR:OH	34:B3:628:ASP:OD2	2.29	0.50
36:BE:155:THR:OG1	36:BE:156:LYS:N	2.44	0.50
39:5C:199:LEU:HD23	39:5C:245:ALA:HB1	1.92	0.50
39:5C:544:ASP:N	39:5C:544:ASP:OD1	2.43	0.50
49:RE:274:LYS:O	49:RE:284:ASN:ND2	2.44	0.50
49:RE:1109:LYS:HZ2	49:RE:1170:GLY:H	1.59	0.50
51:RH:112:VAL:HB	51:RH:124:VAL:HB	1.93	0.50
52:RJ:629:ASP:OD1	52:RJ:629:ASP:N	2.42	0.50
53:RK:30:PRO:HB3	53:RK:77:ARG:HG3	1.91	0.50
55:RO:258:GLU:HA	55:RO:261:TRP:HB2	1.93	0.50
56:RP:120:ASP:O	56:RP:123:LYS:NZ	2.44	0.50
56:RP:1912:ILE:HG13	56:RP:1958:MET:HG2	1.93	0.50
65:R3:239:GLN:HE21	65:R3:291:ILE:HD13	1.76	0.50
72:R4:448:ARG:HH12	72:R4:992:SER:HB3	1.75	0.50
72:R4:682:VAL:O	72:R4:686:GLN:N	2.39	0.50
3:SA:1483:A:O2'	3:SA:1607:G:O2'	2.27	0.50
15:SX:46:TYR:HB3	15:SX:69:LEU:HD12	1.93	0.50
24:3G:58:CYS:HB2	24:3G:98:ILE:HD12	1.92	0.50
25:A4:481:ILE:HD11	25:A4:536:VAL:HG22	1.93	0.50
27:A8:664:LYS:HA	27:A8:667:GLU:HG2	1.93	0.50
29:AE:272:LYS:NZ	29:AE:310:GLY:O	2.44	0.50
30:AF:377:ASP:OD1	30:AF:377:ASP:N	2.44	0.50
31:AG:48:PHE:HB2	31:AG:51:GLN:H	1.75	0.50
32:B1:470:SER:OG	32:B1:471:GLY:N	2.45	0.50
33:B2:297:LYS:HA	33:B2:300:GLU:HB2	1.92	0.50
33:B2:425:ILE:HG22	33:B2:426:ARG:HG2	1.94	0.50
34:B3:553:GLY:HA2	34:B3:577:ALA:HA	1.92	0.50
36:BE:234:ASN:O	36:BE:238:GLY:N	2.45	0.50
36:BE:380:LEU:HD11	36:BE:640:LEU:HD13	1.93	0.50
36:BE:606:ASP:OD1	36:BE:606:ASP:N	2.44	0.50
51:RG:106:LYS:NZ	51:RG:251:ILE:O	2.43	0.50
64:R1:76:VAL:HA	64:R1:126:ILE:HB	1.92	0.50
65:R3:377:SER:O	65:R3:381:SER:N	2.45	0.50
69:R0:70:ASP:OD1	76:M6:100:SER:OG	2.29	0.50
72:R4:61:PRO:HB2	72:R4:65:ASN:HA	1.91	0.50
75:M4:332:PRO:HB2	75:M4:335:GLY:HA3	1.93	0.50
75:M4:461:ILE:HD11	75:M4:480:LEU:HD12	1.92	0.50
3:SA:154:G:H21	7:SH:60:GLY:HA3	1.76	0.50
20:3B:123:ILE:HG23	20:3B:141:TYR:HB2	1.94	0.50
26:A5:130:ASP:OD1	26:A5:130:ASP:N	2.45	0.50
27:A8:587:LEU:HA	27:A8:592:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AE:575:SER:HB3	29:AE:578:VAL:HG22	1.93	0.50
30:AF:288:ASP:OD1	30:AF:288:ASP:N	2.45	0.50
32:B1:35:ASN:OD1	32:B1:35:ASN:N	2.37	0.50
34:B3:496:ALA:HB2	34:B3:538:ASP:HA	1.94	0.50
35:B8:382:GLY:O	35:B8:399:LYS:HA	2.10	0.50
45:5I:398:GLU:HA	45:5I:401:LYS:HE2	1.93	0.50
49:RE:578:ILE:HG21	49:RE:617:LEU:HD12	1.93	0.50
51:RG:77:LEU:HD22	51:RG:84:ILE:HD12	1.94	0.50
64:R1:43:GLU:HG2	64:R1:48:LYS:HG2	1.92	0.50
75:M4:410:ILE:HG12	75:M4:499:LEU:HB3	1.93	0.50
3:SA:238:U:O2'	3:SA:239:C:O4'	2.30	0.50
3:SA:312:A:H62	3:SA:352:A:H1'	1.77	0.50
3:SA:473:A:OP1	10:SK:44:ARG:NH1	2.38	0.50
3:SA:976:G:OP1	12:SO:109:LYS:NZ	2.45	0.50
21:3D:148:GLU:HA	21:3D:151:GLN:HE21	1.77	0.50
24:3H:7:LYS:NZ	24:3H:62:GLU:OE2	2.34	0.50
26:A5:437:VAL:HG13	55:RO:294:LYS:HD2	1.93	0.50
31:AG:765:TRP:HE1	31:AG:777:LEU:HD13	1.76	0.50
32:B1:275:LEU:HD13	32:B1:289:LEU:HD22	1.93	0.50
36:BE:94:TYR:HE1	36:BE:97:LYS:HE2	1.75	0.50
45:5I:290:ASP:OD1	45:5I:291:MET:N	2.41	0.50
49:RE:305:PRO:HB2	49:RE:473:LYS:HD2	1.92	0.50
49:RE:1074:LEU:HD11	49:RE:1087:LEU:HD23	1.93	0.50
51:RH:155:SER:OG	54:RN:716:LYS:NZ	2.40	0.50
52:RJ:895:PRO:HA	52:RJ:918:ILE:HA	1.94	0.50
53:RK:124:SER:OG	53:RK:125:HIS:N	2.43	0.50
53:RK:247:ALA:O	53:RK:255:SER:HA	2.12	0.50
54:RN:475:ARG:NH2	54:RN:516:LEU:O	2.45	0.50
58:RS:273:LYS:HA	58:RS:276:GLN:HE21	1.76	0.50
67:R2:95:ILE:HG12	67:R2:138:VAL:HG22	1.94	0.50
72:R4:150:ASN:O	72:R4:156:THR:OG1	2.29	0.50
75:M4:93:VAL:N	75:M4:113:VAL:O	2.42	0.50
75:M4:93:VAL:HG11	75:M4:325:PRO:HG2	1.92	0.50
75:M4:795:ARG:HA	75:M4:798:ASN:HB2	1.93	0.50
3:SA:347:G:OP1	11:SM:77:SER:OG	2.29	0.50
9:SJ:39:GLY:HA2	9:SJ:61:GLU:HG3	1.93	0.50
16:SY:98:GLU:HG3	53:RK:366:ILE:HG23	1.94	0.50
17:SZ:103:ALA:O	17:SZ:108:ARG:NH1	2.45	0.50
29:AE:254:GLN:NE2	29:AE:285:ASN:O	2.41	0.50
30:AF:33:ALA:HB2	30:AF:330:ARG:HE	1.76	0.50
45:5I:263:ARG:NH2	45:5I:282:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RG:183:ASP:OD2	51:RG:211:ARG:NH2	2.44	0.50
55:RO:374:HIS:ND1	55:RO:454:GLU:O	2.44	0.50
58:RS:261:GLU:HA	58:RS:264:LYS:HG2	1.93	0.50
69:R0:18:PRO:HB2	69:R0:52:VAL:HG22	1.93	0.50
72:R4:161:LEU:N	72:R4:164:GLU:OE1	2.42	0.50
75:M4:169:VAL:HG22	75:M4:317:VAL:HB	1.93	0.50
75:M4:397:ILE:HG23	75:M4:400:MET:HE1	1.93	0.50
1:3A:18:G:H2'	1:3A:19:A:H8	1.76	0.50
5:SF:104:ASP:HB3	5:SF:110:ALA:HB2	1.94	0.50
7:SH:115:LYS:NZ	7:SH:116:LYS:O	2.42	0.50
8:SI:125:ILE:O	8:SI:129:LEU:CB	2.60	0.50
8:SI:138:LYS:HG2	8:SI:152:VAL:HG12	1.93	0.50
17:SZ:78:SER:OG	17:SZ:81:GLU:OE2	2.29	0.50
25:A4:127:ASP:OD1	25:A4:132:LEU:N	2.43	0.50
25:A4:642:ASN:HD22	25:A4:645:ARG:HG3	1.75	0.50
31:AG:17:GLY:HA2	31:AG:50:ASN:HD22	1.76	0.50
33:B2:54:ILE:HA	33:B2:385:ILE:HD11	1.94	0.50
34:B3:128:VAL:HB	34:B3:138:HIS:HB2	1.92	0.50
49:RE:402:ASN:ND2	49:RE:453:PRO:O	2.44	0.50
50:RF:99:ASP:O	50:RF:103:LEU:HB2	2.10	0.50
50:RF:105:SER:OG	50:RF:106:ASP:N	2.44	0.50
53:RK:185:ARG:HH11	53:RK:312:ARG:HH12	1.60	0.50
55:RO:415:MET:HG3	55:RO:463:LEU:HB2	1.94	0.50
56:RP:1949:PRO:HA	56:RP:1985:ARG:HH21	1.76	0.50
59:RT:126:LEU:HD21	59:RT:152:LEU:HA	1.93	0.50
64:R1:69:LYS:HD3	64:R1:114:LEU:HD13	1.93	0.50
72:R4:825:SER:OG	72:R4:826:TYR:N	2.43	0.50
75:M4:94:ASP:O	75:M4:552:ARG:NH2	2.35	0.50
75:M4:433:SER:O	75:M4:437:LYS:N	2.40	0.50
3:SA:925:G:H2'	3:SA:926:A:H8	1.75	0.50
3:SA:1738:U:H5''	33:B2:333:ARG:HH21	1.75	0.50
20:3B:155:ILE:HD11	20:3B:162:LEU:HD11	1.94	0.50
20:3C:236:MET:HG3	22:3E:122:GLU:HB3	1.94	0.50
20:3C:297:ARG:HH12	20:3C:322:ARG:HH21	1.60	0.50
22:3E:167:ILE:HD11	22:3E:298:ARG:HG3	1.94	0.50
25:A4:168:ILE:HA	25:A4:179:HIS:HA	1.94	0.50
26:A5:247:THR:HG21	26:A5:293:ASN:H	1.77	0.50
27:A8:712:ASP:OD1	27:A8:712:ASP:N	2.38	0.50
29:AE:92:LYS:O	29:AE:96:ASN:ND2	2.45	0.50
31:AG:744:ILE:HA	31:AG:755:GLY:O	2.12	0.50
32:B1:457:VAL:HG23	32:B1:466:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B2:503:LYS:O	33:B2:520:LEU:N	2.44	0.50
36:BE:367:LEU:HD23	36:BE:375:LEU:HD21	1.94	0.50
41:5E:379:ASP:OD1	41:5E:379:ASP:N	2.42	0.50
42:5F:109:ARG:NH2	42:5F:155:GLU:OE2	2.44	0.50
44:5H:579:VAL:HG12	47:5K:47:VAL:HG21	1.93	0.50
51:RG:52:THR:OG1	51:RG:54:LYS:NZ	2.45	0.50
53:RK:249:SER:O	53:RK:249:SER:OG	2.29	0.50
54:RN:702:LEU:HD22	55:RO:416:LEU:HD11	1.93	0.50
59:RT:222:THR:OG1	59:RT:223:ARG:N	2.45	0.50
75:M4:504:THR:O	75:M4:508:GLY:N	2.35	0.50
75:M4:960:ALA:O	75:M4:964:LYS:N	2.38	0.50
6:SG:148:ARG:HA	6:SG:157:ARG:HG3	1.94	0.50
14:SR:113:ASP:N	14:SR:113:ASP:OD1	2.45	0.50
22:3E:201:ASP:HB3	22:3E:204:ALA:HB3	1.93	0.50
25:A4:553:LEU:HA	25:A4:560:SER:HA	1.93	0.50
29:AE:583:LYS:HE3	29:AE:627:LEU:HD22	1.94	0.50
31:AG:200:ASN:HD22	31:AG:262:MET:HG3	1.76	0.50
31:AG:313:LEU:HD23	31:AG:323:LEU:HB3	1.94	0.50
36:BE:637:ASN:ND2	36:BE:639:ASP:OD2	2.45	0.50
41:5E:296:ASN:O	52:RJ:264:GLN:NE2	2.45	0.50
45:5I:26:ARG:NH1	57:RQ:867:GLN:O	2.36	0.50
49:RE:428:TYR:O	49:RE:432:MET:HB2	2.12	0.50
53:RK:246:VAL:HA	53:RK:256:TYR:O	2.11	0.50
56:RP:1961:LYS:HB2	56:RP:1998:LEU:HD23	1.94	0.50
58:RS:369:THR:HA	58:RS:372:ILE:HD12	1.93	0.50
63:R5:81:THR:HA	63:R5:138:VAL:HB	1.93	0.50
69:R0:101:ALA:HB1	69:R0:135:GLU:HG2	1.94	0.50
72:R4:376:ASP:HA	72:R4:379:ILE:HD12	1.94	0.50
72:R4:592:THR:OG1	72:R4:593:SER:N	2.44	0.50
75:M4:326:LEU:HD23	75:M4:553:GLY:HA3	1.92	0.50
75:M4:712:THR:HB	75:M4:715:GLU:H	1.77	0.50
75:M4:1022:GLY:O	75:M4:1026:ARG:N	2.42	0.50
4:SC:242:LYS:HD2	34:B3:237:LEU:HD21	1.92	0.50
5:SF:127:LYS:HZ3	5:SF:142:HIS:HB3	1.77	0.50
8:SI:143:LEU:O	15:SX:42:GLN:NE2	2.45	0.50
15:SX:4:SER:OG	15:SX:5:SER:N	2.45	0.50
24:3G:21:LEU:HA	24:3G:24:VAL:HG12	1.93	0.50
25:A4:542:VAL:HA	25:A4:551:ASP:O	2.11	0.50
26:A5:128:GLN:HB2	26:A5:138:GLN:H	1.76	0.50
30:AF:390:ARG:HB2	30:AF:394:GLN:HE22	1.77	0.50
33:B2:645:GLU:HG2	33:B2:646:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B8:384:ILE:HD12	35:B8:423:LEU:HD21	1.93	0.50
35:B8:516:THR:HG21	35:B8:536:ALA:HB3	1.94	0.50
37:B6:178:VAL:HG22	37:B6:180:LYS:H	1.77	0.50
41:5E:357:ILE:HG12	43:5G:169:ASN:HD22	1.77	0.50
53:RK:19:LEU:HA	53:RK:22:VAL:HG12	1.94	0.50
53:RK:285:LYS:HG3	53:RK:316:GLU:HB3	1.93	0.50
53:RK:289:VAL:HG21	53:RK:294:LEU:HD13	1.94	0.50
65:R3:148:GLU:HA	65:R3:151:ILE:HD12	1.93	0.50
71:C4:225:LYS:HE2	71:C4:261:ASN:HD21	1.77	0.50
72:R4:572:ASP:H	72:R4:623:ALA:HA	1.77	0.50
72:R4:678:LEU:HB2	72:R4:726:LEU:HD12	1.93	0.50
75:M4:223:THR:HB	75:M4:226:ILE:H	1.76	0.50
3:SA:315:A:N6	3:SA:350:U:O4'	2.44	0.49
4:SC:160:HIS:HD1	4:SC:205:PHE:HE2	1.59	0.49
12:SO:61:THR:OG1	12:SO:62:GLN:N	2.43	0.49
25:A4:288:THR:OG1	25:A4:289:ASP:N	2.44	0.49
32:B1:210:SER:OG	32:B1:211:LYS:N	2.45	0.49
33:B2:270:SER:HB3	33:B2:286:ILE:HG13	1.94	0.49
35:B8:358:PHE:HA	35:B8:376:LEU:O	2.12	0.49
35:B8:391:SER:OG	35:B8:392:GLY:N	2.44	0.49
36:BE:128:LEU:HB2	36:BE:150:PRO:HG2	1.93	0.49
49:RE:138:ILE:O	49:RE:180:LYS:NZ	2.44	0.49
49:RE:361:GLU:HA	49:RE:364:VAL:HG12	1.94	0.49
49:RE:481:THR:OG1	49:RE:482:VAL:N	2.41	0.49
52:RJ:74:VAL:HG22	52:RJ:139:LEU:HD21	1.94	0.49
71:C4:270:THR:N	71:C4:274:MET:O	2.45	0.49
72:R4:62:ASP:OD1	72:R4:66:GLU:N	2.44	0.49
72:R4:739:ALA:HA	72:R4:742:ILE:HG12	1.93	0.49
75:M4:434:ASP:HA	75:M4:437:LYS:HB2	1.93	0.49
75:M4:503:GLU:O	75:M4:506:SER:OG	2.27	0.49
2:5A:278:G:N2	35:B8:558:SER:O	2.44	0.49
3:SA:593:U:H4'	3:SA:595:G:H4'	1.94	0.49
25:A4:126:TRP:HA	25:A4:133:PRO:HA	1.94	0.49
25:A4:614:TRP:NE1	25:A4:658:ASP:O	2.44	0.49
28:A9:502:ARG:HH11	30:AF:510:LEU:HB2	1.77	0.49
33:B2:215:ASP:N	33:B2:215:ASP:OD1	2.45	0.49
33:B2:403:ASN:OD1	33:B2:403:ASN:N	2.44	0.49
33:B2:446:ILE:HD13	33:B2:456:LEU:HD12	1.94	0.49
35:B8:465:THR:OG1	35:B8:466:THR:N	2.45	0.49
36:BE:21:SER:OG	36:BE:22:LYS:N	2.43	0.49
36:BE:737:LEU:HA	36:BE:740:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5K:183:GLU:HG2	47:5K:184:LYS:HG3	1.94	0.49
49:RE:725:SER:O	49:RE:729:ASN:ND2	2.45	0.49
53:RK:300:TYR:HA	53:RK:303:ILE:HG22	1.93	0.49
55:RO:399:ILE:HD11	55:RO:483:ILE:HD11	1.94	0.49
56:RP:1774:LYS:HA	56:RP:1777:LEU:HB2	1.95	0.49
72:R4:985:SER:O	72:R4:994:ARG:NH2	2.45	0.49
2:5A:474:A:OP2	39:5C:425:ARG:NH2	2.43	0.49
3:SA:919:A:H5'	13:SP:18:ARG:HH12	1.78	0.49
4:SC:129:THR:OG1	4:SC:130:SER:N	2.45	0.49
12:SO:91:LEU:HD22	12:SO:122:ILE:HG12	1.93	0.49
20:3C:96:VAL:HG23	20:3C:106:LEU:HD21	1.94	0.49
20:3C:165:ALA:HB3	20:3C:168:LYS:HB2	1.94	0.49
25:A4:444:ARG:O	25:A4:475:THR:OG1	2.30	0.49
25:A4:560:SER:OG	25:A4:561:LYS:N	2.45	0.49
39:5C:414:LEU:HB2	45:5I:26:ARG:HH22	1.78	0.49
45:5I:224:SER:OG	45:5I:225:LEU:N	2.44	0.49
52:RJ:94:THR:HG21	52:RJ:354:ILE:HB	1.94	0.49
57:RQ:322:ASN:N	57:RQ:322:ASN:OD1	2.45	0.49
66:R6:76:PRO:O	66:R6:128:ASN:ND2	2.35	0.49
72:R4:653:SER:H	72:R4:656:GLN:HB2	1.76	0.49
7:SH:7:TYR:O	7:SH:11:GLY:CA	2.61	0.49
10:SK:109:LEU:HB2	10:SK:146:PHE:HB3	1.94	0.49
25:A4:485:LYS:HA	25:A4:498:VAL:O	2.12	0.49
30:AF:48:ASN:HB3	30:AF:52:PRO:HA	1.93	0.49
30:AF:312:ALA:HB3	30:AF:316:ARG:HE	1.76	0.49
30:AF:390:ARG:O	30:AF:394:GLN:NE2	2.45	0.49
33:B2:634:SER:OG	33:B2:635:LYS:N	2.45	0.49
34:B3:387:HIS:CG	34:B3:407:SER:HB3	2.46	0.49
36:BE:255:SER:OG	36:BE:256:PHE:N	2.45	0.49
51:RH:222:ASP:OD1	51:RH:222:ASP:N	2.44	0.49
56:RP:362:PHE:O	56:RP:366:ILE:CB	2.61	0.49
71:C4:67:GLU:O	71:C4:107:LEU:N	2.45	0.49
75:M4:123:VAL:HA	75:M4:315:HIS:HA	1.93	0.49
75:M4:714:HIS:HA	75:M4:764:LEU:HD12	1.94	0.49
75:M4:985:VAL:HG12	75:M4:988:ASP:H	1.78	0.49
2:5A:87:C:N4	31:AG:333:PHE:O	2.45	0.49
7:SH:39:GLU:HG2	7:SH:46:LYS:HA	1.93	0.49
9:SJ:67:TRP:HD1	9:SJ:70:GLU:H	1.59	0.49
13:SP:53:ASP:OD1	13:SP:53:ASP:N	2.43	0.49
20:3B:127:GLU:OE1	20:3B:137:THR:OG1	2.29	0.49
22:3E:37:LYS:O	22:3E:41:GLU:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3H:26:GLN:NE2	24:3H:113:GLN:OE1	2.45	0.49
29:AE:559:ASN:ND2	29:AE:614:LEU:O	2.42	0.49
30:AF:308:SER:HB2	30:AF:316:ARG:HD3	1.94	0.49
31:AG:591:GLU:HG3	31:AG:593:ASN:HB3	1.93	0.49
33:B2:15:GLY:O	33:B2:360:ASN:ND2	2.46	0.49
34:B3:107:ILE:HD12	34:B3:150:LEU:HD22	1.93	0.49
34:B3:163:LEU:N	34:B3:175:TRP:O	2.45	0.49
39:5C:376:ASN:OD1	39:5C:376:ASN:N	2.43	0.49
40:5D:139:SER:OG	40:5D:140:ARG:N	2.45	0.49
45:5I:77:TYR:HE2	45:5I:229:GLN:HE21	1.59	0.49
50:RF:63:ASN:HD21	50:RF:163:PRO:HB2	1.78	0.49
50:RF:107:LEU:HD21	50:RF:194:ARG:HD3	1.94	0.49
55:RO:279:LEU:HB2	55:RO:318:LEU:HD13	1.94	0.49
58:RS:348:PRO:HG2	58:RS:351:HIS:HB2	1.93	0.49
64:R1:47:ASN:OD1	64:R1:132:ASP:N	2.43	0.49
3:SA:329:G:H2'	3:SA:330:G:H8	1.78	0.49
22:3E:245:THR:OG1	22:3E:246:GLU:N	2.45	0.49
32:B1:536:LYS:O	32:B1:538:GLN:N	2.46	0.49
34:B3:393:SER:OG	34:B3:394:LEU:N	2.45	0.49
34:B3:397:THR:HB	34:B3:399:ASP:H	1.78	0.49
49:RE:777:ASP:OD1	49:RE:777:ASP:N	2.39	0.49
49:RE:842:ILE:O	49:RE:849:GLY:HA2	2.13	0.49
52:RJ:258:ILE:HD13	52:RJ:265:ILE:HG12	1.93	0.49
52:RJ:295:ASP:OD1	52:RJ:295:ASP:N	2.44	0.49
52:RJ:779:ARG:NH1	53:RK:336:GLU:OE1	2.46	0.49
52:RJ:1105:ASP:N	52:RJ:1105:ASP:OD1	2.45	0.49
59:RT:216:ILE:HD13	59:RT:263:LEU:HD21	1.94	0.49
72:R4:780:LEU:HA	72:R4:786:LEU:HD12	1.93	0.49
75:M4:93:VAL:O	75:M4:113:VAL:N	2.43	0.49
3:SA:315:A:N1	3:SA:349:U:O2'	2.39	0.49
11:SM:123:VAL:HG12	11:SM:142:VAL:HG23	1.93	0.49
26:A5:485:ALA:HB2	26:A5:526:LEU:HD12	1.95	0.49
30:AF:284:PHE:HB3	30:AF:290:PHE:HA	1.95	0.49
31:AG:207:LEU:HD23	31:AG:264:ILE:HD12	1.94	0.49
32:B1:69:LEU:HD23	32:B1:127:VAL:HG22	1.93	0.49
34:B3:158:SER:OG	34:B3:159:LYS:N	2.45	0.49
34:B3:509:ALA:HB1	34:B3:536:LEU:HB2	1.93	0.49
38:5B:196:SER:HA	38:5B:199:ILE:HG22	1.95	0.49
39:5C:37:THR:OG1	39:5C:38:LYS:N	2.44	0.49
45:5I:73:ILE:HG22	45:5I:355:LYS:HD2	1.94	0.49
49:RE:1100:VAL:HB	49:RE:1182:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:RK:137:LEU:HD23	53:RK:296:LEU:HD13	1.95	0.49
55:RO:277:ILE:O	55:RO:281:LEU:HB2	2.13	0.49
74:R7:74:SER:HA	74:R7:77:LEU:HB3	1.95	0.49
2:5A:495:G:H2'	2:5A:496:G:C8	2.48	0.49
3:SA:29:U:H2'	3:SA:30:G:H8	1.78	0.49
3:SA:500:C:OP1	3:SA:501:U:N3	2.46	0.49
22:3E:303:SER:OG	22:3E:304:GLY:N	2.45	0.49
23:3F:374:LYS:HG3	23:3F:375:GLU:HG3	1.95	0.49
25:A4:394:TRP:HA	25:A4:399:VAL:HA	1.95	0.49
29:AE:722:ASN:O	29:AE:755:ARG:NH2	2.46	0.49
31:AG:586:SER:O	31:AG:597:LYS:NZ	2.46	0.49
32:B1:70:LEU:HD22	32:B1:84:PHE:HD1	1.77	0.49
42:5F:29:ASP:N	42:5F:29:ASP:OD1	2.46	0.49
49:RE:359:PHE:HZ	49:RE:401:LEU:HD11	1.77	0.49
49:RE:840:LEU:HD23	49:RE:852:PHE:HD2	1.77	0.49
49:RE:1150:VAL:HG21	49:RE:1165:SER:HB2	1.94	0.49
49:RE:1206:PRO:HD2	50:RF:36:PHE:HD2	1.77	0.49
51:RH:111:GLN:NE2	51:RH:123:GLU:OE1	2.45	0.49
67:R2:29:HIS:HA	67:R2:199:LEU:HD13	1.94	0.49
75:M4:277:GLU:OE2	75:M4:609:PHE:N	2.42	0.49
75:M4:1050:LEU:O	75:M4:1054:MET:N	2.45	0.49
1:3A:8:U:H2'	1:3A:9:A:H8	1.78	0.49
5:SF:57:ASN:N	5:SF:57:ASN:OD1	2.45	0.49
9:SJ:36:THR:OG1	9:SJ:59:ARG:N	2.45	0.49
20:3C:303:GLN:HA	20:3C:315:ILE:O	2.12	0.49
25:A4:397:SER:OG	25:A4:426:GLN:O	2.30	0.49
25:A4:514:LEU:HD21	25:A4:562:PRO:HG3	1.95	0.49
29:AE:186:MET:HA	29:AE:189:LEU:HB2	1.94	0.49
31:AG:559:LYS:O	31:AG:576:ALA:HB3	2.13	0.49
33:B2:763:ILE:HD13	33:B2:838:THR:HG21	1.95	0.49
33:B2:861:ILE:HD11	34:B3:805:ILE:HG13	1.94	0.49
36:BE:471:CYS:SG	36:BE:473:ASN:ND2	2.77	0.49
49:RE:1193:ALA:HB1	49:RE:1211:ASN:HB3	1.94	0.49
52:RJ:775:GLU:O	52:RJ:780:ILE:N	2.45	0.49
58:RS:339:GLY:O	58:RS:343:ALA:CB	2.60	0.49
63:R5:144:ASP:OD1	63:R5:225:LEU:N	2.45	0.49
68:M3:193:ALA:HA	68:M3:202:SER:HA	1.94	0.49
71:C4:254:VAL:HB	71:C4:288:CYS:HA	1.94	0.49
3:SA:688:G:H2'	3:SA:689:G:H8	1.78	0.49
11:SM:141:LYS:NZ	11:SM:142:VAL:O	2.46	0.49
17:SZ:103:ALA:HB1	17:SZ:107:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3B:228:GLN:HE21	21:3D:102:ASP:HB3	1.78	0.49
21:3D:90:SER:H	57:RQ:321:HIS:CE1	2.31	0.49
22:3E:356:LYS:HA	22:3E:359:ILE:HG22	1.95	0.49
22:3E:408:THR:O	29:AE:166:ASN:ND2	2.46	0.49
25:A4:33:VAL:HB	27:A8:709:GLU:HB3	1.95	0.49
26:A5:212:LEU:HB2	26:A5:226:LEU:HB2	1.95	0.49
30:AF:145:ASP:OD1	30:AF:172:ARG:NE	2.46	0.49
37:B6:29:VAL:HA	37:B6:32:ILE:HG12	1.95	0.49
43:5G:81:SER:OG	43:5G:82:GLY:N	2.46	0.49
45:5I:420:PRO:HD2	45:5I:423:ILE:HD12	1.95	0.49
49:RE:384:SER:HA	49:RE:584:GLU:HG3	1.95	0.49
49:RE:444:SER:N	49:RE:471:SER:OG	2.40	0.49
51:RG:67:LEU:HD21	51:RG:141:MET:HG3	1.94	0.49
51:RH:47:MET:HG2	51:RH:117:SER:HB3	1.94	0.49
52:RJ:143:ASP:OD1	52:RJ:143:ASP:N	2.46	0.49
52:RJ:170:VAL:HG12	52:RJ:205:PHE:HB2	1.94	0.49
52:RJ:847:LEU:O	52:RJ:853:ARG:HA	2.13	0.49
54:RN:428:VAL:HA	54:RN:431:ARG:HB2	1.94	0.49
63:R5:126:VAL:HG23	63:R5:130:LYS:H	1.78	0.49
66:R6:168:VAL:O	66:R6:172:LYS:N	2.45	0.49
72:R4:559:LEU:HG	72:R4:565:GLU:HB2	1.94	0.49
75:M4:306:ILE:HD13	75:M4:309:ILE:HD11	1.95	0.49
3:SA:155:U:H4'	7:SH:59:GLN:HG3	1.96	0.48
3:SA:1665:U:O2	3:SA:1736:G:C6	2.66	0.48
4:SC:64:ARG:NH2	13:SP:32:ASP:OD2	2.46	0.48
21:3D:74:VAL:HG13	21:3D:78:LEU:HD22	1.93	0.48
22:3E:215:ARG:NH1	22:3E:242:SER:OG	2.46	0.48
22:3E:422:THR:OG1	22:3E:423:GLU:N	2.46	0.48
23:3F:355:THR:OG1	23:3F:356:ARG:N	2.43	0.48
26:A5:362:ARG:NH1	31:AG:591:GLU:OE2	2.46	0.48
27:A8:575:ASN:HA	27:A8:579:LEU:HD22	1.95	0.48
29:AE:576:ILE:HA	29:AE:579:ARG:HB2	1.94	0.48
31:AG:73:LEU:O	31:AG:131:HIS:NE2	2.46	0.48
31:AG:175:ALA:HB3	31:AG:188:ALA:HB3	1.95	0.48
31:AG:501:THR:OG1	31:AG:506:TRP:N	2.46	0.48
33:B2:279:LYS:HD3	33:B2:336:TYR:HA	1.95	0.48
34:B3:519:ASN:ND2	34:B3:526:GLU:OE2	2.45	0.48
35:B8:144:LYS:HB2	35:B8:147:ARG:HH21	1.78	0.48
36:BE:329:SER:O	36:BE:329:SER:OG	2.31	0.48
36:BE:604:SER:OG	36:BE:606:ASP:OD1	2.31	0.48
43:5G:196:THR:HG23	43:5G:199:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:397:MET:HG2	49:RE:425:VAL:HG21	1.95	0.48
51:RH:227:LEU:HD23	51:RH:240:LYS:HE2	1.95	0.48
53:RK:193:GLY:O	53:RK:225:ILE:HA	2.13	0.48
53:RK:315:LYS:HZ3	53:RK:348:GLU:H	1.60	0.48
66:R6:132:ALA:HB1	66:R6:205:LEU:HD23	1.95	0.48
72:R4:12:ARG:NH2	72:R4:18:SER:OG	2.46	0.48
6:SG:120:ILE:HA	6:SG:123:VAL:HG12	1.95	0.48
20:3C:89:GLU:OE1	40:5D:164:ASN:ND2	2.47	0.48
25:A4:147:ILE:HG22	25:A4:158:VAL:HA	1.94	0.48
35:B8:450:GLN:HE21	35:B8:507:PRO:HD3	1.78	0.48
41:5E:346:GLU:O	52:RJ:1005:SER:OG	2.29	0.48
45:5I:252:ASN:ND2	56:RP:1949:PRO:O	2.43	0.48
48:RD:1542:GLN:OE1	49:RE:872:ASN:ND2	2.45	0.48
52:RJ:300:GLN:HG2	52:RJ:792:VAL:HB	1.95	0.48
54:RN:447:SER:O	54:RN:450:ARG:NH2	2.46	0.48
66:R6:217:ILE:O	66:R6:221:LEU:N	2.45	0.48
71:C4:211:ARG:HH11	71:C4:214:ASP:HB3	1.79	0.48
72:R4:10:ARG:HD3	72:R4:18:SER:HB3	1.93	0.48
72:R4:517:ASP:N	72:R4:517:ASP:OD1	2.44	0.48
75:M4:92:GLU:HA	75:M4:114:ARG:HA	1.95	0.48
3:SA:142:G:C2	3:SA:173:A:H2	2.31	0.48
20:3B:189:GLY:O	20:3B:216:ASN:ND2	2.46	0.48
22:3E:138:LYS:HD3	22:3E:141:LEU:HD21	1.95	0.48
26:A5:66:VAL:HG12	26:A5:112:LEU:HD21	1.96	0.48
31:AG:427:LYS:O	31:AG:431:SER:OG	2.28	0.48
31:AG:763:ILE:HD11	31:AG:776:PHE:HB2	1.95	0.48
33:B2:6:GLN:NE2	33:B2:686:GLU:OE1	2.45	0.48
33:B2:435:THR:HG21	33:B2:478:SER:HA	1.94	0.48
35:B8:445:ARG:NH2	35:B8:499:ALA:O	2.42	0.48
36:BE:51:VAL:HG12	36:BE:60:ILE:HG12	1.95	0.48
36:BE:169:SER:OG	36:BE:170:LEU:N	2.46	0.48
39:5C:414:LEU:HD22	45:5I:26:ARG:HH12	1.76	0.48
45:5I:275:PHE:HB3	57:RQ:295:VAL:HG11	1.95	0.48
50:RF:66:HIS:HB2	50:RF:158:TRP:HE1	1.78	0.48
51:RG:116:THR:HB	51:RG:119:GLY:H	1.78	0.48
54:RN:490:PHE:HA	54:RN:493:LEU:HD23	1.94	0.48
54:RN:520:PRO:HA	54:RN:523:ILE:HG12	1.94	0.48
66:R6:15:GLY:O	66:R6:30:VAL:N	2.41	0.48
67:R2:9:SER:O	67:R2:13:ASP:N	2.45	0.48
71:C4:211:ARG:NE	71:C4:213:THR:O	2.47	0.48
72:R4:689:LEU:HD23	72:R4:693:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:M4:793:SER:O	75:M4:797:VAL:N	2.43	0.48
75:M4:903:LEU:HA	75:M4:906:ARG:HD2	1.95	0.48
1:3A:85:G:N7	22:3E:361:ARG:NH1	2.61	0.48
3:SA:867:G:OP1	12:SO:9:LYS:NZ	2.36	0.48
5:SF:54:TYR:O	17:SZ:15:ASN:ND2	2.46	0.48
9:SJ:83:TYR:OH	11:SM:11:ARG:O	2.30	0.48
26:A5:5:VAL:HA	26:A5:21:THR:HG22	1.95	0.48
26:A5:84:GLU:OE1	26:A5:86:TRP:NE1	2.31	0.48
31:AG:595:CYS:SG	31:AG:596:LEU:N	2.86	0.48
45:5I:40:GLU:HG3	45:5I:404:PHE:HE2	1.78	0.48
48:RD:1518:ILE:HG23	48:RD:1552:LYS:HE2	1.95	0.48
49:RE:177:ASN:HB3	49:RE:179:LYS:HZ3	1.78	0.48
49:RE:794:ASP:OD1	49:RE:865:ARG:NH2	2.42	0.48
49:RE:1166:ARG:O	49:RE:1180:ASN:ND2	2.37	0.48
56:RP:185:LYS:HB3	56:RP:188:LEU:HD12	1.95	0.48
58:RS:433:THR:OG1	58:RS:435:ASP:OD1	2.32	0.48
63:R5:198:PHE:CE2	63:R5:264:CYS:HB3	2.48	0.48
72:R4:73:SER:OG	72:R4:74:ASP:OD1	2.30	0.48
75:M4:719:VAL:HB	75:M4:762:ILE:HG13	1.96	0.48
2:5A:296:C:O2'	36:BE:68:LEU:O	2.24	0.48
3:SA:513:U:H2'	3:SA:514:G:C8	2.49	0.48
3:SA:1527:C:OP1	6:SG:106:LYS:NZ	2.37	0.48
23:3F:256:ARG:HD3	23:3F:282:GLU:HG2	1.94	0.48
25:A4:429:SER:OG	25:A4:430:THR:N	2.46	0.48
31:AG:762:TYR:HB3	31:AG:779:ILE:HG12	1.96	0.48
36:BE:569:VAL:HB	36:BE:579:ARG:HB2	1.95	0.48
39:5C:384:VAL:HB	39:5C:389:LEU:O	2.13	0.48
47:5K:153:VAL:O	47:5K:172:LEU:HA	2.13	0.48
53:RK:142:GLU:O	53:RK:147:ARG:NH2	2.40	0.48
56:RP:1919:ILE:HD13	56:RP:1961:LYS:HD3	1.96	0.48
3:SA:448:C:OP2	5:SF:49:ARG:NH1	2.47	0.48
4:SC:175:GLU:O	4:SC:179:SER:OG	2.29	0.48
8:SI:137:GLY:O	8:SI:153:LEU:HB2	2.14	0.48
22:3E:379:ASP:N	22:3E:379:ASP:OD1	2.46	0.48
26:A5:82:ASN:OD1	26:A5:82:ASN:N	2.46	0.48
32:B1:4:ASP:OD1	32:B1:4:ASP:N	2.42	0.48
32:B1:64:ASN:N	32:B1:64:ASN:OD1	2.46	0.48
33:B2:285:ARG:HH22	33:B2:372:ARG:HD2	1.79	0.48
34:B3:15:ILE:HG13	34:B3:33:ALA:HB3	1.96	0.48
34:B3:245:SER:OG	34:B3:262:GLY:N	2.41	0.48
34:B3:469:PRO:HG2	34:B3:475:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B3:513:LYS:HB2	34:B3:532:HIS:HB2	1.95	0.48
35:B8:364:GLN:HG3	35:B8:371:VAL:HG22	1.95	0.48
36:BE:207:ASP:N	36:BE:207:ASP:OD1	2.45	0.48
36:BE:270:SER:O	36:BE:270:SER:OG	2.31	0.48
45:5I:188:HIS:HD1	45:5I:190:GLU:H	1.60	0.48
52:RJ:776:GLN:HA	52:RJ:780:ILE:HG22	1.95	0.48
54:RN:437:SER:HB2	54:RN:499:VAL:HG21	1.96	0.48
54:RN:700:LEU:HD12	55:RO:416:LEU:HA	1.96	0.48
75:M4:187:GLN:O	75:M4:191:ASN:ND2	2.46	0.48
2:5A:495:G:H2'	2:5A:496:G:H8	1.78	0.48
3:SA:66:U:OP2	7:SH:136:LYS:NZ	2.46	0.48
3:SA:844:A:H2'	3:SA:845:G:H8	1.77	0.48
3:SA:874:C:H2'	3:SA:875:G:C8	2.49	0.48
3:SA:1041:G:H2'	3:SA:1042:G:C8	2.48	0.48
3:SA:1685:G:N2	3:SA:1716:C:O2'	2.45	0.48
6:SG:79:ASN:O	32:B1:508:GLN:NE2	2.46	0.48
6:SG:219:ARG:NH2	51:RH:222:ASP:OD2	2.43	0.48
13:SP:81:VAL:HG21	13:SP:102:LEU:HD12	1.94	0.48
21:3D:160:ARG:NH1	37:B6:293:TYR:OH	2.45	0.48
21:3D:194:ARG:NH2	22:3E:172:ASP:OD2	2.47	0.48
25:A4:192:THR:O	25:A4:203:GLY:HA2	2.14	0.48
26:A5:445:LEU:HD11	26:A5:480:LEU:HD13	1.96	0.48
26:A5:467:ASP:O	26:A5:471:ARG:HB2	2.13	0.48
29:AE:697:GLU:O	29:AE:700:SER:OG	2.31	0.48
31:AG:623:PHE:HE2	31:AG:670:LEU:HD11	1.79	0.48
39:5C:340:LEU:O	39:5C:368:TYR:N	2.46	0.48
42:5F:54:ILE:HD11	42:5F:101:VAL:HG21	1.95	0.48
42:5F:169:THR:HA	42:5F:172:ARG:HG2	1.96	0.48
48:RD:1489:SER:O	48:RD:1489:SER:OG	2.32	0.48
50:RF:204:SER:OG	50:RF:205:SER:N	2.47	0.48
64:R1:105:VAL:O	64:R1:109:GLU:N	2.47	0.48
66:R6:138:ILE:O	66:R6:158:LEU:N	2.36	0.48
67:R2:37:PHE:O	67:R2:49:ARG:N	2.45	0.48
72:R4:316:VAL:HA	72:R4:395:ILE:HA	1.95	0.48
72:R4:879:MET:SD	72:R4:882:ARG:NH2	2.87	0.48
2:5A:8:A:H5''	28:A9:487:ARG:HH22	1.79	0.48
3:SA:760:A:N1	3:SA:790:U:C4	2.82	0.48
7:SH:142:ARG:HA	7:SH:147:LEU:HD23	1.96	0.48
23:3F:168:ASN:N	23:3F:174:GLU:O	2.47	0.48
23:3F:398:CYS:H	24:3H:14:ALA:HB1	1.78	0.48
26:A5:156:ALA:HB3	26:A5:159:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A8:493:LYS:HD2	27:A8:493:LYS:HA	1.70	0.48
29:AE:556:LYS:HD2	29:AE:558:VAL:HB	1.95	0.48
31:AG:335:PRO:HB2	31:AG:336:ARG:HD3	1.95	0.48
34:B3:148:SER:OG	34:B3:149:SER:N	2.38	0.48
35:B8:512:ASP:OD1	35:B8:512:ASP:N	2.47	0.48
55:RO:380:ILE:HD12	55:RO:405:LEU:HD22	1.94	0.48
55:RO:380:ILE:HG13	55:RO:402:ILE:HD11	1.96	0.48
59:RT:210:GLY:O	59:RT:214:PHE:HB2	2.13	0.48
63:R5:166:ASP:OD2	63:R5:182:ARG:NE	2.40	0.48
65:R3:362:LEU:HB2	66:R6:180:LEU:HB3	1.96	0.48
67:R2:31:PHE:HE1	67:R2:199:LEU:HB3	1.78	0.48
72:R4:59:VAL:HG13	72:R4:67:LEU:HD23	1.95	0.48
72:R4:830:ARG:NH2	72:R4:837:ASP:OD1	2.46	0.48
72:R4:899:ILE:O	72:R4:903:VAL:N	2.44	0.48
75:M4:87:GLN:N	75:M4:119:VAL:O	2.38	0.48
75:M4:506:SER:O	75:M4:539:GLN:NE2	2.47	0.48
1:3A:266:C:O2'	1:3A:267:A:O4'	2.32	0.48
3:SA:65:A:N6	3:SA:84:A:OP2	2.46	0.48
3:SA:884:A:OP1	4:SC:136:ARG:NH2	2.47	0.48
4:SC:65:VAL:HG21	4:SC:85:LYS:HE2	1.95	0.48
17:SZ:91:LEU:HD22	17:SZ:96:LEU:HD21	1.96	0.48
20:3C:100:ARG:HA	20:3C:104:ASP:HA	1.95	0.48
22:3E:219:SER:OG	37:B6:288:LYS:NZ	2.40	0.48
25:A4:613:GLN:HA	25:A4:616:LYS:HB3	1.95	0.48
27:A8:664:LYS:HD3	28:A9:448:GLU:HG2	1.96	0.48
28:A9:460:LEU:O	28:A9:464:SER:CB	2.58	0.48
31:AG:710:LEU:HG	31:AG:711:ILE:HG23	1.96	0.48
32:B1:441:SER:O	32:B1:441:SER:OG	2.30	0.48
33:B2:476:ILE:HA	33:B2:492:SER:HA	1.95	0.48
45:5I:205:ASP:OD1	45:5I:205:ASP:N	2.43	0.48
47:5K:155:THR:OG1	47:5K:156:ASN:N	2.47	0.48
49:RE:826:SER:OG	49:RE:841:ASN:ND2	2.46	0.48
51:RH:189:VAL:HA	51:RH:192:TYR:HB3	1.95	0.48
56:RP:133:ILE:HD13	56:RP:180:LEU:HG	1.95	0.48
56:RP:193:ALA:O	56:RP:197:SER:HB3	2.13	0.48
60:RW:132:GLU:O	60:RW:136:ARG:CB	2.61	0.48
72:R4:883:ASN:OD1	72:R4:886:ARG:NH1	2.47	0.48
72:R4:903:VAL:HG11	72:R4:935:VAL:HG21	1.95	0.48
8:SI:134:GLU:HB3	8:SI:155:ASP:HB3	1.96	0.48
16:SY:59:ILE:O	16:SY:69:ARG:NH2	2.42	0.48
20:3C:91:HIS:HB3	20:3C:96:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3E:215:ARG:NH2	22:3E:244:GLY:O	2.47	0.48
24:3G:26:GLN:HB3	24:3G:110:ILE:HG21	1.95	0.48
25:A4:417:VAL:HG11	25:A4:460:LEU:HD12	1.96	0.48
29:AE:800:ASP:N	29:AE:800:ASP:OD1	2.46	0.48
30:AF:215:VAL:HA	30:AF:230:GLY:HA3	1.94	0.48
31:AG:378:ASP:O	35:B8:344:ARG:NH2	2.47	0.48
32:B1:261:ALA:HB1	32:B1:279:PHE:HB3	1.95	0.48
32:B1:387:THR:OG1	32:B1:388:SER:N	2.47	0.48
32:B1:538:GLN:HG2	32:B1:554:ASP:HA	1.96	0.48
51:RG:186:VAL:HG22	55:RO:425:PRO:HG2	1.96	0.48
55:RO:290:HIS:CD2	55:RO:291:THR:HG22	2.49	0.48
56:RP:43:GLU:HG3	56:RP:44:SER:H	1.79	0.48
65:R3:131:TYR:CZ	68:M3:11:GLY:HA2	2.49	0.48
69:R0:18:PRO:HD3	76:M6:92:LEU:HD22	1.96	0.48
1:3A:206:C:N3	1:3A:243:U:C4	2.82	0.47
2:5A:295:A:C6	36:BE:381:ARG:HD2	2.49	0.47
16:SY:76:LEU:O	16:SY:80:GLY:HA2	2.13	0.47
20:3B:236:MET:HG2	21:3D:133:LEU:HA	1.95	0.47
20:3C:118:TYR:OH	20:3C:178:GLY:O	2.30	0.47
24:3H:13:ASP:OD1	24:3H:13:ASP:N	2.46	0.47
25:A4:102:LEU:HA	25:A4:115:PHE:O	2.14	0.47
25:A4:305:PHE:HB3	25:A4:325:ASN:HA	1.96	0.47
26:A5:441:LEU:HD22	26:A5:472:LEU:HG	1.96	0.47
29:AE:594:SER:HA	29:AE:614:LEU:HD22	1.96	0.47
31:AG:692:PHE:HE1	31:AG:750:LEU:HB3	1.79	0.47
34:B3:690:HIS:NE2	41:5E:518:GLU:OE2	2.47	0.47
36:BE:405:SER:OG	36:BE:406:THR:N	2.47	0.47
37:B6:67:ARG:NH1	37:B6:84:SER:OG	2.44	0.47
41:5E:316:ASN:O	41:5E:320:ALA:CB	2.62	0.47
43:5G:217:ASP:OD1	43:5G:217:ASP:N	2.44	0.47
43:5G:236:HIS:HA	43:5G:249:GLU:HA	1.95	0.47
45:5I:230:ASN:OD1	45:5I:230:ASN:N	2.43	0.47
52:RJ:268:LYS:HB3	52:RJ:794:GLU:HG3	1.94	0.47
67:R2:207:GLU:O	67:R2:232:ASN:ND2	2.47	0.47
71:C4:259:ALA:O	71:C4:264:GLY:N	2.44	0.47
72:R4:953:PHE:HB2	72:R4:960:LEU:HD13	1.95	0.47
75:M4:722:VAL:HG22	75:M4:759:VAL:HG22	1.95	0.47
1:3A:325:C:N4	22:3E:318:GLN:OE1	2.30	0.47
3:SA:486:G:N3	3:SA:500:C:N4	2.61	0.47
3:SA:524:U:N3	3:SA:527:A:OP2	2.46	0.47
3:SA:596:C:H2'	3:SA:597:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SC:92:GLN:NE2	4:SC:235:GLY:O	2.46	0.47
4:SC:209:ASN:OD1	4:SC:209:ASN:N	2.46	0.47
15:SX:6:VAL:HG23	15:SX:29:PRO:HD2	1.95	0.47
25:A4:62:PRO:HD2	25:A4:65:LEU:HD11	1.94	0.47
25:A4:97:ARG:NH2	38:5B:190:LEU:O	2.45	0.47
25:A4:378:TYR:OH	25:A4:632:ASN:ND2	2.47	0.47
26:A5:336:ASN:OD1	26:A5:336:ASN:N	2.47	0.47
26:A5:541:LEU:HG	30:AF:495:ILE:HD11	1.95	0.47
27:A8:665:GLN:HG3	28:A9:496:LEU:HD22	1.96	0.47
28:A9:437:ILE:HB	28:A9:456:LEU:HD22	1.96	0.47
29:AE:56:LEU:HD22	29:AE:74:PHE:HD2	1.79	0.47
31:AG:138:ASP:OD1	31:AG:140:LYS:NZ	2.38	0.47
36:BE:134:ASP:OD1	36:BE:136:SER:OG	2.32	0.47
36:BE:323:VAL:HB	36:BE:343:LEU:HD22	1.96	0.47
39:5C:170:GLN:NE2	39:5C:177:TYR:OH	2.47	0.47
42:5F:137:ARG:NH2	42:5F:139:GLY:O	2.42	0.47
55:RO:407:ARG:NH2	55:RO:488:PHE:O	2.48	0.47
55:RO:429:PRO:HA	55:RO:432:VAL:HG12	1.96	0.47
56:RP:1893:GLU:HA	56:RP:1896:ILE:HD12	1.96	0.47
56:RP:1957:GLN:NE2	56:RP:1995:ARG:O	2.47	0.47
56:RP:1998:LEU:H	56:RP:1998:LEU:HD12	1.79	0.47
64:R1:176:SER:HA	64:R1:179:GLU:HB2	1.96	0.47
68:M3:118:MET:O	68:M3:122:ASN:ND2	2.47	0.47
72:R4:317:ILE:HD12	72:R4:394:TYR:HD2	1.78	0.47
74:R7:74:SER:O	74:R7:78:GLY:N	2.37	0.47
75:M4:588:ASN:ND2	75:M4:911:ILE:O	2.47	0.47
3:SA:214:G:H4'	3:SA:242:U:H3	1.80	0.47
3:SA:1744:A:N6	3:SA:1746:A:N7	2.62	0.47
23:3F:342:ARG:HH12	24:3H:21:LEU:HB3	1.79	0.47
23:3F:492:TRP:HB3	23:3F:520:VAL:HG22	1.96	0.47
30:AF:238:ASP:OD2	30:AF:241:SER:OG	2.32	0.47
32:B1:36:ARG:NH2	32:B1:53:GLU:OE2	2.46	0.47
33:B2:139:GLY:HA3	33:B2:166:ILE:HD11	1.96	0.47
34:B3:536:LEU:HA	34:B3:552:SER:HB2	1.95	0.47
36:BE:361:SER:HA	36:BE:636:PRO:HB3	1.95	0.47
41:5E:310:GLN:HA	41:5E:313:GLN:HG2	1.96	0.47
41:5E:474:ILE:HG12	41:5E:476:MET:H	1.79	0.47
43:5G:131:CYS:SG	43:5G:136:THR:OG1	2.58	0.47
45:5I:244:ILE:O	45:5I:257:LYS:HA	2.14	0.47
51:RH:77:LEU:HD21	51:RH:84:ILE:HA	1.96	0.47
54:RN:489:HIS:HD2	54:RN:532:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:RN:741:LYS:HA	54:RN:741:LYS:HD2	1.68	0.47
55:RO:206:PRO:HA	55:RO:209:GLN:HG2	1.96	0.47
56:RP:1808:SER:O	56:RP:1808:SER:OG	2.33	0.47
56:RP:1914:THR:HA	56:RP:1917:ILE:HD12	1.96	0.47
65:R3:350:LEU:HB2	65:R3:359:GLN:H	1.78	0.47
72:R4:364:VAL:HG21	72:R4:369:GLN:HB2	1.97	0.47
72:R4:908:ARG:HA	72:R4:994:ARG:HH21	1.80	0.47
75:M4:100:THR:HG23	75:M4:329:TYR:HE1	1.79	0.47
75:M4:411:VAL:HB	75:M4:500:PHE:HA	1.96	0.47
75:M4:533:SER:N	75:M4:536:GLU:OE1	2.47	0.47
2:5A:84:G:H4'	31:AG:295:TRP:HA	1.95	0.47
31:AG:408:THR:HG21	31:AG:488:LEU:HD13	1.96	0.47
32:B1:369:ILE:HB	32:B1:383:PHE:HB2	1.96	0.47
36:BE:509:SER:OG	36:BE:510:LEU:N	2.47	0.47
38:5B:176:PHE:HB3	40:5D:133:HIS:HB3	1.95	0.47
40:5D:18:GLN:HB2	40:5D:28:LEU:H	1.80	0.47
56:RP:35:GLU:O	56:RP:37:ARG:NH2	2.48	0.47
68:M3:83:ILE:HG22	68:M3:85:GLY:H	1.80	0.47
69:R0:6:PHE:N	69:R0:9:ASP:OD2	2.40	0.47
69:R0:161:ASN:HA	69:R0:164:ARG:HD3	1.96	0.47
1:3A:59:G:OP1	32:B1:573:ASN:ND2	2.46	0.47
2:5A:2:U:H2'	2:5A:3:G:C8	2.49	0.47
3:SA:29:U:H2'	3:SA:30:G:C8	2.49	0.47
3:SA:1197:C:OP1	51:RG:135:LYS:NZ	2.40	0.47
4:SC:149:GLN:HE22	4:SC:154:SER:HB3	1.80	0.47
11:SM:64:VAL:HG12	11:SM:129:ARG:HE	1.79	0.47
16:SY:56:LYS:HE2	16:SY:97:ASP:HA	1.95	0.47
16:SY:76:LEU:O	16:SY:80:GLY:N	2.47	0.47
20:3C:166:PRO:HA	20:3C:188:VAL:HA	1.96	0.47
31:AG:317:TRP:HA	31:AG:340:ILE:HG23	1.97	0.47
32:B1:5:PHE:HB3	32:B1:704:TYR:HB3	1.97	0.47
34:B3:34:THR:OG1	34:B3:35:PRO:O	2.28	0.47
34:B3:741:LYS:HG2	34:B3:781:ILE:HD11	1.97	0.47
35:B8:129:ASP:HA	35:B8:132:LYS:HE3	1.97	0.47
35:B8:178:VAL:HG11	36:BE:217:VAL:HG11	1.96	0.47
36:BE:862:VAL:HG21	36:BE:904:ASP:HB2	1.95	0.47
51:RH:154:ASN:ND2	51:RH:156:GLU:OE2	2.48	0.47
69:R0:206:ALA:HB2	69:R0:234:ILE:HG13	1.95	0.47
72:R4:136:CYS:HA	72:R4:145:PHE:HB2	1.96	0.47
72:R4:316:VAL:HA	72:R4:396:GLN:H	1.79	0.47
75:M4:298:ASN:OD1	75:M4:298:ASN:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:M4:971:ALA:O	75:M4:975:LYS:N	2.39	0.47
3:SA:828:U:N3	3:SA:843:U:O2	2.48	0.47
3:SA:1756:A:H62	41:5E:532:LEU:HB2	1.78	0.47
5:SF:206:ASP:OD1	5:SF:206:ASP:N	2.47	0.47
6:SG:146:THR:OG1	6:SG:147:THR:N	2.48	0.47
8:SI:48:GLU:HG2	8:SI:56:LYS:HB3	1.97	0.47
20:3C:90:PRO:HA	20:3C:97:TYR:HD1	1.80	0.47
21:3D:212:ASP:O	21:3D:216:PHE:CB	2.62	0.47
23:3F:411:PHE:HA	23:3F:427:LEU:HD23	1.97	0.47
24:3H:16:LEU:HD21	24:3H:121:ILE:HG22	1.96	0.47
25:A4:101:GLY:HA3	25:A4:117:ILE:HD12	1.96	0.47
33:B2:171:CYS:HB2	33:B2:177:LEU:HD12	1.95	0.47
33:B2:917:ASN:OD1	33:B2:917:ASN:N	2.46	0.47
34:B3:410:ASN:HA	34:B3:435:ALA:HA	1.97	0.47
34:B3:464:LYS:HZ2	34:B3:481:LYS:HB2	1.80	0.47
39:5C:265:GLU:HG3	39:5C:265:GLU:O	2.14	0.47
45:5I:411:LYS:O	45:5I:415:ARG:HB2	2.15	0.47
46:5J:165:ASN:ND2	46:5J:168:GLU:OE1	2.48	0.47
51:RG:49:SER:HB2	51:RG:88:ARG:H	1.80	0.47
54:RN:559:ARG:O	54:RN:651:TRP:NE1	2.43	0.47
58:RS:413:LEU:O	58:RS:447:ARG:NH2	2.43	0.47
69:R0:187:ALA:HB3	69:R0:195:TRP:HB3	1.96	0.47
72:R4:615:LEU:HD22	72:R4:646:ILE:HD11	1.96	0.47
75:M4:343:ASP:OD1	75:M4:343:ASP:N	2.47	0.47
75:M4:946:GLN:HE21	75:M4:1030:ARG:HH12	1.63	0.47
75:M4:1035:VAL:HA	75:M4:1038:LEU:HD12	1.97	0.47
1:3A:30:A:N6	45:5I:342:ILE:O	2.36	0.47
3:SA:252:U:H2'	3:SA:253:A:H8	1.79	0.47
3:SA:1435:G:H5''	58:RS:416:ILE:HG12	1.96	0.47
3:SA:1638:G:OP2	34:B3:751:LYS:NZ	2.37	0.47
4:SC:149:GLN:HE21	4:SC:151:LYS:HG2	1.79	0.47
16:SY:109:ARG:NH2	16:SY:117:ILE:O	2.43	0.47
20:3B:218:ILE:HD12	21:3D:152:LEU:HA	1.96	0.47
20:3B:283:GLU:HG2	47:5K:150:CYS:HB3	1.97	0.47
21:3D:286:ARG:HA	21:3D:289:TYR:HB3	1.97	0.47
23:3F:298:SER:OG	23:3F:325:VAL:O	2.24	0.47
25:A4:121:THR:HA	25:A4:144:ILE:HG22	1.97	0.47
26:A5:472:LEU:HB3	26:A5:476:LEU:HD11	1.96	0.47
27:A8:465:SER:O	27:A8:469:ASP:CB	2.62	0.47
27:A8:507:LEU:HD13	27:A8:538:ARG:HH22	1.80	0.47
29:AE:259:THR:HG23	31:AG:891:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AF:307:VAL:HA	30:AF:318:LEU:HA	1.97	0.47
31:AG:529:LEU:HB2	31:AG:547:VAL:HG23	1.96	0.47
31:AG:768:TRP:HE1	31:AG:772:THR:HA	1.79	0.47
33:B2:218:ILE:HD11	33:B2:226:VAL:HB	1.95	0.47
33:B2:595:LYS:HD2	33:B2:615:GLN:HA	1.97	0.47
34:B3:12:LEU:HD23	34:B3:643:PHE:HE2	1.78	0.47
34:B3:151:LYS:H	34:B3:164:ALA:HB3	1.80	0.47
35:B8:253:SER:HB2	35:B8:297:THR:HA	1.96	0.47
36:BE:896:ILE:HG23	36:BE:905:ILE:HD12	1.95	0.47
37:B6:196:LEU:HA	37:B6:199:ARG:HB3	1.97	0.47
39:5C:69:GLU:OE1	45:5I:13:TYR:OH	2.32	0.47
39:5C:103:ALA:HB2	39:5C:402:ILE:HD11	1.96	0.47
39:5C:138:ASP:OD2	39:5C:141:LYS:NZ	2.44	0.47
46:5J:50:SER:O	46:5J:53:GLN:NE2	2.48	0.47
49:RE:891:ALA:HA	49:RE:894:ARG:HH11	1.80	0.47
49:RE:1087:LEU:O	49:RE:1090:THR:OG1	2.31	0.47
50:RF:64:ILE:HA	50:RF:87:LEU:HD13	1.97	0.47
50:RF:131:ALA:HA	50:RF:134:ILE:HG22	1.97	0.47
51:RH:191:ASP:HA	51:RH:194:GLU:HB3	1.97	0.47
52:RJ:164:MET:HE3	52:RJ:198:VAL:HG23	1.97	0.47
53:RK:302:VAL:HG11	53:RK:329:ILE:HD11	1.96	0.47
54:RN:419:LYS:HE2	54:RN:468:ARG:HE	1.79	0.47
56:RP:47:PHE:HA	56:RP:112:GLN:HG2	1.97	0.47
64:R1:156:ASP:OD1	64:R1:157:TYR:N	2.48	0.47
65:R3:30:SER:O	65:R3:34:HIS:ND1	2.42	0.47
66:R6:190:GLN:O	66:R6:194:LEU:N	2.46	0.47
72:R4:130:THR:O	72:R4:134:THR:N	2.45	0.47
72:R4:218:LEU:O	72:R4:222:ILE:N	2.40	0.47
72:R4:705:MET:HG2	72:R4:712:PRO:HB3	1.97	0.47
74:R7:109:GLU:O	74:R7:113:ASN:ND2	2.48	0.47
75:M4:242:LEU:O	75:M4:246:LEU:N	2.47	0.47
3:SA:455:C:H5'	5:SF:59:ARG:HH22	1.79	0.47
3:SA:461:G:H2'	3:SA:462:G:H8	1.78	0.47
3:SA:867:G:N2	12:SO:87:ASP:OD2	2.48	0.47
3:SA:1060:U:H2'	3:SA:1061:A:H8	1.79	0.47
8:SI:56:LYS:HE2	56:RP:2031:HIS:HE1	1.80	0.47
14:SR:37:THR:O	14:SR:45:ARG:NE	2.47	0.47
23:3F:120:ARG:HH11	56:RP:79:GLN:HA	1.79	0.47
29:AE:672:ASP:OD1	29:AE:672:ASP:N	2.47	0.47
35:B8:149:SER:HB3	35:B8:152:GLU:HG2	1.96	0.47
45:5I:126:LYS:NZ	45:5I:127:LYS:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RD:1701:SER:O	48:RD:1701:SER:OG	2.32	0.47
49:RE:639:SER:OG	49:RE:640:THR:N	2.47	0.47
52:RJ:552:LEU:HD21	52:RJ:566:ARG:HH11	1.80	0.47
53:RK:126:ASN:OD1	53:RK:126:ASN:N	2.47	0.47
55:RO:301:ASP:O	55:RO:305:LEU:CB	2.58	0.47
58:RS:358:TYR:HA	58:RS:361:ARG:HG2	1.96	0.47
66:R6:209:ILE:HA	66:R6:212:ILE:HD12	1.97	0.47
71:C4:254:VAL:HG21	71:C4:286:ARG:HB3	1.96	0.47
3:SA:625:C:O2'	3:SA:939:A:N3	2.44	0.47
13:SP:22:SER:OG	13:SP:23:PHE:N	2.47	0.47
20:3B:144:TRP:CE2	20:3B:152:ALA:HB2	2.49	0.47
22:3E:227:LEU:HD13	22:3E:231:ILE:HB	1.97	0.47
25:A4:198:ASP:OD1	25:A4:198:ASP:N	2.43	0.47
25:A4:516:VAL:HG11	25:A4:529:ASN:HB3	1.96	0.47
26:A5:213:ASN:ND2	26:A5:215:TYR:OH	2.48	0.47
28:A9:466:GLU:O	28:A9:469:SER:OG	2.29	0.47
31:AG:352:ASN:OD1	31:AG:352:ASN:N	2.48	0.47
31:AG:420:SER:HA	31:AG:423:LYS:HE2	1.96	0.47
31:AG:443:ASN:ND2	31:AG:446:ASN:OD1	2.47	0.47
31:AG:586:SER:HB2	31:AG:597:LYS:HZ3	1.80	0.47
31:AG:868:ASN:N	31:AG:868:ASN:OD1	2.44	0.47
32:B1:314:GLY:O	32:B1:332:TRP:NE1	2.39	0.47
34:B3:25:VAL:HG12	34:B3:294:LEU:HD22	1.96	0.47
34:B3:340:ILE:HG12	34:B3:357:THR:HG22	1.97	0.47
34:B3:575:THR:OG1	34:B3:576:ASN:N	2.48	0.47
51:RG:67:LEU:HD23	51:RG:89:PRO:HG3	1.96	0.47
58:RS:452:ILE:O	58:RS:457:ARG:NH2	2.48	0.47
63:R5:68:TYR:HB3	63:R5:70:ASP:H	1.79	0.47
65:R3:360:LEU:HB3	66:R6:182:SER:HB2	1.96	0.47
68:M3:205:LYS:HE3	71:C4:46:TYR:HE1	1.80	0.47
71:C4:45:GLN:HE21	71:C4:52:THR:HB	1.79	0.47
71:C4:139:VAL:HG22	71:C4:158:VAL:HG22	1.97	0.47
72:R4:26:ARG:N	72:R4:33:THR:O	2.43	0.47
3:SA:763:G:H1'	3:SA:787:G:H1'	1.96	0.47
3:SA:1160:A:H2'	3:SA:1161:C:H6	1.80	0.47
3:SA:1751:C:H2'	3:SA:1752:U:C6	2.49	0.47
7:SH:130:PRO:HB3	56:RP:624:VAL:HA	1.97	0.47
29:AE:32:SER:OG	29:AE:35:TYR:O	2.32	0.47
29:AE:772:VAL:HA	29:AE:775:ILE:HG12	1.96	0.47
33:B2:273:TYR:HE2	33:B2:275:GLN:HG3	1.80	0.47
33:B2:412:GLY:HA2	33:B2:431:GLY:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B3:12:LEU:HG	34:B3:641:PHE:HB2	1.96	0.47
34:B3:211:LEU:O	34:B3:222:LEU:HA	2.15	0.47
34:B3:219:ILE:HB	34:B3:235:LYS:HE3	1.96	0.47
37:B6:126:TYR:HA	37:B6:129:ILE:HB	1.96	0.47
43:5G:236:HIS:CE1	43:5G:249:GLU:HB3	2.50	0.47
49:RE:870:ALA:HB2	50:RF:103:LEU:HD21	1.96	0.47
51:RH:64:LYS:NZ	54:RN:721:PHE:O	2.48	0.47
52:RJ:771:GLU:O	52:RJ:777:ARG:NH2	2.47	0.47
52:RJ:1061:GLU:OE1	52:RJ:1063:HIS:NE2	2.47	0.47
53:RK:196:TYR:HA	53:RK:228:ASP:O	2.14	0.47
54:RN:284:ALA:HB2	58:RS:381:ALA:HA	1.96	0.47
72:R4:42:ARG:HB2	72:R4:45:ILE:HD11	1.97	0.47
76:M6:5:ASN:O	76:M6:9:GLY:N	2.48	0.47
1:3A:166:G:H5 <sup>?</sup>	23:3F:266:GLU:HB2	1.96	0.46
3:SA:252:U:H2 <sup>?</sup>	3:SA:253:A:C8	2.51	0.46
3:SA:429:G:H21	52:RJ:225:ARG:HH12	1.63	0.46
3:SA:922:G:H2 <sup>?</sup>	3:SA:923:A:H8	1.80	0.46
8:SI:48:GLU:HA	8:SI:57:ALA:O	2.15	0.46
22:3E:338:LYS:HD3	22:3E:357:GLY:HA3	1.96	0.46
22:3E:355:ASN:HB2	22:3E:401:LEU:HD13	1.97	0.46
25:A4:298:ALA:HB1	25:A4:333:ILE:HG13	1.97	0.46
25:A4:344:ALA:HB2	25:A4:682:THR:HA	1.97	0.46
25:A4:545:ARG:HG2	25:A4:549:VAL:HB	1.98	0.46
29:AE:39:THR:O	29:AE:43:GLN:NE2	2.40	0.46
29:AE:1629:SER:O	29:AE:1633:ASP:CB	2.63	0.46
30:AF:398:SER:O	30:AF:434:ARG:NH2	2.47	0.46
31:AG:524:ASP:OD1	31:AG:524:ASP:N	2.47	0.46
32:B1:295:ILE:HG22	32:B1:296:GLN:HG2	1.96	0.46
32:B1:605:ASP:OD1	32:B1:605:ASP:N	2.42	0.46
33:B2:186:ILE:HG12	33:B2:202:ALA:HB2	1.96	0.46
36:BE:171:GLN:NE2	36:BE:212:ALA:O	2.48	0.46
36:BE:376:TRP:NE1	36:BE:388:GLU:OE1	2.48	0.46
36:BE:664:SER:OG	36:BE:665:THR:N	2.48	0.46
39:5C:183:GLU:HG2	47:5K:16:THR:HG22	1.97	0.46
45:5I:88:ALA:HB1	45:5I:112:LEU:HD23	1.96	0.46
49:RE:184:SER:HB3	49:RE:206:LEU:HB3	1.97	0.46
51:RH:44:VAL:HG22	51:RH:113:TYR:HB2	1.96	0.46
52:RJ:991:PHE:CG	52:RJ:995:ILE:HD11	2.50	0.46
55:RO:326:LEU:HA	55:RO:329:ARG:HG2	1.98	0.46
63:R5:16:LEU:HD11	63:R5:203:PRO:HA	1.97	0.46
65:R3:93:GLY:HA2	65:R3:213:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:512:ALA:HB3	72:R4:620:ASP:HB3	1.97	0.46
72:R4:712:PRO:HG2	72:R4:905:GLN:HB2	1.97	0.46
1:3A:166:G:OP1	23:3F:267:SER:OG	2.26	0.46
3:SA:170:U:H3	3:SA:289:U:HO2'	1.62	0.46
3:SA:903:U:O2'	3:SA:905:A:N7	2.43	0.46
25:A4:147:ILE:HA	25:A4:157:SER:O	2.15	0.46
26:A5:481:LEU:HG	26:A5:526:LEU:HD13	1.95	0.46
32:B1:517:ASP:OD1	32:B1:517:ASP:N	2.35	0.46
32:B1:567:ASP:OD1	32:B1:567:ASP:N	2.47	0.46
33:B2:23:CYS:HB2	33:B2:43:THR:HG22	1.97	0.46
33:B2:373:ASP:N	33:B2:373:ASP:OD1	2.48	0.46
33:B2:584:ASP:N	33:B2:584:ASP:OD1	2.46	0.46
34:B3:215:GLY:N	34:B3:242:GLN:OE1	2.48	0.46
36:BE:914:ASP:O	36:BE:918:LYS:NZ	2.43	0.46
45:5I:359:ASP:N	45:5I:359:ASP:OD1	2.48	0.46
49:RE:692:LYS:HE2	49:RE:692:LYS:HB2	1.81	0.46
51:RG:121:LEU:HD12	51:RG:165:ASN:HA	1.98	0.46
51:RH:192:TYR:HA	51:RH:195:LYS:HE2	1.96	0.46
54:RN:590:ASN:OD1	54:RN:590:ASN:N	2.45	0.46
55:RO:194:TYR:O	55:RO:198:GLU:HB2	2.14	0.46
63:R5:142:ASP:OD2	66:R6:11:ASP:N	2.43	0.46
64:R1:164:GLY:O	64:R1:171:LEU:N	2.43	0.46
75:M4:352:ASN:O	75:M4:356:ALA:N	2.44	0.46
75:M4:516:VAL:HG23	75:M4:544:ALA:HB2	1.96	0.46
75:M4:891:ARG:HE	75:M4:976:ILE:HG21	1.80	0.46
1:3A:247:U:O4	23:3F:151:ARG:NH1	2.49	0.46
10:SK:107:ARG:NH2	10:SK:148:VAL:O	2.41	0.46
12:SO:43:LYS:HB2	12:SO:43:LYS:HE3	1.74	0.46
20:3C:307:GLU:H	40:5D:131:GLY:HA2	1.80	0.46
22:3E:355:ASN:OD1	22:3E:355:ASN:N	2.48	0.46
25:A4:97:ARG:HH12	38:5B:190:LEU:HB2	1.80	0.46
25:A4:274:GLN:HE22	25:A4:319:ARG:HA	1.79	0.46
26:A5:96:THR:OG1	26:A5:97:TYR:N	2.48	0.46
26:A5:231:ASP:O	26:A5:249:GLU:N	2.47	0.46
31:AG:291:ARG:NH1	31:AG:326:LEU:O	2.48	0.46
31:AG:579:ASN:HD21	31:AG:603:ASN:HA	1.80	0.46
31:AG:655:LEU:HD13	31:AG:659:ILE:HG21	1.95	0.46
33:B2:498:LYS:HG3	33:B2:527:THR:HA	1.96	0.46
35:B8:268:TYR:OH	35:B8:296:GLN:NE2	2.48	0.46
36:BE:322:TYR:HE1	36:BE:342:TYR:HD1	1.62	0.46
36:BE:353:PRO:HA	36:BE:370:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BE:719:GLU:OE1	36:BE:719:GLU:N	2.48	0.46
37:B6:144:VAL:HG11	37:B6:178:VAL:HG11	1.97	0.46
51:RG:99:LEU:HD22	51:RG:130:ILE:HD13	1.97	0.46
53:RK:280:LEU:HD13	53:RK:283:ILE:HD11	1.96	0.46
56:RP:135:LEU:HD13	56:RP:138:ALA:HB3	1.97	0.46
68:M3:70:GLN:H	68:M3:145:LYS:HB3	1.80	0.46
75:M4:80:VAL:N	75:M4:125:LEU:H	2.14	0.46
75:M4:166:SER:OG	75:M4:289:TYR:N	2.46	0.46
75:M4:731:PRO:HB3	75:M4:734:LEU:HD12	1.98	0.46
75:M4:889:LEU:HB3	75:M4:894:PHE:HB2	1.98	0.46
8:SI:33:GLU:O	8:SI:35:LYS:NZ	2.39	0.46
23:3F:160:ILE:HG12	23:3F:542:SER:HB3	1.97	0.46
26:A5:344:ASP:OD1	26:A5:348:LYS:N	2.40	0.46
30:AF:104:LEU:HA	30:AF:121:ASN:HA	1.97	0.46
31:AG:57:VAL:HG12	31:AG:383:LEU:HD21	1.96	0.46
31:AG:358:LEU:HB3	31:AG:370:GLN:HB3	1.96	0.46
32:B1:329:VAL:HG13	32:B1:338:ILE:HB	1.97	0.46
33:B2:433:ALA:HB1	33:B2:447:LEU:HD11	1.97	0.46
35:B8:238:LEU:HD13	35:B8:279:GLY:HA2	1.97	0.46
36:BE:626:ASP:N	36:BE:626:ASP:OD1	2.47	0.46
39:5C:23:ARG:HH22	57:RQ:869:TRP:HB3	1.80	0.46
39:5C:387:GLU:HG3	45:5I:6:ILE:HD11	1.96	0.46
45:5I:311:VAL:HA	45:5I:321:VAL:O	2.15	0.46
47:5K:185:LEU:HD12	47:5K:186:PRO:HD2	1.98	0.46
49:RE:462:PHE:HB2	49:RE:466:THR:HG21	1.97	0.46
49:RE:870:ALA:HA	50:RF:103:LEU:HD11	1.98	0.46
49:RE:924:LEU:HG	49:RE:1164:SER:HB3	1.96	0.46
51:RG:115:GLN:HB3	51:RG:121:LEU:HD23	1.98	0.46
56:RP:2023:THR:HA	56:RP:2026:ILE:HG12	1.97	0.46
72:R4:773:ARG:HG2	72:R4:975:VAL:HG12	1.98	0.46
75:M4:153:PHE:O	75:M4:157:ALA:N	2.49	0.46
75:M4:699:ALA:N	75:M4:718:ILE:O	2.48	0.46
1:3A:35:U:O2	45:5I:393:LYS:NZ	2.48	0.46
3:SA:488:G:H1	3:SA:499:U:H3	1.62	0.46
3:SA:592:A:O2'	3:SA:596:C:OP1	2.34	0.46
8:SI:72:LYS:O	8:SI:76:LYS:NZ	2.49	0.46
9:SJ:111:GLN:O	9:SJ:115:ALA:HB3	2.16	0.46
20:3C:98:ILE:HG12	40:5D:164:ASN:HD22	1.80	0.46
20:3C:111:MET:HG3	20:3C:216:ASN:HD22	1.81	0.46
22:3E:238:ALA:O	22:3E:242:SER:HB3	2.15	0.46
26:A5:23:ALA:HB1	35:B8:261:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A9:477:LYS:HA	28:A9:480:LYS:HE2	1.96	0.46
31:AG:408:THR:OG1	31:AG:409:LYS:N	2.49	0.46
33:B2:495:LYS:HA	33:B2:533:ASP:HA	1.98	0.46
42:5F:24:ASP:OD2	42:5F:27:HIS:NE2	2.49	0.46
49:RE:1233:ASN:ND2	49:RE:1235:GLU:OE2	2.49	0.46
52:RJ:61:ARG:NE	52:RJ:277:GLY:O	2.49	0.46
52:RJ:951:MET:SD	52:RJ:987:TYR:OH	2.70	0.46
55:RO:500:ASP:OD1	55:RO:500:ASP:N	2.49	0.46
56:RP:1759:SER:O	56:RP:1759:SER:OG	2.33	0.46
58:RS:266:PHE:O	58:RS:270:LEU:HB2	2.15	0.46
59:RT:174:LEU:HA	59:RT:180:LEU:HD21	1.97	0.46
67:R2:249:ALA:HA	67:R2:252:GLU:HB3	1.96	0.46
75:M4:882:LEU:HG	75:M4:886:LYS:HE3	1.97	0.46
3:SA:862:A:H3'	12:SO:16:ILE:HD11	1.97	0.46
3:SA:898:A:H62	3:SA:914:G:N2	2.13	0.46
7:SH:157:VAL:HB	7:SH:175:ILE:HD11	1.98	0.46
12:SO:49:GLN:HA	12:SO:52:VAL:HG12	1.97	0.46
26:A5:500:VAL:HA	26:A5:503:LYS:HG2	1.96	0.46
27:A8:638:LEU:HD23	28:A9:499:ILE:HD13	1.98	0.46
32:B1:191:ARG:HH12	32:B1:255:PHE:HE2	1.64	0.46
35:B8:426:VAL:HB	35:B8:455:ILE:HD11	1.98	0.46
36:BE:311:VAL:HG22	36:BE:321:GLU:HG2	1.98	0.46
40:5D:104:SER:HB2	40:5D:218:MET:HG3	1.97	0.46
47:5K:52:PHE:HB3	47:5K:55:TYR:HB3	1.96	0.46
51:RG:235:SER:O	51:RG:239:SER:OG	2.30	0.46
52:RJ:138:VAL:HG11	52:RJ:155:PHE:HE2	1.79	0.46
54:RN:385:ASP:HA	54:RN:431:ARG:HG2	1.98	0.46
55:RO:282:HIS:HB2	55:RO:321:ASN:HD22	1.80	0.46
56:RP:1876:LEU:HD23	56:RP:1876:LEU:HA	1.73	0.46
63:R5:130:LYS:HD2	63:R5:174:ILE:HG13	1.98	0.46
63:R5:250:LYS:N	64:R1:199:LEU:O	2.43	0.46
65:R3:44:ARG:HB3	65:R3:48:GLU:HB2	1.98	0.46
72:R4:110:ASP:OD2	72:R4:144:ARG:NH1	2.49	0.46
72:R4:678:LEU:HD12	72:R4:726:LEU:HB2	1.98	0.46
1:3A:18:G:H2'	1:3A:19:A:C8	2.51	0.46
1:3A:168:C:H2'	1:3A:169:A:C8	2.50	0.46
2:5A:87:C:H41	31:AG:334:LEU:HA	1.81	0.46
3:SA:327:U:O3'	11:SM:14:GLN:NE2	2.48	0.46
6:SG:72:HIS:CE1	6:SG:107:LYS:HD3	2.51	0.46
12:SO:99:ARG:HH12	12:SO:141:TYR:HE2	1.64	0.46
21:3D:121:ASN:O	21:3D:125:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A8:555:ILE:HD12	27:A8:582:ILE:HG23	1.97	0.46
30:AF:31:THR:OG1	30:AF:32:SER:N	2.45	0.46
31:AG:46:ILE:HD13	31:AG:385:ILE:HG21	1.96	0.46
31:AG:364:ASN:ND2	31:AG:409:LYS:O	2.49	0.46
31:AG:626:PHE:HB3	31:AG:629:LYS:HG3	1.96	0.46
33:B2:393:ASP:OD1	33:B2:393:ASP:N	2.46	0.46
41:5E:452:SER:O	41:5E:452:SER:OG	2.28	0.46
49:RE:1204:VAL:HG12	50:RF:57:ASN:HD22	1.79	0.46
58:RS:375:LEU:HG	58:RS:380:TYR:HE2	1.81	0.46
63:R5:286:ASP:O	63:R5:290:ARG:N	2.43	0.46
69:R0:67:SER:OG	69:R0:70:ASP:OD2	2.30	0.46
72:R4:894:ALA:O	72:R4:898:SER:N	2.45	0.46
74:R7:84:LYS:O	74:R7:88:ASP:N	2.48	0.46
75:M4:518:PHE:HB2	75:M4:557:MET:HA	1.98	0.46
21:3D:93:LYS:NZ	57:RQ:319:THR:OG1	2.40	0.46
22:3E:279:ARG:HA	22:3E:279:ARG:HD2	1.81	0.46
23:3F:240:LEU:HB2	23:3F:255:GLY:HA2	1.97	0.46
25:A4:121:THR:HB	25:A4:143:VAL:HA	1.97	0.46
25:A4:180:ASP:OD1	25:A4:180:ASP:N	2.49	0.46
29:AE:560:ILE:HB	29:AE:563:LEU:HD21	1.97	0.46
29:AE:797:LEU:HD22	29:AE:801:ILE:HG21	1.97	0.46
31:AG:201:ILE:HD12	31:AG:208:LEU:HB3	1.97	0.46
31:AG:722:LEU:HD13	31:AG:763:ILE:HD13	1.98	0.46
35:B8:206:ASN:O	35:B8:209:THR:OG1	2.30	0.46
37:B6:298:SER:OG	37:B6:299:LYS:N	2.45	0.46
48:RD:1644:LEU:HD21	48:RD:1654:LEU:HD22	1.97	0.46
52:RJ:618:PHE:HA	52:RJ:621:LEU:HD12	1.98	0.46
52:RJ:770:GLN:HA	52:RJ:777:ARG:HH12	1.80	0.46
54:RN:617:HIS:HA	54:RN:620:SER:HB2	1.97	0.46
63:R5:43:GLU:HB2	63:R5:46:ASP:HB2	1.98	0.46
64:R1:8:SER:OG	64:R1:12:LEU:N	2.37	0.46
65:R3:298:GLY:N	65:R3:331:ILE:O	2.39	0.46
69:R0:200:GLU:OE1	69:R0:202:SER:OG	2.32	0.46
71:C4:256:PHE:HZ	71:C4:266:LEU:HD22	1.81	0.46
72:R4:941:LEU:HD13	72:R4:960:LEU:HD21	1.97	0.46
74:R7:92:GLN:HA	74:R7:95:ASN:HD22	1.81	0.46
1:3A:265:C:O2	1:3A:307:G:N2	2.49	0.46
3:SA:34:G:O6	3:SA:475:A:N6	2.48	0.46
3:SA:163:G:OP2	3:SA:163:G:N2	2.39	0.46
3:SA:482:U:H2'	3:SA:483:A:H8	1.81	0.46
3:SA:1731:A:H3'	3:SA:1732:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1735:U:H2'	3:SA:1736:G:C8	2.51	0.46
8:SI:44:LYS:HG3	8:SI:63:PRO:HG3	1.98	0.46
21:3D:382:LYS:HD3	21:3D:382:LYS:HA	1.78	0.46
31:AG:34:ILE:HD12	31:AG:91:ILE:HG13	1.98	0.46
35:B8:464:THR:HG21	35:B8:476:ILE:HG13	1.98	0.46
45:5I:225:LEU:HA	45:5I:237:SER:HA	1.98	0.46
52:RJ:848:SER:O	52:RJ:848:SER:OG	2.34	0.46
56:RP:2095:LEU:O	56:RP:2099:SER:CB	2.64	0.46
64:R1:5:GLU:OE2	72:R4:129:TYR:OH	2.26	0.46
64:R1:72:LEU:HD23	64:R1:105:VAL:HA	1.97	0.46
64:R1:140:ILE:HA	64:R1:143:ILE:HD12	1.98	0.46
72:R4:119:ASP:OD1	72:R4:122:ARG:NH2	2.39	0.46
3:SA:1530:C:N4	3:SA:1531:G:O6	2.49	0.46
8:SI:13:PRO:HB2	8:SI:17:GLU:HB3	1.98	0.46
13:SP:32:ASP:N	13:SP:32:ASP:OD1	2.45	0.46
25:A4:33:VAL:HG22	25:A4:752:LEU:HD13	1.98	0.46
25:A4:79:TRP:HA	25:A4:87:GLN:HA	1.98	0.46
25:A4:740:PRO:O	25:A4:756:GLU:CB	2.64	0.46
27:A8:632:THR:HG21	28:A9:488:SER:HB3	1.98	0.46
28:A9:423:LYS:HG2	28:A9:455:TRP:HZ2	1.81	0.46
30:AF:68:SER:O	30:AF:315:ASN:ND2	2.40	0.46
32:B1:185:THR:OG1	32:B1:186:THR:N	2.49	0.46
32:B1:337:TYR:OH	41:5E:476:MET:SD	2.60	0.46
32:B1:482:SER:OG	32:B1:487:VAL:N	2.49	0.46
33:B2:555:VAL:HG23	33:B2:576:VAL:HG11	1.98	0.46
36:BE:211:THR:HG21	36:BE:253:SER:HA	1.97	0.46
37:B6:25:THR:OG1	37:B6:28:GLU:OE1	2.33	0.46
41:5E:439:GLU:O	41:5E:443:ASN:ND2	2.49	0.46
43:5G:169:ASN:HB2	43:5G:255:GLU:HG2	1.98	0.46
45:5I:265:ASN:N	45:5I:280:ALA:O	2.48	0.46
47:5K:100:ASP:OD1	47:5K:100:ASP:N	2.48	0.46
49:RE:631:GLY:N	49:RE:665:HIS:O	2.47	0.46
49:RE:711:PRO:HG3	49:RE:767:GLN:HB3	1.97	0.46
56:RP:622:CYS:O	56:RP:626:GLU:N	2.41	0.46
56:RP:1900:ARG:HE	56:RP:1933:ILE:HG12	1.81	0.46
72:R4:250:PHE:HE2	72:R4:462:TYR:H	1.62	0.46
75:M4:681:GLU:OE1	75:M4:769:SER:OG	2.30	0.46
75:M4:757:CYS:HB2	75:M4:788:GLU:HG3	1.98	0.46
11:SM:83:THR:HA	11:SM:110:HIS:HA	1.97	0.45
20:3B:164:ILE:HG23	20:3B:170:VAL:HG21	1.98	0.45
25:A4:157:SER:HG	25:A4:195:TRP:HE1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AF:422:ARG:HD2	30:AF:458:ILE:HD11	1.97	0.45
31:AG:767:GLY:O	31:AG:774:PHE:HA	2.16	0.45
31:AG:771:ASP:OD1	31:AG:771:ASP:N	2.42	0.45
34:B3:97:ARG:HD3	34:B3:97:ARG:HA	1.73	0.45
35:B8:264:LEU:HB2	35:B8:300:PHE:HE1	1.81	0.45
40:5D:233:ILE:O	40:5D:241:SER:OG	2.33	0.45
52:RJ:755:LYS:HD3	52:RJ:758:ILE:HD11	1.98	0.45
55:RO:277:ILE:HD12	55:RO:280:ILE:HD11	1.98	0.45
58:RS:360:LEU:HD23	58:RS:389:ASP:HB3	1.98	0.45
72:R4:941:LEU:O	72:R4:945:THR:N	2.47	0.45
3:SA:168:A:O3'	7:SH:176:GLN:NE2	2.39	0.45
3:SA:454:U:H5''	3:SA:455:C:C4	2.51	0.45
3:SA:629:U:H5''	12:SO:127:ARG:HH12	1.80	0.45
3:SA:1210:C:H2'	3:SA:1211:A:C4	2.51	0.45
10:SK:123:HIS:CD2	44:5H:566:ARG:HD2	2.51	0.45
21:3D:30:ARG:HH11	21:3D:122:GLU:HG3	1.82	0.45
23:3F:308:SER:OG	23:3F:310:ASN:OD1	2.34	0.45
24:3H:38:ASN:HA	24:3H:41:THR:HG22	1.97	0.45
25:A4:106:ASN:HB3	25:A4:112:LEU:HG	1.97	0.45
25:A4:349:SER:HB3	25:A4:357:VAL:HG22	1.97	0.45
30:AF:139:ILE:HD11	30:AF:151:LEU:HB3	1.99	0.45
33:B2:163:LYS:HD3	33:B2:163:LYS:HA	1.69	0.45
33:B2:532:ASP:HB3	33:B2:550:LEU:HD23	1.97	0.45
39:5C:96:ASP:OD1	39:5C:96:ASP:N	2.49	0.45
50:RF:19:LYS:HE3	50:RF:160:TYR:H	1.81	0.45
66:R6:74:LEU:HD23	66:R6:77:LEU:HD12	1.97	0.45
67:R2:204:ASN:OD1	67:R2:205:GLU:N	2.47	0.45
72:R4:370:ARG:O	72:R4:374:ALA:N	2.49	0.45
72:R4:767:ASN:O	72:R4:771:ASN:N	2.50	0.45
75:M4:475:HIS:HB2	75:M4:499:LEU:HD11	1.97	0.45
2:5A:296:C:OP2	32:B1:94:ASN:ND2	2.46	0.45
3:SA:150:U:O4'	7:SH:132:ARG:NH1	2.49	0.45
9:SJ:111:GLN:O	9:SJ:115:ALA:CB	2.65	0.45
11:SM:28:SER:O	11:SM:28:SER:OG	2.33	0.45
25:A4:33:VAL:HA	25:A4:752:LEU:HB3	1.98	0.45
27:A8:293:TYR:HA	27:A8:303:GLN:O	2.16	0.45
29:AE:266:THR:HG21	31:AG:895:LEU:HD11	1.99	0.45
29:AE:511:PHE:HE1	29:AE:516:PHE:HB3	1.81	0.45
31:AG:152:ARG:NH1	31:AG:230:LEU:O	2.49	0.45
31:AG:175:ALA:O	31:AG:187:VAL:HA	2.16	0.45
31:AG:496:THR:OG1	31:AG:497:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B2:130:ASP:OD2	33:B2:135:ARG:NE	2.49	0.45
33:B2:421:THR:HG22	33:B2:423:LYS:HG2	1.99	0.45
34:B3:24:THR:HB	34:B3:32:LEU:HD13	1.98	0.45
34:B3:138:HIS:CE1	34:B3:177:LEU:HB2	2.51	0.45
34:B3:362:LEU:HD22	34:B3:405:THR:HG21	1.98	0.45
36:BE:546:ILE:HG21	36:BE:560:LEU:HD23	1.97	0.45
36:BE:616:THR:HG23	36:BE:618:GLY:H	1.81	0.45
46:5J:129:ALA:HB2	52:RJ:1123:LYS:HD3	1.99	0.45
49:RE:128:LEU:HA	49:RE:131:LEU:HB2	1.98	0.45
49:RE:795:GLU:OE2	50:RF:101:SER:OG	2.30	0.45
52:RJ:610:LYS:NZ	52:RJ:612:VAL:O	2.48	0.45
52:RJ:852:ARG:HD2	52:RJ:888:PRO:HG3	1.98	0.45
53:RK:312:ARG:NH2	53:RK:349:ASP:OD2	2.49	0.45
55:RO:281:LEU:HD12	55:RO:285:ILE:HG21	1.97	0.45
57:RQ:301:ILE:HA	57:RQ:304:GLN:HG2	1.99	0.45
63:R5:58:CYS:SG	63:R5:59:ARG:N	2.89	0.45
67:R2:138:VAL:HA	67:R2:141:ILE:HD12	1.96	0.45
72:R4:225:LEU:HB2	72:R4:228:ALA:HB2	1.97	0.45
75:M4:171:ALA:H	75:M4:177:LYS:HD3	1.82	0.45
75:M4:778:PRO:HG2	75:M4:786:GLN:HB3	1.98	0.45
1:3A:164:C:H2'	1:3A:165:G:H8	1.81	0.45
3:SA:493:U:OP2	52:RJ:1138:ARG:NH1	2.49	0.45
7:SH:126:ASP:OD1	7:SH:126:ASP:N	2.41	0.45
9:SJ:74:LYS:HA	9:SJ:74:LYS:HD2	1.78	0.45
12:SO:69:ASN:OD1	12:SO:69:ASN:N	2.49	0.45
17:SZ:6:THR:HG23	17:SZ:28:LEU:HB2	1.98	0.45
17:SZ:118:ILE:HG22	17:SZ:120:GLY:H	1.81	0.45
24:3G:120:LYS:O	24:3G:123:THR:OG1	2.34	0.45
25:A4:120:SER:OG	25:A4:121:THR:N	2.49	0.45
25:A4:519:THR:OG1	25:A4:520:LYS:N	2.48	0.45
31:AG:85:ASN:O	31:AG:112:ASN:ND2	2.50	0.45
32:B1:459:SER:OG	32:B1:462:THR:O	2.28	0.45
33:B2:107:ASP:OD2	33:B2:110:SER:OG	2.32	0.45
34:B3:669:LEU:HD23	34:B3:693:ARG:HH21	1.82	0.45
36:BE:97:LYS:HG3	36:BE:111:GLU:HA	1.98	0.45
36:BE:854:SER:HB3	36:BE:858:PHE:HD1	1.81	0.45
41:5E:316:ASN:HA	41:5E:319:VAL:HG12	1.97	0.45
41:5E:350:THR:HG21	52:RJ:975:GLU:HB2	1.98	0.45
43:5G:233:VAL:HB	43:5G:254:PHE:HB2	1.97	0.45
53:RK:143:LYS:NZ	53:RK:180:MET:SD	2.89	0.45
63:R5:162:PHE:HD2	63:R5:187:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:62:ASP:OD1	72:R4:62:ASP:N	2.48	0.45
75:M4:537:TYR:HA	75:M4:540:MET:HB2	1.97	0.45
1:3A:294:U:H2'	1:3A:295:A:C8	2.52	0.45
5:SF:201:HIS:H	5:SF:206:ASP:HB3	1.82	0.45
6:SG:118:LEU:HB2	6:SG:129:PRO:HB2	1.98	0.45
7:SH:46:LYS:H	7:SH:119:GLN:HB2	1.81	0.45
8:SI:49:ILE:HG12	8:SI:175:LYS:HE3	1.98	0.45
15:SX:18:GLU:HB3	15:SX:65:LEU:HD11	1.98	0.45
15:SX:68:ARG:NH1	45:5I:68:ASP:OD1	2.47	0.45
20:3B:269:ILE:O	20:3B:315:ILE:HA	2.17	0.45
21:3D:83:ASP:HB3	21:3D:113:PHE:HE1	1.81	0.45
23:3F:529:SER:OG	23:3F:530:GLY:N	2.50	0.45
25:A4:477:LEU:HD22	25:A4:534:LEU:H	1.82	0.45
25:A4:489:CYS:HB2	25:A4:534:LEU:HD23	1.98	0.45
26:A5:528:SER:HA	26:A5:531:LYS:HG2	1.97	0.45
29:AE:745:TYR:HB3	29:AE:748:LEU:HB3	1.97	0.45
33:B2:121:LYS:HD3	33:B2:121:LYS:HA	1.79	0.45
33:B2:806:MET:HE2	33:B2:806:MET:HB2	1.78	0.45
49:RE:282:ASP:N	49:RE:282:ASP:OD1	2.50	0.45
51:RG:171:LEU:HD22	51:RG:203:CYS:HB3	1.98	0.45
52:RJ:138:VAL:HG11	52:RJ:155:PHE:CE2	2.52	0.45
52:RJ:1051:ASP:OD1	52:RJ:1051:ASP:N	2.45	0.45
54:RN:510:THR:O	54:RN:557:SER:OG	2.35	0.45
64:R1:171:LEU:HD23	64:R1:171:LEU:HA	1.82	0.45
65:R3:387:ASP:O	65:R3:391:ARG:N	2.49	0.45
67:R2:86:ARG:HG2	67:R2:88:ASP:H	1.81	0.45
75:M4:583:PHE:HB3	75:M4:610:PHE:HB2	1.99	0.45
75:M4:941:SER:HB3	75:M4:1001:VAL:HG21	1.98	0.45
3:SA:126:A:H62	3:SA:291:G:H21	1.65	0.45
3:SA:794:U:H5''	3:SA:796:A:H62	1.80	0.45
15:SX:105:THR:O	15:SX:105:THR:OG1	2.31	0.45
25:A4:488:ILE:HB	25:A4:496:PHE:HB2	1.98	0.45
29:AE:295:ALA:HA	29:AE:298:THR:HG22	1.98	0.45
31:AG:110:PHE:HE1	31:AG:116:VAL:HG13	1.82	0.45
32:B1:802:LEU:HD23	32:B1:802:LEU:HA	1.79	0.45
34:B3:461:LEU:HD13	34:B3:485:TYR:HB2	1.99	0.45
36:BE:114:THR:OG1	36:BE:115:ASP:N	2.50	0.45
37:B6:201:LYS:HD2	46:5J:55:ILE:HG21	1.99	0.45
43:5G:183:SER:HB3	54:RN:6:LEU:HD11	1.98	0.45
45:5I:18:SER:O	45:5I:18:SER:OG	2.29	0.45
45:5I:309:MET:H	45:5I:324:SER:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:5J:134:ARG:HA	46:5J:134:ARG:HD2	1.86	0.45
49:RE:925:LEU:HD22	49:RE:1064:LEU:HD12	1.98	0.45
51:RH:186:VAL:HG23	51:RH:227:LEU:HA	1.99	0.45
52:RJ:761:GLN:O	52:RJ:765:ASN:HB2	2.16	0.45
52:RJ:1027:THR:OG1	52:RJ:1028:GLU:N	2.47	0.45
52:RJ:1106:GLU:HG3	52:RJ:1110:ARG:HH12	1.81	0.45
53:RK:97:GLY:HA2	53:RK:100:VAL:HG12	1.99	0.45
54:RN:537:LEU:HB3	54:RN:624:THR:HB	1.98	0.45
54:RN:607:THR:HG23	54:RN:610:ARG:HB2	1.98	0.45
56:RP:1963:LEU:HD22	56:RP:2002:PHE:HE1	1.82	0.45
65:R3:297:TYR:N	65:R3:347:ILE:O	2.49	0.45
1:3A:329:C:H2'	1:3A:330:A:C8	2.49	0.45
2:5A:70:A:P	31:AG:426:ARG:HH22	2.40	0.45
3:SA:748:U:H3	3:SA:801:G:H22	1.64	0.45
7:SH:3:LEU:HB3	7:SH:5:ILE:HD11	1.97	0.45
9:SJ:60:ILE:HD11	9:SJ:173:PRO:HB3	1.99	0.45
20:3B:175:ALA:HB1	20:3B:181:VAL:HG21	1.99	0.45
20:3B:294:ARG:HH21	20:3B:300:PRO:HG2	1.82	0.45
20:3C:225:ARG:HG2	20:3C:252:ILE:HG12	1.99	0.45
25:A4:625:GLU:O	25:A4:629:LEU:HB2	2.17	0.45
32:B1:576:ARG:HG2	42:5F:142:LEU:HD22	1.99	0.45
32:B1:710:ILE:HG13	36:BE:596:GLU:HG2	1.98	0.45
33:B2:16:VAL:HG21	33:B2:46:LEU:HG	1.99	0.45
33:B2:487:ARG:HA	33:B2:500:TRP:O	2.16	0.45
34:B3:439:ALA:HB3	34:B3:497:LEU:HB3	1.98	0.45
34:B3:464:LYS:HZ3	34:B3:481:LYS:HD2	1.81	0.45
35:B8:390:THR:OG1	35:B8:391:SER:N	2.49	0.45
36:BE:421:ASN:ND2	36:BE:429:ASN:HD21	2.15	0.45
36:BE:590:ALA:O	36:BE:602:SER:HA	2.16	0.45
41:5E:298:SER:OG	41:5E:299:SER:N	2.50	0.45
49:RE:673:SER:OG	49:RE:674:SER:N	2.49	0.45
49:RE:1227:GLY:O	49:RE:1231:VAL:N	2.41	0.45
54:RN:438:ASN:OD1	54:RN:438:ASN:N	2.48	0.45
58:RS:271:THR:O	58:RS:275:SER:CB	2.59	0.45
64:R1:185:VAL:HG22	64:R1:201:VAL:HG22	1.97	0.45
65:R3:378:LEU:HB3	65:R3:382:ARG:HH12	1.82	0.45
72:R4:413:ASP:OD2	72:R4:416:SER:N	2.50	0.45
3:SA:677:G:H2'	3:SA:678:A:C8	2.52	0.45
3:SA:689:G:H2'	3:SA:690:G:H8	1.81	0.45
3:SA:960:U:H5'	12:SO:55:ARG:HD3	1.98	0.45
4:SC:178:GLY:HA2	49:RE:897:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SJ:37:LYS:HB2	9:SJ:59:ARG:HG2	1.98	0.45
15:SX:70:ASN:N	15:SX:70:ASN:OD1	2.49	0.45
15:SX:89:TRP:O	15:SX:93:LEU:CB	2.64	0.45
20:3B:90:PRO:HA	20:3B:97:TYR:HD1	1.82	0.45
20:3B:92:ARG:NH1	20:3B:159:LEU:O	2.49	0.45
20:3C:242:ALA:HB3	20:3C:269:ILE:HG23	1.99	0.45
20:3C:281:ASP:O	20:3C:284:THR:OG1	2.27	0.45
21:3D:173:HIS:NE2	22:3E:251:ASP:OD2	2.50	0.45
22:3E:132:SER:HB2	22:3E:135:ASP:HB3	1.99	0.45
23:3F:156:ASN:HD21	23:3F:545:LYS:HG3	1.82	0.45
31:AG:80:GLN:NE2	31:AG:83:GLU:O	2.44	0.45
34:B3:175:TRP:HD1	34:B3:182:CYS:HA	1.80	0.45
36:BE:568:VAL:HG13	36:BE:577:VAL:HG13	1.99	0.45
39:5C:437:LEU:HD21	45:5I:39:ARG:HG3	1.98	0.45
45:5I:68:ASP:HB2	45:5I:89:ASP:HB3	1.99	0.45
46:5J:68:GLY:O	46:5J:72:LEU:HB2	2.15	0.45
49:RE:858:ARG:HD2	49:RE:861:ILE:HD11	1.99	0.45
52:RJ:864:ASP:OD1	52:RJ:864:ASP:N	2.45	0.45
53:RK:109:PHE:HB3	53:RK:361:ASN:HB3	1.99	0.45
56:RP:1952:SER:O	56:RP:1952:SER:OG	2.34	0.45
59:RT:224:ILE:HG22	59:RT:233:ILE:HG23	1.98	0.45
63:R5:101:GLU:OE1	63:R5:101:GLU:N	2.38	0.45
64:R1:66:ASP:OD2	64:R1:68:SER:OG	2.32	0.45
67:R2:213:LEU:HD23	67:R2:228:SER:HA	1.99	0.45
71:C4:141:THR:HG22	71:C4:155:ILE:HA	1.99	0.45
72:R4:178:CYS:HB2	72:R4:213:ILE:HD11	1.99	0.45
72:R4:227:ASN:OD1	72:R4:227:ASN:N	2.46	0.45
72:R4:406:GLN:HG2	72:R4:425:ILE:HB	1.97	0.45
75:M4:401:ILE:O	75:M4:405:LYS:N	2.50	0.45
75:M4:449:ALA:HA	75:M4:456:ARG:HH21	1.82	0.45
1:3A:12:U:O4	52:RJ:1158:LYS:NZ	2.39	0.45
1:3A:30:A:N6	45:5I:341:GLU:OE2	2.49	0.45
3:SA:1068:C:H2'	3:SA:1069:A:C8	2.52	0.45
22:3E:359:ILE:HD12	22:3E:398:LEU:HD13	1.99	0.45
24:3H:20:ILE:HD12	24:3H:53:ILE:HD12	1.99	0.45
24:3H:28:ALA:HB2	24:3H:33:LEU:HD23	1.99	0.45
25:A4:184:MET:HB2	25:A4:224:ARG:HA	1.99	0.45
29:AE:463:ALA:HA	29:AE:504:LYS:HG2	1.99	0.45
31:AG:484:VAL:HG12	31:AG:485:ARG:H	1.82	0.45
31:AG:870:ASN:OD1	31:AG:870:ASN:N	2.50	0.45
33:B2:322:SER:HA	33:B2:325:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B3:340:ILE:HG21	34:B3:355:LEU:HG	1.98	0.45
45:5I:93:LYS:HG2	45:5I:105:SER:HB2	1.98	0.45
45:5I:358:MET:HB3	57:RQ:890:VAL:HG23	1.99	0.45
45:5I:396:TYR:HE1	57:RQ:865:ILE:HG13	1.82	0.45
45:5I:409:GLU:HA	45:5I:412:ARG:HG2	1.98	0.45
45:5I:458:LYS:HE3	45:5I:458:LYS:HB2	1.81	0.45
49:RE:736:ASP:OD1	49:RE:821:TYR:OH	2.35	0.45
49:RE:1169:ILE:HG22	49:RE:1180:ASN:HD22	1.81	0.45
51:RH:189:VAL:HG13	51:RH:227:LEU:HD13	1.98	0.45
52:RJ:752:GLU:HA	52:RJ:755:LYS:HB2	1.99	0.45
55:RO:223:VAL:HG11	55:RO:261:TRP:HZ2	1.82	0.45
55:RO:382:LYS:HE3	55:RO:382:LYS:HB3	1.84	0.45
56:RP:1822:SER:O	56:RP:1822:SER:OG	2.31	0.45
56:RP:1975:LYS:HB3	56:RP:1978:ALA:HB3	1.99	0.45
63:R5:262:MET:HE1	64:R1:210:LEU:HB3	1.98	0.45
75:M4:1023:SER:HA	75:M4:1026:ARG:HB2	1.99	0.45
3:SA:-1:G:O6	45:5I:457:ARG:NE	2.40	0.45
3:SA:144:U:O4	7:SH:137:ARG:NH1	2.50	0.45
3:SA:890:C:H2'	3:SA:891:A:H8	1.82	0.45
20:3B:116:SER:OG	20:3B:120:GLU:OE1	2.35	0.45
20:3B:142:ARG:NH2	20:3B:182:SER:OG	2.47	0.45
23:3F:224:SER:OG	23:3F:227:GLU:OE1	2.35	0.45
25:A4:458:ASN:N	25:A4:458:ASN:OD1	2.50	0.45
29:AE:148:PHE:HA	29:AE:151:ILE:HG22	1.98	0.45
32:B1:83:ASN:H	32:B1:90:LEU:HD23	1.81	0.45
33:B2:152:GLY:HA3	33:B2:154:VAL:HG12	1.99	0.45
35:B8:532:MET:O	35:B8:541:LEU:HA	2.17	0.45
37:B6:24:PHE:HE1	37:B6:70:ARG:HD3	1.82	0.45
42:5F:174:ARG:NH2	52:RJ:1077:LEU:O	2.50	0.45
49:RE:434:LEU:O	49:RE:466:THR:OG1	2.34	0.45
49:RE:687:GLN:NE2	49:RE:694:ALA:O	2.40	0.45
50:RF:123:THR:O	50:RF:123:THR:OG1	2.35	0.45
50:RF:151:HIS:HD2	50:RF:154:GLU:H	1.65	0.45
51:RG:91:ILE:HA	51:RG:94:GLN:HG2	1.99	0.45
51:RH:123:GLU:OE2	51:RH:161:LYS:NZ	2.39	0.45
53:RK:263:ASP:O	53:RK:266:SER:OG	2.31	0.45
58:RS:304:TYR:O	58:RS:308:LYS:HB2	2.17	0.45
71:C4:149:GLN:HG2	71:C4:150:ARG:HH11	1.81	0.45
75:M4:956:LYS:HA	75:M4:957:PRO:HD3	1.82	0.45
3:SA:1677:C:H2'	3:SA:1678:A:C8	2.52	0.44
3:SA:1775:U:H3	3:SA:1786:G:H1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SF:89:VAL:HA	5:SF:99:PHE:O	2.18	0.44
5:SF:127:LYS:HD3	5:SF:127:LYS:HA	1.77	0.44
6:SG:97:LEU:HD21	6:SG:113:ILE:HD11	1.98	0.44
12:SO:60:VAL:HB	12:SO:66:ILE:HD12	1.98	0.44
20:3B:118:TYR:OH	20:3B:148:ARG:NH2	2.50	0.44
24:3G:12:ALA:HB1	24:3G:16:LEU:HG	1.99	0.44
25:A4:490:SER:HG	25:A4:494:ASP:H	1.65	0.44
30:AF:372:HIS:H	35:B8:287:SER:HG	1.64	0.44
32:B1:74:ASP:OD1	32:B1:74:ASP:N	2.38	0.44
36:BE:274:ILE:HG13	36:BE:286:VAL:HG23	1.99	0.44
36:BE:441:ARG:HA	36:BE:454:THR:HA	1.99	0.44
36:BE:495:ARG:HA	36:BE:495:ARG:HD3	1.75	0.44
43:5G:93:SER:OG	43:5G:94:ARG:N	2.50	0.44
45:5I:327:LYS:HE3	45:5I:349:GLN:HG2	1.99	0.44
45:5I:351:VAL:HA	45:5I:367:SER:HA	1.98	0.44
48:RD:1672:GLU:HG2	48:RD:1695:TRP:HH2	1.81	0.44
49:RE:337:LEU:HD12	49:RE:337:LEU:HA	1.85	0.44
56:RP:29:GLU:HB3	56:RP:32:ARG:HB2	1.98	0.44
56:RP:130:LYS:O	56:RP:134:ASN:ND2	2.50	0.44
59:RT:248:VAL:HA	59:RT:251:ILE:HG12	1.99	0.44
63:R5:163:LYS:HA	63:R5:186:PRO:HA	1.98	0.44
63:R5:256:MET:O	64:R1:196:LEU:N	2.45	0.44
69:R0:80:PHE:HB2	69:R0:85:LYS:HG2	1.97	0.44
71:C4:40:GLY:HA3	71:C4:110:VAL:HB	1.99	0.44
72:R4:764:GLU:HA	72:R4:767:ASN:HB2	1.99	0.44
75:M4:445:ASN:O	75:M4:449:ALA:N	2.50	0.44
75:M4:1039:VAL:O	75:M4:1043:ASN:ND2	2.50	0.44
1:3A:331:A:H2'	1:3A:332:G:C8	2.52	0.44
2:5A:88:U:H2'	2:5A:89:C:C2	2.52	0.44
3:SA:1220:C:N3	3:SA:1264:G:N2	2.66	0.44
5:SF:69:HIS:HE1	5:SF:94:ALA:HB3	1.82	0.44
10:SK:48:GLN:HA	10:SK:51:LYS:HG2	1.99	0.44
23:3F:450:ASP:OD1	23:3F:450:ASP:N	2.50	0.44
24:3G:34:LYS:HB3	24:3G:39:GLU:HG2	1.98	0.44
24:3H:23:VAL:HA	24:3H:26:GLN:HE21	1.82	0.44
26:A5:226:LEU:HD13	26:A5:273:LYS:HB2	2.00	0.44
31:AG:669:ASN:HA	31:AG:681:ILE:O	2.17	0.44
34:B3:76:LEU:HG	34:B3:87:ILE:HB	1.99	0.44
34:B3:417:TYR:HA	34:B3:424:PHE:HD1	1.81	0.44
34:B3:433:HIS:HD2	34:B3:436:ALA:HB2	1.83	0.44
34:B3:542:CYS:HB3	34:B3:547:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BE:100:ILE:HD13	36:BE:149:TYR:HB2	1.98	0.44
37:B6:34:LYS:HE3	37:B6:34:LYS:HB2	1.86	0.44
39:5C:111:PHE:HD1	39:5C:131:LYS:HB2	1.81	0.44
49:RE:507:PHE:HA	49:RE:510:ILE:HG22	2.00	0.44
51:RH:76:LEU:HA	51:RH:79:LYS:HG2	1.99	0.44
52:RJ:251:ASP:HA	52:RJ:269:VAL:HG22	1.98	0.44
66:R6:3:VAL:HG12	66:R6:21:SER:HA	1.98	0.44
68:M3:75:THR:HG21	68:M3:175:SER:CB	2.47	0.44
72:R4:627:ILE:HB	72:R4:640:ASN:HB2	1.99	0.44
72:R4:736:ILE:HG23	72:R4:838:ILE:HG23	1.99	0.44
72:R4:766:LEU:O	72:R4:770:LEU:N	2.48	0.44
2:5A:69:U:H2'	2:5A:70:A:C4	2.52	0.44
5:SF:129:VAL:HG12	5:SF:139:VAL:HA	2.00	0.44
11:SM:14:GLN:HB3	11:SM:54:ILE:HG21	1.99	0.44
23:3F:416:GLY:HA3	23:3F:475:ILE:HD11	1.99	0.44
25:A4:231:VAL:HG22	25:A4:265:TRP:HZ2	1.82	0.44
25:A4:326:ARG:HH11	25:A4:365:SER:HA	1.83	0.44
26:A5:356:TYR:HB2	31:AG:472:TYR:HB2	2.00	0.44
27:A8:659:THR:HA	27:A8:662:ILE:HG22	1.98	0.44
28:A9:508:ARG:HA	28:A9:511:LYS:HD3	1.98	0.44
29:AE:142:TYR:O	29:AE:145:THR:OG1	2.24	0.44
30:AF:27:TRP:HH2	30:AF:268:MET:HB3	1.81	0.44
31:AG:206:LYS:HB3	31:AG:206:LYS:HE2	1.82	0.44
31:AG:401:GLN:HB3	31:AG:411:SER:HB2	1.99	0.44
32:B1:156:GLN:H	32:B1:203:GLN:HE21	1.65	0.44
32:B1:329:VAL:HG12	32:B1:339:LEU:HG	2.00	0.44
34:B3:622:ALA:HB3	34:B3:636:ASP:HB3	1.99	0.44
40:5D:211:LEU:HA	40:5D:214:VAL:HG12	1.99	0.44
43:5G:173:ARG:HE	43:5G:173:ARG:HB2	1.67	0.44
45:5I:15:PRO:HB3	45:5I:20:GLN:HG2	1.99	0.44
45:5I:69:GLY:HA2	45:5I:370:GLY:HA2	1.98	0.44
49:RE:218:ASP:O	49:RE:223:ARG:NH2	2.51	0.44
49:RE:309:LEU:HD12	49:RE:310:PRO:HD2	1.99	0.44
49:RE:549:SER:HA	49:RE:552:ARG:HG2	1.99	0.44
52:RJ:856:THR:OG1	52:RJ:857:LEU:N	2.47	0.44
54:RN:512:ASP:OD1	54:RN:512:ASP:N	2.45	0.44
54:RN:534:PHE:HA	54:RN:539:ARG:HD2	1.98	0.44
54:RN:577:VAL:HG21	54:RN:596:TYR:HA	1.98	0.44
56:RP:1960:LEU:HD23	56:RP:1960:LEU:HA	1.87	0.44
59:RT:261:GLY:HA2	59:RT:264:ARG:HE	1.82	0.44
65:R3:147:GLU:O	65:R3:150:THR:OG1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:R3:360:LEU:HD21	65:R3:362:LEU:HD13	1.98	0.44
68:M3:106:ASN:OD1	68:M3:107:THR:N	2.50	0.44
72:R4:764:GLU:HA	72:R4:767:ASN:HD22	1.82	0.44
75:M4:222:MET:HB2	75:M4:237:MET:HB3	1.99	0.44
1:3A:152:U:O2	1:3A:161:G:N2	2.48	0.44
4:SC:132:ASP:HB2	4:SC:221:PRO:HB3	1.99	0.44
5:SF:116:ASP:OD1	5:SF:116:ASP:N	2.50	0.44
7:SH:48:TYR:HD1	7:SH:117:GLY:H	1.64	0.44
9:SJ:97:THR:OG1	9:SJ:98:LYS:N	2.50	0.44
14:SR:22:VAL:HG22	14:SR:65:ILE:HG12	2.00	0.44
20:3B:267:VAL:HG21	20:3B:298:ILE:HD13	1.99	0.44
23:3F:263:TRP:CZ3	23:3F:270:PRO:HD3	2.36	0.44
30:AF:464:ALA:O	30:AF:468:GLU:HB2	2.17	0.44
32:B1:359:ARG:HA	32:B1:373:ASP:HA	1.98	0.44
33:B2:218:ILE:HG23	33:B2:259:ILE:HD12	1.99	0.44
34:B3:296:ILE:HB	34:B3:301:GLN:HB2	2.00	0.44
44:5H:564:LYS:HE3	44:5H:564:LYS:HB2	1.75	0.44
45:5I:278:VAL:HG11	45:5I:311:VAL:HG21	1.98	0.44
49:RE:151:SER:HA	49:RE:154:LYS:HB2	1.99	0.44
54:RN:475:ARG:HH22	54:RN:517:VAL:HA	1.83	0.44
55:RO:213:LEU:HD11	55:RO:264:LEU:HA	1.99	0.44
58:RS:221:LEU:HA	58:RS:224:TRP:CD1	2.50	0.44
58:RS:430:ASN:ND2	58:RS:431:ASP:OD1	2.51	0.44
68:M3:75:THR:CG2	68:M3:175:SER:OG	2.63	0.44
72:R4:539:ILE:HD13	72:R4:555:HIS:HB3	2.00	0.44
72:R4:692:GLY:O	72:R4:783:SER:OG	2.22	0.44
72:R4:777:SER:OG	72:R4:778:ILE:N	2.49	0.44
3:SA:1792:G:O2'	3:SA:1793:G:O4'	2.35	0.44
4:SC:51:SER:HA	4:SC:57:ALA:HB3	2.00	0.44
6:SG:26:ALA:N	14:SR:27:GLY:O	2.50	0.44
22:3E:377:ALA:HB3	22:3E:380:ARG:HD2	1.98	0.44
28:A9:403:LEU:O	28:A9:407:MET:CB	2.65	0.44
31:AG:427:LYS:O	31:AG:431:SER:CB	2.66	0.44
31:AG:725:ASN:H	31:AG:740:LYS:HE2	1.81	0.44
32:B1:60:ALA:HB3	32:B1:73:ILE:HB	2.00	0.44
32:B1:337:TYR:HD2	32:B1:340:LYS:HD3	1.82	0.44
33:B2:214:ASP:OD1	33:B2:214:ASP:N	2.50	0.44
33:B2:267:ASP:OD1	33:B2:267:ASP:N	2.44	0.44
34:B3:539:VAL:HG22	34:B3:550:THR:HA	1.99	0.44
34:B3:593:CYS:HB2	34:B3:620:LEU:HB2	2.00	0.44
34:B3:672:TYR:HB3	34:B3:681:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BE:184:THR:HG1	36:BE:187:ASN:H	1.66	0.44
36:BE:379:SER:OG	36:BE:382:LYS:O	2.36	0.44
38:5B:180:LEU:HD11	40:5D:143:MET:HG3	1.99	0.44
41:5E:373:ILE:HD12	41:5E:373:ILE:HA	1.86	0.44
42:5F:91:LYS:HE2	42:5F:91:LYS:HB2	1.90	0.44
52:RJ:906:ASP:OD1	52:RJ:906:ASP:N	2.51	0.44
53:RK:154:LEU:HD13	53:RK:165:GLU:HB3	1.98	0.44
53:RK:245:LEU:O	53:RK:257:PHE:HA	2.18	0.44
56:RP:177:LEU:HD22	56:RP:180:LEU:HD12	1.99	0.44
65:R3:221:SER:HB2	68:M3:53:ILE:HG23	1.99	0.44
67:R2:223:THR:OG1	67:R2:224:SER:N	2.51	0.44
72:R4:606:MET:O	72:R4:610:THR:OG1	2.25	0.44
72:R4:669:GLU:HA	72:R4:672:MET:HB2	1.98	0.44
72:R4:959:LYS:HD3	72:R4:974:TYR:CZ	2.53	0.44
75:M4:699:ALA:O	75:M4:718:ILE:N	2.43	0.44
75:M4:940:LEU:HD22	75:M4:1034:LEU:HD21	1.98	0.44
3:SA:689:G:H2'	3:SA:690:G:C8	2.53	0.44
3:SA:1052:U:H5''	45:5I:449:LYS:HE2	2.00	0.44
3:SA:1666:U:H2'	3:SA:1667:A:H8	1.83	0.44
7:SH:57:ASP:HB2	7:SH:105:ASP:HB3	2.00	0.44
21:3D:21:LYS:HD2	21:3D:49:GLU:HB2	1.98	0.44
25:A4:451:PHE:HD1	25:A4:464:LYS:HA	1.82	0.44
26:A5:213:ASN:OD1	26:A5:213:ASN:N	2.50	0.44
26:A5:222:THR:HG21	36:BE:586:ASN:HD21	1.82	0.44
32:B1:274:LEU:HD11	32:B1:286:LEU:HB2	2.00	0.44
34:B3:283:LYS:HD2	34:B3:284:PRO:HD2	2.00	0.44
35:B8:133:ILE:HD13	36:BE:194:ARG:HH22	1.82	0.44
35:B8:229:PRO:HA	35:B8:230:PRO:HD3	1.92	0.44
35:B8:310:GLN:HB3	35:B8:326:LEU:HG	2.00	0.44
36:BE:629:ALA:HA	36:BE:645:HIS:HA	1.99	0.44
36:BE:869:THR:HG23	36:BE:915:VAL:HG11	1.98	0.44
39:5C:23:ARG:NH1	57:RQ:863:MET:SD	2.91	0.44
42:5F:120:MET:HG3	42:5F:160:TRP:CZ2	2.52	0.44
49:RE:585:MET:HB3	49:RE:610:PHE:HB2	2.00	0.44
49:RE:756:VAL:HA	49:RE:896:THR:HG21	1.99	0.44
49:RE:1167:LYS:HB2	49:RE:1167:LYS:HE3	1.82	0.44
53:RK:8:TYR:CG	53:RK:30:PRO:HG2	2.52	0.44
58:RS:366:PRO:HA	58:RS:369:THR:HG22	1.98	0.44
65:R3:61:ARG:HB3	65:R3:72:ASN:HB3	2.00	0.44
65:R3:78:ASN:ND2	65:R3:236:TYR:HB2	2.33	0.44
71:C4:34:ASN:N	71:C4:104:LYS:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:667:ASN:OD1	72:R4:675:ARG:NH2	2.50	0.44
75:M4:619:PRO:HA	75:M4:622:GLU:HB2	2.00	0.44
1:3A:73:A:H2'	1:3A:74:A:C8	2.52	0.44
2:5A:20:C:H2'	2:5A:21:A:C8	2.52	0.44
3:SA:482:U:H2'	3:SA:483:A:C8	2.53	0.44
3:SA:961:U:H2'	3:SA:962:C:C6	2.53	0.44
4:SC:180:THR:O	4:SC:183:GLN:N	2.51	0.44
15:SX:11:LEU:HD22	15:SX:74:VAL:HG13	1.99	0.44
15:SX:28:ARG:HB3	15:SX:60:LYS:HG2	2.00	0.44
20:3C:194:VAL:HB	20:3C:217:ILE:HD13	1.99	0.44
22:3E:319:ILE:HD12	22:3E:326:LEU:HD22	2.00	0.44
23:3F:252:VAL:HA	23:3F:261:ILE:O	2.17	0.44
25:A4:167:LEU:HD23	25:A4:183:LEU:HD13	2.00	0.44
29:AE:591:LYS:HG3	29:AE:592:ARG:HG3	2.00	0.44
29:AE:797:LEU:HA	29:AE:801:ILE:HD12	2.00	0.44
31:AG:140:LYS:HE2	31:AG:157:PHE:HE1	1.82	0.44
32:B1:102:VAL:HG23	32:B1:113:LEU:HB3	1.99	0.44
32:B1:796:LEU:HD23	32:B1:796:LEU:HA	1.82	0.44
35:B8:263:LEU:HB2	35:B8:277:ILE:HD13	2.00	0.44
36:BE:175:THR:O	36:BE:175:THR:OG1	2.32	0.44
36:BE:254:LEU:HG	36:BE:266:VAL:HG12	1.99	0.44
36:BE:443:TRP:HA	36:BE:451:GLY:H	1.82	0.44
37:B6:124:THR:OG1	37:B6:125:SER:N	2.49	0.44
51:RG:94:GLN:O	51:RG:235:SER:OG	2.29	0.44
53:RK:141:MET:HG2	53:RK:300:TYR:CE2	2.50	0.44
53:RK:309:GLY:O	53:RK:353:THR:HA	2.18	0.44
55:RO:328:LYS:HA	55:RO:328:LYS:HD2	1.82	0.44
59:RT:242:MET:HB3	59:RT:266:VAL:HG21	2.00	0.44
63:R5:216:SER:N	63:R5:217:GLU:OE1	2.44	0.44
69:R0:76:ILE:O	69:R0:116:GLY:N	2.50	0.44
72:R4:431:LEU:HA	72:R4:432:PRO:HD3	1.84	0.44
72:R4:555:HIS:HD2	72:R4:557:LYS:HG3	1.82	0.44
72:R4:681:SER:O	72:R4:685:LYS:N	2.48	0.44
3:SA:58:U:OP1	3:SA:456:A:O2'	2.35	0.44
3:SA:82:U:OP1	56:RP:15:ARG:NH1	2.48	0.44
3:SA:1160:A:H2'	3:SA:1161:C:C6	2.52	0.44
4:SC:164:ILE:HD11	4:SC:204:ILE:HB	2.00	0.44
20:3C:157:GLY:HA3	20:3C:304:LEU:HD11	2.00	0.44
25:A4:427:ASN:OD1	25:A4:427:ASN:N	2.48	0.44
25:A4:490:SER:OG	25:A4:494:ASP:N	2.50	0.44
25:A4:741:LEU:CD2	25:A4:741:LEU:C	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AG:46:ILE:HG23	31:AG:53:LYS:HB2	2.00	0.44
34:B3:680:ASN:N	34:B3:680:ASN:OD1	2.50	0.44
35:B8:388:HIS:HB3	35:B8:392:GLY:H	1.82	0.44
36:BE:190:LEU:HD12	36:BE:235:MET:HE2	1.99	0.44
40:5D:235:ASP:OD1	40:5D:235:ASP:N	2.51	0.44
41:5E:322:LYS:HD2	41:5E:327:LYS:HB2	2.00	0.44
42:5F:57:LEU:HD22	42:5F:78:LEU:HD22	1.98	0.44
42:5F:114:ILE:HD13	42:5F:150:VAL:HG21	1.99	0.44
43:5G:166:SER:O	43:5G:256:MET:HA	2.18	0.44
48:RD:1607:ASN:HD22	48:RD:1610:LYS:NZ	2.16	0.44
49:RE:535:LYS:H	49:RE:538:ASN:HB3	1.82	0.44
49:RE:1176:LYS:HD3	49:RE:1178:ASP:HB2	2.00	0.44
51:RG:96:LEU:HD13	51:RG:130:ILE:HG21	1.99	0.44
53:RK:192:THR:HA	53:RK:224:ASN:O	2.17	0.44
55:RO:402:ILE:HD12	55:RO:405:LEU:HD13	1.99	0.44
61:X1:707:UNK:O	61:X1:711:UNK:CB	2.66	0.44
67:R2:256:PRO:HA	67:R2:259:VAL:HB	2.00	0.44
71:C4:211:ARG:HA	71:C4:248:ALA:HA	2.00	0.44
72:R4:525:ASP:HB3	72:R4:528:LEU:HB2	2.00	0.44
74:R7:111:ALA:HA	74:R7:114:ILE:HD12	2.00	0.44
75:M4:400:MET:O	75:M4:404:LYS:N	2.44	0.44
75:M4:419:CYS:HB3	75:M4:500:PHE:HB3	1.99	0.44
75:M4:486:VAL:HA	75:M4:489:ILE:HD12	1.99	0.44
75:M4:719:VAL:N	75:M4:762:ILE:O	2.38	0.44
75:M4:938:ALA:O	75:M4:941:SER:OG	2.25	0.44
75:M4:1032:GLU:OE2	75:M4:1062:HIS:ND1	2.35	0.44
3:SA:329:G:H2'	3:SA:330:G:C8	2.52	0.44
3:SA:1773:C:H2'	3:SA:1774:G:H8	1.83	0.44
14:SR:117:LEU:HD23	14:SR:117:LEU:HA	1.85	0.44
20:3C:231:ARG:HA	20:3C:260:PHE:HZ	1.83	0.44
23:3F:301:ASP:O	23:3F:303:LYS:NZ	2.44	0.44
25:A4:167:LEU:HD13	25:A4:167:LEU:HA	1.87	0.44
25:A4:431:CYS:HA	25:A4:441:VAL:O	2.18	0.44
25:A4:453:LEU:HD12	25:A4:460:LEU:HB3	2.00	0.44
29:AE:107:SER:HB2	29:AE:108:LYS:HZ2	1.83	0.44
30:AF:23:GLU:HG3	30:AF:267:PRO:HB2	1.99	0.44
32:B1:495:LYS:HA	32:B1:517:ASP:HA	2.00	0.44
32:B1:846:TYR:HE1	36:BE:909:LEU:HB3	1.82	0.44
33:B2:586:LYS:HG3	33:B2:587:MET:HB2	1.99	0.44
34:B3:239:VAL:HG12	49:RE:636:GLU:HG2	1.99	0.44
36:BE:713:LEU:HD11	36:BE:716:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5E:325:SER:O	41:5E:325:SER:OG	2.36	0.44
49:RE:372:GLN:O	49:RE:516:SER:OG	2.33	0.44
51:RH:129:ARG:N	54:RN:713:HIS:O	2.45	0.44
53:RK:221:CYS:SG	53:RK:222:GLU:N	2.91	0.44
56:RP:1224:LEU:O	56:RP:1228:LEU:CB	2.66	0.44
63:R5:102:VAL:HA	63:R5:105:SER:HB3	1.99	0.44
72:R4:88:VAL:HB	72:R4:111:VAL:HG22	2.00	0.44
72:R4:167:ASN:HA	72:R4:170:ASN:HD22	1.82	0.44
72:R4:735:ASN:OD1	72:R4:842:PHE:N	2.51	0.44
74:R7:79:GLU:OE1	74:R7:82:ARG:NH1	2.43	0.44
75:M4:296:ILE:HD11	75:M4:299:ALA:HA	2.00	0.44
75:M4:407:ASN:N	75:M4:407:ASN:OD1	2.49	0.44
75:M4:567:VAL:O	75:M4:571:MET:N	2.41	0.44
3:SA:577:G:H5''	52:RJ:1047:PRO:HG2	2.00	0.43
3:SA:1140:G:H2'	3:SA:1141:G:H8	1.82	0.43
13:SP:61:MET:HB2	13:SP:104:ALA:HB2	2.00	0.43
16:SY:126:LYS:HG2	16:SY:131:SER:HA	2.00	0.43
20:3C:241:PHE:HA	20:3C:268:VAL:O	2.18	0.43
20:3C:252:ILE:HA	20:3C:252:ILE:HD12	1.75	0.43
23:3F:253:THR:HG22	23:3F:261:ILE:HB	2.00	0.43
25:A4:346:PHE:HA	25:A4:360:SER:HA	2.00	0.43
26:A5:464:VAL:O	26:A5:468:THR:OG1	2.26	0.43
31:AG:337:LEU:HD23	31:AG:337:LEU:HA	1.87	0.43
33:B2:186:ILE:O	33:B2:199:THR:HA	2.17	0.43
36:BE:25:SER:HB2	36:BE:657:ARG:HH21	1.82	0.43
36:BE:132:THR:OG1	36:BE:136:SER:OG	2.35	0.43
41:5E:497:ASN:OD1	41:5E:497:ASN:N	2.49	0.43
48:RD:1181:ASP:HA	48:RD:1191:GLY:HA2	2.00	0.43
49:RE:949:PHE:O	49:RE:960:LYS:NZ	2.51	0.43
50:RF:58:LEU:HD21	50:RF:124:ALA:H	1.83	0.43
51:RH:174:LYS:HD2	51:RH:174:LYS:HA	1.74	0.43
52:RJ:998:SER:O	52:RJ:998:SER:OG	2.33	0.43
55:RO:507:LEU:HA	55:RO:510:GLU:HG2	2.00	0.43
57:RQ:309:ASP:N	57:RQ:309:ASP:OD1	2.48	0.43
58:RS:263:THR:HG21	58:RS:306:ALA:HA	1.99	0.43
66:R6:70:LEU:HD13	66:R6:113:ILE:HG12	1.99	0.43
66:R6:187:ASN:OD1	66:R6:189:ASP:N	2.51	0.43
69:R0:150:LEU:HD13	69:R0:195:TRP:CD2	2.53	0.43
71:C4:32:ILE:HB	71:C4:103:VAL:HG12	2.00	0.43
71:C4:223:CYS:HA	71:C4:286:ARG:HA	1.99	0.43
75:M4:329:TYR:N	75:M4:555:VAL:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SC:136:ARG:HE	4:SC:136:ARG:HB3	1.61	0.43
5:SF:125:LYS:HE2	5:SF:157:ASN:HD22	1.83	0.43
9:SJ:166:TYR:HB3	9:SJ:184:LEU:HD21	2.00	0.43
9:SJ:172:ARG:HB2	9:SJ:175:GLN:HB2	1.99	0.43
11:SM:124:THR:O	11:SM:124:THR:OG1	2.37	0.43
25:A4:420:LEU:HB3	25:A4:422:LEU:HD23	1.99	0.43
29:AE:648:LYS:HD3	29:AE:648:LYS:HA	1.78	0.43
30:AF:211:HIS:CE1	30:AF:235:LYS:HD3	2.53	0.43
31:AG:140:LYS:HE2	31:AG:157:PHE:CE1	2.53	0.43
31:AG:294:LYS:HB2	31:AG:294:LYS:HE3	1.79	0.43
32:B1:355:PRO:HD2	32:B1:399:GLY:HA2	2.00	0.43
33:B2:912:TRP:CD2	34:B3:779:VAL:HG21	2.53	0.43
34:B3:362:LEU:HG	34:B3:384:TYR:HB2	1.99	0.43
34:B3:662:GLN:HA	34:B3:665:GLN:HE21	1.83	0.43
35:B8:541:LEU:HD22	35:B8:562:LEU:HD21	2.00	0.43
36:BE:544:ALA:HB3	36:BE:562:LEU:HD22	1.99	0.43
37:B6:273:ILE:HA	37:B6:276:VAL:HG22	2.00	0.43
43:5G:107:ILE:HD11	43:5G:254:PHE:HZ	1.82	0.43
47:5K:97:LEU:HD23	47:5K:128:LEU:HD11	2.00	0.43
48:RD:1522:ASN:HD22	48:RD:1556:ILE:HD11	1.83	0.43
48:RD:1686:LYS:HB2	48:RD:1686:LYS:HE3	1.71	0.43
49:RE:1159:ASN:OD1	49:RE:1159:ASN:N	2.47	0.43
51:RH:130:ILE:HD12	51:RH:131:PRO:HD2	1.99	0.43
52:RJ:102:GLN:NE2	52:RJ:358:MET:O	2.47	0.43
54:RN:425:PHE:HA	54:RN:428:VAL:HG12	1.98	0.43
55:RO:382:LYS:HG3	55:RO:448:VAL:HG13	2.00	0.43
56:RP:180:LEU:HD13	56:RP:192:SER:HB3	2.00	0.43
56:RP:1777:LEU:HB3	56:RP:1867:THR:HG22	2.00	0.43
65:R3:345:SER:OG	65:R3:366:GLY:N	2.48	0.43
71:C4:17:ILE:HD11	71:C4:58:ALA:HB2	2.00	0.43
72:R4:13:LEU:N	72:R4:17:LEU:O	2.39	0.43
72:R4:52:CYS:HG	72:R4:184:HIS:CE1	2.29	0.43
75:M4:220:GLY:N	75:M4:234:CYS:O	2.37	0.43
75:M4:790:VAL:O	75:M4:794:LEU:N	2.44	0.43
1:3A:47:G:H2'	1:3A:48:A:C8	2.52	0.43
21:3D:15:TYR:CZ	21:3D:78:LEU:HD12	2.53	0.43
21:3D:263:ILE:HG22	21:3D:265:GLU:HB2	2.01	0.43
23:3F:162:CYS:N	23:3F:525:GLN:OE1	2.47	0.43
29:AE:725:SER:HB3	29:AE:728:GLU:HB3	2.00	0.43
30:AF:302:VAL:HA	30:AF:322:LEU:HG	2.00	0.43
31:AG:71:ASN:HB3	31:AG:73:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AG:501:THR:HG1	31:AG:506:TRP:HD1	1.66	0.43
33:B2:116:ASN:OD1	33:B2:116:ASN:N	2.50	0.43
34:B3:485:TYR:CZ	34:B3:514:THR:HB	2.53	0.43
36:BE:880:LEU:HA	36:BE:880:LEU:HD23	1.78	0.43
39:5C:114:TYR:N	39:5C:379:GLU:OE2	2.50	0.43
39:5C:295:ASP:OD1	39:5C:295:ASP:N	2.48	0.43
49:RE:703:LYS:HD3	49:RE:1082:GLN:HG2	1.99	0.43
52:RJ:104:PRO:HA	52:RJ:117:PHE:O	2.18	0.43
66:R6:14:ASP:OD2	66:R6:32:GLY:N	2.50	0.43
66:R6:28:CYS:SG	66:R6:29:SER:N	2.91	0.43
66:R6:36:PRO:HB3	66:R6:87:LEU:HB2	2.00	0.43
69:R0:183:LYS:HE3	76:M6:118:ASN:H	1.82	0.43
72:R4:193:VAL:HG22	72:R4:214:ILE:HG21	1.99	0.43
72:R4:237:GLN:HG3	72:R4:464:LEU:HB3	1.99	0.43
72:R4:318:VAL:HA	72:R4:392:VAL:HA	1.99	0.43
75:M4:177:LYS:HB3	75:M4:292:LEU:HD13	1.99	0.43
75:M4:245:MET:HB3	75:M4:250:SER:HB3	2.01	0.43
75:M4:268:ARG:HB3	75:M4:579:LEU:HD12	1.99	0.43
75:M4:405:LYS:O	75:M4:514:LYS:NZ	2.50	0.43
75:M4:678:ARG:HA	75:M4:774:ARG:HG2	2.00	0.43
75:M4:683:SER:HA	75:M4:689:ASN:HA	2.00	0.43
2:5A:286:U:H2'	2:5A:287:G:H8	1.83	0.43
3:SA:327:U:H2'	3:SA:328:A:C8	2.53	0.43
3:SA:591:A:H2'	3:SA:592:A:C8	2.53	0.43
3:SA:688:G:H2'	3:SA:689:G:C8	2.53	0.43
21:3D:173:HIS:HD2	21:3D:295:LYS:HE2	1.82	0.43
23:3F:185:LEU:H	23:3F:202:THR:HB	1.82	0.43
25:A4:400:LYS:NZ	25:A4:401:ILE:O	2.52	0.43
25:A4:565:ARG:HB2	29:AE:639:ARG:HH12	1.83	0.43
31:AG:616:SER:OG	31:AG:620:SER:N	2.39	0.43
31:AG:674:THR:OG1	31:AG:675:ARG:N	2.49	0.43
31:AG:851:GLU:OE1	35:B8:475:LYS:NZ	2.40	0.43
32:B1:60:ALA:HB1	32:B1:102:VAL:HG12	2.00	0.43
33:B2:185:MET:HA	33:B2:200:HIS:O	2.18	0.43
33:B2:231:LEU:HD12	33:B2:233:ILE:HD11	2.01	0.43
33:B2:633:CYS:HA	33:B2:639:VAL:HG12	2.00	0.43
34:B3:16:TYR:OH	34:B3:21:ALA:O	2.31	0.43
36:BE:822:ARG:O	36:BE:826:GLN:NE2	2.52	0.43
37:B6:106:ASP:OD1	37:B6:106:ASP:N	2.39	0.43
40:5D:29:GLU:OE1	52:RJ:1062:ARG:NH1	2.51	0.43
45:5I:146:LYS:HG2	45:5I:175:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:307:LYS:HG2	49:RE:312:ARG:HG3	2.00	0.43
49:RE:909:TYR:OH	49:RE:935:GLU:O	2.36	0.43
51:RH:227:LEU:HB3	51:RH:240:LYS:HE2	2.00	0.43
52:RJ:97:THR:OG1	52:RJ:98:LEU:N	2.51	0.43
53:RK:45:LEU:HG	53:RK:49:GLU:HG3	2.00	0.43
53:RK:171:ASP:N	53:RK:171:ASP:OD1	2.49	0.43
54:RN:716:LYS:HB3	54:RN:716:LYS:HE2	1.90	0.43
65:R3:165[B]:LEU:HA	65:R3:165[B]:LEU:HD12	1.80	0.43
67:R2:189:ILE:HG23	67:R2:201:PRO:HD2	1.99	0.43
2:5A:84:G:O2'	31:AG:295:TRP:O	2.36	0.43
3:SA:454:U:H2'	3:SA:455:C:C2	2.53	0.43
3:SA:488:G:H2'	3:SA:489:C:C6	2.53	0.43
4:SC:32:ILE:HG12	4:SC:96:LEU:HD12	2.00	0.43
8:SI:36:ALA:HA	8:SI:39:ARG:HH21	1.83	0.43
9:SJ:103:GLN:NE2	9:SJ:166:TYR:OH	2.52	0.43
23:3F:160:ILE:HD13	23:3F:160:ILE:HA	1.93	0.43
26:A5:231:ASP:HB3	26:A5:249:GLU:HB2	2.01	0.43
26:A5:491:GLN:NE2	26:A5:494:ARG:O	2.50	0.43
27:A8:314:LEU:HA	27:A8:321:ILE:HA	2.01	0.43
27:A8:549:ARG:O	27:A8:553:GLN:NE2	2.52	0.43
29:AE:48:ILE:HG13	29:AE:120:TRP:HD1	1.84	0.43
29:AE:194:SER:HB3	36:BE:335:VAL:HG11	2.00	0.43
29:AE:238:LEU:O	29:AE:242:SER:OG	2.33	0.43
29:AE:526:LEU:HD11	29:AE:547:ILE:HD13	2.00	0.43
29:AE:773:GLN:HA	29:AE:808:GLN:HE22	1.82	0.43
32:B1:604:TYR:HD1	32:B1:611:LEU:HA	1.84	0.43
33:B2:339:LYS:HE3	33:B2:358:SER:HA	2.01	0.43
33:B2:390:GLN:HG2	33:B2:394:VAL:HB	2.01	0.43
33:B2:551:LEU:HA	33:B2:575:PRO:HB3	2.00	0.43
35:B8:146:LEU:HD12	35:B8:163:ARG:HB3	1.99	0.43
37:B6:92:ILE:HA	37:B6:95:ILE:HD12	2.00	0.43
39:5C:412:ASP:OD1	45:5I:27:ASN:N	2.50	0.43
39:5C:454:LYS:HD3	39:5C:454:LYS:HA	1.78	0.43
51:RH:100:LEU:O	51:RH:106:LYS:NZ	2.39	0.43
52:RJ:175:ASP:OD1	52:RJ:175:ASP:N	2.50	0.43
55:RO:249:ASN:HB3	55:RO:252:LYS:HB3	1.99	0.43
56:RP:1709:ASP:OD1	56:RP:1803:ASN:ND2	2.51	0.43
57:RQ:334:PRO:HB3	57:RQ:340:GLU:HB3	2.00	0.43
64:R1:166:TYR:O	64:R1:169:THR:N	2.39	0.43
65:R3:357:TYR:OH	65:R3:382:ARG:NH1	2.51	0.43
67:R2:17:SER:HB3	67:R2:20:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:M3:47:SER:OG	68:M3:49:HIS:NE2	2.37	0.43
72:R4:760:SER:O	72:R4:764:GLU:N	2.47	0.43
74:R7:95:ASN:O	74:R7:98:THR:OG1	2.26	0.43
3:SA:803:A:O2'	15:SX:107:SER:O	2.37	0.43
3:SA:898:A:H62	3:SA:914:G:H21	1.65	0.43
3:SA:933:A:OP1	4:SC:116:LYS:NZ	2.49	0.43
3:SA:1068:C:H2'	3:SA:1069:A:H8	1.83	0.43
4:SC:165:ARG:HA	4:SC:168:ILE:HG22	2.00	0.43
11:SM:78:THR:HA	11:SM:84:ILE:HG22	2.01	0.43
22:3E:214:ILE:HG22	22:3E:216:SER:H	1.83	0.43
25:A4:32:ILE:HG23	25:A4:751:GLU:HA	2.00	0.43
25:A4:83:ASN:HB3	25:A4:86:PHE:HE2	1.83	0.43
25:A4:500:LEU:HD12	25:A4:500:LEU:HA	1.90	0.43
29:AE:101:TYR:HE2	29:AE:118:THR:HG23	1.83	0.43
29:AE:134:MET:O	29:AE:138:SER:HB3	2.19	0.43
31:AG:144:VAL:HA	31:AG:153:ILE:HA	2.01	0.43
32:B1:280:THR:HA	32:B1:304:PRO:HB3	2.01	0.43
33:B2:624:LEU:HA	33:B2:625:PRO:HD3	1.85	0.43
39:5C:23:ARG:HH21	45:5I:30:PRO:HG3	1.83	0.43
39:5C:417:ASN:HB3	39:5C:420:GLU:HB2	2.00	0.43
41:5E:448:LEU:HA	41:5E:451:LEU:HD23	2.00	0.43
53:RK:14:SER:O	53:RK:14:SER:OG	2.35	0.43
58:RS:442:GLU:HG2	58:RS:445:ARG:HE	1.82	0.43
65:R3:380:LEU:HD23	65:R3:380:LEU:HA	1.86	0.43
72:R4:755:HIS:HD2	72:R4:816:ALA:HB2	1.84	0.43
74:R7:98:THR:O	74:R7:102:GLU:N	2.38	0.43
3:SA:1474:G:N2	3:SA:1535:U:O4	2.40	0.43
4:SC:18:LYS:HB3	4:SC:18:LYS:HE2	4.16	0.43
4:SC:240:LYS:HD2	4:SC:240:LYS:HA	1.75	0.43
10:SK:41:GLU:HA	10:SK:44:ARG:HE	1.82	0.43
10:SK:124:HIS:HA	10:SK:127:VAL:HG12	2.00	0.43
14:SR:121:SER:OG	14:SR:122:ARG:N	2.52	0.43
25:A4:433:LEU:HB2	25:A4:440:LEU:HD12	2.01	0.43
26:A5:368:ASN:HB2	26:A5:524:SER:HB2	2.01	0.43
27:A8:558:CYS:O	27:A8:585:ARG:NH1	2.52	0.43
29:AE:1213:SER:O	29:AE:1217:THR:CB	2.67	0.43
30:AF:266:SER:OG	30:AF:268:MET:O	2.36	0.43
31:AG:90:LYS:HE2	31:AG:144:VAL:HB	2.00	0.43
31:AG:271:LEU:HD23	31:AG:285:LEU:HD21	1.99	0.43
32:B1:190:HIS:HD2	32:B1:210:SER:HB2	1.84	0.43
32:B1:200:SER:OG	32:B1:202:ASP:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B1:621:MET:N	32:B1:621:MET:SD	2.91	0.43
33:B2:415:LYS:HB2	33:B2:417:TRP:HE1	1.83	0.43
33:B2:746:LEU:HD12	33:B2:750:GLU:HG3	2.00	0.43
45:5I:265:ASN:HD22	45:5I:309:MET:HA	1.84	0.43
47:5K:69:THR:HG23	47:5K:102:VAL:HG22	2.01	0.43
49:RE:1018:LYS:HD3	49:RE:1018:LYS:HA	1.68	0.43
49:RE:1205:LYS:HA	49:RE:1205:LYS:HD2	1.78	0.43
52:RJ:863:THR:HB	52:RJ:866:ARG:HA	2.00	0.43
53:RK:95:PRO:HG3	53:RK:124:SER:HB3	2.00	0.43
64:R1:157:TYR:OH	64:R1:229:ASP:OD1	2.28	0.43
69:R0:119:VAL:HA	69:R0:149:ILE:HA	2.00	0.43
72:R4:419:THR:HA	72:R4:439:ARG:HA	2.01	0.43
75:M4:399:LYS:HA	75:M4:402:TRP:HB3	2.00	0.43
1:3A:152:U:H3	1:3A:161:G:H1	1.67	0.43
3:SA:1630:U:O4	41:5E:510:LYS:NZ	2.40	0.43
11:SM:77:SER:HB3	11:SM:85:VAL:HB	1.99	0.43
20:3B:135:PRO:HA	20:3B:136:PRO:HD3	1.86	0.43
21:3D:209:LEU:HD22	21:3D:250:ARG:HH12	1.84	0.43
21:3D:281:LEU:HD12	21:3D:281:LEU:HA	1.87	0.43
27:A8:491:THR:HA	27:A8:528:THR:HA	2.01	0.43
29:AE:521:SER:O	29:AE:521:SER:OG	2.37	0.43
31:AG:670:LEU:HB3	31:AG:681:ILE:HB	2.01	0.43
32:B1:203:GLN:HB2	61:X1:1503:UNK:HA	2.01	0.43
32:B1:330:TYR:OH	32:B1:335:GLU:OE2	2.33	0.43
32:B1:645:ASP:OD2	39:5C:171:LYS:NZ	2.44	0.43
33:B2:163:LYS:HD3	41:5E:522:ARG:HH21	1.83	0.43
35:B8:546:LEU:HA	35:B8:549:CYS:H	1.82	0.43
36:BE:257:ARG:NE	36:BE:259:ASP:OD1	2.51	0.43
39:5C:96:ASP:OD1	39:5C:99:THR:OG1	2.26	0.43
39:5C:321:ASN:ND2	39:5C:379:GLU:O	2.52	0.43
45:5I:399:LYS:HG2	57:RQ:879:ILE:HG22	2.01	0.43
49:RE:1202:CYS:SG	49:RE:1203:ASN:N	2.88	0.43
58:RS:305:ARG:HD3	58:RS:309:LYS:HB2	2.01	0.43
58:RS:314:PRO:HA	58:RS:317:PHE:HB3	2.00	0.43
59:RT:115:LYS:HZ3	59:RT:168:LEU:HD22	1.84	0.43
63:R5:120:VAL:HA	63:R5:123:LEU:HD13	2.00	0.43
66:R6:13:VAL:HG11	66:R6:29:SER:HB2	2.01	0.43
68:M3:195:GLU:OE2	68:M3:198:GLY:N	2.52	0.43
71:C4:60:LEU:HD23	71:C4:60:LEU:HA	1.85	0.43
72:R4:653:SER:OG	72:R4:654:TYR:N	2.51	0.43
1:3A:206:C:O2	1:3A:243:U:N3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:309:A:OP2	22:3E:426:ALA:N	2.45	0.43
3:SA:560:U:H2'	3:SA:561:G:H8	1.84	0.43
3:SA:891:A:H2'	3:SA:892:A:H8	1.83	0.43
3:SA:1615:C:N4	6:SG:80:LYS:O	2.52	0.43
9:SJ:84:HIS:ND1	9:SJ:87:ASN:O	2.39	0.43
14:SR:46:PHE:HA	14:SR:49:TYR:HB2	1.99	0.43
25:A4:171:SER:O	25:A4:171:SER:OG	2.30	0.43
26:A5:4:PRO:HD2	26:A5:306:LEU:HD22	2.01	0.43
29:AE:225:SER:OG	29:AE:226:ASN:N	2.52	0.43
29:AE:746:GLU:OE2	29:AE:788:THR:OG1	2.36	0.43
32:B1:212:ASP:OD1	32:B1:212:ASP:N	2.52	0.43
34:B3:679:THR:HG21	34:B3:723:GLU:HB2	2.00	0.43
36:BE:423:ARG:HD3	36:BE:427:TRP:CZ2	2.54	0.43
36:BE:564:ASP:OD1	36:BE:564:ASP:N	2.47	0.43
39:5C:330:LEU:O	39:5C:340:LEU:HA	2.18	0.43
45:5I:290:ASP:HB2	45:5I:298:LEU:HD23	1.99	0.43
48:RD:1511:ALA:HA	48:RD:1514:LEU:HD12	2.00	0.43
49:RE:1144:ASP:OD1	49:RE:1144:ASP:N	2.51	0.43
52:RJ:68:PRO:HB3	52:RJ:274:TYR:HE1	1.83	0.43
52:RJ:964:ALA:HB3	52:RJ:976:ILE:HD11	2.00	0.43
63:R5:240:ASN:ND2	63:R5:244:GLU:HG2	2.33	0.43
67:R2:15:LEU:HD21	67:R2:205:GLU:HG2	2.01	0.43
72:R4:20:THR:O	72:R4:39:HIS:N	2.49	0.43
72:R4:288:GLY:O	72:R4:301:ILE:N	2.40	0.43
75:M4:139:ARG:HH22	75:M4:155:ASP:HA	1.83	0.43
75:M4:466:PRO:HA	75:M4:469:ARG:HB2	2.01	0.43
75:M4:727:TYR:CE2	75:M4:729:ASP:HB2	2.53	0.43
2:5A:68:U:H3'	31:AG:426:ARG:HH12	1.84	0.43
3:SA:89:G:H21	3:SA:452:A:H5''	1.84	0.43
3:SA:953:G:H2'	3:SA:954:G:C8	2.52	0.43
3:SA:1615:C:OP1	6:SG:81:ARG:NH2	2.49	0.43
3:SA:1666:U:H2'	3:SA:1667:A:C8	2.53	0.43
17:SZ:8:ARG:NH2	23:3F:316:GLU:OE1	2.48	0.43
23:3F:168:ASN:H	23:3F:174:GLU:HA	1.84	0.43
25:A4:106:ASN:OD1	25:A4:106:ASN:N	2.51	0.43
25:A4:390:LEU:HB3	25:A4:403:THR:HG22	2.01	0.43
25:A4:770:ILE:HD11	38:5B:212:ASN:HB3	2.01	0.43
29:AE:102:LEU:HD23	29:AE:102:LEU:HA	1.89	0.43
29:AE:135:LEU:HD21	29:AE:151:ILE:HD11	2.01	0.43
29:AE:778:SER:O	29:AE:784:SER:OG	2.28	0.43
31:AG:75:SER:O	31:AG:79:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B2:549:SER:HA	33:B2:555:VAL:HG22	2.00	0.43
33:B2:630:PHE:O	33:B2:641:TYR:HA	2.19	0.43
39:5C:213:TRP:HZ3	39:5C:227:GLU:HB3	1.84	0.43
45:5I:50:LEU:HD23	45:5I:50:LEU:HA	1.86	0.43
45:5I:179:GLU:HB3	56:RP:1783:LEU:HD23	2.01	0.43
49:RE:260:ASP:HB3	49:RE:378:ASN:HA	2.01	0.43
49:RE:270:ILE:HB	49:RE:292:ILE:HG13	2.00	0.43
49:RE:580:TYR:HB2	49:RE:618:ILE:HD11	2.01	0.43
49:RE:871:ARG:HB3	49:RE:874:LEU:HD12	2.01	0.43
51:RG:48:ALA:HA	51:RG:208:ALA:HB3	2.01	0.43
52:RJ:69:PRO:HD2	52:RJ:274:TYR:CE1	2.54	0.43
52:RJ:629:ASP:HA	52:RJ:632:LYS:HB2	2.01	0.43
53:RK:243:ILE:HG23	53:RK:275:VAL:HG21	1.99	0.43
54:RN:522:LEU:HA	54:RN:525:MET:HG3	2.01	0.43
58:RS:267:VAL:HG21	58:RS:310:SER:HA	2.00	0.43
58:RS:415:VAL:HA	58:RS:418:HIS:HB2	2.01	0.43
68:M3:169:ILE:HB	68:M3:200:VAL:HG21	2.00	0.43
72:R4:531:ARG:NH2	72:R4:572:ASP:OD2	2.46	0.43
72:R4:763:PHE:HB3	72:R4:778:ILE:HD12	2.00	0.43
1:3A:168:C:H2'	1:3A:169:A:H8	1.84	0.42
3:SA:844:A:H2'	3:SA:845:G:C8	2.53	0.42
3:SA:895:G:H21	13:SP:38:THR:HG21	1.84	0.42
3:SA:1463:C:H5''	54:RN:64:ARG:HG2	2.01	0.42
3:SA:1594:G:HO2'	3:SA:1600:A:N6	2.17	0.42
20:3B:241:PHE:HE2	20:3B:243:ASP:HB2	1.85	0.42
25:A4:135:ARG:NH1	25:A4:175:GLY:O	2.47	0.42
25:A4:338:ALA:HB1	25:A4:361:LEU:HD11	2.00	0.42
25:A4:645:ARG:NE	25:A4:656:ARG:HH21	2.17	0.42
26:A5:214:VAL:HG23	26:A5:224:CYS:H	1.83	0.42
26:A5:548:ASP:HA	26:A5:551:ILE:HG22	2.01	0.42
30:AF:252:ASN:HB2	30:AF:278:ASP:HB3	2.01	0.42
31:AG:52:ILE:HB	31:AG:66:LEU:HB2	2.00	0.42
31:AG:303:LEU:HD22	31:AG:312:LEU:HD11	2.00	0.42
31:AG:536:ASP:OD1	31:AG:536:ASP:N	2.50	0.42
32:B1:109:ARG:HG3	32:B1:110:LEU:HG	2.01	0.42
32:B1:743:PHE:HZ	32:B1:778:ILE:HD13	1.84	0.42
33:B2:525:ASP:OD1	33:B2:525:ASP:N	2.50	0.42
33:B2:821:LEU:HB2	33:B2:860:ILE:HD11	2.01	0.42
35:B8:485:GLY:HA3	35:B8:518:ILE:HD11	2.01	0.42
37:B6:50:ILE:HD13	37:B6:50:ILE:HA	1.84	0.42
43:5G:153:THR:HG21	43:5G:266:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5G:200:LYS:HA	43:5G:203:VAL:HG12	2.00	0.42
45:5I:146:LYS:HB3	45:5I:148:TRP:NE1	2.34	0.42
45:5I:264:THR:HA	45:5I:281:ASN:HB3	2.01	0.42
49:RE:115:LYS:HD3	49:RE:117:LYS:HE3	2.01	0.42
49:RE:338:SER:O	49:RE:342:HIS:ND1	2.51	0.42
49:RE:818:SER:O	49:RE:818:SER:OG	2.30	0.42
52:RJ:940:LYS:HB3	52:RJ:947:PHE:HB2	2.01	0.42
53:RK:185:ARG:HD2	53:RK:312:ARG:HH12	1.82	0.42
53:RK:244:THR:OG1	53:RK:244:THR:O	2.36	0.42
53:RK:249:SER:HB2	53:RK:251:GLN:HE22	1.84	0.42
56:RP:88:PHE:HZ	56:RP:128:ALA:HB2	1.83	0.42
56:RP:1718:VAL:HA	56:RP:1721:ILE:HD12	2.01	0.42
56:RP:1797:LEU:HD23	56:RP:1797:LEU:HA	1.84	0.42
64:R1:168:THR:HG22	64:R1:209:ARG:HH21	1.84	0.42
72:R4:632:ASP:OD1	72:R4:679:LYS:NZ	2.52	0.42
75:M4:394:ILE:HA	75:M4:397:ILE:HD12	2.00	0.42
75:M4:537:TYR:O	75:M4:541:SER:OG	2.27	0.42
75:M4:592:ASN:HA	75:M4:595:ARG:HB3	2.00	0.42
75:M4:895:CYS:HA	75:M4:902:GLU:HG2	2.01	0.42
1:3A:47:G:H2'	1:3A:48:A:H8	1.84	0.42
1:3A:204:U:H3'	1:3A:205:G:C8	2.54	0.42
3:SA:233:C:O2	3:SA:234:G:N2	2.52	0.42
3:SA:429:G:H21	52:RJ:225:ARG:NH1	2.16	0.42
3:SA:1112:G:O6	52:RJ:1158:LYS:NZ	2.52	0.42
3:SA:1199:G:N1	51:RH:72:ASP:O	2.40	0.42
3:SA:1693:A:H3'	3:SA:1694:A:C8	2.54	0.42
20:3B:198:GLU:OE2	20:3B:199:PHE:N	2.52	0.42
25:A4:58:ASN:OD1	25:A4:58:ASN:N	2.42	0.42
26:A5:46:TRP:HE1	26:A5:48:GLU:HG3	1.83	0.42
29:AE:11:VAL:HA	29:AE:14:ASN:HB2	2.01	0.42
31:AG:423:LYS:O	31:AG:427:LYS:HB2	2.19	0.42
32:B1:190:HIS:CD2	32:B1:210:SER:HB2	2.54	0.42
34:B3:228:LYS:HA	34:B3:228:LYS:HD3	1.80	0.42
34:B3:303:PHE:HE1	34:B3:313:LEU:HD12	1.84	0.42
35:B8:175:PRO:HD2	36:BE:217:VAL:HG23	2.00	0.42
37:B6:78:LYS:HA	37:B6:78:LYS:HD3	1.80	0.42
37:B6:114:LEU:O	37:B6:118:LYS:HG2	2.19	0.42
37:B6:319:TYR:O	37:B6:323:PHE:CB	2.62	0.42
39:5C:272:SER:OG	39:5C:301:TRP:NE1	2.51	0.42
43:5G:177:ILE:HG21	54:RN:57:PRO:HB2	2.01	0.42
49:RE:254:LEU:HD11	49:RE:268:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:593:PRO:HD2	49:RE:596:LYS:HB2	2.00	0.42
49:RE:633:ALA:HA	49:RE:664:THR:HA	2.00	0.42
51:RG:151:ARG:HD3	51:RG:155:SER:HA	2.01	0.42
51:RG:180:LEU:HD13	51:RG:207:GLY:H	1.84	0.42
51:RH:119:GLY:O	51:RH:165:ASN:ND2	2.47	0.42
52:RJ:1049:ASN:HA	52:RJ:1050:PRO:HD3	1.93	0.42
53:RK:255:SER:O	53:RK:293:GLN:NE2	2.50	0.42
54:RN:561:ILE:HD12	54:RN:562:PRO:HD2	2.01	0.42
54:RN:698:ILE:O	55:RO:464:TRP:NE1	2.45	0.42
64:R1:23:ARG:HH22	64:R1:47:ASN:HD22	1.67	0.42
72:R4:377:ALA:O	72:R4:381:GLN:N	2.45	0.42
72:R4:783:SER:HB3	72:R4:832:TYR:CZ	2.53	0.42
75:M4:170:SER:OG	75:M4:294:ALA:O	2.37	0.42
75:M4:883:ARG:HA	75:M4:886:LYS:HD2	2.01	0.42
9:SJ:187:GLU:H	11:SM:30:ARG:NE	2.17	0.42
21:3D:195:VAL:HG12	21:3D:216:PHE:HE2	1.84	0.42
21:3D:283:ASP:OD1	21:3D:286:ARG:NH1	2.51	0.42
22:3E:113:THR:HA	22:3E:116:ILE:HG12	2.01	0.42
23:3F:156:ASN:HD22	23:3F:544:ALA:HB1	1.84	0.42
25:A4:31:MET:HG2	25:A4:752:LEU:HD12	2.01	0.42
31:AG:347:LEU:HD22	31:AG:355:SER:HB3	2.00	0.42
31:AG:412:ASN:ND2	31:AG:416:SER:O	2.52	0.42
31:AG:878:ASN:OD1	31:AG:878:ASN:N	2.51	0.42
33:B2:436:CYS:HB3	33:B2:447:LEU:HD12	2.00	0.42
33:B2:468:ILE:HD11	33:B2:522:LEU:HB2	2.01	0.42
39:5C:107:SER:O	39:5C:107:SER:OG	2.37	0.42
42:5F:71:ARG:NH1	42:5F:75:GLU:OE2	2.52	0.42
48:RD:1592:LEU:HB3	48:RD:1597:GLU:HB2	2.00	0.42
49:RE:853:ARG:CZ	49:RE:888:LYS:HE2	2.49	0.42
50:RF:23:HIS:HD2	50:RF:26:LEU:HG	1.84	0.42
51:RG:36:LYS:HE3	51:RG:172:PRO:HB3	2.01	0.42
56:RP:2021:ASP:OD1	56:RP:2024:ARG:NH1	2.53	0.42
59:RT:141:THR:OG1	59:RT:142:ASN:N	2.53	0.42
63:R5:44:PHE:HA	63:R5:161:HIS:CE1	2.53	0.42
72:R4:104:ASN:HD21	72:R4:106:ASN:HB2	1.84	0.42
74:R7:51:ASN:O	74:R7:55:TYR:N	2.49	0.42
75:M4:781:ILE:HG13	75:M4:782:ARG:H	1.84	0.42
75:M4:876:VAL:HB	75:M4:879:LEU:HG	2.01	0.42
1:3A:50:U:O2'	2:5A:467:A:N6	2.46	0.42
3:SA:789:A:H61	10:SK:71:PHE:HB3	1.85	0.42
3:SA:1154:G:H2'	3:SA:1155:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1695:G:H2'	3:SA:1696:G:H8	1.84	0.42
3:SA:1751:C:H2'	3:SA:1752:U:H6	1.83	0.42
10:SK:127:VAL:O	10:SK:131:GLN:NE2	2.52	0.42
22:3E:381:ASP:N	22:3E:381:ASP:OD1	2.50	0.42
23:3F:481:ILE:HD11	23:3F:526:VAL:HG21	2.02	0.42
29:AE:546:ASN:HA	29:AE:549:LYS:HE2	2.01	0.42
29:AE:699:ARG:CZ	29:AE:720:LEU:HD11	2.49	0.42
30:AF:139:ILE:HG12	30:AF:151:LEU:HD22	2.01	0.42
31:AG:311:TYR:HD2	31:AG:323:LEU:HD12	1.83	0.42
32:B1:9:ASN:OD1	32:B1:10:LEU:N	2.53	0.42
34:B3:4:LYS:HA	34:B3:649:GLU:HG3	2.01	0.42
34:B3:126:ILE:HD11	34:B3:147:ILE:HG12	2.02	0.42
36:BE:343:LEU:HD12	36:BE:343:LEU:HA	1.87	0.42
36:BE:387:GLN:HE21	36:BE:448:LYS:HD2	1.84	0.42
41:5E:369:ILE:HD11	43:5G:190:ILE:HD13	2.02	0.42
41:5E:507:ILE:HD11	41:5E:528:LEU:HD13	2.01	0.42
42:5F:61:LEU:HD23	42:5F:61:LEU:HA	1.87	0.42
42:5F:114:ILE:HA	42:5F:117:ARG:HB3	2.01	0.42
45:5I:270:ASN:HB2	45:5I:276:ASN:O	2.19	0.42
51:RG:122:ILE:HG12	51:RG:144:LEU:HD11	2.01	0.42
54:RN:552:GLN:HE22	54:RN:555:ARG:HE	1.66	0.42
55:RO:314:VAL:HG12	55:RO:318:LEU:HG	2.01	0.42
55:RO:375:LEU:HD23	55:RO:453:PRO:HB2	2.00	0.42
65:R3:388:LEU:HD23	65:R3:388:LEU:HA	1.85	0.42
72:R4:23:VAL:HB	72:R4:36:VAL:HG23	2.01	0.42
72:R4:93:ASN:O	72:R4:97:GLN:N	2.45	0.42
72:R4:655:GLU:HG2	72:R4:659:LEU:HD23	2.00	0.42
72:R4:753:ARG:N	72:R4:839:TYR:O	2.42	0.42
72:R4:894:ALA:HA	72:R4:897:ALA:HB3	2.01	0.42
75:M4:153:PHE:HB2	75:M4:317:VAL:HG11	2.01	0.42
75:M4:892:LEU:HA	75:M4:892:LEU:HD13	1.83	0.42
1:3A:331:A:O2'	22:3E:404:ARG:NH2	2.52	0.42
2:5A:66:C:H2'	2:5A:67:G:H8	1.84	0.42
3:SA:914:G:H4'	3:SA:915:A:H8	1.84	0.42
3:SA:922:G:H2'	3:SA:923:A:C8	2.54	0.42
3:SA:1222:C:H2'	3:SA:1223:A:C8	2.54	0.42
3:SA:1578:U:H2'	3:SA:1579:U:C6	2.54	0.42
3:SA:1796:C:H1'	3:SA:1797:A:H5'	2.01	0.42
5:SF:67:GLN:HB3	5:SF:69:HIS:HB2	2.02	0.42
8:SI:64:VAL:HB	8:SI:67:LEU:HD22	2.01	0.42
11:SM:58:CYS:SG	11:SM:61:THR:OG1	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SO:45:LEU:HB2	12:SO:50:ILE:CG2	2.49	0.42
16:SY:114:LYS:HB2	16:SY:114:LYS:HE3	1.85	0.42
25:A4:568:ASN:OD1	25:A4:568:ASN:N	2.53	0.42
25:A4:624:LYS:HD3	25:A4:627:LYS:HD2	2.01	0.42
27:A8:346:HIS:HA	27:A8:353:ARG:HA	2.02	0.42
29:AE:483:MET:HG2	29:AE:490:ARG:HB2	2.00	0.42
29:AE:620:GLU:HA	29:AE:622:TRP:HE3	1.84	0.42
31:AG:224:SER:HA	31:AG:240:PRO:HA	2.01	0.42
32:B1:54:HIS:NE2	32:B1:72:SER:OG	2.45	0.42
33:B2:223:ASP:OD1	33:B2:223:ASP:N	2.52	0.42
34:B3:625:THR:HG22	34:B3:633:VAL:HG23	2.02	0.42
36:BE:171:GLN:HE22	36:BE:213:GLU:HA	1.84	0.42
45:5I:145:VAL:HB	45:5I:176:PHE:HB2	2.01	0.42
45:5I:185:ILE:HA	45:5I:185:ILE:HD13	1.84	0.42
52:RJ:824:ILE:HD13	52:RJ:926:ILE:HG12	2.00	0.42
53:RK:154:LEU:HD11	53:RK:167:HIS:HB2	2.00	0.42
56:RP:1942:LEU:HD21	56:RP:1978:ALA:HB1	2.02	0.42
58:RS:286:ARG:NE	58:RS:290:ASN:OD1	2.47	0.42
64:R1:22:LEU:HD23	64:R1:173:ASP:HB2	2.01	0.42
65:R3:345:SER:HA	65:R3:365:GLY:H	1.84	0.42
67:R2:154:LEU:HA	67:R2:155:PRO:HD3	1.92	0.42
72:R4:229:ASP:HA	72:R4:232:ARG:HE	1.84	0.42
72:R4:736:ILE:O	72:R4:740:ARG:N	2.45	0.42
75:M4:240:GLU:HG3	75:M4:275:VAL:HG11	2.00	0.42
1:3A:329:C:N4	40:5D:250:ARG:O	2.51	0.42
3:SA:75:U:N3	3:SA:76:A:N3	2.47	0.42
3:SA:958:U:H2'	12:SO:14:SER:HB3	2.02	0.42
3:SA:1767:G:OP2	59:RT:200:ARG:NH1	2.53	0.42
6:SG:222:LYS:HE3	6:SG:222:LYS:HB3	1.84	0.42
10:SK:45:ILE:HD11	10:SK:105:LEU:HD23	2.02	0.42
12:SO:45:LEU:HB2	12:SO:50:ILE:HG22	2.01	0.42
20:3C:188:VAL:HG22	20:3C:192:GLY:HA3	2.01	0.42
23:3F:353:ASP:OD1	23:3F:353:ASP:N	2.49	0.42
24:3H:20:ILE:HG22	24:3H:117:VAL:HG13	2.01	0.42
24:3H:54:MET:O	24:3H:80:PHE:HA	2.19	0.42
26:A5:148:LEU:HD22	26:A5:165:VAL:HG12	2.01	0.42
26:A5:470:PHE:HB2	26:A5:508:ILE:HD13	2.02	0.42
29:AE:280:GLU:HB3	29:AE:319:ILE:HD12	2.01	0.42
31:AG:530:LYS:HB2	31:AG:543:LEU:HD11	2.02	0.42
33:B2:52:TRP:CD1	33:B2:59:LEU:HA	2.54	0.42
33:B2:180:THR:HB	33:B2:186:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5G:107:ILE:HD13	43:5G:107:ILE:HA	1.87	0.42
49:RE:590:SER:O	49:RE:590:SER:OG	2.31	0.42
51:RG:47:MET:H	51:RG:115:GLN:HE21	1.68	0.42
54:RN:701:ALA:O	54:RN:704:ASN:ND2	2.53	0.42
63:R5:137:ASP:OD2	66:R6:57:GLY:N	2.52	0.42
64:R1:23:ARG:HD2	64:R1:45:GLY:HA3	2.02	0.42
72:R4:26:ARG:HB3	72:R4:33:THR:HB	2.02	0.42
72:R4:454:ASP:H	72:R4:465:GLY:HA2	1.83	0.42
72:R4:968:ASP:OD1	72:R4:968:ASP:N	2.51	0.42
75:M4:168:LEU:HA	75:M4:291:PHE:HB2	2.02	0.42
75:M4:724:ASN:HB3	75:M4:791:GLY:HA3	2.00	0.42
1:3A:8:U:H2'	1:3A:9:A:C8	2.54	0.42
3:SA:174:U:O4	3:SA:266:A:N7	2.53	0.42
3:SA:1736:G:H2'	3:SA:1737:G:C8	2.55	0.42
6:SG:92:ARG:NH1	6:SG:169:ASN:OD1	2.45	0.42
7:SH:121:LEU:HD23	7:SH:121:LEU:HA	1.85	0.42
8:SI:7:LYS:HG3	8:SI:41:LEU:HD21	2.02	0.42
8:SI:159:VAL:HA	8:SI:162:ILE:HB	2.02	0.42
25:A4:322:ASN:O	31:AG:329:ASN:ND2	2.53	0.42
25:A4:580:LYS:HG3	25:A4:596:MET:HB2	2.01	0.42
26:A5:166:ALA:HB2	26:A5:170:ILE:HG23	2.01	0.42
27:A8:668:ILE:HA	27:A8:671:ARG:HG2	2.02	0.42
29:AE:44:ASP:OD1	29:AE:45:TYR:N	2.49	0.42
29:AE:236:PRO:HA	35:B8:212:LEU:HD21	2.01	0.42
29:AE:635:TYR:HB3	29:AE:639:ARG:HH21	1.83	0.42
30:AF:282:LYS:HZ2	30:AF:292:VAL:HG21	1.83	0.42
31:AG:408:THR:HG23	31:AG:411:SER:H	1.84	0.42
31:AG:669:ASN:OD1	31:AG:669:ASN:N	2.53	0.42
32:B1:273:ARG:HD2	32:B1:290:PRO:HG2	2.02	0.42
32:B1:849:LEU:HG	36:BE:897:HIS:HB2	2.02	0.42
33:B2:411:ASN:ND2	33:B2:413:SER:OG	2.53	0.42
34:B3:457:ALA:HB2	34:B3:497:LEU:HD22	2.01	0.42
37:B6:148:ILE:HD13	37:B6:148:ILE:HA	1.88	0.42
42:5F:64:LEU:HD23	42:5F:64:LEU:HA	1.85	0.42
44:5H:544:ILE:HD13	52:RJ:834:TRP:CD2	2.55	0.42
45:5I:285:ASN:N	45:5I:285:ASN:OD1	2.50	0.42
49:RE:899:LEU:HA	49:RE:902:ILE:HG22	2.02	0.42
49:RE:920:LEU:HG	49:RE:925:LEU:HB2	2.01	0.42
49:RE:1187:LYS:HA	49:RE:1187:LYS:HD3	1.80	0.42
51:RG:150:ILE:HG22	51:RG:160:LEU:HB2	2.02	0.42
52:RJ:302:GLU:HB2	52:RJ:790:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RJ:827:ALA:HA	52:RJ:920:GLU:H	1.85	0.42
53:RK:55:LEU:HD12	53:RK:88:HIS:CD2	2.54	0.42
54:RN:64:ARG:NH1	54:RN:65:ASN:O	2.42	0.42
56:RP:2069:GLN:H	56:RP:2069:GLN:HG3	1.71	0.42
65:R3:21:VAL:HA	71:C4:190:VAL:HG11	2.01	0.42
65:R3:40:ARG:NH2	65:R3:333:ASP:O	2.38	0.42
66:R6:51:ILE:HB	66:R6:91:THR:HG23	2.01	0.42
67:R2:65:LYS:O	67:R2:123:LYS:N	2.52	0.42
72:R4:292:LEU:HD23	72:R4:292:LEU:HA	1.84	0.42
75:M4:186:ALA:HA	75:M4:189:LEU:HB2	2.00	0.42
75:M4:461:ILE:HA	75:M4:464:ILE:HG22	2.02	0.42
75:M4:957:PRO:HA	75:M4:960:ALA:HB3	2.02	0.42
3:SA:890:C:H2'	3:SA:891:A:C8	2.55	0.42
3:SA:1146:G:H2'	3:SA:1147:A:C8	2.55	0.42
3:SA:1752:U:H2'	3:SA:1753:A:C8	2.55	0.42
4:SC:124:ASN:N	4:SC:124:ASN:OD1	2.51	0.42
5:SF:105:VAL:HG13	5:SF:245:LYS:HB3	2.02	0.42
10:SK:123:HIS:CD2	44:5H:566:ARG:HH21	2.38	0.42
11:SM:40:LEU:HD21	11:SM:70:ILE:HG12	2.02	0.42
13:SP:70:LYS:HA	13:SP:70:LYS:HD2	1.79	0.42
23:3F:310:ASN:OD1	23:3F:310:ASN:N	2.53	0.42
25:A4:167:LEU:HD11	25:A4:195:TRP:HZ2	1.85	0.42
25:A4:332:ASP:HB2	25:A4:352:VAL:HG12	2.02	0.42
26:A5:120:ILE:HD11	26:A5:148:LEU:HB3	2.00	0.42
29:AE:661:ILE:HA	29:AE:662:PRO:HD3	1.90	0.42
31:AG:86:GLU:OE2	31:AG:111:THR:OG1	2.31	0.42
31:AG:408:THR:HG23	31:AG:410:ASN:H	1.85	0.42
31:AG:891:VAL:HA	31:AG:894:VAL:HG12	2.01	0.42
32:B1:848:PHE:O	32:B1:852:THR:OG1	2.32	0.42
35:B8:284:LEU:HD21	35:B8:287:SER:HB3	2.01	0.42
35:B8:526:ASP:OD1	35:B8:526:ASP:N	2.46	0.42
36:BE:132:THR:OG1	36:BE:134:ASP:OD1	2.32	0.42
36:BE:354:SER:O	36:BE:631:ASN:ND2	2.52	0.42
37:B6:75:LEU:HB3	37:B6:77:VAL:HG22	2.02	0.42
39:5C:463:ALA:HA	39:5C:466:LEU:HD23	2.01	0.42
40:5D:192:LYS:O	40:5D:196:LYS:NZ	2.51	0.42
47:5K:70:ASN:HD21	47:5K:157:ASP:HB2	1.85	0.42
47:5K:139:ASP:HA	47:5K:142:VAL:HG12	2.02	0.42
49:RE:524:ASP:HB3	49:RE:618:ILE:HA	2.02	0.42
52:RJ:879:THR:OG1	52:RJ:880:TYR:N	2.53	0.42
52:RJ:1104:GLY:H	52:RJ:1107:LYS:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:RK:319:ASP:N	53:RK:319:ASP:OD1	2.52	0.42
56:RP:98:HIS:CG	56:RP:135:LEU:HD11	2.55	0.42
58:RS:233:PHE:HA	58:RS:236:ILE:HG12	2.01	0.42
58:RS:356:LEU:HD13	58:RS:375:LEU:HD23	2.00	0.42
63:R5:31:ASP:OD1	63:R5:31:ASP:N	2.35	0.42
65:R3:51:ASP:OD1	65:R3:52:VAL:N	2.52	0.42
65:R3:348:SER:O	65:R3:361:THR:N	2.51	0.42
66:R6:163:LEU:HD13	66:R6:180:LEU:HD13	2.01	0.42
67:R2:26:ARG:HD2	67:R2:30:GLN:HB2	2.01	0.42
72:R4:519:PRO:O	72:R4:523:SER:N	2.45	0.42
72:R4:715:VAL:HG23	72:R4:906:VAL:HG11	2.02	0.42
75:M4:407:ASN:HB2	75:M4:497:LYS:HD2	2.01	0.42
3:SA:314:C:H42	3:SA:354:C:H42	1.68	0.42
3:SA:1465:C:O2	43:5G:146:ARG:NH2	2.53	0.42
4:SC:106:THR:HG23	4:SC:109:LYS:H	1.85	0.42
5:SF:155:LYS:HA	5:SF:155:LYS:HD3	1.87	0.42
13:SP:83:ILE:HD11	13:SP:102:LEU:HD13	2.02	0.42
22:3E:322:ALA:H	22:3E:340:GLY:HA2	1.85	0.42
25:A4:565:ARG:NH1	29:AE:628:ASN:HB3	2.34	0.42
25:A4:649:TRP:CD1	25:A4:744:VAL:HB	2.55	0.42
27:A8:455:LEU:HA	27:A8:497:ILE:HD12	2.01	0.42
29:AE:328:ASP:O	29:AE:331:SER:OG	2.36	0.42
29:AE:390:LEU:HA	29:AE:393:ILE:HG22	2.02	0.42
30:AF:458:ILE:HD12	30:AF:458:ILE:HA	1.83	0.42
31:AG:615:TRP:CD1	31:AG:622:ILE:HG12	2.55	0.42
32:B1:718:ASP:O	36:BE:579:ARG:NH1	2.47	0.42
33:B2:799:LYS:HE2	33:B2:799:LYS:HB2	1.86	0.42
33:B2:836:ILE:HA	33:B2:839:VAL:HG12	2.01	0.42
35:B8:534:SER:OG	35:B8:535:ARG:N	2.53	0.42
36:BE:501:HIS:CD2	36:BE:521:GLY:HA3	2.55	0.42
39:5C:128:THR:O	39:5C:128:THR:OG1	2.32	0.42
49:RE:329:THR:O	49:RE:333:ASN:ND2	2.52	0.42
49:RE:413:LEU:HG	49:RE:415:GLY:H	1.85	0.42
49:RE:495:THR:HA	49:RE:498:MET:HG2	2.01	0.42
49:RE:808:LEU:HD12	49:RE:825:PHE:CZ	2.55	0.42
50:RF:219:ASN:OD1	50:RF:219:ASN:N	2.53	0.42
51:RH:105:ASN:HD22	51:RH:110:LEU:HD23	1.85	0.42
52:RJ:42:THR:OG1	52:RJ:43:MET:N	2.53	0.42
52:RJ:247:ASP:OD1	52:RJ:247:ASP:N	2.52	0.42
53:RK:228:ASP:OD2	53:RK:230:TRP:NE1	2.43	0.42
54:RN:561:ILE:HG13	54:RN:563:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:RN:752:MET:HA	54:RN:755:ILE:HG12	2.00	0.42
59:RT:255:PRO:HB2	59:RT:258:LYS:HD3	2.01	0.42
63:R5:229:LEU:HD23	63:R5:229:LEU:HA	1.84	0.42
65:R3:40:ARG:HD3	65:R3:44:ARG:HB2	2.02	0.42
69:R0:122:ARG:O	69:R0:135:GLU:N	2.41	0.42
69:R0:217:LYS:HD3	69:R0:217:LYS:HA	1.88	0.42
71:C4:36:VAL:N	71:C4:106:ILE:O	2.43	0.42
75:M4:339:TYR:HB3	75:M4:352:ASN:HB3	2.02	0.42
75:M4:670:ALA:HB3	75:M4:764:LEU:HD22	2.01	0.42
75:M4:792:LYS:O	75:M4:796:GLU:N	2.49	0.42
75:M4:931:LEU:HD23	75:M4:931:LEU:HA	1.83	0.42
3:SA:34:G:C6	3:SA:475:A:C6	3.08	0.42
3:SA:333:A:OP1	9:SJ:49:ARG:NH1	2.52	0.42
3:SA:939:A:H2'	3:SA:940:A:C8	2.55	0.42
3:SA:1112:G:H2'	3:SA:1113:A:H8	1.85	0.42
3:SA:1150:G:H2'	3:SA:1151:A:C8	2.55	0.42
16:SY:77:ILE:HB	52:RJ:54:LEU:HD13	2.02	0.42
20:3B:229:LYS:HB3	20:3B:229:LYS:HE2	1.66	0.42
24:3H:20:ILE:HA	24:3H:23:VAL:HG12	2.01	0.42
24:3H:53:ILE:HG22	24:3H:87:LEU:HD11	2.02	0.42
24:3H:68:PRO:HA	24:3H:71:CYS:SG	2.60	0.42
25:A4:183:LEU:HG	25:A4:223:GLY:HA2	2.01	0.42
25:A4:581:SER:HA	25:A4:594:PHE:O	2.20	0.42
26:A5:233:LYS:HD3	26:A5:233:LYS:HA	1.85	0.42
29:AE:151:ILE:O	29:AE:155:ILE:HB	2.20	0.42
30:AF:123:SER:HG	30:AF:144:SER:HG	1.61	0.42
31:AG:559:LYS:HD2	31:AG:559:LYS:HA	1.75	0.42
34:B3:279:LYS:NZ	34:B3:326:THR:O	2.48	0.42
39:5C:39:ASP:HB3	39:5C:42:LEU:HB3	2.01	0.42
41:5E:432:LYS:HD2	41:5E:432:LYS:HA	1.81	0.42
48:RD:1513:LYS:HA	48:RD:1516:ILE:HG22	2.02	0.42
48:RD:1549:ILE:HD13	48:RD:1549:ILE:HA	1.91	0.42
49:RE:1224:ALA:HB1	49:RE:1231:VAL:HG11	2.02	0.42
51:RG:102:SER:HB3	51:RG:110:LEU:HD13	2.02	0.42
51:RH:90:ASP:OD1	51:RH:90:ASP:N	2.49	0.42
54:RN:488:ASN:HD22	54:RN:492:ALA:H	1.68	0.42
56:RP:1003:ILE:O	56:RP:1005:ASN:N	2.53	0.42
63:R5:55:LYS:HB3	63:R5:141:LEU:HD12	2.02	0.42
66:R6:132:ALA:HB3	66:R6:202:CYS:HB3	2.02	0.42
68:M3:46:LEU:HD13	68:M3:48:LEU:HD11	2.02	0.42
68:M3:71:THR:OG1	68:M3:144:ASP:OD1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:507:GLY:HA2	72:R4:607:LEU:HD11	2.01	0.42
75:M4:158:ILE:HG23	75:M4:183:TYR:CE2	2.55	0.42
75:M4:459:PRO:O	75:M4:463:HIS:ND1	2.52	0.42
75:M4:680:VAL:HG12	75:M4:770:ILE:HG12	2.02	0.42
3:SA:1731:A:H3'	3:SA:1732:A:C8	2.55	0.41
4:SC:141:ALA:HB2	4:SC:210:ILE:HG23	2.01	0.41
20:3B:202:ARG:HB3	24:3H:69:LEU:HD12	2.01	0.41
21:3D:247:ILE:HG12	21:3D:250:ARG:HH21	1.85	0.41
22:3E:331:LYS:HA	40:5D:106:TYR:CE1	2.55	0.41
23:3F:194:LEU:O	23:3F:215:LYS:HA	2.20	0.41
23:3F:488:ILE:HG22	23:3F:498:VAL:HG22	2.02	0.41
25:A4:150:ASN:HD22	25:A4:155:LYS:HB2	1.84	0.41
25:A4:157:SER:OG	25:A4:195:TRP:NE1	2.51	0.41
25:A4:334:ARG:H	25:A4:351:GLY:HA2	1.84	0.41
27:A8:592:ARG:HD3	27:A8:640:LEU:HD21	2.01	0.41
30:AF:165:THR:N	30:AF:202:GLY:O	2.53	0.41
31:AG:506:TRP:HA	31:AG:532:TRP:O	2.18	0.41
31:AG:577:ASP:OD1	31:AG:578:ASN:N	2.53	0.41
32:B1:19:ASN:OD1	32:B1:19:ASN:N	2.53	0.41
32:B1:44:ASN:O	32:B1:46:LYS:N	2.53	0.41
33:B2:413:SER:OG	33:B2:413:SER:O	2.33	0.41
34:B3:258:ILE:HG23	34:B3:269:LEU:HD12	2.02	0.41
37:B6:277:CYS:O	37:B6:281:LEU:HB2	2.20	0.41
43:5G:106:GLU:OE1	43:5G:172:MET:HB2	2.20	0.41
49:RE:781:ASP:HA	49:RE:851:LYS:HB2	2.01	0.41
51:RG:80:MET:H	51:RG:80:MET:HG2	1.68	0.41
52:RJ:980:LEU:HD23	52:RJ:980:LEU:HA	1.88	0.41
54:RN:546:LEU:HA	54:RN:549:ILE:HG22	2.01	0.41
54:RN:646:THR:O	54:RN:650:VAL:HB	2.20	0.41
55:RO:261:TRP:O	55:RO:265:LEU:HB2	2.20	0.41
58:RS:407:GLU:HB2	58:RS:411:ARG:HB2	2.02	0.41
66:R6:4:GLN:HG3	66:R6:20:VAL:HB	2.02	0.41
3:SA:1712:A:H8	3:SA:1713:G:H4'	1.86	0.41
3:SA:1769:U:O2	59:RT:213:LYS:NZ	2.48	0.41
3:SA:1773:C:H2'	3:SA:1774:G:C8	2.55	0.41
8:SI:140:VAL:HA	8:SI:149:ILE:O	2.20	0.41
10:SK:154:LYS:HD3	23:3F:322:HIS:CE1	2.55	0.41
25:A4:345:ASP:N	25:A4:345:ASP:OD1	2.52	0.41
29:AE:19:ALA:HB3	29:AE:25:ARG:HH11	1.86	0.41
29:AE:363:LEU:HD23	29:AE:403:LEU:HD21	2.02	0.41
30:AF:34:GLN:OE1	30:AF:71:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AF:49:PRO:HG2	30:AF:91:SER:HA	2.02	0.41
30:AF:182:HIS:ND1	30:AF:197:ASP:OD1	2.53	0.41
30:AF:193:ILE:HB	30:AF:209:LEU:HB2	2.02	0.41
31:AG:340:ILE:HG13	31:AG:361:THR:HG22	2.03	0.41
31:AG:698:VAL:HG12	31:AG:724:ILE:HB	2.02	0.41
32:B1:286:LEU:HG	32:B1:296:GLN:HB2	2.02	0.41
32:B1:441:SER:O	32:B1:443:GLU:N	2.53	0.41
33:B2:432:TYR:HB3	33:B2:450:ARG:HD2	2.01	0.41
33:B2:747:LYS:HE3	33:B2:747:LYS:HB2	1.80	0.41
49:RE:978:ASP:OD1	49:RE:978:ASP:N	2.48	0.41
50:RF:20:LEU:N	50:RF:33:SER:OG	2.52	0.41
52:RJ:556:ASP:OD1	52:RJ:556:ASP:N	2.43	0.41
55:RO:254:LYS:HD3	55:RO:254:LYS:HA	1.75	0.41
55:RO:334:TYR:HB2	55:RO:337:PHE:HD2	1.85	0.41
63:R5:101:GLU:O	63:R5:105:SER:N	2.51	0.41
63:R5:146:GLY:O	63:R5:150:ALA:N	2.48	0.41
64:R1:24:ARG:HG3	72:R4:13:LEU:HD21	2.00	0.41
72:R4:987:MET:HA	72:R4:994:ARG:HA	2.01	0.41
75:M4:138:LYS:HD3	75:M4:138:LYS:HA	1.87	0.41
75:M4:903:LEU:HA	75:M4:906:ARG:HB2	2.02	0.41
1:3A:174:U:H4'	60:RW:44:SER:HA	2.02	0.41
3:SA:23:G:H2'	3:SA:24:U:C6	2.55	0.41
3:SA:925:G:H2'	3:SA:926:A:C8	2.54	0.41
4:SC:189:ILE:HD13	4:SC:189:ILE:HA	1.91	0.41
15:SX:105:THR:HG23	15:SX:126:LEU:HB2	2.01	0.41
21:3D:181:LEU:HB3	21:3D:288:LEU:HD23	2.01	0.41
22:3E:191:HIS:CE1	22:3E:246:GLU:HA	2.55	0.41
22:3E:279:ARG:O	22:3E:283:ILE:HG12	2.20	0.41
25:A4:81:PRO:HA	25:A4:85:TRP:HA	2.02	0.41
25:A4:85:TRP:HZ3	25:A4:376:GLU:HG2	1.86	0.41
25:A4:467:ASN:HB2	25:A4:470:LEU:HB3	2.02	0.41
25:A4:485:LYS:HD3	25:A4:497:ILE:HG23	2.02	0.41
26:A5:22:VAL:HG13	35:B8:278:ASP:HB2	2.01	0.41
27:A8:293:TYR:HA	27:A8:304:GLN:HA	2.02	0.41
29:AE:81:LEU:HD11	29:AE:86:GLN:HE22	1.85	0.41
31:AG:383:LEU:HD13	31:AG:385:ILE:HD11	2.02	0.41
31:AG:568:ASN:HB3	31:AG:571:GLN:HB2	2.02	0.41
31:AG:614:ALA:HB3	31:AG:623:PHE:HB2	2.01	0.41
32:B1:641:LEU:HD23	32:B1:641:LEU:HA	1.88	0.41
33:B2:41:LEU:HD13	33:B2:54:ILE:HG21	2.01	0.41
34:B3:147:ILE:HD12	34:B3:167:ASP:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B6:16:ASP:OD2	39:5C:15:ARG:NH1	2.43	0.41
40:5D:137:VAL:HG12	40:5D:138:ASP:H	1.84	0.41
45:5I:347:ARG:HG2	47:5K:108:LYS:HG3	2.00	0.41
49:RE:100:SER:HA	49:RE:103:PHE:HE1	1.85	0.41
49:RE:193:ALA:O	49:RE:367:ARG:NH2	2.54	0.41
50:RF:64:ILE:HD11	50:RF:68:LYS:HE3	2.03	0.41
52:RJ:996:LEU:HD23	52:RJ:996:LEU:HA	1.89	0.41
58:RS:229:LEU:HB2	58:RS:261:GLU:HG3	2.02	0.41
65:R3:261:THR:HG22	65:R3:262:ARG:H	1.84	0.41
67:R2:57:GLU:HB3	67:R2:131:ILE:HB	2.01	0.41
75:M4:449:ALA:O	75:M4:456:ARG:NH2	2.52	0.41
75:M4:458:LEU:HD23	75:M4:458:LEU:HA	1.84	0.41
75:M4:499:LEU:HD12	75:M4:499:LEU:HA	1.87	0.41
75:M4:791:GLY:HA2	75:M4:794:LEU:HD12	2.02	0.41
1:3A:61:G:O6	32:B1:630:LEU:N	2.43	0.41
2:5A:476:A:H2'	2:5A:477:G:C8	2.55	0.41
3:SA:142:G:N7	7:SH:177:ARG:NH1	2.68	0.41
3:SA:325:G:H21	11:SM:81:HIS:CD2	2.39	0.41
3:SA:334:G:C8	3:SA:335:U:H5	2.39	0.41
3:SA:656:G:C2	3:SA:678:A:H2	2.36	0.41
3:SA:800:U:H2'	3:SA:801:G:C8	2.56	0.41
8:SI:67:LEU:HD23	8:SI:68:ALA:H	1.85	0.41
17:SZ:105:ARG:O	17:SZ:109:LYS:HB2	2.20	0.41
20:3B:155:ILE:HD13	20:3B:155:ILE:HA	1.85	0.41
20:3C:309:TYR:OH	40:5D:129:SER:OG	2.29	0.41
21:3D:140:LYS:HD2	37:B6:104:PRO:HD2	2.02	0.41
22:3E:285:PRO:HG3	22:3E:382:ASP:HA	2.01	0.41
25:A4:312:ASN:HA	25:A4:315:GLN:HG2	2.02	0.41
25:A4:741:LEU:CG	25:A4:744:VAL:CG2	2.98	0.41
26:A5:490:ARG:HA	26:A5:490:ARG:HD3	1.78	0.41
29:AE:6:ASP:N	29:AE:6:ASP:OD1	2.41	0.41
29:AE:376:GLU:CD	29:AE:377:ARG:H	2.24	0.41
29:AE:377:ARG:HH11	31:AG:856:GLU:HG3	1.85	0.41
29:AE:547:ILE:HD12	29:AE:550:TYR:HB2	2.03	0.41
31:AG:124:LYS:HA	31:AG:124:LYS:HD2	1.72	0.41
32:B1:11:LEU:HA	32:B1:11:LEU:HD23	1.82	0.41
32:B1:291:ASP:N	32:B1:291:ASP:OD1	2.51	0.41
32:B1:598:ASN:OD1	32:B1:598:ASN:N	2.49	0.41
33:B2:159:LEU:HD12	33:B2:159:LEU:HA	1.88	0.41
35:B8:380:ASN:N	35:B8:380:ASN:OD1	2.52	0.41
39:5C:192:GLU:OE2	39:5C:211:THR:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RE:628:VAL:HG13	49:RE:666:CYS:HB2	2.02	0.41
49:RE:800:GLU:O	49:RE:804:THR:HG23	2.21	0.41
49:RE:1094:LYS:HD3	61:X1:1304:UNK:HA	2.03	0.41
49:RE:1111:SER:HA	49:RE:1129:PRO:HD3	2.02	0.41
49:RE:1221:HIS:NE2	50:RF:21:PRO:O	2.52	0.41
50:RF:150:LYS:HE2	50:RF:150:LYS:HB3	1.74	0.41
51:RH:39:LYS:HB2	51:RH:198:ASP:HA	2.02	0.41
53:RK:151:LEU:HD13	53:RK:168:LEU:HB3	2.01	0.41
53:RK:177:PRO:HD2	53:RK:304:GLY:HA2	2.01	0.41
54:RN:585:PRO:HB2	54:RN:586:LEU:H	1.72	0.41
65:R3:257:MET:O	65:R3:268:ILE:N	2.48	0.41
65:R3:257:MET:HA	72:R4:294:ARG:HH11	1.85	0.41
67:R2:68:ASP:HB3	67:R2:71:VAL:HG22	2.01	0.41
68:M3:180:LEU:HA	68:M3:180:LEU:HD23	1.84	0.41
72:R4:703:VAL:HG11	72:R4:902:TYR:HB3	2.03	0.41
75:M4:703:ASN:HB2	75:M4:711:TYR:HE2	1.85	0.41
1:3A:204:U:N3	1:3A:245:U:O2	2.54	0.41
1:3A:249:G:H2'	1:3A:250:C:H6	1.84	0.41
3:SA:1461:C:H2'	3:SA:1462:G:H8	1.85	0.41
3:SA:1742:U:H2'	3:SA:1743:U:H4'	2.03	0.41
7:SH:139:ASN:HA	7:SH:142:ARG:HB2	2.03	0.41
11:SM:54:ILE:HG23	11:SM:55:ASP:H	1.85	0.41
22:3E:19:ASP:HA	22:3E:44:ILE:HA	2.02	0.41
27:A8:637:LEU:HA	27:A8:640:LEU:HD12	2.01	0.41
29:AE:760:PHE:HD1	29:AE:763:LEU:HD12	1.86	0.41
31:AG:25:LEU:HB3	31:AG:28:VAL:HB	2.02	0.41
31:AG:483:LYS:HA	31:AG:483:LYS:HD3	1.85	0.41
32:B1:68:THR:HB	32:B1:127:VAL:HG21	2.02	0.41
32:B1:288:ASP:HB2	32:B1:295:ILE:HD11	2.02	0.41
33:B2:53:ASP:OD1	33:B2:53:ASP:N	2.50	0.41
33:B2:750:GLU:HA	33:B2:753:MET:HB3	2.03	0.41
34:B3:496:ALA:HB3	34:B3:509:ALA:HB3	2.03	0.41
34:B3:683:LEU:HD23	34:B3:683:LEU:HA	1.92	0.41
35:B8:168:PHE:HA	35:B8:171:ILE:HG22	2.02	0.41
35:B8:239:LYS:HE2	35:B8:243:ALA:HB3	2.03	0.41
35:B8:439:LYS:HG3	35:B8:442:HIS:HE1	1.85	0.41
36:BE:632:VAL:HG13	36:BE:641:LEU:HD11	2.02	0.41
40:5D:17:SER:OG	40:5D:18:GLN:N	2.53	0.41
42:5F:34:ARG:NH2	47:5K:16:THR:O	2.50	0.41
49:RE:712:ASN:N	49:RE:1113:GLY:O	2.47	0.41
49:RE:769:VAL:HG11	49:RE:1113:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:RF:41:ARG:HD2	50:RF:138:TRP:HB2	2.02	0.41
52:RJ:839:LEU:HD23	52:RJ:839:LEU:HA	1.91	0.41
55:RO:185:TYR:HA	55:RO:191:ILE:HG21	2.02	0.41
55:RO:352:VAL:HG12	55:RO:354:TYR:H	1.85	0.41
59:RT:120:LEU:HD12	59:RT:124:LEU:HB3	2.02	0.41
64:R1:163:VAL:HG22	64:R1:172:LEU:HA	2.03	0.41
69:R0:220:THR:HA	69:R0:223:PHE:CD2	2.55	0.41
69:R0:231:PHE:O	69:R0:235:LEU:N	2.35	0.41
74:R7:40:LEU:HD23	74:R7:45:ALA:HB1	2.02	0.41
75:M4:506:SER:HA	75:M4:543:ARG:HH11	1.85	0.41
3:SA:153:G:H2'	3:SA:154:G:C8	2.56	0.41
3:SA:1575:G:H2'	3:SA:1576:A:C8	2.56	0.41
20:3C:89:GLU:HB3	20:3C:98:ILE:HB	2.03	0.41
20:3C:103:GLU:HA	40:5D:194:LYS:HZ3	1.84	0.41
20:3C:185:SER:HA	20:3C:188:VAL:HG12	2.03	0.41
21:3D:400:PHE:HA	21:3D:403:VAL:HG12	2.03	0.41
23:3F:419:ASN:HA	23:3F:472:PRO:HG3	2.02	0.41
24:3H:5:ASN:OD1	24:3H:5:ASN:N	2.52	0.41
24:3H:70:LEU:HA	24:3H:70:LEU:HD23	1.86	0.41
25:A4:87:GLN:HB3	25:A4:378:TYR:CD2	2.56	0.41
26:A5:169:SER:O	26:A5:169:SER:OG	2.38	0.41
29:AE:596:LYS:HZ1	29:AE:649:VAL:HG22	1.86	0.41
30:AF:108:TYR:HE2	30:AF:113:PRO:HA	1.86	0.41
32:B1:458:TRP:CD1	32:B1:465:LEU:HA	2.55	0.41
33:B2:660:VAL:HA	33:B2:676:SER:HA	2.03	0.41
34:B3:210:ASN:HD22	34:B3:222:LEU:HD21	1.86	0.41
34:B3:280:ARG:HH12	34:B3:283:LYS:H	1.67	0.41
36:BE:420:GLU:HG3	36:BE:470:GLN:HA	2.01	0.41
36:BE:605:LEU:HD23	36:BE:628:VAL:HG11	2.02	0.41
37:B6:60:GLU:HA	37:B6:63:VAL:HG12	2.03	0.41
37:B6:75:LEU:HD12	37:B6:75:LEU:HA	1.94	0.41
47:5K:164:ILE:HD12	47:5K:170:ILE:HD11	2.02	0.41
49:RE:146:LEU:HD12	49:RE:146:LEU:HA	1.90	0.41
49:RE:207:LEU:HD11	49:RE:294:LEU:HD12	2.02	0.41
49:RE:227:LYS:O	49:RE:231:TYR:HB2	2.21	0.41
49:RE:950:ILE:HA	49:RE:951:PRO:HD3	1.93	0.41
51:RG:71:ASP:OD2	51:RH:136:ARG:NE	2.49	0.41
52:RJ:930:LYS:HE3	52:RJ:930:LYS:HB2	1.87	0.41
55:RO:224:ASN:HD22	55:RO:280:ILE:HG21	1.86	0.41
58:RS:242:TRP:HA	58:RS:245:VAL:HB	2.02	0.41
58:RS:254:TRP:CD1	58:RS:286:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:R5:248:VAL:H	64:R1:201:VAL:HB	1.85	0.41
65:R3:97:GLU:HA	65:R3:209:TRP:CD1	2.55	0.41
72:R4:555:HIS:CD2	72:R4:557:LYS:HG3	2.55	0.41
72:R4:826:TYR:HA	72:R4:829:PHE:CD2	2.55	0.41
75:M4:87:GLN:HB3	75:M4:119:VAL:HB	2.01	0.41
75:M4:513:ALA:O	75:M4:545:GLY:N	2.39	0.41
75:M4:747:ARG:NH1	75:M4:753:GLU:OE1	2.51	0.41
3:SA:891:A:H2'	3:SA:892:A:C8	2.56	0.41
3:SA:1485:C:N3	3:SA:1592:A:H1'	2.36	0.41
3:SA:1745:G:O2'	3:SA:1746:A:O4'	2.39	0.41
9:SJ:184:LEU:HD22	9:SJ:192:TYR:HD2	1.86	0.41
20:3B:247:PRO:HA	20:3B:276:ILE:HD13	2.02	0.41
21:3D:409:GLU:HA	21:3D:412:LEU:HD22	2.03	0.41
22:3E:195:LEU:HA	22:3E:198:ILE:HG12	2.02	0.41
25:A4:44:ALA:HB3	25:A4:71:ARG:HB3	2.03	0.41
26:A5:308:ASN:HB2	26:A5:311:MET:HG2	2.03	0.41
27:A8:475:PHE:HA	27:A8:514:PHE:HZ	1.85	0.41
27:A8:638:LEU:HG	27:A8:642:LEU:HD12	2.03	0.41
28:A9:502:ARG:HG2	30:AF:510:LEU:HD22	2.03	0.41
29:AE:414:LEU:HD23	29:AE:414:LEU:HA	1.88	0.41
30:AF:278:ASP:OD1	30:AF:278:ASP:N	2.53	0.41
31:AG:560:ILE:HD13	31:AG:575:THR:HG22	2.01	0.41
31:AG:678:LEU:HD12	31:AG:678:LEU:HA	1.91	0.41
34:B3:548:LEU:HB3	34:B3:560:TRP:HB2	2.02	0.41
34:B3:597:GLY:O	34:B3:613:LEU:HB2	2.20	0.41
34:B3:678:TRP:HB3	34:B3:697:VAL:HG22	2.01	0.41
36:BE:131:SER:HB3	36:BE:170:LEU:HD21	2.02	0.41
39:5C:220:SER:OG	39:5C:221:THR:N	2.54	0.41
40:5D:18:GLN:OE1	40:5D:19:LEU:N	2.53	0.41
49:RE:565:LYS:HD3	49:RE:690:VAL:HG12	2.02	0.41
52:RJ:860:TYR:HA	52:RJ:883:ALA:HA	2.02	0.41
54:RN:620:SER:HA	54:RN:623:ASP:HB2	2.03	0.41
63:R5:80:SER:N	63:R5:136:ALA:O	2.51	0.41
68:M3:231:LYS:HG2	68:M3:235:ASN:HD21	1.86	0.41
72:R4:258:TYR:OH	72:R4:308:ASN:O	2.26	0.41
75:M4:83:ASP:OD2	75:M4:131:TYR:OH	2.38	0.41
75:M4:581:SER:HB2	75:M4:609:PHE:HD2	1.86	0.41
3:SA:38:C:H2'	3:SA:39:A:C4	2.56	0.41
3:SA:1604:U:H2'	3:SA:1605:G:H8	1.86	0.41
6:SG:15:GLU:HG2	36:BE:499:LYS:HB3	2.03	0.41
11:SM:19:ILE:HG22	11:SM:32:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SO:37:ILE:HG21	12:SO:74:ILE:HD11	2.02	0.41
14:SR:113:ASP:HB2	14:SR:115:THR:HG22	2.01	0.41
17:SZ:16:PRO:HA	17:SZ:19:ALA:HA	2.02	0.41
20:3C:228:GLN:O	20:3C:231:ARG:NE	2.34	0.41
30:AF:75:LYS:HE3	30:AF:75:LYS:HB3	1.93	0.41
32:B1:31:SER:HA	32:B1:32:PRO:HD3	1.91	0.41
32:B1:486:SER:HB3	32:B1:503:PHE:HE2	1.86	0.41
32:B1:539:ILE:HG23	32:B1:553:ILE:HB	2.02	0.41
32:B1:707:ASN:OD1	32:B1:707:ASN:N	2.52	0.41
32:B1:721:VAL:HG23	32:B1:741:MET:HG2	2.02	0.41
32:B1:814:LYS:NZ	36:BE:938:THR:O	2.53	0.41
32:B1:833:LYS:HG3	36:BE:930:MET:HE1	2.02	0.41
33:B2:88:HIS:CE1	33:B2:90:ASP:HB2	2.55	0.41
34:B3:377:LEU:O	34:B3:379:LEU:N	2.54	0.41
36:BE:229:GLU:HA	36:BE:244:ILE:O	2.21	0.41
42:5F:60:LYS:HA	42:5F:60:LYS:HD2	1.89	0.41
42:5F:128:VAL:O	42:5F:132:GLU:HB2	2.20	0.41
47:5K:84:ARG:HG2	56:RP:1850:LEU:HD11	2.03	0.41
49:RE:235:LEU:HA	49:RE:235:LEU:HD23	1.85	0.41
49:RE:1169:ILE:HG13	49:RE:1170:GLY:H	1.85	0.41
52:RJ:248:ARG:HB3	52:RJ:272:TYR:HB2	2.02	0.41
52:RJ:552:LEU:HD23	52:RJ:552:LEU:HA	1.84	0.41
52:RJ:775:GLU:HA	52:RJ:779:ARG:HG2	2.03	0.41
54:RN:652:LYS:HE2	54:RN:652:LYS:HB2	1.87	0.41
54:RN:681:PRO:HA	54:RN:684:ILE:HG22	2.02	0.41
55:RO:254:LYS:HB3	55:RO:290:HIS:CD2	2.56	0.41
56:RP:1979:LEU:HD12	56:RP:2013:LEU:HD11	2.02	0.41
56:RP:2085:LEU:HA	56:RP:2085:LEU:HD12	1.85	0.41
57:RQ:274:LEU:H	57:RQ:274:LEU:HG	1.70	0.41
64:R1:157:TYR:HD2	64:R1:225:ARG:HB2	1.86	0.41
72:R4:198:ASP:O	72:R4:202:ARG:N	2.53	0.41
72:R4:217:SER:N	72:R4:220:GLN:HB3	2.34	0.41
72:R4:586:GLU:HA	72:R4:589:ALA:HB3	2.03	0.41
72:R4:921:VAL:HG12	72:R4:953:PHE:HE1	1.86	0.41
72:R4:930:VAL:HB	72:R4:933:PHE:HB2	2.02	0.41
75:M4:197:TYR:HD2	75:M4:236:VAL:HG13	1.86	0.41
75:M4:777:MET:HA	75:M4:778:PRO:HD3	1.93	0.41
2:5A:6:A:H5'	31:AG:609:ASN:HD21	1.85	0.41
3:SA:560:U:H2'	3:SA:561:G:C8	2.56	0.41
3:SA:639:U:OP1	8:SI:117:THR:N	2.54	0.41
3:SA:810:G:H2'	3:SA:811:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:864:U:H6	3:SA:864:U:H2'	1.74	0.41
3:SA:1718:G:H2'	3:SA:1719:A:C4	2.55	0.41
3:SA:1752:U:H2'	3:SA:1753:A:H8	1.85	0.41
4:SC:19:ARG:HH22	34:B3:359:SER:N	2.18	0.41
4:SC:55:LYS:HA	4:SC:55:LYS:HD2	1.96	0.41
9:SJ:39:GLY:O	9:SJ:59:ARG:HB3	2.21	0.41
9:SJ:164:ARG:HD3	9:SJ:164:ARG:HA	1.88	0.41
10:SK:64:GLU:HG3	10:SK:65:LYS:HG3	2.03	0.41
11:SM:109:VAL:HG21	11:SM:125:VAL:HG11	2.02	0.41
13:SP:110:LEU:HD12	13:SP:110:LEU:HA	1.91	0.41
15:SX:109:GLY:HA2	56:RP:1737:ASN:HD22	1.86	0.41
16:SY:113:ALA:HB3	16:SY:116:ASP:HB2	2.01	0.41
17:SZ:101:GLU:OE1	17:SZ:108:ARG:NH2	2.54	0.41
20:3C:236:MET:HG2	22:3E:121:LYS:HB3	2.02	0.41
23:3F:142:ILE:HD13	23:3F:142:ILE:HA	1.97	0.41
23:3F:342:ARG:HA	23:3F:342:ARG:HD3	1.84	0.41
24:3G:89:ARG:HH22	35:B8:492:ASN:HD21	1.69	0.41
25:A4:281:ALA:HB1	25:A4:300:VAL:HG23	2.03	0.41
25:A4:436:ASP:OD1	25:A4:483:ASN:ND2	2.54	0.41
25:A4:774:LEU:HD11	31:AG:297:ILE:HD12	2.03	0.41
26:A5:306:LEU:HD23	26:A5:310:THR:HA	2.03	0.41
26:A5:436:THR:HG23	55:RO:294:LYS:HE3	2.01	0.41
26:A5:546:ARG:HA	26:A5:549:CYS:HB3	2.03	0.41
28:A9:441:ILE:HG21	28:A9:482:LEU:HG	2.02	0.41
29:AE:472:HIS:HB3	29:AE:497:LEU:HD22	2.03	0.41
29:AE:623:LEU:HD23	29:AE:641:LEU:HD21	2.02	0.41
30:AF:46:SER:OG	30:AF:47:PHE:N	2.53	0.41
30:AF:103:GLY:HA2	30:AF:127:THR:HG22	2.03	0.41
30:AF:234:PHE:CE1	30:AF:248:ARG:HB2	2.55	0.41
30:AF:436:GLU:HA	30:AF:439:LEU:HB2	2.02	0.41
31:AG:90:LYS:HD2	31:AG:144:VAL:H	1.86	0.41
31:AG:426:ARG:HA	31:AG:429:ILE:HB	2.03	0.41
32:B1:480:SER:OG	32:B1:481:PHE:N	2.53	0.41
32:B1:491:ALA:HB2	32:B1:521:LEU:HD12	2.03	0.41
35:B8:231:LYS:O	35:B8:553:SER:OG	2.39	0.41
35:B8:233:LEU:HD23	35:B8:552:PHE:CG	2.56	0.41
35:B8:258:PRO:HB3	35:B8:469:PRO:HG2	2.01	0.41
36:BE:396:LYS:HE2	36:BE:396:LYS:HB3	1.83	0.41
36:BE:918:LYS:HE2	36:BE:918:LYS:HB2	1.87	0.41
36:BE:923:ASP:HA	36:BE:926:VAL:HG12	2.03	0.41
37:B6:128:LYS:HB2	37:B6:128:LYS:HE2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5E:447:LYS:HA	41:5E:450:VAL:HG12	2.03	0.41
42:5F:183:SER:O	42:5F:183:SER:OG	2.33	0.41
48:RD:1642:GLU:HA	48:RD:1645:VAL:HG22	2.02	0.41
48:RD:1674:LEU:O	48:RD:1678:ILE:HG13	2.21	0.41
49:RE:387:GLY:HA3	49:RE:480:MET:HB3	2.03	0.41
49:RE:566:ILE:HA	49:RE:569:VAL:HG22	2.03	0.41
49:RE:712:ASN:HA	49:RE:1115:LEU:HD23	2.03	0.41
50:RF:62:SER:HA	50:RF:66:HIS:CE1	2.55	0.41
51:RH:35:ASP:OD1	51:RH:35:ASP:N	2.54	0.41
52:RJ:69:PRO:HD2	52:RJ:274:TYR:CZ	2.56	0.41
52:RJ:824:ILE:HD12	52:RJ:1011:VAL:HG11	2.03	0.41
52:RJ:1151:GLN:HA	52:RJ:1154:LYS:HE3	2.02	0.41
53:RK:307:ASP:O	53:RK:355:LYS:HA	2.20	0.41
53:RK:364:LYS:HB2	53:RK:364:LYS:HE2	1.82	0.41
56:RP:1738:TYR:HE2	56:RP:1741:LYS:HE3	1.86	0.41
56:RP:1941:VAL:HA	56:RP:1944:ILE:HD12	2.03	0.41
57:RQ:277:ARG:HG3	57:RQ:278:ILE:HD12	2.02	0.41
58:RS:379:LYS:HB3	58:RS:427:ARG:NH2	2.36	0.41
59:RT:263:LEU:HA	59:RT:266:VAL:HG12	2.03	0.41
63:R5:29:SER:OG	63:R5:30:PHE:N	2.53	0.41
63:R5:238:THR:HB	63:R5:246:VAL:HB	2.02	0.41
64:R1:104:LEU:HD13	64:R1:143:ILE:HD11	2.03	0.41
64:R1:196:LEU:HD23	64:R1:196:LEU:HA	1.85	0.41
65:R3:150:THR:HB	65:R3:154:LYS:HE3	2.01	0.41
66:R6:120:LEU:HA	66:R6:120:LEU:HD23	1.86	0.41
66:R6:164:ALA:HB3	66:R6:179:LEU:H	1.86	0.41
67:R2:101:LYS:NZ	67:R2:227:ARG:HH11	2.19	0.41
67:R2:146:TYR:O	67:R2:150:ASN:ND2	2.54	0.41
68:M3:203:PHE:HB3	68:M3:207:GLY:HA2	2.02	0.41
71:C4:235:LEU:HD23	71:C4:235:LEU:HA	1.88	0.41
72:R4:99:ILE:HA	72:R4:102:LEU:HD12	2.03	0.41
72:R4:323:GLN:HA	72:R4:326:TRP:CG	2.56	0.41
72:R4:652:PHE:HD1	72:R4:656:GLN:HB3	1.86	0.41
75:M4:212:LEU:HA	75:M4:215:GLU:HB3	2.03	0.41
75:M4:341:VAL:HA	75:M4:349:ARG:HB2	2.03	0.41
75:M4:587:TYR:CG	75:M4:917:LEU:HD21	2.55	0.41
75:M4:696:VAL:HB	75:M4:720:ASN:HB2	2.02	0.41
75:M4:793:SER:HA	75:M4:796:GLU:HB2	2.02	0.41
1:3A:43:C:H2'	1:3A:44:U:H6	1.86	0.41
1:3A:107:C:HO2'	1:3A:108:A:P	2.44	0.41
3:SA:775:G:H1	3:SA:785:U:H2'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1146:G:H2'	3:SA:1147:A:H8	1.86	0.41
4:SC:87:ARG:HH21	4:SC:101:HIS:HD2	1.69	0.41
4:SC:126:THR:HA	4:SC:135:LEU:O	2.21	0.41
5:SF:86:PHE:CE2	5:SF:87:MET:HG2	2.56	0.41
6:SG:83:ARG:HH12	32:B1:546:ASP:HA	1.85	0.41
7:SH:147:LEU:HG	7:SH:153:VAL:HG12	2.03	0.41
8:SI:175:LYS:HB2	8:SI:175:LYS:HE2	1.86	0.41
22:3E:193:PRO:HG2	22:3E:243:MET:HG3	2.03	0.41
25:A4:196:LYS:HG2	25:A4:197:LYS:HG3	2.03	0.41
25:A4:358:ILE:HB	25:A4:370:ARG:HB3	2.03	0.41
25:A4:421:THR:H	26:A5:581:ASN:HA	1.85	0.41
27:A8:312:ASP:HA	27:A8:324:GLN:HA	2.03	0.41
27:A8:333:LEU:O	27:A8:345:LEU:HA	2.21	0.41
27:A8:650:LEU:HD13	27:A8:655:LEU:HD21	2.03	0.41
29:AE:193:THR:HG22	29:AE:241:ILE:HD13	2.03	0.41
30:AF:402:ASP:OD1	30:AF:434:ARG:NH2	2.43	0.41
30:AF:426:LYS:NZ	31:AG:486:PHE:O	2.43	0.41
31:AG:367:SER:O	31:AG:367:SER:OG	2.38	0.41
33:B2:181:SER:OG	33:B2:183:ASP:O	2.39	0.41
33:B2:550:LEU:HD13	33:B2:554:THR:HG23	2.03	0.41
34:B3:117:LEU:HB2	34:B3:131:ILE:HD11	2.03	0.41
36:BE:264:LEU:HB2	36:BE:278:LEU:HD11	2.02	0.41
40:5D:202:LYS:HA	40:5D:202:LYS:HD2	1.88	0.41
41:5E:448:LEU:HD11	42:5F:81:LYS:HE3	2.03	0.41
43:5G:192:ASP:HB3	43:5G:225:ALA:HA	2.02	0.41
49:RE:858:ARG:HD2	49:RE:858:ARG:HA	1.94	0.41
51:RG:174:LYS:HA	51:RG:174:LYS:HD2	1.82	0.41
52:RJ:111:LYS:HA	52:RJ:311:PRO:HG2	2.02	0.41
52:RJ:177:PHE:HB3	52:RJ:179:SER:H	1.86	0.41
52:RJ:568:ARG:HA	52:RJ:568:ARG:HD2	1.85	0.41
55:RO:463:LEU:HD21	55:RO:466:LEU:HD13	2.03	0.41
58:RS:441:LEU:HA	58:RS:444:VAL:HG22	2.02	0.41
63:R5:236:THR:HG22	63:R5:247:GLN:HE22	1.86	0.41
64:R1:18:ARG:NH2	72:R4:44:ASP:OD2	2.54	0.41
64:R1:41:TYR:CE2	64:R1:43:GLU:HG3	2.56	0.41
65:R3:97:GLU:HG2	65:R3:209:TRP:HE1	1.86	0.41
65:R3:348:SER:HB2	65:R3:361:THR:HB	2.02	0.41
67:R2:48:SER:HB3	67:R2:148:ALA:HB2	2.02	0.41
75:M4:411:VAL:HA	75:M4:517:VAL:HB	2.03	0.41
75:M4:475:HIS:CE1	75:M4:505:PHE:HB2	2.56	0.41
75:M4:778:PRO:HB3	75:M4:786:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:M4:889:LEU:O	75:M4:893:GLY:N	2.54	0.41
1:3A:1:G:N2	3:SA:1125:A:O3'	2.53	0.40
1:3A:278:U:H3	1:3A:289:A:H61	1.69	0.40
3:SA:1123:C:H2'	3:SA:1124:A:C8	2.56	0.40
3:SA:1584:G:O2'	3:SA:1610:G:O6	2.34	0.40
3:SA:1591:C:H2'	3:SA:1592:A:C8	2.56	0.40
8:SI:58:LEU:HD11	8:SI:85:PHE:HE2	1.86	0.40
8:SI:131:PHE:CD2	8:SI:133:THR:HG23	2.56	0.40
8:SI:162:ILE:HD13	8:SI:162:ILE:HA	1.88	0.40
15:SX:20:THR:OG1	15:SX:22:LYS:NZ	2.52	0.40
20:3B:193:VAL:HA	20:3B:216:ASN:O	2.21	0.40
22:3E:173:LEU:O	22:3E:177:LEU:HB2	2.21	0.40
23:3F:168:ASN:O	23:3F:170:TYR:N	2.54	0.40
24:3G:50:GLU:OE2	24:3G:118:LYS:NZ	2.41	0.40
25:A4:71:ARG:HB2	25:A4:75:ASN:OD1	2.21	0.40
28:A9:477:LYS:HA	28:A9:480:LYS:HB3	2.04	0.40
29:AE:477:ASN:HB2	29:AE:516:PHE:HE1	1.85	0.40
31:AG:666:ASN:OD1	31:AG:666:ASN:N	2.52	0.40
31:AG:780:GLU:O	31:AG:782:THR:N	2.54	0.40
32:B1:269:HIS:NE2	32:B1:312:GLN:O	2.37	0.40
32:B1:387:THR:OG1	32:B1:408:ASP:OD1	2.34	0.40
32:B1:418:ARG:NH2	41:5E:490:LEU:O	2.54	0.40
35:B8:226:LYS:HA	35:B8:226:LYS:HD2	1.83	0.40
35:B8:244:SER:OG	35:B8:245:HIS:N	2.54	0.40
35:B8:439:LYS:HB3	35:B8:439:LYS:HE2	1.75	0.40
36:BE:273:LEU:HD12	36:BE:273:LEU:HA	1.93	0.40
36:BE:285:HIS:ND1	36:BE:286:VAL:O	2.54	0.40
36:BE:464:LYS:HD2	36:BE:504:ALA:HB1	2.03	0.40
36:BE:533:LYS:HE2	36:BE:533:LYS:HB2	1.93	0.40
43:5G:149:PRO:HG2	43:5G:170:VAL:HG11	2.04	0.40
45:5I:449:LYS:HD3	45:5I:449:LYS:HA	1.82	0.40
49:RE:390:THR:O	49:RE:394:THR:HG23	2.21	0.40
49:RE:435:CYS:HB2	49:RE:485:TYR:CD2	2.56	0.40
54:RN:691:LEU:HD12	54:RN:691:LEU:HA	1.93	0.40
55:RO:259:LYS:HD2	55:RO:259:LYS:HA	1.80	0.40
55:RO:271:LEU:HD11	55:RO:312:ALA:HB2	2.02	0.40
56:RP:1872:ALA:HB3	56:RP:1910:VAL:HG21	2.02	0.40
56:RP:2052:GLN:HB3	56:RP:2057:LEU:HD12	2.02	0.40
56:RP:2070:TYR:HB3	56:RP:2076:ARG:HG3	2.03	0.40
68:M3:189:ASP:OD1	68:M3:190:MET:N	2.55	0.40
69:R0:11:PHE:HA	69:R0:12:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:R4:783:SER:HA	72:R4:786:LEU:HB3	2.03	0.40
72:R4:857:GLN:HG2	72:R4:867:LEU:HD11	2.02	0.40
2:5A:88:U:H3	35:B8:344:ARG:CZ	2.34	0.40
3:SA:78:A:H1'	7:SH:175:ILE:HG12	2.03	0.40
3:SA:809:A:C6	3:SA:810:G:H1'	2.57	0.40
3:SA:1143:A:H2'	3:SA:1144:U:O4'	2.21	0.40
9:SJ:184:LEU:HD13	9:SJ:189:LEU:HA	2.03	0.40
9:SJ:196:LEU:HD23	9:SJ:199:LYS:HZ1	1.86	0.40
10:SK:17:ARG:HA	10:SK:17:ARG:HD2	1.88	0.40
10:SK:37:LYS:HE3	10:SK:37:LYS:HB2	1.76	0.40
22:3E:177:LEU:HD21	22:3E:265:PHE:HB3	2.04	0.40
23:3F:142:ILE:HG21	23:3F:512:GLY:HA3	2.03	0.40
25:A4:66:ARG:HH12	25:A4:82:ARG:HH12	1.68	0.40
25:A4:193:LEU:HA	25:A4:202:ILE:O	2.21	0.40
25:A4:247:LEU:HD12	25:A4:292:ASN:HB3	2.03	0.40
25:A4:640:ILE:HG21	25:A4:749:SER:HA	2.03	0.40
29:AE:227:ASN:HB3	29:AE:230:LYS:HB3	2.03	0.40
29:AE:723:LEU:HD23	29:AE:723:LEU:HA	1.97	0.40
30:AF:198:THR:HG23	30:AF:199:ARG:HD3	2.04	0.40
31:AG:23:ASN:HB2	31:AG:32:LYS:HA	2.03	0.40
31:AG:693:ASP:OD1	31:AG:693:ASP:N	2.53	0.40
33:B2:145:ILE:O	33:B2:159:LEU:HB3	2.21	0.40
33:B2:268:LYS:HD3	33:B2:268:LYS:HA	1.94	0.40
33:B2:283:THR:OG1	33:B2:330:GLN:O	2.39	0.40
33:B2:538:ARG:HG2	33:B2:581:ILE:HD12	2.03	0.40
34:B3:350:LEU:HD12	34:B3:350:LEU:HA	1.84	0.40
34:B3:402:TRP:HA	34:B3:415:TRP:O	2.20	0.40
34:B3:432:GLY:O	34:B3:433:HIS:ND1	2.54	0.40
35:B8:545:HIS:HB2	35:B8:552:PHE:CZ	2.56	0.40
36:BE:230:VAL:O	36:BE:243:THR:HA	2.21	0.40
36:BE:482:GLY:HA2	36:BE:505:VAL:HG23	2.03	0.40
36:BE:846:ASP:HA	36:BE:849:ILE:HG22	2.03	0.40
39:5C:257:SER:OG	39:5C:259:TRP:NE1	2.33	0.40
44:5H:571:LYS:O	44:5H:575:LYS:N	2.55	0.40
45:5I:429:ILE:HA	45:5I:432:ILE:HG12	2.03	0.40
49:RE:273:SER:O	49:RE:284:ASN:ND2	2.45	0.40
49:RE:476:ILE:H	49:RE:476:ILE:HG13	1.57	0.40
49:RE:779:PHE:HB3	49:RE:851:LYS:HG3	2.03	0.40
56:RP:2026:ILE:O	56:RP:2030:ASN:HB2	2.20	0.40
58:RS:452:ILE:HG12	58:RS:457:ARG:HH22	1.86	0.40
63:R5:164:LYS:N	63:R5:185:VAL:O	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:R6:206:VAL:HA	66:R6:209:ILE:HD12	2.03	0.40
71:C4:259:ALA:N	71:C4:265:GLY:O	2.48	0.40
72:R4:310:ALA:HA	72:R4:398:ARG:HH12	1.87	0.40
75:M4:480:LEU:HD23	75:M4:480:LEU:HA	1.86	0.40
3:SA:646:C:H2'	3:SA:647:G:C8	2.57	0.40
3:SA:1151:A:H2'	3:SA:1152:A:H8	1.85	0.40
20:3B:231:ARG:NE	21:3D:10:GLU:OE2	2.33	0.40
20:3C:112:ALA:HA	20:3C:113:PRO:HD3	1.93	0.40
20:3C:212:LYS:HE2	20:3C:212:LYS:HB2	1.85	0.40
21:3D:397:SER:OG	21:3D:398:ASN:N	2.54	0.40
22:3E:419:VAL:HG21	36:BE:323:VAL:HG21	2.03	0.40
25:A4:464:LYS:HB3	25:A4:464:LYS:HE2	1.82	0.40
30:AF:146:ASP:OD1	30:AF:146:ASP:N	2.39	0.40
30:AF:424:ARG:HA	31:AG:477:VAL:HG21	2.03	0.40
32:B1:176:ASP:OD1	32:B1:176:ASP:N	2.53	0.40
32:B1:221:THR:OG1	32:B1:222:LYS:N	2.52	0.40
32:B1:317:LEU:O	32:B1:329:VAL:HA	2.21	0.40
33:B2:884:LYS:HE3	33:B2:884:LYS:HB3	1.83	0.40
35:B8:245:HIS:O	35:B8:275:TYR:OH	2.38	0.40
35:B8:345:LEU:HD23	35:B8:345:LEU:HA	1.88	0.40
39:5C:104:LEU:HD21	39:5C:139:TRP:HB2	2.03	0.40
39:5C:116:ILE:HG23	39:5C:125:LEU:HD11	2.03	0.40
39:5C:259:TRP:CE2	39:5C:266:PRO:HB3	2.56	0.40
44:5H:544:ILE:O	52:RJ:193:ARG:NH1	2.33	0.40
49:RE:143:GLU:HB2	49:RE:177:ASN:ND2	2.36	0.40
49:RE:326:LEU:HD23	49:RE:326:LEU:HA	1.92	0.40
51:RG:123:GLU:HB3	51:RG:161:LYS:HB2	2.03	0.40
51:RG:211:ARG:HD2	51:RG:211:ARG:HA	1.83	0.40
51:RH:240:LYS:O	51:RH:243:HIS:ND1	2.54	0.40
56:RP:177:LEU:HA	56:RP:177:LEU:HD23	1.90	0.40
56:RP:2016:LEU:HA	56:RP:2019:ILE:HB	2.02	0.40
58:RS:376:LEU:HD13	58:RS:424:PHE:HB3	2.03	0.40
72:R4:212:ASN:OD1	72:R4:212:ASN:N	2.52	0.40
72:R4:539:ILE:HB	72:R4:648:SER:HA	2.03	0.40
75:M4:137:HIS:NE2	75:M4:162:ASP:OD2	2.37	0.40
75:M4:939:LEU:HD12	75:M4:939:LEU:HA	1.84	0.40
2:5A:14:U:H5''	2:5A:15:G:H5''	2.02	0.40
3:SA:1682:U:O2'	3:SA:1683:C:O4'	2.31	0.40
3:SA:1756:A:C8	41:5E:536:ARG:HD3	2.56	0.40
4:SC:242:LYS:HG3	4:SC:244:VAL:HG12	2.03	0.40
6:SG:130:ILE:H	6:SG:130:ILE:HG12	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SH:48:TYR:CZ	7:SH:119:GLN:HB3	2.57	0.40
17:SZ:27:VAL:HG21	17:SZ:35:VAL:HG21	2.04	0.40
21:3D:178:ILE:HG12	21:3D:314:ARG:HD2	2.03	0.40
24:3G:41:THR:HG21	24:3G:66:HIS:CE1	2.56	0.40
25:A4:34:HIS:ND1	25:A4:404:MET:SD	2.90	0.40
29:AE:699:ARG:HE	29:AE:699:ARG:HB2	1.48	0.40
30:AF:27:TRP:HZ2	30:AF:264:PHE:HZ	1.69	0.40
30:AF:256:THR:OG1	30:AF:257:CYS:N	2.55	0.40
30:AF:375:HIS:CD2	35:B8:339:ILE:HD11	2.56	0.40
30:AF:391:ASN:O	30:AF:396:LYS:N	2.43	0.40
30:AF:474:LEU:HD12	30:AF:474:LEU:HA	1.90	0.40
31:AG:79:LEU:HA	31:AG:79:LEU:HD23	1.89	0.40
31:AG:375:ASN:OD1	31:AG:380:THR:N	2.54	0.40
31:AG:467:GLN:HE22	31:AG:470:TYR:HD2	1.70	0.40
31:AG:678:LEU:N	31:AG:692:PHE:O	2.54	0.40
32:B1:717:LEU:HD12	36:BE:578:VAL:HB	2.02	0.40
33:B2:243:THR:OG1	33:B2:244:GLU:N	2.54	0.40
33:B2:478:SER:HB3	33:B2:537:VAL:H	1.86	0.40
33:B2:585:SER:O	33:B2:585:SER:OG	2.35	0.40
36:BE:717:ASP:OD1	36:BE:717:ASP:N	2.54	0.40
39:5C:44:ALA:HA	39:5C:47:LYS:HG2	2.04	0.40
40:5D:233:ILE:HG21	40:5D:243:LYS:HE3	2.02	0.40
42:5F:65:PRO:HA	42:5F:66:PRO:HD3	1.94	0.40
42:5F:181:ASP:OD1	42:5F:181:ASP:N	2.54	0.40
44:5H:550:LEU:HD12	44:5H:550:LEU:HA	1.95	0.40
45:5I:139:CYS:SG	45:5I:185:ILE:HG12	2.61	0.40
46:5J:111:ASP:OD1	46:5J:111:ASP:N	2.42	0.40
49:RE:941:PRO:HG3	49:RE:961:VAL:HG22	2.03	0.40
49:RE:1101:ASP:OD2	49:RE:1233:ASN:ND2	2.54	0.40
50:RF:94:GLY:HA3	50:RF:121:ARG:HH12	1.87	0.40
51:RH:146:HIS:HB3	54:RN:723:PRO:HG3	2.03	0.40
54:RN:513:GLN:HB2	55:RO:475:PRO:HG3	2.04	0.40
55:RO:359:PHE:HA	55:RO:362:MET:HB2	2.04	0.40
57:RQ:880:LYS:HD3	57:RQ:884:MET:HE1	2.03	0.40
63:R5:5:ILE:HD11	63:R5:90:GLN:HE21	1.85	0.40
65:R3:22:LEU:HG	65:R3:30:SER:HB2	2.02	0.40
72:R4:194:LEU:HA	72:R4:194:LEU:HD23	4.47	0.40
75:M4:437:LYS:HE2	75:M4:469:ARG:NH2	2.36	0.40
75:M4:480:LEU:HB2	75:M4:483:LEU:HG	2.04	0.40
3:SA:246:G:H2'	3:SA:247:A:C8	2.56	0.40
3:SA:1211:A:N6	3:SA:1452:U:O4	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1695:G:H2'	3:SA:1696:G:C8	2.57	0.40
4:SC:87:ARG:HD3	4:SC:101:HIS:CD2	2.57	0.40
6:SG:26:ALA:HB3	14:SR:28:LEU:HB3	2.03	0.40
13:SP:47:LYS:HA	13:SP:47:LYS:HD3	1.81	0.40
17:SZ:36:SER:O	17:SZ:39:GLU:N	2.55	0.40
22:3E:302:HIS:ND1	22:3E:320:LEU:O	2.54	0.40
26:A5:191:VAL:HA	26:A5:206:ALA:HA	2.03	0.40
28:A9:505:MET:HG2	28:A9:508:ARG:NH1	2.37	0.40
29:AE:115:LEU:HD12	29:AE:115:LEU:HA	1.86	0.40
30:AF:235:LYS:HG3	30:AF:247:GLU:HG2	2.03	0.40
32:B1:88:ASN:ND2	36:BE:659:GLN:HG2	2.36	0.40
32:B1:429:GLU:HG2	32:B1:431:ILE:HG23	2.02	0.40
32:B1:770:ILE:HA	32:B1:771:PRO:HD3	1.98	0.40
33:B2:88:HIS:NE2	33:B2:132:THR:OG1	2.42	0.40
33:B2:617:SER:OG	33:B2:618:ILE:O	2.38	0.40
34:B3:340:ILE:H	34:B3:340:ILE:HG13	1.46	0.40
43:5G:285:ASN:OD1	43:5G:285:ASN:N	2.50	0.40
46:5J:180:ASP:O	46:5J:183:SER:OG	2.37	0.40
49:RE:501:ASN:HD21	49:RE:506:GLN:HE22	1.69	0.40
52:RJ:841:THR:HB	52:RJ:859:ILE:HD12	2.04	0.40
53:RK:198:THR:OG1	53:RK:235:SER:O	2.40	0.40
53:RK:357:ILE:H	53:RK:357:ILE:HG12	1.70	0.40
63:R5:243:ARG:HA	63:R5:269:TYR:HE1	1.86	0.40
67:R2:154:LEU:HA	67:R2:154:LEU:HD23	1.94	0.40
72:R4:314:ASP:OD1	72:R4:399:SER:OG	2.31	0.40
72:R4:591:GLY:HA3	72:R4:887:LYS:HG3	2.04	0.40
75:M4:105:LEU:HD11	75:M4:344:GLU:HB2	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	SC	230/255 (90%)	190 (83%)	39 (17%)	1 (0%)	34	70
5	SF	248/261 (95%)	211 (85%)	37 (15%)	0	100	100
6	SG	211/225 (94%)	194 (92%)	17 (8%)	0	100	100
7	SH	178/236 (75%)	158 (89%)	17 (10%)	3 (2%)	9	43
8	SI	160/190 (84%)	136 (85%)	24 (15%)	0	100	100
9	SJ	136/200 (68%)	113 (83%)	23 (17%)	0	100	100
10	SK	169/197 (86%)	155 (92%)	14 (8%)	0	100	100
11	SM	135/156 (86%)	119 (88%)	16 (12%)	0	100	100
12	SO	132/151 (87%)	119 (90%)	13 (10%)	0	100	100
13	SP	116/137 (85%)	103 (89%)	13 (11%)	0	100	100
14	SR	123/143 (86%)	110 (89%)	13 (11%)	0	100	100
15	SX	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
16	SY	104/145 (72%)	91 (88%)	13 (12%)	0	100	100
17	SZ	121/135 (90%)	104 (86%)	17 (14%)	0	100	100
18	Sc	78/82 (95%)	66 (85%)	12 (15%)	0	100	100
19	Sd	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
20	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
20	3C	221/327 (68%)	204 (92%)	17 (8%)	0	100	100
21	3D	372/504 (74%)	343 (92%)	29 (8%)	0	100	100
22	3E	428/511 (84%)	389 (91%)	39 (9%)	0	100	100
23	3F	431/573 (75%)	365 (85%)	65 (15%)	1 (0%)	47	79
24	3G	119/126 (94%)	109 (92%)	10 (8%)	0	100	100
24	3H	119/126 (94%)	112 (94%)	6 (5%)	1 (1%)	19	57
25	A4	650/776 (84%)	583 (90%)	67 (10%)	0	100	100
26	A5	501/643 (78%)	453 (90%)	48 (10%)	0	100	100
27	A8	534/713 (75%)	423 (79%)	109 (20%)	2 (0%)	34	70
28	A9	126/575 (22%)	114 (90%)	12 (10%)	0	100	100
29	AE	1496/1769 (85%)	1372 (92%)	124 (8%)	0	100	100
30	AF	473/513 (92%)	427 (90%)	46 (10%)	0	100	100
31	AG	812/896 (91%)	694 (86%)	118 (14%)	0	100	100
32	B1	800/900 (89%)	720 (90%)	80 (10%)	0	100	100
33	B2	813/943 (86%)	731 (90%)	82 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	B3	733/817 (90%)	608 (83%)	123 (17%)	2 (0%)	41	74
35	B8	469/594 (79%)	423 (90%)	45 (10%)	1 (0%)	47	79
36	BE	817/939 (87%)	746 (91%)	71 (9%)	0	100	100
37	B6	368/440 (84%)	343 (93%)	25 (7%)	0	100	100
38	5B	58/214 (27%)	52 (90%)	6 (10%)	0	100	100
39	5C	452/554 (82%)	400 (88%)	52 (12%)	0	100	100
40	5D	198/250 (79%)	172 (87%)	25 (13%)	1 (0%)	29	66
41	5E	187/593 (32%)	173 (92%)	14 (8%)	0	100	100
42	5F	180/183 (98%)	165 (92%)	15 (8%)	0	100	100
43	5G	214/290 (74%)	196 (92%)	18 (8%)	0	100	100
44	5H	72/610 (12%)	63 (88%)	9 (12%)	0	100	100
45	5I	456/489 (93%)	422 (92%)	33 (7%)	1 (0%)	47	79
46	5J	130/217 (60%)	121 (93%)	9 (7%)	0	100	100
47	5K	162/189 (86%)	149 (92%)	13 (8%)	0	100	100
48	RD	310/1729 (18%)	278 (90%)	32 (10%)	0	100	100
49	RE	1080/1237 (87%)	996 (92%)	84 (8%)	0	100	100
50	RF	233/297 (78%)	203 (87%)	30 (13%)	0	100	100
51	RG	212/252 (84%)	193 (91%)	19 (9%)	0	100	100
51	RH	226/252 (90%)	208 (92%)	18 (8%)	0	100	100
52	RJ	719/1183 (61%)	649 (90%)	69 (10%)	1 (0%)	51	83
53	RK	358/367 (98%)	335 (94%)	23 (6%)	0	100	100
54	RN	539/810 (66%)	482 (89%)	57 (11%)	0	100	100
55	RO	523/552 (95%)	473 (90%)	49 (9%)	1 (0%)	47	79
56	RP	2112/2493 (85%)	1903 (90%)	203 (10%)	6 (0%)	41	74
57	RQ	220/899 (24%)	197 (90%)	23 (10%)	0	100	100
58	RS	247/480 (52%)	218 (88%)	29 (12%)	0	100	100
59	RT	165/326 (51%)	152 (92%)	13 (8%)	0	100	100
60	RW	146/206 (71%)	140 (96%)	6 (4%)	0	100	100
63	R5	297/305 (97%)	276 (93%)	21 (7%)	0	100	100
64	R1	242/246 (98%)	225 (93%)	17 (7%)	0	100	100
65	R3	332/394 (84%)	304 (92%)	27 (8%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	R6	221/223 (99%)	208 (94%)	13 (6%)	0	100	100
67	R2	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
68	M3	209/250 (84%)	190 (91%)	19 (9%)	0	100	100
69	R0	235/240 (98%)	216 (92%)	19 (8%)	0	100	100
70	r4	287/359 (80%)	262 (91%)	25 (9%)	0	100	100
71	C4	214/292 (73%)	198 (92%)	16 (8%)	0	100	100
72	R4	942/1001 (94%)	875 (93%)	67 (7%)	0	100	100
73	r6	98/733 (13%)	91 (93%)	7 (7%)	0	100	100
74	R7	83/184 (45%)	82 (99%)	1 (1%)	0	100	100
75	M4	866/1073 (81%)	806 (93%)	60 (7%)	0	100	100
76	M6	36/186 (19%)	32 (89%)	4 (11%)	0	100	100
All	All	26369/36145 (73%)	23774 (90%)	2573 (10%)	22 (0%)	54	83

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	B8	226	LYS
55	RO	75	PRO
24	3H	6	PRO
27	A8	309	PRO
56	RP	37	ARG
56	RP	1004	VAL
4	SC	213	ARG
7	SH	173	PRO
23	3F	270	PRO
34	B3	71	PRO
34	B3	474	SER
56	RP	77	LEU
56	RP	204	PRO
7	SH	154	ARG
27	A8	308	PHE
40	5D	11	LYS
52	RJ	900	GLN
65	R3	337	GLU
56	RP	76	THR
56	RP	1997	GLY
7	SH	153	VAL
45	5I	34	PRO



### 5.3.2 Protein sidechains [i](#)

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	SC	205/224 (92%)	203 (99%)	2 (1%)	76	86
5	SF	199/222 (90%)	196 (98%)	3 (2%)	65	81
6	SG	180/191 (94%)	179 (99%)	1 (1%)	86	92
7	SH	153/201 (76%)	152 (99%)	1 (1%)	84	91
8	SI	145/170 (85%)	144 (99%)	1 (1%)	84	91
9	SJ	114/161 (71%)	114 (100%)	0	100	100
10	SK	147/166 (89%)	146 (99%)	1 (1%)	84	91
11	SM	124/137 (90%)	122 (98%)	2 (2%)	62	79
12	SO	117/128 (91%)	114 (97%)	3 (3%)	46	69
13	SP	90/105 (86%)	89 (99%)	1 (1%)	73	85
14	SR	105/119 (88%)	104 (99%)	1 (1%)	76	86
15	SX	108/111 (97%)	108 (100%)	0	100	100
16	SY	88/120 (73%)	86 (98%)	2 (2%)	50	72
17	SZ	103/113 (91%)	98 (95%)	5 (5%)	25	55
18	Sc	69/71 (97%)	66 (96%)	3 (4%)	29	58
19	Sd	56/60 (93%)	56 (100%)	0	100	100
20	3B	201/240 (84%)	201 (100%)	0	100	100
20	3C	190/240 (79%)	187 (98%)	3 (2%)	62	79
21	3D	322/435 (74%)	320 (99%)	2 (1%)	86	92
22	3E	265/433 (61%)	263 (99%)	2 (1%)	81	89
23	3F	382/503 (76%)	374 (98%)	8 (2%)	53	74
24	3G	100/104 (96%)	100 (100%)	0	100	100
24	3H	100/104 (96%)	100 (100%)	0	100	100
25	A4	593/713 (83%)	585 (99%)	8 (1%)	69	82
26	A5	431/574 (75%)	428 (99%)	3 (1%)	84	91
27	A8	174/657 (26%)	170 (98%)	4 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	A9	89/533 (17%)	86 (97%)	3 (3%)	37	64
29	AE	708/1633 (43%)	705 (100%)	3 (0%)	91	95
30	AF	424/454 (93%)	420 (99%)	4 (1%)	78	88
31	AG	750/826 (91%)	744 (99%)	6 (1%)	81	89
32	B1	707/789 (90%)	703 (99%)	4 (1%)	86	92
33	B2	712/832 (86%)	701 (98%)	11 (2%)	65	81
34	B3	665/719 (92%)	657 (99%)	8 (1%)	71	84
35	B8	421/529 (80%)	419 (100%)	2 (0%)	88	94
36	BE	721/819 (88%)	713 (99%)	8 (1%)	73	85
37	B6	251/414 (61%)	248 (99%)	3 (1%)	71	84
38	5B	57/196 (29%)	56 (98%)	1 (2%)	59	77
39	5C	394/480 (82%)	390 (99%)	4 (1%)	76	86
40	5D	192/234 (82%)	191 (100%)	1 (0%)	88	94
41	5E	175/535 (33%)	174 (99%)	1 (1%)	86	92
42	5F	171/172 (99%)	171 (100%)	0	100	100
43	5G	191/258 (74%)	191 (100%)	0	100	100
44	5H	63/538 (12%)	63 (100%)	0	100	100
45	5I	415/443 (94%)	408 (98%)	7 (2%)	60	78
46	5J	124/200 (62%)	121 (98%)	3 (2%)	49	71
47	5K	148/169 (88%)	147 (99%)	1 (1%)	84	91
48	RD	226/1544 (15%)	225 (100%)	1 (0%)	91	95
49	RE	994/1125 (88%)	986 (99%)	8 (1%)	81	89
50	RF	221/274 (81%)	216 (98%)	5 (2%)	50	72
51	RG	195/222 (88%)	191 (98%)	4 (2%)	53	74
51	RH	206/222 (93%)	206 (100%)	0	100	100
52	RJ	649/1039 (62%)	644 (99%)	5 (1%)	81	89
53	RK	307/312 (98%)	302 (98%)	5 (2%)	62	79
54	RN	379/732 (52%)	375 (99%)	4 (1%)	73	85
55	RO	329/506 (65%)	327 (99%)	2 (1%)	86	92
56	RP	550/2307 (24%)	545 (99%)	5 (1%)	78	88
57	RQ	149/808 (18%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	RS	225/421 (53%)	219 (97%)	6 (3%)	44	69
59	RT	148/282 (52%)	148 (100%)	0	100	100
63	R5	255/266 (96%)	255 (100%)	0	100	100
64	R1	210/218 (96%)	207 (99%)	3 (1%)	67	81
65	R3	282/349 (81%)	281 (100%)	1 (0%)	91	95
66	R6	195/197 (99%)	195 (100%)	0	100	100
67	R2	236/240 (98%)	236 (100%)	0	100	100
68	M3	181/219 (83%)	180 (99%)	1 (1%)	86	92
69	R0	194/209 (93%)	193 (100%)	1 (0%)	88	94
70	r4	243/311 (78%)	242 (100%)	1 (0%)	91	95
71	C4	174/240 (72%)	172 (99%)	2 (1%)	73	85
72	R4	812/901 (90%)	808 (100%)	4 (0%)	88	94
73	r6	89/671 (13%)	89 (100%)	0	100	100
74	R7	76/168 (45%)	75 (99%)	1 (1%)	69	82
75	M4	729/953 (76%)	725 (100%)	4 (0%)	88	94
76	M6	25/168 (15%)	25 (100%)	0	100	100
All	All	20418/31979 (64%)	20229 (99%)	189 (1%)	79	88

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SC	61	LEU
4	SC	162	ARG
5	SF	78	THR
5	SF	192	ILE
5	SF	211	LYS
6	SG	157	ARG
7	SH	51	LYS
8	SI	66	SER
10	SK	128	LEU
11	SM	46	LYS
11	SM	67	ARG
12	SO	54	LEU
12	SO	91	LEU
12	SO	130	ARG
13	SP	127	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	SR	123	ARG
16	SY	93	LEU
16	SY	121	ARG
17	SZ	35	VAL
17	SZ	49	LYS
17	SZ	109	LYS
17	SZ	112	LYS
17	SZ	123	LYS
18	Sc	65	THR
18	Sc	67	THR
18	Sc	77	THR
20	3C	100	ARG
20	3C	144	TRP
20	3C	306	LEU
21	3D	285	ARG
21	3D	412	LEU
22	3E	370	SER
22	3E	380	ARG
23	3F	197	THR
23	3F	242	VAL
23	3F	262	VAL
23	3F	396	PHE
23	3F	397	PHE
23	3F	405	VAL
23	3F	425	TRP
23	3F	524	ILE
25	A4	30	ARG
25	A4	121	THR
25	A4	429	SER
25	A4	459	LYS
25	A4	472	ARG
25	A4	485	LYS
25	A4	558	ARG
25	A4	565	ARG
26	A5	167	SER
26	A5	240	GLN
26	A5	494	ARG
27	A8	505	LYS
27	A8	549	ARG
27	A8	576	ARG
27	A8	664	LYS
28	A9	476	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	A9	502	ARG
28	A9	508	ARG
29	AE	87	THR
29	AE	321	LYS
29	AE	597	HIS
30	AF	199	ARG
30	AF	255	VAL
30	AF	446	CYS
30	AF	490	LYS
31	AG	336	ARG
31	AG	421	LYS
31	AG	528	ILE
31	AG	629	LYS
31	AG	740	LYS
31	AG	893	LYS
32	B1	117	ARG
32	B1	119	LEU
32	B1	517	ASP
32	B1	582	THR
33	B2	17	ILE
33	B2	75	ARG
33	B2	213	LYS
33	B2	301	LYS
33	B2	343	TRP
33	B2	450	ARG
33	B2	487	ARG
33	B2	503	LYS
33	B2	569	LEU
33	B2	576	VAL
33	B2	811	ARG
34	B3	280	ARG
34	B3	344	ARG
34	B3	346	VAL
34	B3	438	THR
34	B3	465	LYS
34	B3	534	ARG
34	B3	555	LYS
34	B3	698	LEU
35	B8	406	ASP
35	B8	534	SER
36	BE	98	VAL
36	BE	177	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	BE	500	LEU
36	BE	576	ARG
36	BE	661	LYS
36	BE	747	LYS
36	BE	888	LEU
36	BE	923	ASP
37	B6	18	LEU
37	B6	133	TYR
37	B6	196	LEU
38	5B	160	ARG
39	5C	228	LEU
39	5C	291	THR
39	5C	443	THR
39	5C	455	ARG
40	5D	165	ARG
41	5E	451	LEU
45	5I	100	ARG
45	5I	186	ASP
45	5I	204	TRP
45	5I	238	THR
45	5I	255	THR
45	5I	356	TYR
45	5I	464	THR
46	5J	69	PHE
46	5J	115	ARG
46	5J	156	LYS
47	5K	124	ARG
48	RD	1466	ARG
49	RE	223	ARG
49	RE	227	LYS
49	RE	245	LYS
49	RE	316	ARG
49	RE	351	LYS
49	RE	474	VAL
49	RE	477	LEU
49	RE	626	LYS
50	RF	19	LYS
50	RF	69	LYS
50	RF	176	ASP
50	RF	263	ARG
50	RF	266	LYS
51	RG	40	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	RG	72	ASP
51	RG	116	THR
51	RG	136	ARG
52	RJ	113	ARG
52	RJ	188	LYS
52	RJ	214	ARG
52	RJ	290	ILE
52	RJ	973	ARG
53	RK	8	TYR
53	RK	77	ARG
53	RK	207	ARG
53	RK	214	LYS
53	RK	246	VAL
54	RN	431	ARG
54	RN	450	ARG
54	RN	468	ARG
54	RN	690	LYS
55	RO	150	LYS
55	RO	355	ARG
56	RP	26	LEU
56	RP	37	ARG
56	RP	1716	MET
56	RP	1882	ARG
56	RP	1963	LEU
58	RS	210	VAL
58	RS	258	VAL
58	RS	312	TYR
58	RS	319	LYS
58	RS	427	ARG
58	RS	450	LYS
64	R1	77	ASN
64	R1	86	ARG
64	R1	225	ARG
65	R3	73	ASN
68	M3	55	ASN
69	R0	3	THR
70	r4	212	ASN
71	C4	51	ARG
71	C4	130	ASN
72	R4	29	ASN
72	R4	144	ARG
72	R4	169	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
72	R4	775	ASN
74	R7	64	ASN
75	M4	470	ARG
75	M4	530	ARG
75	M4	543	ARG
75	M4	614	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (286) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	SC	101	HIS
4	SC	199	ASN
5	SF	69	HIS
5	SF	157	ASN
6	SG	104	ASN
6	SG	131	GLN
7	SH	4	ASN
8	SI	11	GLN
8	SI	147	ASN
9	SJ	103	GLN
10	SK	123	HIS
10	SK	131	GLN
11	SM	81	HIS
12	SO	58	HIS
13	SP	29	HIS
14	SR	100	GLN
17	SZ	29	HIS
17	SZ	31	ASN
17	SZ	34	ASN
17	SZ	113	ASN
18	Sc	9	HIS
19	Sd	27	GLN
19	Sd	51	ASN
20	3B	228	GLN
20	3C	228	GLN
21	3D	39	ASN
21	3D	65	ASN
21	3D	85	ASN
21	3D	125	GLN
21	3D	151	GLN
21	3D	213	ASN
22	3E	261	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	3E	286	ASN
22	3E	396	ASN
23	3F	156	ASN
23	3F	230	ASN
23	3F	322	HIS
23	3F	561	ASN
24	3G	5	ASN
24	3H	5	ASN
24	3H	18	GLN
24	3H	26	GLN
25	A4	53	HIS
25	A4	274	GLN
25	A4	315	GLN
25	A4	317	ASN
25	A4	340	GLN
25	A4	589	ASN
25	A4	632	ASN
25	A4	642	ASN
25	A4	766	GLN
26	A5	7	GLN
26	A5	302	ASN
26	A5	308	ASN
26	A5	316	ASN
26	A5	495	GLN
26	A5	509	HIS
26	A5	552	ASN
27	A8	504	ASN
27	A8	539	ASN
27	A8	597	GLN
28	A9	509	GLN
29	AE	7	GLN
29	AE	10	GLN
29	AE	96	ASN
29	AE	208	ASN
29	AE	219	ASN
29	AE	258	HIS
29	AE	477	ASN
29	AE	545	ASN
29	AE	675	ASN
29	AE	773	GLN
29	AE	808	GLN
30	AF	161	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	AF	263	ASN
30	AF	289	ASN
30	AF	394	GLN
30	AF	472	ASN
31	AG	50	ASN
31	AG	166	ASN
31	AG	236	ASN
31	AG	331	GLN
31	AG	370	GLN
31	AG	467	GLN
31	AG	489	ASN
31	AG	549	ASN
31	AG	569	ASN
31	AG	690	ASN
32	B1	88	ASN
32	B1	92	HIS
32	B1	120	GLN
32	B1	296	GLN
32	B1	394	GLN
32	B1	400	GLN
32	B1	837	ASN
32	B1	842	ASN
33	B2	10	GLN
33	B2	195	GLN
33	B2	383	HIS
33	B2	455	GLN
33	B2	677	HIS
33	B2	798	ASN
33	B2	856	ASN
33	B2	881	ASN
33	B2	913	ASN
33	B2	916	HIS
34	B3	81	GLN
34	B3	337	HIS
34	B3	444	ASN
34	B3	579	GLN
34	B3	589	GLN
34	B3	665	GLN
34	B3	671	ASN
34	B3	749	ASN
34	B3	757	GLN
34	B3	767	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	B8	162	ASN
35	B8	167	GLN
35	B8	296	GLN
35	B8	308	ASN
35	B8	311	ASN
35	B8	348	HIS
35	B8	362	HIS
35	B8	385	ASN
35	B8	440	ASN
35	B8	450	GLN
35	B8	513	GLN
35	B8	545	HIS
35	B8	581	ASN
36	BE	67	HIS
36	BE	263	HIS
36	BE	421	ASN
36	BE	429	ASN
36	BE	473	ASN
36	BE	490	GLN
36	BE	586	ASN
36	BE	826	GLN
36	BE	916	HIS
37	B6	10	GLN
37	B6	41	HIS
37	B6	115	ASN
37	B6	166	ASN
37	B6	287	ASN
38	5B	207	ASN
38	5B	212	ASN
39	5C	36	GLN
39	5C	78	ASN
39	5C	88	GLN
39	5C	151	ASN
39	5C	170	GLN
39	5C	321	ASN
39	5C	337	HIS
39	5C	394	HIS
39	5C	424	GLN
39	5C	435	ASN
40	5D	45	GLN
41	5E	316	ASN
41	5E	443	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	5F	39	GLN
42	5F	163	ASN
43	5G	118	ASN
43	5G	145	HIS
43	5G	193	ASN
45	5I	46	ASN
45	5I	96	ASN
45	5I	207	ASN
45	5I	242	ASN
45	5I	276	ASN
45	5I	293	ASN
45	5I	353	GLN
45	5I	371	ASN
45	5I	392	ASN
45	5I	431	ASN
46	5J	126	HIS
46	5J	165	ASN
47	5K	43	ASN
47	5K	148	HIS
47	5K	162	GLN
48	RD	1515	ASN
48	RD	1522	ASN
48	RD	1525	ASN
48	RD	1542	GLN
48	RD	1607	ASN
49	RE	129	HIS
49	RE	261	ASN
49	RE	372	GLN
49	RE	441	GLN
49	RE	500	ASN
49	RE	588	GLN
49	RE	665	HIS
49	RE	743	GLN
49	RE	841	ASN
49	RE	872	ASN
49	RE	1023	ASN
49	RE	1125	ASN
49	RE	1148	GLN
50	RF	66	HIS
50	RF	122	ASN
50	RF	146	ASN
50	RF	187	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	RF	232	ASN
50	RF	268	GLN
51	RG	105	ASN
51	RG	111	GLN
51	RG	115	GLN
51	RG	146	HIS
51	RH	69	ASN
51	RH	105	ASN
51	RH	125	ASN
51	RH	215	ASN
52	RJ	99	ASN
52	RJ	126	ASN
52	RJ	300	GLN
52	RJ	1037	GLN
52	RJ	1049	ASN
53	RK	88	HIS
53	RK	234	ASN
53	RK	317	GLN
54	RN	467	ASN
54	RN	488	ASN
54	RN	489	HIS
54	RN	515	HIS
54	RN	552	GLN
54	RN	554	GLN
54	RN	683	ASN
54	RN	705	HIS
55	RO	273	GLN
55	RO	321	ASN
55	RO	418	ASN
55	RO	472	HIS
56	RP	112	GLN
56	RP	115	HIS
56	RP	134	ASN
56	RP	146	ASN
56	RP	1801	ASN
56	RP	1802	HIS
57	RQ	303	GLN
57	RQ	316	ASN
57	RQ	836	ASN
57	RQ	856	GLN
58	RS	276	GLN
58	RS	449	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	RT	218	ASN
59	RT	262	ASN
64	R1	30	ASN
64	R1	64	GLN
64	R1	77	ASN
65	R3	73	ASN
65	R3	153	GLN
65	R3	239	GLN
65	R3	287	ASN
66	R6	81	HIS
66	R6	216	ASN
67	R2	150	ASN
67	R2	183	ASN
67	R2	219	ASN
68	M3	55	ASN
68	M3	235	ASN
70	r4	212	ASN
71	C4	45	GLN
72	R4	29	ASN
72	R4	170	ASN
72	R4	197	ASN
72	R4	555	HIS
72	R4	775	ASN
72	R4	855	HIS
72	R4	857	GLN
73	r6	83	ASN
73	r6	604	GLN
73	r6	612	ASN
74	R7	64	ASN
74	R7	95	ASN
74	R7	113	ASN
75	M4	191	ASN
75	M4	206	ASN
75	M4	445	ASN
75	M4	475	HIS
75	M4	539	GLN
75	M4	588	ASN
75	M4	614	ASN
75	M4	669	ASN
75	M4	786	GLN
75	M4	874	GLN
75	M4	929	ASN

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Mol	Chain	Res	Type
75	M4	946	GLN
75	M4	1043	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	222/333 (66%)	86 (38%)	3 (1%)
2	5A	144/700 (20%)	62 (43%)	2 (1%)
3	SA	1227/1809 (67%)	466 (37%)	20 (1%)
All	All	1593/2842 (56%)	614 (38%)	25 (1%)

All (614) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	4	G
1	3A	12	U
1	3A	15	U
1	3A	24	U
1	3A	25	U
1	3A	28	A
1	3A	30	A
1	3A	31	G
1	3A	33	A
1	3A	34	A
1	3A	35	U
1	3A	37	G
1	3A	38	U
1	3A	39	C
1	3A	46	U
1	3A	47	G
1	3A	49	C
1	3A	51	C
1	3A	53	U
1	3A	54	C
1	3A	56	A
1	3A	59	G
1	3A	61	G
1	3A	67	G
1	3A	81	U
1	3A	82	G
1	3A	87	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3A	88	U
1	3A	89	C
1	3A	90	C
1	3A	91	C
1	3A	92	A
1	3A	93	U
1	3A	94	A
1	3A	95	A
1	3A	101	G
1	3A	103	A
1	3A	104	C
1	3A	105	C
1	3A	107	C
1	3A	108	A
1	3A	109	G
1	3A	110	A
1	3A	111	G
1	3A	114	A
1	3A	115	G
1	3A	116	A
1	3A	138	A
1	3A	142	U
1	3A	147	C
1	3A	151	A
1	3A	165	G
1	3A	173	A
1	3A	174	U
1	3A	175	A
1	3A	198	U
1	3A	199	G
1	3A	203	U
1	3A	204	U
1	3A	205	G
1	3A	206	C
1	3A	207	A
1	3A	243	U
1	3A	247	U
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	255	U
1	3A	256	G

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3A	261	U
1	3A	262	G
1	3A	263	A
1	3A	265	C
1	3A	266	C
1	3A	267	A
1	3A	268	U
1	3A	270	C
1	3A	290	G
1	3A	311	G
1	3A	313	A
1	3A	314	C
1	3A	315	A
1	3A	320	G
1	3A	324	U
1	3A	325	C
1	3A	329	C
2	5A	4	C
2	5A	6	A
2	5A	7	A
2	5A	8	A
2	5A	9	G
2	5A	10	C
2	5A	11	A
2	5A	12	G
2	5A	14	U
2	5A	15	G
2	5A	59	U
2	5A	63	G
2	5A	64	U
2	5A	83	U
2	5A	86	C
2	5A	87	C
2	5A	88	U
2	5A	89	C
2	5A	90	G
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	292	A
2	5A	296	C
2	5A	297	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5A	299	G
2	5A	302	A
2	5A	305	A
2	5A	306	G
2	5A	310	U
2	5A	311	C
2	5A	312	U
2	5A	313	A
2	5A	465	G
2	5A	466	A
2	5A	468	A
2	5A	469	C
2	5A	470	U
2	5A	471	C
2	5A	474	A
2	5A	475	G
2	5A	479	G
2	5A	481	U
2	5A	482	A
2	5A	484	G
2	5A	497	A
2	5A	500	G
2	5A	501	C
2	5A	536	A
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	542	U
2	5A	544	C
2	5A	548	A
2	5A	553	A
2	5A	555	A
2	5A	583	U
2	5A	585	C
2	5A	586	A
2	5A	587	G
2	5A	590	G
3	SA	-4	A
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	6	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	10	G
3	SA	17	C
3	SA	18	C
3	SA	20	G
3	SA	21	U
3	SA	25	C
3	SA	26	A
3	SA	31	C
3	SA	34	G
3	SA	38	C
3	SA	40	A
3	SA	50	C
3	SA	57	G
3	SA	60	U
3	SA	63	G
3	SA	66	U
3	SA	68	A
3	SA	69	G
3	SA	71	A
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	75	U
3	SA	76	A
3	SA	77	U
3	SA	78	A
3	SA	80	A
3	SA	92	A
3	SA	107	C
3	SA	108	A
3	SA	114	C
3	SA	116	U
3	SA	127	G
3	SA	140	A
3	SA	143	G
3	SA	146	U
3	SA	152	U
3	SA	153	G
3	SA	155	U
3	SA	157	A
3	SA	160	C
3	SA	161	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	166	C
3	SA	167	U
3	SA	169	A
3	SA	176	C
3	SA	177	U
3	SA	182	A
3	SA	184	C
3	SA	185	U
3	SA	186	C
3	SA	187	G
3	SA	189	C
3	SA	191	C
3	SA	192	U
3	SA	194	U
3	SA	195	G
3	SA	196	G
3	SA	198	A
3	SA	199	G
3	SA	200	A
3	SA	201	G
3	SA	204	G
3	SA	215	A
3	SA	231	U
3	SA	233	C
3	SA	234	G
3	SA	236	A
3	SA	238	U
3	SA	239	C
3	SA	241	U
3	SA	243	G
3	SA	246	G
3	SA	248	U
3	SA	249	U
3	SA	250	C
3	SA	257	A
3	SA	259	U
3	SA	260	U
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	270	C
3	SA	271	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	272	U
3	SA	275	C
3	SA	277	U
3	SA	278	U
3	SA	279	G
3	SA	281	G
3	SA	285	G
3	SA	288	A
3	SA	299	A
3	SA	301	A
3	SA	312	A
3	SA	313	U
3	SA	314	C
3	SA	316	A
3	SA	318	U
3	SA	320	U
3	SA	321	C
3	SA	322	G
3	SA	325	G
3	SA	328	A
3	SA	329	G
3	SA	333	A
3	SA	334	G
3	SA	336	G
3	SA	337	G
3	SA	338	C
3	SA	341	A
3	SA	350	U
3	SA	351	C
3	SA	352	A
3	SA	354	C
3	SA	433	C
3	SA	434	G
3	SA	435	C
3	SA	437	A
3	SA	438	A
3	SA	439	U
3	SA	440	U
3	SA	444	C
3	SA	445	A
3	SA	448	C
3	SA	453	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	454	U
3	SA	455	C
3	SA	456	A
3	SA	468	A
3	SA	469	C
3	SA	477	A
3	SA	480	G
3	SA	484	C
3	SA	485	A
3	SA	487	G
3	SA	488	G
3	SA	492	A
3	SA	493	U
3	SA	494	U
3	SA	495	C
3	SA	500	C
3	SA	501	U
3	SA	502	U
3	SA	504	U
3	SA	506	A
3	SA	507	U
3	SA	508	U
3	SA	510	G
3	SA	511	A
3	SA	514	G
3	SA	519	C
3	SA	520	A
3	SA	525	A
3	SA	534	A
3	SA	536	C
3	SA	538	A
3	SA	539	G
3	SA	540	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	545	A
3	SA	548	G
3	SA	557	G
3	SA	563	U
3	SA	570	A
3	SA	572	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	573	C
3	SA	574	G
3	SA	575	C
3	SA	579	A
3	SA	580	A
3	SA	583	C
3	SA	584	C
3	SA	585	A
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	602	U
3	SA	603	U
3	SA	634	G
3	SA	635	A
3	SA	638	U
3	SA	639	U
3	SA	640	U
3	SA	641	G
3	SA	642	G
3	SA	643	G
3	SA	644	C
3	SA	649	U
3	SA	653	C
3	SA	654	C
3	SA	655	G
3	SA	656	G
3	SA	657	U
3	SA	678	A
3	SA	684	A
3	SA	685	A
3	SA	686	C
3	SA	687	G
3	SA	692	C
3	SA	693	U
3	SA	694	U
3	SA	696	C
3	SA	747	C
3	SA	748	U
3	SA	751	G
3	SA	752	A
3	SA	754	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	755	A
3	SA	758	U
3	SA	759	U
3	SA	763	G
3	SA	765	G
3	SA	766	U
3	SA	771	A
3	SA	772	G
3	SA	774	A
3	SA	775	G
3	SA	778	G
3	SA	779	U
3	SA	780	A
3	SA	781	U
3	SA	782	U
3	SA	783	G
3	SA	784	C
3	SA	785	U
3	SA	786	C
3	SA	787	G
3	SA	788	A
3	SA	789	A
3	SA	790	U
3	SA	794	U
3	SA	802	G
3	SA	803	A
3	SA	804	A
3	SA	805	U
3	SA	809	A
3	SA	810	G
3	SA	811	A
3	SA	812	A
3	SA	813	U
3	SA	814	A
3	SA	815	G
3	SA	822	U
3	SA	824	G
3	SA	827	C
3	SA	828	U
3	SA	841	U
3	SA	845	G
3	SA	858	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	859	A
3	SA	860	U
3	SA	863	A
3	SA	864	U
3	SA	873	U
3	SA	876	G
3	SA	877	G
3	SA	894	U
3	SA	898	A
3	SA	905	A
3	SA	906	A
3	SA	913	G
3	SA	914	G
3	SA	928	U
3	SA	929	A
3	SA	933	A
3	SA	935	U
3	SA	944	A
3	SA	951	A
3	SA	960	U
3	SA	966	A
3	SA	969	C
3	SA	971	A
3	SA	976	G
3	SA	1052	U
3	SA	1053	G
3	SA	1056	U
3	SA	1057	U
3	SA	1058	U
3	SA	1059	U
3	SA	1060	U
3	SA	1063	U
3	SA	1064	G
3	SA	1076	A
3	SA	1080	U
3	SA	1110	G
3	SA	1111	G
3	SA	1114	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	1127	G
3	SA	1128	C
3	SA	1131	A
3	SA	1132	A
3	SA	1133	A
3	SA	1134	C
3	SA	1135	U
3	SA	1141	G
3	SA	1142	A
3	SA	1143	A
3	SA	1146	G
3	SA	1158	C
3	SA	1164	G
3	SA	1191	U
3	SA	1192	C
3	SA	1193	A
3	SA	1195	C
3	SA	1196	A
3	SA	1197	C
3	SA	1198	G
3	SA	1200	G
3	SA	1201	G
3	SA	1202	A
3	SA	1203	A
3	SA	1205	C
3	SA	1207	C
3	SA	1208	A
3	SA	1209	C
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1220	C
3	SA	1221	A
3	SA	1223	A
3	SA	1226	A
3	SA	1227	A
3	SA	1228	G
3	SA	1229	G
3	SA	1230	A
3	SA	1233	G
3	SA	1236	A
3	SA	1252	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	1253	U
3	SA	1254	U
3	SA	1256	A
3	SA	1257	U
3	SA	1258	U
3	SA	1261	G
3	SA	1264	G
3	SA	1266	U
3	SA	1267	G
3	SA	1268	G
3	SA	1269	U
3	SA	1271	G
3	SA	1276	U
3	SA	1435	G
3	SA	1436	A
3	SA	1437	U
3	SA	1440	C
3	SA	1443	U
3	SA	1449	U
3	SA	1451	C
3	SA	1452	U
3	SA	1454	G
3	SA	1455	G
3	SA	1456	C
3	SA	1469	A
3	SA	1471	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1476	C
3	SA	1477	G
3	SA	1488	G
3	SA	1489	U
3	SA	1531	G
3	SA	1535	U
3	SA	1536	G
3	SA	1537	C
3	SA	1538	U
3	SA	1539	G
3	SA	1573	A
3	SA	1575	G
3	SA	1577	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	1584	G
3	SA	1590	G
3	SA	1592	A
3	SA	1595	U
3	SA	1596	C
3	SA	1600	A
3	SA	1601	G
3	SA	1602	C
3	SA	1614	A
3	SA	1618	C
3	SA	1619	C
3	SA	1622	G
3	SA	1628	U
3	SA	1630	U
3	SA	1631	A
3	SA	1639	C
3	SA	1651	A
3	SA	1654	G
3	SA	1657	U
3	SA	1658	G
3	SA	1664	C
3	SA	1665	U
3	SA	1666	U
3	SA	1668	G
3	SA	1671	A
3	SA	1672	G
3	SA	1678	A
3	SA	1679	G
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1686	C
3	SA	1687	U
3	SA	1689	A
3	SA	1694	A
3	SA	1698	G
3	SA	1702	A
3	SA	1703	C
3	SA	1704	U
3	SA	1708	U
3	SA	1709	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	SA	1710	U
3	SA	1711	C
3	SA	1712	A
3	SA	1713	G
3	SA	1714	A
3	SA	1715	G
3	SA	1716	C
3	SA	1717	G
3	SA	1718	G
3	SA	1719	A
3	SA	1721	A
3	SA	1724	U
3	SA	1725	U
3	SA	1732	A
3	SA	1734	U
3	SA	1735	U
3	SA	1736	G
3	SA	1743	U
3	SA	1745	G
3	SA	1747	G
3	SA	1749	A
3	SA	1751	C
3	SA	1755	A
3	SA	1756	A
3	SA	1757	G
3	SA	1768	G
3	SA	1769	U
3	SA	1780	G
3	SA	1781	A
3	SA	1782	A
3	SA	1789	G
3	SA	1791	A
3	SA	1792	G
3	SA	1793	G
3	SA	1794	A
3	SA	1795	U
3	SA	1797	A
3	SA	1798	U
3	SA	1799	U
3	SA	1800	A
3	SA	1801	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	102	U
1	3A	107	C
1	3A	248	G
2	5A	6	A
2	5A	311	C
3	SA	0	U
3	SA	68	A
3	SA	139	C
3	SA	278	U
3	SA	280	U
3	SA	454	U
3	SA	484	C
3	SA	503	G
3	SA	542	A
3	SA	579	A
3	SA	602	U
3	SA	637	C
3	SA	685	A
3	SA	773	C
3	SA	781	U
3	SA	1052	U
3	SA	1063	U
3	SA	1471	A
3	SA	1594	G
3	SA	1754	A

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
78	GTP	RJ	1201	79	26,34,34	1.18	2 (7%)	32,54,54	1.78	7 (21%)

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
78	GTP	RJ	1201	79	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	RJ	1201	GTP	C5-C6	-4.13	1.39	1.47
78	RJ	1201	GTP	C2-N3	2.02	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	RJ	1201	GTP	PA-O3A-PB	-5.07	115.43	132.83
78	RJ	1201	GTP	PB-O3B-PG	-3.88	119.52	132.83
78	RJ	1201	GTP	C5-C6-N1	3.52	120.16	113.95
78	RJ	1201	GTP	C8-N7-C5	3.16	109.02	102.99
78	RJ	1201	GTP	C2-N1-C6	-3.14	119.31	125.10
78	RJ	1201	GTP	C3'-C2'-C1'	2.88	105.32	100.98
78	RJ	1201	GTP	O6-C6-C5	-2.09	120.29	124.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

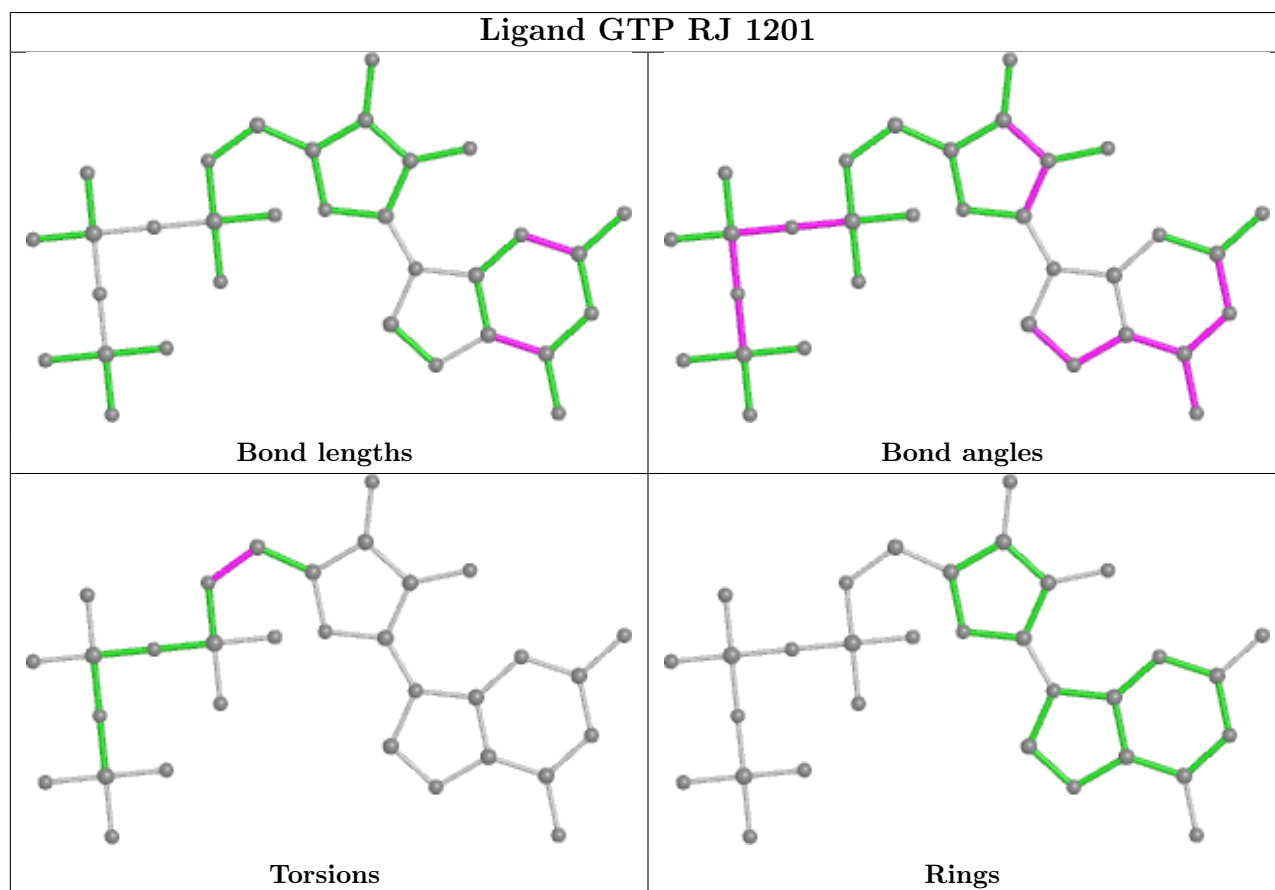
Mol	Chain	Res	Type	Atoms
78	RJ	1201	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

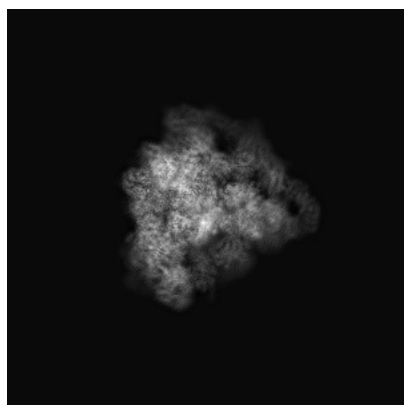
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0952. These allow visual inspection of the internal detail of the map and identification of artifacts.

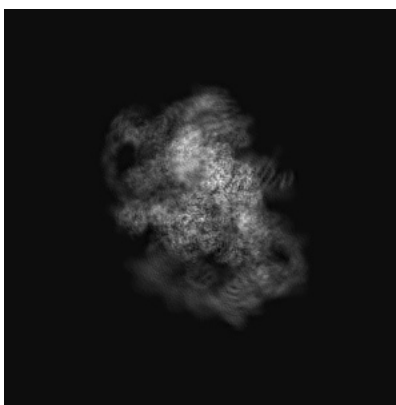
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

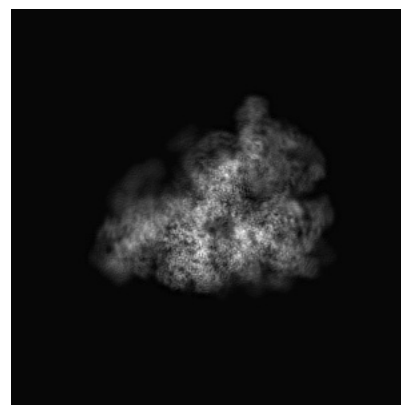
#### 6.1.1 Primary map



X



Y

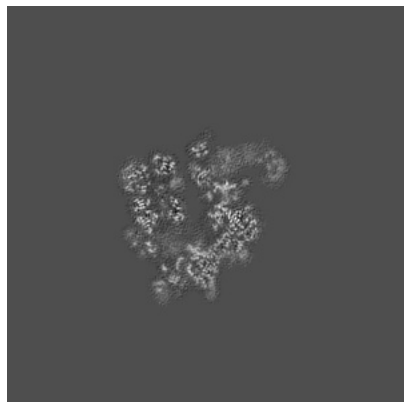


Z

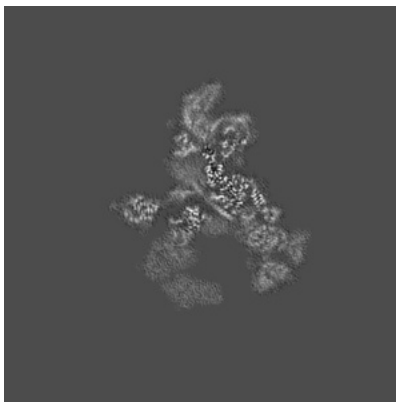
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

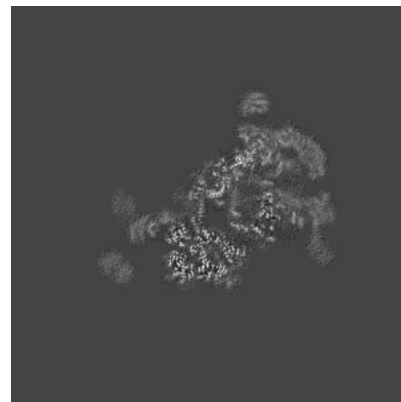
#### 6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224



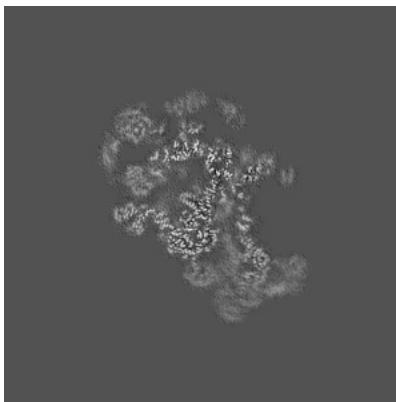
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

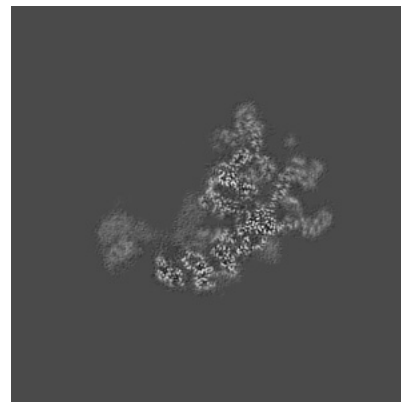
### 6.3.1 Primary map



X Index: 212



Y Index: 189

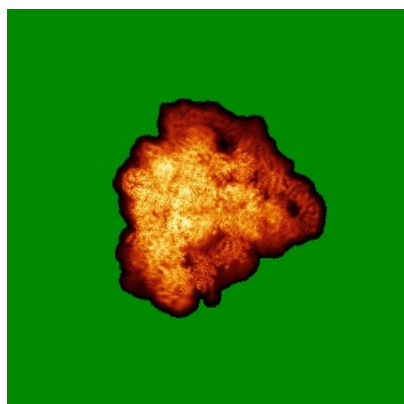


Z Index: 245

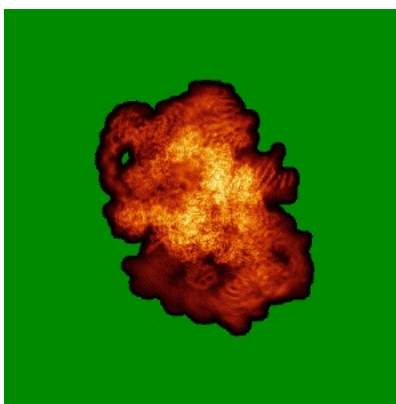
The images above show the largest variance slices of the map in three orthogonal directions.

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

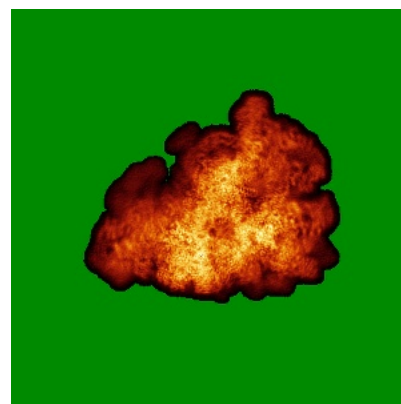
### 6.4.1 Primary map



X



Y

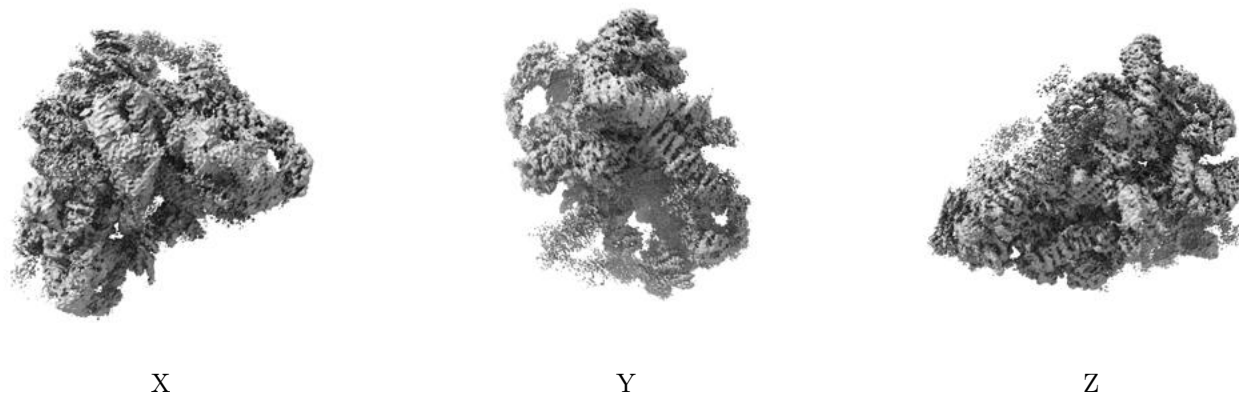


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

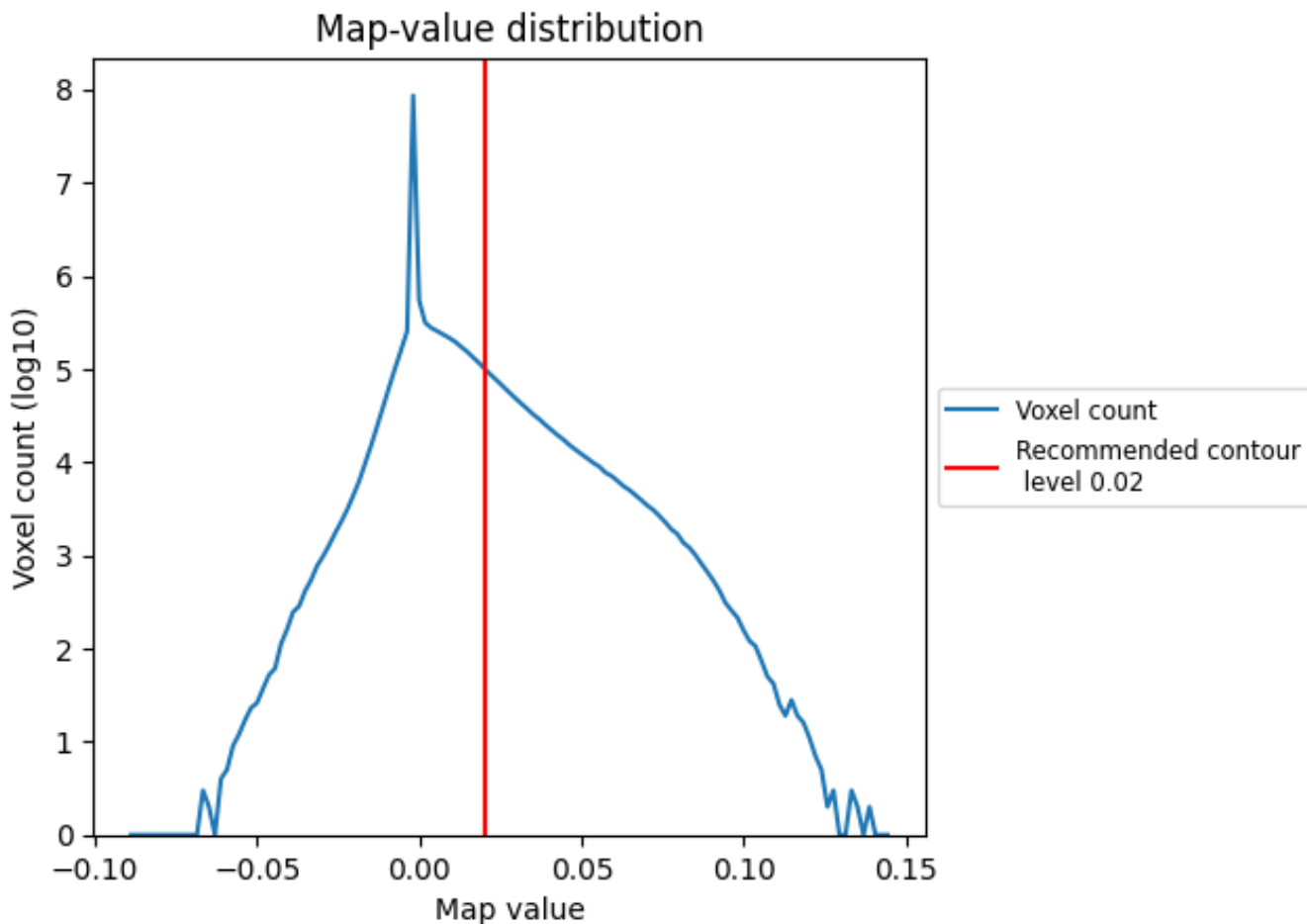
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

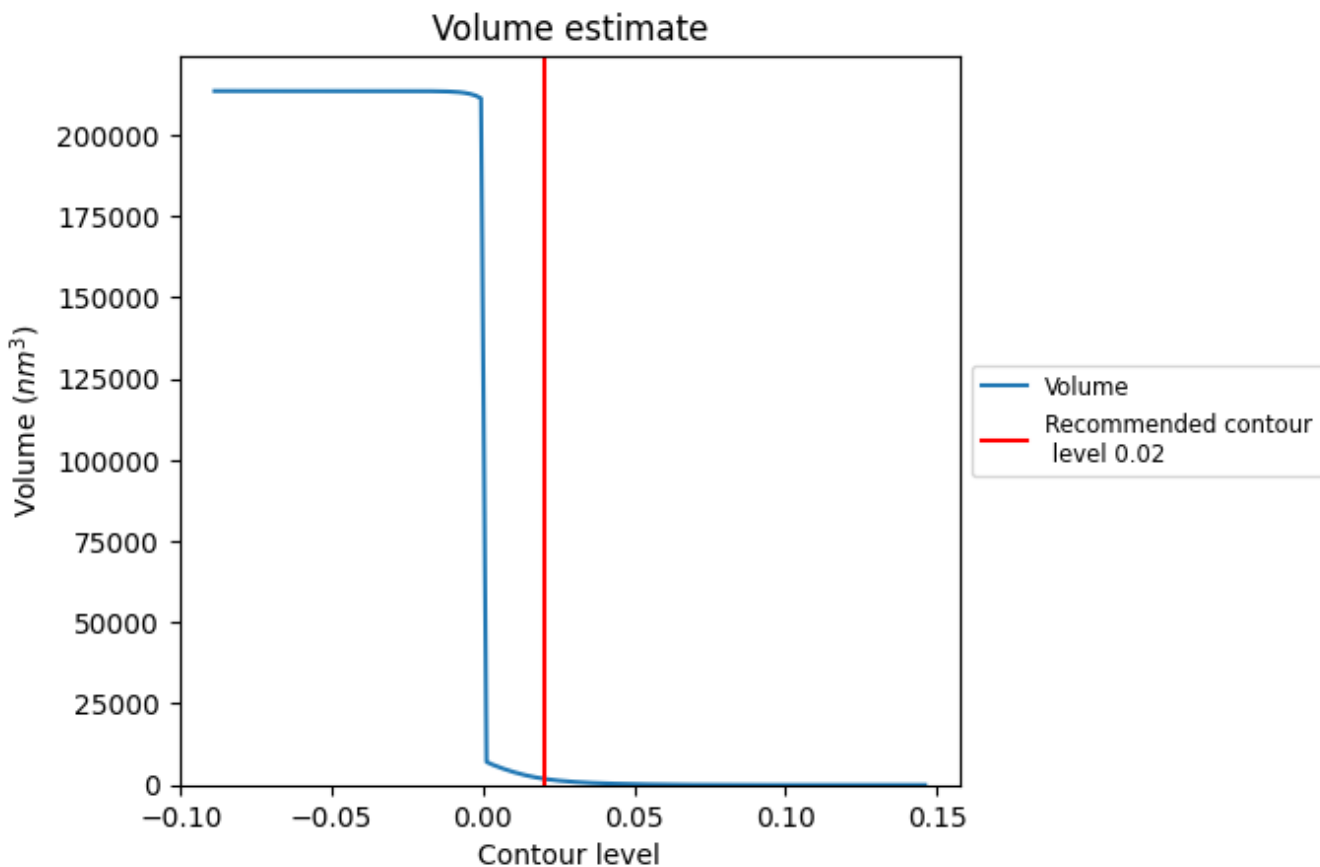
This section contains the results of statistical analysis of the map.

### 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.

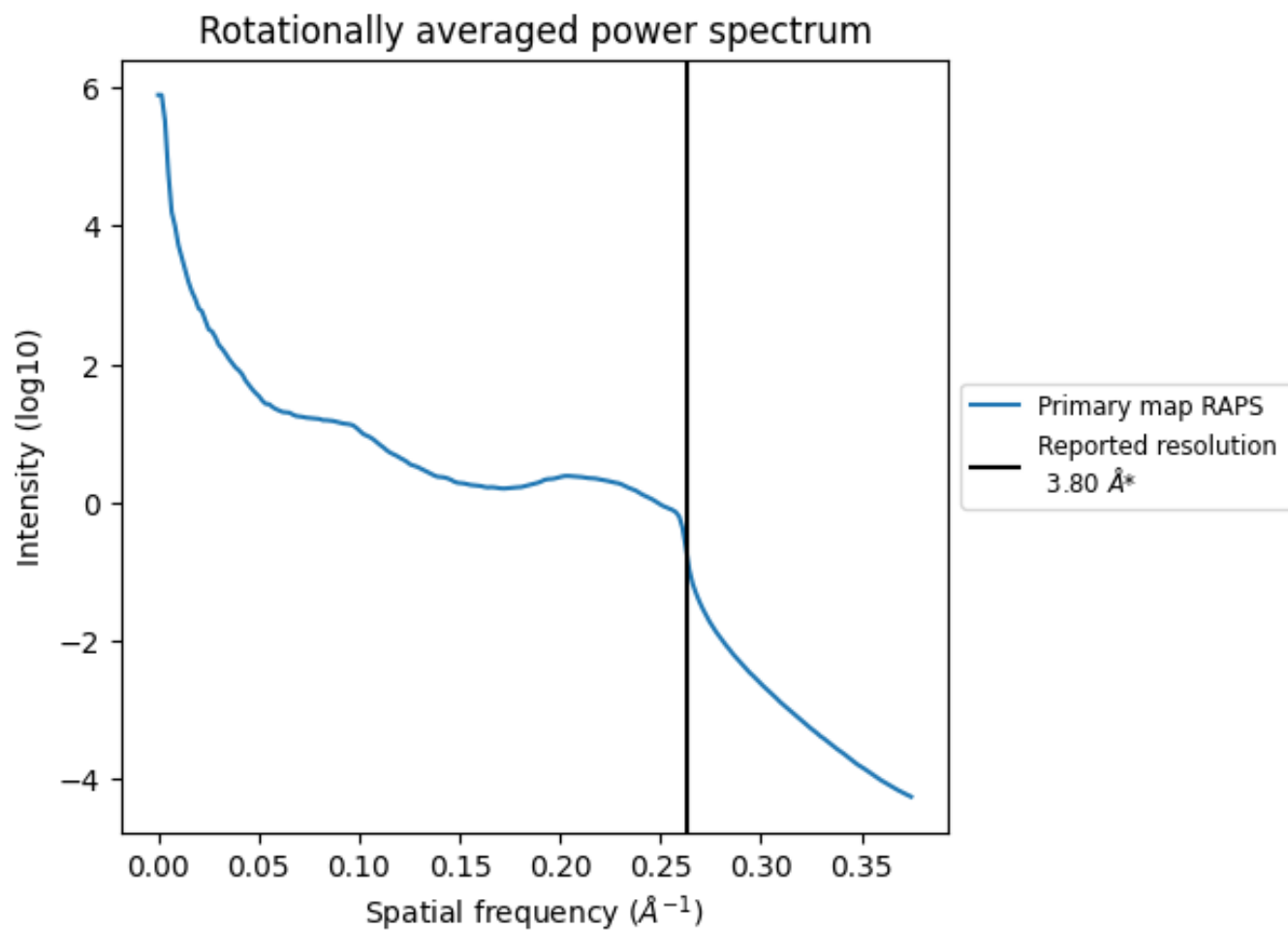
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1925  $\text{nm}^3$ ; this corresponds to an approximate mass of 1739 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 [i](#)

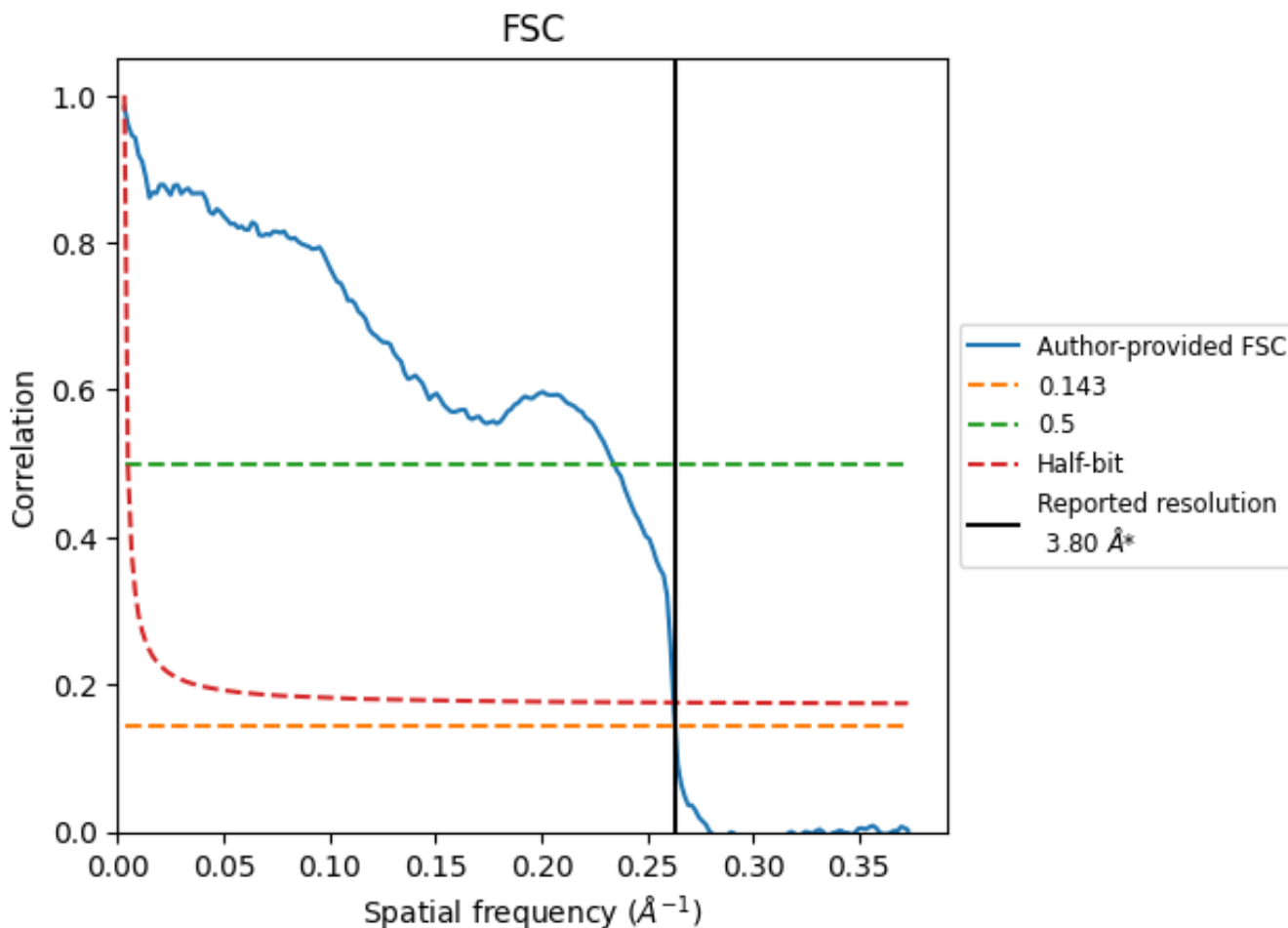


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

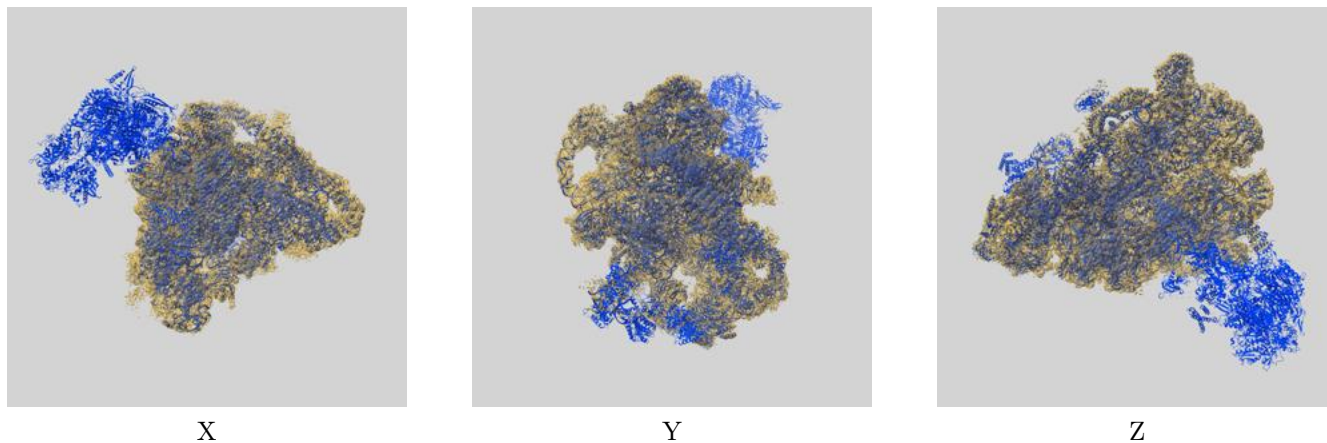
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.27	3.81
Unmasked-calculated*	-	-	-

\*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-0952 and PDB model 6LQS. Per-residue inclusion information can be found in section 3 on page 18.

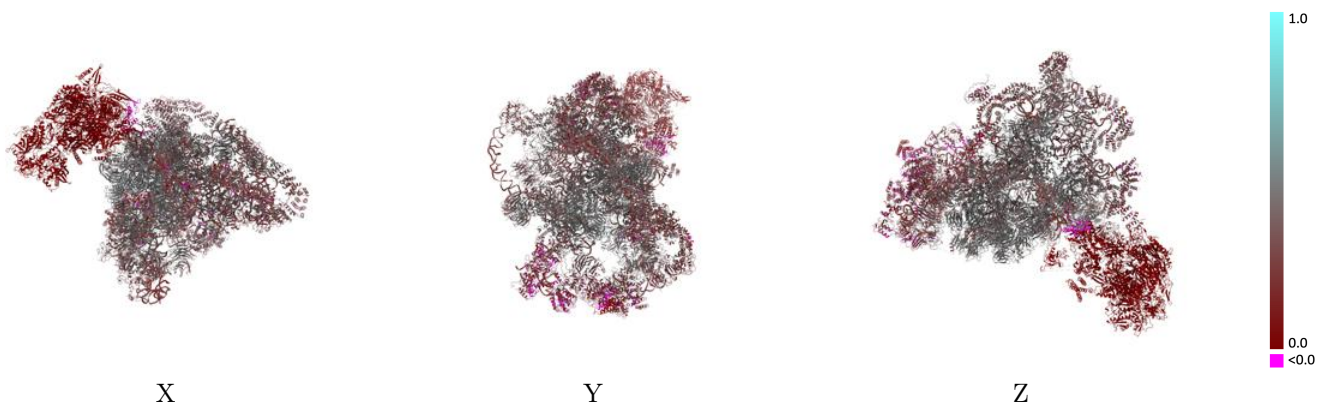
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

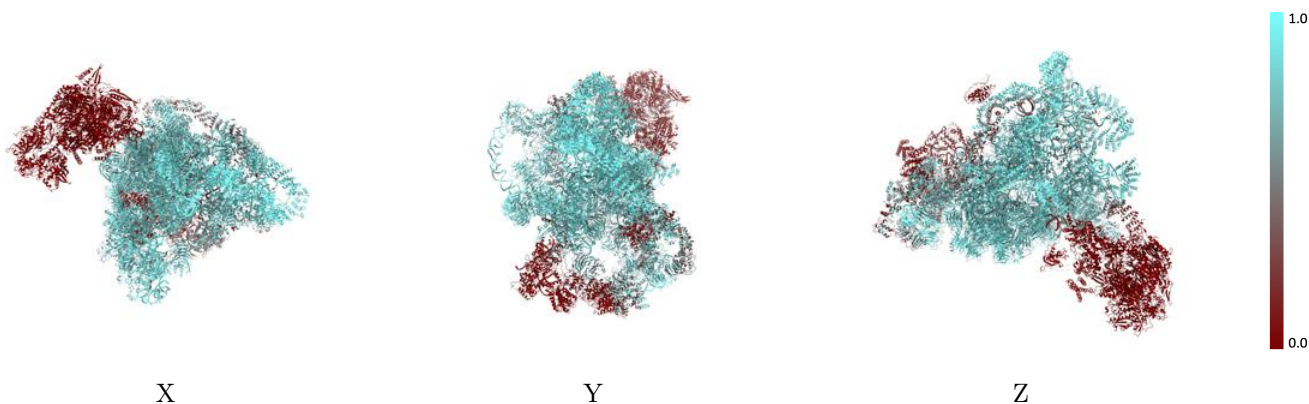


## 9.2 Q-score mapped to coordinate model [i](#)



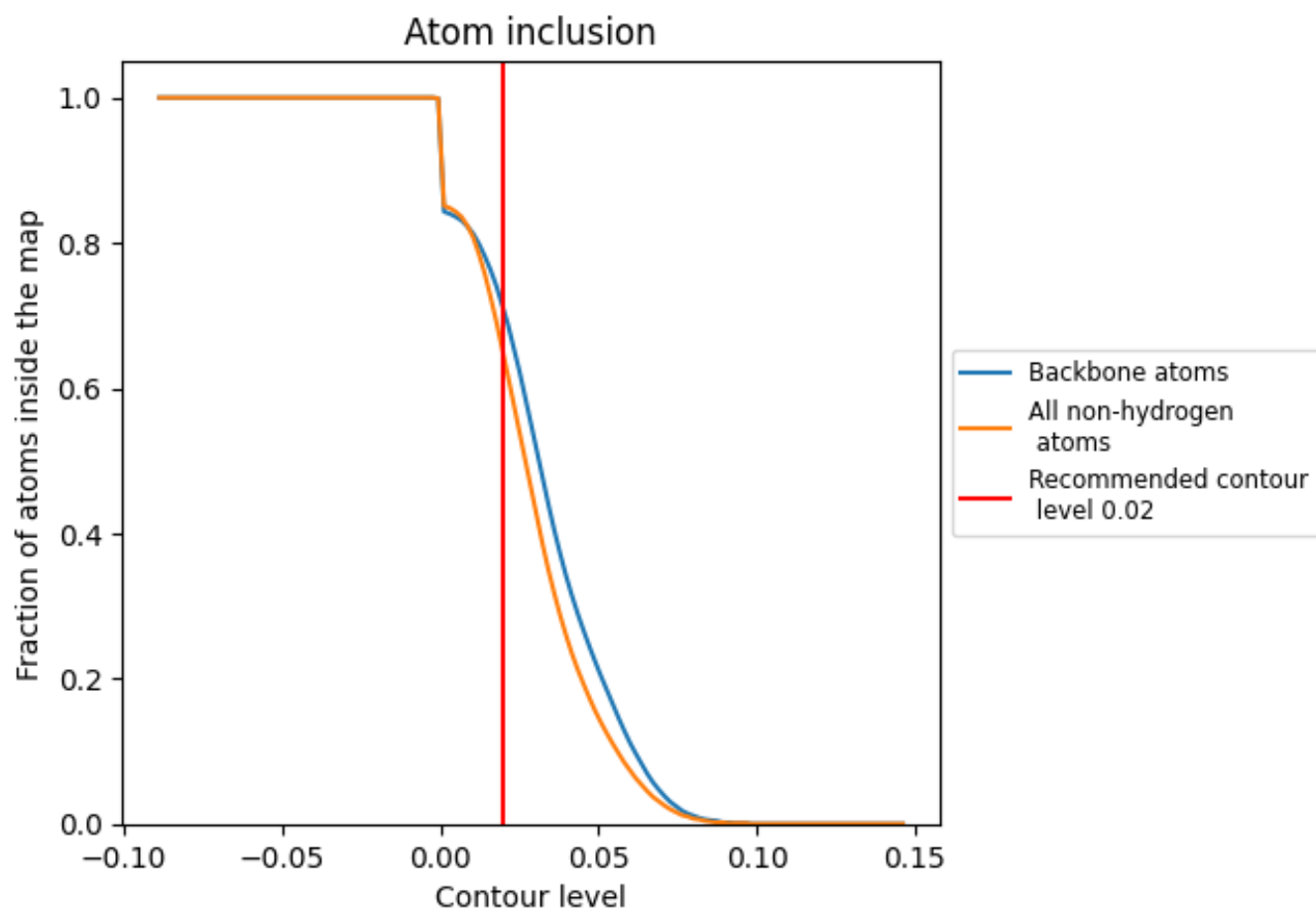
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.3160
3A	 0.7970	 0.3500
3B	 0.8650	 0.4750
3C	 0.7380	 0.3690
3D	 0.8620	 0.4290
3E	 0.8280	 0.3910
3F	 0.8760	 0.4550
3G	 0.8010	 0.3890
3H	 0.8550	 0.4590
5A	 0.7230	 0.2890
5B	 0.4290	 0.3480
5C	 0.8620	 0.4790
5D	 0.5030	 0.3770
5E	 0.8250	 0.4170
5F	 0.8530	 0.4590
5G	 0.8430	 0.4690
5H	 0.8860	 0.4730
5I	 0.9090	 0.4910
5J	 0.7600	 0.4050
5K	 0.8640	 0.4790
A4	 0.7920	 0.3530
A5	 0.7020	 0.3800
A8	 0.3990	 0.2010
A9	 0.5750	 0.2150
AE	 0.6750	 0.3380
AF	 0.6480	 0.2880
AG	 0.7940	 0.3350
B1	 0.8910	 0.4750
B2	 0.8750	 0.4080
B3	 0.8640	 0.3710
B6	 0.8660	 0.4110
B8	 0.8570	 0.4480
BE	 0.9020	 0.4730
C4	 0.0000	 0.0000
M3	 0.0000	 0.0000









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Chain	Atom inclusion	Q-score
M4	 0.0000	 -0.0040
M6	 0.0000	 0.0000
R0	 0.0000	 0.0000
R1	 0.0000	 0.0000
R2	 0.0000	 0.0000
R3	 0.0000	 0.0000
R4	 0.0000	 0.0000
R5	 0.0000	 0.0000
R6	 0.0000	 0.0000
R7	 0.0000	 0.0000
RD	 0.3260	 0.2790
RE	 0.8000	 0.3500
RF	 0.7710	 0.3320
RG	 0.1070	 0.2420
RH	 0.2340	 0.2920
RJ	 0.8410	 0.4200
RK	 0.8420	 0.4100
RN	 0.1150	 0.1960
RO	 0.0210	 0.1810
RP	 0.8800	 0.3400
RQ	 0.7950	 0.4200
RS	 0.0490	 0.1750
RT	 0.6990	 0.3620
RW	 0.2640	 0.3010
SA	 0.8380	 0.3440
SC	 0.8500	 0.4530
SF	 0.8280	 0.3990
SG	 0.8520	 0.4490
SH	 0.6680	 0.3150
SI	 0.7830	 0.3650
SJ	 0.6470	 0.2950
SK	 0.8750	 0.4690
SM	 0.5590	 0.2910
SO	 0.8750	 0.4310
SP	 0.8570	 0.4260
SR	 0.8830	 0.4690
SX	 0.8700	 0.4550
SY	 0.8140	 0.4470
SZ	 0.8770	 0.4470
Sc	 0.9040	 0.4690
Sd	 0.8850	 0.4670
X1	 0.8530	 0.3890

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Chain	Atom inclusion	Q-score
X2	 0.0840	 0.2990
r4	 0.0000	 0.0000
r6	 0.0000	 0.0000