Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 01:21 AM JST

PDB ID	:	7D5T
EMDB ID	:	EMD-30585
Title	:	Cryo-EM structure of 90S preribosome with inactive Utp24 (state F1)
Authors	:	Du, Y.; Zhang, J.; An, W.; Ye, K.
Deposited on	:	2020-09-28
Resolution	:	6.00 Å(reported)
Based on initial model	:	7D4I

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

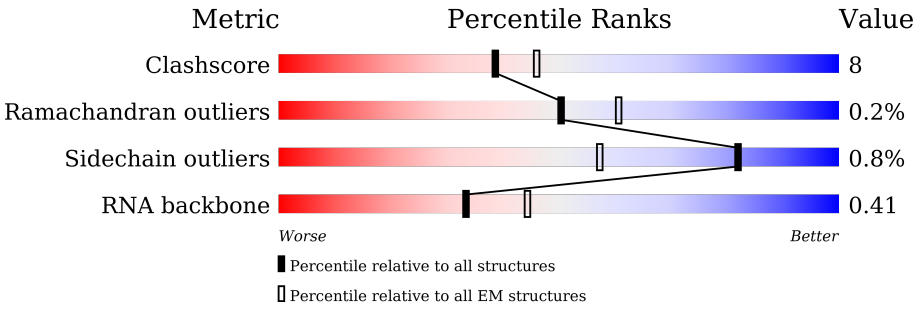
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.00 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 >=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 <=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	5% 20% 23% 6% 50%
2	5A	700	94%
3	SA	1812	27% 30% 8% 34%
4	SC	255	71% 24% 5%
5	SF	261	17% 72% 22% 5%
6	SG	225	79% 16% 5%
7	SH	236	30% 59% 18% 23%

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Mol	Chain	Length	Quality of chain
8	SI	190	8% 59% 26% 13%
9	SJ	200	24% 55% 18% 26%
10	SK	197	67% 20% 12%
11	SM	156	54% 66% 22% 12%
12	SO	151	72% 17% 11%
13	SP	137	62% 23% 15%
14	SR	143	66% 20% 13%
15	SX	130	11% 75% 23%
16	SY	145	10% 61% 10% 28%
17	SZ	135	67% 24% 9%
18	Sc	82	96%
19	Sd	67	93% 6%
20	3B	327	8% 60% 14% 26%
20	3C	327	51% 52% 16% 31%
21	3D	504	6% 59% 16% 25%
22	3E	511	10% 45% 10% 46%
23	3F	573	59% 17% 24%
24	3G	126	43% 73% 22%
24	3H	126	76% 19%
25	A5	643	34% 36% 11% 52%
26	AE	1769	6% 20% 5% 76%
27	AG	896	5% 95%
28	B1	900	10% 70% 17% 12%
29	B2	943	64% 23% 13%
30	B3	817	65% 27% 7%

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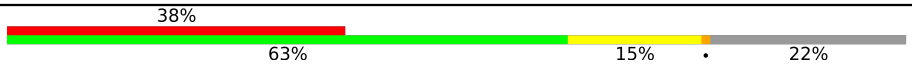
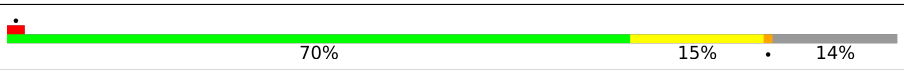
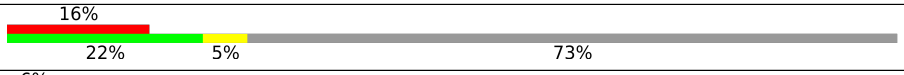
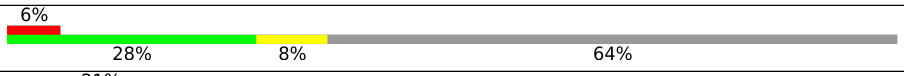
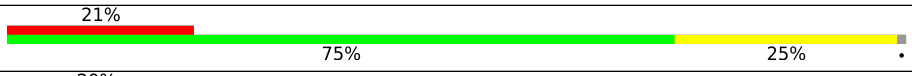
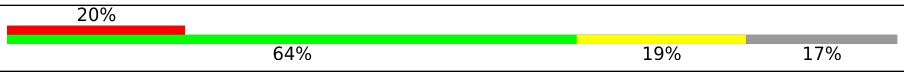
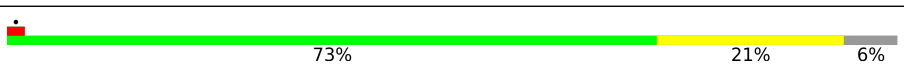
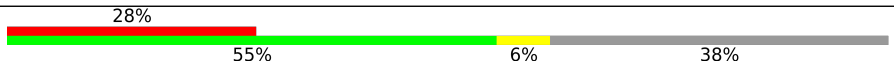
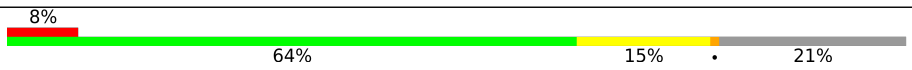
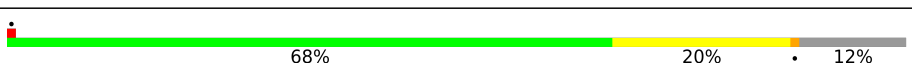
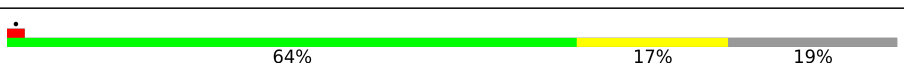
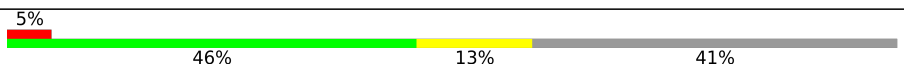
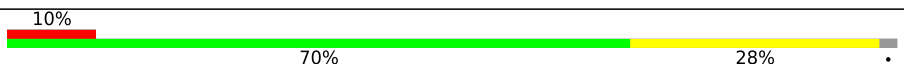
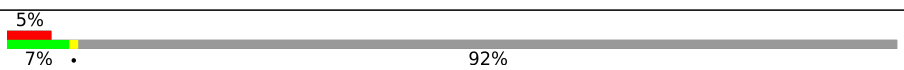
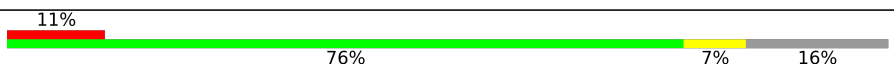
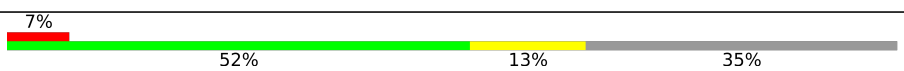
Mol	Chain	Length	Quality of chain
31	B8	594	
32	BE	939	
33	B6	440	
34	5C	554	
35	5D	250	
36	5E	593	
37	5F	183	
38	5G	290	
39	5H	610	
40	5I	489	
41	5J	217	
42	5K	189	
43	RD	1729	
44	RE	1237	
45	RF	297	
46	RJ	1183	
47	RK	367	
48	RN	810	
49	RP	2493	
50	RQ	899	
51	RT	326	
52	RZ	1267	
53	X1	300	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 163485 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	167	3534	1581	606	1180	167	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	43	926	413	173	297	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	1189	25332	11327	4490	8326	1189	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	242	1923	1214	356	349	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	247	1915	1223	351	338	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
7	SH	182	Total	C	N	O	S	0	0
			1456	916	273	266	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	SI	165	Total	C	N	O	0	0
			1321	853	226	242		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SJ	148	Total	C	N	O	S	0	0
			1181	739	228	212	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	174	Total	C	N	O	S	0	0
			1410	892	272	245	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SP	116	Total	C	N	O	S	0	0
			848	524	158	163	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SY	104	Total 792	C 506	N 145	O 139	S 2	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3B	242	Total 1878	C 1190	N 338	O 340	S 10	0	0
20	3C	224	Total 1754	C 1114	N 314	O 316	S 10	0	0

- 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	277	Total	C	N	O	S	0	0
			2130	1335	374	414	7		

- 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 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A5	309	Total	C	N	O	S	0	0
			2452	1573	397	472	10		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AE	431	Total	C	N	O	S	0	0
			3443	2224	566	641	12		

- Molecule 27 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AG	48	Total	C	N	O	S	0	0
			394	248	62	80	4		

- Molecule 28 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B1	791	Total	C	N	O	S	0	0
			6316	4037	1082	1179	18		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B2	824	Total	C	N	O	S	0	0
			6497	4153	1095	1222	27		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B3	757	Total	C	N	O	S	0	0
			5906	3763	993	1123	27		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	463	Total	C	N	O	S	0	0
			3648	2314	640	684	10		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BE	890	Total	C	N	O	S	0	0
			6876	4356	1191	1308	21		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B6	377	Total	C	N	O	S	0	0
			3077	1984	529	549	15		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5C	482	Total	C	N	O	S	0	0
			3825	2409	684	721	11		

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5D	68	Total	C	N	O	S	0	0
			589	365	120	103	1		

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5E	213	Total	C	N	O	S	0	0
			1728	1072	304	348	4		

- Molecule 37 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 38 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5G	241	Total	C	N	O	S	0	0
			1956	1228	368	353	7		

- Molecule 39 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	5H	74	Total	C	N	O	0	0
			596	373	122	101		

- Molecule 40 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5I	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 41 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5J	134	Total	C	N	O	S	0	0
			1127	712	205	207	3		

- Molecule 42 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5K	150	Total	C	N	O	S	0	0
			1190	765	212	203	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5K	138	ASN	ASP	conflict	UNP Q05498

- Molecule 43 is a protein called rRNA biogenesis protein RRP5.

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

- Molecule 44 is a protein called U3 small nucleolar RNA-associated protein 22.

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

- Molecule 45 is a protein called Ribosomal RNA-processing protein 7.

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

- Molecule 46 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	RJ	702	Total	C	N	O	S	0	0
			5709	3669	1008	1006	26		

- Molecule 47 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 48 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	RN	61	Total	C	N	O	S	0	0
			523	320	102	99	2		

- Molecule 49 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	RP	2084	Total	C	N	O	S	0	0
			12263	7556	2298	2392	17		

- Molecule 50 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RQ	339	Total	C	N	O	S	0	0
			2411	1487	456	466	2		

- Molecule 51 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	RT	213	Total	C	N	O	S	0	0
			1652	1051	300	297	4		

- Molecule 52 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RZ	838	Total	C	N	O	S	1	0
			6598	4212	1145	1206	35		

- Molecule 53 is a protein called Unassigned peptides 1.

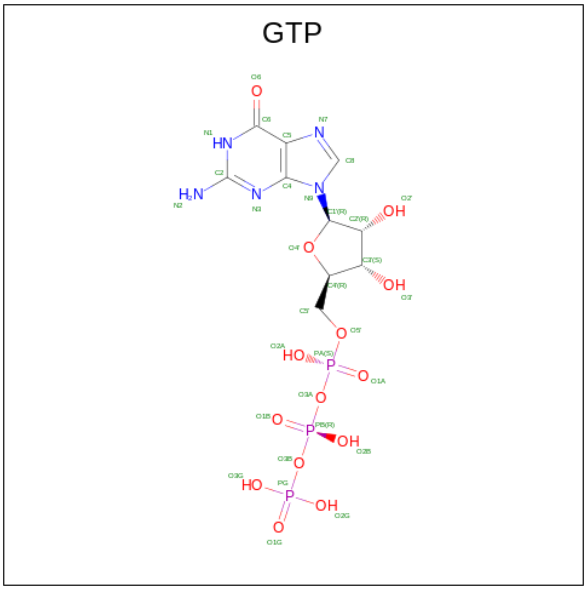
Mol	Chain	Residues	Atoms				AltConf	Trace
53	X1	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	Sc	1	Total	Zn	0
			1	1	
54	5K	1	Total	Zn	0
			1	1	

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$C_{10}H_{16}N_5O_{14}P_3$).

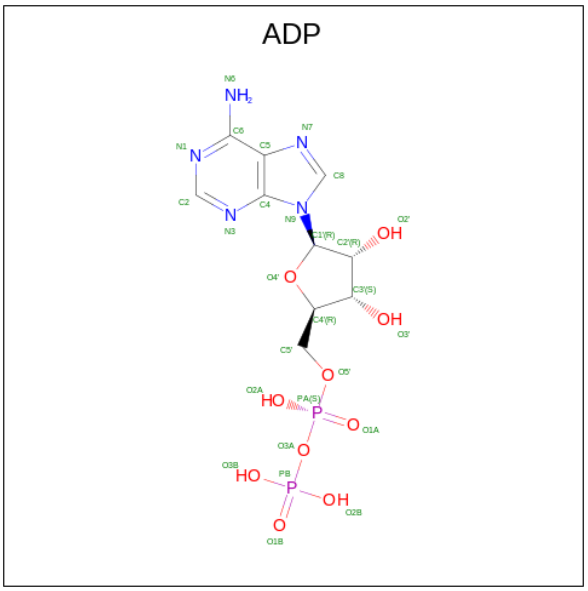


Mol	Chain	Residues	Atoms					AltConf
55	RJ	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



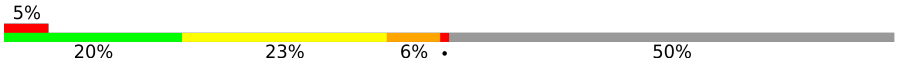
Mol	Chain	Residues	Atoms					AltConf
57	RZ	1	Total	C	N	O	P	0
			27	10	5	10	2	

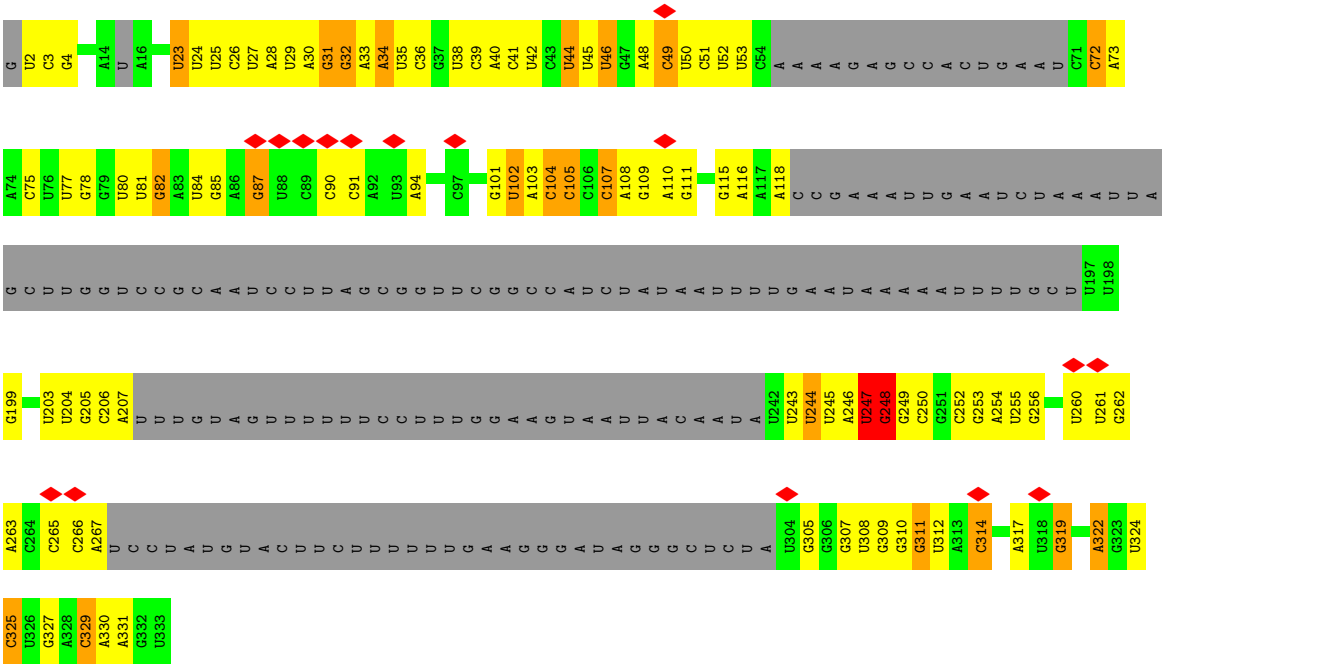
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: U3 snoRNA

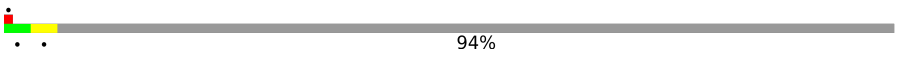
Chain 3A:

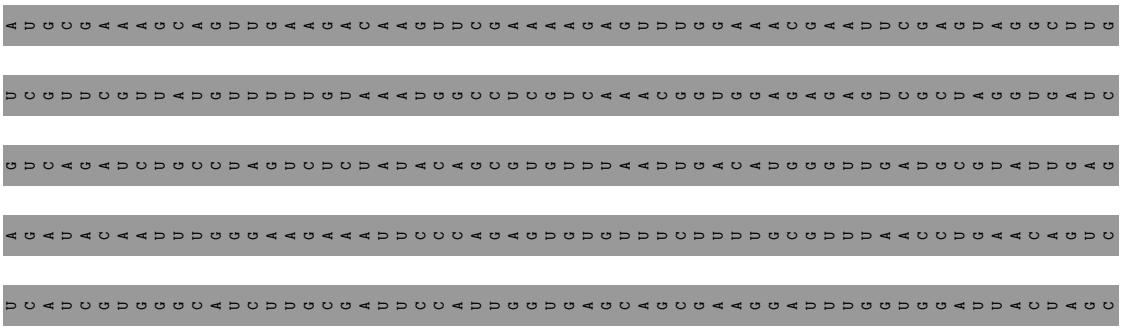


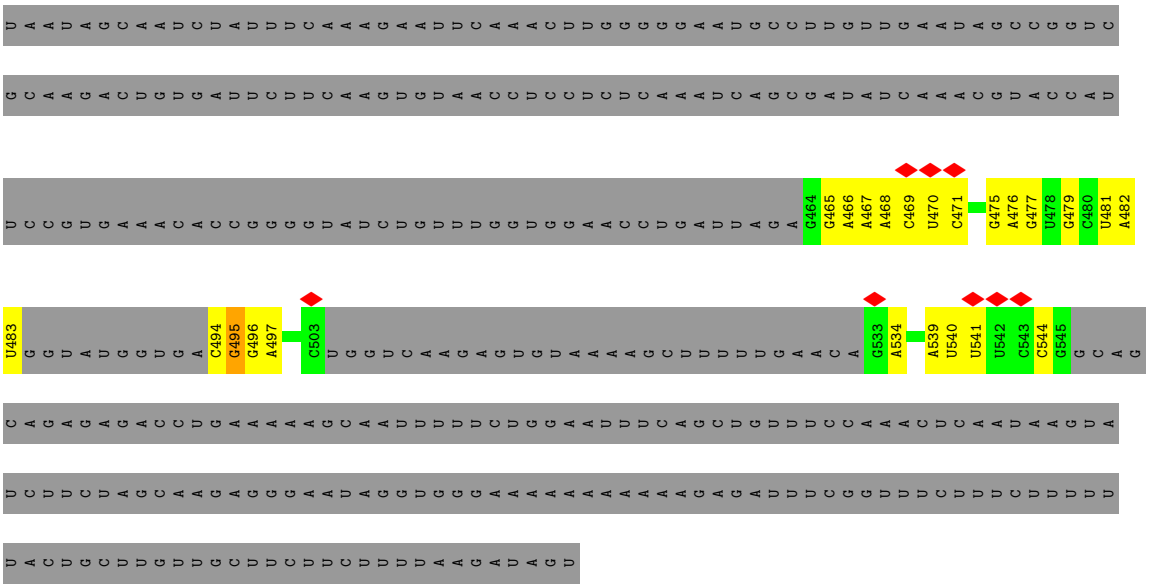


• Molecule 2: 5' ETS

Chain 5A:

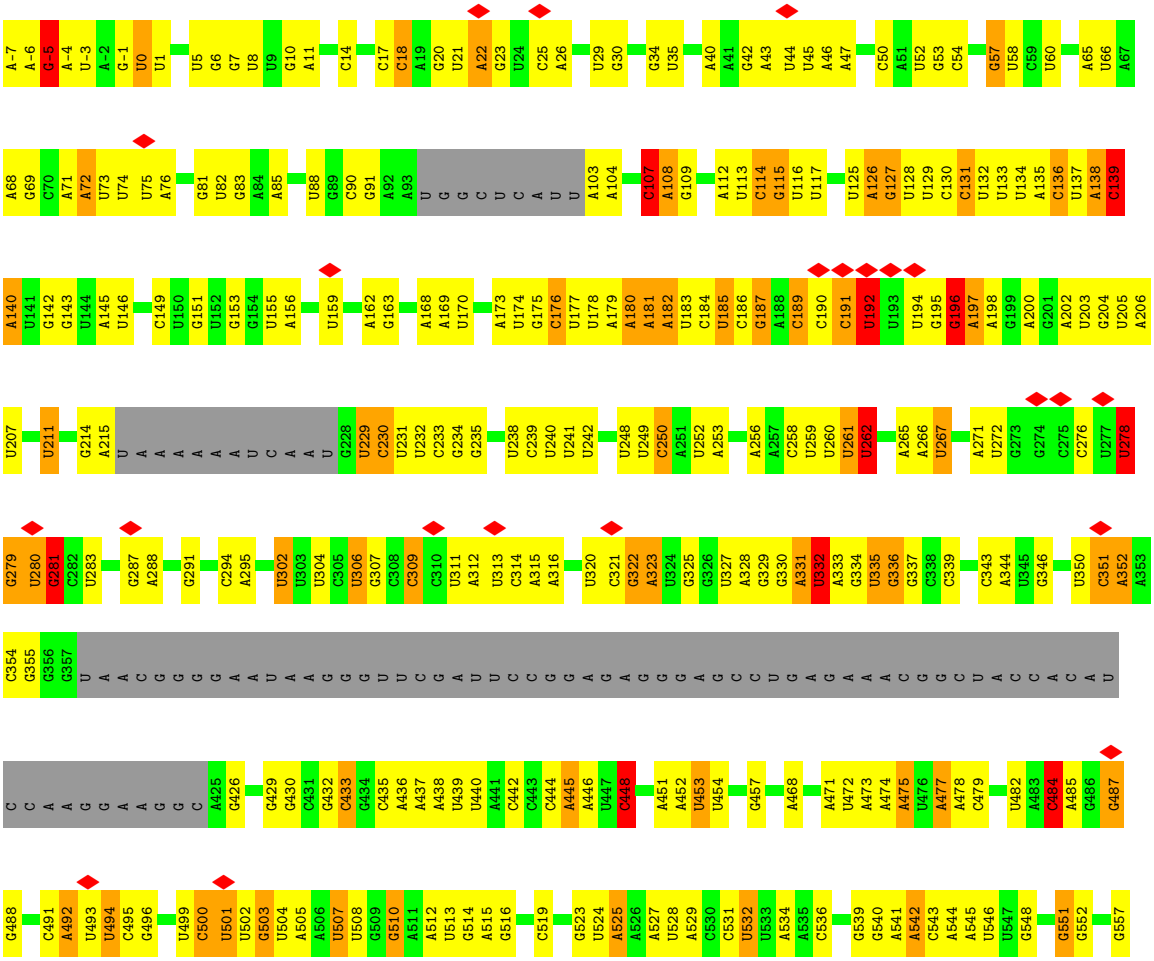


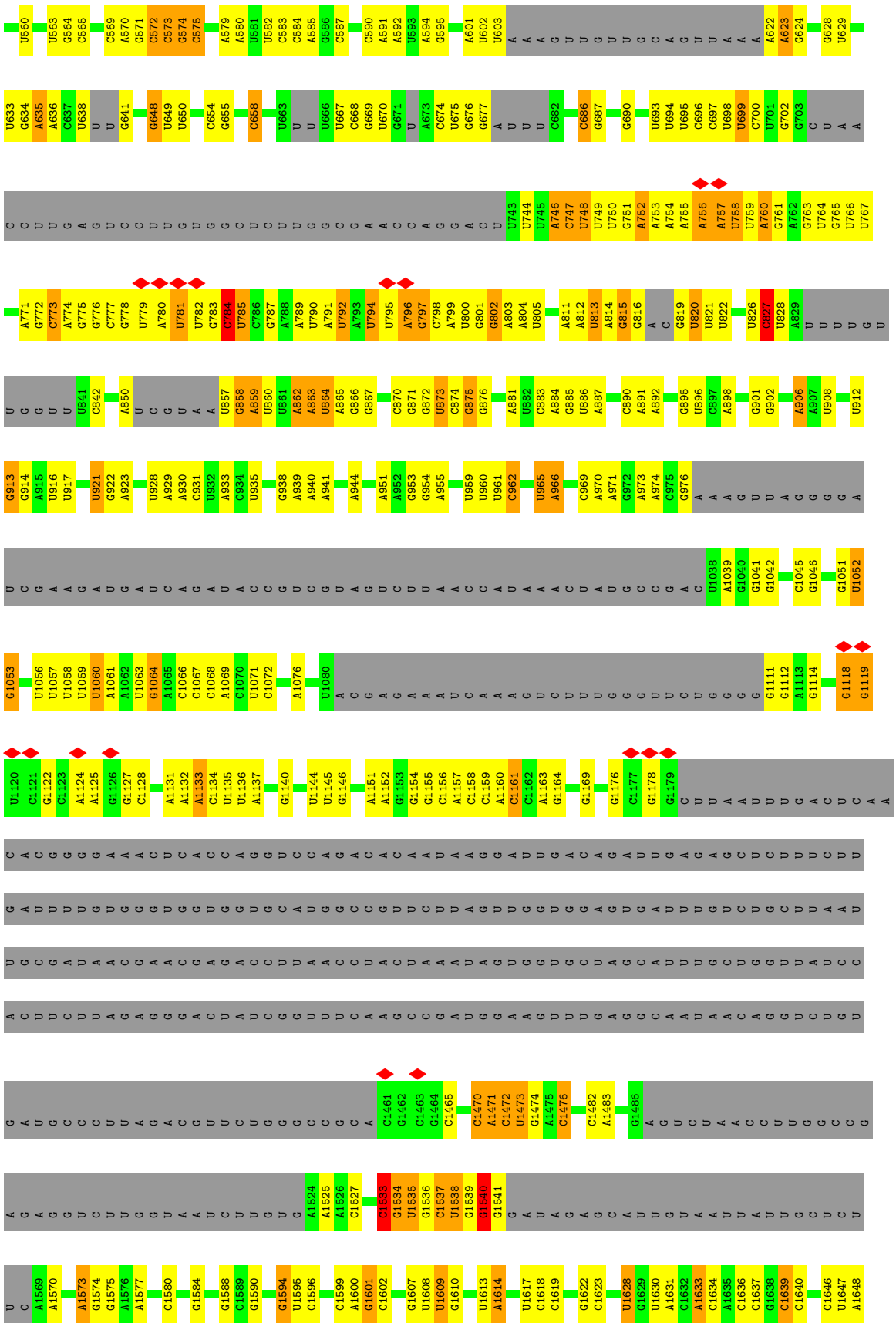


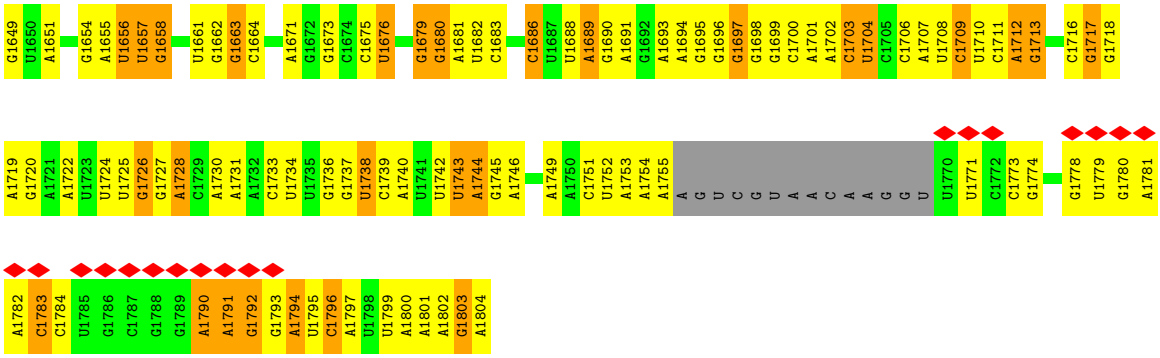


• Molecule 3: 18S rRNA

Chain SA:





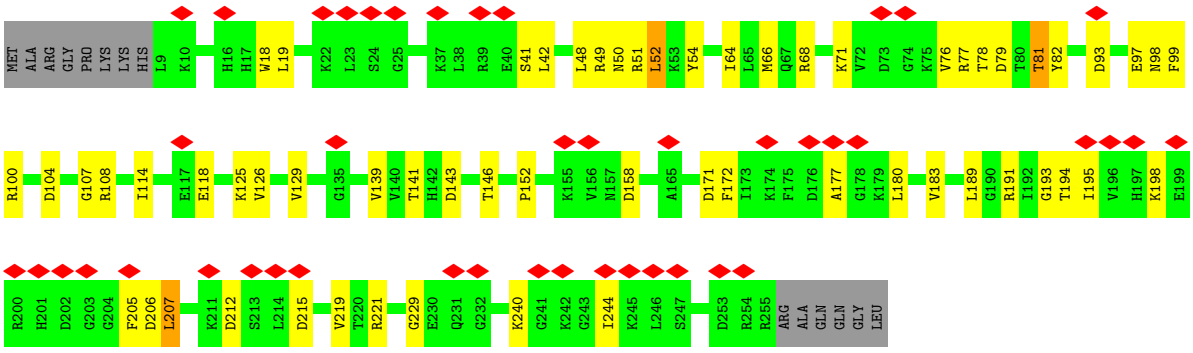


• Molecule 4: 40S ribosomal protein S1-A

Chain SC:

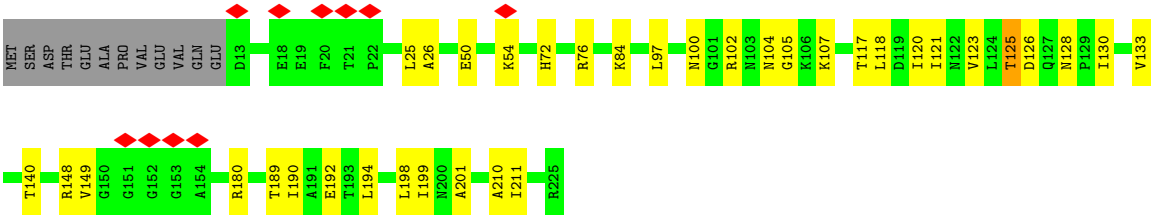
• Molecule 5: 40S ribosomal protein S4-A

Chain SF:



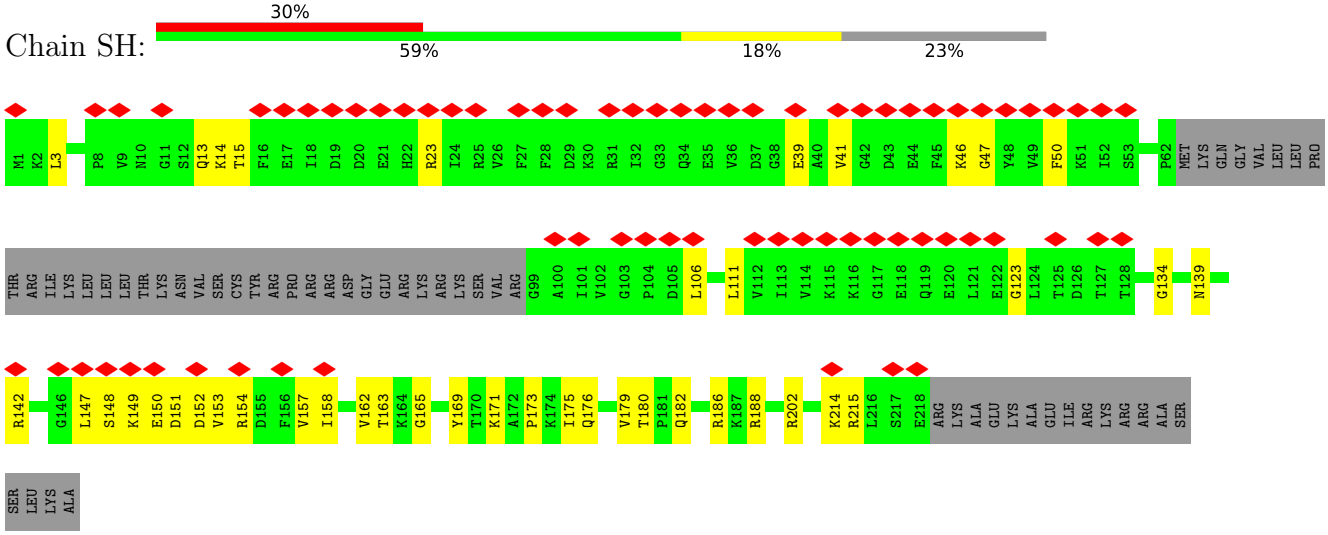
• Molecule 6: 40S ribosomal protein S5

Chain SG:



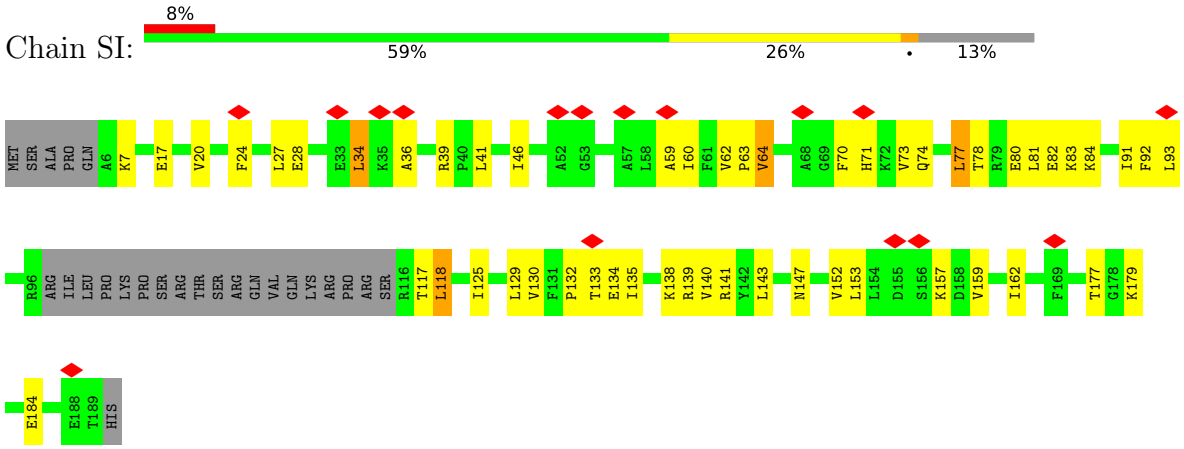
• Molecule 7: 40S ribosomal protein S6-A

Chain SH:



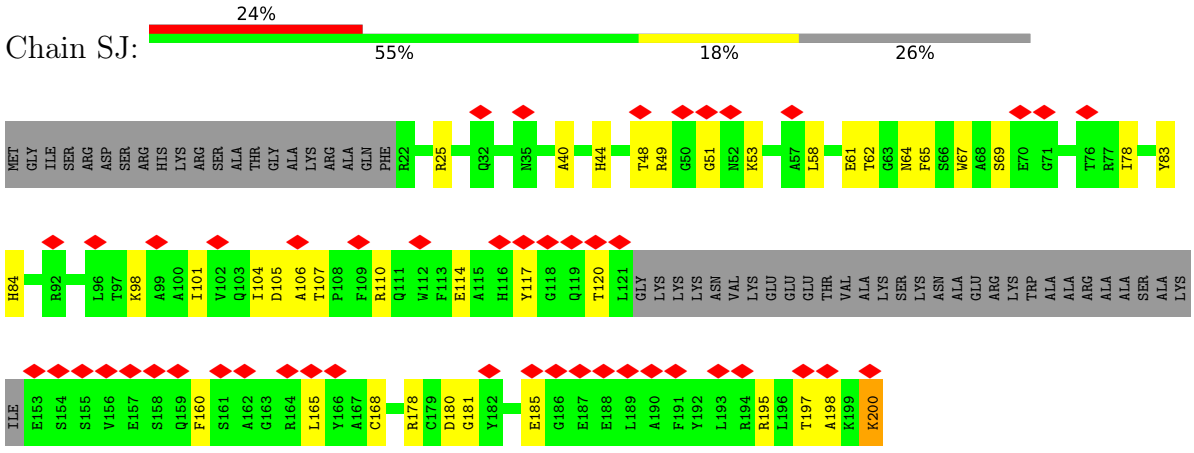
• Molecule 8: 40S ribosomal protein S7-A

Chain SI:



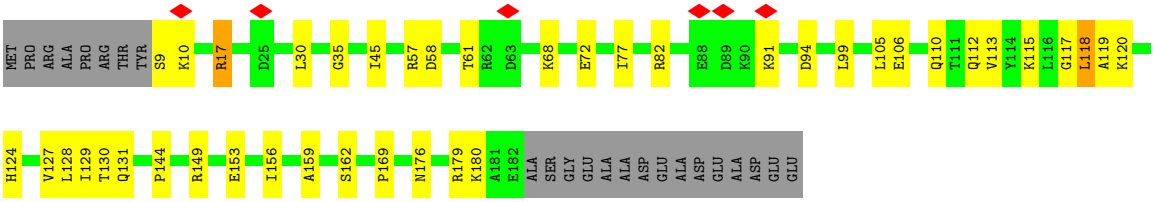
• Molecule 9: 40S ribosomal protein S8-A

Chain SJ:



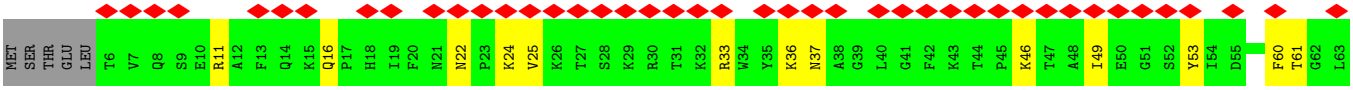
• Molecule 10: 40S ribosomal protein S9-A

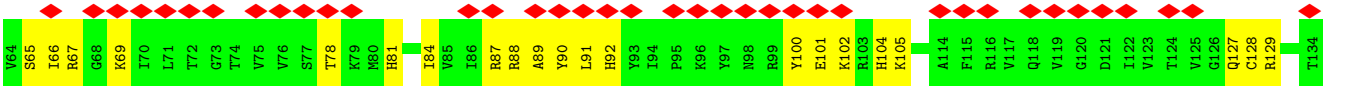
Chain SK:

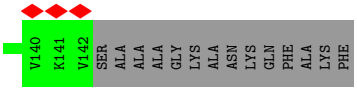


• Molecule 11: 40S ribosomal protein S11-A

Chain SM:





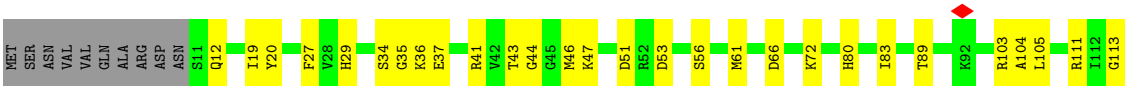


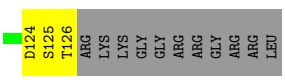
• Molecule 12: 40S ribosomal protein S13

Chain SO:

• Molecule 13: 40S ribosomal protein S14-A

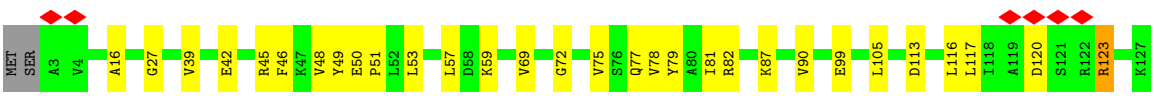
Chain SP:





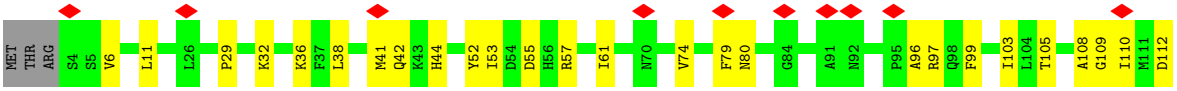
• Molecule 14: 40S ribosomal protein S16-A

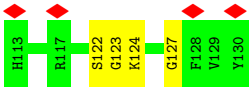
Chain SR:



• Molecule 15: 40S ribosomal protein S22-B

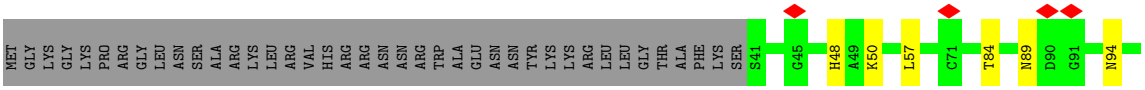
Chain SX:

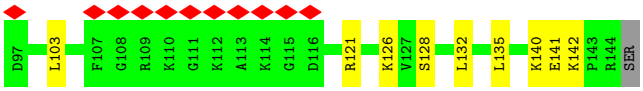




• Molecule 16: 40S ribosomal protein S23-A

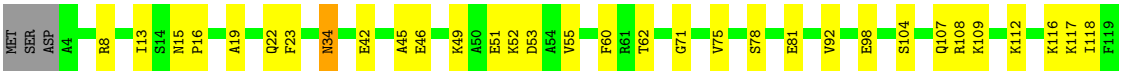
Chain SY:

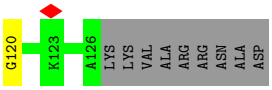




• Molecule 17: 40S ribosomal protein S24-A

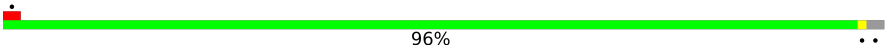
Chain SZ:

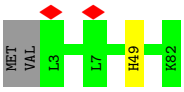




• Molecule 18: 40S ribosomal protein S27-A

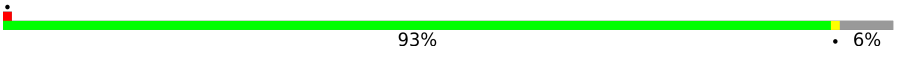
Chain Sc:

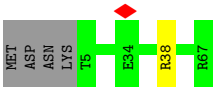




• Molecule 19: 40S ribosomal protein S28-A

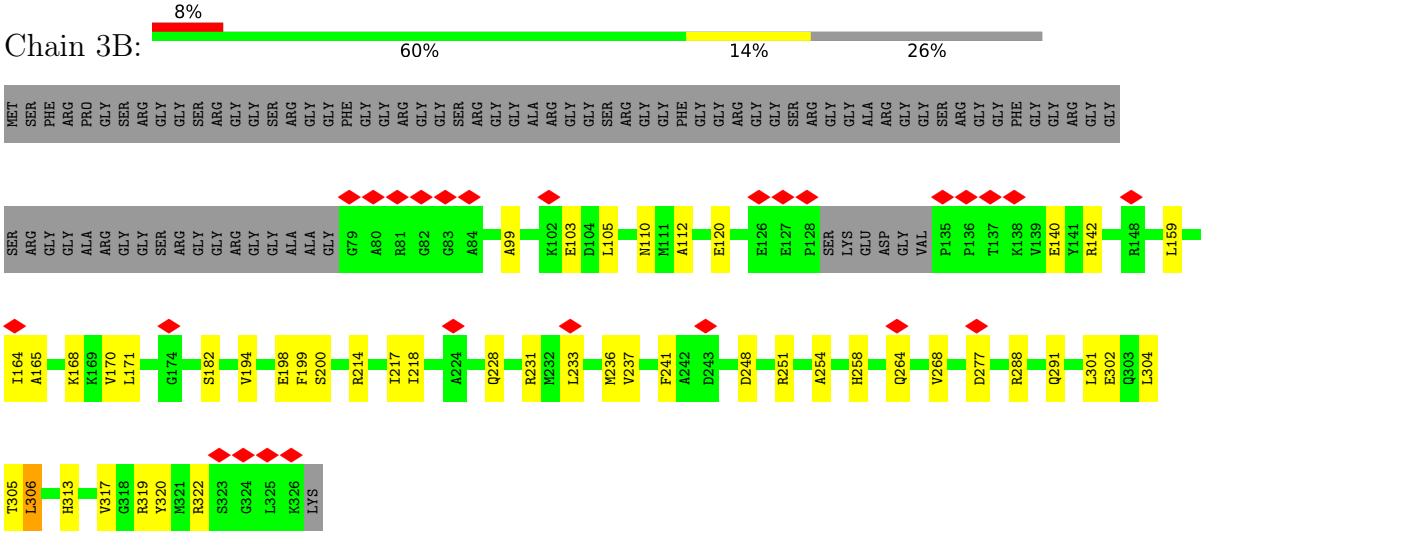
Chain Sd:





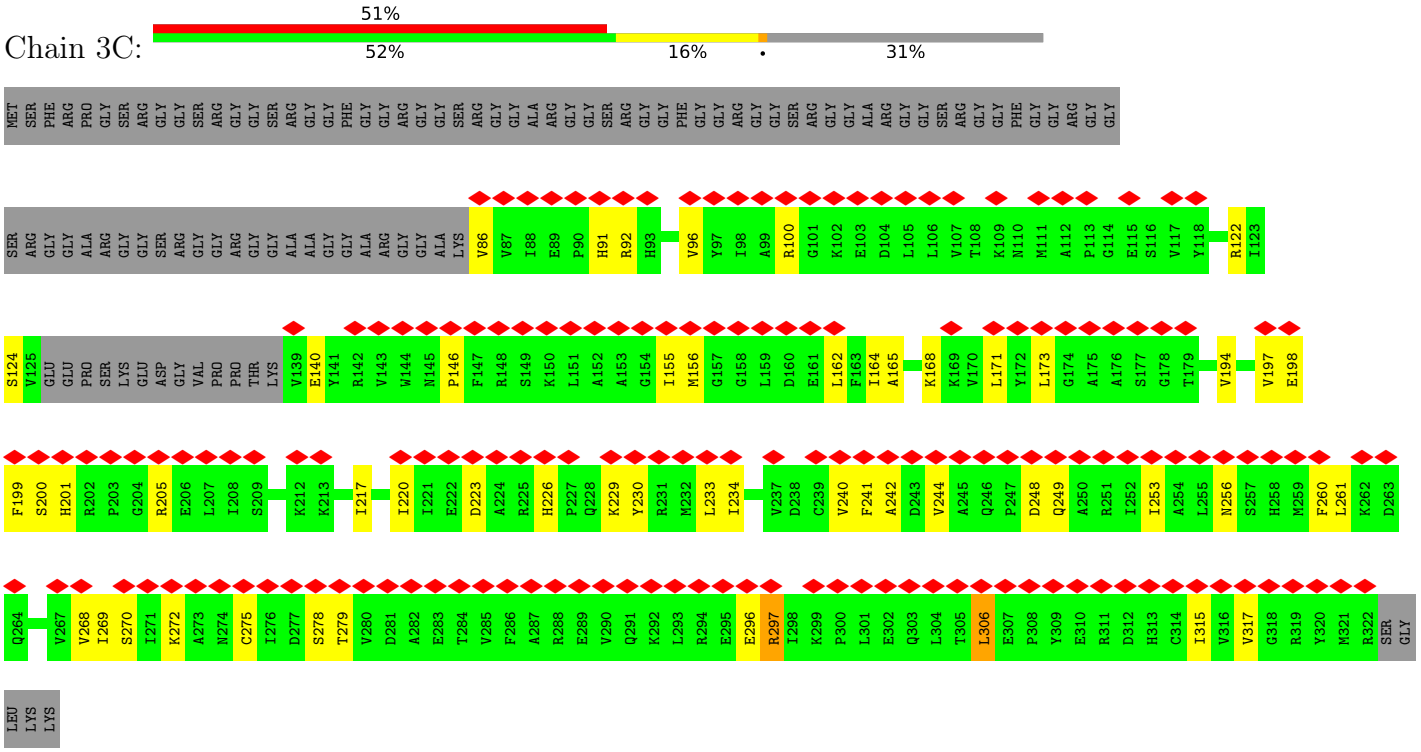
• Molecule 20: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:



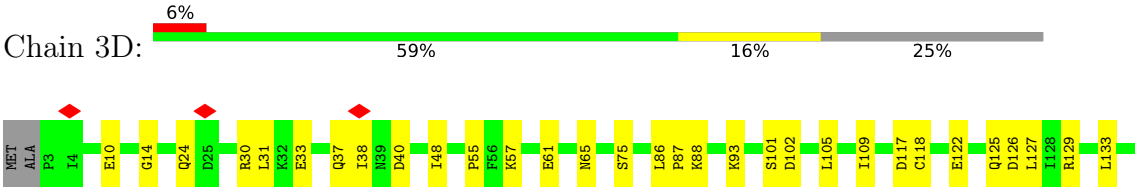
• Molecule 20: rRNA 2'-O-methyltransferase fibrillarin

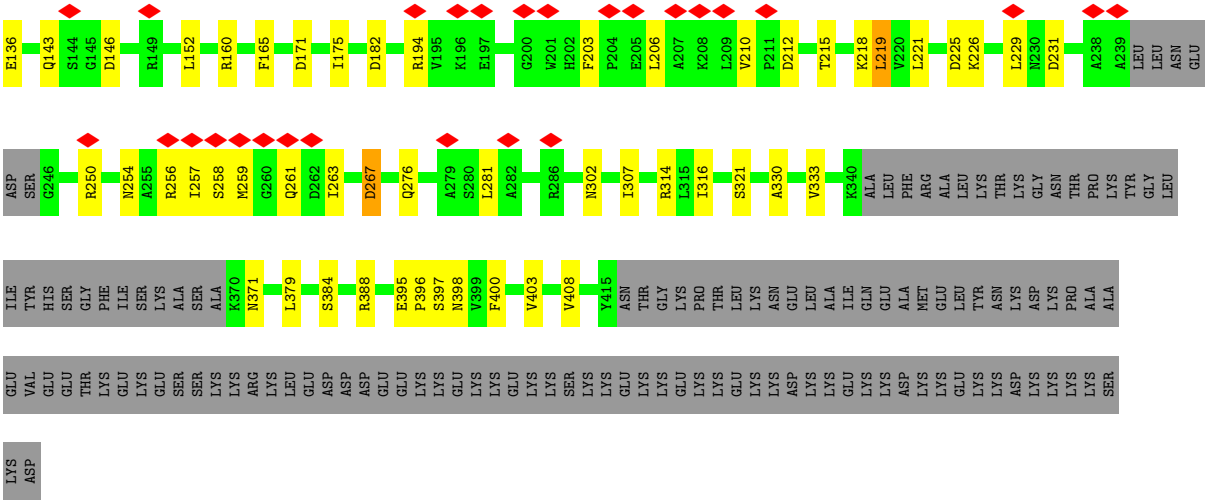
Chain 3C:



• Molecule 21: Nucleolar protein 56

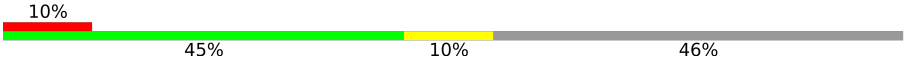
Chain 3D:

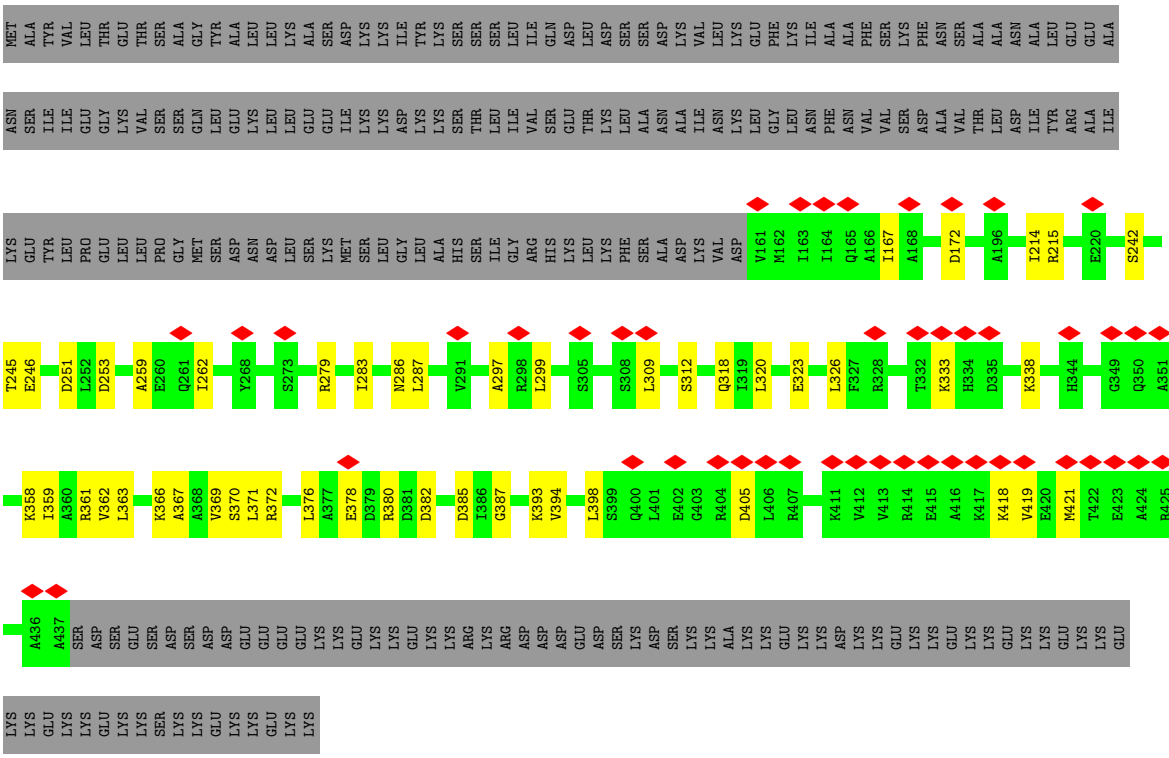




• Molecule 22: Nucleolar protein 58

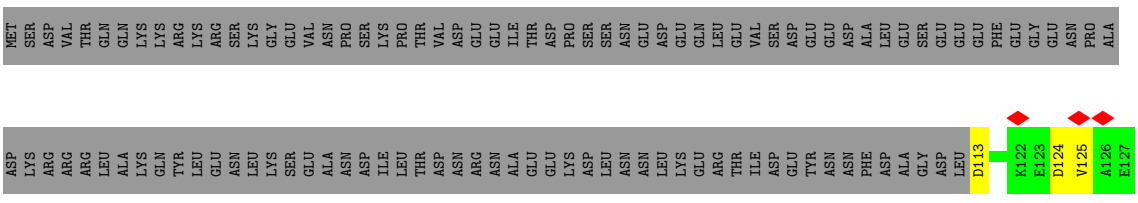
Chain 3E:

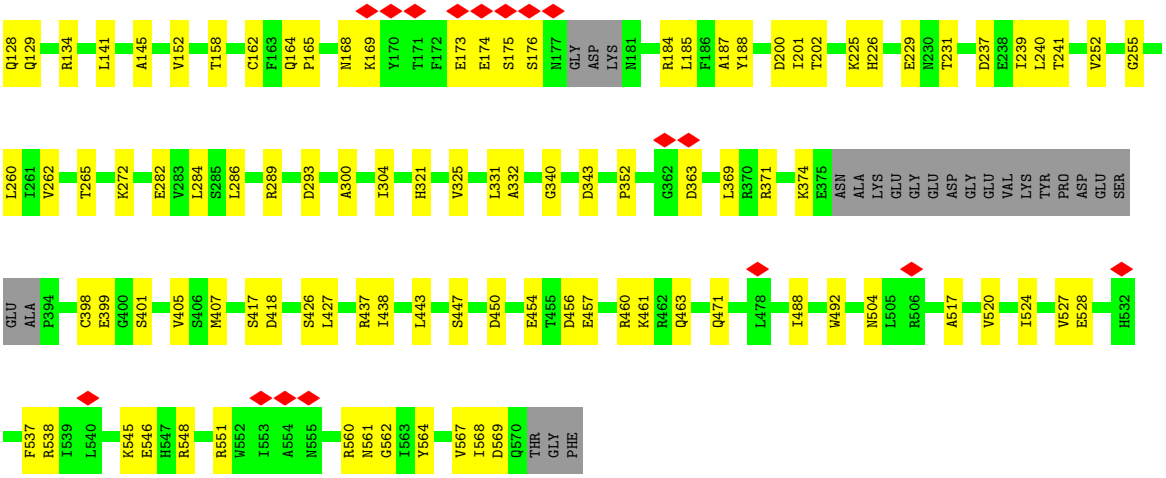




• Molecule 23: Ribosomal RNA-processing protein 9

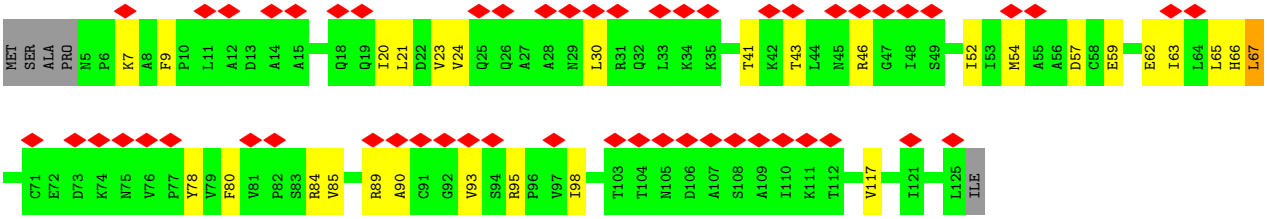
Chain 3F:





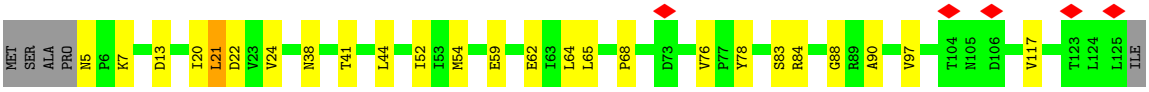
• Molecule 24: 13 kDa ribonucleoprotein-associated protein

Chain 3G:



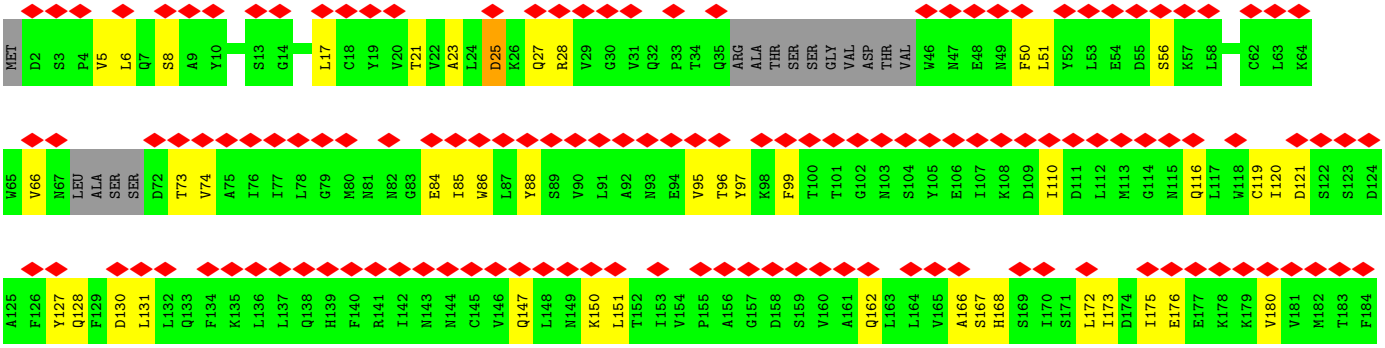
• Molecule 24: 13 kDa ribonucleoprotein-associated protein

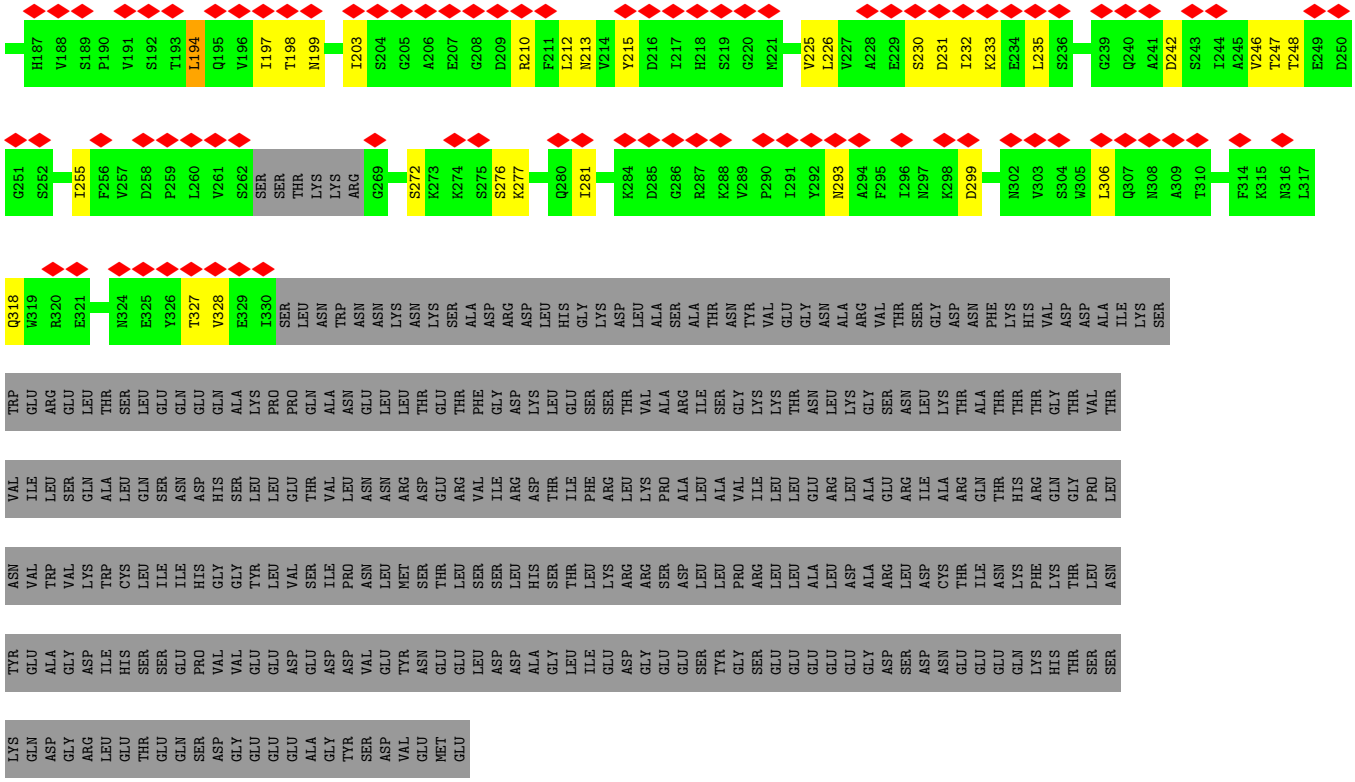
Chain 3H:



• Molecule 25: U3 small nucleolar RNA-associated protein 5

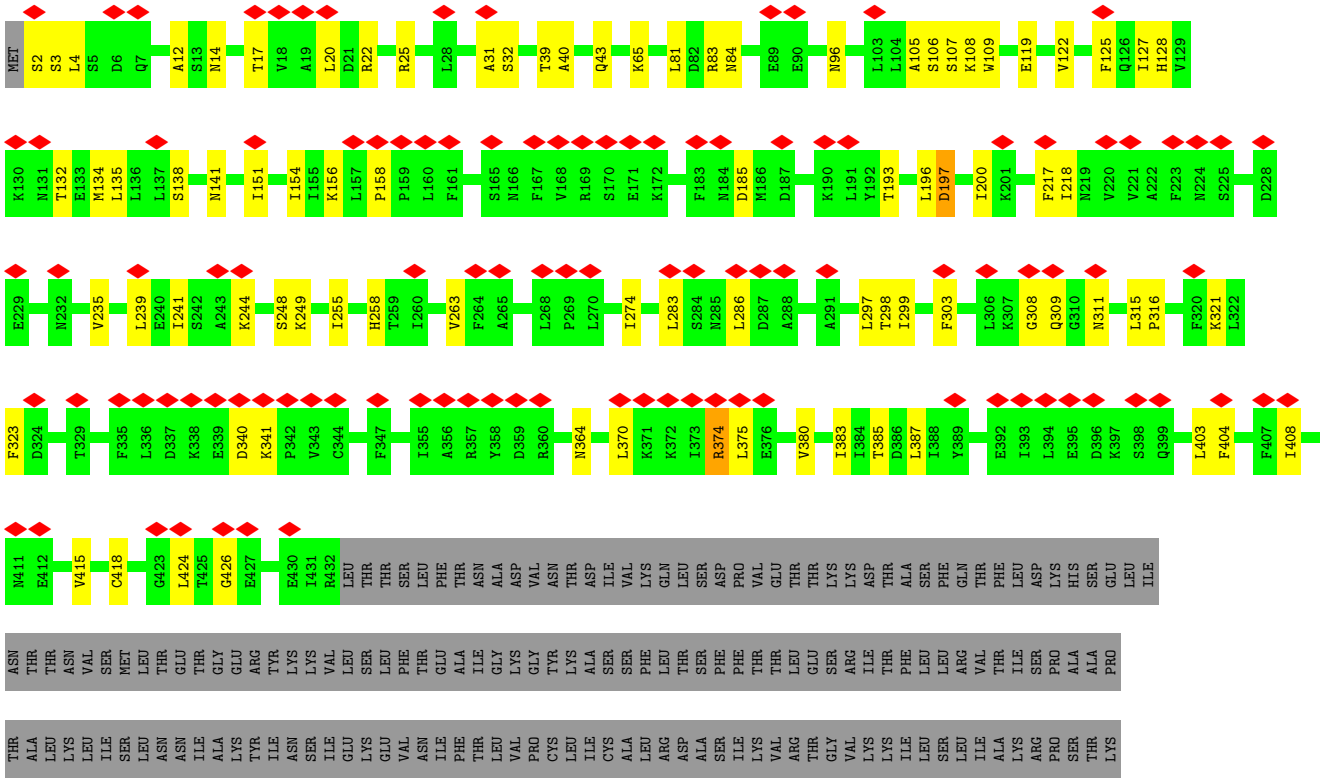
Chain A5:

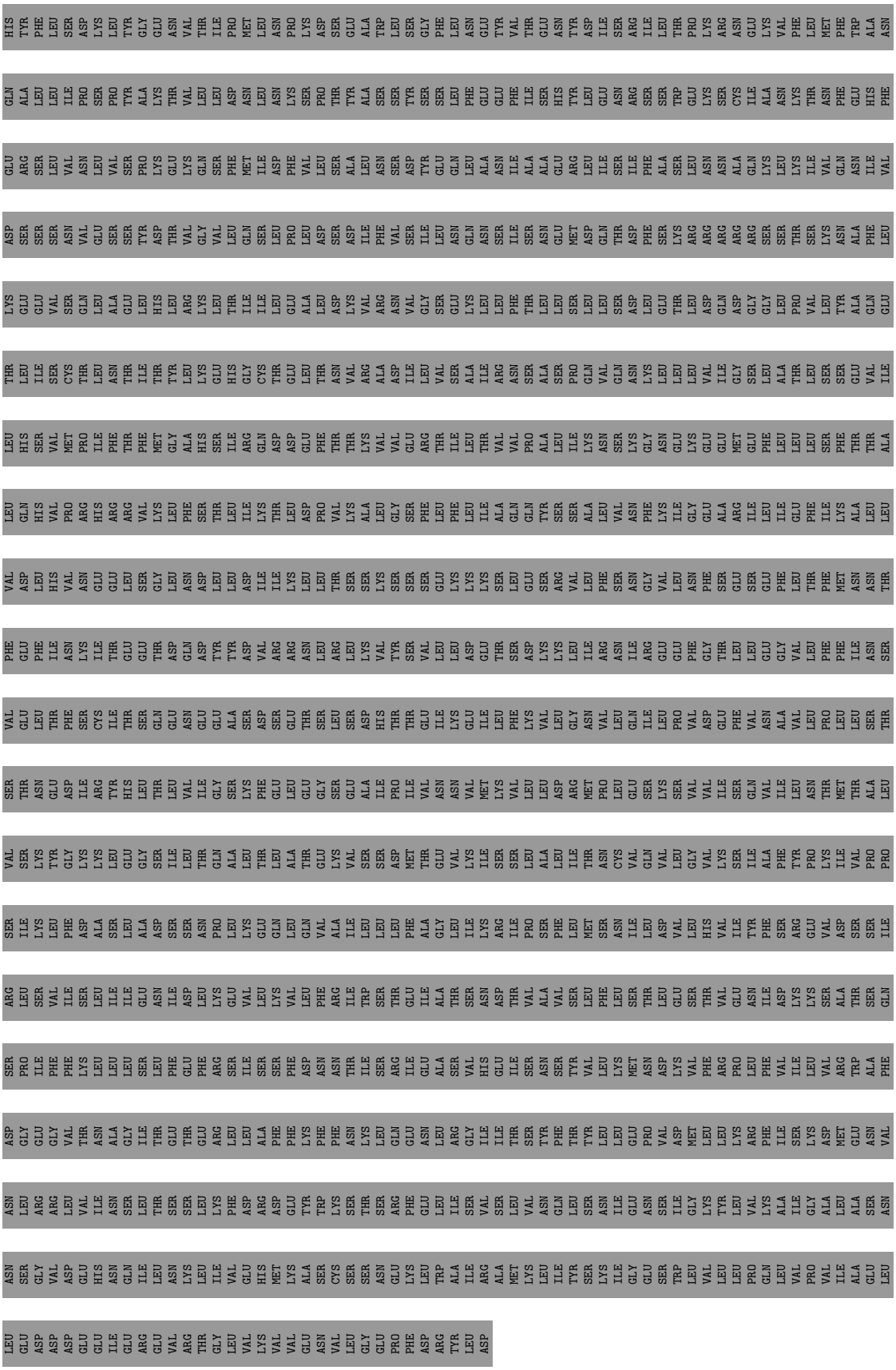




• Molecule 26: U3 small nucleolar RNA-associated protein 10

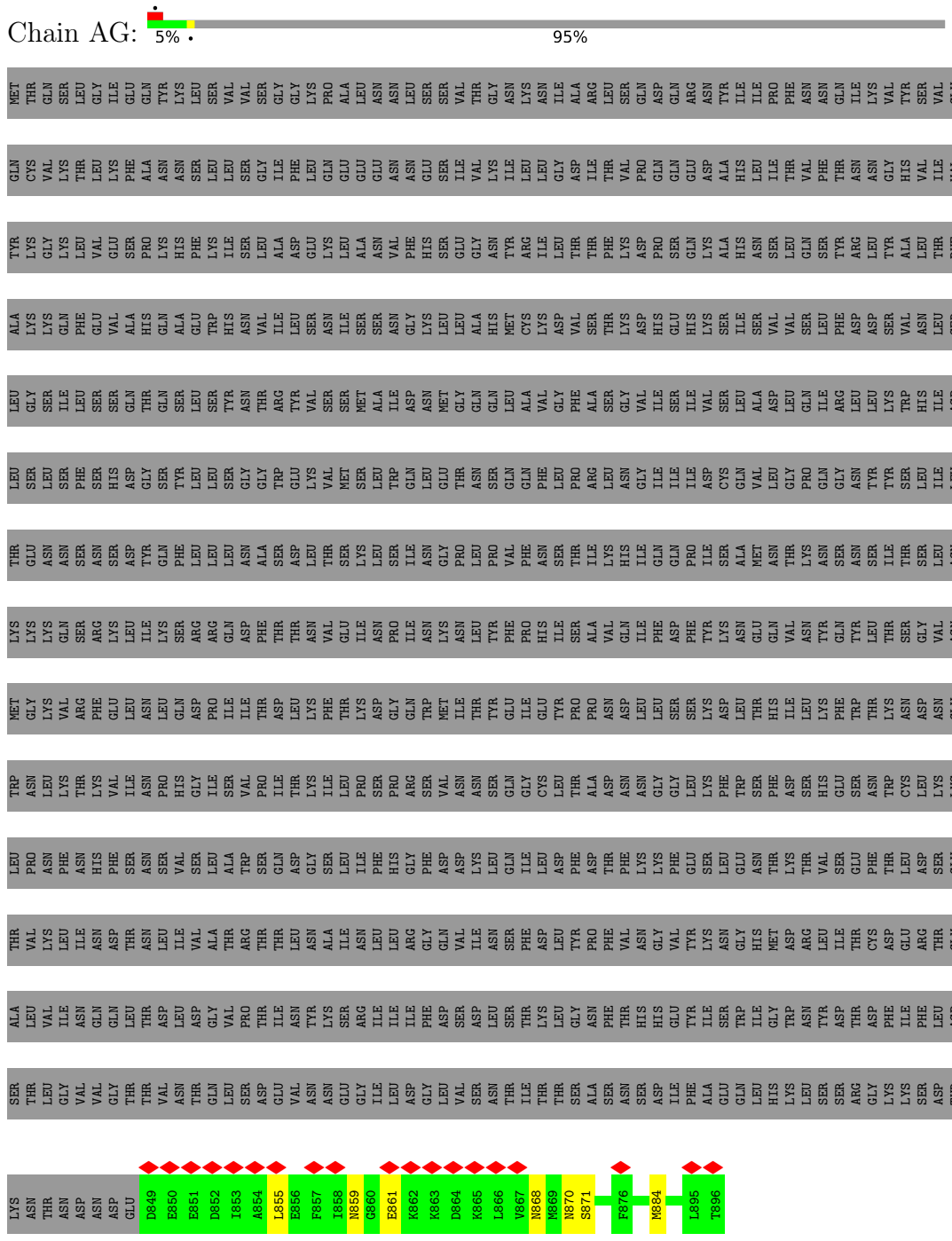
Chain AE:





• Molecule 27: NET1-associated nuclear protein 1

Chain AG:


5%
95%
MET THR GLN SER LEU GLY ILE GLU GLN TYR LYS LEU SER VAL VAL SER GLY GLY LYS PRO ALA LEU ASN ASN LEU SER SER VAL THR GLY ASN LYS ASN ILE ALA ARG LEU SER GLN ASP GLN ARG ASN TYR ILE ILE PRO PHE ASN ASN GLN ILE LYS VAL TYR SER VAL GLU THR ARG
GLN CYS VAL LYS THR LEU LYS PHE ALA ASN ASN SER LEU LEU SER GLY ILE PHE LEU GLN GLU GLU ASN ASN GLU SER ILE VAL LYS ILE LEU LEU GLY ASP ILE THR VAL PRO GLN GLN GLU ASP ALA HIS LEU ILE THR VAL PHE THR ASN ASN GLY HIS VAL ILE VAL LEU ASN
TYR LYS GLY LYS LEU VAL GLU SER PRO LYS HIS PHE LYS ILE SER LEU ALA ASP GLU LYS LEU ALA ASN VAL PHE HIS SER GLU GLY ASN TYR ARG ILE LEU THR THR PHE LYS ASP PRO SER GLN LYS ALA HIS ASN SER LEU GLN SER TYR ARG LEU TYR ALA LEU THR PHE ASP ASP
ALA LYS LYS GLN PHE GLU VAL ALA HIS GLN ALA GLU TRP HIS ASN VAL ILE LEU SER ASN ILE SER SER ASN GLY LYS LEU LEU ALA HIS MET CYS LYS ASP VAL SER THR LYS ASP HIS GLU HIS LYS SER ILE SER VAL VAL SER LEU PHE ASP ASP SER VAL ASN LEU SER PHE PRO
LEU GLY SER ILE LEU SER SER GLN THR GLN SER LEU SER TYR ASN THR ARG TYR VAL SER SER MET ALA ILE ASP ASN MET GLY GLN GLN LEU ALA VAL GLY PHE ALA SER GLY VAL ILE SER ILE VAL SER LEU ALA ASP LEU GLN ILE ARG LEU LEU LYS TRP HIS ILE ASP SER VAL
LEU SER LEU SER PHE SER HIS ASP GLY SER TYR LEU LEU SER GLY GLY TRP GLU LYS VAL MET SER LEU TRP GLN LEU GLU THR ASN SER GLN GLN LEU ALA VAL GLN PHE LEU PRO ARG LEU ASN GLY ILE ILE ILE ASP CYS GLN VAL LEU GLY PRO GLN GLN GLY ASN TYR TYR SER LEU ILE LEU GLN LEU
THR GLU ASN ASN SER ASN SER ASP TYR GLN PHE LEU LEU LEU ASN ALA SER ASP LEU THR SER LYS LEU SER ILE ASN GLY PRO LEU PRO VAL PHE ASN SER THR ILE LYS HIS ILE GLN GLN PRO ILE SER ALA MET ASP ASN THR LYS ASN SER GLN GLN GLY ASN SER ASN SER ILE THR SER LEU ILE GLN ILE ARG LEU LEU GLN PRO GLN GLY ASN HIS SER
LYS LYS LYS GLN SER ARG LYS LEU ILE LYS SER ARG ARG GLN ASP PHE THR THR ASN VAL GLU ILE ASN PRO ILE ASN ASN LYS ASN LEU TYR PHE PRO HIS ILE SER ALA VAL GLN ILE PHE ASP PHE TYR LYS ASN GLU GLN VAL ASN TYR GLN TYR LEU LEU THR SER GLY VAL ASN ASN SER
MET GLY LYS VAL ARG PHE GLU LEU ASN LEU GLN ASP PRO ILE ILE THR ASP LEU LYS PHE THR LYS ASP GLY GLN TRP MET ILE THR TYR GLU ILE GLU TYR PRO PRO ASN ASP LEU LEU SER SER LYS ASP LEU THR HIS ILE LEU LYS PHE TRP THR LYS ASN ASP ASN GLU THR ASN
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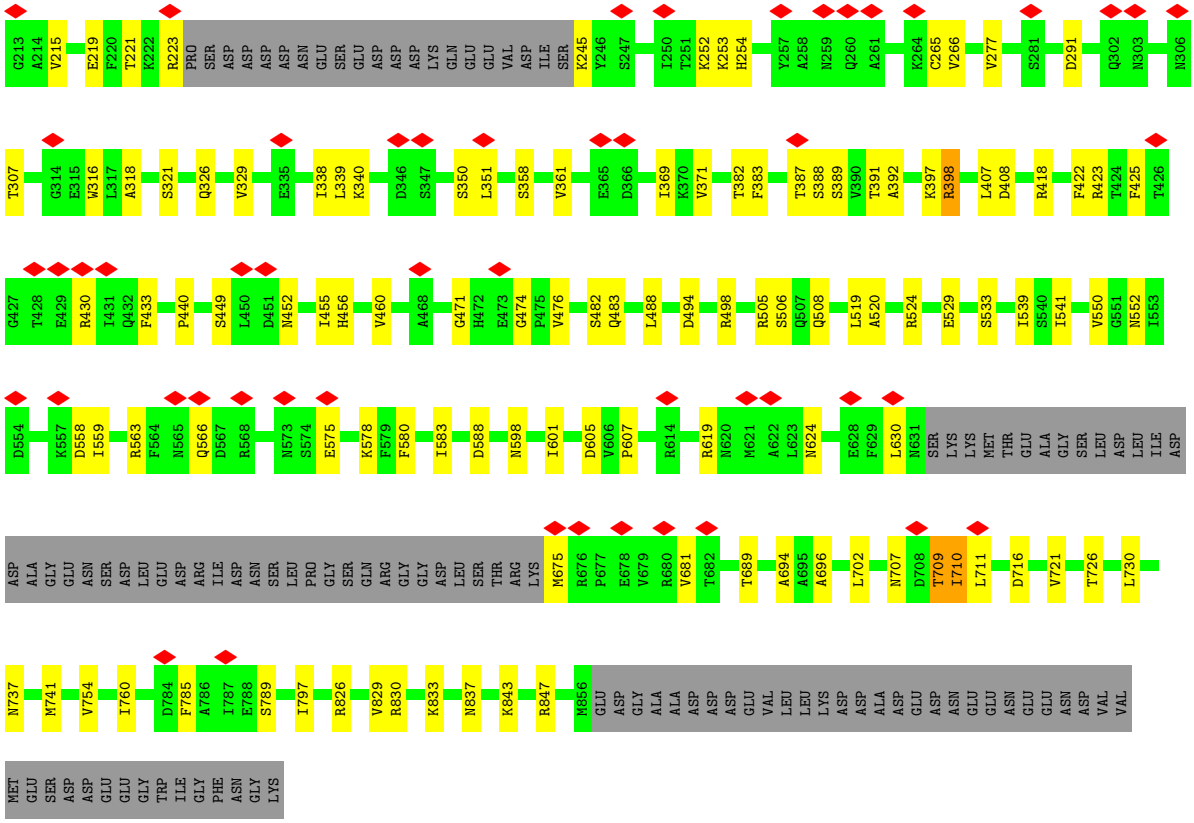
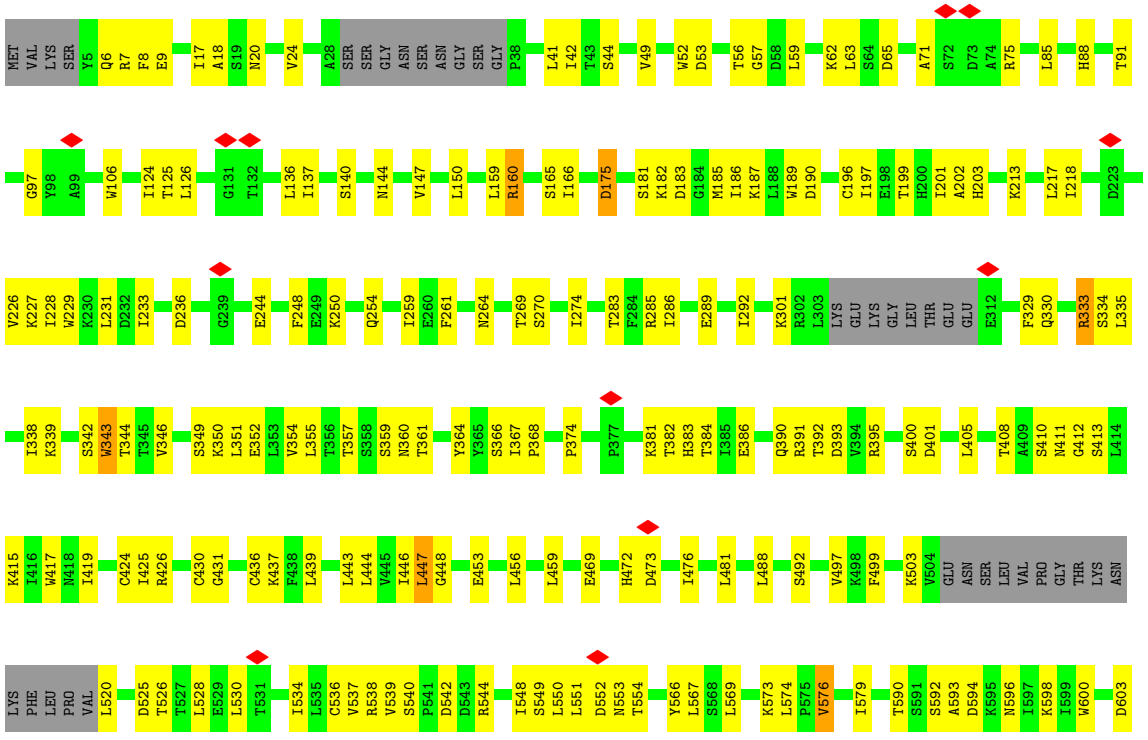
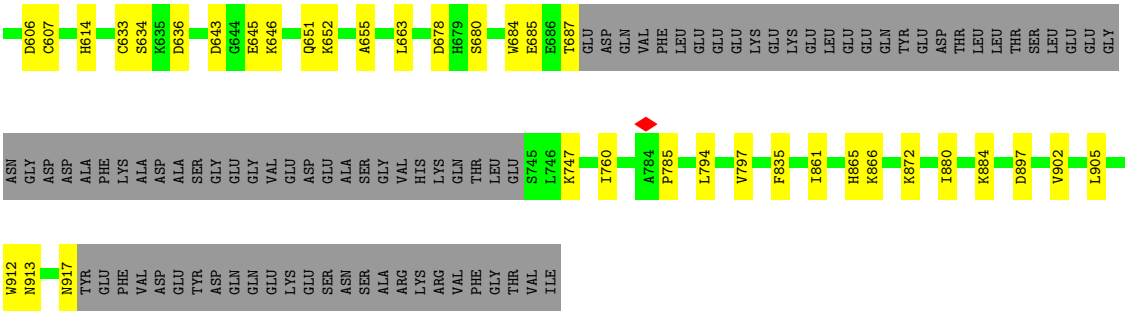


• Molecule 29: U3 small nucleolar RNA-associated protein 12

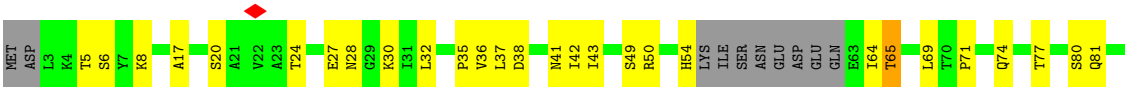
Chain B2:

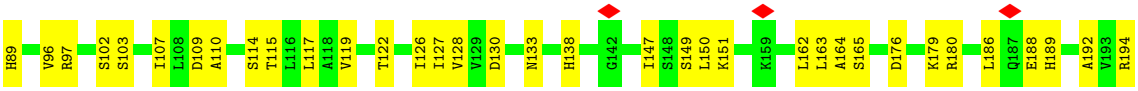


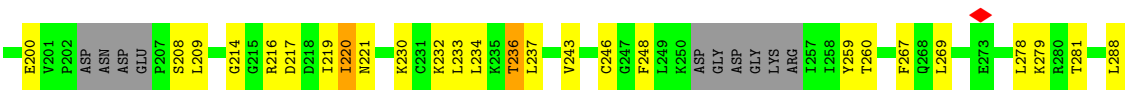


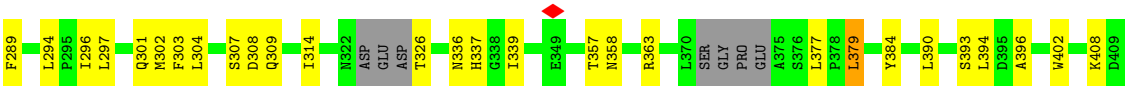
• Molecule 30: U3 small nucleolar RNA-associated protein 13

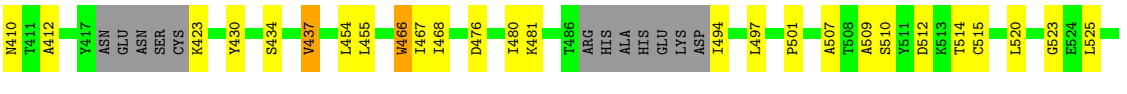
Chain B3:

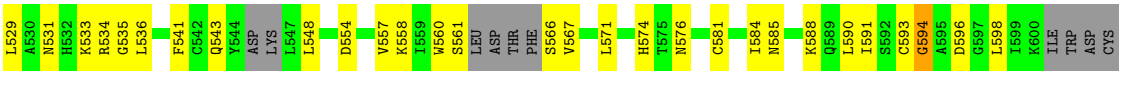


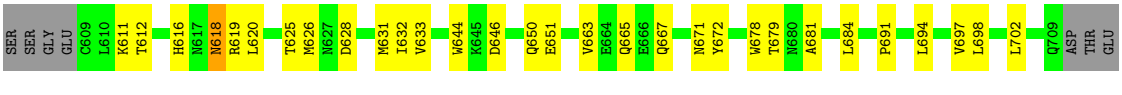


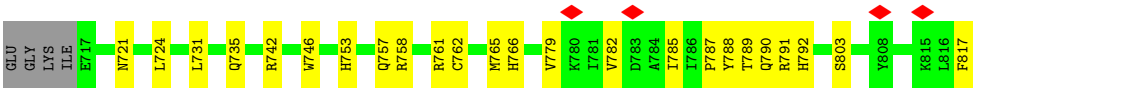


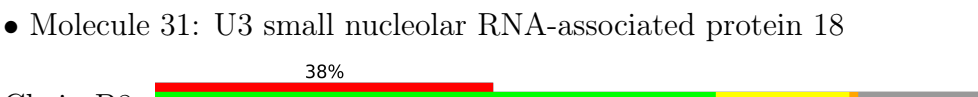






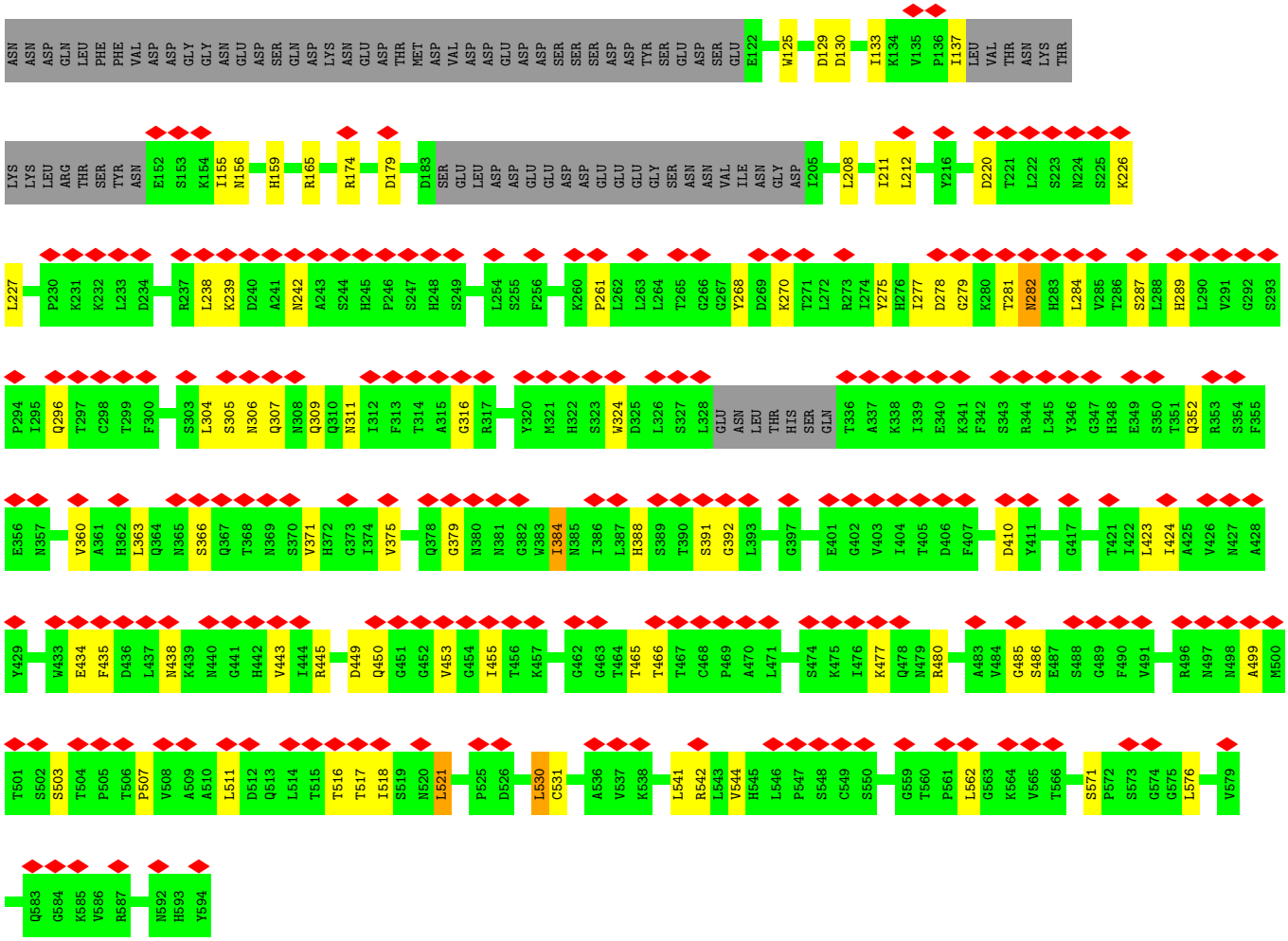






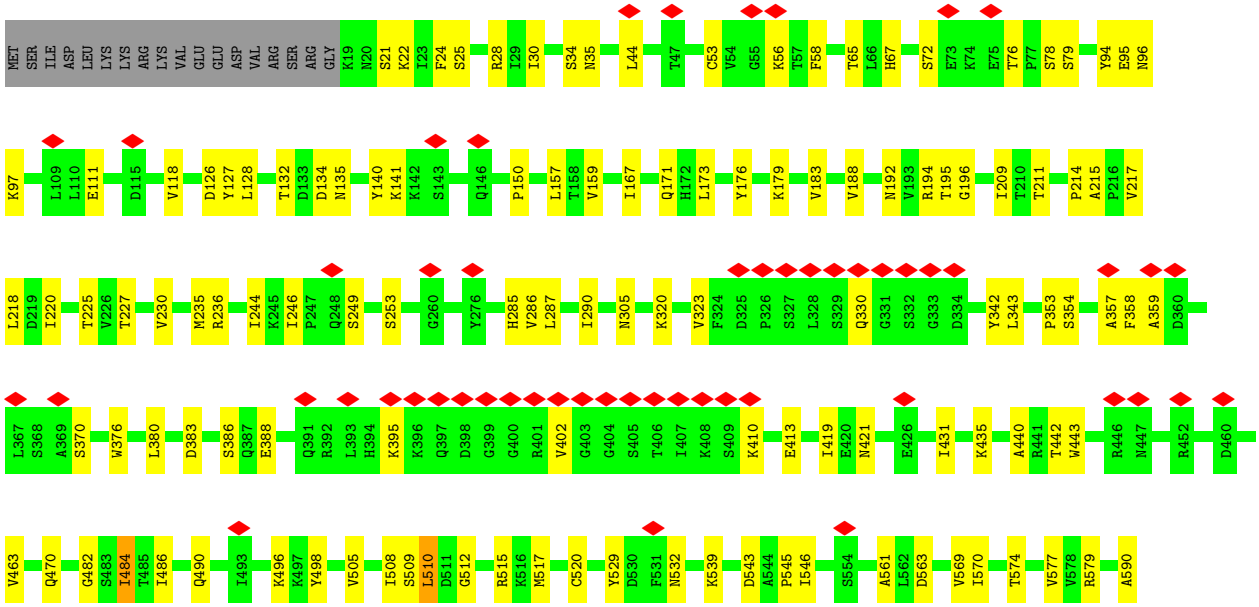
• Molecule 31: U3 small nucleolar RNA-associated protein 18

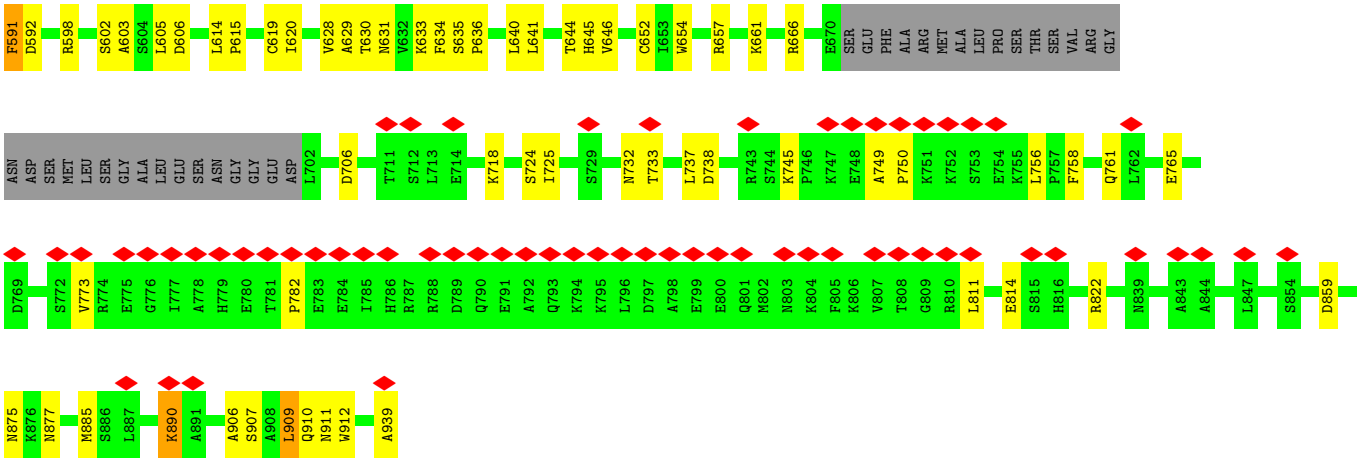
Chain B8:



• Molecule 32: U3 small nucleolar RNA-associated protein 21

Chain BE:





• Molecule 33: U3 small nucleolar RNA-associated protein 6

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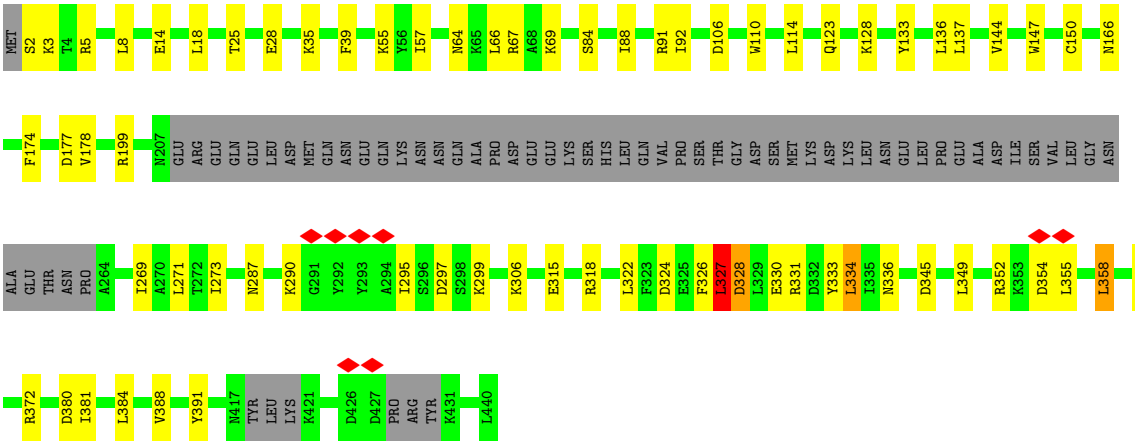
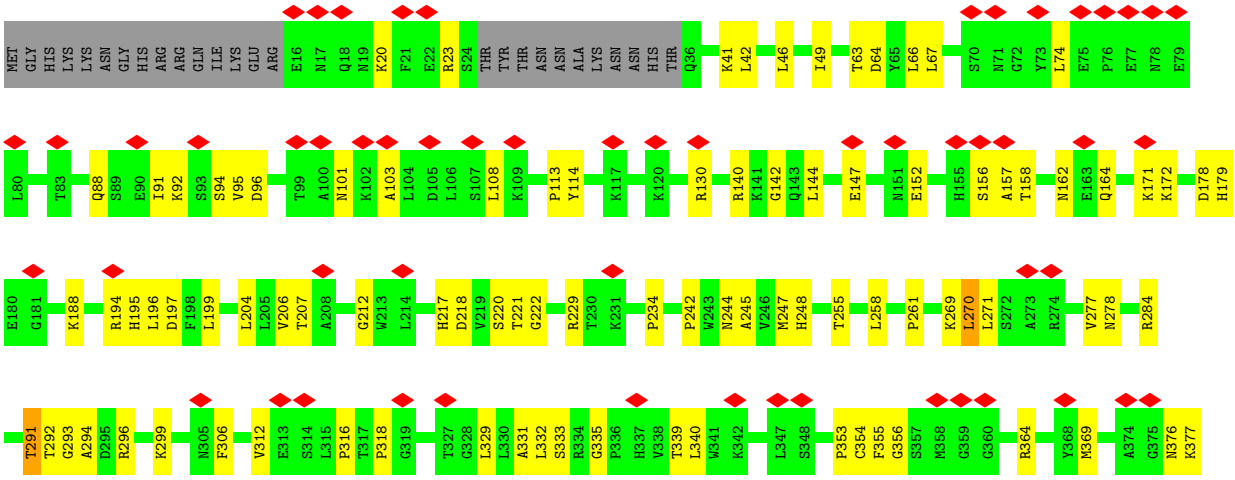
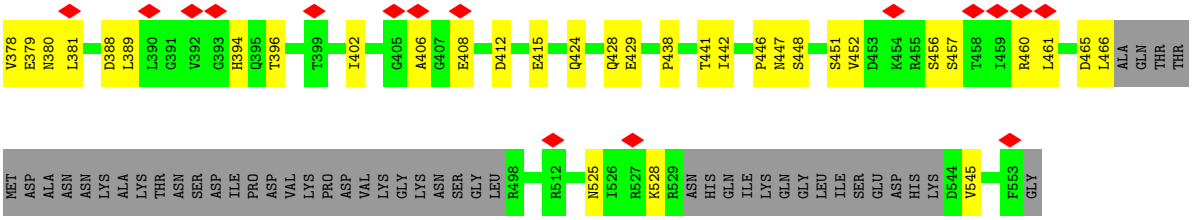


• Molecule 34: U3 small nucleolar RNA-associated protein 7

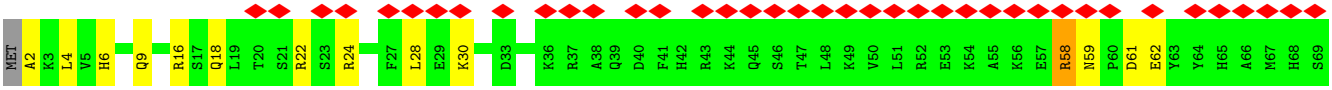
Chain 5C:





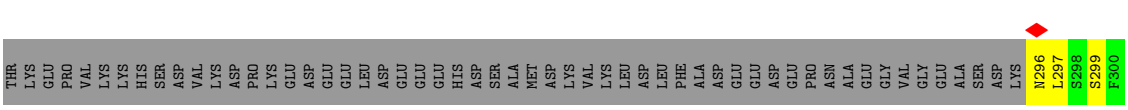
• Molecule 35: U3 small nucleolar RNA-associated protein 11

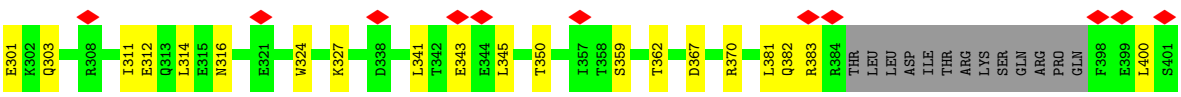
Chain 5D:

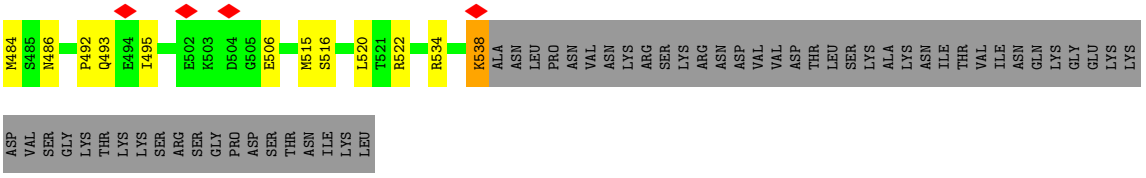


• Molecule 36: U3 small nucleolar RNA-associated protein MPP10

Chain 5E:

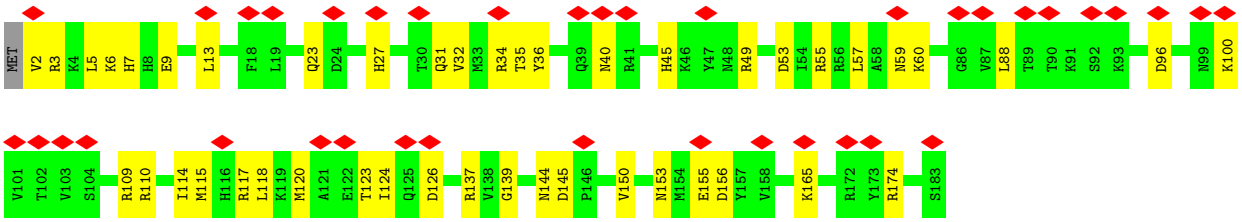






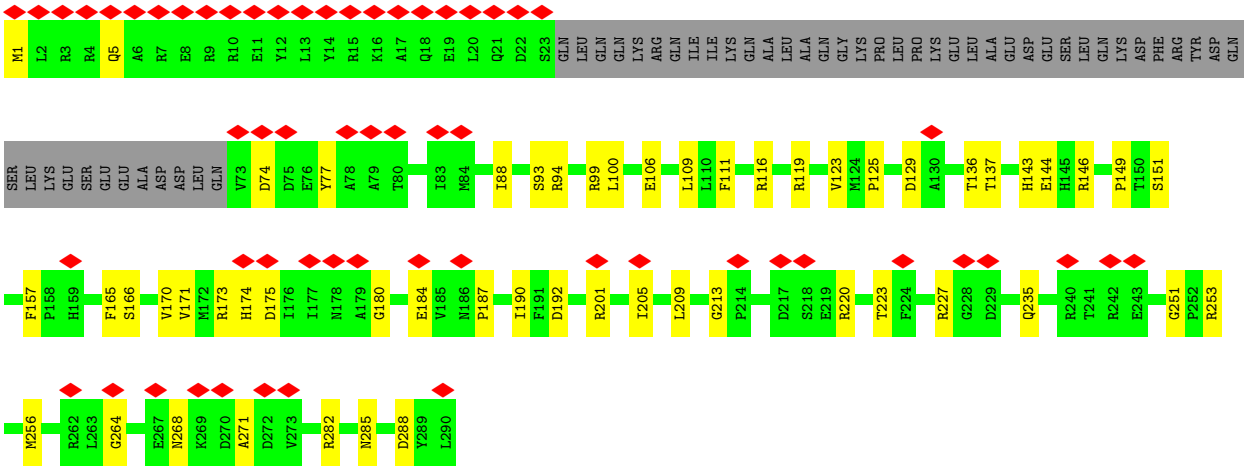
• Molecule 37: U3 small nucleolar ribonucleoprotein protein IMP3

Chain 5F:



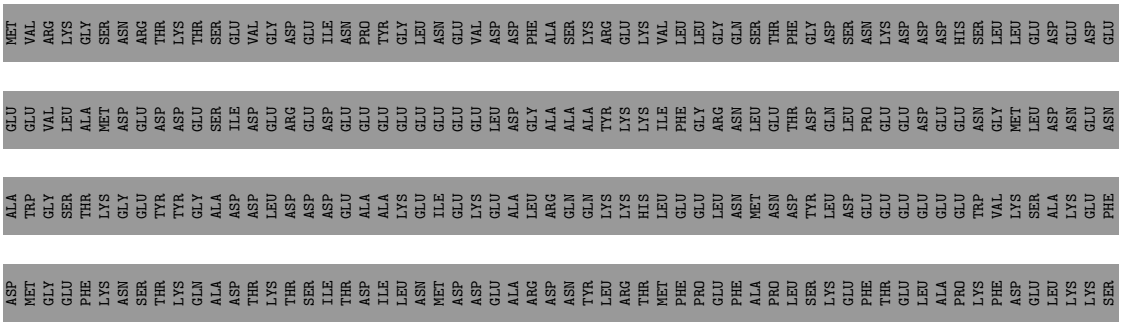
• Molecule 38: U3 small nucleolar ribonucleoprotein protein IMP4

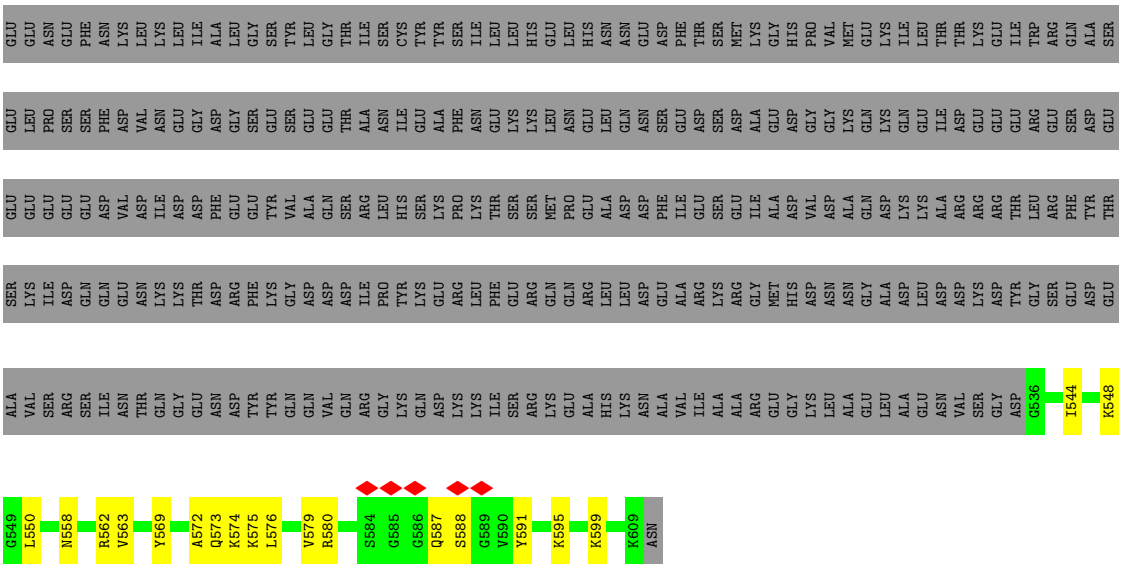
Chain 5G:



• Molecule 39: Something about silencing protein 10

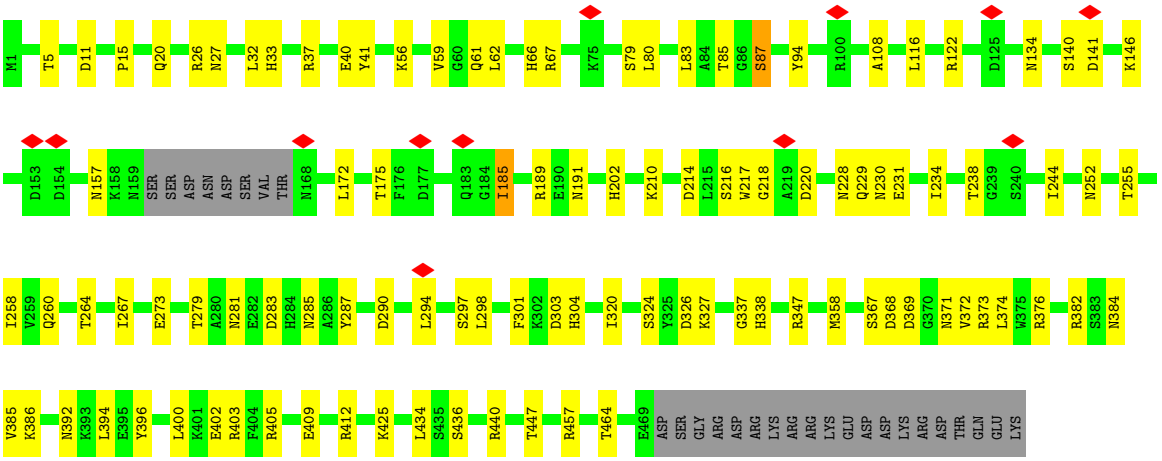
Chain 5H:





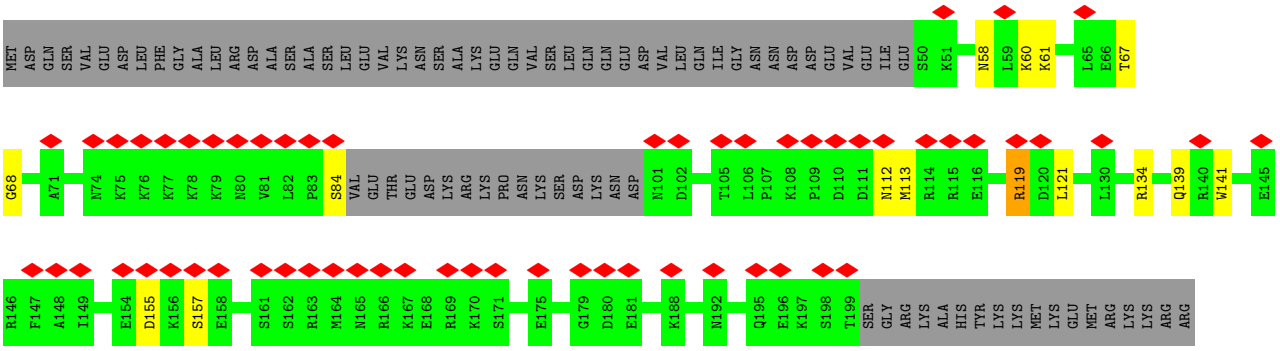
• Molecule 40: Protein SOF1

Chain 5I:



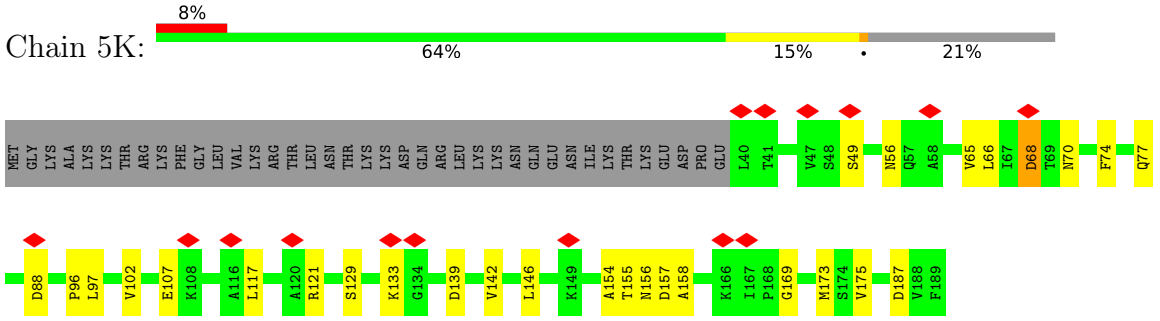
• Molecule 41: rRNA-processing protein FCF2

Chain 5J:



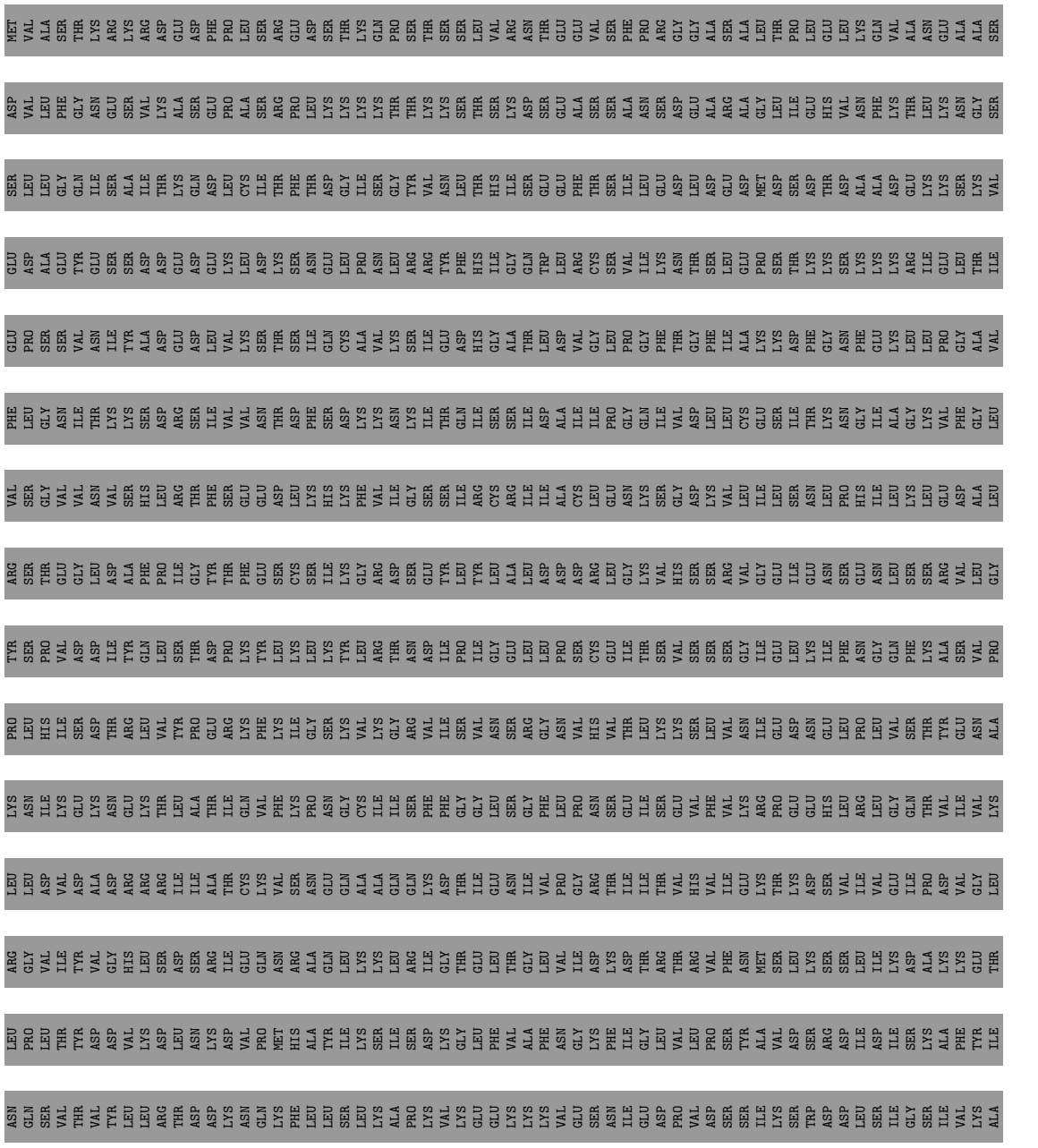
• Molecule 42: rRNA-processing protein FCF1

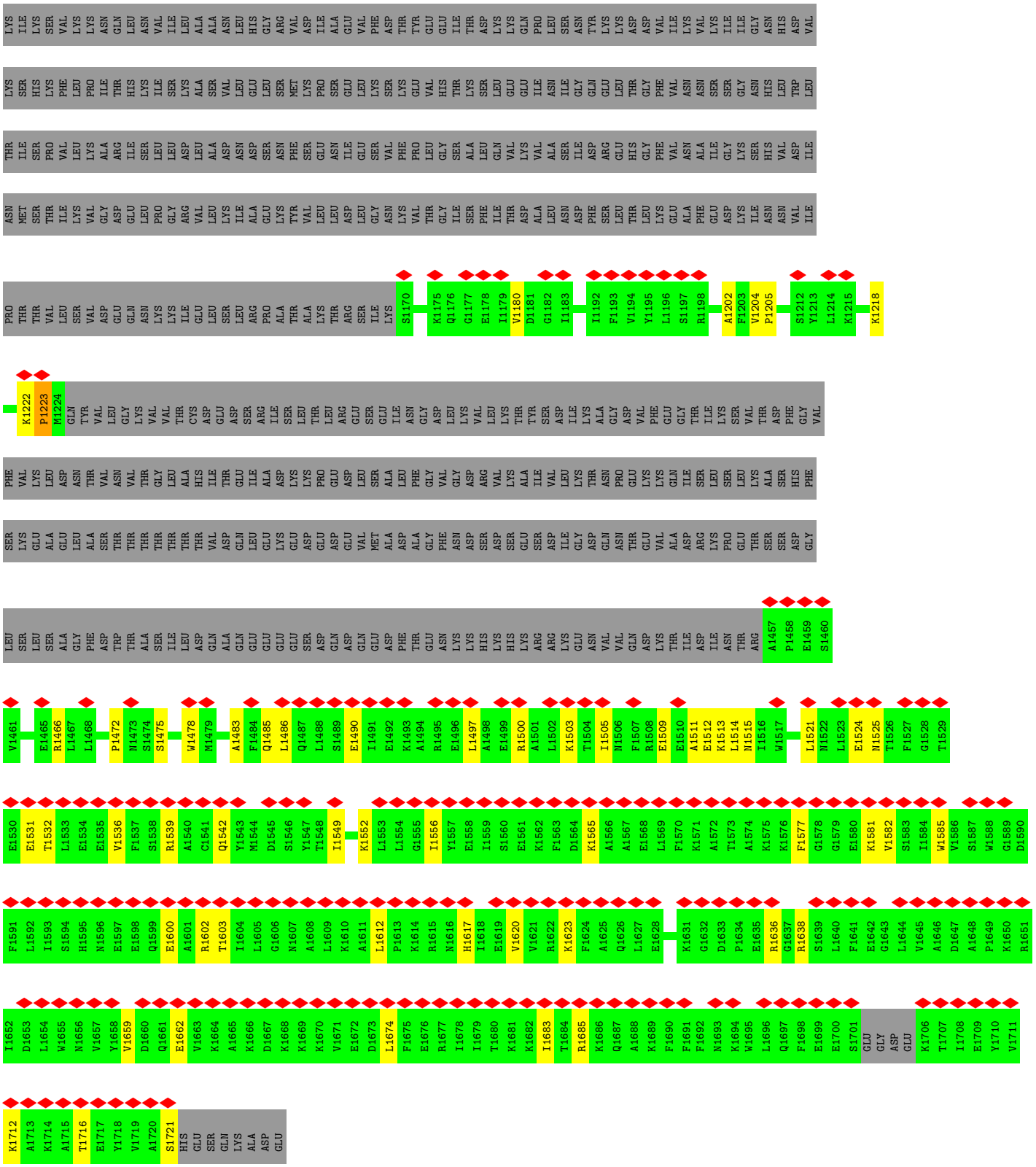
Chain 5K:



• Molecule 43: rRNA biogenesis protein RRP5

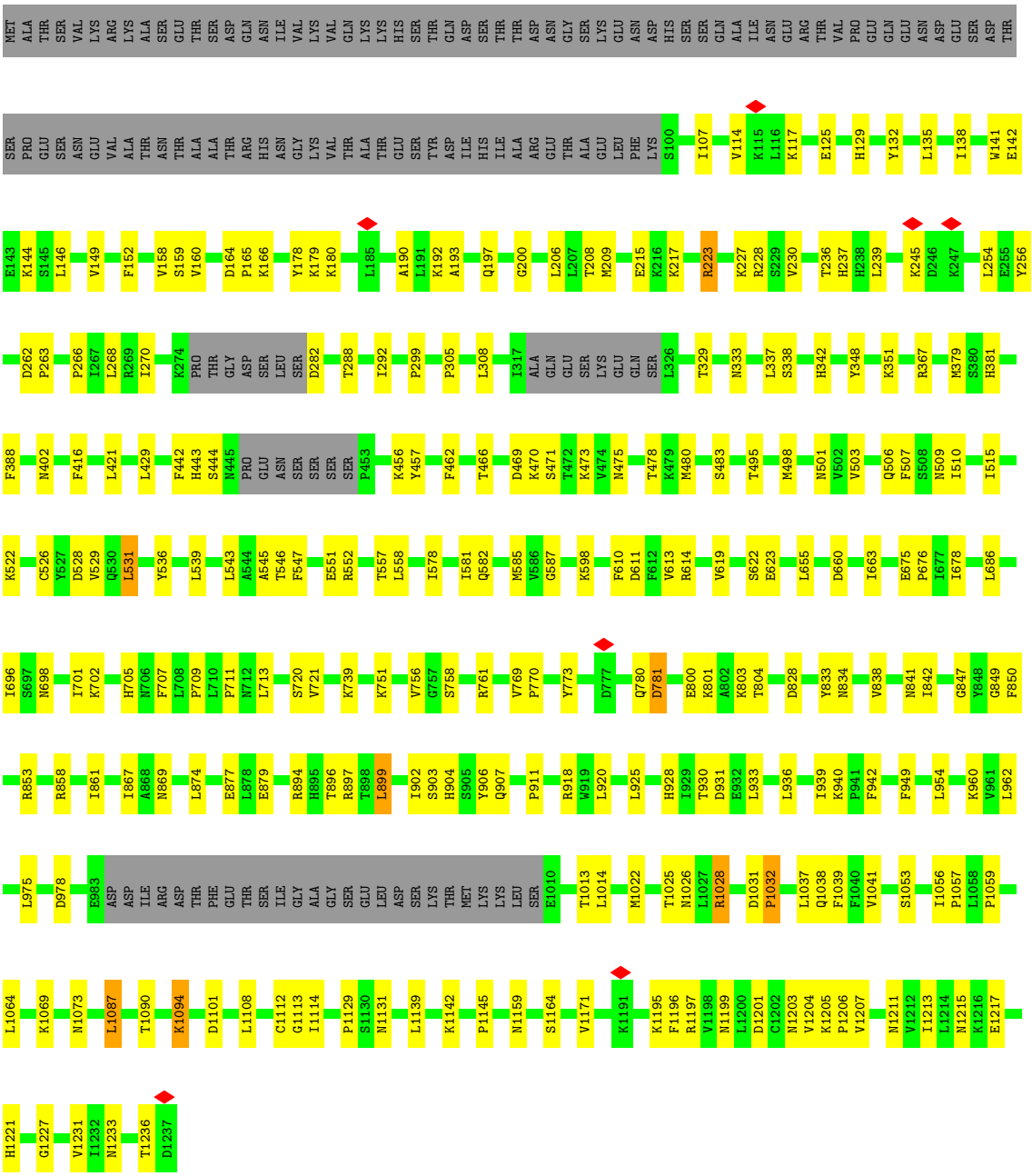
Chain RD:





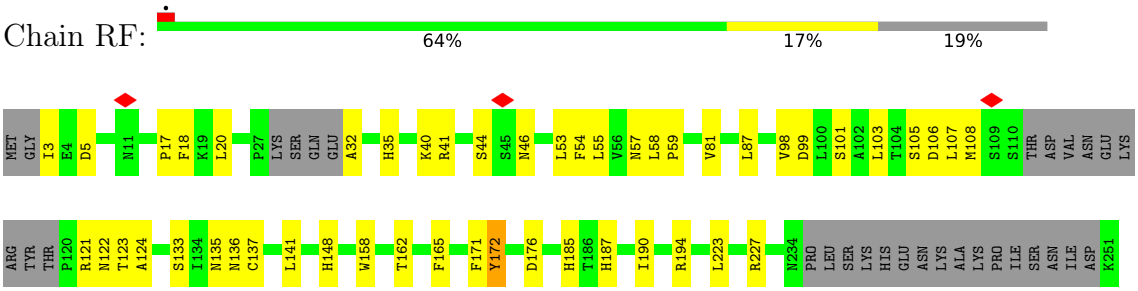
• Molecule 44: U3 small nucleolar RNA-associated protein 22

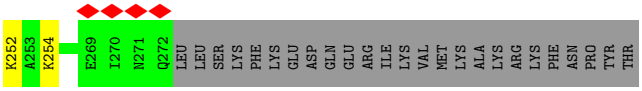
Chain RE:



• Molecule 45: Ribosomal RNA-processing protein 7

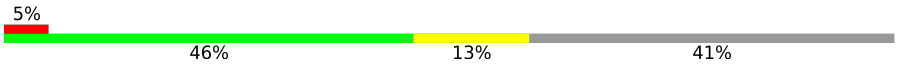
Chain RF:

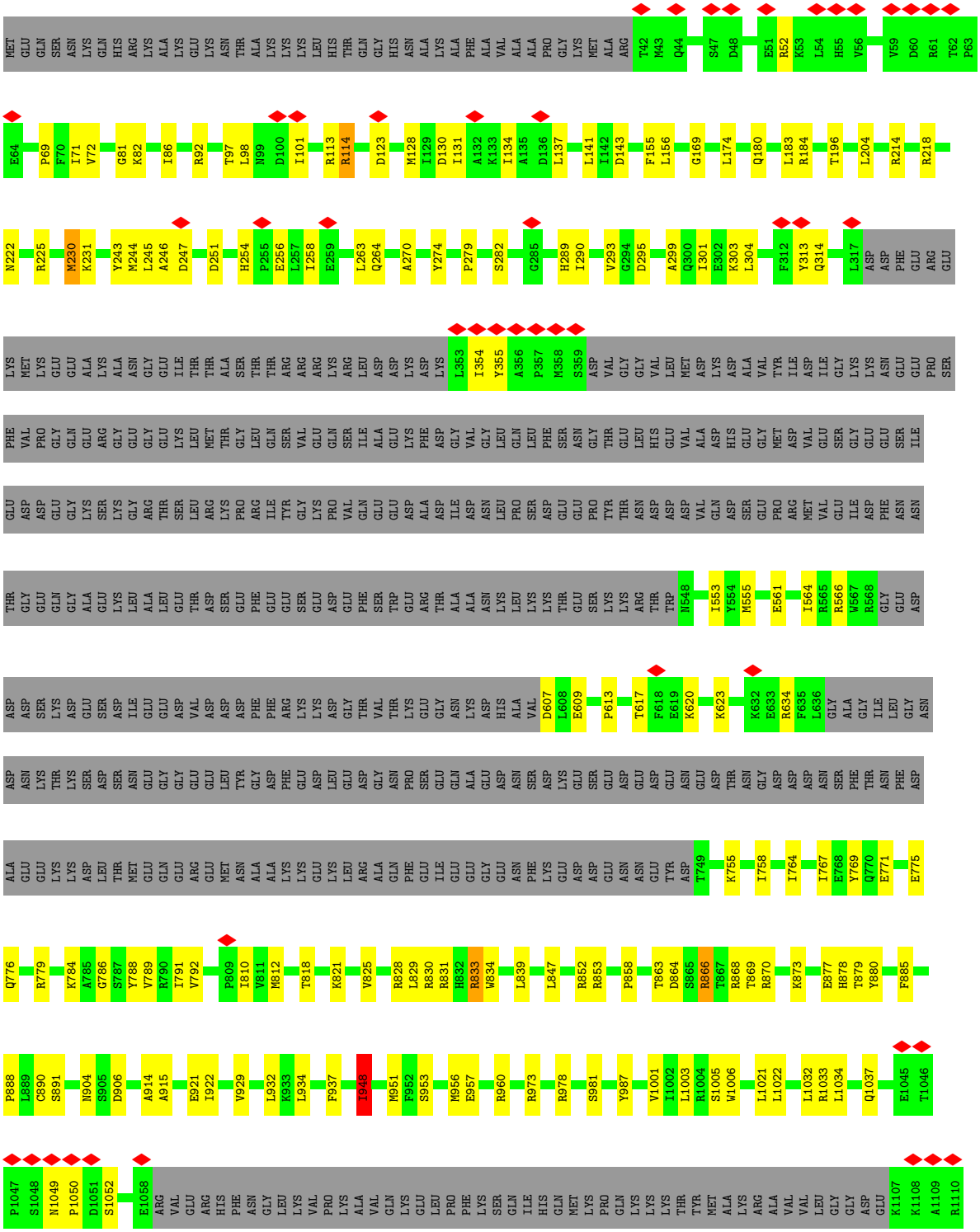


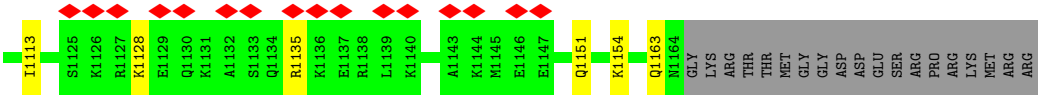


• Molecule 46: Ribosome biogenesis protein BMS1

Chain RJ:

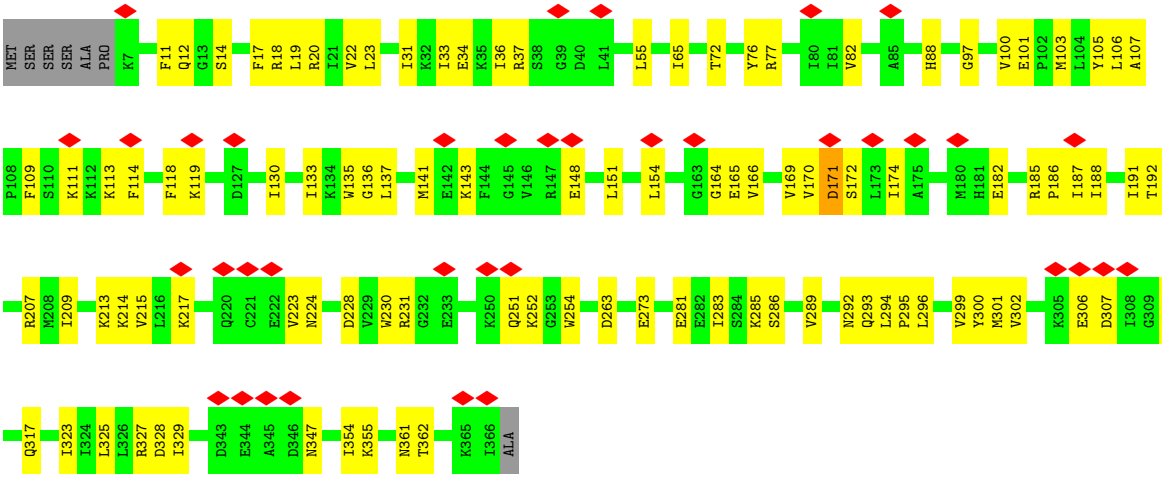






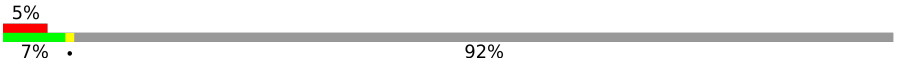
• Molecule 47: RNA 3'-terminal phosphate cyclase-like protein

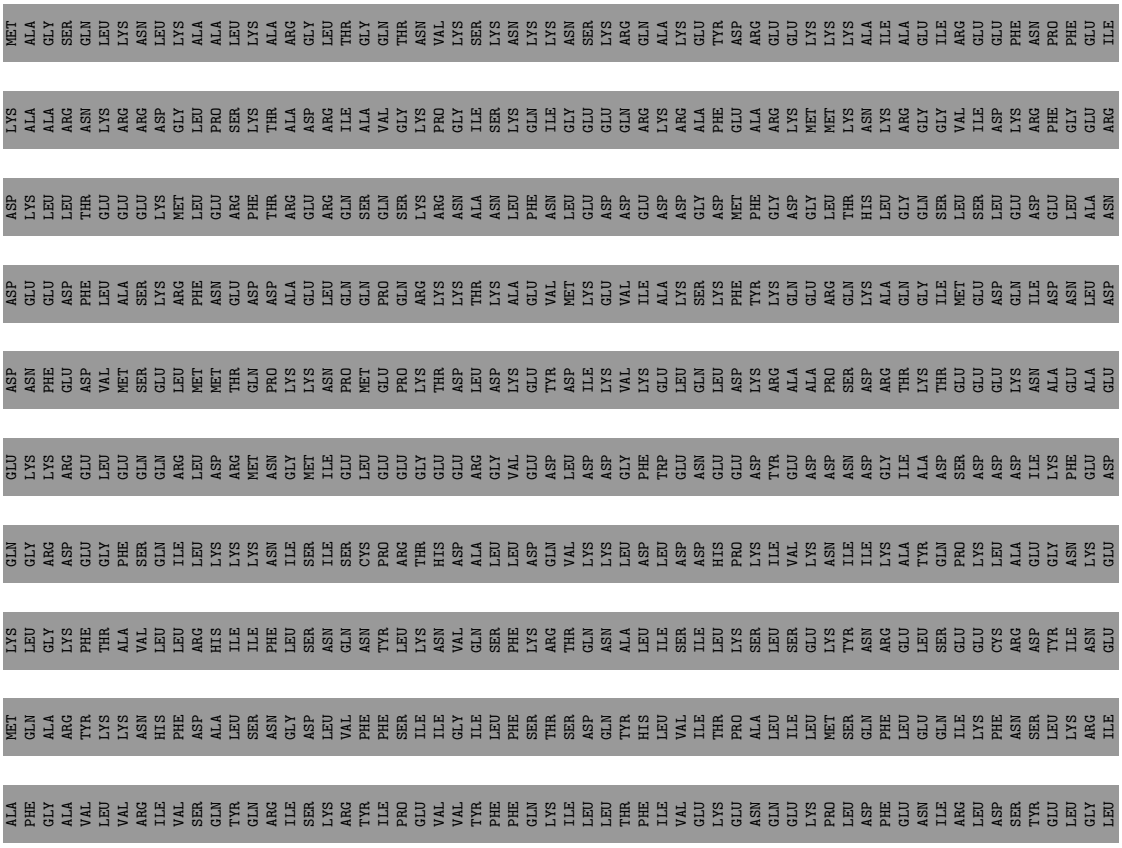
Chain RK:

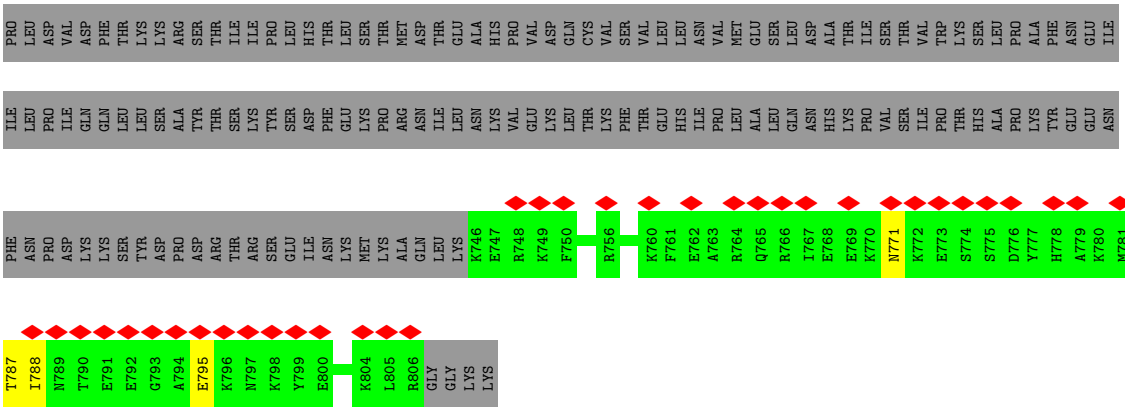


• Molecule 48: Nucleolar complex protein 14

Chain RN:

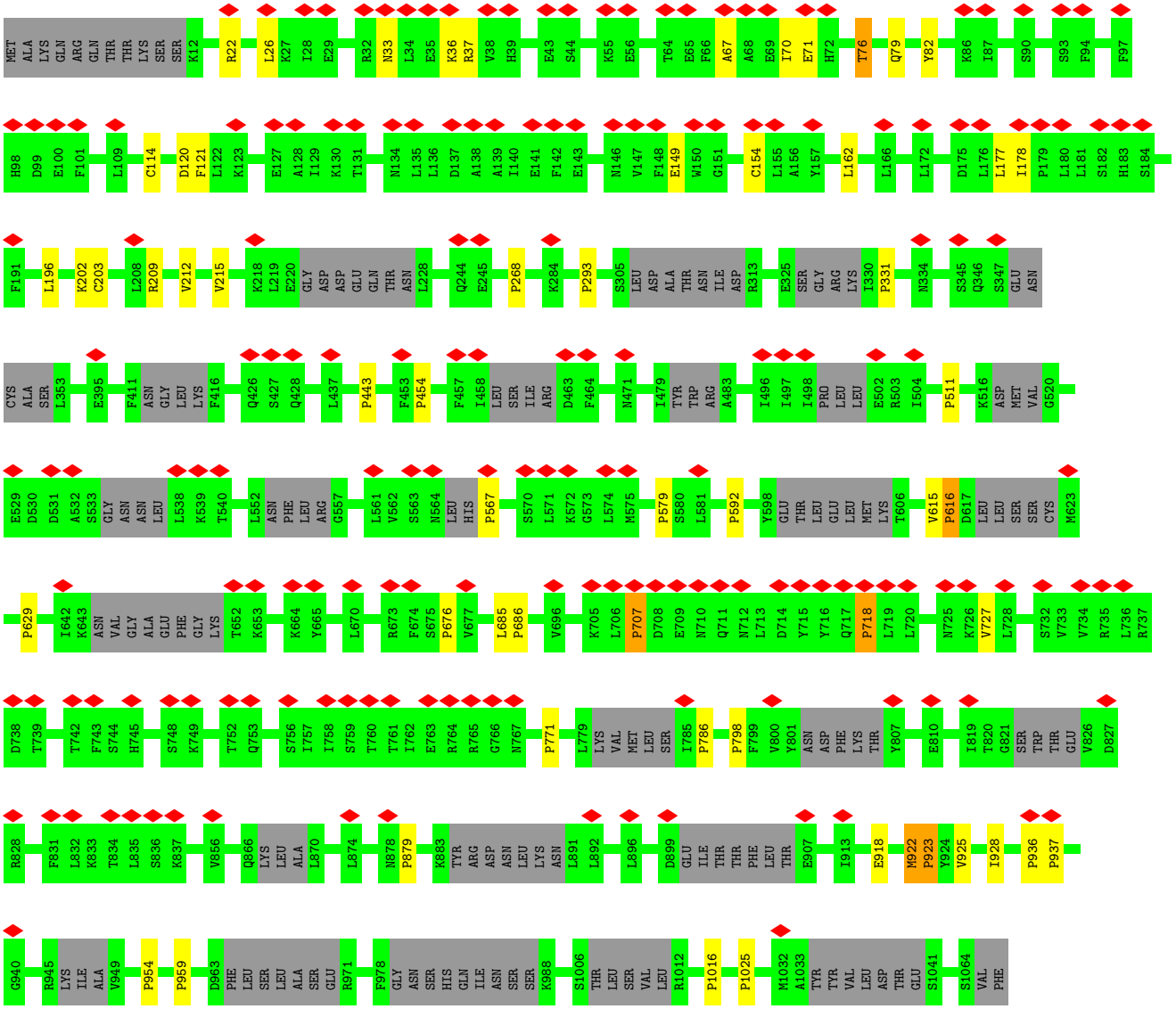


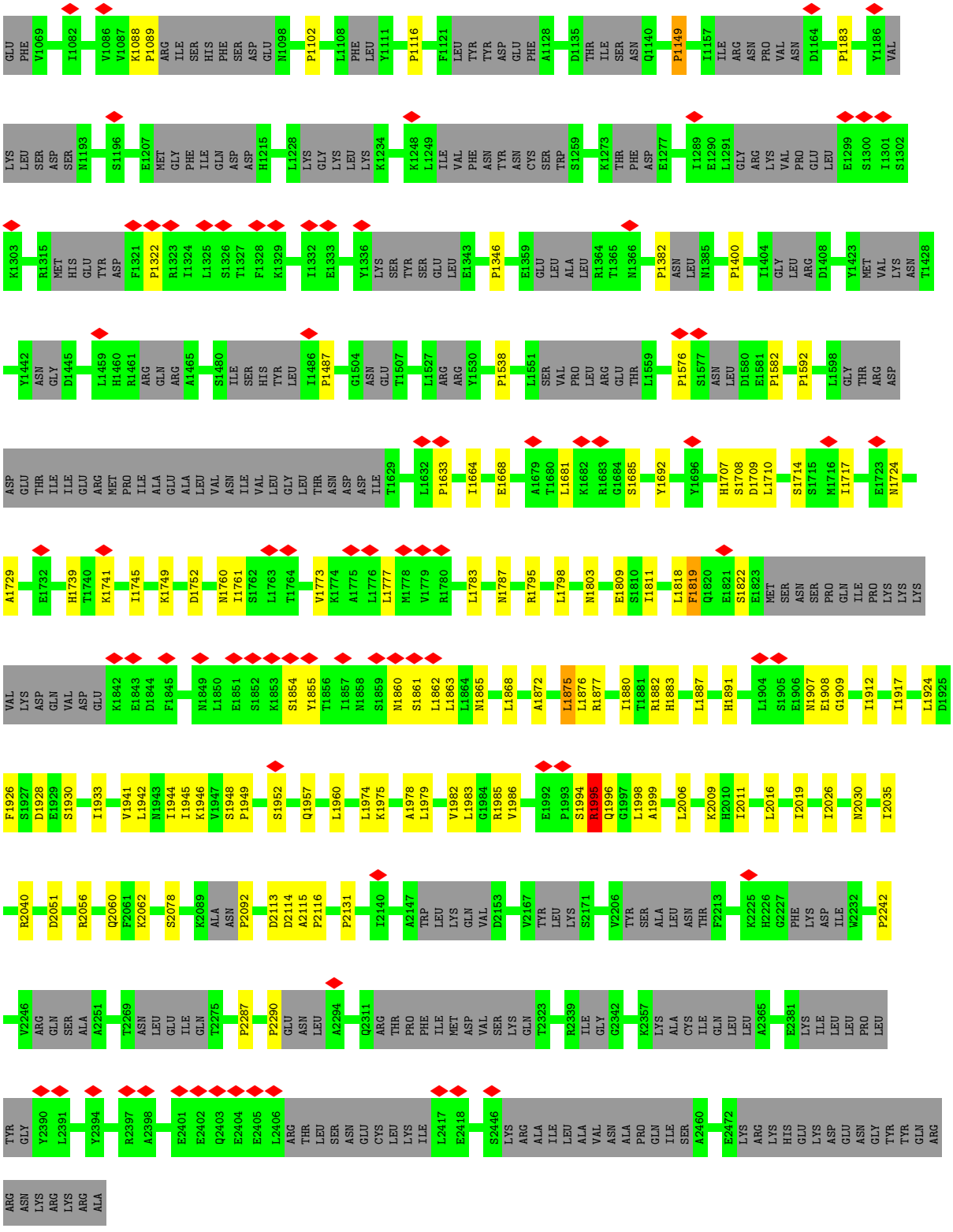




• Molecule 49: U3 small nucleolar RNA-associated protein 20

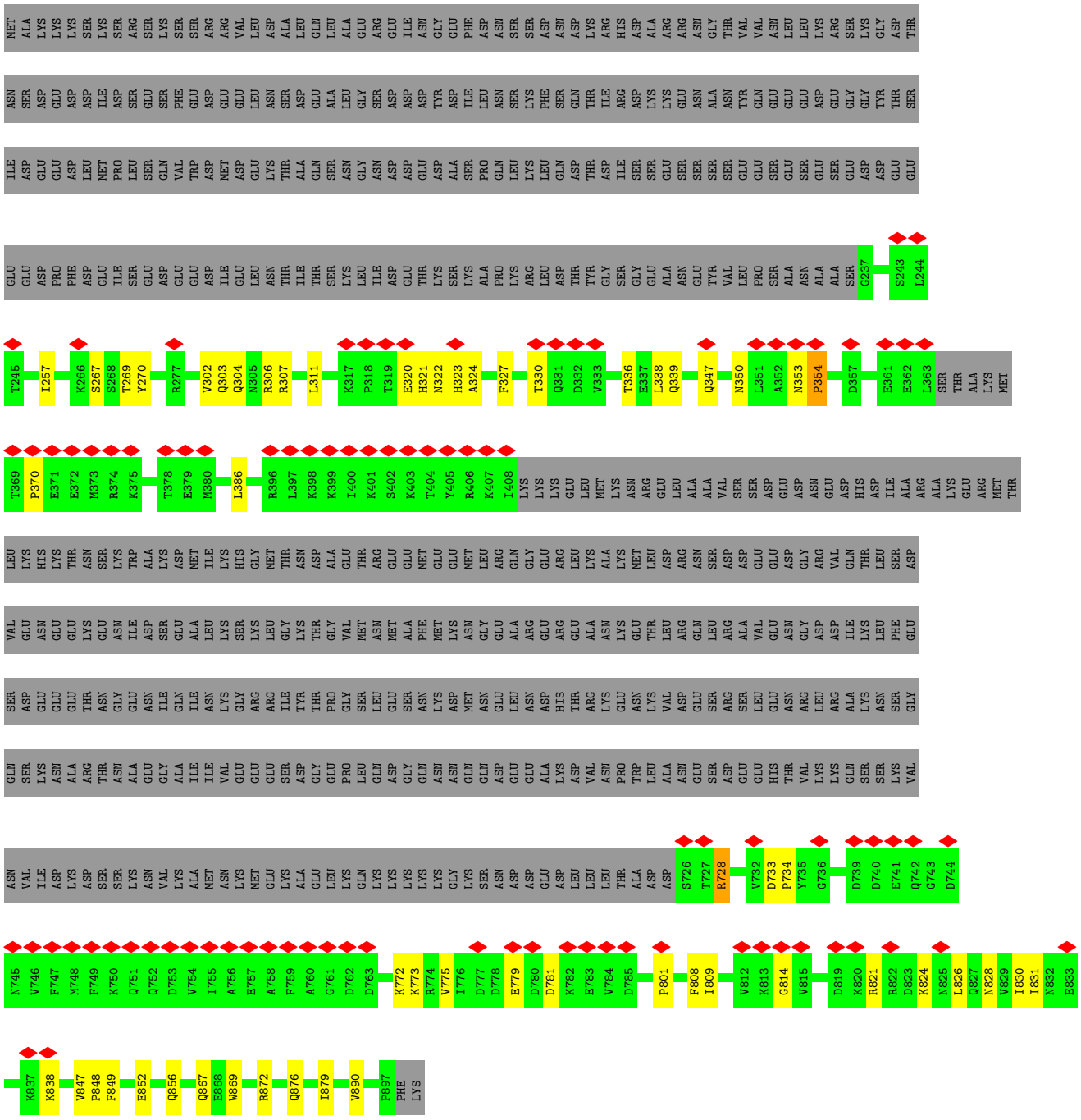
Chain RP:



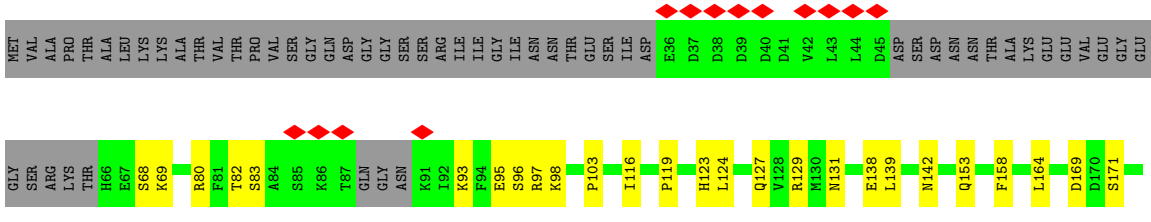


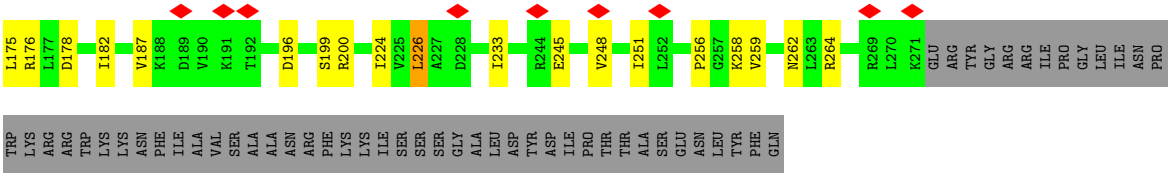
• Molecule 50: U3 small nucleolar RNA-associated protein 14

Chain RQ:

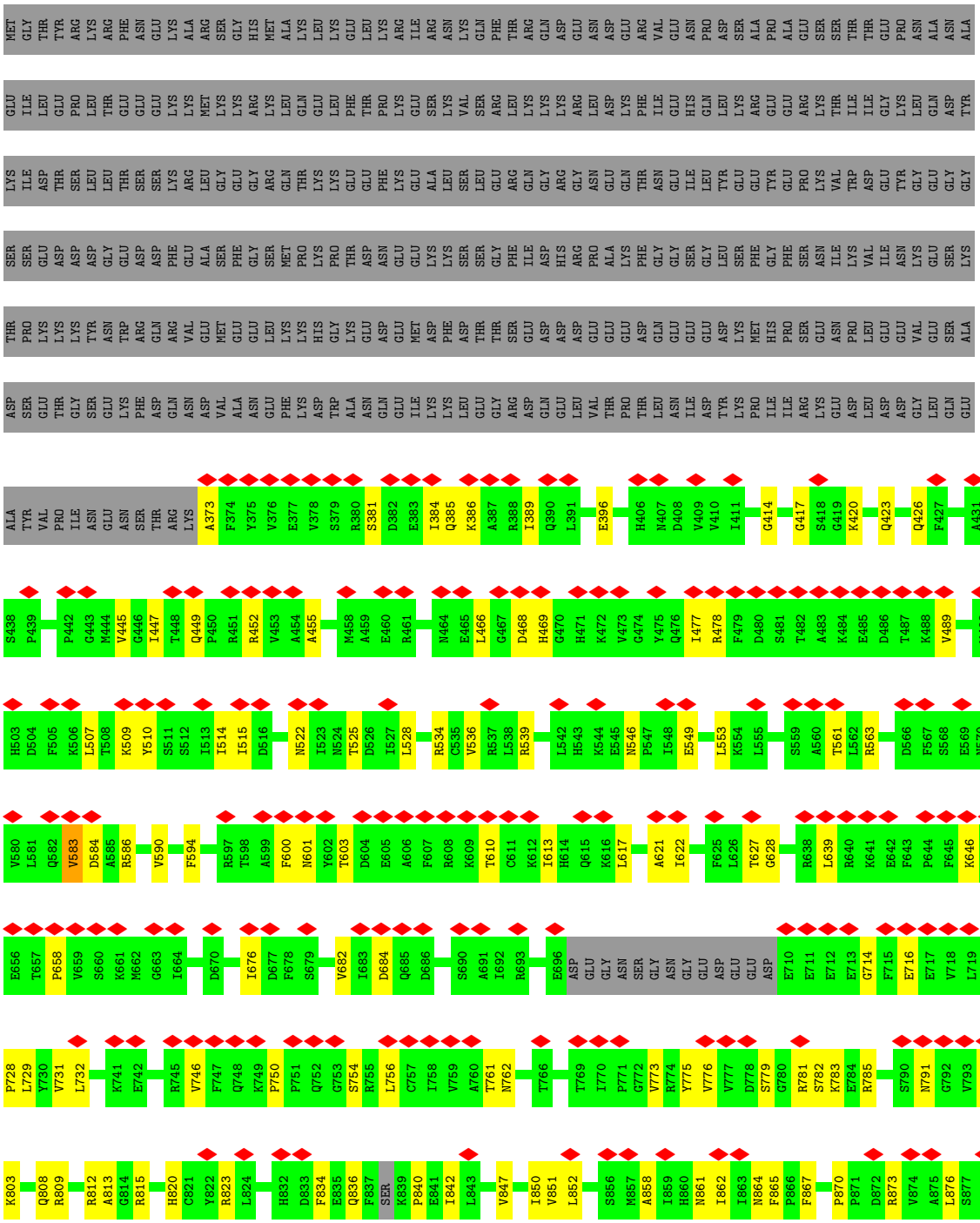


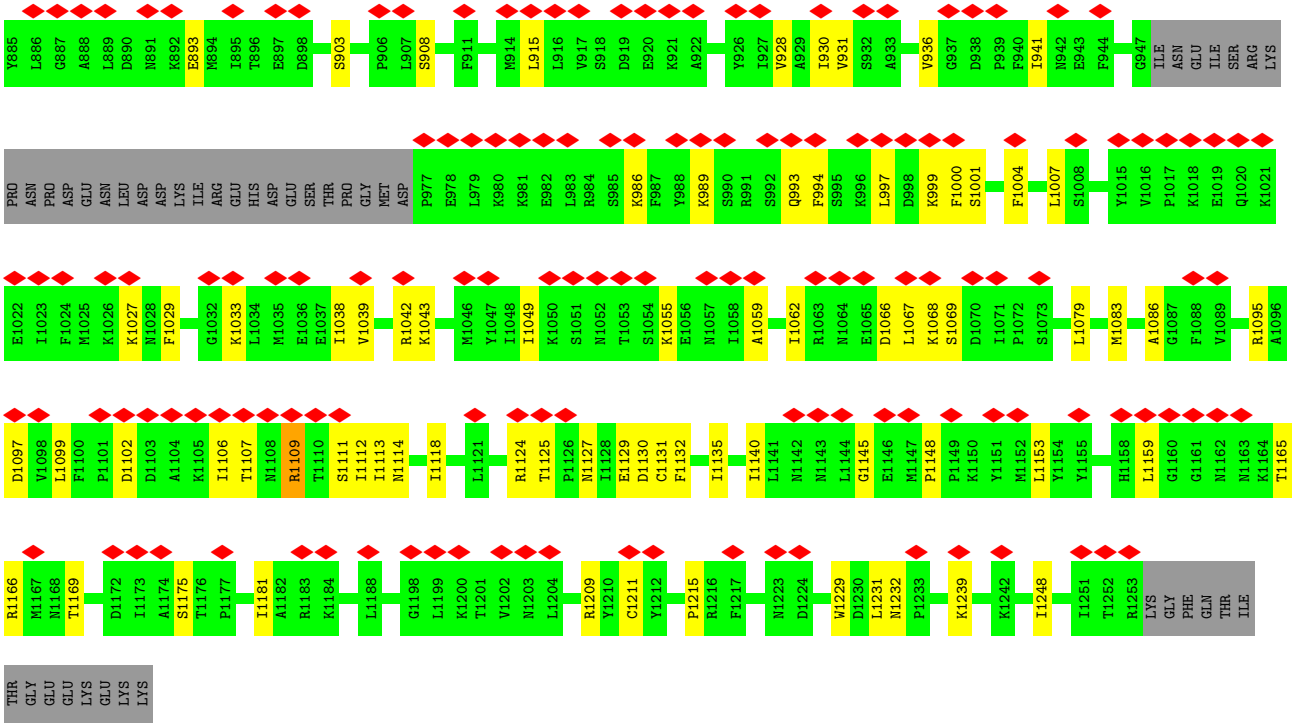
- Molecule 51: Pno1





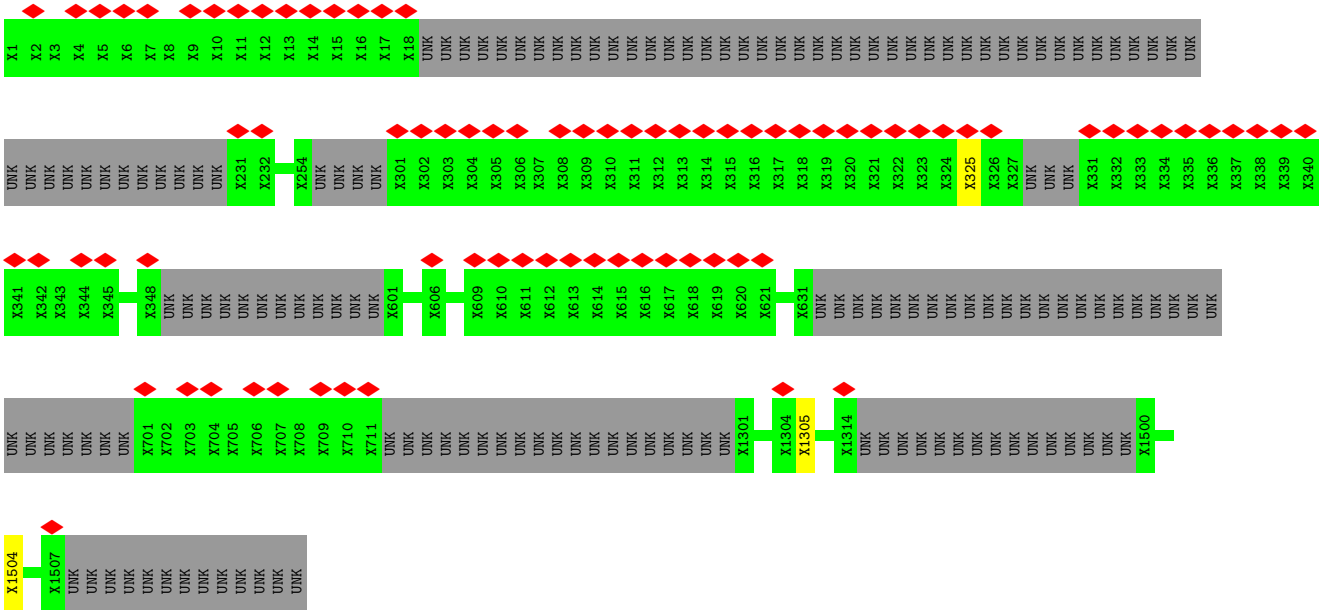
• Molecule 52: Probable ATP-dependent RNA helicase DHR1





• Molecule 53: Unassigned peptides 1

Chain X1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62400	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 ($e^-/Å^2$)	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	0.051	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	531.19995, 531.19995, 531.19995	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3279998, 1.3279998, 1.3279998	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, ADP, 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	0/3940	1.21	37/6120 (0.6%)
2	5A	0.42	0/1035	1.22	7/1608 (0.4%)
3	SA	0.58	0/28317	1.18	194/44080 (0.4%)
4	SC	0.39	0/1949	0.66	2/2609 (0.1%)
5	SF	0.37	0/1954	0.65	1/2640 (0.0%)
6	SG	0.38	0/1690	0.61	0/2285
7	SH	0.29	0/1476	0.56	1/1975 (0.1%)
8	SI	0.36	0/1341	0.76	3/1806 (0.2%)
9	SJ	0.30	0/1202	0.58	0/1610
10	SK	0.41	0/1432	0.65	2/1917 (0.1%)
11	SM	0.29	0/1139	0.52	0/1535
12	SO	0.37	0/1109	0.57	0/1495
13	SP	0.37	0/859	0.63	0/1161
14	SR	0.46	0/990	0.63	0/1335
15	SX	0.39	0/1020	0.64	0/1371
16	SY	0.40	0/804	0.57	0/1074
17	SZ	0.44	0/1000	0.66	0/1334
18	Sc	0.38	0/613	0.62	0/828
19	Sd	0.41	0/499	0.60	0/670
20	3B	0.50	0/1914	0.66	1/2582 (0.0%)
20	3C	0.41	0/1787	0.66	2/2413 (0.1%)
21	3D	0.41	0/3020	0.60	2/4066 (0.0%)
22	3E	0.40	0/2155	0.62	1/2910 (0.0%)
23	3F	0.45	0/3569	0.62	0/4806
24	3G	0.42	0/928	0.74	2/1262 (0.2%)
24	3H	0.46	0/928	0.74	2/1262 (0.2%)
25	A5	0.41	0/2500	0.64	2/3393 (0.1%)
26	AE	0.39	0/3500	0.59	1/4736 (0.0%)
27	AG	0.37	0/398	0.53	0/532
28	B1	0.43	0/6459	0.63	0/8744
29	B2	0.38	0/6624	0.65	3/8950 (0.0%)
30	B3	0.37	0/6001	0.66	3/8120 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	B8	0.44	0/3730	0.63	3/5058 (0.1%)
32	BE	0.42	0/7012	0.63	5/9493 (0.1%)
33	B6	0.40	0/3138	0.60	2/4226 (0.0%)
34	5C	0.40	0/3902	0.61	3/5265 (0.1%)
35	5D	0.36	0/601	0.55	0/798
36	5E	0.34	0/1745	0.62	1/2335 (0.0%)
37	5F	0.37	0/1559	0.60	0/2097
38	5G	0.42	0/1993	0.65	2/2689 (0.1%)
39	5H	0.42	0/601	0.58	0/789
40	5I	0.49	0/3844	0.61	0/5174
41	5J	0.37	0/1147	0.56	0/1531
42	5K	0.44	0/1213	0.63	1/1638 (0.1%)
43	RD	0.30	0/2454	0.56	3/3310 (0.1%)
44	RE	0.34	0/9015	0.58	4/12195 (0.0%)
45	RF	0.32	0/2004	0.62	0/2697
46	RJ	0.41	0/5836	0.60	1/7859 (0.0%)
47	RK	0.38	0/2832	0.61	0/3825
48	RN	0.33	0/528	0.53	0/695
49	RP	0.31	0/12292	0.58	48/16822 (0.3%)
50	RQ	0.35	0/2446	0.61	3/3323 (0.1%)
51	RT	0.34	0/1679	0.63	1/2261 (0.0%)
52	RZ	0.31	0/6730	0.58	1/9088 (0.0%)
All	All	0.43	0/168453	0.78	344/234397 (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	2
5	SF	0	1
7	SH	0	2
8	SI	0	2
14	SR	0	1
15	SX	0	1
17	SZ	0	1
18	Sc	0	1
23	3F	0	3
24	3G	0	2
24	3H	0	1
25	A5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	B1	0	2
29	B2	0	2
30	B3	0	7
32	BE	0	3
33	B6	0	2
39	5H	0	1
40	5I	0	2
42	5K	0	1
44	RE	0	2
45	RF	0	1
46	RJ	0	1
49	RP	0	9
50	RQ	0	1
52	RZ	0	2
All	All	0	54

There are no bond length outliers.

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5A	494	C	C2-N1-C1'	14.08	134.28	118.80
3	SA	185	U	C2-N1-C1'	10.48	130.27	117.70
3	SA	185	U	N1-C2-O2	10.12	129.88	122.80
3	SA	1473	U	C2-N1-C1'	10.10	129.82	117.70
3	SA	1473	U	N1-C2-O2	9.84	129.69	122.80
2	5A	494	C	C6-N1-C1'	-9.80	109.04	120.80
3	SA	75	U	N1-C2-O2	9.60	129.52	122.80
3	SA	185	U	N3-C2-O2	-9.60	115.48	122.20
3	SA	75	U	C2-N1-C1'	9.53	129.14	117.70
2	5A	494	C	C6-N1-C2	-9.33	116.57	120.30
3	SA	75	U	N3-C2-O2	-9.25	115.72	122.20
3	SA	767	U	N3-C2-O2	-9.15	115.80	122.20
3	SA	1784	C	N3-C2-O2	-9.14	115.50	121.90
3	SA	658	C	N1-C2-O2	9.09	124.35	118.90
3	SA	1473	U	N3-C2-O2	-8.89	115.97	122.20
24	3H	21	LEU	CA-CB-CG	8.80	135.54	115.30
3	SA	658	C	C2-N1-C1'	8.66	128.33	118.80
3	SA	827	C	C2-N1-C1'	8.63	128.29	118.80
20	3C	306	LEU	CA-CB-CG	8.46	134.76	115.30
4	SC	54	LEU	CA-CB-CG	8.43	134.68	115.30
3	SA	190	C	N3-C2-O2	-8.28	116.10	121.90
3	SA	827	C	N1-C2-O2	8.23	123.84	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	767	U	C2-N1-C1'	8.19	127.52	117.70
3	SA	767	U	N1-C2-O2	8.10	128.47	122.80
3	SA	827	C	N3-C2-O2	-8.02	116.28	121.90
2	5A	494	C	C5-C6-N1	8.02	125.01	121.00
3	SA	1472	C	C2-N1-C1'	7.99	127.59	118.80
25	A5	25	ASP	CB-CG-OD1	7.98	125.48	118.30
3	SA	1533	C	P-O3'-C3'	7.84	129.11	119.70
3	SA	230	C	C5-C6-N1	7.83	124.91	121.00
1	3A	105	C	C2-N1-C1'	7.80	127.39	118.80
3	SA	820	U	C2-N1-C1'	7.73	126.98	117.70
3	SA	287	G	O4'-C1'-N9	7.72	114.38	108.20
20	3B	306	LEU	CA-CB-CG	7.71	133.03	115.30
24	3G	65	LEU	CA-CB-CG	7.68	132.97	115.30
2	5A	494	C	N1-C2-O2	7.59	123.45	118.90
3	SA	1664	C	C2-N1-C1'	7.53	127.08	118.80
3	SA	648	G	C4-N9-C1'	7.52	136.28	126.50
3	SA	648	G	N3-C4-N9	7.47	130.48	126.00
38	5G	129	ASP	CB-CG-OD1	7.38	124.95	118.30
3	SA	532	U	N3-C2-O2	-7.32	117.08	122.20
3	SA	864	U	N1-C2-O2	7.29	127.91	122.80
3	SA	820	U	N1-C2-O2	7.28	127.89	122.80
24	3G	67	LEU	CA-CB-CG	7.23	131.92	115.30
3	SA	185	U	C6-N1-C1'	-7.22	111.10	121.20
3	SA	864	U	C2-N1-C1'	7.19	126.33	117.70
3	SA	139	C	P-O3'-C3'	7.16	128.29	119.70
3	SA	302	U	C2-N1-C1'	7.15	126.28	117.70
3	SA	1472	C	N1-C2-O2	7.11	123.16	118.90
3	SA	136	C	N1-C2-O2	7.10	123.16	118.90
3	SA	864	U	N3-C2-O2	-7.04	117.27	122.20
1	3A	102	U	N3-C2-O2	-7.01	117.29	122.20
3	SA	536	C	N1-C2-O2	6.98	123.09	118.90
3	SA	1657	U	C2-N1-C1'	6.93	126.02	117.70
3	SA	648	G	C8-N9-C1'	-6.89	118.04	127.00
3	SA	1053	G	O5'-P-OP1	-6.88	99.51	105.70
1	3A	314	C	C2-N1-C1'	6.86	126.35	118.80
3	SA	569	C	C6-N1-C2	-6.84	117.56	120.30
8	SI	118	LEU	CA-CB-CG	6.82	130.98	115.30
3	SA	1784	C	C6-N1-C2	-6.80	117.58	120.30
3	SA	1675	C	N1-C2-O2	6.78	122.97	118.90
1	3A	46	U	N3-C2-O2	-6.78	117.45	122.20
3	SA	773	C	O4'-C1'-N1	6.77	113.62	108.20
1	3A	104	C	C2-N1-C1'	6.77	126.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	784	C	N3-C2-O2	-6.73	117.19	121.90
3	SA	1476	C	C2-N1-C1'	6.73	126.21	118.80
3	SA	747	C	N1-C2-O2	6.73	122.94	118.90
3	SA	1803	G	P-O3'-C3'	6.71	127.75	119.70
3	SA	507	U	C2-N1-C1'	6.70	125.75	117.70
3	SA	1476	C	C6-N1-C2	-6.69	117.62	120.30
3	SA	532	U	N1-C2-O2	6.69	127.48	122.80
3	SA	487	G	C2-N3-C4	6.68	115.24	111.90
1	3A	27	U	N1-C2-O2	6.67	127.47	122.80
49	RP	923	PRO	N-CA-CB	6.65	111.28	103.30
3	SA	815	G	N3-C4-C5	-6.64	125.28	128.60
3	SA	1066	C	N3-C2-O2	-6.61	117.27	121.90
3	SA	815	G	C4-N9-C1'	6.61	135.09	126.50
3	SA	258	C	C6-N1-C2	-6.59	117.66	120.30
1	3A	104	C	C6-N1-C2	-6.59	117.66	120.30
3	SA	189	C	C2-N1-C1'	6.58	126.04	118.80
3	SA	658	C	C6-N1-C2	-6.58	117.67	120.30
43	RD	1223	PRO	N-CA-CB	6.57	111.19	103.30
3	SA	532	U	C2-N1-C1'	6.56	125.57	117.70
22	3E	253	ASP	CB-CG-OD1	6.53	124.18	118.30
3	SA	658	C	N3-C2-O2	-6.52	117.33	121.90
3	SA	1473	U	C6-N1-C1'	-6.52	112.07	121.20
3	SA	1657	U	N1-C2-O2	6.51	127.36	122.80
29	B2	443	LEU	CA-CB-CG	6.51	130.27	115.30
3	SA	136	C	C2-N1-C1'	6.50	125.96	118.80
3	SA	747	C	C2-N1-C1'	6.50	125.95	118.80
24	3H	22	ASP	CB-CG-OD1	6.50	124.15	118.30
3	SA	1784	C	N1-C2-O2	6.44	122.76	118.90
3	SA	189	C	N1-C2-O2	6.42	122.75	118.90
3	SA	453	U	C2-N1-C1'	6.40	125.38	117.70
3	SA	777	C	C2-N1-C1'	6.38	125.82	118.80
1	3A	46	U	N1-C2-O2	6.36	127.25	122.80
3	SA	1664	C	N1-C2-O2	6.36	122.71	118.90
49	RP	707	PRO	N-CA-CB	6.34	110.91	103.30
1	3A	27	U	C2-N1-C1'	6.31	125.27	117.70
3	SA	339	C	C2-N1-C1'	6.30	125.73	118.80
1	3A	102	U	N1-C2-O2	6.26	127.18	122.80
3	SA	827	C	C6-N1-C2	-6.26	117.80	120.30
34	5C	74	LEU	CA-CB-CG	6.25	129.67	115.30
3	SA	230	C	C2-N1-C1'	6.24	125.66	118.80
3	SA	1476	C	C5-C6-N1	6.24	124.12	121.00
3	SA	190	C	C6-N1-C2	-6.24	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1657	U	N3-C2-O2	-6.22	117.84	122.20
3	SA	1472	C	N3-C2-O2	-6.20	117.56	121.90
49	RP	2116	PRO	N-CA-CB	6.20	110.74	103.30
1	3A	105	C	C6-N1-C2	-6.20	117.82	120.30
3	SA	229	U	C2-N1-C1'	6.19	125.13	117.70
3	SA	507	U	N1-C2-O2	6.19	127.13	122.80
1	3A	42	U	C5-C6-N1	6.19	125.79	122.70
3	SA	50	C	C2-N1-C1'	6.18	125.60	118.80
3	SA	176	C	C6-N1-C2	-6.18	117.83	120.30
3	SA	1527	C	C2-N1-C1'	6.16	125.58	118.80
1	3A	248	G	P-O3'-C3'	6.16	127.09	119.70
3	SA	230	C	N1-C2-O2	6.13	122.58	118.90
3	SA	1053	G	C8-N9-C4	-6.13	103.95	106.40
3	SA	815	G	N3-C4-N9	6.12	129.68	126.00
3	SA	35	U	N3-C2-O2	-6.11	117.92	122.20
3	SA	1473	U	C5-C6-N1	6.11	125.76	122.70
3	SA	75	U	C6-N1-C1'	-6.09	112.67	121.20
3	SA	777	C	C6-N1-C2	-6.07	117.87	120.30
49	RP	2092	PRO	N-CA-CB	6.05	110.56	103.30
3	SA	262	U	N1-C2-O2	6.04	127.03	122.80
1	3A	27	U	N3-C2-O2	-6.03	117.98	122.20
3	SA	487	G	C8-N9-C4	-6.02	103.99	106.40
34	5C	389	LEU	CA-CB-CG	6.02	129.15	115.30
1	3A	260	U	C2-N1-C1'	6.01	124.92	117.70
49	RP	616	PRO	N-CA-CB	6.01	110.51	103.30
10	SK	118	LEU	CA-CB-CG	6.00	129.11	115.30
32	BE	756	LEU	CA-CB-CG	6.00	129.10	115.30
32	BE	782	PRO	N-CA-CB	6.00	110.50	103.30
49	RP	567	PRO	N-CA-CB	5.98	110.47	103.30
49	RP	629	PRO	N-CA-CB	5.98	110.47	103.30
1	3A	105	C	N1-C2-O2	5.98	122.49	118.90
32	BE	750	PRO	N-CA-CB	5.98	110.47	103.30
3	SA	873	U	C2-N1-C1'	5.96	124.86	117.70
3	SA	820	U	N3-C2-O2	-5.95	118.03	122.20
3	SA	332	U	N1-C2-O2	5.94	126.96	122.80
3	SA	302	U	N1-C2-O2	5.94	126.96	122.80
3	SA	873	U	N1-C2-O2	5.94	126.96	122.80
49	RP	718	PRO	N-CA-CB	5.93	110.42	103.30
3	SA	962	C	N3-C2-O2	-5.93	117.75	121.90
1	3A	260	U	N1-C2-O2	5.92	126.94	122.80
49	RP	1089	PRO	N-CA-CB	5.92	110.40	103.30
3	SA	484	C	P-O3'-C3'	5.91	126.79	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B2	785	PRO	N-CA-CB	5.90	110.38	103.30
49	RP	293	PRO	N-CA-CB	5.90	110.38	103.30
3	SA	280	U	P-O3'-C3'	5.90	126.78	119.70
3	SA	648	G	N3-C4-C5	-5.89	125.65	128.60
49	RP	1633	PRO	N-CA-CB	5.89	110.37	103.30
3	SA	230	C	C6-N1-C2	-5.89	117.94	120.30
7	SH	171	LYS	C-N-CA	5.89	136.43	121.70
3	SA	773	C	P-O3'-C3'	5.89	126.77	119.70
3	SA	1594	G	P-O3'-C3'	5.89	126.76	119.70
3	SA	1709	C	N3-C2-O2	-5.89	117.78	121.90
52	RZ	658	PRO	N-CA-CB	5.88	110.36	103.30
43	RD	1205	PRO	N-CA-CB	5.87	110.34	103.30
49	RP	2290	PRO	N-CA-CB	5.87	110.34	103.30
49	RP	1183	PRO	N-CA-CB	5.87	110.34	103.30
49	RP	798	PRO	N-CA-CB	5.85	110.32	103.30
3	SA	302	U	N3-C2-O2	-5.85	118.11	122.20
49	RP	1382	PRO	N-CA-CB	5.84	110.31	103.30
49	RP	268	PRO	N-CA-CB	5.84	110.30	103.30
3	SA	1709	C	N1-C2-O2	5.82	122.39	118.90
3	SA	658	C	C6-N1-C1'	-5.82	113.82	120.80
49	RP	676	PRO	N-CA-CB	5.82	110.28	103.30
49	RP	786	PRO	N-CA-CB	5.81	110.28	103.30
3	SA	1527	C	C6-N1-C2	-5.80	117.98	120.30
33	B6	334	LEU	CA-CB-CG	5.79	128.62	115.30
49	RP	1149	PRO	N-CA-CB	5.79	110.25	103.30
1	3A	248	G	O4'-C1'-N9	5.79	112.83	108.20
3	SA	542	A	P-O3'-C3'	5.79	126.65	119.70
49	RP	1487	PRO	N-CA-CB	5.79	110.24	103.30
3	SA	332	U	N3-C2-O2	-5.78	118.15	122.20
49	RP	954	PRO	N-CA-CB	5.78	110.24	103.30
1	3A	204	U	N3-C2-O2	-5.78	118.15	122.20
3	SA	332	U	C2-N1-C1'	5.78	124.64	117.70
49	RP	936	PRO	N-CA-CB	5.78	110.23	103.30
1	3A	105	C	C5-C6-N1	5.78	123.89	121.00
3	SA	0	U	P-O3'-C3'	5.78	126.63	119.70
3	SA	773	C	C2-N1-C1'	-5.77	112.46	118.80
3	SA	781	U	P-O3'-C3'	5.76	126.61	119.70
49	RP	1322	PRO	N-CA-CB	5.76	110.21	103.30
49	RP	443	PRO	N-CA-CB	5.75	110.21	103.30
49	RP	592	PRO	N-CA-CB	5.75	110.20	103.30
3	SA	1472	C	C6-N1-C1'	-5.75	113.90	120.80
49	RP	686	PRO	N-CA-CB	5.75	110.20	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	RQ	801	PRO	N-CA-CB	5.74	110.19	103.30
3	SA	827	C	C6-N1-C1'	-5.74	113.92	120.80
2	5A	494	C	N3-C2-O2	-5.74	117.89	121.90
49	RP	511	PRO	N-CA-CB	5.73	110.18	103.30
49	RP	1116	PRO	N-CA-CB	5.73	110.18	103.30
49	RP	454	PRO	N-CA-CB	5.73	110.17	103.30
3	SA	487	G	N3-C4-C5	-5.72	125.74	128.60
3	SA	448	C	C6-N1-C2	-5.72	118.01	120.30
42	5K	146	LEU	CA-CB-CG	5.72	128.45	115.30
3	SA	278	U	P-O3'-C3'	5.71	126.56	119.70
1	3A	247	U	C2-N1-C1'	5.71	124.55	117.70
3	SA	1664	C	C6-N1-C1'	-5.70	113.96	120.80
31	B8	521	LEU	CA-CB-CG	5.70	128.40	115.30
49	RP	2287	PRO	N-CA-CB	5.69	110.13	103.30
49	RP	1576	PRO	N-CA-CB	5.69	110.13	103.30
49	RP	331	PRO	N-CA-CB	5.67	110.11	103.30
49	RP	1016	PRO	N-CA-CB	5.67	110.10	103.30
50	RQ	354	PRO	N-CA-CB	5.67	110.10	103.30
49	RP	1025	PRO	N-CA-CB	5.66	110.09	103.30
49	RP	1102	PRO	N-CA-CB	5.66	110.09	103.30
3	SA	784	C	N1-C2-O2	5.66	122.29	118.90
3	SA	1717	G	C4-N9-C1'	5.66	133.85	126.50
32	BE	614	LEU	CA-CB-CG	5.64	128.28	115.30
32	BE	909	LEU	CA-CB-CG	5.64	128.27	115.30
3	SA	1733	C	N1-C2-O2	5.64	122.28	118.90
3	SA	197	A	O4'-C1'-N9	5.63	112.70	108.20
49	RP	879	PRO	N-CA-CB	5.63	110.06	103.30
3	SA	149	C	C2-N1-C1'	5.63	124.99	118.80
3	SA	908	U	N1-C2-O2	5.63	126.74	122.80
3	SA	281	G	N1-C6-O6	-5.62	116.53	119.90
3	SA	262	U	N3-C2-O2	-5.61	118.27	122.20
3	SA	536	C	N3-C2-O2	-5.61	117.97	121.90
1	3A	46	U	C2-N1-C1'	5.60	124.42	117.70
30	B3	698	LEU	CA-CB-CG	5.60	128.18	115.30
3	SA	1661	U	N3-C2-O2	-5.60	118.28	122.20
30	B3	525	LEU	CA-CB-CG	5.59	128.15	115.30
3	SA	883	C	C6-N1-C2	-5.58	118.07	120.30
43	RD	1514	LEU	CA-CB-CG	5.58	128.13	115.30
49	RP	2242	PRO	N-CA-CB	5.58	109.99	103.30
49	RP	1400	PRO	N-CA-CB	5.58	109.99	103.30
49	RP	1582	PRO	N-CA-CB	5.58	109.99	103.30
3	SA	107	C	C2-N1-C1'	5.57	124.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	686	C	N1-C2-O2	5.57	122.24	118.90
3	SA	536	C	C2-N1-C1'	5.56	124.92	118.80
3	SA	747	C	N3-C2-O2	-5.56	118.01	121.90
49	RP	1346	PRO	N-CA-CB	5.56	109.97	103.30
3	SA	658	C	C5-C6-N1	5.56	123.78	121.00
1	3A	204	U	N1-C2-O2	5.55	126.69	122.80
49	RP	937	PRO	N-CA-CB	5.54	109.95	103.30
49	RP	771	PRO	N-CA-CB	5.53	109.93	103.30
3	SA	196	G	N1-C6-O6	-5.53	116.58	119.90
49	RP	959	PRO	N-CA-CB	5.52	109.93	103.30
49	RP	1592	PRO	N-CA-CB	5.51	109.92	103.30
3	SA	176	C	C6-N1-C1'	5.51	127.41	120.80
3	SA	267	U	N3-C2-O2	-5.50	118.35	122.20
31	B8	530	LEU	CA-CB-CG	5.50	127.95	115.30
21	3D	219	LEU	CA-CB-CG	5.50	127.95	115.30
10	SK	128	LEU	CA-CB-CG	5.49	127.92	115.30
3	SA	908	U	N3-C2-O2	-5.48	118.36	122.20
31	B8	449	ASP	CB-CG-OD1	5.48	123.23	118.30
36	5E	314	LEU	CA-CB-CG	5.47	127.89	115.30
49	RP	2131	PRO	N-CA-CB	5.47	109.86	103.30
50	RQ	370	PRO	N-CA-CB	5.47	109.86	103.30
3	SA	686	C	C2-N1-C1'	5.46	124.80	118.80
1	3A	314	C	C6-N1-C2	-5.42	118.13	120.30
3	SA	211	U	C2-N1-C1'	5.42	124.21	117.70
3	SA	1161	C	C5-C6-N1	5.42	123.71	121.00
1	3A	41	C	C6-N1-C2	-5.41	118.14	120.30
3	SA	75	U	C5-C6-N1	5.40	125.40	122.70
44	RE	531	LEU	CA-CB-CG	5.39	127.71	115.30
1	3A	311	G	C4-N9-C1'	5.39	133.51	126.50
3	SA	88	U	N3-C2-O2	-5.38	118.44	122.20
34	5C	270	LEU	CA-CB-CG	5.38	127.67	115.30
3	SA	650	U	C5-C6-N1	5.37	125.39	122.70
4	SC	172	LEU	CA-CB-CG	5.37	127.64	115.30
2	5A	479	G	N1-C6-O6	-5.37	116.68	119.90
3	SA	185	U	C5-C6-N1	5.36	125.38	122.70
3	SA	192	U	C2-N1-C1'	5.36	124.14	117.70
49	RP	579	PRO	N-CA-CB	5.36	109.74	103.30
3	SA	901	G	C4-N9-C1'	5.36	133.47	126.50
3	SA	916	U	N1-C2-O2	5.35	126.55	122.80
3	SA	815	G	C8-N9-C1'	-5.34	120.05	127.00
8	SI	77	LEU	CA-CB-CG	5.34	127.59	115.30
1	3A	104	C	C5-C6-N1	5.32	123.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	777	C	N1-C2-O2	5.31	122.09	118.90
3	SA	1067	C	C6-N1-C2	-5.31	118.18	120.30
3	SA	335	U	P-O3'-C3'	5.30	126.06	119.70
3	SA	482	U	N3-C2-O2	-5.30	118.49	122.20
3	SA	767	U	C6-N1-C1'	-5.30	113.79	121.20
25	A5	51	LEU	CA-CB-CG	5.30	127.48	115.30
3	SA	648	G	C6-C5-N7	-5.28	127.23	130.40
29	B2	551	LEU	CA-CB-CG	5.28	127.44	115.30
3	SA	136	C	N3-C2-O2	-5.28	118.20	121.90
1	3A	308	U	N1-C2-O2	5.28	126.49	122.80
1	3A	44	U	N3-C2-O2	-5.26	118.52	122.20
3	SA	633	U	N3-C2-O2	-5.26	118.52	122.20
49	RP	1538	PRO	N-CA-CB	5.25	109.60	103.30
44	RE	1087	LEU	CA-CB-CG	5.25	127.37	115.30
3	SA	1161	C	C6-N1-C2	-5.24	118.21	120.30
3	SA	870	C	C6-N1-C2	-5.23	118.21	120.30
5	SF	193	GLY	N-CA-C	5.23	126.18	113.10
3	SA	453	U	N3-C2-O2	-5.22	118.54	122.20
3	SA	302	U	C5-C6-N1	5.22	125.31	122.70
46	RJ	1021	LEU	CA-CB-CG	5.22	127.31	115.30
3	SA	35	U	N1-C2-O2	5.22	126.45	122.80
3	SA	820	U	C6-N1-C1'	-5.22	113.90	121.20
3	SA	1052	U	O4'-C1'-N1	5.21	112.37	108.20
33	B6	327	LEU	CB-CG-CD1	5.21	119.86	111.00
1	3A	260	U	N3-C2-O2	-5.20	118.56	122.20
44	RE	655	LEU	CA-CB-CG	5.20	127.25	115.30
3	SA	1646	C	N1-C2-O2	5.19	122.01	118.90
3	SA	916	U	N3-C2-O2	-5.19	118.57	122.20
3	SA	921	U	C2-N1-C1'	5.19	123.92	117.70
3	SA	448	C	C2-N1-C1'	5.18	124.50	118.80
3	SA	1609	U	N3-C2-O2	-5.17	118.58	122.20
3	SA	1783	C	C6-N1-C2	-5.17	118.23	120.30
3	SA	196	G	C5-C6-O6	5.17	131.70	128.60
3	SA	309	C	N1-C2-O2	5.17	122.00	118.90
1	3A	107	C	P-O3'-C3'	5.16	125.89	119.70
3	SA	448	C	C5-C6-N1	5.15	123.58	121.00
21	3D	40	ASP	CB-CG-OD1	5.14	122.92	118.30
3	SA	873	U	N3-C2-O2	-5.13	118.61	122.20
3	SA	1540	G	N3-C4-C5	-5.13	126.03	128.60
38	5G	209	LEU	CA-CB-CG	5.13	127.10	115.30
3	SA	331	A	C8-N9-C4	-5.12	103.75	105.80
3	SA	453	U	C5-C6-N1	5.12	125.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3A	107	C	OP1-P-O3'	5.11	116.44	105.20
1	3A	32	G	C2-N3-C4	5.11	114.45	111.90
3	SA	262	U	C2-N1-C1'	5.09	123.81	117.70
1	3A	314	C	C5-C6-N1	5.08	123.54	121.00
51	RT	226	LEU	CA-CB-CG	5.08	126.99	115.30
20	3C	233	LEU	CA-CB-CG	5.08	126.99	115.30
3	SA	1064	G	C4-N9-C1'	5.07	133.09	126.50
1	3A	46	U	C5-C6-N1	5.07	125.23	122.70
26	AE	403	LEU	CA-CB-CG	5.06	126.94	115.30
1	3A	105	C	C6-N1-C1'	-5.06	114.73	120.80
3	SA	280	U	OP2-P-O3'	5.06	116.33	105.20
3	SA	1703	C	N1-C2-O2	5.05	121.93	118.90
44	RE	429	LEU	CA-CB-CG	5.05	126.91	115.30
8	SI	64	VAL	CA-CB-CG1	5.04	118.47	110.90
3	SA	507	U	C6-N1-C1'	-5.04	114.14	121.20
3	SA	575	C	N1-C2-O2	5.03	121.92	118.90
30	B3	379	LEU	CA-CB-CG	5.03	126.87	115.30
49	RP	202	LYS	C-N-CA	5.03	134.27	121.70
3	SA	1594	G	OP2-P-O3'	5.02	116.25	105.20
3	SA	14	C	N3-C2-O2	-5.02	118.39	121.90
3	SA	1686	C	C6-N1-C2	-5.02	118.29	120.30
3	SA	965	U	C2-N1-C1'	5.01	123.72	117.70
3	SA	1623	C	C6-N1-C2	-5.01	118.30	120.30
1	3A	75	C	C6-N1-C2	-5.01	118.30	120.30
3	SA	-5	G	C4-N9-C1'	5.01	133.01	126.50
3	SA	453	U	N1-C2-O2	5.01	126.30	122.80
3	SA	1633	A	C4-N9-C1'	5.00	135.30	126.30
3	SA	1706	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	3F	141	LEU	Peptide
23	3F	173	GLU	Peptide
23	3F	237	ASP	Peptide
24	3G	59	GLU	Peptide
24	3G	9	PHE	Peptide
24	3H	59	GLU	Peptide
39	5H	576	LEU	Peptide
40	5I	185	ILE	Peptide
40	5I	87	SER	Peptide

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Mol	Chain	Res	Type	Group
42	5K	68	ASP	Peptide
25	A5	50	PHE	Peptide
28	B1	519	LEU	Peptide
28	B1	709	THR	Peptide
29	B2	160	ARG	Peptide
29	B2	552	ASP	Peptide
30	B3	220	ILE	Peptide
30	B3	236	THR	Peptide
30	B3	410	ASN	Peptide
30	B3	437	VAL	Peptide
30	B3	50	ARG	Peptide
30	B3	567	VAL	Peptide
30	B3	594	GLY	Peptide
33	B6	322	LEU	Peptide
33	B6	326	PHE	Peptide
32	BE	591	PHE	Peptide
32	BE	811	LEU	Peptide
32	BE	94	TYR	Peptide
44	RE	1028	ARG	Peptide
44	RE	1094	LYS	Peptide
45	RF	171	PHE	Peptide
46	RJ	948	ILE	Peptide
49	RP	1739	HIS	Peptide
49	RP	1745	ILE	Peptide
49	RP	1907	ASN	Peptide
49	RP	1995	ARG	Peptide
49	RP	2009	LYS	Peptide
49	RP	203	CYS	Peptide
49	RP	2113	ASP	Peptide
49	RP	2114	ASP	Peptide
49	RP	33	ASN	Peptide
50	RQ	728	ARG	Peptide
52	RZ	1001	SER	Peptide
52	RZ	1069	SER	Peptide
4	SC	16	GLN	Peptide
4	SC	18	LYS	Peptide
5	SF	207	LEU	Peptide
7	SH	147	LEU	Peptide
7	SH	152	ASP	Peptide
8	SI	134	GLU	Peptide
8	SI	64	VAL	Peptide
14	SR	123	ARG	Peptide

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Mol	Chain	Res	Type	Group
15	SX	108	ALA	Peptide
17	SZ	34	ASN	Peptide
18	Sc	49	HIS	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	3534	0	1792	32	0
2	5A	926	0	468	8	0
3	SA	25332	0	12769	275	0
4	SC	1923	0	2029	41	0
5	SF	1915	0	1941	38	0
6	SG	1669	0	1724	25	0
7	SH	1456	0	1505	24	0
8	SI	1321	0	1387	34	0
9	SJ	1181	0	1198	22	0
10	SK	1410	0	1492	28	0
11	SM	1113	0	1181	24	0
12	SO	1087	0	1152	22	0
13	SP	848	0	868	21	0
14	SR	973	0	1029	21	0
15	SX	1003	0	1040	21	0
16	SY	792	0	847	14	0
17	SZ	986	0	1042	23	0
18	Sc	603	0	621	0	0
19	Sd	497	0	535	0	0
20	3B	1878	0	1923	28	0
20	3C	1754	0	1792	35	0
21	3D	2974	0	3001	55	0
22	3E	2130	0	2187	33	0
23	3F	3498	0	3515	67	0
24	3G	916	0	964	15	0
24	3H	916	0	964	18	0
25	A5	2452	0	2435	48	0
26	AE	3443	0	3564	57	0
27	AG	394	0	380	6	0
28	B1	6316	0	6218	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B2	6497	0	6492	147	0
30	B3	5906	0	5983	150	0
31	B8	3648	0	3626	64	0
32	BE	6876	0	6734	115	0
33	B6	3077	0	3022	46	0
34	5C	3825	0	3829	87	0
35	5D	589	0	590	13	0
36	5E	1728	0	1739	35	0
37	5F	1530	0	1572	33	0
38	5G	1956	0	1971	36	0
39	5H	596	0	661	17	0
40	5I	3765	0	3714	74	0
41	5J	1127	0	1150	11	0
42	5K	1190	0	1252	22	0
43	RD	2413	0	2264	33	0
44	RE	8805	0	8911	157	0
45	RF	1963	0	1942	35	0
46	RJ	5709	0	5870	111	0
47	RK	2781	0	2878	68	0
48	RN	523	0	530	7	0
49	RP	12263	0	8039	80	0
50	RQ	2411	0	2092	44	0
51	RT	1652	0	1706	32	0
52	RZ	6598	0	6631	112	0
53	X1	755	0	179	3	0
54	5K	1	0	0	0	0
54	Sc	1	0	0	0	0
55	RJ	32	0	12	0	0
56	RJ	1	0	0	0	0
57	RZ	27	0	12	1	0
All	All	163485	0	144964	2382	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 8.

All (2382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1663:G:H1	3:SA:1738:U:H3	0.94	0.93
47:RK:213:LYS:O	47:RK:217:LYS:HB3	1.71	0.91
3:SA:174:U:H3	3:SA:266:A:H62	0.92	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1697:G:H1	3:SA:1704:U:H3	1.08	0.90
45:RF:101:SER:O	45:RF:105:SER:HB3	1.73	0.88
3:SA:1688:U:H3	3:SA:1713:G:H1	1.21	0.86
3:SA:174:U:H3	3:SA:266:A:N6	1.74	0.86
52:RZ:600:PHE:CE1	52:RZ:684:ASP:O	2.32	0.82
30:B3:384:TYR:HH	30:B3:423:LYS:N	1.77	0.82
3:SA:917:U:HO2'	13:SP:29:HIS:HE2	1.28	0.81
30:B3:412:ALA:O	30:B3:430:TYR:HB2	1.80	0.80
33:B6:380:ASP:O	33:B6:384:LEU:HB2	1.80	0.80
47:RK:114:PHE:O	47:RK:169:VAL:HA	1.86	0.76
3:SA:311:U:H3	3:SA:355:G:H1	1.29	0.76
3:SA:1541:G:N2	3:SA:1570:A:H62	1.85	0.74
15:SX:36:LYS:HB3	15:SX:110:ILE:HG13	1.69	0.74
36:5E:449:ASP:O	36:5E:453:SER:HB3	1.88	0.72
1:3A:31:G:H1	40:5I:61:GLN:HE21	1.35	0.72
32:BE:569:VAL:HG22	32:BE:579:ARG:HB2	1.73	0.71
31:B8:435:PHE:HB3	31:B8:443:VAL:HA	1.72	0.71
3:SA:628:G:H21	3:SA:971:A:H62	1.39	0.70
3:SA:1541:G:H21	3:SA:1570:A:N6	1.88	0.70
3:SA:126:A:H62	3:SA:291:G:N2	1.89	0.70
29:B2:9:GLU:O	29:B2:684:TRP:HA	1.92	0.69
49:RP:1749:LYS:HB3	49:RP:1795:ARG:HG3	1.74	0.69
3:SA:622:A:HO2'	3:SA:976:G:H1	1.41	0.69
31:B8:296:GLN:H	31:B8:316:GLY:HA2	1.58	0.68
37:5F:115:MET:HG3	37:5F:120:MET:HB2	1.75	0.68
37:5F:49:ARG:O	37:5F:53:ASP:HB2	1.93	0.68
3:SA:126:A:N6	3:SA:291:G:N2	2.41	0.68
3:SA:1673:G:H1	3:SA:1728:A:N6	1.91	0.68
3:SA:794:U:H2'	3:SA:796:A:H62	1.59	0.68
23:3F:125:VAL:O	23:3F:129:GLN:HB2	1.94	0.68
44:RE:701:ILE:O	44:RE:705:HIS:HB2	1.94	0.68
47:RK:14:SER:HB3	47:RK:36:ILE:HG23	1.76	0.68
1:3A:250:C:H41	23:3F:560:ARG:HH12	1.42	0.67
31:B8:455:ILE:HA	31:B8:486:SER:HA	1.74	0.67
3:SA:187:G:H21	3:SA:198:A:H62	1.41	0.67
30:B3:107:ILE:HG12	30:B3:149:SER:HA	1.75	0.67
26:AE:218:ILE:HG22	26:AE:263:VAL:HG11	1.76	0.67
7:SH:3:LEU:O	7:SH:15:THR:HA	1.95	0.67
32:BE:733:THR:O	32:BE:737:LEU:HB3	1.95	0.66
45:RF:41:ARG:HH22	45:RF:135:ASN:HA	1.59	0.66
29:B2:41:LEU:HD11	29:B2:354:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B2:349:SER:O	29:B2:368:PRO:HA	1.95	0.66
33:B6:144:VAL:HG11	33:B6:178:VAL:HG21	1.78	0.66
28:B1:785:PHE:O	28:B1:789:SER:HB3	1.95	0.66
23:3F:125:VAL:HA	23:3F:128:GLN:HE21	1.61	0.66
43:RD:1509:GLU:HG3	43:RD:1512:GLU:HB2	1.76	0.66
21:3D:87:PRO:HB3	50:RQ:323:HIS:HA	1.78	0.65
34:5C:158:THR:HG21	34:5C:197:ASP:HA	1.79	0.65
3:SA:1673:G:N1	3:SA:1728:A:N6	2.42	0.65
17:SZ:118:ILE:HG22	17:SZ:120:GLY:H	1.61	0.65
52:RZ:785:ARG:HH22	52:RZ:794:GLN:HE21	1.45	0.65
23:3F:168:ASN:H	23:3F:174:GLU:HG2	1.61	0.65
52:RZ:396:GLU:HB2	52:RZ:583:VAL:CG2	2.27	0.65
7:SH:14:LYS:HD2	7:SH:123:GLY:HA3	1.78	0.65
34:5C:91:ILE:O	34:5C:95:VAL:HB	1.97	0.64
33:B6:14:GLU:O	33:B6:18:LEU:HB2	1.98	0.64
40:5I:27:ASN:HD22	40:5I:32:LEU:HD12	1.63	0.64
46:RJ:114:ARG:NH2	46:RJ:274:TYR:OH	2.30	0.64
52:RZ:1097:ASP:HB3	52:RZ:1106:ILE:HG21	1.79	0.64
51:RT:224:ILE:HG22	51:RT:233:ILE:HG23	1.80	0.64
30:B3:267:PHE:H	30:B3:281:THR:HG22	1.62	0.64
3:SA:1691:A:N3	3:SA:1712:A:N6	2.46	0.64
14:SR:50:GLU:HA	14:SR:53:LEU:HB2	1.80	0.64
23:3F:252:VAL:HG12	23:3F:262:VAL:HG12	1.79	0.63
31:B8:352:GLN:HE22	31:B8:379:GLY:HA2	1.61	0.63
4:SC:132:ASP:HB2	4:SC:221:PRO:HB3	1.80	0.63
22:3E:309:LEU:HG	22:3E:371:LEU:HD21	1.79	0.63
44:RE:578:ILE:HG22	44:RE:619:VAL:HG12	1.79	0.63
13:SP:80:HIS:HA	13:SP:113:GLY:O	1.97	0.63
44:RE:529:VAL:HB	44:RE:613:VAL:HB	1.81	0.63
44:RE:894:ARG:HA	44:RE:897:ARG:HE	1.64	0.63
21:3D:267:ASP:OD1	21:3D:267:ASP:N	2.31	0.63
49:RP:177:LEU:HD13	49:RP:196:LEU:HD21	1.81	0.62
3:SA:113:U:H5"	3:SA:114:C:H5'	1.81	0.62
45:RF:81:VAL:HG12	45:RF:136:ASN:HD22	1.64	0.62
30:B3:501:PRO:HG3	30:B3:543:GLN:HA	1.80	0.62
30:B3:594:GLY:O	30:B3:619:ARG:NH2	2.31	0.62
32:BE:176:TYR:HB3	32:BE:179:LYS:HB2	1.82	0.62
33:B6:355:LEU:HB3	33:B6:358:LEU:HB3	1.81	0.62
44:RE:149:VAL:HA	44:RE:152:PHE:HB3	1.82	0.62
23:3F:443:LEU:HD21	23:3F:492:TRP:HE1	1.65	0.62
29:B2:333:ARG:NH1	29:B2:334:SER:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RJ:279:PRO:HB3	46:RJ:784:LYS:HA	1.82	0.62
46:RJ:775:GLU:HA	46:RJ:779:ARG:HG2	1.81	0.62
34:5C:242:PRO:HG2	34:5C:284:ARG:HA	1.80	0.62
3:SA:573:C:O2'	46:RJ:870:ARG:NH2	2.33	0.61
29:B2:264:ASN:H	29:B2:269:THR:HG1	1.45	0.61
33:B6:106:ASP:OD1	33:B6:106:ASP:N	2.33	0.61
43:RD:1475:SER:HA	43:RD:1478:TRP:HB2	1.82	0.61
21:3D:37:GLN:NE2	40:5I:385:VAL:O	2.34	0.61
23:3F:398:CYS:SG	23:3F:399:GLU:N	2.74	0.61
30:B3:288:LEU:HB3	30:B3:307:SER:HB2	1.83	0.61
32:BE:590:ALA:O	32:BE:602:SER:HA	2.01	0.61
3:SA:474:A:H5"	10:SK:144:PRO:HD2	1.82	0.61
24:3G:93:VAL:HG12	24:3G:95:ARG:H	1.66	0.61
34:5C:162:ASN:ND2	34:5C:429:GLU:OE2	2.33	0.61
44:RE:526:CYS:O	44:RE:698:ASN:ND2	2.34	0.61
44:RE:701:ILE:O	44:RE:705:HIS:CB	2.49	0.61
28:B1:716:ASP:HB3	32:BE:574:THR:HG21	1.83	0.61
8:SI:27:LEU:HD13	8:SI:80:GLU:HG3	1.81	0.61
28:B1:369:ILE:HB	28:B1:383:PHE:HB2	1.82	0.61
49:RP:1926:PHE:HB2	49:RP:1930:SER:HB3	1.82	0.61
52:RZ:999:LYS:HD3	52:RZ:1000:PHE:H	1.66	0.61
32:BE:724:SER:HA	32:BE:877:ASN:HD22	1.65	0.60
44:RE:761:ARG:HD2	44:RE:899:LEU:HD21	1.82	0.60
46:RJ:890:CYS:SG	46:RJ:891:SER:N	2.75	0.60
21:3D:229:LEU:HG	21:3D:256:ARG:HH21	1.66	0.60
28:B1:223:ARG:NH2	28:B1:245:LYS:O	2.34	0.60
33:B6:14:GLU:HG2	33:B6:91:ARG:HH12	1.65	0.60
30:B3:757:GLN:NE2	30:B3:789:THR:OG1	2.34	0.60
3:SA:574:G:OP2	46:RJ:873:LYS:NZ	2.35	0.60
6:SG:76:ARG:HH22	14:SR:123:ARG:HH12	1.47	0.60
34:5C:354:CYS:SG	34:5C:355:PHE:N	2.74	0.60
45:RF:105:SER:OG	45:RF:106:ASP:N	2.34	0.60
49:RP:1945:ILE:HG21	49:RP:1982:VAL:HG23	1.83	0.60
50:RQ:336:THR:HG23	50:RQ:339:GLN:H	1.67	0.60
16:SY:141:GLU:HB2	46:RJ:833:ARG:HH12	1.66	0.60
32:BE:287:LEU:HB3	32:BE:290:ILE:HD11	1.83	0.60
23:3F:569:ASP:N	23:3F:569:ASP:OD1	2.33	0.60
28:B1:601:ILE:HD11	28:B1:681:VAL:HG11	1.84	0.60
29:B2:160:ARG:HH22	36:5E:522:ARG:HD2	1.66	0.60
30:B3:593:CYS:SG	30:B3:619:ARG:NH1	2.74	0.60
46:RJ:830:ARG:NH2	46:RJ:878:HIS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AE:96:ASN:OD1	31:B8:41:ASN:ND2	2.35	0.60
29:B2:861:ILE:O	29:B2:865:HIS:HB2	2.02	0.60
30:B3:200:GLU:HB3	30:B3:209:LEU:HD23	1.82	0.60
49:RP:2026:ILE:O	49:RP:2030:ASN:HB2	2.02	0.60
13:SP:53:ASP:HB2	13:SP:56:SER:HB2	1.84	0.60
29:B2:439:LEU:HD13	29:B2:481:LEU:HD21	1.83	0.60
30:B3:557:VAL:O	30:B3:571:LEU:HA	2.01	0.60
32:BE:570:ILE:HG22	32:BE:577:VAL:HA	1.83	0.60
36:5E:367:ASP:HA	36:5E:370:ARG:HG2	1.84	0.60
3:SA:1673:G:C6	3:SA:1728:A:N6	2.70	0.60
7:SH:163:THR:HG22	7:SH:165:GLY:H	1.67	0.60
25:A5:225:VAL:O	25:A5:272:SER:HA	2.02	0.60
29:B2:436:CYS:HB3	29:B2:447:LEU:HD12	1.84	0.60
30:B3:69:LEU:HD23	30:B3:110:ALA:H	1.65	0.60
30:B3:598:LEU:HD13	30:B3:612:THR:HG22	1.84	0.60
3:SA:1663:G:N2	3:SA:1738:U:O2	2.30	0.59
21:3D:254:ASN:HA	21:3D:257:ILE:HG22	1.84	0.59
29:B2:392:THR:HG21	29:B2:410:SER:HB3	1.84	0.59
31:B8:521:LEU:HA	31:B8:531:CYS:O	2.02	0.59
52:RZ:941:ILE:HB	52:RZ:1029:PHE:HB3	1.84	0.59
32:BE:395:LYS:HA	32:BE:402:VAL:HG12	1.84	0.59
49:RP:1909:GLY:HA2	49:RP:1912:ILE:HD12	1.83	0.59
3:SA:-7:A:N1	50:RQ:306:ARG:NH2	2.49	0.59
3:SA:207:U:O2	9:SJ:178:ARG:NH1	2.35	0.59
10:SK:9:SER:OG	10:SK:10:LYS:N	2.34	0.59
10:SK:106:GLU:OE2	10:SK:115:LYS:NZ	2.35	0.59
28:B1:110:LEU:HD21	28:B1:121:ILE:HG23	1.85	0.59
30:B3:590:LEU:HD11	30:B3:633:VAL:HG21	1.84	0.59
29:B2:536:CYS:HB3	29:B2:549:SER:HB3	1.83	0.59
34:5C:277:VAL:HA	34:5C:293:GLY:HA2	1.83	0.59
38:5G:1:MET:SD	38:5G:5:GLN:NE2	2.76	0.59
47:RK:171:ASP:N	47:RK:171:ASP:OD1	2.32	0.59
20:3B:228:GLN:NE2	21:3D:101:SER:O	2.35	0.59
23:3F:113:ASP:N	49:RP:82:TYR:HH	2.00	0.59
23:3F:282:GLU:HB3	23:3F:300:ALA:HB3	1.85	0.59
45:RF:20:LEU:HD12	45:RF:32:ALA:HB1	1.84	0.59
3:SA:1541:G:H21	3:SA:1570:A:H62	1.45	0.59
10:SK:45:ILE:HG21	10:SK:105:LEU:HB3	1.83	0.59
34:5C:356:GLY:O	34:5C:364:ARG:NH1	2.36	0.59
47:RK:20:ARG:NH1	47:RK:328:ASP:OD1	2.36	0.59
22:3E:245:THR:OG1	22:3E:246:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AE:20:LEU:HD13	34:5C:140:ARG:HG3	1.85	0.59
47:RK:192:THR:HA	47:RK:224:ASN:O	2.03	0.59
46:RJ:301:ILE:HG22	46:RJ:791:ILE:HG23	1.85	0.59
47:RK:114:PHE:HB2	47:RK:170:VAL:HG22	1.84	0.59
20:3C:86:VAL:N	20:3C:100:ARG:O	2.36	0.58
30:B3:454:LEU:HD23	30:B3:466:TRP:HE1	1.68	0.58
33:B6:345:ASP:HB2	33:B6:349:LEU:HA	1.83	0.58
40:5I:252:ASN:ND2	49:RP:1949:PRO:O	2.35	0.58
29:B2:351:LEU:O	29:B2:366:SER:HA	2.02	0.58
32:BE:65:THR:HG23	32:BE:67:HIS:H	1.68	0.58
37:5F:117:ARG:NH1	37:5F:155:GLU:OE1	2.36	0.58
29:B2:334:SER:OG	29:B2:335:LEU:N	2.36	0.58
30:B3:584:ILE:HG22	30:B3:585:ASN:HD22	1.68	0.58
45:RF:18:PHE:H	45:RF:35:HIS:H	1.51	0.58
46:RJ:847:LEU:O	46:RJ:853:ARG:HA	2.03	0.58
26:AE:17:THR:O	26:AE:84:ASN:ND2	2.36	0.58
38:5G:123:VAL:HG12	38:5G:125:PRO:HD2	1.86	0.58
3:SA:477:A:H5'	39:5H:563:VAL:HG21	1.84	0.58
32:BE:128:LEU:HB2	32:BE:150:PRO:HG2	1.85	0.58
3:SA:57:G:OP1	17:SZ:112:LYS:NZ	2.36	0.58
8:SI:132:PRO:O	12:SO:21:ASN:ND2	2.36	0.58
20:3C:242:ALA:HB3	20:3C:269:ILE:HG22	1.86	0.58
35:5D:59:ASN:ND2	37:5F:118:LEU:O	2.37	0.58
44:RE:1205:LYS:HB2	44:RE:1215:ASN:HB3	1.85	0.58
3:SA:151:G:N3	7:SH:13:GLN:NE2	2.50	0.58
14:SR:42:GLU:HG2	14:SR:45:ARG:HH22	1.68	0.58
28:B1:471:GLY:O	28:B1:498:ARG:NH2	2.37	0.58
30:B3:96:VAL:HG12	30:B3:97:ARG:HG2	1.85	0.58
34:5C:206:VAL:HG21	34:5C:247:MET:HG3	1.85	0.58
44:RE:587:GLY:HA3	44:RE:611:ASP:H	1.69	0.58
45:RF:3:ILE:HG12	45:RF:5:ASP:H	1.69	0.58
51:RT:124:LEU:HD22	51:RT:175:LEU:HD11	1.85	0.58
14:SR:51:PRO:HG3	14:SR:116:LEU:HD11	1.84	0.58
34:5C:415:GLU:O	34:5C:428:GLN:NE2	2.36	0.58
3:SA:896:U:O2	13:SP:41:ARG:NH1	2.37	0.58
8:SI:138:LYS:HG2	8:SI:152:VAL:HG12	1.85	0.58
29:B2:49:VAL:HG11	29:B2:85:LEU:HD11	1.85	0.58
46:RJ:864:ASP:OD2	46:RJ:868:ARG:NH2	2.36	0.58
3:SA:103:A:O2'	3:SA:309:C:N4	2.37	0.57
29:B2:412:GLY:HA3	29:B2:430:CYS:H	1.69	0.57
32:BE:25:SER:OG	32:BE:657:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:5F:137:ARG:NH2	37:5F:139:GLY:O	2.37	0.57
40:5I:228:ASN:ND2	40:5I:234:ILE:O	2.37	0.57
49:RP:1760:ASN:ND2	49:RP:1803:ASN:OD1	2.37	0.57
25:A5:88:TYR:HB2	25:A5:95:VAL:HG12	1.86	0.57
25:A5:247:THR:HG21	25:A5:293:ASN:H	1.68	0.57
33:B6:324:ASP:OD2	33:B6:372:ARG:NH1	2.36	0.57
8:SI:159:VAL:HA	8:SI:162:ILE:HG22	1.84	0.57
25:A5:212:LEU:HB2	25:A5:226:LEU:HB2	1.85	0.57
29:B2:289:GLU:HA	29:B2:292:ILE:HG12	1.86	0.57
38:5G:136:THR:HG23	38:5G:157:PHE:HZ	1.69	0.57
46:RJ:299:ALA:HB3	46:RJ:792:VAL:HG23	1.85	0.57
52:RZ:1095:ARG:NH1	52:RZ:1148:PRO:O	2.37	0.57
3:SA:205:U:H2'	3:SA:206:A:H8	1.70	0.57
30:B3:24:THR:HG22	30:B3:32:LEU:HD13	1.87	0.57
38:5G:285:ASN:O	48:RN:771:ASN:ND2	2.37	0.57
20:3B:254:ALA:O	20:3B:258:HIS:ND1	2.37	0.57
23:3F:325:VAL:HA	23:3F:340:GLY:HA2	1.86	0.57
6:SG:117:THR:HG21	6:SG:194:LEU:HD23	1.87	0.57
49:RP:2026:ILE:HG23	49:RP:2030:ASN:HD22	1.69	0.57
51:RT:164:LEU:HD22	51:RT:182:ILE:HD11	1.86	0.57
15:SX:96:ALA:HB3	15:SX:99:PHE:HB3	1.86	0.57
28:B1:689:THR:HG21	28:B1:826:ARG:HD3	1.87	0.57
28:B1:707:ASN:ND2	28:B1:709:THR:OG1	2.37	0.57
40:5I:189:ARG:NH1	40:5I:229:GLN:OE1	2.38	0.57
52:RZ:600:PHE:CZ	52:RZ:684:ASP:O	2.57	0.57
30:B3:128:VAL:HG12	30:B3:138:HIS:HB2	1.86	0.57
49:RP:1880:ILE:O	49:RP:1883:HIS:ND1	2.35	0.57
3:SA:623:A:H62	3:SA:976:G:H21	1.52	0.57
10:SK:176:ASN:O	10:SK:180:LYS:HB2	2.05	0.57
11:SM:91:LEU:HD11	11:SM:100:TYR:HB3	1.85	0.57
22:3E:251:ASP:N	22:3E:251:ASP:OD1	2.35	0.57
44:RE:209:MET:HB3	44:RE:299:PRO:HD3	1.87	0.57
44:RE:254:LEU:HD13	44:RE:270:ILE:HG13	1.87	0.57
44:RE:308:LEU:HG	44:RE:337:LEU:HD21	1.86	0.57
45:RF:252:LYS:O	45:RF:254:LYS:NZ	2.37	0.57
47:RK:214:LYS:HA	47:RK:217:LYS:HD3	1.87	0.57
15:SX:122:SER:OG	15:SX:123:GLY:N	2.36	0.57
34:5C:415:GLU:OE2	40:5I:33:HIS:ND1	2.38	0.57
40:5I:228:ASN:HD21	40:5I:234:ILE:HG12	1.70	0.57
45:RF:162:THR:HG22	45:RF:165:PHE:H	1.70	0.57
47:RK:188:ILE:HG13	47:RK:283:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:87:G:OP2	22:3E:338:LYS:NZ	2.37	0.56
3:SA:304:U:O2'	11:SM:69:LYS:NZ	2.38	0.56
3:SA:433:C:N4	3:SA:436:A:OP1	2.38	0.56
7:SH:134:GLY:HA3	7:SH:158:ILE:HD12	1.85	0.56
8:SI:133:THR:HA	12:SO:21:ASN:HD21	1.69	0.56
9:SJ:114:GLU:HG2	9:SJ:120:THR:HA	1.87	0.56
12:SO:87:ASP:N	12:SO:87:ASP:OD1	2.36	0.56
13:SP:20:TYR:HB3	13:SP:27:PHE:HB2	1.87	0.56
26:AE:258:HIS:HB3	26:AE:298:THR:HG21	1.87	0.56
44:RE:585:MET:HB3	44:RE:610:PHE:HB3	1.85	0.56
51:RT:96:SER:HA	51:RT:139:LEU:O	2.05	0.56
3:SA:142:G:H22	3:SA:173:A:H2	1.53	0.56
3:SA:805:U:OP1	15:SX:32:LYS:NZ	2.37	0.56
16:SY:132:LEU:HA	16:SY:135:LEU:HB2	1.85	0.56
28:B1:121:ILE:HG22	28:B1:139:HIS:HB3	1.87	0.56
44:RE:483:SER:OG	44:RE:582:GLN:NE2	2.37	0.56
44:RE:756:VAL:O	44:RE:761:ARG:NH2	2.38	0.56
44:RE:801:LYS:HG3	45:RF:187:HIS:HD2	1.69	0.56
1:3A:84:U:OP2	22:3E:361:ARG:NH2	2.37	0.56
3:SA:939:A:OP1	12:SO:114:ARG:NH2	2.38	0.56
5:SF:66:MET:SD	5:SF:78:THR:OG1	2.64	0.56
12:SO:129:TYR:HB3	12:SO:135:LEU:HD22	1.86	0.56
26:AE:83:ARG:NH1	26:AE:125:PHE:O	2.38	0.56
29:B2:344:THR:O	29:B2:352:GLU:HB2	2.05	0.56
30:B3:194:ARG:HG2	30:B3:243:VAL:HG13	1.86	0.56
30:B3:509:ALA:HB1	30:B3:536:LEU:HD13	1.86	0.56
33:B6:327:LEU:HD12	33:B6:328:ASP:H	1.70	0.56
34:5C:447:ASN:O	40:5I:37:ARG:NH1	2.38	0.56
34:5C:460:ARG:NH2	50:RQ:848:PRO:O	2.38	0.56
40:5I:376:ARG:HH12	40:5I:382:ARG:HA	1.71	0.56
45:RF:18:PHE:HB2	45:RF:35:HIS:HB3	1.87	0.56
21:3D:65:ASN:ND2	21:3D:75:SER:OG	2.39	0.56
30:B3:64:ILE:O	30:B3:81:GLN:NE2	2.34	0.56
44:RE:675:GLU:HG3	44:RE:702:LYS:HD2	1.86	0.56
3:SA:343:C:H2'	3:SA:344:A:H8	1.70	0.56
21:3D:88:LYS:HE2	50:RQ:330:THR:HG22	1.86	0.56
1:3A:82:G:O2'	1:3A:327:G:N2	2.36	0.56
4:SC:19:ARG:NH2	30:B3:308:ASP:OD1	2.38	0.56
17:SZ:46:GLU:HA	49:RP:37:ARG:HH22	1.69	0.56
21:3D:258:SER:OG	21:3D:259:MET:N	2.39	0.56
44:RE:770:PRO:HB3	44:RE:847:GLY:HA3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RZ:776:VAL:HG22	52:RZ:813:ALA:HB2	1.86	0.56
3:SA:1541:G:N2	3:SA:1570:A:N6	2.49	0.56
26:AE:31:ALA:HB1	26:AE:154:ILE:HG23	1.88	0.56
32:BE:118:VAL:HA	32:BE:132:THR:HA	1.87	0.56
50:RQ:772:LYS:HA	50:RQ:830:ILE:HD12	1.87	0.56
3:SA:1797:A:N6	51:RT:226:LEU:O	2.39	0.56
5:SF:71:LYS:NZ	5:SF:93:ASP:OD2	2.39	0.56
23:3F:492:TRP:HB3	23:3F:520:VAL:HG12	1.87	0.56
25:A5:255:ILE:HB	25:A5:277:LYS:HB2	1.88	0.56
34:5C:461:LEU:HD21	34:5C:466:LEU:HG	1.87	0.56
38:5G:100:LEU:HD13	38:5G:144:GLU:HB3	1.87	0.56
47:RK:295:PRO:HG3	47:RK:325:LEU:HD11	1.88	0.56
13:SP:125:SER:OG	13:SP:126:THR:N	2.38	0.56
14:SR:120:ASP:O	14:SR:123:ARG:NH2	2.37	0.56
22:3E:359:ILE:HG13	22:3E:398:LEU:HD12	1.87	0.56
28:B1:219:GLU:HG3	28:B1:221:THR:HG23	1.87	0.56
28:B1:506:SER:HB2	28:B1:508:GLN:HG2	1.86	0.56
32:BE:78:SER:OG	32:BE:79:SER:N	2.39	0.56
3:SA:805:U:O2	15:SX:124:LYS:NZ	2.39	0.56
6:SG:97:LEU:O	6:SG:180:ARG:NH2	2.39	0.56
6:SG:201:ALA:HA	6:SG:211:ILE:HD11	1.87	0.56
9:SJ:117:TYR:OH	11:SM:24:LYS:NZ	2.38	0.56
14:SR:39:VAL:HG21	14:SR:48:VAL:HG11	1.87	0.56
33:B6:5:ARG:HH12	34:5C:63:THR:HG23	1.69	0.56
44:RE:305:PRO:HA	44:RE:308:LEU:HB2	1.87	0.56
22:3E:385:ASP:N	22:3E:385:ASP:OD1	2.39	0.55
28:B1:316:TRP:HE1	28:B1:338:ILE:HG13	1.71	0.55
40:5I:140:SER:OG	40:5I:141:ASP:N	2.36	0.55
44:RE:711:PRO:HB2	44:RE:713:LEU:HD23	1.87	0.55
47:RK:82:VAL:HG23	47:RK:111:LYS:HD3	1.86	0.55
49:RP:1946:LYS:NZ	53:X1:325:UNK:O	2.39	0.55
3:SA:126:A:N6	3:SA:291:G:H21	2.03	0.55
3:SA:512:A:N3	10:SK:131:GLN:NE2	2.53	0.55
29:B2:381:LYS:NZ	29:B2:384:THR:OG1	2.40	0.55
30:B3:494:ILE:N	30:B3:510:SER:HG	2.04	0.55
34:5C:103:ALA:HB2	34:5C:402:ILE:HD11	1.87	0.55
44:RE:215:GLU:OE2	44:RE:223:ARG:NH1	2.39	0.55
44:RE:858:ARG:HD2	44:RE:861:ILE:HD11	1.88	0.55
44:RE:1069:LYS:O	44:RE:1073:ASN:ND2	2.39	0.55
44:RE:1101:ASP:HB2	44:RE:1233:ASN:HB3	1.88	0.55
47:RK:12:GLN:NE2	47:RK:34:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:974:A:O3'	12:SO:112:LYS:NZ	2.39	0.55
5:SF:18:TRP:O	5:SF:51:ARG:NH2	2.38	0.55
20:3B:264:GLN:OE1	20:3B:319:ARG:NH1	2.40	0.55
23:3F:134:ARG:NH2	23:3F:528:GLU:OE2	2.39	0.55
25:A5:5:VAL:HA	25:A5:21:THR:HG22	1.87	0.55
32:BE:97:LYS:HG3	32:BE:111:GLU:HA	1.88	0.55
32:BE:126:ASP:OD2	32:BE:141:LYS:NZ	2.39	0.55
43:RD:1525:ASN:HD22	43:RD:1556:ILE:HG22	1.70	0.55
10:SK:119:ALA:O	10:SK:124:HIS:ND1	2.37	0.55
20:3C:155:ILE:HD11	20:3C:162:LEU:HD22	1.87	0.55
29:B2:549:SER:OG	29:B2:576:VAL:O	2.24	0.55
40:5I:62:LEU:HD23	40:5I:374:LEU:HD11	1.89	0.55
40:5I:367:SER:OG	40:5I:368:ASP:N	2.39	0.55
46:RJ:906:ASP:N	46:RJ:906:ASP:OD1	2.39	0.55
52:RZ:840:PRO:HB2	52:RZ:842:ILE:HG22	1.87	0.55
8:SI:143:LEU:O	15:SX:42:GLN:NE2	2.40	0.55
20:3C:244:VAL:O	20:3C:249:GLN:NE2	2.38	0.55
25:A5:84:GLU:OE1	25:A5:86:TRP:NE1	2.38	0.55
28:B1:65:LYS:HG3	28:B1:106:PRO:HA	1.88	0.55
30:B3:721:ASN:OD1	30:B3:721:ASN:N	2.39	0.55
32:BE:732:ASN:ND2	36:5E:484:MET:SD	2.79	0.55
43:RD:1582:VAL:HA	43:RD:1585:TRP:HD1	1.71	0.55
46:RJ:304:LEU:HB2	46:RJ:788:TYR:O	2.06	0.55
11:SM:46:LYS:HD3	11:SM:49:ILE:HD12	1.88	0.55
25:A5:212:LEU:HD21	25:A5:232:ILE:HD13	1.88	0.55
29:B2:401:ASP:OD1	29:B2:401:ASP:N	2.40	0.55
29:B2:913:ASN:O	29:B2:917:ASN:HB3	2.06	0.55
30:B3:17:ALA:HB3	30:B3:35:PRO:HA	1.88	0.55
32:BE:211:THR:HG21	32:BE:253:SER:HA	1.88	0.55
37:5F:45:HIS:O	37:5F:49:ARG:HB2	2.07	0.55
38:5G:74:ASP:OD2	38:5G:201:ARG:NH1	2.39	0.55
1:3A:253:G:N7	23:3F:551:ARG:NH2	2.55	0.55
3:SA:886:U:H2'	3:SA:887:A:H8	1.72	0.55
30:B3:162:LEU:HA	30:B3:176:ASP:HA	1.89	0.55
30:B3:679:THR:HA	30:B3:724:LEU:HD13	1.89	0.55
44:RE:114:VAL:O	44:RE:117:LYS:NZ	2.38	0.55
46:RJ:1034:LEU:H	46:RJ:1037:GLN:HE21	1.54	0.55
47:RK:174:ILE:O	47:RK:361:ASN:ND2	2.39	0.55
47:RK:281:GLU:HG2	47:RK:285:LYS:HD2	1.86	0.55
29:B2:250:LYS:NZ	29:B2:254:GLN:O	2.36	0.55
33:B6:330:GLU:HB3	33:B6:333:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1679:G:O3'	3:SA:1722:A:N6	2.40	0.55
13:SP:29:HIS:HB3	13:SP:41:ARG:HA	1.89	0.55
9:SJ:48:THR:OG1	9:SJ:51:GLY:O	2.23	0.55
29:B2:229:TRP:HA	29:B2:244:GLU:HA	1.89	0.55
33:B6:2:SER:O	50:RQ:872:ARG:NH1	2.36	0.55
44:RE:141:TRP:O	44:RE:179:LYS:NZ	2.39	0.55
49:RP:2051:ASP:OD1	49:RP:2051:ASP:N	2.38	0.55
52:RZ:732:LEU:HD13	52:RZ:746:VAL:HA	1.89	0.55
21:3D:182:ASP:HB3	21:3D:314:ARG:HH21	1.72	0.54
31:B8:130:ASP:OD1	31:B8:130:ASP:N	2.40	0.54
3:SA:484:C:H42	3:SA:503:G:H1	1.54	0.54
12:SO:61:THR:OG1	12:SO:62:GLN:N	2.39	0.54
26:AE:193:THR:HB	26:AE:241:ILE:HG21	1.88	0.54
28:B1:559:ILE:HD12	28:B1:598:ASN:HD21	1.71	0.54
29:B2:338:ILE:HB	29:B2:355:LEU:HD11	1.89	0.54
47:RK:23:LEU:HD21	47:RK:329:ILE:HG22	1.90	0.54
47:RK:137:LEU:HD23	47:RK:296:LEU:HD13	1.90	0.54
52:RZ:534:ARG:NH2	52:RZ:864:ASN:O	2.40	0.54
3:SA:472:U:H2'	3:SA:473:A:H8	1.72	0.54
3:SA:494:U:O2	46:RJ:1135:ARG:NH2	2.40	0.54
3:SA:1796:C:H2'	3:SA:1797:A:H8	1.72	0.54
28:B1:707:ASN:HB2	28:B1:709:THR:HG23	1.89	0.54
44:RE:142:GLU:O	44:RE:144:LYS:NZ	2.38	0.54
44:RE:709:PRO:HB2	44:RE:1114:ILE:HG12	1.87	0.54
49:RP:2056:ARG:HE	49:RP:2060:GLN:HE21	1.54	0.54
3:SA:445:A:H2'	3:SA:446:A:H8	1.71	0.54
3:SA:590:C:H2'	3:SA:591:A:H8	1.73	0.54
22:3E:419:VAL:HG11	32:BE:323:VAL:HG21	1.89	0.54
28:B1:482:SER:OG	28:B1:483:GLN:N	2.39	0.54
30:B3:246:CYS:SG	30:B3:260:THR:OG1	2.65	0.54
30:B3:515:CYS:HB2	30:B3:529:LEU:HB2	1.90	0.54
32:BE:619:CYS:SG	32:BE:620:ILE:N	2.80	0.54
34:5C:188:LYS:HE2	37:5F:23:GLN:HB2	1.90	0.54
39:5H:569:TYR:O	39:5H:573:GLN:N	2.39	0.54
49:RP:1783:LEU:O	49:RP:1787:ASN:ND2	2.41	0.54
1:3A:34:A:N7	37:5F:7:HIS:ND1	2.55	0.54
3:SA:138:A:N6	3:SA:175:G:O2'	2.39	0.54
3:SA:551:G:N7	35:5D:2:ALA:N	2.55	0.54
28:B1:176:ASP:OD1	28:B1:176:ASP:N	2.40	0.54
29:B2:417:TRP:NE1	29:B2:424:CYS:SG	2.78	0.54
30:B3:38:ASP:N	30:B3:38:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B3:481:LYS:HE3	30:B3:523:GLY:H	1.71	0.54
31:B8:366:SER:OG	31:B8:438:ASN:ND2	2.40	0.54
52:RZ:1209:ARG:HG2	52:RZ:1211:CYS:HB3	1.90	0.54
31:B8:242:ASN:ND2	31:B8:275:TYR:OH	2.41	0.54
32:BE:28:ARG:HG2	32:BE:30:ILE:HG22	1.89	0.54
44:RE:506:GLN:HB2	44:RE:509:ASN:HB2	1.89	0.54
52:RZ:1124:ARG:NH1	52:RZ:1127:ASN:O	2.40	0.54
3:SA:859:A:OP1	12:SO:73:ARG:NH1	2.40	0.54
23:3F:289:ARG:NH2	23:3F:332:ALA:O	2.39	0.54
28:B1:23:SER:HA	28:B1:63:LEU:HD21	1.89	0.54
29:B2:426:ARG:NH2	29:B2:459:LEU:O	2.41	0.54
30:B3:176:ASP:OD2	30:B3:179:LYS:N	2.39	0.54
32:BE:209:ILE:HA	32:BE:225:THR:HA	1.89	0.54
42:5K:107:GLU:OE1	42:5K:121:ARG:NH1	2.41	0.54
47:RK:228:ASP:OD2	47:RK:230:TRP:NE1	2.40	0.54
47:RK:306:GLU:OE2	47:RK:355:LYS:NZ	2.40	0.54
51:RT:258:LYS:O	51:RT:262:ASN:ND2	2.40	0.54
52:RZ:1113:ILE:HD12	52:RZ:1166:ARG:HH22	1.71	0.54
30:B3:618:ASN:OD1	30:B3:618:ASN:N	2.38	0.54
30:B3:791:ARG:HH12	36:5E:493:GLN:HE22	1.56	0.54
31:B8:268:TYR:OH	31:B8:296:GLN:NE2	2.41	0.54
32:BE:21:SER:OG	32:BE:22:LYS:N	2.41	0.54
32:BE:718:LYS:O	32:BE:875:ASN:ND2	2.39	0.54
46:RJ:934:LEU:HB2	46:RJ:1003:LEU:HB2	1.88	0.54
50:RQ:303:GLN:HE21	50:RQ:307:ARG:HD3	1.73	0.54
3:SA:478:A:N1	3:SA:510:G:O6	2.40	0.54
3:SA:1118:G:H2'	48:RN:786:ASN:HD21	1.73	0.54
20:3B:306:LEU:HD11	20:3B:313:HIS:HB2	1.90	0.54
30:B3:246:CYS:HG	30:B3:260:THR:HG1	1.55	0.54
30:B3:279:LYS:NZ	30:B3:326:THR:OG1	2.41	0.54
30:B3:396:ALA:HA	30:B3:402:TRP:O	2.08	0.54
32:BE:78:SER:HB3	32:BE:95:GLU:HG2	1.90	0.54
32:BE:758:PHE:HA	51:RT:176:ARG:HH21	1.73	0.54
34:5C:164:GLN:HA	34:5C:179:HIS:HB3	1.90	0.54
38:5G:187:PRO:HB3	38:5G:220:ARG:HG3	1.90	0.54
46:RJ:254:HIS:HD2	46:RJ:256:GLU:H	1.56	0.54
22:3E:215:ARG:NH2	22:3E:242:SER:OG	2.41	0.54
22:3E:421:MET:N	22:3E:421:MET:SD	2.81	0.54
23:3F:241:THR:HG21	23:3F:286:LEU:H	1.73	0.54
25:A5:231:ASP:OD1	25:A5:231:ASP:N	2.38	0.54
28:B1:737:ASN:O	28:B1:741:MET:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B3:296:ILE:HG22	30:B3:297:LEU:HG	1.90	0.54
42:5K:74:PHE:HB3	42:5K:175:VAL:HG11	1.90	0.54
49:RP:1880:ILE:HD13	49:RP:1917:ILE:HG12	1.90	0.54
52:RZ:445:VAL:HB	52:RZ:489:VAL:HA	1.90	0.54
3:SA:478:A:H5'	39:5H:562:ARG:HH22	1.73	0.53
15:SX:112:ASP:OD1	15:SX:112:ASP:N	2.33	0.53
20:3C:306:LEU:HD22	20:3C:315:ILE:HG12	1.90	0.53
23:3F:417:SER:OG	23:3F:418:ASP:N	2.40	0.53
28:B1:117:ARG:NH2	28:B1:145:HIS:O	2.41	0.53
28:B1:329:VAL:HG12	28:B1:339:LEU:H	1.72	0.53
28:B1:391:THR:OG1	28:B1:392:ALA:N	2.41	0.53
29:B2:537:VAL:HG22	29:B2:548:ILE:HG22	1.89	0.53
40:5I:396:TYR:HB2	50:RQ:879:ILE:HD13	1.90	0.53
3:SA:1471:A:N7	6:SG:102:ARG:NH2	2.53	0.53
6:SG:133:VAL:HG23	6:SG:198:LEU:HD11	1.90	0.53
20:3B:320:TYR:HE1	20:3B:322:ARG:HD2	1.71	0.53
29:B2:236:ASP:OD1	29:B2:236:ASP:N	2.41	0.53
35:5D:58:ARG:HE	37:5F:174:ARG:HH12	1.55	0.53
38:5G:143:HIS:HB2	38:5G:151:SER:HB2	1.90	0.53
43:RD:1602:ARG:HE	43:RD:1636:ARG:HD2	1.74	0.53
45:RF:87:LEU:HD23	45:RF:124:ALA:HB1	1.89	0.53
3:SA:819:G:N2	3:SA:857:U:OP1	2.41	0.53
3:SA:1794:A:OP2	51:RT:200:ARG:NH1	2.41	0.53
4:SC:113:MET:SD	4:SC:209:ASN:ND2	2.81	0.53
6:SG:50:GLU:OE2	6:SG:128:ASN:ND2	2.41	0.53
21:3D:126:ASP:HA	21:3D:129:ARG:HB3	1.90	0.53
21:3D:210:VAL:HG21	21:3D:219:LEU:HD21	1.90	0.53
26:AE:39:THR:O	26:AE:43:GLN:NE2	2.34	0.53
26:AE:134:MET:O	26:AE:138:SER:HB3	2.08	0.53
26:AE:217:PHE:HE2	26:AE:241:ILE:HD11	1.74	0.53
31:B8:18:GLU:OE1	33:B6:69:LYS:NZ	2.41	0.53
32:BE:359:ALA:O	32:BE:421:ASN:ND2	2.41	0.53
33:B6:177:ASP:N	33:B6:177:ASP:OD1	2.40	0.53
36:5E:440:LEU:HG	37:5F:57:LEU:HD23	1.90	0.53
40:5I:228:ASN:ND2	40:5I:231:GLU:O	2.41	0.53
10:SK:82:ARG:HH11	10:SK:149:ARG:HH21	1.55	0.53
22:3E:405:ASP:OD1	22:3E:405:ASP:N	2.40	0.53
23:3F:457:GLU:OE1	23:3F:461:LYS:NZ	2.41	0.53
29:B2:124:ILE:HA	29:B2:140:SER:HA	1.90	0.53
30:B3:219:ILE:HG22	30:B3:221:ASN:HB2	1.90	0.53
32:BE:543:ASP:OD1	32:BE:543:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B6:297:ASP:OD1	33:B6:297:ASP:N	2.40	0.53
33:B6:315:GLU:OE1	33:B6:318:ARG:NH1	2.41	0.53
34:5C:23:ARG:HH22	50:RQ:869:TRP:HB3	1.74	0.53
37:5F:27:HIS:O	37:5F:31:GLN:HB2	2.09	0.53
40:5I:244:ILE:HD11	40:5I:264:THR:HG21	1.90	0.53
40:5I:402:GLU:O	40:5I:405:ARG:NH2	2.41	0.53
25:A5:210:ARG:NH1	32:BE:563:ASP:OD2	2.38	0.53
28:B1:30:LEU:HD21	28:B1:63:LEU:HD22	1.90	0.53
28:B1:558:ASP:N	28:B1:558:ASP:OD1	2.41	0.53
29:B2:49:VAL:HG23	29:B2:63:LEU:HB3	1.89	0.53
29:B2:186:ILE:HG12	29:B2:202:ALA:HB2	1.90	0.53
40:5I:202:HIS:NE2	40:5I:214:ASP:OD2	2.42	0.53
3:SA:1696:G:H2'	3:SA:1697:G:H8	1.74	0.53
38:5G:173:ARG:NH2	38:5G:180:GLY:O	2.41	0.53
43:RD:1511:ALA:O	43:RD:1515:ASN:ND2	2.41	0.53
44:RE:190:ALA:O	44:RE:192:LYS:NZ	2.41	0.53
44:RE:978:ASP:OD1	44:RE:978:ASP:N	2.41	0.53
52:RZ:779:SER:O	52:RZ:781:ARG:NH1	2.42	0.53
52:RZ:884:GLN:NE2	52:RZ:893:GLU:OE2	2.42	0.53
4:SC:59:ASP:N	4:SC:59:ASP:OD1	2.40	0.53
4:SC:87:ARG:HH21	4:SC:101:HIS:HD2	1.57	0.53
6:SG:126:ASP:N	6:SG:126:ASP:OD1	2.37	0.53
16:SY:141:GLU:OE1	46:RJ:833:ARG:NH2	2.41	0.53
22:3E:286:ASN:HD22	22:3E:387:GLY:H	1.55	0.53
29:B2:395:ARG:N	29:B2:408:THR:O	2.41	0.53
46:RJ:81:GLY:HA3	46:RJ:141:LEU:HD13	1.90	0.53
3:SA:930:A:H62	4:SC:120:LEU:HD11	1.74	0.53
5:SF:143:ASP:OD1	5:SF:143:ASP:N	2.38	0.53
28:B1:350:SER:OG	28:B1:351:LEU:N	2.42	0.53
28:B1:675:MET:N	28:B1:675:MET:SD	2.82	0.53
44:RE:498:MET:O	44:RE:506:GLN:NE2	2.41	0.53
44:RE:551:GLU:OE2	44:RE:552:ARG:NH1	2.42	0.53
52:RZ:808:GLN:OE1	52:RZ:812:ARG:NH1	2.42	0.53
1:3A:255:U:O4	24:3H:84:ARG:NH1	2.42	0.53
30:B3:42:ILE:HG22	30:B3:49:SER:HA	1.91	0.53
38:5G:288:ASP:OD1	38:5G:288:ASP:N	2.41	0.53
40:5I:436:SER:OG	40:5I:440:ARG:NH2	2.42	0.53
52:RZ:594:PHE:HE1	52:RZ:823:ARG:HH11	1.57	0.53
3:SA:557:G:N2	3:SA:571:G:O2'	2.42	0.53
3:SA:1159:C:N4	38:5G:184:GLU:OE2	2.42	0.53
5:SF:54:TYR:O	17:SZ:15:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SK:176:ASN:OD1	10:SK:179:ARG:NH1	2.42	0.53
22:3E:287:LEU:HD22	22:3E:371:LEU:HD13	1.90	0.53
23:3F:239:ILE:HA	23:3F:255:GLY:HA3	1.90	0.53
28:B1:16:ARG:HB3	28:B1:34:GLY:H	1.74	0.53
31:B8:516:THR:OG1	31:B8:517:THR:N	2.41	0.53
32:BE:353:PRO:HA	32:BE:370:SER:HA	1.91	0.53
34:5C:64:ASP:HA	34:5C:67:LEU:HB2	1.91	0.53
38:5G:93:SER:O	38:5G:119:ARG:NH2	2.42	0.53
44:RE:138:ILE:O	44:RE:180:LYS:NZ	2.41	0.53
49:RP:1760:ASN:OD1	49:RP:1760:ASN:N	2.42	0.53
52:RZ:447:ILE:HG13	52:RZ:514:ILE:HD13	1.89	0.53
3:SA:-6:A:H1'	34:5C:41:LYS:HB3	1.90	0.52
3:SA:29:U:H2'	3:SA:30:G:H8	1.73	0.52
3:SA:622:A:O2'	3:SA:976:G:N1	2.40	0.52
5:SF:194:THR:HG23	5:SF:195:ILE:HG23	1.90	0.52
7:SH:180:THR:HG23	7:SH:182:GLN:H	1.72	0.52
20:3B:165:ALA:HB3	20:3B:168:LYS:HG2	1.89	0.52
24:3G:7:LYS:NZ	24:3G:62:GLU:OE1	2.41	0.52
28:B1:408:ASP:OD1	28:B1:430:ARG:NH1	2.41	0.52
29:B2:166:ILE:HA	29:B2:181:SER:HA	1.90	0.52
29:B2:600:TRP:NE1	29:B2:607:CYS:SG	2.81	0.52
30:B3:779:VAL:HA	30:B3:782:VAL:HG22	1.92	0.52
37:5F:109:ARG:NH2	37:5F:155:GLU:OE2	2.42	0.52
43:RD:1536:VAL:HA	43:RD:1539:ARG:HG2	1.91	0.52
51:RT:97:ARG:NH1	51:RT:153:GLN:OE1	2.40	0.52
51:RT:187:VAL:HG13	51:RT:251:ILE:HD11	1.90	0.52
52:RZ:1042:ARG:NH1	52:RZ:1067:LEU:O	2.42	0.52
3:SA:131:C:N3	3:SA:180:A:O2'	2.42	0.52
6:SG:25:LEU:HD11	14:SR:57:LEU:HD22	1.90	0.52
20:3B:194:VAL:HB	20:3B:217:ILE:HG22	1.91	0.52
20:3C:230:TYR:OH	20:3C:256:ASN:ND2	2.42	0.52
21:3D:397:SER:OG	21:3D:398:ASN:N	2.40	0.52
33:B6:306:LYS:HE2	33:B6:354:ASP:HB2	1.91	0.52
50:RQ:269:THR:OG1	50:RQ:270:TYR:N	2.42	0.52
33:B6:25:THR:N	33:B6:28:GLU:OE2	2.39	0.52
33:B6:271:LEU:HD21	33:B6:334:LEU:HB2	1.90	0.52
49:RP:76:THR:O	49:RP:79:GLN:N	2.43	0.52
49:RP:1708:SER:OG	49:RP:1709:ASP:N	2.42	0.52
52:RZ:851:VAL:HG23	52:RZ:862:ILE:HG21	1.91	0.52
1:3A:49:C:N4	1:3A:50:U:O4	2.43	0.52
24:3G:57:ASP:O	24:3G:84:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A5:281:ILE:HG12	25:A5:328:VAL:HB	1.89	0.52
28:B1:440:PRO:HG2	28:B1:483:GLN:HA	1.90	0.52
30:B3:788:TYR:O	30:B3:792:HIS:ND1	2.42	0.52
34:5C:465:ASP:N	34:5C:465:ASP:OD1	2.41	0.52
40:5I:303:ASP:OD2	40:5I:338:HIS:ND1	2.43	0.52
44:RE:329:THR:OG1	44:RE:333:ASN:ND2	2.42	0.52
49:RP:1811:ILE:HB	49:RP:1882:ARG:HH12	1.73	0.52
52:RZ:794:GLN:HE22	52:RZ:908:SER:HB3	1.74	0.52
5:SF:126:VAL:HG22	5:SF:158:ASP:H	1.75	0.52
28:B1:159:ARG:NH2	53:X1:1504:UNK:O	2.43	0.52
28:B1:252:LYS:NZ	28:B1:253:LYS:O	2.43	0.52
28:B1:563:ARG:NH1	28:B1:630:LEU:O	2.43	0.52
29:B2:430:CYS:SG	29:B2:431:GLY:N	2.83	0.52
29:B2:444:LEU:HG	29:B2:456:LEU:HD11	1.91	0.52
32:BE:320:LYS:NZ	32:BE:342:TYR:OH	2.36	0.52
38:5G:99:ARG:NH1	38:5G:175:ASP:OD2	2.42	0.52
3:SA:500:C:OP1	3:SA:501:U:N3	2.43	0.52
3:SA:1628:U:OP2	36:5E:534:ARG:NH1	2.42	0.52
8:SI:91:ILE:HG21	8:SI:129:LEU:HD12	1.91	0.52
28:B1:121:ILE:HB	28:B1:140:ARG:O	2.10	0.52
30:B3:384:TYR:OH	30:B3:423:LYS:N	2.42	0.52
32:BE:354:SER:O	32:BE:631:ASN:ND2	2.39	0.52
34:5C:329:LEU:HD22	34:5C:406:ALA:HB2	1.92	0.52
36:5E:299:SER:O	36:5E:303:GLN:NE2	2.42	0.52
44:RE:1196:PHE:O	44:RE:1197:ARG:NH1	2.37	0.52
49:RP:1948:SER:O	49:RP:1985:ARG:NH2	2.43	0.52
51:RT:256:PRO:HA	51:RT:259:VAL:HG12	1.91	0.52
3:SA:168:A:O2'	7:SH:176:GLN:NE2	2.41	0.52
20:3C:205:ARG:NH1	22:3E:378:GLU:OE1	2.42	0.52
26:AE:2:SER:OG	26:AE:3:SER:N	2.40	0.52
28:B1:138:ARG:NH1	50:RQ:733:ASP:OD2	2.43	0.52
28:B1:202:ASP:N	28:B1:202:ASP:OD1	2.42	0.52
29:B2:196:CYS:SG	30:B3:667:GLN:NE2	2.83	0.52
30:B3:337:HIS:HD2	30:B3:363:ARG:HE	1.56	0.52
40:5I:260:GLN:HE22	40:5I:279:THR:HG21	1.75	0.52
40:5I:281:ASN:HD21	40:5I:287:TYR:HE2	1.56	0.52
2:5A:467:A:N3	2:5A:469:C:N4	2.57	0.52
3:SA:531:C:O2'	17:SZ:62:THR:O	2.26	0.52
3:SA:1169:G:N1	3:SA:1575:G:OP2	2.43	0.52
8:SI:117:THR:OG1	8:SI:118:LEU:N	2.43	0.52
29:B2:183:ASP:N	29:B2:183:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B2:190:ASP:OD1	29:B2:190:ASP:N	2.40	0.52
29:B2:525:ASP:OD1	29:B2:525:ASP:N	2.43	0.52
29:B2:540:SER:OG	29:B2:542:ASP:OD1	2.28	0.52
30:B3:731:LEU:HB2	30:B3:735:GLN:HE22	1.74	0.52
34:5C:217:HIS:NE2	34:5C:222:GLY:O	2.37	0.52
36:5E:383:ARG:NH2	38:5G:213:GLY:O	2.43	0.52
44:RE:1087:LEU:HA	44:RE:1090:THR:HG23	1.90	0.52
47:RK:31:ILE:HG22	47:RK:76:TYR:HB3	1.92	0.52
47:RK:182:GLU:OE1	47:RK:254:TRP:NE1	2.38	0.52
8:SI:77:LEU:HD11	8:SI:92:PHE:HZ	1.73	0.52
11:SM:33:ARG:NH1	11:SM:53:TYR:O	2.42	0.52
25:A5:110:ILE:HG22	25:A5:119:CYS:HB3	1.91	0.52
35:5D:61:ASP:N	35:5D:61:ASP:OD1	2.39	0.52
44:RE:338:SER:O	44:RE:342:HIS:ND1	2.43	0.52
3:SA:572:C:H5'	35:5D:9:GLN:HG3	1.90	0.52
29:B2:448:GLY:HA3	29:B2:476:ILE:HD11	1.91	0.52
30:B3:237:LEU:HD21	44:RE:663:ILE:HG21	1.92	0.52
43:RD:1612:LEU:O	43:RD:1617:HIS:NE2	2.43	0.52
44:RE:515:ILE:HG13	44:RE:522:LYS:HE2	1.91	0.52
52:RZ:936:VAL:HG11	52:RZ:1038:ILE:HB	1.92	0.52
10:SK:68:LYS:O	10:SK:72:GLU:HB2	2.10	0.51
31:B8:311:ASN:HA	31:B8:324:TRP:O	2.10	0.51
37:5F:96:ASP:O	37:5F:100:LYS:NZ	2.43	0.51
38:5G:166:SER:O	38:5G:256:MET:HA	2.09	0.51
44:RE:348:TYR:OH	44:RE:402:ASN:OD1	2.28	0.51
3:SA:546:U:O4	39:5H:558:ASN:ND2	2.43	0.51
4:SC:108:ASP:N	4:SC:108:ASP:OD1	2.42	0.51
6:SG:125:THR:HG21	6:SG:199:ILE:HG12	1.92	0.51
8:SI:81:LEU:HA	8:SI:84:LYS:HB3	1.91	0.51
12:SO:71:ILE:HA	12:SO:74:ILE:HG22	1.93	0.51
29:B2:24:VAL:HG22	29:B2:42:ILE:HG12	1.93	0.51
29:B2:606:ASP:N	29:B2:606:ASP:OD1	2.41	0.51
30:B3:109:ASP:N	30:B3:109:ASP:OD1	2.43	0.51
30:B3:476:ASP:OD1	30:B3:476:ASP:N	2.38	0.51
34:5C:284:ARG:HH22	34:5C:408:GLU:HG3	1.76	0.51
44:RE:442:PHE:O	44:RE:470:LYS:N	2.41	0.51
46:RJ:143:ASP:N	46:RJ:143:ASP:OD1	2.43	0.51
49:RP:212:VAL:HA	49:RP:215:VAL:HG12	1.92	0.51
3:SA:7:G:H5'	3:SA:8:U:H5'	1.92	0.51
3:SA:429:G:O2'	46:RJ:225:ARG:NH2	2.43	0.51
3:SA:628:G:N2	3:SA:971:A:H62	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SM:16:GLN:NE2	11:SM:61:THR:O	2.43	0.51
23:3F:331:LEU:HD23	23:3F:407:MET:HB2	1.91	0.51
28:B1:533:SER:HB2	28:B1:583:ILE:HD11	1.93	0.51
29:B2:576:VAL:HA	29:B2:592:SER:HA	1.92	0.51
31:B8:360:VAL:HG22	31:B8:375:VAL:HG12	1.92	0.51
32:BE:738:ASP:N	32:BE:738:ASP:OD1	2.40	0.51
39:5H:580:ARG:NH2	42:5K:49:SER:O	2.42	0.51
44:RE:193:ALA:O	44:RE:367:ARG:NH1	2.43	0.51
46:RJ:555:MET:O	47:RK:327:ARG:NH2	2.44	0.51
46:RJ:951:MET:SD	46:RJ:987:TYR:OH	2.57	0.51
46:RJ:956:MET:N	46:RJ:956:MET:SD	2.84	0.51
52:RZ:507:LEU:O	52:RZ:539:ARG:NH2	2.43	0.51
3:SA:322:G:N2	3:SA:325:G:O6	2.44	0.51
5:SF:19:LEU:HB2	5:SF:51:ARG:HH22	1.74	0.51
5:SF:100:ARG:NH1	5:SF:118:GLU:OE1	2.43	0.51
6:SG:148:ARG:NH1	6:SG:149:VAL:O	2.38	0.51
9:SJ:110:ARG:NH1	9:SJ:160:PHE:O	2.43	0.51
28:B1:391:THR:HG22	28:B1:407:LEU:HD12	1.93	0.51
32:BE:509:SER:OG	32:BE:510:LEU:N	2.43	0.51
42:5K:65:VAL:HG22	42:5K:96:PRO:HA	1.91	0.51
44:RE:720:SER:OG	44:RE:721:VAL:N	2.42	0.51
52:RZ:396:GLU:HB2	52:RZ:583:VAL:HG23	1.91	0.51
52:RZ:423:GLN:OE1	52:RZ:426:GLN:NE2	2.42	0.51
3:SA:973:A:H2'	3:SA:974:A:H8	1.76	0.51
3:SA:1792:G:OP2	51:RT:200:ARG:NH1	2.44	0.51
16:SY:48:HIS:HB3	16:SY:103:LEU:HD11	1.93	0.51
32:BE:484:ILE:HG23	32:BE:498:TYR:HB2	1.91	0.51
36:5E:312:GLU:O	36:5E:316:ASN:ND2	2.43	0.51
37:5F:57:LEU:HA	37:5F:60:LYS:HB2	1.92	0.51
44:RE:483:SER:OG	44:RE:581:ILE:O	2.25	0.51
44:RE:1094:LYS:NZ	53:X1:1305:UNK:O	2.42	0.51
45:RF:176:ASP:N	45:RF:176:ASP:OD1	2.39	0.51
52:RZ:775:TYR:HD1	52:RZ:820:HIS:HB2	1.75	0.51
3:SA:311:U:O4	3:SA:355:G:O6	2.27	0.51
9:SJ:67:TRP:HD1	9:SJ:69:SER:H	1.58	0.51
20:3C:256:ASN:O	20:3C:260:PHE:HB2	2.11	0.51
23:3F:426:SER:OG	23:3F:427:LEU:N	2.44	0.51
36:5E:381:LEU:O	36:5E:382:GLN:NE2	2.44	0.51
40:5I:392:ASN:HD21	50:RQ:876:GLN:HE21	1.58	0.51
49:RP:67:ALA:HA	49:RP:70:ILE:HG22	1.91	0.51
52:RZ:561:THR:OG1	52:RZ:563:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RZ:1107:THR:OG1	52:RZ:1109:ARG:NH2	2.44	0.51
3:SA:655:G:H1	3:SA:675:U:H3	1.57	0.51
5:SF:48:LEU:HD23	5:SF:52:LEU:HD21	1.93	0.51
16:SY:94:ASN:O	46:RJ:828:ARG:NH2	2.44	0.51
20:3C:296:GLU:O	20:3C:297:ARG:NH2	2.37	0.51
30:B3:296:ILE:HB	30:B3:301:GLN:HB2	1.93	0.51
33:B6:39:PHE:HE1	33:B6:55:LYS:HG3	1.75	0.51
38:5G:93:SER:OG	38:5G:94:ARG:N	2.43	0.51
44:RE:904:HIS:O	44:RE:907:GLN:NE2	2.44	0.51
47:RK:215:VAL:HG21	47:RK:273:GLU:HG2	1.93	0.51
3:SA:174:U:O4	3:SA:266:A:N7	2.44	0.51
4:SC:16:GLN:HG3	30:B3:339:ILE:HD11	1.92	0.51
10:SK:159:ALA:O	10:SK:162:SER:OG	2.29	0.51
30:B3:36:VAL:HG23	30:B3:37:LEU:HG	1.93	0.51
49:RP:1724:ASN:HA	49:RP:1729:ALA:HB3	1.91	0.51
1:3A:23:U:O2	1:3A:26:C:N4	2.43	0.51
23:3F:537:PHE:HB2	23:3F:568:ILE:HG22	1.92	0.51
28:B1:524:ARG:NH2	28:B1:529:GLU:OE2	2.44	0.51
28:B1:566:GLN:OE1	28:B1:624:ASN:ND2	2.42	0.51
32:BE:606:ASP:N	32:BE:606:ASP:OD1	2.38	0.51
34:5C:269:LYS:HB2	50:RQ:830:ILE:HG23	1.92	0.51
44:RE:495:THR:HA	44:RE:498:MET:HG2	1.91	0.51
45:RF:40:LYS:HB3	45:RF:54:PHE:HB2	1.92	0.51
52:RZ:468:ASP:N	52:RZ:468:ASP:OD1	2.44	0.51
52:RZ:1042:ARG:NH1	52:RZ:1068:LYS:O	2.43	0.51
11:SM:22:ASN:HB3	11:SM:25:VAL:HG22	1.92	0.51
21:3D:231:ASP:OD1	21:3D:231:ASP:N	2.41	0.51
25:A5:6:LEU:HD12	25:A5:27:GLN:HE22	1.75	0.51
28:B1:148:ASP:OD1	28:B1:148:ASP:N	2.44	0.51
29:B2:197:ILE:O	30:B3:671:ASN:ND2	2.39	0.51
30:B3:509:ALA:HA	30:B3:514:THR:O	2.11	0.51
32:BE:515:ARG:HE	32:BE:532:ASN:HD22	1.59	0.51
3:SA:329:G:H5"	9:SJ:98:LYS:HB3	1.93	0.50
3:SA:448:C:OP2	5:SF:49:ARG:NH2	2.42	0.50
17:SZ:34:ASN:N	17:SZ:34:ASN:OD1	2.44	0.50
23:3F:401:SER:HB3	23:3F:418:ASP:HB2	1.93	0.50
26:AE:374:ARG:NH1	26:AE:375:LEU:O	2.45	0.50
29:B2:97:GLY:HA3	29:B2:124:ILE:HD11	1.93	0.50
32:BE:215:ALA:HB3	32:BE:220:ILE:HG13	1.92	0.50
32:BE:517:MET:HG2	32:BE:529:TYR:HB2	1.93	0.50
43:RD:1472:PRO:O	43:RD:1478:TRP:NE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RD:1500:ARG:HH11	44:RE:1032:PRO:HG3	1.76	0.50
46:RJ:71:ILE:HD12	46:RJ:245:LEU:HD22	1.93	0.50
47:RK:18:ARG:NH2	47:RK:101:GLU:OE2	2.44	0.50
52:RZ:546:ASN:ND2	52:RZ:549:GLU:OE2	2.44	0.50
1:3A:319:G:OP1	20:3C:122:ARG:NH2	2.44	0.50
3:SA:528:U:O2'	46:RJ:184:ARG:NH2	2.44	0.50
4:SC:124:ASN:N	4:SC:124:ASN:OD1	2.44	0.50
23:3F:124:ASP:OD2	23:3F:128:GLN:NE2	2.45	0.50
23:3F:260:LEU:HD11	23:3F:286:LEU:HD11	1.93	0.50
23:3F:456:ASP:OD1	23:3F:456:ASP:N	2.36	0.50
25:A5:8:SER:OG	25:A5:293:ASN:ND2	2.41	0.50
29:B2:342:SER:OG	29:B2:343:TRP:N	2.42	0.50
29:B2:603:ASP:OD1	29:B2:603:ASP:N	2.43	0.50
32:BE:192:ASN:ND2	32:BE:195:THR:OG1	2.44	0.50
34:5C:271:LEU:HB3	50:RQ:828:ASN:HB3	1.92	0.50
38:5G:100:LEU:HD22	38:5G:144:GLU:HG2	1.92	0.50
44:RE:1057:PRO:HB2	44:RE:1059:PRO:HD2	1.91	0.50
49:RP:1783:LEU:HD23	49:RP:1787:ASN:HD22	1.76	0.50
3:SA:140:A:H1'	7:SH:179:VAL:HG11	1.92	0.50
8:SI:141:ARG:NH2	40:5I:220:ASP:OD2	2.44	0.50
21:3D:384:SER:OG	21:3D:388:ARG:NH1	2.44	0.50
23:3F:168:ASN:HA	23:3F:174:GLU:HA	1.94	0.50
23:3F:284:LEU:O	23:3F:548:ARG:NH2	2.44	0.50
24:3H:7:LYS:NZ	24:3H:62:GLU:OE2	2.45	0.50
29:B2:538:ARG:NH1	29:B2:539:VAL:O	2.44	0.50
31:B8:277:ILE:HA	31:B8:282:ASN:HB3	1.92	0.50
34:5C:451:SER:OG	34:5C:452:VAL:N	2.44	0.50
37:5F:32:VAL:HA	37:5F:35:THR:HG22	1.93	0.50
44:RE:528:ASP:OD1	44:RE:614:ARG:NH1	2.44	0.50
44:RE:1217:GLU:O	44:RE:1221:HIS:HB2	2.12	0.50
46:RJ:246:ALA:HB3	46:RJ:810:ILE:HB	1.93	0.50
3:SA:634:G:N2	3:SA:965:U:OP2	2.40	0.50
3:SA:866:G:H2'	3:SA:867:G:C8	2.46	0.50
3:SA:1533:C:O2'	3:SA:1534:G:O4'	2.28	0.50
5:SF:191:ARG:NH2	5:SF:244:ILE:O	2.44	0.50
11:SM:37:ASN:OD1	11:SM:37:ASN:N	2.43	0.50
26:AE:40:ALA:HA	26:AE:43:GLN:HG2	1.94	0.50
30:B3:217:ASP:OD1	30:B3:217:ASP:N	2.41	0.50
30:B3:455:LEU:HD11	30:B3:520:LEU:HD13	1.92	0.50
34:5C:296:ARG:NH1	34:5C:316:PRO:O	2.44	0.50
36:5E:475:SER:OG	36:5E:476:MET:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RD:1485:GLN:HG3	43:RD:1490:GLU:HB2	1.94	0.50
43:RD:1539:ARG:HA	43:RD:1542:GLN:HG2	1.93	0.50
46:RJ:293:VAL:HG23	46:RJ:1022:LEU:HD11	1.94	0.50
5:SF:68:ARG:HD3	5:SF:76:VAL:HG11	1.93	0.50
21:3D:250:ARG:O	21:3D:254:ASN:HB2	2.12	0.50
29:B2:760:ILE:HD11	29:B2:835:PHE:HB2	1.93	0.50
43:RD:1497:LEU:HD22	43:RD:1500:ARG:HH21	1.77	0.50
46:RJ:764:ILE:HD12	47:RK:310:ARG:HH12	1.76	0.50
3:SA:315:A:N6	3:SA:350:U:O4'	2.45	0.50
3:SA:655:G:N2	3:SA:675:U:O2	2.40	0.50
3:SA:699:U:N3	3:SA:813:U:OP2	2.37	0.50
3:SA:1068:C:H2'	3:SA:1069:A:H8	1.77	0.50
3:SA:1119:G:H5"	48:RN:783:HIS:HD2	1.76	0.50
16:SY:140:LYS:NZ	46:RJ:196:THR:O	2.45	0.50
29:B2:361:THR:OG1	29:B2:391:ARG:NE	2.44	0.50
32:BE:666:ARG:NH1	32:BE:706:ASP:OD2	2.44	0.50
37:5F:36:TYR:O	37:5F:110:ARG:NH1	2.32	0.50
43:RD:1549:ILE:HA	43:RD:1552:LYS:HG2	1.94	0.50
43:RD:1712:LYS:NZ	43:RD:1716:THR:OG1	2.42	0.50
46:RJ:289:HIS:HA	46:RJ:295:ASP:HA	1.93	0.50
47:RK:14:SER:OG	47:RK:37:ARG:NH2	2.45	0.50
3:SA:479:C:H4'	10:SK:120:LYS:HD3	1.93	0.50
3:SA:529:A:H5'	46:RJ:184:ARG:HH22	1.77	0.50
3:SA:913:G:OP2	30:B3:408:LYS:NZ	2.41	0.50
7:SH:162:VAL:HG23	7:SH:169:TYR:HB2	1.94	0.50
20:3B:248:ASP:OD2	20:3B:251:ARG:NH1	2.40	0.50
23:3F:454:GLU:HB2	23:3F:460:ARG:HG3	1.93	0.50
28:B1:760:ILE:HD11	28:B1:797:ILE:HD13	1.93	0.50
30:B3:133:ASN:ND2	52:RZ:1055:LYS:O	2.44	0.50
33:B6:166:ASN:ND2	50:RQ:327:PHE:O	2.42	0.50
34:5C:340:LEU:HD13	34:5C:369:MET:HG3	1.94	0.50
40:5I:94:TYR:OH	40:5I:134:ASN:ND2	2.44	0.50
44:RE:159:SER:OG	44:RE:160:VAL:N	2.44	0.50
44:RE:906:TYR:HB3	44:RE:942:PHE:HD2	1.77	0.50
3:SA:181:A:H3'	3:SA:182:A:C8	2.47	0.50
3:SA:432:G:OP1	46:RJ:231:LYS:NZ	2.44	0.50
3:SA:776:G:N2	3:SA:785:U:O2	2.45	0.50
17:SZ:78:SER:O	17:SZ:81:GLU:N	2.44	0.50
20:3B:236:MET:HG2	21:3D:133:LEU:HA	1.93	0.50
30:B3:27:GLU:OE1	30:B3:28:ASN:ND2	2.38	0.50
31:B8:278:ASP:N	31:B8:278:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B8:424:ILE:HG12	31:B8:434:GLU:HB3	1.93	0.50
33:B6:381:ILE:HD13	33:B6:384:LEU:HD13	1.93	0.50
44:RE:781:ASP:OD1	44:RE:781:ASP:N	2.45	0.50
44:RE:869:ASN:ND2	45:RF:103:LEU:O	2.44	0.50
5:SF:50:ASN:OD1	5:SF:50:ASN:N	2.44	0.50
28:B1:120:GLN:HB3	28:B1:122:TRP:HE1	1.76	0.50
29:B2:201:ILE:HG13	30:B3:663:VAL:HG11	1.94	0.50
34:5C:412:ASP:OD2	40:5I:26:ARG:NH2	2.45	0.50
40:5I:56:LYS:HB2	40:5I:382:ARG:HH22	1.77	0.50
44:RE:536:TYR:OH	44:RE:552:ARG:NE	2.43	0.50
47:RK:113:LYS:HD2	47:RK:171:ASP:HA	1.94	0.50
49:RP:1928:ASP:OD1	49:RP:1928:ASP:N	2.43	0.50
8:SI:177:THR:HG23	8:SI:179:LYS:H	1.76	0.49
12:SO:69:ASN:N	12:SO:69:ASN:OD1	2.45	0.49
14:SR:16:ALA:HB2	14:SR:72:GLY:HA3	1.94	0.49
20:3B:231:ARG:NE	21:3D:10:GLU:OE2	2.35	0.49
20:3B:277:ASP:OD2	20:3B:288:ARG:NH2	2.44	0.49
30:B3:561:SER:O	30:B3:566:SER:N	2.45	0.49
33:B6:2:SER:OG	33:B6:3:LYS:N	2.45	0.49
37:5F:145:ASP:N	37:5F:145:ASP:OD1	2.42	0.49
40:5I:175:THR:H	49:RP:1862:LEU:HD22	1.77	0.49
43:RD:1505:ILE:HG21	43:RD:1513:LYS:HD3	1.93	0.49
49:RP:1809:GLU:OE1	49:RP:1891:HIS:NE2	2.45	0.49
52:RZ:750:PRO:HD3	52:RZ:756:LEU:HD12	1.94	0.49
25:A5:299:ASP:O	25:A5:318:GLN:NE2	2.45	0.49
30:B3:626:MET:HB2	30:B3:632:ILE:HG22	1.94	0.49
32:BE:96:ASN:ND2	32:BE:111:GLU:OE1	2.45	0.49
32:BE:484:ILE:HD12	32:BE:508:ILE:HD12	1.93	0.49
40:5I:273:GLU:HA	50:RQ:302:VAL:HG21	1.93	0.49
49:RP:1957:GLN:HE22	49:RP:1999:ALA:H	1.60	0.49
52:RZ:534:ARG:HH12	52:RZ:861:ASN:HB3	1.77	0.49
3:SA:29:U:H2'	3:SA:30:G:C8	2.47	0.49
4:SC:199:ASN:HA	4:SC:202:LYS:HE3	1.94	0.49
28:B1:53:GLU:OE2	28:B1:619:ARG:N	2.39	0.49
29:B2:181:SER:OG	29:B2:183:ASP:O	2.29	0.49
29:B2:405:LEU:HD11	29:B2:419:ILE:HG23	1.94	0.49
30:B3:192:ALA:HB3	30:B3:216:ARG:HG3	1.94	0.49
31:B8:156:ASN:HB3	31:B8:159:HIS:HD2	1.77	0.49
36:5E:296:ASN:OD1	46:RJ:264:GLN:NE2	2.45	0.49
44:RE:841:ASN:HA	44:RE:850:PHE:O	2.12	0.49
44:RE:1207:VAL:HG23	45:RF:3:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RT:196:ASP:N	51:RT:196:ASP:OD1	2.42	0.49
3:SA:283:U:H5"	7:SH:188:ARG:HD3	1.94	0.49
3:SA:959:U:H5"	12:SO:14:SER:HB2	1.94	0.49
8:SI:93:LEU:HD23	8:SI:125:ILE:HB	1.94	0.49
30:B3:650:GLN:NE2	30:B3:651:GLU:OE2	2.45	0.49
31:B8:165:ARG:HH22	32:BE:236:ARG:HH22	1.59	0.49
32:BE:24:PHE:HB3	32:BE:654:TRP:HB3	1.95	0.49
32:BE:442:THR:OG1	32:BE:443:TRP:N	2.45	0.49
34:5C:46:LEU:HD13	34:5C:49:ILE:HD11	1.95	0.49
45:RF:107:LEU:HD12	45:RF:108:MET:HG2	1.94	0.49
52:RZ:522:ASN:HB2	52:RZ:525:THR:HG23	1.93	0.49
3:SA:10:G:H2'	3:SA:11:A:H8	1.77	0.49
25:A5:116:GLN:OE1	25:A5:128:GLN:NE2	2.45	0.49
28:B1:155:SER:OG	28:B1:157:ASP:OD1	2.30	0.49
29:B2:655:ALA:HB3	29:B2:684:TRP:HH2	1.78	0.49
30:B3:220:ILE:HD11	30:B3:236:THR:HG23	1.93	0.49
32:BE:246:ILE:O	32:BE:249:SER:OG	2.29	0.49
40:5I:230:ASN:OD1	40:5I:230:ASN:N	2.45	0.49
46:RJ:818:THR:HG21	47:RK:362:THR:HG21	1.95	0.49
49:RP:1996:GLN:HB3	49:RP:2035:ILE:HD12	1.95	0.49
52:RZ:1086:ALA:HB2	52:RZ:1181:ILE:HD12	1.94	0.49
3:SA:18:C:N4	42:5K:158:ALA:O	2.45	0.49
3:SA:54:C:O3'	17:SZ:109:LYS:NZ	2.44	0.49
13:SP:12:GLN:OE1	13:SP:111:ARG:NH1	2.46	0.49
17:SZ:104:SER:OG	17:SZ:107:GLN:NE2	2.45	0.49
21:3D:302:ASN:ND2	21:3D:397:SER:O	2.46	0.49
23:3F:546:GLU:OE2	23:3F:551:ARG:NE	2.46	0.49
24:3G:90:ALA:HB2	31:B8:453:VAL:HG21	1.94	0.49
25:A5:162:GLN:HG2	25:A5:172:LEU:HD11	1.95	0.49
26:AE:255:ILE:HD11	27:AG:884:MET:HB3	1.95	0.49
29:B2:364:TYR:HB3	29:B2:383:HIS:HB2	1.95	0.49
29:B2:400:SER:OG	29:B2:401:ASP:N	2.45	0.49
38:5G:88:ILE:HG21	38:5G:111:PHE:HE1	1.77	0.49
42:5K:56:ASN:ND2	42:5K:169:GLY:O	2.33	0.49
43:RD:1620:VAL:HG23	43:RD:1623:LYS:HZ3	1.78	0.49
47:RK:307:ASP:O	47:RK:355:LYS:HA	2.12	0.49
51:RT:93:LYS:HB3	51:RT:95:GLU:HG3	1.94	0.49
3:SA:560:U:OP2	38:5G:282:ARG:NH2	2.44	0.49
13:SP:19:ILE:HD11	13:SP:105:LEU:HD21	1.94	0.49
17:SZ:45:ALA:HB2	17:SZ:55:VAL:HG11	1.94	0.49
21:3D:175:ILE:HD11	21:3D:316:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A5:203:ILE:HD11	25:A5:212:LEU:HD13	1.93	0.49
26:AE:193:THR:HG22	26:AE:241:ILE:HD13	1.94	0.49
28:B1:125:PRO:HB3	28:B1:135:PRO:HB2	1.95	0.49
29:B2:643:ASP:OD2	29:B2:646:LYS:NZ	2.43	0.49
30:B3:232:LYS:NZ	30:B3:233:LEU:O	2.43	0.49
40:5I:290:ASP:HB2	40:5I:298:LEU:HD22	1.94	0.49
44:RE:933:LEU:HD11	44:RE:1053:SER:HA	1.93	0.49
44:RE:1108:LEU:O	44:RE:1112:CYS:CB	2.61	0.49
52:RZ:1039:VAL:HG12	52:RZ:1042:ARG:HH21	1.77	0.49
3:SA:1771:U:O4	3:SA:1791:A:N6	2.45	0.49
5:SF:126:VAL:HA	5:SF:141:THR:HA	1.94	0.49
9:SJ:44:HIS:HD2	9:SJ:58:LEU:HD12	1.77	0.49
13:SP:103:ARG:NH1	51:RT:178:ASP:O	2.42	0.49
17:SZ:60:PHE:HD1	17:SZ:71:GLY:HA3	1.77	0.49
20:3C:124:SER:HA	20:3C:140:GLU:HA	1.95	0.49
24:3H:54:MET:HB3	24:3H:64:LEU:HD13	1.94	0.49
28:B1:382:THR:HG21	36:5E:479:ALA:HB1	1.94	0.49
30:B3:6:SER:HA	30:B3:611:LYS:HE2	1.95	0.49
31:B8:304:LEU:HD23	31:B8:371:VAL:HG11	1.93	0.49
36:5E:343:GLU:HG2	36:5E:345:LEU:HD23	1.95	0.49
44:RE:1038:GLN:NE2	44:RE:1056:ILE:O	2.39	0.49
46:RJ:355:TYR:HH	46:RJ:788:TYR:HH	1.61	0.49
49:RP:1664:ILE:O	49:RP:1668:GLU:CB	2.61	0.49
1:3A:85:G:OP2	22:3E:358:LYS:NZ	2.37	0.49
1:3A:205:G:N3	1:3A:244:U:N3	2.48	0.49
15:SX:44:HIS:NE2	15:SX:112:ASP:OD2	2.33	0.49
20:3C:171:LEU:HB3	20:3C:240:VAL:HG12	1.93	0.49
21:3D:93:LYS:HE3	50:RQ:320:GLU:H	1.78	0.49
23:3F:185:LEU:HD12	23:3F:202:THR:HA	1.95	0.49
26:AE:197:ASP:HA	26:AE:200:ILE:HD12	1.94	0.49
28:B1:566:GLN:O	37:5F:144:ASN:ND2	2.46	0.49
29:B2:18:ALA:HB3	29:B2:360:ASN:HA	1.94	0.49
29:B2:413:SER:HB2	29:B2:415:LYS:HD3	1.95	0.49
30:B3:309:GLN:HB3	30:B3:336:ASN:HB3	1.94	0.49
30:B3:574:HIS:HE1	30:B3:594:GLY:HA3	1.78	0.49
31:B8:208:LEU:HA	31:B8:211:ILE:HG12	1.94	0.49
31:B8:281:THR:OG1	31:B8:282:ASN:N	2.45	0.49
31:B8:571:SER:HB3	31:B8:576:LEU:HB2	1.94	0.49
32:BE:290:ILE:HG23	32:BE:320:LYS:HD2	1.94	0.49
32:BE:907:SER:O	32:BE:911:ASN:ND2	2.46	0.49
34:5C:144:LEU:HD21	34:5C:147:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:5I:85:THR:HG21	40:5I:372:VAL:HG21	1.94	0.49
44:RE:282:ASP:N	44:RE:282:ASP:OD1	2.45	0.49
46:RJ:921:GLU:OE2	47:RK:111:LYS:NZ	2.43	0.49
49:RP:1862:LEU:HD11	49:RP:1865:ASN:HD22	1.77	0.49
52:RZ:414:GLY:HA3	52:RZ:420:LYS:HD3	1.95	0.49
52:RZ:1239:LYS:HB2	52:RZ:1248:ILE:HD11	1.95	0.49
3:SA:1482:C:O2'	14:SR:77:GLN:NE2	2.46	0.49
3:SA:1588:G:H1	3:SA:1608:U:H3	1.61	0.49
3:SA:1679:G:O2'	3:SA:1722:A:N7	2.41	0.49
8:SI:70:PHE:O	8:SI:74:GLN:NE2	2.42	0.49
26:AE:105:ALA:O	26:AE:109:TRP:NE1	2.46	0.49
41:5J:67:THR:OG1	41:5J:68:GLY:N	2.46	0.49
42:5K:187:ASP:N	42:5K:187:ASP:OD1	2.46	0.49
49:RP:1862:LEU:O	49:RP:1865:ASN:N	2.36	0.49
3:SA:261:U:H1'	3:SA:262:U:H5'	1.94	0.48
3:SA:954:G:H2'	3:SA:955:A:C8	2.48	0.48
4:SC:64:ARG:NH2	13:SP:37:GLU:OE1	2.46	0.48
4:SC:174:LYS:NZ	4:SC:175:GLU:OE2	2.46	0.48
8:SI:28:GLU:OE1	8:SI:39:ARG:NH2	2.46	0.48
16:SY:84:THR:HG21	48:RN:788:ILE:HD12	1.95	0.48
23:3F:175:SER:OG	23:3F:176:SER:N	2.43	0.48
44:RE:443:HIS:HD2	44:RE:470:LYS:HE3	1.78	0.48
46:RJ:553:ILE:HG12	47:RK:323:ILE:HD12	1.95	0.48
47:RK:301:MET:HE3	47:RK:354:ILE:HD12	1.95	0.48
3:SA:442:C:O2'	3:SA:525:A:N1	2.39	0.48
3:SA:1137:A:C6	29:B2:573:LYS:HD3	2.48	0.48
5:SF:48:LEU:HD13	5:SF:64:ILE:HD11	1.94	0.48
14:SR:59:LYS:HD2	14:SR:105:LEU:HD21	1.95	0.48
20:3B:291:GLN:NE2	42:5K:129:SER:OG	2.46	0.48
21:3D:221:LEU:HD13	21:3D:276:GLN:HB3	1.96	0.48
30:B3:434:SER:O	30:B3:434:SER:OG	2.30	0.48
33:B6:273:ILE:HG22	50:RQ:338:LEU:HD11	1.94	0.48
1:3A:50:U:O2'	2:5A:467:A:N1	2.41	0.48
3:SA:1041:G:H2'	3:SA:1042:G:C8	2.49	0.48
5:SF:206:ASP:OD1	5:SF:206:ASP:N	2.46	0.48
22:3E:167:ILE:HG21	22:3E:297:ALA:HB1	1.94	0.48
24:3H:65:LEU:HD12	24:3H:68:PRO:HG2	1.95	0.48
32:BE:592:ASP:OD2	32:BE:634:PHE:N	2.47	0.48
38:5G:144:GLU:HA	38:5G:149:PRO:HA	1.95	0.48
42:5K:139:ASP:HA	42:5K:142:VAL:HG12	1.94	0.48
46:RJ:72:VAL:HG12	46:RJ:137:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RJ:755:LYS:HD2	46:RJ:758:ILE:HD11	1.95	0.48
47:RK:191:ILE:HG23	47:RK:223:VAL:HA	1.95	0.48
49:RP:2006:LEU:HD12	49:RP:2011:ILE:HD11	1.95	0.48
51:RT:129:ARG:NE	51:RT:131:ASN:OD1	2.44	0.48
52:RZ:783:LYS:HB2	52:RZ:798:VAL:HG22	1.95	0.48
3:SA:1688:U:O4	3:SA:1713:G:O6	2.31	0.48
4:SC:36:SER:OG	4:SC:41:ARG:NH1	2.40	0.48
11:SM:92:HIS:ND1	11:SM:101:GLU:OE2	2.40	0.48
20:3C:253:ILE:HD13	20:3C:269:ILE:HG21	1.95	0.48
28:B1:539:ILE:HD11	28:B1:580:PHE:HD2	1.78	0.48
30:B3:581:CYS:HB3	30:B3:591:ILE:HG22	1.95	0.48
30:B3:765:MET:HG3	30:B3:766:HIS:HD2	1.78	0.48
34:5C:545:VAL:HG13	45:RF:185:HIS:HB2	1.96	0.48
38:5G:171:VAL:HB	38:5G:253:ARG:HG2	1.94	0.48
44:RE:305:PRO:HB3	44:RE:473:LYS:HG2	1.95	0.48
7:SH:39:GLU:HB2	7:SH:47:GLY:H	1.78	0.48
20:3B:99:ALA:HB3	20:3B:105:LEU:HB2	1.94	0.48
21:3D:333:VAL:HG21	21:3D:384:SER:HB2	1.95	0.48
25:A5:130:ASP:OD1	25:A5:130:ASP:N	2.46	0.48
29:B2:866:LYS:NZ	32:BE:939:ALA:O	2.47	0.48
29:B2:902:VAL:HG21	30:B3:790:GLN:HG3	1.95	0.48
30:B3:377:LEU:HG	30:B3:379:LEU:HD23	1.96	0.48
32:BE:217:VAL:HB	32:BE:220:ILE:HD11	1.95	0.48
32:BE:285:HIS:ND1	32:BE:286:VAL:O	2.42	0.48
37:5F:123:THR:OG1	37:5F:124:ILE:N	2.46	0.48
40:5I:40:GLU:OE2	40:5I:403:ARG:NH1	2.46	0.48
43:RD:1202:ALA:N	43:RD:1218:LYS:O	2.46	0.48
46:RJ:1049:ASN:HB3	46:RJ:1052:SER:HB3	1.93	0.48
1:3A:325:C:N4	22:3E:318:GLN:OE1	2.43	0.48
3:SA:71:A:H2'	3:SA:72:A:C8	2.49	0.48
3:SA:758:U:H3	3:SA:792:U:H3	1.62	0.48
9:SJ:168:CYS:O	9:SJ:181:GLY:HA2	2.12	0.48
20:3C:220:ILE:HD11	20:3C:234:ILE:HD11	1.96	0.48
25:A5:25:ASP:HB2	25:A5:56:SER:HB2	1.94	0.48
28:B1:54:HIS:NE2	28:B1:72:SER:OG	2.43	0.48
28:B1:397:LYS:O	28:B1:398:ARG:NH2	2.36	0.48
29:B2:7:ARG:HH21	29:B2:71:ALA:HB1	1.78	0.48
29:B2:651:GLN:NE2	29:B2:652:LYS:O	2.35	0.48
36:5E:483:TYR:O	36:5E:486:ASN:ND2	2.39	0.48
44:RE:164:ASP:OD1	44:RE:598:LYS:NZ	2.37	0.48
46:RJ:609:GLU:OE2	47:RK:17:PHE:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SC:115:ARG:HH21	51:RT:103:PRO:HG3	1.79	0.48
20:3B:228:GLN:O	20:3B:231:ARG:NH2	2.47	0.48
23:3F:401:SER:O	23:3F:418:ASP:N	2.44	0.48
23:3F:471:GLN:HG3	24:3H:83:SER:HB2	1.94	0.48
24:3G:21:LEU:HA	24:3G:24:VAL:HG12	1.95	0.48
29:B2:270:SER:O	29:B2:285:ARG:HA	2.14	0.48
30:B3:510:SER:O	30:B3:514:THR:OG1	2.26	0.48
43:RD:1512:GLU:HA	43:RD:1515:ASN:HD22	1.78	0.48
47:RK:286:SER:OG	47:RK:289:VAL:O	2.27	0.48
2:5A:475:G:H2'	2:5A:476:A:C8	2.48	0.48
3:SA:306:U:H2'	3:SA:307:G:C8	2.49	0.48
26:AE:158:PRO:HB3	32:BE:330:GLN:HE22	1.79	0.48
30:B3:114:SER:OG	30:B3:115:THR:N	2.47	0.48
32:BE:135:ASN:HB3	32:BE:159:VAL:HG13	1.94	0.48
37:5F:153:ASN:OD1	37:5F:153:ASN:N	2.45	0.48
40:5I:172:LEU:HD23	49:RP:1861:SER:HB3	1.94	0.48
52:RZ:583:VAL:HG13	52:RZ:583:VAL:O	2.12	0.48
1:3A:110:A:N6	39:5H:587:GLN:O	2.47	0.48
3:SA:332:U:O2'	3:SA:334:G:OP2	2.32	0.48
3:SA:1538:U:H2'	3:SA:1540:G:H8	1.79	0.48
5:SF:180:LEU:N	5:SF:229:GLY:O	2.46	0.48
26:AE:274:ILE:HA	31:B8:211:ILE:HD11	1.95	0.48
32:BE:725:ILE:HD12	32:BE:877:ASN:HD21	1.79	0.48
33:B6:35:LYS:HE3	33:B6:39:PHE:HE2	1.79	0.48
33:B6:64:ASN:HB2	33:B6:88:ILE:HG21	1.95	0.48
3:SA:668:C:H2'	3:SA:669:G:C8	2.49	0.48
3:SA:1617:U:OP2	28:B1:505:ARG:NH1	2.47	0.48
6:SG:140:THR:HG23	6:SG:210:ALA:HB1	1.96	0.48
20:3C:91:HIS:HB3	20:3C:96:VAL:HG13	1.96	0.48
21:3D:379:LEU:HD13	21:3D:408:VAL:HG21	1.96	0.48
29:B2:566:TYR:O	47:RK:207:ARG:NH2	2.41	0.48
31:B8:445:ARG:NH2	31:B8:499:ALA:O	2.41	0.48
33:B6:8:LEU:HB3	34:5C:66:LEU:HD11	1.96	0.48
35:5D:58:ARG:HH22	35:5D:62:GLU:HG2	1.78	0.48
43:RD:1509:GLU:OE2	44:RE:1199:ASN:ND2	2.47	0.48
44:RE:761:ARG:NH1	44:RE:931:ASP:OD2	2.47	0.48
44:RE:925:LEU:HD21	44:RE:1064:LEU:HB2	1.96	0.48
49:RP:1795:ARG:HD2	49:RP:1798:LEU:HD21	1.95	0.48
1:3A:77:U:H2'	1:3A:78:G:H8	1.79	0.47
3:SA:1634:C:OP1	28:B1:418:ARG:NH2	2.47	0.47
8:SI:125:ILE:O	8:SI:129:LEU:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SX:6:VAL:HG23	15:SX:29:PRO:HB2	1.96	0.47
16:SY:89:ASN:ND2	35:5D:4:LEU:O	2.47	0.47
20:3C:241:PHE:HA	20:3C:268:VAL:O	2.14	0.47
23:3F:162:CYS:HA	23:3F:187:ALA:HA	1.95	0.47
23:3F:488:ILE:HG22	23:3F:524:ILE:HD13	1.95	0.47
24:3H:44:LEU:HD11	24:3H:76:VAL:HG11	1.94	0.47
27:AG:861:GLU:HG3	31:B8:227:LEU:HD21	1.96	0.47
28:B1:351:LEU:HD23	28:B1:696:ALA:HB2	1.95	0.47
29:B2:228:ILE:HD11	29:B2:248:PHE:HE1	1.79	0.47
29:B2:425:ILE:HG22	29:B2:426:ARG:HG2	1.96	0.47
29:B2:437:LYS:HD3	29:B2:481:LEU:H	1.79	0.47
29:B2:645:GLU:HG2	29:B2:646:LYS:HG3	1.95	0.47
30:B3:269:LEU:HB2	30:B3:279:LYS:HB2	1.96	0.47
32:BE:357:ALA:HB1	32:BE:419:ILE:HG21	1.95	0.47
44:RE:456:LYS:NZ	44:RE:457:TYR:O	2.41	0.47
44:RE:911:PRO:HB2	44:RE:954:LEU:HD13	1.96	0.47
49:RP:918:GLU:O	49:RP:922:MET:CB	2.62	0.47
52:RZ:815:ARG:O	52:RZ:815:ARG:NH1	2.41	0.47
23:3F:184:ARG:NH1	23:3F:200:ASP:OD2	2.47	0.47
26:AE:185:ASP:OD1	26:AE:185:ASP:N	2.42	0.47
28:B1:58:ILE:HD11	28:B1:72:SER:HB2	1.95	0.47
28:B1:452:ASN:HD21	28:B1:456:HIS:CE1	2.33	0.47
31:B8:306:ASN:ND2	31:B8:309:GLN:OE1	2.45	0.47
40:5I:116:LEU:HA	40:5I:185:ILE:HD11	1.96	0.47
42:5K:68:ASP:HA	42:5K:102:VAL:HG11	1.96	0.47
44:RE:578:ILE:HA	44:RE:619:VAL:HA	1.96	0.47
45:RF:81:VAL:HG13	45:RF:133:SER:HA	1.96	0.47
46:RJ:313:TYR:HD1	46:RJ:314:GLN:HE21	1.61	0.47
46:RJ:932:LEU:O	46:RJ:1005:SER:OG	2.30	0.47
52:RZ:477:ILE:HG13	52:RZ:478:ARG:HG3	1.96	0.47
52:RZ:761:THR:HG22	52:RZ:762:ASN:H	1.78	0.47
3:SA:-5:G:OP1	50:RQ:306:ARG:NH2	2.46	0.47
3:SA:1688:U:O2	3:SA:1713:G:N2	2.47	0.47
3:SA:1699:G:N2	3:SA:1702:A:OP2	2.44	0.47
13:SP:53:ASP:OD1	13:SP:53:ASP:N	2.46	0.47
28:B1:843:LYS:HG2	28:B1:847:ARG:HH12	1.79	0.47
30:B3:665:GLN:HB2	30:B3:684:LEU:HD22	1.96	0.47
33:B6:336:ASN:HD21	33:B6:369:LEU:HD22	1.79	0.47
40:5I:67:ARG:NH1	42:5K:121:ARG:O	2.46	0.47
40:5I:301:PHE:HD1	40:5I:337:GLY:HA2	1.80	0.47
44:RE:930:THR:OG1	44:RE:931:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RT:158:PHE:O	51:RT:171:SER:OG	2.32	0.47
52:RZ:417:GLY:O	52:RZ:815:ARG:NH2	2.44	0.47
52:RZ:1102:ASP:N	52:RZ:1102:ASP:OD1	2.47	0.47
52:RZ:1112:ILE:HG13	52:RZ:1145:GLY:HA3	1.96	0.47
2:5A:495:G:H2'	2:5A:496:G:H8	1.79	0.47
3:SA:524:U:N3	3:SA:527:A:OP2	2.42	0.47
3:SA:1163:A:N3	3:SA:1613:U:O2'	2.45	0.47
13:SP:47:LYS:NZ	13:SP:66:ASP:OD2	2.43	0.47
20:3B:268:VAL:HG22	20:3B:317:VAL:HG13	1.96	0.47
22:3E:259:ALA:HA	22:3E:262:ILE:HG22	1.97	0.47
25:A5:230:SER:HB3	25:A5:248:THR:HB	1.96	0.47
27:AG:859:ASN:O	31:B8:480:ARG:NH2	2.48	0.47
28:B1:19:ASN:OD1	28:B1:19:ASN:N	2.48	0.47
28:B1:291:ASP:OD1	28:B1:291:ASP:N	2.40	0.47
29:B2:439:LEU:HB2	29:B2:444:LEU:HB3	1.96	0.47
37:5F:55:ARG:O	37:5F:59:ASN:ND2	2.46	0.47
46:RJ:98:LEU:HD13	46:RJ:101:ILE:HD13	1.96	0.47
52:RZ:600:PHE:HE1	52:RZ:684:ASP:O	1.92	0.47
52:RZ:1135:ILE:HG23	52:RZ:1169:THR:HG21	1.95	0.47
3:SA:1656:U:OP2	29:B2:395:ARG:NH1	2.46	0.47
7:SH:148:SER:O	7:SH:148:SER:OG	2.30	0.47
9:SJ:197:THR:HG22	9:SJ:200:LYS:HE3	1.94	0.47
11:SM:36:LYS:N	11:SM:60:PHE:O	2.46	0.47
20:3B:103:GLU:HB2	39:5H:595:LYS:HA	1.95	0.47
20:3B:164:ILE:HG23	20:3B:170:VAL:HG21	1.96	0.47
25:A5:66:VAL:HG21	25:A5:131:LEU:HD11	1.96	0.47
25:A5:85:ILE:HB	25:A5:99:PHE:HB2	1.97	0.47
28:B1:389:SER:HB3	28:B1:407:LEU:HD13	1.97	0.47
29:B2:411:ASN:HD21	29:B2:413:SER:HB3	1.79	0.47
29:B2:473:ASP:OD1	29:B2:473:ASP:N	2.42	0.47
30:B3:501:PRO:HB3	30:B3:543:GLN:HG3	1.96	0.47
32:BE:383:ASP:OD1	32:BE:386:SER:OG	2.32	0.47
39:5H:572:ALA:HA	39:5H:575:LYS:HB2	1.95	0.47
39:5H:599:LYS:HE2	41:5J:139:GLN:HB3	1.96	0.47
44:RE:469:ASP:HB2	44:RE:473:LYS:H	1.79	0.47
46:RJ:128:MET:HG2	46:RJ:155:PHE:HD1	1.80	0.47
50:RQ:852:GLU:OE2	50:RQ:856:GLN:NE2	2.47	0.47
52:RZ:373:ALA:N	52:RZ:437:ASP:OD1	2.46	0.47
52:RZ:381:SER:H	52:RZ:384:ILE:HD11	1.78	0.47
3:SA:641:G:O6	3:SA:693:U:O2	2.32	0.47
5:SF:104:ASP:OD1	5:SF:108:ARG:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SM:88:ARG:HH11	11:SM:105:LYS:HD2	1.80	0.47
20:3B:198:GLU:OE2	20:3B:200:SER:N	2.39	0.47
26:AE:283:LEU:HD11	26:AE:323:PHE:HD1	1.79	0.47
28:B1:710:ILE:O	32:BE:598:ARG:NH2	2.46	0.47
29:B2:530:LEU:HD13	29:B2:550:LEU:HD11	1.95	0.47
29:B2:872:LYS:HE2	30:B3:817:PHE:HB3	1.96	0.47
32:BE:641:LEU:HB2	32:BE:654:TRP:HB2	1.96	0.47
32:BE:909:LEU:HA	32:BE:912:TRP:HB3	1.96	0.47
40:5I:258:ILE:HD13	40:5I:294:LEU:HD22	1.95	0.47
44:RE:842:ILE:O	44:RE:849:GLY:HA2	2.13	0.47
46:RJ:282:SER:HA	46:RJ:301:ILE:HD11	1.96	0.47
49:RP:1773:VAL:O	49:RP:1777:LEU:HB2	2.15	0.47
49:RP:1979:LEU:HA	49:RP:1982:VAL:HG12	1.96	0.47
3:SA:295:A:H1'	5:SF:146:THR:HG21	1.96	0.47
3:SA:312:A:N6	3:SA:352:A:O2'	2.46	0.47
3:SA:329:G:H2'	3:SA:330:G:H8	1.79	0.47
3:SA:654:C:H2'	3:SA:655:G:H8	1.79	0.47
3:SA:1671:A:N6	3:SA:1730:A:O2'	2.47	0.47
4:SC:144:ARG:HB3	4:SC:206:PRO:HB2	1.97	0.47
8:SI:28:GLU:HA	8:SI:34:LEU:HD11	1.97	0.47
8:SI:140:VAL:HG13	15:SX:52:TYR:HB3	1.97	0.47
16:SY:135:LEU:HD11	16:SY:142:LYS:HB2	1.96	0.47
21:3D:109:ILE:HD11	21:3D:118:CYS:HB3	1.97	0.47
23:3F:164:GLN:HB3	23:3F:527:VAL:HG23	1.97	0.47
26:AE:340:ASP:OD1	26:AE:340:ASP:N	2.47	0.47
28:B1:117:ARG:HH21	28:B1:146:PHE:HA	1.80	0.47
30:B3:130:ASP:OD1	30:B3:130:ASP:N	2.48	0.47
31:B8:511:LEU:HD13	31:B8:544:VAL:HG11	1.97	0.47
37:5F:156:ASP:N	37:5F:156:ASP:OD1	2.47	0.47
40:5I:26:ARG:NH1	50:RQ:867:GLN:O	2.48	0.47
44:RE:209:MET:SD	44:RE:227:LYS:NZ	2.71	0.47
44:RE:800:GLU:OE1	44:RE:834:ASN:ND2	2.48	0.47
44:RE:949:PHE:O	44:RE:960:LYS:NZ	2.41	0.47
44:RE:1022:MET:O	44:RE:1026:ASN:ND2	2.48	0.47
44:RE:1028:ARG:NH2	44:RE:1037:LEU:O	2.47	0.47
46:RJ:270:ALA:HA	46:RJ:791:ILE:O	2.13	0.47
47:RK:103:MET:O	47:RK:107:ALA:HB2	2.14	0.47
50:RQ:821:ARG:NH2	50:RQ:831:ILE:O	2.47	0.47
51:RT:127:GLN:NE2	51:RT:142:ASN:OD1	2.48	0.47
52:RZ:852:LEU:HG	52:RZ:903:SER:HB2	1.97	0.47
8:SI:153:LEU:HA	8:SI:184:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AE:364:ASN:OD1	26:AE:364:ASN:N	2.47	0.47
29:B2:897:ASP:OD1	30:B3:761:ARG:NH2	2.48	0.47
32:BE:28:ARG:NH2	32:BE:380:LEU:O	2.48	0.47
33:B6:67:ARG:NE	33:B6:84:SER:O	2.48	0.47
40:5I:108:ALA:O	40:5I:146:LYS:NZ	2.38	0.47
40:5I:122:ARG:HH12	40:5I:191:ASN:HA	1.79	0.47
1:3A:330:A:H2'	1:3A:331:A:H8	1.80	0.47
3:SA:22:A:H4'	10:SK:17:ARG:HB3	1.96	0.47
3:SA:871:G:H2'	3:SA:872:G:C8	2.50	0.47
3:SA:1614:A:OP2	6:SG:84:LYS:NZ	2.43	0.47
9:SJ:83:TYR:HB3	9:SJ:101:ILE:HB	1.97	0.47
10:SK:58:ASP:HA	10:SK:61:THR:HG22	1.97	0.47
11:SM:66:ILE:HD12	11:SM:128:CYS:HB2	1.96	0.47
13:SP:34:SER:OG	13:SP:35:GLY:N	2.48	0.47
20:3C:268:VAL:HG12	20:3C:317:VAL:HG12	1.96	0.47
21:3D:117:ASP:OD1	40:5I:157:ASN:ND2	2.47	0.47
25:A5:121:ASP:OD2	25:A5:127:TYR:OH	2.30	0.47
28:B1:113:LEU:HB3	28:B1:120:GLN:HB2	1.96	0.47
29:B2:137:ILE:HG22	29:B2:147:VAL:HG13	1.97	0.47
29:B2:390:GLN:NE2	29:B2:413:SER:OG	2.47	0.47
31:B8:445:ARG:HH11	31:B8:503:SER:H	1.61	0.47
32:BE:605:LEU:HD23	32:BE:628:VAL:HG11	1.97	0.47
34:5C:312:VAL:HG21	34:5C:353:PRO:HG2	1.97	0.47
36:5E:341:LEU:O	46:RJ:960:ARG:NH2	2.48	0.47
40:5I:15:PRO:HB3	40:5I:20:GLN:HE21	1.78	0.47
45:RF:123:THR:OG1	45:RF:124:ALA:N	2.48	0.47
4:SC:64:ARG:HG2	13:SP:36:LYS:HE2	1.97	0.47
14:SR:113:ASP:N	14:SR:113:ASP:OD1	2.45	0.47
24:3H:5:ASN:OD1	24:3H:5:ASN:N	2.48	0.47
34:5C:461:LEU:HD11	34:5C:466:LEU:HA	1.97	0.47
38:5G:235:GLN:HE21	38:5G:251:GLY:HA3	1.80	0.47
44:RE:206:LEU:HD23	44:RE:208:THR:HG22	1.97	0.47
46:RJ:69:PRO:HD2	46:RJ:274:TYR:CE1	2.50	0.47
52:RZ:610:THR:HA	52:RZ:613:ILE:HD12	1.96	0.47
7:SH:148:SER:O	7:SH:150:GLU:N	2.43	0.46
20:3B:110:ASN:ND2	20:3B:112:ALA:O	2.48	0.46
28:B1:520:ALA:HB3	28:B1:533:SER:HB3	1.98	0.46
34:5C:354:CYS:SG	34:5C:364:ARG:NH1	2.87	0.46
36:5E:324:TRP:HA	36:5E:327:LYS:HE2	1.98	0.46
46:RJ:295:ASP:OD1	46:RJ:295:ASP:N	2.43	0.46
8:SI:71:HIS:HE1	12:SO:28:LEU:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3E:309:LEU:O	22:3E:312:SER:OG	2.26	0.46
26:AE:107:SER:OG	26:AE:108:LYS:NZ	2.48	0.46
28:B1:41:ASP:O	28:B1:45:ASN:HA	2.16	0.46
29:B2:56:THR:OG1	29:B2:57:GLY:N	2.47	0.46
29:B2:329:PHE:HB2	29:B2:374:PRO:HD3	1.97	0.46
31:B8:238:LEU:HD13	31:B8:279:GLY:HA2	1.96	0.46
31:B8:485:GLY:HA3	31:B8:518:ILE:HD11	1.96	0.46
34:5C:199:LEU:HB2	34:5C:204:LEU:HB2	1.96	0.46
40:5I:409:GLU:HA	40:5I:412:ARG:HG2	1.97	0.46
46:RJ:613:PRO:HD3	47:RK:292:ASN:HB3	1.97	0.46
3:SA:351:C:H42	11:SM:87:ARG:HH22	1.63	0.46
4:SC:243:LYS:HB3	30:B3:234:LEU:HA	1.96	0.46
8:SI:139:ARG:HE	15:SX:53:ILE:HD13	1.81	0.46
20:3C:199:PHE:HB2	20:3C:223:ASP:HA	1.97	0.46
21:3D:102:ASP:OD2	21:3D:105:LEU:N	2.49	0.46
28:B1:209:VAL:HG12	28:B1:215:VAL:HG22	1.96	0.46
28:B1:433:PHE:HA	28:B1:449:SER:HA	1.98	0.46
29:B2:794:LEU:HA	29:B2:797:VAL:HG12	1.97	0.46
30:B3:74:GLN:HA	30:B3:89:HIS:CD2	2.50	0.46
46:RJ:879:THR:OG1	46:RJ:880:TYR:N	2.47	0.46
49:RP:121:PHE:HD2	49:RP:162:LEU:HD11	1.81	0.46
1:3A:2:U:H1'	3:SA:1124:A:H61	1.80	0.46
3:SA:65:A:N7	3:SA:85:A:N6	2.63	0.46
3:SA:115:G:OP2	11:SM:67:ARG:NH1	2.48	0.46
3:SA:895:G:H22	3:SA:917:U:H3	1.62	0.46
3:SA:1663:G:O6	3:SA:1738:U:O4	2.32	0.46
5:SF:183:VAL:HG22	5:SF:191:ARG:H	1.80	0.46
21:3D:24:GLN:HE22	21:3D:38:ILE:HD11	1.80	0.46
34:5C:255:THR:HA	34:5C:270:LEU:O	2.16	0.46
44:RE:217:LYS:O	44:RE:223:ARG:NH1	2.48	0.46
46:RJ:953:SER:N	46:RJ:957:GLU:OE1	2.48	0.46
8:SI:17:GLU:HA	8:SI:20:VAL:HG22	1.97	0.46
24:3H:21:LEU:HD13	24:3H:90:ALA:HB2	1.96	0.46
26:AE:12:ALA:HB2	34:5C:142:GLY:HA3	1.97	0.46
29:B2:196:CYS:O	30:B3:667:GLN:NE2	2.49	0.46
30:B3:42:ILE:HD12	30:B3:379:LEU:HD22	1.98	0.46
32:BE:132:THR:OG1	32:BE:134:ASP:OD1	2.33	0.46
32:BE:183:VAL:HG12	32:BE:188:VAL:HG22	1.97	0.46
34:5C:94:SER:O	34:5C:94:SER:OG	2.33	0.46
41:5J:84:SER:O	41:5J:84:SER:OG	2.34	0.46
46:RJ:829:LEU:O	46:RJ:880:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:77:U:O2'	27:AG:870:ASN:ND2	2.48	0.46
3:SA:953:G:H2'	3:SA:954:G:H8	1.79	0.46
8:SI:130:VAL:HG11	8:SI:135:ILE:HG23	1.97	0.46
21:3D:194:ARG:NH1	22:3E:172:ASP:OD2	2.43	0.46
23:3F:371:ARG:O	23:3F:374:LYS:NZ	2.43	0.46
25:A5:175:ILE:HG13	25:A5:176:GLU:HG3	1.98	0.46
28:B1:575:GLU:HG3	28:B1:578:LYS:HB2	1.97	0.46
29:B2:165:SER:HB3	29:B2:182:LYS:HB2	1.97	0.46
29:B2:259:ILE:HG22	29:B2:274:ILE:HA	1.97	0.46
30:B3:138:HIS:CD2	30:B3:180:ARG:HG2	2.51	0.46
30:B3:512:ASP:HA	30:B3:535:GLY:HA2	1.97	0.46
30:B3:596:ASP:OD1	30:B3:596:ASP:N	2.49	0.46
33:B6:114:LEU:HD23	33:B6:114:LEU:HA	1.81	0.46
34:5C:378:VAL:HA	34:5C:394:HIS:HB3	1.96	0.46
43:RD:1659:VAL:HG12	43:RD:1674:LEU:HD23	1.97	0.46
44:RE:622:SER:OG	44:RE:623:GLU:OE1	2.34	0.46
44:RE:1205:LYS:N	44:RE:1213:ILE:O	2.45	0.46
49:RP:1811:ILE:HB	49:RP:1882:ARG:HH22	1.80	0.46
52:RZ:1175:SER:OG	52:RZ:1232:ASN:ND2	2.49	0.46
3:SA:140:A:N6	3:SA:281:G:OP1	2.48	0.46
3:SA:252:U:H2'	3:SA:253:A:C8	2.50	0.46
4:SC:32:ILE:HB	4:SC:43:VAL:HG22	1.97	0.46
10:SK:57:ARG:NH2	42:5K:88:ASP:OD1	2.48	0.46
10:SK:77:ILE:HD12	10:SK:91:LYS:HE2	1.98	0.46
28:B1:361:VAL:HG22	28:B1:371:VAL:HG22	1.97	0.46
32:BE:34:SER:OG	32:BE:35:ASN:N	2.49	0.46
38:5G:264:GLY:HA3	38:5G:268:ASN:HD21	1.81	0.46
44:RE:1145:PRO:HA	45:RF:172:TYR:HE2	1.81	0.46
51:RT:116:ILE:HG23	51:RT:158:PHE:HE2	1.80	0.46
52:RZ:502:MET:HG3	52:RZ:858:ALA:HB3	1.98	0.46
1:3A:110:A:N6	39:5H:588:SER:O	2.49	0.46
16:SY:128:SER:OG	16:SY:142:LYS:NZ	2.48	0.46
24:3H:88:GLY:HA2	24:3H:97:VAL:HG12	1.97	0.46
25:A5:150:LYS:HB2	25:A5:166:ALA:HB3	1.98	0.46
28:B1:387:THR:OG1	28:B1:388:SER:N	2.49	0.46
29:B2:574:LEU:HD23	29:B2:593:ALA:HB3	1.98	0.46
32:BE:814:GLU:OE1	32:BE:822:ARG:NH1	2.46	0.46
33:B6:290:LYS:HD2	33:B6:295:ILE:HG22	1.96	0.46
34:5C:388:ASP:HB2	40:5I:5:THR:HG23	1.96	0.46
52:RZ:1118:ILE:HG23	52:RZ:1131:CYS:HB3	1.98	0.46
3:SA:1580:C:OP1	38:5G:174:HIS:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1773:C:H2'	3:SA:1774:G:C8	2.51	0.46
24:3G:20:ILE:HA	24:3G:23:VAL:HG12	1.98	0.46
26:AE:239:LEU:HB3	31:B8:212:LEU:HD11	1.97	0.46
29:B2:497:VAL:HG13	29:B2:528:LEU:HB2	1.98	0.46
30:B3:208:SER:OG	30:B3:209:LEU:N	2.49	0.46
30:B3:691:PRO:HB3	30:B3:742:ARG:HE	1.79	0.46
36:5E:449:ASP:O	36:5E:453:SER:CB	2.62	0.46
39:5H:595:LYS:O	41:5J:134:ARG:NH1	2.46	0.46
40:5I:297:SER:OG	40:5I:457:ARG:O	2.27	0.46
41:5J:119:ARG:HG3	46:RJ:1113:ILE:HG13	1.98	0.46
44:RE:903:SER:O	44:RE:903:SER:OG	2.31	0.46
45:RF:58:LEU:HD12	45:RF:59:PRO:HD2	1.98	0.46
46:RJ:607:ASP:OD1	46:RJ:607:ASP:N	2.48	0.46
46:RJ:858:PRO:HA	46:RJ:885:PHE:HB3	1.98	0.46
47:RK:36:ILE:N	47:RK:72:THR:OG1	2.49	0.46
47:RK:119:LYS:HA	47:RK:164:GLY:O	2.16	0.46
47:RK:136:GLY:O	47:RK:293:GLN:NE2	2.49	0.46
49:RP:1681:LEU:O	49:RP:1685:SER:CB	2.64	0.46
49:RP:1714:SER:HA	49:RP:1717:ILE:HD13	1.97	0.46
3:SA:748:U:O2	3:SA:802:G:N2	2.49	0.46
6:SG:130:ILE:HA	6:SG:133:VAL:HG12	1.98	0.46
6:SG:189:THR:OG1	6:SG:190:ILE:N	2.49	0.46
8:SI:78:THR:O	8:SI:82:GLU:HB2	2.16	0.46
16:SY:57:LEU:HD21	48:RN:788:ILE:HG13	1.98	0.46
20:3B:182:SER:OG	20:3B:214:ARG:NH1	2.49	0.46
25:A5:235:LEU:HB3	25:A5:246:VAL:HG12	1.98	0.46
28:B1:157:ASP:OD2	28:B1:159:ARG:NE	2.39	0.46
28:B1:605:ASP:HB2	28:B1:607:PRO:HD2	1.98	0.46
28:B1:694:ALA:HA	28:B1:702:LEU:O	2.15	0.46
31:B8:384:ILE:HD12	31:B8:423:LEU:HD21	1.98	0.46
34:5C:212:GLY:O	34:5C:229:ARG:NH1	2.49	0.46
37:5F:165:LYS:HE2	37:5F:165:LYS:HB3	1.82	0.46
44:RE:501:ASN:OD1	44:RE:506:GLN:NE2	2.49	0.46
2:5A:475:G:H2'	2:5A:476:A:H8	1.81	0.45
3:SA:127:G:O6	7:SH:202:ARG:NH1	2.49	0.45
3:SA:523:G:N1	3:SA:528:U:OP2	2.45	0.45
3:SA:1628:U:H5"	36:5E:538:LYS:HE2	1.96	0.45
3:SA:1676:U:N3	3:SA:1726:G:O6	2.49	0.45
4:SC:28:GLU:OE1	4:SC:29:TRP:N	2.49	0.45
13:SP:19:ILE:HB	13:SP:83:ILE:HD13	1.98	0.45
14:SR:99:GLU:H	32:BE:490:GLN:NE2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SZ:49:LYS:HA	17:SZ:49:LYS:HD3	1.84	0.45
20:3B:110:ASN:ND2	20:3B:140:GLU:OE2	2.49	0.45
20:3C:226:HIS:HB3	20:3C:229:LYS:HB2	1.97	0.45
25:A5:242:ASP:OD1	25:A5:242:ASP:N	2.49	0.45
26:AE:122:VAL:HA	26:AE:127:ILE:HG12	1.98	0.45
26:AE:248:SER:OG	26:AE:249:LYS:N	2.48	0.45
28:B1:826:ARG:HA	28:B1:829:VAL:HG22	1.98	0.45
31:B8:220:ASP:N	31:B8:220:ASP:OD1	2.44	0.45
32:BE:561:ALA:HB2	32:BE:591:PHE:HE2	1.81	0.45
34:5C:248:HIS:CG	34:5C:258:LEU:HD22	2.51	0.45
45:RF:55:LEU:HG	45:RF:124:ALA:HB3	1.98	0.45
46:RJ:247:ASP:N	46:RJ:247:ASP:OD1	2.48	0.45
46:RJ:1034:LEU:HB2	46:RJ:1037:GLN:HG2	1.98	0.45
47:RK:141:MET:HG2	47:RK:300:TYR:HE2	1.79	0.45
3:SA:114:C:O2'	11:SM:65:SER:OG	2.32	0.45
3:SA:1538:U:H2'	3:SA:1540:G:C8	2.50	0.45
3:SA:1779:U:O2	3:SA:1782:A:N6	2.43	0.45
6:SG:72:HIS:O	14:SR:79:TYR:OH	2.33	0.45
8:SI:46:ILE:HA	8:SI:59:ALA:O	2.15	0.45
9:SJ:197:THR:HA	9:SJ:200:LYS:HG3	1.98	0.45
11:SM:89:ALA:HA	11:SM:104:HIS:HA	1.97	0.45
12:SO:18:TYR:HE1	15:SX:55:ASP:HA	1.81	0.45
28:B1:730:LEU:HD13	28:B1:754:VAL:HG23	1.98	0.45
29:B2:747:LYS:HB2	29:B2:747:LYS:HE3	1.75	0.45
30:B3:278:LEU:HD12	30:B3:279:LYS:HG2	1.98	0.45
30:B3:294:LEU:HB2	30:B3:303:PHE:HB2	1.99	0.45
31:B8:530:LEU:HB3	31:B8:544:VAL:HG22	1.97	0.45
34:5C:162:ASN:HB2	34:5C:164:GLN:H	1.81	0.45
44:RE:125:GLU:O	44:RE:129:HIS:ND1	2.49	0.45
44:RE:164:ASP:HA	44:RE:165:PRO:HA	1.82	0.45
44:RE:1022:MET:HA	44:RE:1025:THR:HG22	1.98	0.45
44:RE:1028:ARG:HA	44:RE:1031:ASP:HB3	1.97	0.45
46:RJ:123:ASP:O	46:RJ:904:ASN:ND2	2.47	0.45
46:RJ:130:ASP:OD1	46:RJ:130:ASP:N	2.48	0.45
49:RP:1818:LEU:HB3	49:RP:1875:LEU:HD22	1.97	0.45
52:RZ:515:ILE:HD12	52:RZ:528:LEU:HD21	1.97	0.45
52:RZ:873:ARG:HA	52:RZ:876:LEU:HG	1.98	0.45
3:SA:29:U:OP1	46:RJ:52:ARG:NH1	2.46	0.45
4:SC:126:THR:HB	4:SC:136:ARG:HD2	1.99	0.45
20:3C:91:HIS:CD2	20:3C:92:ARG:H	2.35	0.45
20:3C:272:LYS:HE3	20:3C:275:CYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B1:552:ASN:OD1	28:B1:552:ASN:N	2.47	0.45
30:B3:408:LYS:HG3	30:B3:437:VAL:HG13	1.99	0.45
32:BE:127:TYR:HA	32:BE:140:TYR:O	2.16	0.45
36:5E:359:SER:HA	36:5E:362:THR:HG22	1.99	0.45
38:5G:106:GLU:OE1	38:5G:173:ARG:N	2.43	0.45
45:RF:190:ILE:HD12	45:RF:194:ARG:HH21	1.80	0.45
47:RK:195:ALA:HB2	47:RK:209:ILE:HD11	1.99	0.45
52:RZ:803:LYS:HB2	52:RZ:836:GLN:HA	1.98	0.45
1:3A:31:G:H5"	1:3A:32:G:C4	2.52	0.45
3:SA:191:C:O2'	3:SA:192:U:O4'	2.33	0.45
3:SA:1465:C:O2	38:5G:146:ARG:NE	2.48	0.45
20:3B:120:GLU:OE2	20:3B:142:ARG:NE	2.49	0.45
29:B2:634:SER:OG	29:B2:636:ASP:N	2.49	0.45
30:B3:803:SER:O	30:B3:803:SER:OG	2.34	0.45
32:BE:630:THR:N	32:BE:644:THR:O	2.49	0.45
40:5I:216:SER:OG	40:5I:217:TRP:N	2.50	0.45
46:RJ:825:VAL:HG23	46:RJ:922:ILE:HG22	1.98	0.45
3:SA:746:A:O2'	15:SX:80:ASN:ND2	2.49	0.45
3:SA:966:A:OP2	12:SO:124:ARG:NH1	2.49	0.45
11:SM:89:ALA:HB1	11:SM:102:LYS:HE2	1.98	0.45
15:SX:97:ARG:HD3	15:SX:97:ARG:HA	1.74	0.45
20:3B:198:GLU:OE2	20:3B:199:PHE:N	2.49	0.45
20:3C:91:HIS:HB2	20:3C:96:VAL:O	2.16	0.45
24:3G:52:ILE:HG21	24:3G:67:LEU:HD11	1.98	0.45
25:A5:212:LEU:HD11	25:A5:246:VAL:HG11	1.98	0.45
29:B2:503:LYS:O	29:B2:520:LEU:N	2.49	0.45
30:B3:30:LYS:HB3	30:B3:43:ILE:HG12	1.99	0.45
30:B3:41:ASN:OD1	30:B3:41:ASN:N	2.44	0.45
34:5C:156:SER:OG	34:5C:157:ALA:N	2.50	0.45
34:5C:278:ASN:HD21	34:5C:294:ALA:HB2	1.80	0.45
34:5C:380:ASN:ND2	34:5C:381:LEU:O	2.49	0.45
44:RE:834:ASN:N	44:RE:834:ASN:OD1	2.48	0.45
45:RF:99:ASP:O	45:RF:103:LEU:HB2	2.17	0.45
46:RJ:258:ILE:HD11	46:RJ:263:LEU:HD23	1.98	0.45
47:RK:294:LEU:HD22	47:RK:317:GLN:HE21	1.81	0.45
52:RZ:622:ILE:HA	52:RZ:775:TYR:O	2.16	0.45
1:3A:26:C:O2'	1:3A:29:U:O4	2.34	0.45
3:SA:635:A:O4'	3:SA:863:A:N6	2.50	0.45
3:SA:1680:G:N2	3:SA:1720:G:O6	2.38	0.45
13:SP:43:THR:HG23	13:SP:46:MET:H	1.82	0.45
14:SR:79:TYR:HD1	14:SR:82:ARG:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SZ:23:PHE:HE2	17:SZ:75:VAL:HG12	1.81	0.45
24:3G:41:THR:HG21	24:3G:66:HIS:CE1	2.51	0.45
25:A5:8:SER:HB2	25:A5:17:LEU:HD11	1.98	0.45
28:B1:541:ILE:HG13	28:B1:550:VAL:HB	1.99	0.45
30:B3:584:ILE:HB	30:B3:588:LYS:HG3	1.98	0.45
31:B8:284:LEU:HD11	31:B8:287:SER:HB3	1.98	0.45
31:B8:363:LEU:HD11	31:B8:438:ASN:HA	1.99	0.45
40:5I:210:LYS:HB3	40:5I:210:LYS:HE2	1.78	0.45
44:RE:444:SER:N	44:RE:471:SER:OG	2.48	0.45
44:RE:507:PHE:HA	44:RE:510:ILE:HG22	1.99	0.45
45:RF:137:CYS:O	45:RF:141:LEU:HB2	2.17	0.45
46:RJ:230:MET:HG3	46:RJ:231:LYS:H	1.82	0.45
47:RK:97:GLY:HA2	47:RK:100:VAL:HG12	1.99	0.45
49:RP:1692:TYR:HE1	49:RP:1741:LYS:HG2	1.82	0.45
3:SA:325:G:O2'	11:SM:81:HIS:O	2.32	0.45
3:SA:938:G:N2	3:SA:941:A:OP2	2.47	0.45
24:3H:38:ASN:HA	24:3H:41:THR:HG22	1.97	0.45
26:AE:81:LEU:HD22	31:B8:33:LEU:HD21	1.97	0.45
29:B2:446:ILE:HG12	29:B2:488:LEU:HD11	1.97	0.45
34:5C:335:GLY:HA2	34:5C:377:LYS:HG3	1.98	0.45
45:RF:44:SER:OG	45:RF:46:ASN:OD1	2.34	0.45
46:RJ:134:ILE:HG13	46:RJ:243:TYR:HD2	1.82	0.45
46:RJ:244:MET:HE1	46:RJ:791:ILE:HD11	1.99	0.45
47:RK:22:VAL:HG23	47:RK:106:LEU:HD12	1.99	0.45
49:RP:1952:SER:OG	49:RP:1994:SER:OG	2.33	0.45
3:SA:752:A:H2'	3:SA:753:A:C8	2.52	0.45
3:SA:794:U:OP2	3:SA:797:G:N1	2.34	0.45
3:SA:1739:C:H2'	3:SA:1740:A:C8	2.52	0.45
20:3B:171:LEU:HB2	20:3B:237:VAL:HG21	1.97	0.45
21:3D:14:GLY:HA3	21:3D:55:PRO:HA	1.97	0.45
33:B6:67:ARG:HE	33:B6:84:SER:HG	1.64	0.45
41:5J:58:ASN:HA	41:5J:61:LYS:HG2	1.97	0.45
49:RP:67:ALA:O	49:RP:71:GLU:HB2	2.16	0.45
3:SA:1610:G:H5"	6:SG:107:LYS:HE3	1.98	0.45
28:B1:721:VAL:HG23	28:B1:741:MET:HG2	1.99	0.45
30:B3:20:SER:O	30:B3:20:SER:OG	2.33	0.45
31:B8:174:ARG:NH1	31:B8:179:ASP:OD1	2.50	0.45
35:5D:18:GLN:HB2	35:5D:28:LEU:H	1.82	0.45
36:5E:311:ILE:HG23	46:RJ:1032:LEU:HD13	1.97	0.45
44:RE:379:MET:HG2	44:RE:381:HIS:H	1.82	0.45
45:RF:252:LYS:HD2	45:RF:252:LYS:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RJ:251:ASP:OD1	46:RJ:251:ASP:N	2.49	0.45
47:RK:22:VAL:HG11	47:RK:105:TYR:HE1	1.82	0.45
49:RP:1983:LEU:HA	49:RP:1986:VAL:HG12	1.99	0.45
3:SA:163:G:OP2	3:SA:163:G:N2	2.42	0.45
3:SA:475:A:H5"	10:SK:130:THR:HG21	1.98	0.45
21:3D:30:ARG:HD3	21:3D:30:ARG:HA	1.78	0.45
23:3F:538:ARG:HD2	23:3F:567:VAL:HG22	1.98	0.45
26:AE:380:VAL:HA	26:AE:383:ILE:HG12	1.99	0.45
30:B3:454:LEU:HB2	30:B3:468:ILE:HD11	1.97	0.45
32:BE:56:LYS:O	32:BE:76:THR:OG1	2.29	0.45
38:5G:149:PRO:HG2	38:5G:170:VAL:HG11	1.98	0.45
47:RK:133:ILE:HA	47:RK:137:LEU:HD13	1.98	0.45
49:RP:1710:LEU:HD22	49:RP:1761:ILE:HG22	1.99	0.45
49:RP:2040:ARG:HH21	49:RP:2078:SER:HA	1.82	0.45
51:RT:245:GLU:HA	51:RT:248:VAL:HG12	1.98	0.45
52:RZ:646:LYS:HA	52:RZ:646:LYS:HD2	1.79	0.45
3:SA:327:U:H2'	3:SA:328:A:C8	2.52	0.44
5:SF:107:GLY:HA2	5:SF:189:LEU:HD22	1.99	0.44
6:SG:100:ASN:O	6:SG:104:ASN:ND2	2.51	0.44
15:SX:38:LEU:HA	15:SX:41:MET:HG2	2.00	0.44
27:AG:855:LEU:HD13	31:B8:477:LYS:HE2	1.99	0.44
30:B3:576:ASN:OD1	30:B3:576:ASN:N	2.50	0.44
32:BE:35:ASN:ND2	32:BE:53:CYS:SG	2.86	0.44
32:BE:225:THR:OG1	32:BE:227:THR:O	2.27	0.44
33:B6:327:LEU:HD22	33:B6:331:ARG:HD3	2.00	0.44
40:5I:216:SER:OG	40:5I:218:GLY:O	2.32	0.44
52:RZ:590:VAL:HG23	52:RZ:813:ALA:HB3	1.99	0.44
3:SA:676:G:H2'	3:SA:677:G:C8	2.53	0.44
3:SA:764:U:OP1	10:SK:82:ARG:NH1	2.51	0.44
21:3D:371:ASN:OD1	21:3D:371:ASN:N	2.47	0.44
30:B3:103:SER:OG	30:B3:122:THR:OG1	2.33	0.44
30:B3:188:GLU:OE2	30:B3:189:HIS:ND1	2.40	0.44
32:BE:482:GLY:HA2	32:BE:505:VAL:HG23	2.00	0.44
32:BE:539:LYS:HB3	32:BE:539:LYS:HE2	1.76	0.44
37:5F:6:LYS:NZ	37:5F:9:GLU:OE2	2.49	0.44
38:5G:136:THR:OG1	38:5G:137:THR:N	2.49	0.44
40:5I:281:ASN:ND2	40:5I:283:ASP:OD1	2.49	0.44
44:RE:158:VAL:HG11	44:RE:237:HIS:HB2	1.99	0.44
45:RF:101:SER:O	45:RF:105:SER:CB	2.56	0.44
49:RP:120:ASP:OD1	49:RP:120:ASP:N	2.46	0.44
52:RZ:420:LYS:N	57:RZ:1301:ADP:O1B	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RZ:728:PRO:O	52:RZ:754:SER:HA	2.16	0.44
3:SA:126:A:N6	3:SA:291:G:C2	2.85	0.44
3:SA:159:U:H5'	17:SZ:117:LYS:HB3	1.99	0.44
5:SF:41:SER:OG	5:SF:42:LEU:N	2.50	0.44
7:SH:50:PHE:HB3	7:SH:111:LEU:HD22	1.98	0.44
9:SJ:195:ARG:HD3	9:SJ:198:ALA:HB3	1.99	0.44
17:SZ:16:PRO:HA	17:SZ:19:ALA:HA	2.00	0.44
23:3F:152:VAL:HG12	23:3F:562:GLY:HA2	1.99	0.44
28:B1:30:LEU:HB3	28:B1:39:VAL:HG22	2.00	0.44
29:B2:590:THR:HG23	29:B2:598:LYS:HB2	1.99	0.44
30:B3:8:LYS:O	30:B3:644:TRP:HA	2.18	0.44
30:B3:138:HIS:HD2	30:B3:180:ARG:HG2	1.81	0.44
30:B3:541:PHE:HB3	30:B3:548:LEU:HA	2.00	0.44
31:B8:165:ARG:HH12	32:BE:236:ARG:HH12	1.66	0.44
34:5C:113:PRO:HG2	34:5C:130:ARG:HG3	1.98	0.44
34:5C:218:ASP:OD2	34:5C:221:THR:N	2.41	0.44
43:RD:1513:LYS:HA	43:RD:1513:LYS:HD2	1.83	0.44
46:RJ:97:THR:OG1	46:RJ:98:LEU:N	2.50	0.44
3:SA:591:A:H2'	3:SA:592:A:H8	1.82	0.44
4:SC:131:ASP:OD2	4:SC:180:THR:OG1	2.36	0.44
5:SF:152:PRO:HG2	7:SH:215:ARG:HD2	1.99	0.44
6:SG:118:LEU:HA	6:SG:121:ILE:HG12	1.99	0.44
22:3E:366:LYS:HE2	22:3E:393:LYS:HD2	1.99	0.44
25:A5:197:ILE:HG13	25:A5:198:THR:HG23	1.99	0.44
26:AE:370:LEU:HD23	26:AE:370:LEU:HA	1.89	0.44
30:B3:102:SER:OG	30:B3:103:SER:N	2.49	0.44
30:B3:787:PRO:HG3	36:5E:495:ILE:HG21	2.00	0.44
31:B8:450:GLN:HB3	31:B8:507:PRO:HD3	2.00	0.44
44:RE:543:LEU:HD12	44:RE:545:ALA:H	1.82	0.44
50:RQ:779:GLU:HG2	50:RQ:821:ARG:HD2	1.99	0.44
52:RZ:1043:LYS:NZ	52:RZ:1062:ILE:O	2.44	0.44
3:SA:886:U:OP2	4:SC:216:LYS:NZ	2.49	0.44
3:SA:1160:A:H2'	3:SA:1161:C:C6	2.52	0.44
4:SC:192:VAL:HG21	44:RE:751:LYS:HA	1.99	0.44
6:SG:120:ILE:HA	6:SG:123:VAL:HG12	2.00	0.44
14:SR:87:LYS:HA	14:SR:90:VAL:HG12	1.98	0.44
28:B1:107:ASP:OD1	28:B1:107:ASP:N	2.46	0.44
28:B1:358:SER:HB3	28:B1:826:ARG:HE	1.83	0.44
28:B1:726:THR:HG22	28:B1:741:MET:HB3	1.98	0.44
29:B2:330:GLN:HG2	29:B2:367:ILE:HG21	1.99	0.44
30:B3:150:LEU:HB2	30:B3:165:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RE:529:VAL:HG12	44:RE:531:LEU:HD22	1.99	0.44
44:RE:773:TYR:OH	44:RE:1131:ASN:O	2.35	0.44
49:RP:1822:SER:HA	49:RP:1868:LEU:HD22	2.00	0.44
52:RZ:1066:ASP:N	52:RZ:1066:ASP:OD1	2.49	0.44
3:SA:139:C:H42	3:SA:175:G:H21	1.66	0.44
3:SA:457:G:OP1	17:SZ:108:ARG:NH2	2.50	0.44
3:SA:629:U:H3	3:SA:970:A:H62	1.65	0.44
3:SA:826:U:O2'	3:SA:827:C:O2	2.23	0.44
4:SC:50:LYS:HD2	4:SC:50:LYS:HA	1.77	0.44
9:SJ:64:ASN:O	9:SJ:180:ASP:HA	2.17	0.44
12:SO:13:SER:OG	12:SO:14:SER:N	2.50	0.44
17:SZ:8:ARG:HD2	23:3F:352:PRO:HA	1.99	0.44
20:3C:198:GLU:OE2	20:3C:200:SER:N	2.49	0.44
23:3F:450:ASP:OD1	23:3F:450:ASP:N	2.48	0.44
24:3H:20:ILE:HG22	24:3H:117:VAL:HG13	1.98	0.44
28:B1:265:CYS:SG	28:B1:266:VAL:N	2.91	0.44
29:B2:678:ASP:OD1	29:B2:680:SER:OG	2.35	0.44
30:B3:785:ILE:HD13	30:B3:785:ILE:HA	1.88	0.44
34:5C:438:PRO:O	34:5C:441:THR:OG1	2.34	0.44
34:5C:460:ARG:HH22	50:RQ:849:PHE:HA	1.82	0.44
44:RE:141:TRP:HB3	44:RE:178:TYR:HB3	1.99	0.44
47:RK:148:GLU:H	47:RK:172:SER:HB3	1.82	0.44
47:RK:347:ASN:OD1	47:RK:347:ASN:N	2.51	0.44
49:RP:1995:ARG:HD3	49:RP:1996:GLN:HG3	2.00	0.44
51:RT:248:VAL:HA	51:RT:251:ILE:HG22	1.98	0.44
3:SA:676:G:H2'	3:SA:677:G:H8	1.82	0.44
3:SA:1051:G:H21	40:5I:447:THR:HG21	1.83	0.44
21:3D:400:PHE:HA	21:3D:403:VAL:HG22	2.00	0.44
28:B1:266:VAL:HG12	28:B1:277:VAL:HG22	1.98	0.44
30:B3:248:PHE:H	30:B3:259:TYR:HD1	1.66	0.44
30:B3:357:THR:HG21	30:B3:363:ARG:HD3	1.99	0.44
42:5K:70:ASN:OD1	42:5K:70:ASN:N	2.50	0.44
44:RE:160:VAL:HG21	44:RE:230:VAL:HG22	2.00	0.44
44:RE:503:VAL:HA	44:RE:1014:LEU:HD13	1.99	0.44
44:RE:761:ARG:HB2	44:RE:899:LEU:HD11	1.99	0.44
49:RP:1887:LEU:HB3	49:RP:1924:LEU:HD11	1.99	0.44
52:RZ:613:ILE:HG23	52:RZ:617:LEU:HD12	1.99	0.44
52:RZ:1129:GLU:HA	52:RZ:1132:PHE:HB2	2.00	0.44
3:SA:1068:C:H2'	3:SA:1069:A:C8	2.53	0.44
3:SA:1647:U:H2'	3:SA:1648:A:H8	1.83	0.44
9:SJ:65:PHE:HA	9:SJ:181:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3C:173:LEU:HD13	20:3C:256:ASN:HD22	1.83	0.44
22:3E:363:LEU:HD12	22:3E:394:VAL:HG11	1.99	0.44
25:A5:233:LYS:HB2	25:A5:247:THR:HG23	2.00	0.44
28:B1:23:SER:OG	28:B1:25:ASP:OD1	2.36	0.44
29:B2:203:HIS:CE1	29:B2:227:LYS:HG3	2.52	0.44
29:B2:884:LYS:HE3	29:B2:884:LYS:HB3	1.92	0.44
30:B3:302:MET:HB2	30:B3:314:ILE:HB	2.00	0.44
31:B8:305:SER:OG	31:B8:306:ASN:N	2.50	0.44
32:BE:590:ALA:HB3	32:BE:603:ALA:HB3	2.00	0.44
34:5C:525:ASN:HA	34:5C:528:LYS:HG2	1.98	0.44
36:5E:297:LEU:HD22	36:5E:301:GLU:HG2	1.98	0.44
36:5E:444:LEU:HD13	37:5F:57:LEU:HD21	2.00	0.44
39:5H:579:VAL:HG23	39:5H:580:ARG:HG3	1.99	0.44
44:RE:660:ASP:N	44:RE:660:ASP:OD1	2.51	0.44
44:RE:739:LYS:HA	44:RE:739:LYS:HD3	1.79	0.44
46:RJ:829:LEU:HD22	46:RJ:915:ALA:HB1	1.99	0.44
49:RP:1957:GLN:HE21	49:RP:1998:LEU:HB2	1.83	0.44
52:RZ:507:LEU:HD21	52:RZ:510:TYR:HB2	1.99	0.44
5:SF:98:ASN:ND2	5:SF:114:ILE:O	2.43	0.44
8:SI:157:LYS:HD2	8:SI:157:LYS:HA	1.69	0.44
11:SM:78:THR:HG23	11:SM:84:ILE:HG22	2.00	0.44
16:SY:121:ARG:NH1	48:RN:795:GLU:OE2	2.45	0.44
22:3E:380:ARG:NH1	22:3E:382:ASP:OD1	2.50	0.44
22:3E:418:LYS:HD3	22:3E:418:LYS:HA	1.78	0.44
24:3H:62:GLU:HA	24:3H:65:LEU:HB3	1.99	0.44
25:A5:255:ILE:O	25:A5:276:SER:OG	2.31	0.44
28:B1:474:GLY:N	28:B1:494:ASP:OD2	2.50	0.44
29:B2:213:LYS:HZ2	29:B2:261:PHE:HB3	1.82	0.44
30:B3:672:TYR:HB3	30:B3:681:ALA:HB2	2.00	0.44
30:B3:702:LEU:HD11	30:B3:758:ARG:HE	1.82	0.44
32:BE:171:GLN:HG3	32:BE:214:PRO:HG3	1.98	0.44
36:5E:311:ILE:HD12	46:RJ:1032:LEU:HD13	2.00	0.44
43:RD:1485:GLN:HE21	43:RD:1497:LEU:HD11	1.83	0.44
44:RE:270:ILE:HB	44:RE:292:ILE:HG12	1.99	0.44
46:RJ:169:GLY:HA3	46:RJ:204:LEU:HD12	2.00	0.44
46:RJ:1151:GLN:HA	46:RJ:1154:LYS:HG2	1.99	0.44
47:RK:154:LEU:HD21	47:RK:165:GLU:HG2	2.00	0.44
52:RZ:930:ILE:HD11	52:RZ:1007:LEU:HB2	1.99	0.44
3:SA:58:U:O2'	3:SA:451:A:N3	2.50	0.43
3:SA:1658:G:N2	3:SA:1743:U:O2	2.37	0.43
5:SF:97:GLU:OE1	5:SF:99:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SK:112:GLN:NE2	10:SK:153:GLU:OE2	2.50	0.43
11:SM:69:LYS:HB2	11:SM:127:GLN:HB2	1.99	0.43
20:3B:241:PHE:HA	20:3B:268:VAL:O	2.18	0.43
25:A5:166:ALA:HB2	25:A5:194:LEU:HD13	2.00	0.43
26:AE:32:SER:OG	26:AE:119:GLU:OE2	2.36	0.43
26:AE:241:ILE:HA	26:AE:244:LYS:HG2	2.00	0.43
26:AE:308:GLY:O	26:AE:311:ASN:HB3	2.18	0.43
34:5C:261:PRO:O	50:RQ:838:LYS:NZ	2.48	0.43
37:5F:114:ILE:HD13	37:5F:114:ILE:HA	1.89	0.43
43:RD:1531:GLU:H	43:RD:1531:GLU:HG2	1.66	0.43
44:RE:874:LEU:HD13	45:RF:98:VAL:HG12	2.00	0.43
47:RK:118:PHE:HB2	47:RK:166:VAL:HG22	1.99	0.43
52:RZ:627:THR:OG1	52:RZ:628:GLY:N	2.51	0.43
3:SA:112:A:O2'	11:SM:67:ARG:NE	2.44	0.43
3:SA:323:A:O2'	3:SA:346:G:N2	2.51	0.43
3:SA:654:C:H2'	3:SA:655:G:C8	2.54	0.43
4:SC:30:PHE:HE1	4:SC:94:LYS:HD2	1.82	0.43
9:SJ:40:ALA:N	9:SJ:61:GLU:OE1	2.51	0.43
12:SO:16:ILE:HD12	12:SO:62:GLN:HE22	1.83	0.43
21:3D:330:ALA:HB3	24:3H:38:ASN:HD22	1.83	0.43
22:3E:359:ILE:HA	22:3E:362:VAL:HG12	2.01	0.43
26:AE:309:GLN:H	31:B8:226:LYS:HZ1	1.67	0.43
29:B2:144:ASN:OD1	29:B2:160:ARG:NE	2.34	0.43
44:RE:769:VAL:HG11	44:RE:1113:GLY:HA3	2.00	0.43
44:RE:773:TYR:HE2	44:RE:1129:PRO:HG2	1.82	0.43
50:RQ:781:ASP:HA	50:RQ:814:GLY:HA3	2.00	0.43
52:RZ:601:ASN:OD1	52:RZ:603:THR:OG1	2.34	0.43
1:3A:39:C:H2'	1:3A:40:A:C8	2.54	0.43
3:SA:874:C:H2'	3:SA:875:G:C8	2.54	0.43
3:SA:1696:G:H2'	3:SA:1697:G:C8	2.52	0.43
4:SC:165:ARG:HA	4:SC:168:ILE:HG22	2.00	0.43
9:SJ:78:ILE:HA	9:SJ:104:ILE:HG22	2.01	0.43
10:SK:35:GLY:O	10:SK:110:GLN:NE2	2.46	0.43
10:SK:129:ILE:HD11	10:SK:144:PRO:HA	2.00	0.43
20:3C:248:ASP:OD1	20:3C:248:ASP:N	2.45	0.43
26:AE:122:VAL:HG13	26:AE:128:HIS:HB3	2.00	0.43
29:B2:17:ILE:HG13	29:B2:360:ASN:HB2	1.99	0.43
29:B2:88:HIS:ND1	29:B2:91:THR:OG1	2.38	0.43
29:B2:392:THR:OG1	29:B2:393:ASP:N	2.51	0.43
30:B3:393:SER:OG	30:B3:394:LEU:N	2.50	0.43
30:B3:531:ASN:O	30:B3:558:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5H:544:ILE:HD13	46:RJ:834:TRP:CD2	2.54	0.43
39:5H:587:GLN:HE21	39:5H:591:TYR:HB2	1.83	0.43
40:5I:258:ILE:HG22	40:5I:464:THR:HG23	2.00	0.43
40:5I:386:LYS:HE3	40:5I:394:LEU:HD12	1.99	0.43
44:RE:804:THR:HG22	44:RE:838:VAL:HB	2.00	0.43
46:RJ:561:GLU:HA	46:RJ:564:ILE:HG12	1.99	0.43
51:RT:80:ARG:HG2	52:RZ:1059:ALA:HB2	1.99	0.43
52:RZ:781:ARG:HB2	52:RZ:798:VAL:HG12	2.00	0.43
52:RZ:1099:LEU:HD21	52:RZ:1229:TRP:HB3	1.99	0.43
3:SA:884:A:H2'	3:SA:885:G:C8	2.54	0.43
3:SA:1599:C:OP1	46:RJ:978:ARG:NH2	2.51	0.43
4:SC:129:THR:OG1	4:SC:130:SER:N	2.51	0.43
9:SJ:67:TRP:NE1	9:SJ:185:GLU:OE1	2.50	0.43
13:SP:43:THR:OG1	13:SP:44:GLY:N	2.50	0.43
14:SR:69:VAL:HG21	14:SR:81:ILE:HG12	2.00	0.43
24:3G:54:MET:O	24:3G:80:PHE:HA	2.18	0.43
25:A5:173:ILE:HG22	25:A5:180:VAL:HA	2.00	0.43
29:B2:8:PHE:HA	29:B2:685:GLU:O	2.17	0.43
30:B3:593:CYS:O	30:B3:619:ARG:NH1	2.48	0.43
31:B8:305:SER:O	31:B8:307:GLN:NE2	2.51	0.43
32:BE:159:VAL:HG11	32:BE:167:ILE:HD11	2.00	0.43
32:BE:545:PRO:HD2	32:BE:563:ASP:HB2	2.00	0.43
36:5E:506:GLU:HA	36:5E:516:SER:HA	2.01	0.43
44:RE:254:LEU:HD21	44:RE:268:LEU:HD13	2.00	0.43
46:RJ:174:LEU:HD13	46:RJ:183:LEU:HD11	1.99	0.43
49:RP:1818:LEU:HD23	49:RP:1818:LEU:HA	1.89	0.43
49:RP:1941:VAL:HA	49:RP:1944:ILE:HG12	2.00	0.43
3:SA:502:U:H5"	39:5H:574:LYS:HD2	2.01	0.43
3:SA:635:A:H2'	3:SA:636:A:C8	2.52	0.43
3:SA:784:C:H2'	3:SA:785:U:C2	2.53	0.43
3:SA:902:G:H22	3:SA:906:A:H5"	1.81	0.43
3:SA:1609:U:O2'	6:SG:105:GLY:O	2.26	0.43
15:SX:105:THR:HA	15:SX:109:GLY:O	2.18	0.43
24:3G:43:THR:HA	24:3G:46:ARG:HG2	2.01	0.43
24:3H:13:ASP:OD1	24:3H:13:ASP:N	2.36	0.43
25:A5:5:VAL:HG23	25:A5:306:LEU:HD11	1.99	0.43
25:A5:168:HIS:CE1	32:BE:646:VAL:HB	2.54	0.43
25:A5:327:THR:O	25:A5:327:THR:OG1	2.37	0.43
30:B3:625:THR:OG1	30:B3:628:ASP:OD1	2.36	0.43
34:5C:96:ASP:OD1	34:5C:96:ASP:N	2.51	0.43
34:5C:452:VAL:HG11	50:RQ:847:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RE:197:GLN:HB2	44:RE:200:GLY:H	1.83	0.43
44:RE:462:PHE:HB2	44:RE:466:THR:HG21	2.01	0.43
52:RZ:600:PHE:CZ	52:RZ:684:ASP:C	2.91	0.43
52:RZ:847:VAL:HA	52:RZ:850:ILE:HB	2.00	0.43
3:SA:491:C:H2'	3:SA:492:A:C8	2.54	0.43
3:SA:891:A:H2'	3:SA:892:A:H8	1.82	0.43
17:SZ:118:ILE:HD13	17:SZ:118:ILE:HA	1.92	0.43
22:3E:299:LEU:HD23	22:3E:320:LEU:HD23	1.99	0.43
24:3H:52:ILE:O	24:3H:78:TYR:HA	2.19	0.43
32:BE:761:GLN:H	32:BE:761:GLN:HG3	1.54	0.43
42:5K:66:LEU:HD23	42:5K:97:LEU:HB2	2.01	0.43
44:RE:475:ASN:O	44:RE:478:THR:OG1	2.26	0.43
44:RE:920:LEU:HD11	44:RE:925:LEU:HD22	2.00	0.43
44:RE:1013:THR:OG1	44:RE:1014:LEU:N	2.52	0.43
44:RE:1195:LYS:HA	44:RE:1211:ASN:HA	1.99	0.43
46:RJ:755:LYS:HD2	46:RJ:755:LYS:HA	1.84	0.43
49:RP:1975:LYS:HB3	49:RP:1978:ALA:HB3	2.00	0.43
52:RZ:842:ILE:HG13	52:RZ:850:ILE:HD13	2.01	0.43
3:SA:1780:G:H2'	3:SA:1781:A:H8	1.83	0.43
7:SH:139:ASN:HA	7:SH:142:ARG:HB2	2.00	0.43
7:SH:157:VAL:HG12	7:SH:175:ILE:HD11	2.00	0.43
9:SJ:53:LYS:HE3	9:SJ:53:LYS:HB3	1.93	0.43
14:SR:46:PHE:HA	14:SR:49:TYR:HB2	1.99	0.43
21:3D:395:GLU:HA	21:3D:396:PRO:HD3	1.81	0.43
22:3E:367:ALA:O	22:3E:371:LEU:HB3	2.18	0.43
23:3F:145:ALA:HB2	23:3F:568:ILE:HD12	1.99	0.43
26:AE:65:LYS:HE3	26:AE:65:LYS:HB3	1.89	0.43
28:B1:19:ASN:HA	28:B1:307:THR:HG21	2.01	0.43
28:B1:62:ASP:N	28:B1:62:ASP:OD1	2.51	0.43
29:B2:44:SER:HA	29:B2:49:VAL:HG12	2.00	0.43
29:B2:136:LEU:HB2	29:B2:150:LEU:HD11	2.00	0.43
29:B2:264:ASN:N	29:B2:269:THR:HG1	2.14	0.43
34:5C:331:ALA:HA	34:5C:339:THR:O	2.18	0.43
34:5C:376:ASN:HD22	34:5C:396:THR:HG22	1.82	0.43
38:5G:165:PHE:HB3	38:5G:256:MET:HB2	1.99	0.43
44:RE:928:HIS:HE1	44:RE:1164:SER:HB2	1.84	0.43
46:RJ:82:LYS:HB2	46:RJ:82:LYS:HE3	1.79	0.43
49:RP:26:LEU:HD21	49:RP:149:GLU:HB2	1.99	0.43
50:RQ:311:LEU:HD23	50:RQ:311:LEU:HA	1.90	0.43
3:SA:1154:G:H2'	3:SA:1155:G:H8	1.83	0.43
7:SH:23:ARG:HG2	7:SH:41:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3C:201:HIS:O	20:3C:205:ARG:NH2	2.52	0.43
21:3D:127:LEU:HD12	21:3D:127:LEU:HA	1.81	0.43
24:3G:54:MET:HE1	24:3G:78:TYR:HB2	2.00	0.43
24:3G:98:ILE:HD13	24:3G:98:ILE:HA	1.87	0.43
28:B1:321:SER:HB3	28:B1:326:GLN:HG2	2.00	0.43
28:B1:760:ILE:HD11	28:B1:797:ILE:HG21	2.00	0.43
30:B3:77:THR:HG21	30:B3:117:LEU:HD22	2.01	0.43
32:BE:230:VAL:HB	32:BE:244:ILE:HG13	2.01	0.43
32:BE:486:ILE:HB	32:BE:496:LYS:HG3	2.01	0.43
32:BE:520:CYS:SG	32:BE:546:ILE:HG21	2.59	0.43
40:5I:304:HIS:CE1	40:5I:324:SER:HB3	2.53	0.43
44:RE:1108:LEU:O	44:RE:1112:CYS:HB2	2.18	0.43
46:RJ:634:ARG:NH1	47:RK:283:ILE:O	2.51	0.43
47:RK:299:VAL:HA	47:RK:302:VAL:HG12	2.01	0.43
3:SA:336:G:OP1	11:SM:129:ARG:NH2	2.52	0.43
3:SA:940:A:H2'	3:SA:941:A:H8	1.84	0.43
10:SK:113:VAL:HG12	10:SK:156:ILE:HG21	2.01	0.43
12:SO:132:VAL:HG13	12:SO:134:VAL:HG13	2.00	0.43
17:SZ:51:GLU:HB3	17:SZ:53:ASP:H	1.83	0.43
20:3C:197:VAL:HG23	20:3C:220:ILE:HB	2.01	0.43
21:3D:33:GLU:OE2	40:5I:376:ARG:NH2	2.46	0.43
29:B2:20:ASN:HD22	29:B2:339:LYS:HE3	1.84	0.43
29:B2:65:ASP:HA	29:B2:106:TRP:HH2	1.84	0.43
30:B3:243:VAL:HG21	30:B3:289:PHE:HE2	1.84	0.43
38:5G:109:LEU:HD23	38:5G:109:LEU:HA	1.87	0.43
46:RJ:771:GLU:HB2	46:RJ:776:GLN:HG2	2.00	0.43
50:RQ:304:GLN:HA	50:RQ:307:ARG:HE	1.83	0.43
51:RT:68:SER:HB3	51:RT:82:THR:HG21	2.01	0.43
3:SA:90:C:H2'	3:SA:91:G:C8	2.54	0.43
3:SA:1601:G:OP1	46:RJ:981:SER:OG	2.31	0.43
3:SA:1790:A:O2'	3:SA:1792:G:N2	2.52	0.43
4:SC:16:GLN:HB3	30:B3:390:LEU:HD11	2.01	0.43
5:SF:240:LYS:HA	5:SF:240:LYS:HD2	1.75	0.43
14:SR:75:VAL:HA	14:SR:78:VAL:HG12	2.01	0.43
22:3E:372:ARG:O	22:3E:376:LEU:HB2	2.19	0.43
23:3F:293:ASP:N	23:3F:293:ASP:OD1	2.52	0.43
25:A5:73:THR:OG1	25:A5:74:VAL:N	2.51	0.43
25:A5:213:ASN:OD1	25:A5:213:ASN:N	2.49	0.43
25:A5:230:SER:OG	25:A5:231:ASP:N	2.52	0.43
28:B1:163:THR:O	28:B1:163:THR:OG1	2.37	0.43
28:B1:709:THR:O	28:B1:711:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B8:125:TRP:NE1	32:BE:235:MET:O	2.40	0.43
33:B6:137:LEU:HD23	33:B6:137:LEU:HA	1.85	0.43
40:5I:41:TYR:OH	40:5I:409:GLU:OE2	2.34	0.43
43:RD:1721:SER:O	43:RD:1721:SER:OG	2.32	0.43
46:RJ:86:ILE:HD13	46:RJ:86:ILE:HA	1.85	0.43
46:RJ:218:ARG:O	46:RJ:222:ASN:ND2	2.52	0.43
52:RZ:1027:LYS:O	52:RZ:1027:LYS:NZ	2.43	0.43
3:SA:306:U:H2'	3:SA:307:G:H8	1.84	0.42
4:SC:13:LYS:HB3	4:SC:13:LYS:HE2	1.76	0.42
6:SG:133:VAL:HA	6:SG:198:LEU:HD21	2.01	0.42
10:SK:99:LEU:HD12	10:SK:99:LEU:HA	1.92	0.42
23:3F:545:LYS:HG2	23:3F:561:ASN:HD21	1.84	0.42
30:B3:5:THR:OG1	30:B3:6:SER:N	2.52	0.42
31:B8:22:LEU:HB3	33:B6:66:LEU:HD12	2.01	0.42
34:5C:113:PRO:HB2	34:5C:379:GLU:HG3	2.00	0.42
34:5C:424:GLN:H	34:5C:424:GLN:HG2	1.73	0.42
45:RF:121:ARG:HA	45:RF:121:ARG:HD2	1.83	0.42
46:RJ:131:ILE:HD13	46:RJ:131:ILE:HA	1.80	0.42
46:RJ:180:GLN:OE1	46:RJ:184:ARG:NE	2.38	0.42
49:RP:209:ARG:HA	49:RP:212:VAL:HG12	2.01	0.42
3:SA:294:C:H2'	3:SA:295:A:H8	1.85	0.42
3:SA:940:A:H2'	3:SA:941:A:C8	2.54	0.42
3:SA:1648:A:H2'	3:SA:1649:G:H8	1.84	0.42
3:SA:1690:G:H2'	3:SA:1691:A:H8	1.84	0.42
3:SA:1744:A:H2'	3:SA:1745:G:C8	2.54	0.42
6:SG:120:ILE:HD11	6:SG:192:GLU:HA	2.01	0.42
11:SM:90:TYR:HE2	11:SM:92:HIS:HD2	1.67	0.42
12:SO:19:SER:OG	12:SO:21:ASN:OD1	2.37	0.42
17:SZ:13:ILE:HG13	17:SZ:22:GLN:HG3	2.00	0.42
17:SZ:92:VAL:HG23	17:SZ:98:GLU:HA	2.00	0.42
23:3F:165:PRO:HD2	23:3F:185:LEU:HD23	2.01	0.42
23:3F:343:ASP:OD1	23:3F:343:ASP:N	2.51	0.42
28:B1:340:LYS:HE3	36:5E:478:ASP:HA	2.01	0.42
28:B1:830:ARG:HD3	28:B1:830:ARG:HA	1.90	0.42
29:B2:544:ARG:HD2	29:B2:544:ARG:HA	1.76	0.42
29:B2:614:HIS:HD2	29:B2:634:SER:HB3	1.84	0.42
30:B3:678:TRP:HD1	30:B3:697:VAL:HG23	1.84	0.42
31:B8:133:ILE:HD13	32:BE:194:ARG:HH22	1.83	0.42
32:BE:388:GLU:OE2	32:BE:410:LYS:NZ	2.44	0.42
34:5C:448:SER:O	34:5C:448:SER:OG	2.30	0.42
36:5E:400:LEU:HD23	51:RT:264:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RE:1204:VAL:HG23	44:RE:1206:PRO:HD3	2.02	0.42
45:RF:17:PRO:HD2	45:RF:148:HIS:CD2	2.54	0.42
52:RZ:714:GLY:N	52:RZ:716:GLU:OE2	2.48	0.42
3:SA:143:G:OP2	7:SH:139:ASN:ND2	2.45	0.42
3:SA:862:A:H4'	15:SX:57:ARG:HG2	2.01	0.42
3:SA:1045:C:H2'	3:SA:1046:G:H8	1.84	0.42
3:SA:1071:U:H2'	3:SA:1072:C:C6	2.54	0.42
3:SA:1482:C:H4'	14:SR:77:GLN:HE22	1.85	0.42
4:SC:8:ARG:HD3	4:SC:8:ARG:HA	1.88	0.42
21:3D:48:ILE:HD13	21:3D:48:ILE:HA	1.91	0.42
21:3D:122:GLU:HA	21:3D:125:GLN:HB2	2.00	0.42
26:AE:286:LEU:HD23	26:AE:286:LEU:HA	1.85	0.42
28:B1:588:ASP:OD1	28:B1:588:ASP:N	2.51	0.42
29:B2:125:THR:HG23	29:B2:126:LEU:HD23	2.01	0.42
29:B2:880:ILE:HD13	29:B2:880:ILE:HA	1.90	0.42
31:B8:388:HIS:HB3	31:B8:392:GLY:H	1.85	0.42
33:B6:133:TYR:CZ	33:B6:150:CYS:HB2	2.54	0.42
38:5G:192:ASP:OD2	38:5G:227:ARG:NH2	2.50	0.42
38:5G:264:GLY:H	38:5G:271:ALA:HB1	1.85	0.42
44:RE:707:PHE:O	44:RE:918:ARG:NH1	2.52	0.42
44:RE:758:SER:N	44:RE:780:GLN:OE1	2.52	0.42
44:RE:833:TYR:OH	44:RE:877:GLU:OE2	2.25	0.42
45:RF:40:LYS:O	45:RF:53:LEU:HA	2.19	0.42
47:RK:133:ILE:HD11	47:RK:151:LEU:HD22	2.00	0.42
49:RP:2016:LEU:HA	49:RP:2019:ILE:HG12	2.01	0.42
51:RT:196:ASP:O	51:RT:199:SER:OG	2.32	0.42
52:RZ:800:TRP:HB3	52:RZ:834:PHE:HE1	1.84	0.42
52:RZ:815:ARG:HA	52:RZ:815:ARG:HD2	1.79	0.42
8:SI:34:LEU:O	8:SI:36:ALA:N	2.51	0.42
20:3C:220:ILE:HG21	20:3C:230:TYR:HB2	2.02	0.42
24:3H:21:LEU:HA	24:3H:24:VAL:HB	2.01	0.42
29:B2:567:LEU:HD23	29:B2:567:LEU:HA	1.91	0.42
30:B3:163:LEU:HD12	30:B3:163:LEU:HA	1.93	0.42
31:B8:465:THR:OG1	31:B8:466:THR:N	2.49	0.42
34:5C:291:THR:HG23	34:5C:299:LYS:HB2	2.01	0.42
37:5F:40:ASN:OD1	37:5F:40:ASN:N	2.52	0.42
41:5J:121:LEU:HD22	41:5J:141:TRP:HH2	1.85	0.42
43:RD:1600:GLU:HA	43:RD:1603:THR:HG22	2.01	0.42
44:RE:1203:ASN:ND2	45:RF:57:ASN:OD1	2.52	0.42
47:RK:55:LEU:HD12	47:RK:88:HIS:CG	2.55	0.42
47:RK:65:ILE:HG12	47:RK:76:TYR:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RP:1819:PHE:HZ	49:RP:1876:LEU:HD21	1.84	0.42
49:RP:1883:HIS:HB2	49:RP:1887:LEU:HD21	2.02	0.42
49:RP:1960:LEU:HD23	49:RP:1960:LEU:HA	1.88	0.42
52:RZ:1079:LEU:O	52:RZ:1083:MET:HG2	2.19	0.42
3:SA:1133:A:OP1	47:RK:231:ARG:NH2	2.49	0.42
3:SA:1537:C:O2'	3:SA:1540:G:O6	2.28	0.42
3:SA:1689:A:H3'	3:SA:1690:G:H8	1.84	0.42
4:SC:7:LYS:NZ	13:SP:51:ASP:OD2	2.50	0.42
8:SI:73:VAL:HG22	8:SI:77:LEU:HD23	2.00	0.42
16:SY:103:LEU:HD23	16:SY:126:LYS:HD3	2.00	0.42
20:3B:301:LEU:HG	20:3B:302:GLU:HG2	2.02	0.42
23:3F:229:GLU:HB2	23:3F:231:THR:HG23	2.00	0.42
23:3F:272:LYS:HA	23:3F:272:LYS:HD2	1.88	0.42
26:AE:141:ASN:OD1	26:AE:141:ASN:N	2.52	0.42
29:B2:6:GLN:HB3	29:B2:687:THR:HG22	2.02	0.42
29:B2:52:TRP:CD1	29:B2:59:LEU:HA	2.54	0.42
29:B2:596:ASN:N	29:B2:596:ASN:OD1	2.52	0.42
30:B3:533:LYS:N	30:B3:554:ASP:OD2	2.44	0.42
32:BE:470:GLN:HG2	32:BE:512:GLY:HA2	2.02	0.42
35:5D:16:ARG:O	35:5D:30:LYS:NZ	2.51	0.42
36:5E:350:THR:O	38:5G:285:ASN:ND2	2.52	0.42
36:5E:515:MET:HE2	36:5E:520:LEU:HD21	2.02	0.42
38:5G:190:ILE:HG13	38:5G:223:THR:HA	2.00	0.42
40:5I:327:LYS:H	40:5I:327:LYS:HG3	1.70	0.42
40:5I:384:ASN:OD1	40:5I:384:ASN:N	2.52	0.42
43:RD:1638:ARG:NH2	43:RD:1662:GLU:OE1	2.42	0.42
44:RE:756:VAL:HA	44:RE:896:THR:HG21	2.02	0.42
51:RT:98:LYS:HG2	51:RT:138:GLU:HB3	2.01	0.42
52:RZ:449:GLN:HG3	52:RZ:455:ALA:HA	2.01	0.42
3:SA:1639:C:H42	36:5E:515:MET:HE3	1.84	0.42
4:SC:27:LYS:HB3	4:SC:47:LEU:HD22	2.02	0.42
5:SF:177:ALA:HA	5:SF:198:LYS:HE2	2.02	0.42
20:3C:194:VAL:HB	20:3C:217:ILE:HD13	2.02	0.42
21:3D:136:GLU:OE1	21:3D:143:GLN:NE2	2.52	0.42
23:3F:437:ARG:HA	23:3F:437:ARG:HD3	1.78	0.42
26:AE:341:LYS:HE2	26:AE:341:LYS:HB2	1.93	0.42
29:B2:283:THR:OG1	29:B2:330:GLN:O	2.34	0.42
29:B2:361:THR:HG23	29:B2:386:GLU:HB3	2.01	0.42
30:B3:65:THR:HA	30:B3:80:SER:HB3	2.01	0.42
30:B3:467:ILE:HG13	30:B3:480:ILE:HD11	2.00	0.42
32:BE:758:PHE:HA	51:RT:176:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BE:885:MET:HG2	32:BE:912:TRP:CZ2	2.55	0.42
40:5I:347:ARG:HB3	42:5K:107:GLU:HB3	2.02	0.42
42:5K:107:GLU:HG2	42:5K:117:LEU:HD11	2.02	0.42
44:RE:557:THR:OG1	44:RE:558:LEU:N	2.53	0.42
44:RE:940:LYS:HD3	44:RE:975:LEU:HD11	2.01	0.42
44:RE:1159:ASN:ND2	44:RE:1201:ASP:O	2.41	0.42
47:RK:11:PHE:HB2	47:RK:33:ILE:HG12	2.02	0.42
50:RQ:321:HIS:ND1	50:RQ:322:ASN:O	2.46	0.42
1:3A:247:U:H2'	1:3A:248:G:C8	2.54	0.42
3:SA:142:G:N2	3:SA:174:U:O2	2.53	0.42
3:SA:752:A:H5"	5:SF:219:VAL:HG23	2.02	0.42
5:SF:77:ARG:HG2	5:SF:82:TYR:CZ	2.55	0.42
7:SH:148:SER:OG	7:SH:151:ASP:OD2	2.37	0.42
21:3D:87:PRO:HA	50:RQ:324:ALA:HB2	2.02	0.42
25:A5:120:ILE:HG23	25:A5:151:LEU:HD13	2.01	0.42
29:B2:499:PHE:HD2	29:B2:526:THR:HB	1.84	0.42
29:B2:633:CYS:HB3	29:B2:663:LEU:HD22	2.02	0.42
29:B2:912:TRP:CD2	30:B3:779:VAL:HG21	2.54	0.42
30:B3:38:ASP:HB3	30:B3:54:HIS:HA	2.02	0.42
31:B8:137:ILE:HG22	31:B8:155:ILE:HD11	2.01	0.42
32:BE:765:GLU:HB2	32:BE:773:VAL:HG21	2.02	0.42
34:5C:172:LYS:HB2	34:5C:172:LYS:HE2	1.90	0.42
37:5F:126:ASP:OD1	37:5F:126:ASP:N	2.48	0.42
40:5I:61:GLN:OE1	40:5I:371:ASN:ND2	2.52	0.42
40:5I:244:ILE:HD12	40:5I:267:ILE:HD12	2.00	0.42
43:RD:1483:ALA:HA	43:RD:1486:LEU:HB2	2.01	0.42
44:RE:962:LEU:HA	44:RE:962:LEU:HD23	1.82	0.42
46:RJ:831:ARG:NH1	46:RJ:877:GLU:O	2.49	0.42
47:RK:19:LEU:HA	47:RK:22:VAL:HG12	2.01	0.42
47:RK:187:ILE:O	47:RK:251:GLN:NE2	2.49	0.42
52:RZ:729:LEU:HD23	52:RZ:731:VAL:HG22	2.01	0.42
2:5A:476:A:H2'	2:5A:477:G:C8	2.54	0.42
3:SA:82:U:H2'	3:SA:83:G:C4	2.54	0.42
3:SA:628:G:N1	3:SA:970:A:OP2	2.36	0.42
3:SA:1686:C:N4	3:SA:1716:C:N3	2.67	0.42
3:SA:1693:A:H3'	3:SA:1694:A:H8	1.85	0.42
5:SF:205:PHE:H	5:SF:221:ARG:HD3	1.84	0.42
23:3F:504:ASN:OD1	23:3F:504:ASN:N	2.52	0.42
32:BE:440:ALA:HB2	32:BE:463:VAL:HG21	2.01	0.42
32:BE:629:ALA:HA	32:BE:645:HIS:HA	2.02	0.42
33:B6:128:LYS:HA	33:B6:128:LYS:HD3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B6:199:ARG:NH2	50:RQ:386:LEU:O	2.49	0.42
37:5F:2:VAL:HG12	37:5F:3:ARG:HB2	2.02	0.42
37:5F:114:ILE:HG21	37:5F:150:VAL:HG11	2.01	0.42
46:RJ:617:THR:HG22	46:RJ:620:LYS:H	1.85	0.42
47:RK:143:LYS:NZ	47:RK:252:LYS:O	2.39	0.42
48:RN:784:ILE:HA	48:RN:787:THR:HG22	2.01	0.42
3:SA:756:A:H3'	3:SA:757:A:H8	1.85	0.42
3:SA:760:A:H2'	3:SA:761:G:H8	1.84	0.42
20:3C:146:PRO:HG3	20:3C:156:MET:HG3	2.02	0.42
21:3D:212:ASP:HB3	21:3D:215:THR:HG22	2.00	0.42
23:3F:241:THR:OG1	23:3F:548:ARG:NH2	2.53	0.42
34:5C:42:LEU:HD12	34:5C:42:LEU:HA	1.88	0.42
41:5J:113:MET:HE3	41:5J:113:MET:HB3	1.87	0.42
44:RE:107:ILE:HD13	44:RE:107:ILE:HA	1.93	0.42
46:RJ:929:VAL:HB	46:RJ:1006:TRP:HB3	2.01	0.42
46:RJ:948:ILE:HG21	46:RJ:1001:VAL:HG11	2.02	0.42
49:RP:1908:GLU:HG3	49:RP:1912:ILE:HD11	2.02	0.42
51:RT:169:ASP:OD1	51:RT:169:ASP:N	2.53	0.42
52:RZ:1153:LEU:O	52:RZ:1169:THR:HA	2.19	0.42
3:SA:107:C:H2'	3:SA:108:A:H8	1.85	0.42
3:SA:196:G:O2'	3:SA:197:A:O4'	2.37	0.42
3:SA:922:G:H2'	3:SA:923:A:H8	1.84	0.42
3:SA:1060:U:H2'	3:SA:1061:A:C8	2.55	0.42
7:SH:111:LEU:HD23	7:SH:111:LEU:HA	1.87	0.42
8:SI:17:GLU:HB3	8:SI:46:ILE:HG12	2.02	0.42
9:SJ:84:HIS:O	11:SM:11:ARG:NH2	2.53	0.42
9:SJ:105:ASP:HB3	9:SJ:107:THR:HG22	2.02	0.42
14:SR:117:LEU:HD23	14:SR:117:LEU:HA	1.92	0.42
15:SX:61:ILE:HD13	15:SX:61:ILE:HA	1.89	0.42
20:3B:218:ILE:HD12	21:3D:152:LEU:HA	2.01	0.42
21:3D:203:PHE:CD2	21:3D:206:LEU:HB2	2.55	0.42
21:3D:281:LEU:HD12	21:3D:281:LEU:HA	1.93	0.42
22:3E:333:LYS:HD2	22:3E:333:LYS:HA	1.81	0.42
23:3F:437:ARG:HB3	23:3F:438:ILE:H	1.72	0.42
27:AG:868:ASN:OD1	27:AG:871:SER:OG	2.27	0.42
29:B2:183:ASP:O	29:B2:185:MET:N	2.53	0.42
30:B3:631:MET:HA	30:B3:646:ASP:HB2	2.02	0.42
31:B8:388:HIS:ND1	31:B8:391:SER:OG	2.46	0.42
32:BE:431:ILE:HA	32:BE:442:THR:HA	2.01	0.42
34:5C:152:GLU:HB2	34:5C:171:LYS:HB2	2.00	0.42
34:5C:456:SER:OG	34:5C:457:SER:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5E:405:SER:OG	36:5E:406:SER:N	2.52	0.42
40:5I:400:LEU:HD23	40:5I:400:LEU:HA	1.86	0.42
42:5K:133:LYS:HD2	42:5K:133:LYS:HA	1.93	0.42
44:RE:867:ILE:HD12	44:RE:879:GLU:HG3	2.01	0.42
44:RE:1039:PHE:HB2	44:RE:1053:SER:HB2	2.02	0.42
46:RJ:839:LEU:HD11	46:RJ:914:ALA:HB1	2.01	0.42
47:RK:130:ILE:HG21	47:RK:166:VAL:HG11	2.02	0.42
52:RZ:993:GLN:HB3	52:RZ:994:PHE:H	1.74	0.42
1:3A:330:A:H2'	1:3A:331:A:C8	2.55	0.41
5:SF:81:THR:OG1	5:SF:81:THR:O	2.36	0.41
5:SF:129:VAL:HG22	5:SF:139:VAL:HG12	2.02	0.41
16:SY:50:LYS:HE3	16:SY:50:LYS:HB3	1.86	0.41
20:3C:240:VAL:HG22	20:3C:261:LEU:HD22	2.02	0.41
21:3D:146:ASP:OD1	21:3D:146:ASP:N	2.53	0.41
21:3D:261:GLN:HE21	21:3D:263:ILE:HA	1.84	0.41
28:B1:520:ALA:HB1	28:B1:583:ILE:HG12	2.02	0.41
29:B2:159:LEU:HD21	29:B2:189:TRP:CD2	2.55	0.41
32:BE:305:ASN:OD1	32:BE:305:ASN:N	2.50	0.41
32:BE:745:LYS:HE3	32:BE:745:LYS:HB2	1.89	0.41
34:5C:88:GLN:O	34:5C:92:LYS:HB2	2.20	0.41
44:RE:1139:LEU:HD13	44:RE:1142:LYS:HD2	2.02	0.41
45:RF:223:LEU:HG	45:RF:227:ARG:HH21	1.85	0.41
47:RK:263:ASP:OD1	47:RK:263:ASP:N	2.53	0.41
49:RP:1752:ASP:N	49:RP:1752:ASP:OD1	2.53	0.41
52:RZ:791:ASN:OD1	52:RZ:791:ASN:N	2.52	0.41
1:3A:39:C:O3'	26:AE:22:ARG:NH1	2.52	0.41
3:SA:799:A:H2'	3:SA:800:U:C6	2.56	0.41
22:3E:323:GLU:HA	22:3E:326:LEU:HB3	2.02	0.41
25:A5:23:ALA:HB1	31:B8:261:PRO:HG3	2.02	0.41
26:AE:196:LEU:HD12	26:AE:196:LEU:HA	1.85	0.41
26:AE:299:ILE:O	26:AE:303:PHE:HB2	2.21	0.41
28:B1:423:ARG:NH2	28:B1:460:VAL:O	2.53	0.41
30:B3:304:LEU:HD23	30:B3:304:LEU:HA	1.91	0.41
30:B3:480:ILE:HG22	30:B3:481:LYS:H	1.84	0.41
32:BE:413:GLU:O	32:BE:435:LYS:N	2.48	0.41
3:SA:800:U:H2'	3:SA:801:G:C4	2.56	0.41
3:SA:1151:A:H2'	3:SA:1152:A:H8	1.86	0.41
6:SG:26:ALA:H	14:SR:27:GLY:HA3	1.84	0.41
9:SJ:106:ALA:HB2	9:SJ:165:LEU:HG	2.02	0.41
28:B1:425:PHE:HZ	28:B1:460:VAL:HG23	1.86	0.41
29:B2:231:LEU:HD12	29:B2:233:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B2:351:LEU:HB2	29:B2:367:ILE:HG13	2.02	0.41
30:B3:186:LEU:HD21	30:B3:230:LYS:HE3	2.00	0.41
30:B3:616:HIS:CG	30:B3:620:LEU:HD21	2.56	0.41
32:BE:173:LEU:HB3	32:BE:214:PRO:HB3	2.02	0.41
32:BE:738:ASP:OD2	32:BE:890:LYS:NZ	2.53	0.41
32:BE:906:ALA:O	32:BE:910:GLN:HB2	2.21	0.41
33:B6:144:VAL:HA	33:B6:147:TRP:HD1	1.85	0.41
34:5C:88:GLN:HA	34:5C:91:ILE:HG22	2.02	0.41
40:5I:285:ASN:OD1	40:5I:285:ASN:N	2.52	0.41
41:5J:60:LYS:HA	41:5J:60:LYS:HD2	1.84	0.41
41:5J:112:ASN:OD1	41:5J:112:ASN:N	2.52	0.41
42:5K:155:THR:OG1	42:5K:156:ASN:N	2.53	0.41
43:RD:1577:PHE:HD2	43:RD:1581:LYS:HE2	1.85	0.41
47:RK:300:TYR:HD1	47:RK:300:TYR:HA	1.74	0.41
49:RP:1974:LEU:HG	49:RP:1975:LYS:HG3	2.02	0.41
3:SA:814:A:N6	3:SA:858:G:O4'	2.41	0.41
10:SK:117:GLY:O	10:SK:119:ALA:N	2.53	0.41
28:B1:488:LEU:HA	28:B1:488:LEU:HD12	1.84	0.41
29:B2:217:LEU:HB3	29:B2:229:TRP:HB2	2.01	0.41
29:B2:360:ASN:OD1	29:B2:360:ASN:N	2.52	0.41
32:BE:157:LEU:HD21	32:BE:196:GLY:HA2	2.03	0.41
34:5C:244:ASN:HB3	34:5C:446:PRO:HD3	2.02	0.41
34:5C:333:SER:O	34:5C:333:SER:OG	2.38	0.41
44:RE:236:THR:HG21	44:RE:256:TYR:HE1	1.86	0.41
46:RJ:290:ILE:HG22	46:RJ:812:MET:HB3	2.02	0.41
46:RJ:623:LYS:HA	46:RJ:623:LYS:HD2	1.87	0.41
51:RT:82:THR:OG1	51:RT:83:SER:N	2.54	0.41
52:RZ:536:VAL:HA	52:RZ:553:LEU:HD23	2.03	0.41
52:RZ:621:ALA:HB3	52:RZ:773:VAL:HA	2.03	0.41
1:3A:44:U:H2'	1:3A:45:U:H6	1.85	0.41
6:SG:130:ILE:H	6:SG:130:ILE:HG12	1.65	0.41
8:SI:24:PHE:HE1	8:SI:77:LEU:HD13	1.84	0.41
20:3C:165:ALA:HB3	20:3C:168:LYS:HB2	2.01	0.41
22:3E:214:ILE:H	22:3E:214:ILE:HG13	1.69	0.41
23:3F:188:TYR:OH	23:3F:265:THR:OG1	2.33	0.41
24:3G:85:VAL:HB	24:3G:89:ARG:HH12	1.86	0.41
26:AE:315:LEU:HA	26:AE:316:PRO:HD3	1.90	0.41
26:AE:408:ILE:HD13	26:AE:415:VAL:HG11	2.02	0.41
29:B2:175:ASP:O	29:B2:190:ASP:HA	2.20	0.41
29:B2:301:LYS:HD2	29:B2:301:LYS:HA	1.80	0.41
29:B2:472:HIS:CG	29:B2:492:SER:HG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B2:544:ARG:NH1	29:B2:544:ARG:O	2.54	0.41
30:B3:735:GLN:H	30:B3:735:GLN:HG3	1.66	0.41
31:B8:384:ILE:HD11	31:B8:435:PHE:HZ	1.85	0.41
32:BE:343:LEU:HD23	32:BE:343:LEU:HA	1.81	0.41
32:BE:652:CYS:SG	32:BE:654:TRP:NE1	2.90	0.41
33:B6:199:ARG:HA	33:B6:199:ARG:HD2	1.82	0.41
33:B6:388:VAL:HA	33:B6:391:TYR:HB3	2.02	0.41
34:5C:20:LYS:HD3	34:5C:20:LYS:HA	1.85	0.41
34:5C:220:SER:OG	34:5C:221:THR:N	2.53	0.41
35:5D:24:ARG:H	35:5D:24:ARG:HG2	1.67	0.41
44:RE:135:LEU:HD21	44:RE:239:LEU:HD11	2.01	0.41
44:RE:146:LEU:HA	44:RE:149:VAL:HG22	2.01	0.41
46:RJ:1128:LYS:HE2	46:RJ:1128:LYS:HB3	1.88	0.41
50:RQ:775:VAL:HG12	50:RQ:821:ARG:HH12	1.85	0.41
3:SA:52:U:H2'	3:SA:53:G:C8	2.55	0.41
3:SA:229:U:H2'	3:SA:230:C:H6	1.85	0.41
3:SA:953:G:H2'	3:SA:954:G:C8	2.56	0.41
3:SA:1111:G:H2'	3:SA:1112:G:C8	2.56	0.41
4:SC:52:THR:OG1	4:SC:53:GLY:N	2.53	0.41
4:SC:78:ASP:N	4:SC:78:ASP:OD1	2.53	0.41
10:SK:94:ASP:OD1	10:SK:94:ASP:N	2.52	0.41
13:SP:72:LYS:HB2	13:SP:72:LYS:HE3	1.86	0.41
21:3D:31:LEU:HD21	40:5I:59:VAL:HG23	2.02	0.41
21:3D:86:LEU:HD13	21:3D:86:LEU:HA	1.91	0.41
21:3D:194:ARG:HA	21:3D:194:ARG:HD3	1.93	0.41
21:3D:307:ILE:HD12	21:3D:307:ILE:HA	1.96	0.41
28:B1:833:LYS:O	28:B1:837:ASN:ND2	2.54	0.41
29:B2:59:LEU:HD21	29:B2:62:LYS:HB2	2.03	0.41
29:B2:553:ASN:OD1	29:B2:553:ASN:N	2.53	0.41
31:B8:541:LEU:HB3	31:B8:562:LEU:HD13	2.02	0.41
32:BE:657:ARG:HB2	32:BE:661:LYS:HZ3	1.85	0.41
34:5C:296:ARG:HG3	34:5C:318:PRO:HG3	2.01	0.41
35:5D:28:LEU:HD23	35:5D:30:LYS:HZ1	1.86	0.41
38:5G:77:TYR:HE2	38:5G:205:ILE:HG22	1.84	0.41
40:5I:320:ILE:HA	40:5I:320:ILE:HD13	1.83	0.41
42:5K:74:PHE:HA	42:5K:77:GLN:HG2	2.02	0.41
46:RJ:1049:ASN:HA	46:RJ:1050:PRO:HD3	1.96	0.41
49:RP:1994:SER:H	49:RP:1996:GLN:HE22	1.68	0.41
50:RQ:350:ASN:OD1	50:RQ:350:ASN:N	2.51	0.41
52:RZ:385:GLN:O	52:RZ:389:ILE:HG12	2.20	0.41
52:RZ:1000:PHE:HA	52:RZ:1140:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RZ:1215:PRO:HG2	52:RZ:1231:LEU:HB2	2.02	0.41
3:SA:214:G:N2	3:SA:250:C:OP2	2.53	0.41
3:SA:278:U:OP1	3:SA:279:G:N2	2.54	0.41
3:SA:890:C:H2'	3:SA:891:A:C8	2.55	0.41
3:SA:1151:A:H2'	3:SA:1152:A:C8	2.55	0.41
3:SA:1658:G:H1	3:SA:1743:U:H3	1.69	0.41
4:SC:26:ARG:HG2	4:SC:50:LYS:HB2	2.02	0.41
23:3F:463:GLN:HE22	24:3H:7:LYS:H	1.66	0.41
23:3F:517:ALA:HB2	23:3F:564:TYR:CG	2.55	0.41
28:B1:155:SER:OG	28:B1:156:GLN:N	2.53	0.41
29:B2:187:LYS:HG2	29:B2:199:THR:HG22	2.03	0.41
29:B2:357:THR:OG1	29:B2:359:SER:O	2.29	0.41
29:B2:400:SER:OG	29:B2:401:ASP:OD1	2.34	0.41
30:B3:214:GLY:HA2	30:B3:220:ILE:HA	2.02	0.41
31:B8:270:LYS:HG3	31:B8:289:HIS:CE1	2.55	0.41
33:B6:57:ILE:HD12	33:B6:92:ILE:HG23	2.01	0.41
40:5I:281:ASN:N	40:5I:281:ASN:OD1	2.54	0.41
41:5J:155:ASP:OD1	41:5J:157:SER:OG	2.32	0.41
44:RE:129:HIS:HD2	44:RE:132:TYR:HE1	1.67	0.41
44:RE:800:GLU:HA	44:RE:803:LYS:HE2	2.02	0.41
46:RJ:764:ILE:HA	46:RJ:767:ILE:HG22	2.02	0.41
3:SA:182:A:H2'	3:SA:183:U:C6	2.55	0.41
3:SA:973:A:H2'	3:SA:974:A:C8	2.56	0.41
3:SA:1636:C:H2'	3:SA:1637:C:C6	2.55	0.41
7:SH:182:GLN:HE21	7:SH:186:ARG:NE	2.19	0.41
8:SI:62:VAL:HA	8:SI:63:PRO:HD3	1.94	0.41
12:SO:70:LYS:H	12:SO:70:LYS:HG2	1.65	0.41
20:3C:278:SER:OG	20:3C:279:THR:N	2.53	0.41
23:3F:304:ILE:HD11	23:3F:325:VAL:HG21	2.02	0.41
23:3F:363:ASP:OD1	23:3F:363:ASP:N	2.43	0.41
29:B2:453:GLU:HG2	29:B2:469:GLU:HG3	2.03	0.41
30:B3:126:ILE:HG12	30:B3:147:ILE:HD13	2.03	0.41
31:B8:366:SER:HG	31:B8:438:ASN:HD22	1.69	0.41
32:BE:859:ASP:OD1	32:BE:859:ASP:N	2.52	0.41
33:B6:269:ILE:H	33:B6:269:ILE:HG13	1.64	0.41
33:B6:287:ASN:HD22	33:B6:287:ASN:HA	1.65	0.41
34:5C:306:PHE:HB2	50:RQ:826:LEU:HD13	2.03	0.41
37:5F:36:TYR:HB3	37:5F:110:ARG:HH12	1.85	0.41
40:5I:324:SER:OG	40:5I:326:ASP:O	2.28	0.41
44:RE:388:PHE:HD1	44:RE:480:MET:HE1	1.86	0.41
44:RE:936:LEU:HA	44:RE:939:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RE:975:LEU:HD23	44:RE:1041:VAL:HG12	2.02	0.41
44:RE:1227:GLY:O	44:RE:1231:VAL:N	2.43	0.41
46:RJ:274:TYR:CE1	46:RJ:786:GLY:HA2	2.56	0.41
49:RP:178:ILE:HD13	49:RP:178:ILE:HA	1.89	0.41
52:RZ:997:LEU:H	52:RZ:1004:PHE:HE2	1.68	0.41
1:3A:317:A:O2'	1:3A:319:G:OP1	2.38	0.41
2:5A:495:G:O2'	33:B6:123:GLN:O	2.39	0.41
3:SA:961:U:H2'	3:SA:962:C:C6	2.56	0.41
3:SA:1782:A:H3'	3:SA:1783:C:H6	1.86	0.41
4:SC:29:TRP:HB3	4:SC:45:LYS:HE3	2.01	0.41
5:SF:125:LYS:HE2	5:SF:125:LYS:HB3	1.92	0.41
8:SI:7:LYS:HB3	8:SI:41:LEU:HD11	2.02	0.41
10:SK:124:HIS:HA	10:SK:127:VAL:HG12	2.03	0.41
13:SP:61:MET:HG3	13:SP:104:ALA:HB2	2.01	0.41
15:SX:74:VAL:HA	15:SX:127:GLY:HA2	2.03	0.41
20:3C:162:LEU:HG	20:3C:164:ILE:H	1.86	0.41
20:3C:270:SER:OG	20:3C:270:SER:O	2.38	0.41
21:3D:160:ARG:HG3	21:3D:165:PHE:HB3	2.03	0.41
22:3E:279:ARG:O	22:3E:283:ILE:HG22	2.21	0.41
23:3F:113:ASP:N	23:3F:113:ASP:OD1	2.52	0.41
23:3F:201:ILE:HD12	23:3F:201:ILE:HA	1.93	0.41
24:3H:44:LEU:HD12	24:3H:44:LEU:HA	1.87	0.41
25:A5:213:ASN:ND2	25:A5:215:TYR:OH	2.54	0.41
26:AE:25:ARG:NH2	40:5I:11:ASP:OD1	2.41	0.41
26:AE:297:LEU:HA	26:AE:297:LEU:HD23	1.84	0.41
26:AE:424:LEU:HG	26:AE:426:GLY:H	1.86	0.41
28:B1:422:PHE:HD1	28:B1:423:ARG:HG2	1.84	0.41
29:B2:218:ILE:HD11	29:B2:226:VAL:HB	2.01	0.41
30:B3:151:LYS:H	30:B3:164:ALA:HB3	1.86	0.41
30:B3:534:ARG:N	30:B3:554:ASP:OD1	2.43	0.41
30:B3:762:CYS:O	30:B3:766:HIS:HB2	2.21	0.41
31:B8:129:ASP:OD2	32:BE:194:ARG:NH2	2.52	0.41
31:B8:226:LYS:HE2	31:B8:226:LYS:HB2	1.80	0.41
32:BE:633:LYS:HA	32:BE:633:LYS:HD3	1.90	0.41
34:5C:194:ARG:O	34:5C:195:HIS:ND1	2.53	0.41
39:5H:548:LYS:HB3	39:5H:548:LYS:HE2	1.82	0.41
40:5I:358:MET:HB3	50:RQ:890:VAL:HG23	2.01	0.41
43:RD:1524:GLU:OE1	43:RD:1532:THR:OG1	2.33	0.41
44:RE:228:ARG:NH1	44:RE:266:PRO:O	2.35	0.41
44:RE:416:PHE:HE1	44:RE:421:LEU:HB3	1.85	0.41
46:RJ:303:LYS:HA	46:RJ:789:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RJ:863:THR:HB	46:RJ:866:ARG:HA	2.02	0.41
49:RP:1854:SER:OG	49:RP:1855:TYR:N	2.52	0.41
49:RP:1942:LEU:HD21	49:RP:1978:ALA:HB1	2.02	0.41
50:RQ:347:GLN:H	50:RQ:347:GLN:HG3	1.71	0.41
52:RZ:466:LEU:HB3	52:RZ:469:HIS:HB2	2.03	0.41
52:RZ:915:LEU:HD13	52:RZ:1049:ILE:HG21	2.03	0.41
52:RZ:928:VAL:HA	52:RZ:931:VAL:HG12	2.02	0.41
52:RZ:986:LYS:HA	52:RZ:989:LYS:HD2	2.02	0.41
2:5A:465:G:C2	2:5A:466:A:H1'	2.56	0.41
3:SA:329:G:H2'	3:SA:330:G:C8	2.56	0.41
3:SA:930:A:H8	4:SC:114:VAL:HG11	1.85	0.41
4:SC:88:VAL:HG21	4:SC:96:LEU:HD13	2.03	0.41
10:SK:169:PRO:HB3	23:3F:226:HIS:HE1	1.86	0.41
12:SO:46:THR:OG1	12:SO:86:GLU:OE2	2.36	0.41
15:SX:103:ILE:HA	15:SX:112:ASP:HA	2.02	0.41
17:SZ:42:GLU:HB3	17:SZ:52:LYS:HE2	2.03	0.41
21:3D:225:ASP:OD1	21:3D:226:LYS:N	2.53	0.41
22:3E:369:VAL:HG13	24:3G:63:ILE:HD13	2.04	0.41
23:3F:447:SER:OG	23:3F:450:ASP:OD1	2.39	0.41
28:B1:192:ASP:HB3	34:5C:234:PRO:HD3	2.03	0.41
28:B1:318:ALA:HB2	28:B1:329:VAL:HG23	2.01	0.41
29:B2:554:THR:OG1	29:B2:569:LEU:O	2.30	0.41
29:B2:905:LEU:HD12	30:B3:782:VAL:HB	2.03	0.41
32:BE:376:TRP:CE2	32:BE:388:GLU:HB2	2.56	0.41
32:BE:579:ARG:NH2	32:BE:615:PRO:O	2.54	0.41
33:B6:110:TRP:CD2	33:B6:136:LEU:HD13	2.56	0.41
40:5I:79:SER:OG	40:5I:80:LEU:N	2.54	0.41
42:5K:157:ASP:OD1	42:5K:157:ASP:N	2.43	0.41
43:RD:1712:LYS:HA	43:RD:1712:LYS:HD2	1.94	0.41
44:RE:902:ILE:HD12	44:RE:902:ILE:HA	1.91	0.41
49:RP:1933:ILE:HD13	49:RP:1933:ILE:HA	1.92	0.41
52:RZ:782:SER:HB3	52:RZ:809:ARG:HH22	1.85	0.41
52:RZ:1033:LYS:HD3	52:RZ:1033:LYS:HA	1.86	0.41
52:RZ:1159:LEU:HA	52:RZ:1165:THR:HA	2.03	0.41
1:3A:329:C:H2'	1:3A:330:A:C8	2.56	0.40
3:SA:107:C:H2'	3:SA:108:A:C8	2.56	0.40
3:SA:1137:A:H1'	29:B2:594:ASP:HB3	2.03	0.40
3:SA:1535:U:H1'	3:SA:1536:G:N2	2.36	0.40
5:SF:171:ASP:OD1	5:SF:172:PHE:N	2.52	0.40
23:3F:321:HIS:CE1	23:3F:340:GLY:HA3	2.56	0.40
25:A5:96:THR:OG1	25:A5:97:TYR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A5:199:ASN:OD1	25:A5:199:ASN:N	2.50	0.40
26:AE:106:SER:HA	26:AE:109:TRP:HE1	1.86	0.40
28:B1:194:VAL:HA	28:B1:210:SER:HA	2.03	0.40
28:B1:215:VAL:HB	28:B1:254:HIS:HB2	2.03	0.40
29:B2:382:THR:OG1	29:B2:383:HIS:N	2.54	0.40
29:B2:534:ILE:H	29:B2:534:ILE:HG22	1.66	0.40
29:B2:549:SER:HB2	29:B2:579:ILE:HD11	2.02	0.40
30:B3:119:VAL:HG13	30:B3:127:ILE:HG13	2.03	0.40
30:B3:179:LYS:O	51:RT:69:LYS:NZ	2.44	0.40
30:B3:497:LEU:HA	30:B3:507:ALA:O	2.20	0.40
31:B8:37:LEU:O	31:B8:41:ASN:HB2	2.20	0.40
35:5D:6:HIS:CE1	39:5H:550:LEU:HD23	2.55	0.40
35:5D:22:ARG:NH1	46:RJ:937:PHE:HB3	2.36	0.40
40:5I:66:HIS:CE1	40:5I:87:SER:HG	2.38	0.40
42:5K:154:ALA:HA	42:5K:173:MET:HG2	2.03	0.40
44:RE:539:LEU:HD22	44:RE:547:PHE:HB2	2.04	0.40
44:RE:709:PRO:HB3	44:RE:1171:VAL:HG23	2.02	0.40
44:RE:800:GLU:O	44:RE:804:THR:HG23	2.21	0.40
46:RJ:869:THR:O	46:RJ:869:THR:OG1	2.35	0.40
46:RJ:1163:GLN:H	46:RJ:1163:GLN:HG3	1.66	0.40
47:RK:252:LYS:HG3	47:RK:254:TRP:HD1	1.86	0.40
49:RP:1872:ALA:HA	49:RP:1875:LEU:HD23	2.02	0.40
50:RQ:809:ILE:HD12	50:RQ:809:ILE:HA	1.99	0.40
52:RZ:494:ASP:O	52:RZ:498:LEU:HG	2.21	0.40
52:RZ:1125:THR:OG1	52:RZ:1130:ASP:OD2	2.32	0.40
3:SA:890:C:H2'	3:SA:891:A:H8	1.87	0.40
3:SA:1739:C:H2'	3:SA:1740:A:H8	1.85	0.40
4:SC:48:VAL:HG23	4:SC:49:ASN:H	1.87	0.40
8:SI:143:LEU:HD12	8:SI:147:ASN:HB2	2.03	0.40
10:SK:30:LEU:HA	10:SK:30:LEU:HD23	1.90	0.40
15:SX:11:LEU:HD13	15:SX:11:LEU:HA	1.96	0.40
21:3D:171:ASP:OD2	21:3D:321:SER:OG	2.32	0.40
23:3F:158:THR:HG21	23:3F:240:LEU:HA	2.04	0.40
24:3G:20:ILE:HG22	24:3G:117:VAL:HG13	2.02	0.40
25:A5:203:ILE:HD13	25:A5:235:LEU:HD22	2.03	0.40
26:AE:14:ASN:HB3	34:5C:101:ASN:HD21	1.85	0.40
26:AE:387:LEU:HA	26:AE:387:LEU:HD12	1.87	0.40
28:B1:455:ILE:HD11	28:B1:476:VAL:HG11	2.03	0.40
30:B3:423:LYS:HA	30:B3:423:LYS:HD2	1.84	0.40
30:B3:548:LEU:HB3	30:B3:560:TRP:HB2	2.02	0.40
34:5C:199:LEU:HD22	34:5C:245:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:5F:36:TYR:HB3	37:5F:110:ARG:NH1	2.37	0.40
43:RD:1521:LEU:O	43:RD:1525:ASN:HB2	2.20	0.40
43:RD:1683:ILE:HD13	43:RD:1683:ILE:HA	1.95	0.40
49:RP:1860:ASN:HA	49:RP:1863:LEU:HB2	2.03	0.40
49:RP:1877:ARG:HA	49:RP:1880:ILE:HG22	2.04	0.40
49:RP:2062:LYS:HG3	50:RQ:267:SER:HB3	2.03	0.40
50:RQ:773:LYS:HD2	50:RQ:773:LYS:HA	1.81	0.40
52:RZ:867:PHE:HD2	52:RZ:870:PRO:HA	1.86	0.40
3:SA:1156:C:H2'	3:SA:1157:A:C8	2.56	0.40
3:SA:1695:G:H2'	3:SA:1696:G:C8	2.55	0.40
5:SF:207:LEU:HA	5:SF:207:LEU:HD12	1.85	0.40
12:SO:84:ILE:HB	12:SO:88:LEU:HD23	2.03	0.40
21:3D:57:LYS:N	21:3D:61:GLU:OE2	2.54	0.40
26:AE:14:ASN:ND2	34:5C:101:ASN:OD1	2.55	0.40
28:B1:27:LYS:HB2	28:B1:27:LYS:HE3	1.82	0.40
30:B3:694:LEU:HG	30:B3:746:TRP:HH2	1.87	0.40
31:B8:239:LYS:HD2	31:B8:281:THR:HA	2.03	0.40
32:BE:44:LEU:HD13	50:RQ:734:PRO:HA	2.04	0.40
36:5E:492:PRO:HA	36:5E:495:ILE:HG22	2.03	0.40
37:5F:88:LEU:HD23	37:5F:88:LEU:HA	1.92	0.40
40:5I:369:ASP:OD2	40:5I:373:ARG:NH2	2.44	0.40
44:RE:262:ASP:HA	44:RE:263:PRO:HD3	1.97	0.40
44:RE:348:TYR:HA	44:RE:351:LYS:HG2	2.03	0.40
44:RE:676:PRO:HB2	44:RE:678:ILE:HG22	2.03	0.40
44:RE:858:ARG:HD2	44:RE:858:ARG:HA	1.94	0.40
46:RJ:98:LEU:HD11	46:RJ:354:ILE:HD11	2.03	0.40
46:RJ:821:LYS:HE2	46:RJ:821:LYS:HB3	1.95	0.40
51:RT:119:PRO:HA	51:RT:123:HIS:HB2	2.03	0.40
52:RZ:509:LYS:HE3	52:RZ:509:LYS:HB2	1.94	0.40
52:RZ:865:PHE:HB3	52:RZ:867:PHE:CZ	2.55	0.40
1:3A:72:C:H2'	1:3A:73:A:H8	1.87	0.40
3:SA:1751:C:H2'	3:SA:1752:U:C6	2.56	0.40
20:3B:159:LEU:HG	20:3B:304:LEU:HD13	2.04	0.40
25:A5:147:GLN:O	25:A5:167:SER:OG	2.29	0.40
26:AE:4:LEU:HD13	34:5C:108:LEU:HD11	2.03	0.40
26:AE:135:LEU:HD21	26:AE:151:ILE:HD12	2.02	0.40
26:AE:385:THR:OG1	26:AE:418:CYS:SG	2.73	0.40
28:B1:164:THR:HG21	28:B1:196:GLY:HA2	2.03	0.40
32:BE:58:PHE:CE1	32:BE:72:SER:HB3	2.57	0.40
32:BE:358:PHE:HD2	32:BE:636:PRO:HD3	1.87	0.40
34:5C:108:LEU:HB2	34:5C:114:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5E:482:LEU:HG	36:5E:484:MET:H	1.87	0.40
42:5K:66:LEU:HD23	42:5K:66:LEU:HA	1.87	0.40
44:RE:686:LEU:HD12	44:RE:696:ILE:HD11	2.03	0.40
46:RJ:290:ILE:HA	46:RJ:812:MET:HA	2.04	0.40
47:RK:361:ASN:OD1	47:RK:361:ASN:N	2.54	0.40
50:RQ:824:LYS:HE3	50:RQ:824:LYS:HB3	1.93	0.40
52:RZ:1111:SER:OG	52:RZ:1114:ASN:OD1	2.39	0.40
1:3A:94:A:H61	1:3A:322:A:H61	1.70	0.40
3:SA:862:A:H5"	12:SO:16:ILE:HG21	2.04	0.40
3:SA:1470:C:H3'	3:SA:1573:A:H62	1.86	0.40
4:SC:19:ARG:NH1	30:B3:358:ASN:OD1	2.50	0.40
4:SC:138:PHE:HB2	4:SC:214:LYS:HB3	2.03	0.40
5:SF:79:ASP:HB3	5:SF:82:TYR:HB2	2.03	0.40
5:SF:212:ASP:H	5:SF:215:ASP:HA	1.86	0.40
7:SH:106:LEU:HD12	7:SH:106:LEU:HA	1.93	0.40
8:SI:46:ILE:HG22	8:SI:60:ILE:HG23	2.04	0.40
17:SZ:116:LYS:HE2	17:SZ:116:LYS:HB3	1.81	0.40
23:3F:363:ASP:HB2	23:3F:437:ARG:HH22	1.85	0.40
23:3F:369:LEU:HD23	23:3F:369:LEU:HA	1.93	0.40
26:AE:235:VAL:O	26:AE:239:LEU:HB2	2.21	0.40
29:B2:53:ASP:OD1	29:B2:53:ASP:N	2.54	0.40
29:B2:346:VAL:HB	29:B2:350:LYS:HB2	2.03	0.40
31:B8:238:LEU:HD23	31:B8:238:LEU:HA	1.94	0.40
32:BE:635:SER:HB2	32:BE:640:LEU:HB2	2.03	0.40
34:5C:178:ASP:OD1	34:5C:179:HIS:ND1	2.54	0.40
34:5C:196:LEU:HD12	34:5C:207:THR:HG23	2.02	0.40
34:5C:292:THR:HG21	34:5C:332:LEU:HD21	2.03	0.40
38:5G:149:PRO:HD2	38:5G:170:VAL:HG21	2.03	0.40
40:5I:425:LYS:HD3	40:5I:425:LYS:HA	1.87	0.40
40:5I:434:LEU:HD12	40:5I:434:LEU:HA	1.85	0.40
44:RE:166:LYS:HE3	44:RE:166:LYS:HB2	1.90	0.40
44:RE:828:ASP:OD2	44:RE:853:ARG:NH1	2.38	0.40
46:RJ:156:LEU:HA	46:RJ:156:LEU:HD23	1.79	0.40
46:RJ:852:ARG:HD2	46:RJ:888:PRO:HG3	2.04	0.40
47:RK:109:PHE:HB3	47:RK:361:ASN:HB3	2.04	0.40
47:RK:185:ARG:HA	47:RK:186:PRO:HD3	1.94	0.40
49:RP:22:ARG:O	49:RP:26:LEU:HB2	2.21	0.40
49:RP:1707:HIS:HB3	49:RP:1708:SER:H	1.78	0.40
49:RP:1877:ARG:HA	49:RP:1877:ARG:HD2	1.92	0.40
50:RQ:338:LEU:HD12	50:RQ:338:LEU:HA	1.87	0.40
52:RZ:639:LEU:HD23	52:RZ:639:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RZ:802:SER:OG	52:RZ:803:LYS:N	2.55	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	240/255 (94%)	210 (88%)	30 (12%)	0	100	100
5	SF	245/261 (94%)	198 (81%)	47 (19%)	0	100	100
6	SG	211/225 (94%)	194 (92%)	17 (8%)	0	100	100
7	SH	178/236 (75%)	159 (89%)	15 (8%)	4 (2%)	6	35
8	SI	161/190 (85%)	137 (85%)	24 (15%)	0	100	100
9	SJ	144/200 (72%)	126 (88%)	18 (12%)	0	100	100
10	SK	172/197 (87%)	154 (90%)	17 (10%)	1 (1%)	25	66
11	SM	135/156 (86%)	117 (87%)	18 (13%)	0	100	100
12	SO	132/151 (87%)	123 (93%)	9 (7%)	0	100	100
13	SP	114/137 (83%)	96 (84%)	18 (16%)	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	102/145 (70%)	88 (86%)	14 (14%)	0	100	100
17	SZ	121/135 (90%)	106 (88%)	15 (12%)	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	238/327 (73%)	215 (90%)	23 (10%)	0	100	100
20	3C	220/327 (67%)	200 (91%)	20 (9%)	0	100	100
21	3D	372/504 (74%)	342 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	3E	275/511 (54%)	262 (95%)	13 (5%)	0	100	100
23	3F	431/573 (75%)	394 (91%)	37 (9%)	0	100	100
24	3G	119/126 (94%)	114 (96%)	5 (4%)	0	100	100
24	3H	119/126 (94%)	110 (92%)	9 (8%)	0	100	100
25	A5	301/643 (47%)	269 (89%)	32 (11%)	0	100	100
26	AE	429/1769 (24%)	408 (95%)	21 (5%)	0	100	100
27	AG	46/896 (5%)	43 (94%)	3 (6%)	0	100	100
28	B1	785/900 (87%)	709 (90%)	75 (10%)	1 (0%)	51	85
29	B2	814/943 (86%)	716 (88%)	98 (12%)	0	100	100
30	B3	733/817 (90%)	585 (80%)	147 (20%)	1 (0%)	51	85
31	B8	453/594 (76%)	397 (88%)	56 (12%)	0	100	100
32	BE	886/939 (94%)	804 (91%)	81 (9%)	1 (0%)	51	85
33	B6	369/440 (84%)	341 (92%)	26 (7%)	2 (0%)	29	69
34	5C	474/554 (86%)	424 (90%)	50 (10%)	0	100	100
35	5D	66/250 (26%)	56 (85%)	10 (15%)	0	100	100
36	5E	205/593 (35%)	187 (91%)	18 (9%)	0	100	100
37	5F	180/183 (98%)	169 (94%)	11 (6%)	0	100	100
38	5G	237/290 (82%)	215 (91%)	22 (9%)	0	100	100
39	5H	72/610 (12%)	67 (93%)	5 (7%)	0	100	100
40	5I	457/489 (94%)	413 (90%)	44 (10%)	0	100	100
41	5J	130/217 (60%)	117 (90%)	13 (10%)	0	100	100
42	5K	148/189 (78%)	134 (90%)	14 (10%)	0	100	100
43	RD	310/1729 (18%)	281 (91%)	25 (8%)	4 (1%)	12	48
44	RE	1080/1237 (87%)	998 (92%)	81 (8%)	1 (0%)	51	85
45	RF	233/297 (78%)	205 (88%)	26 (11%)	2 (1%)	17	56
46	RJ	690/1183 (58%)	636 (92%)	54 (8%)	0	100	100
47	RK	358/367 (98%)	332 (93%)	26 (7%)	0	100	100
48	RN	59/810 (7%)	59 (100%)	0	0	100	100
49	RP	1948/2493 (78%)	1778 (91%)	156 (8%)	14 (1%)	22	62
50	RQ	333/899 (37%)	289 (87%)	41 (12%)	3 (1%)	17	56
51	RT	207/326 (64%)	188 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	RZ	831/1267 (66%)	737 (89%)	91 (11%)	3 (0%)	34 72
All	All	16950/27128 (62%)	15248 (90%)	1665 (10%)	37 (0%)	50 81

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	RD	1223	PRO
49	RP	707	PRO
49	RP	718	PRO
49	RP	922	MET
49	RP	923	PRO
49	RP	925	VAL
49	RP	2115	ALA
50	RQ	257	ILE
50	RQ	353	ASN
52	RZ	583	VAL
52	RZ	676	ILE
52	RZ	682	VAL
28	B1	710	ILE
45	RF	122	ASN
45	RF	172	TYR
49	RP	727	VAL
49	RP	1149	PRO
7	SH	154	ARG
7	SH	173	PRO
49	RP	616	PRO
7	SH	149	LYS
30	B3	71	PRO
33	B6	327	LEU
43	RD	1204	VAL
49	RP	76	THR
49	RP	685	LEU
10	SK	118	LEU
33	B6	328	ASP
43	RD	1222	LYS
49	RP	1088	LYS
49	RP	615	VAL
49	RP	928	ILE
32	BE	749	ALA
43	RD	1180	VAL
44	RE	1032	PRO
7	SH	153	VAL

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Mol	Chain	Res	Type
50	RQ	354	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	213/224 (95%)	210 (99%)	3 (1%)	67 80
5	SF	199/222 (90%)	197 (99%)	2 (1%)	76 86
6	SG	180/191 (94%)	178 (99%)	2 (1%)	73 84
7	SH	153/201 (76%)	151 (99%)	2 (1%)	69 82
8	SI	146/170 (86%)	144 (99%)	2 (1%)	67 80
9	SJ	122/161 (76%)	118 (97%)	4 (3%)	38 61
10	SK	150/166 (90%)	149 (99%)	1 (1%)	84 90
11	SM	124/137 (90%)	124 (100%)	0	100 100
12	SO	117/128 (91%)	117 (100%)	0	100 100
13	SP	88/105 (84%)	86 (98%)	2 (2%)	50 71
14	SR	105/119 (88%)	105 (100%)	0	100 100
15	SX	108/111 (97%)	107 (99%)	1 (1%)	78 88
16	SY	86/120 (72%)	86 (100%)	0	100 100
17	SZ	103/113 (91%)	103 (100%)	0	100 100
18	Sc	69/71 (97%)	69 (100%)	0	100 100
19	Sd	56/60 (93%)	55 (98%)	1 (2%)	59 77
20	3B	201/240 (84%)	199 (99%)	2 (1%)	76 86
20	3C	189/240 (79%)	188 (100%)	1 (0%)	88 93
21	3D	322/435 (74%)	320 (99%)	2 (1%)	86 92
22	3E	222/433 (51%)	221 (100%)	1 (0%)	88 93
23	3F	382/503 (76%)	379 (99%)	3 (1%)	81 89
24	3G	100/104 (96%)	99 (99%)	1 (1%)	76 86
24	3H	100/104 (96%)	100 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	A5	280/574 (49%)	278 (99%)	2 (1%)	84	90
26	AE	391/1633 (24%)	385 (98%)	6 (2%)	65	80
27	AG	46/826 (6%)	46 (100%)	0	100	100
28	B1	694/789 (88%)	691 (100%)	3 (0%)	91	94
29	B2	712/832 (86%)	705 (99%)	7 (1%)	76	86
30	B3	659/719 (92%)	655 (99%)	4 (1%)	86	92
31	B8	407/529 (77%)	403 (99%)	4 (1%)	76	86
32	BE	741/819 (90%)	737 (100%)	4 (0%)	88	93
33	B6	323/414 (78%)	319 (99%)	4 (1%)	71	84
34	5C	418/480 (87%)	416 (100%)	2 (0%)	88	93
35	5D	63/234 (27%)	62 (98%)	1 (2%)	62	79
36	5E	193/535 (36%)	192 (100%)	1 (0%)	88	93
37	5F	171/172 (99%)	168 (98%)	3 (2%)	59	77
38	5G	214/258 (83%)	213 (100%)	1 (0%)	88	93
39	5H	63/538 (12%)	63 (100%)	0	100	100
40	5I	416/443 (94%)	413 (99%)	3 (1%)	84	90
41	5J	124/200 (62%)	123 (99%)	1 (1%)	81	89
42	5K	133/169 (79%)	133 (100%)	0	100	100
43	RD	226/1544 (15%)	222 (98%)	4 (2%)	59	77
44	RE	994/1125 (88%)	987 (99%)	7 (1%)	84	90
45	RF	221/274 (81%)	220 (100%)	1 (0%)	88	93
46	RJ	624/1039 (60%)	612 (98%)	12 (2%)	57	75
47	RK	307/312 (98%)	304 (99%)	3 (1%)	76	86
48	RN	55/732 (8%)	55 (100%)	0	100	100
49	RP	556/2307 (24%)	550 (99%)	6 (1%)	73	84
50	RQ	206/808 (26%)	204 (99%)	2 (1%)	76	86
51	RT	178/282 (63%)	178 (100%)	0	100	100
52	RZ	717/1140 (63%)	712 (99%)	5 (1%)	84	90
All	All	13667/24085 (57%)	13551 (99%)	116 (1%)	82	89

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SC	22	ASP
4	SC	59	ASP
4	SC	162	ARG
5	SF	52	LEU
5	SF	81	THR
6	SG	54	LYS
6	SG	125	THR
7	SH	46	LYS
7	SH	214	LYS
8	SI	34	LEU
8	SI	83	LYS
9	SJ	25	ARG
9	SJ	49	ARG
9	SJ	62	THR
9	SJ	200	LYS
10	SK	17	ARG
13	SP	89	THR
13	SP	124	ASP
15	SX	79	PHE
19	Sd	38	ARG
20	3B	233	LEU
20	3B	305	THR
20	3C	297	ARG
21	3D	218	LYS
21	3D	267	ASP
22	3E	370	SER
23	3F	169	LYS
23	3F	225	LYS
23	3F	405	VAL
24	3G	30	LEU
25	A5	28	ARG
25	A5	194	LEU
26	AE	132	THR
26	AE	156	LYS
26	AE	197	ASP
26	AE	321	LYS
26	AE	374	ARG
26	AE	404	PHE
28	B1	163	THR
28	B1	192	ASP
28	B1	398	ARG
29	B2	75	ARG
29	B2	175	ASP

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Mol	Chain	Res	Type
29	B2	286	ILE
29	B2	333	ARG
29	B2	343	TRP
29	B2	447	LEU
29	B2	576	VAL
30	B3	65	THR
30	B3	466	TRP
30	B3	618	ASN
30	B3	753	HIS
31	B8	282	ASN
31	B8	384	ILE
31	B8	410	ASP
31	B8	542	ARG
32	BE	218	LEU
32	BE	484	ILE
32	BE	510	LEU
32	BE	890	LYS
33	B6	174	PHE
33	B6	299	LYS
33	B6	352	ARG
33	B6	358	LEU
34	5C	291	THR
34	5C	442	ILE
35	5D	58	ARG
36	5E	538	LYS
37	5F	5	LEU
37	5F	13	LEU
37	5F	34	ARG
38	5G	116	ARG
40	5I	83	LEU
40	5I	238	THR
40	5I	255	THR
41	5J	119	ARG
43	RD	1466	ARG
43	RD	1503	LYS
43	RD	1565	LYS
43	RD	1685	ARG
44	RE	223	ARG
44	RE	245	LYS
44	RE	288	THR
44	RE	546	THR
44	RE	781	ASP

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Mol	Chain	Res	Type
44	RE	899	LEU
44	RE	1236	THR
45	RF	158	TRP
46	RJ	92	ARG
46	RJ	113	ARG
46	RJ	114	ARG
46	RJ	214	ARG
46	RJ	230	MET
46	RJ	566	ARG
46	RJ	769	TYR
46	RJ	833	ARG
46	RJ	866	ARG
46	RJ	948	ILE
46	RJ	973	ARG
46	RJ	1033	ARG
47	RK	77	ARG
47	RK	135	TRP
47	RK	171	ASP
49	RP	36	LYS
49	RP	114	CYS
49	RP	154	CYS
49	RP	1819	PHE
49	RP	1875	LEU
49	RP	1995	ARG
50	RQ	728	ARG
50	RQ	808	PHE
52	RZ	386	LYS
52	RZ	452	ARG
52	RZ	584	ASP
52	RZ	586	ARG
52	RZ	1109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
4	SC	101	HIS
4	SC	211	HIS
5	SF	142	HIS
6	SG	95	ASN
6	SG	131	GLN
7	SH	176	GLN
7	SH	182	GLN

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Mol	Chain	Res	Type
7	SH	201	GLN
8	SI	174	ASN
8	SI	180	GLN
9	SJ	32	GLN
9	SJ	44	HIS
10	SK	112	GLN
11	SM	8	GLN
11	SM	106	ASN
14	SR	77	GLN
15	SX	39	GLN
15	SX	80	ASN
16	SY	99	ASN
17	SZ	29	HIS
17	SZ	107	GLN
18	Sc	9	HIS
18	Sc	19	HIS
20	3B	291	GLN
20	3C	91	HIS
20	3C	216	ASN
20	3C	256	ASN
20	3C	291	GLN
21	3D	24	GLN
21	3D	65	ASN
21	3D	85	ASN
21	3D	172	ASN
21	3D	213	ASN
22	3E	261	GLN
22	3E	286	ASN
23	3F	128	GLN
23	3F	181	ASN
23	3F	226	HIS
23	3F	230	ASN
23	3F	310	ASN
23	3F	321	HIS
23	3F	366	GLN
23	3F	463	GLN
23	3F	471	GLN
23	3F	547	HIS
23	3F	561	ASN
24	3G	32	GLN
24	3G	38	ASN
24	3G	75	ASN

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Mol	Chain	Res	Type
24	3H	5	ASN
24	3H	18	GLN
25	A5	27	GLN
25	A5	168	HIS
25	A5	293	ASN
25	A5	316	ASN
26	AE	14	ASN
26	AE	219	ASN
28	B1	45	ASN
28	B1	128	ASN
28	B1	421	ASN
28	B1	464	GLN
28	B1	597	ASN
28	B1	707	ASN
28	B1	734	GLN
28	B1	837	ASN
28	B1	842	ASN
29	B2	20	ASN
29	B2	264	ASN
29	B2	327	HIS
29	B2	390	GLN
29	B2	629	ASN
30	B3	210	ASN
30	B3	337	HIS
30	B3	585	ASN
30	B3	616	HIS
30	B3	667	GLN
30	B3	696	ASN
30	B3	757	GLN
30	B3	766	HIS
30	B3	767	HIS
31	B8	159	HIS
31	B8	162	ASN
31	B8	242	ASN
31	B8	282	ASN
31	B8	283	HIS
31	B8	296	GLN
31	B8	310	GLN
31	B8	352	GLN
31	B8	362	HIS
31	B8	381	ASN
31	B8	438	ASN

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Mol	Chain	Res	Type
31	B8	492	ASN
31	B8	593	HIS
32	BE	96	ASN
32	BE	192	ASN
32	BE	421	ASN
32	BE	481	ASN
32	BE	490	GLN
32	BE	532	ASN
32	BE	820	GLN
32	BE	877	ASN
32	BE	903	GLN
33	B6	10	GLN
33	B6	90	GLN
33	B6	287	ASN
33	B6	336	ASN
33	B6	383	GLN
34	5C	36	GLN
34	5C	101	ASN
34	5C	151	ASN
34	5C	162	ASN
34	5C	251	HIS
34	5C	253	ASN
34	5C	278	ASN
34	5C	394	HIS
34	5C	424	GLN
34	5C	435	ASN
36	5E	303	GLN
37	5F	8	HIS
37	5F	59	ASN
37	5F	74	HIS
38	5G	5	GLN
38	5G	181	ASN
39	5H	573	GLN
39	5H	587	GLN
40	5I	20	GLN
40	5I	23	GLN
40	5I	27	ASN
40	5I	46	ASN
40	5I	61	GLN
40	5I	109	HIS
40	5I	134	ASN
40	5I	207	ASN

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Mol	Chain	Res	Type
40	5I	228	ASN
40	5I	242	ASN
40	5I	260	GLN
40	5I	276	ASN
40	5I	293	ASN
40	5I	371	ASN
40	5I	466	HIS
41	5J	118	GLN
41	5J	135	HIS
41	5J	184	ASN
41	5J	195	GLN
42	5K	46	GLN
42	5K	138	ASN
43	RD	1485	GLN
43	RD	1515	ASN
43	RD	1525	ASN
44	RE	261	ASN
44	RE	333	ASN
44	RE	407	ASN
44	RE	414	HIS
44	RE	443	HIS
44	RE	582	GLN
44	RE	588	GLN
44	RE	647	ASN
44	RE	811	GLN
44	RE	1073	ASN
44	RE	1078	HIS
44	RE	1203	ASN
44	RE	1228	ASN
45	RF	57	ASN
45	RF	122	ASN
45	RF	136	ASN
45	RF	148	HIS
45	RF	187	HIS
46	RJ	222	ASN
46	RJ	254	HIS
46	RJ	314	GLN
46	RJ	1037	GLN
47	RK	317	GLN
48	RN	783	HIS
49	RP	33	ASN
49	RP	112	GLN

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Mol	Chain	Res	Type
49	RP	1787	ASN
49	RP	1865	ASN
49	RP	1957	GLN
50	RQ	303	GLN
50	RQ	876	GLN
51	RT	127	GLN
51	RT	142	ASN
52	RZ	385	GLN
52	RZ	794	GLN
52	RZ	884	GLN
52	RZ	1114	ASN
52	RZ	1232	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	161/333 (48%)	69 (42%)	4 (2%)
2	5A	40/700 (5%)	13 (32%)	0
3	SA	1170/1812 (64%)	440 (37%)	18 (1%)
All	All	1371/2845 (48%)	522 (38%)	22 (1%)

All (522) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	3	C
1	3A	4	G
1	3A	23	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	36	C
1	3A	38	U
1	3A	46	U
1	3A	48	A
1	3A	49	C
1	3A	51	C

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Mol	Chain	Res	Type
1	3A	52	U
1	3A	53	U
1	3A	72	C
1	3A	80	U
1	3A	81	U
1	3A	82	G
1	3A	87	G
1	3A	90	C
1	3A	91	C
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	111	G
1	3A	115	G
1	3A	116	A
1	3A	118	A
1	3A	199	G
1	3A	203	U
1	3A	206	C
1	3A	207	A
1	3A	243	U
1	3A	244	U
1	3A	245	U
1	3A	246	A
1	3A	247	U
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	254	A
1	3A	256	G
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	305	G
1	3A	307	G

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Mol	Chain	Res	Type
1	3A	309	G
1	3A	310	G
1	3A	311	G
1	3A	312	U
1	3A	314	C
1	3A	319	G
1	3A	322	A
1	3A	324	U
1	3A	325	C
1	3A	329	C
2	5A	468	A
2	5A	470	U
2	5A	471	C
2	5A	481	U
2	5A	482	A
2	5A	483	U
2	5A	495	G
2	5A	497	A
2	5A	534	A
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	544	C
3	SA	-5	G
3	SA	-4	A
3	SA	-3	U
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	5	U
3	SA	6	G
3	SA	17	C
3	SA	18	C
3	SA	20	G
3	SA	21	U
3	SA	22	A
3	SA	23	G
3	SA	25	C
3	SA	26	A
3	SA	34	G
3	SA	40	A
3	SA	42	G

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Mol	Chain	Res	Type
3	SA	43	A
3	SA	44	U
3	SA	45	U
3	SA	46	A
3	SA	47	A
3	SA	57	G
3	SA	60	U
3	SA	66	U
3	SA	68	A
3	SA	69	G
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	76	A
3	SA	81	G
3	SA	104	A
3	SA	107	C
3	SA	108	A
3	SA	109	G
3	SA	114	C
3	SA	115	G
3	SA	116	U
3	SA	117	U
3	SA	125	U
3	SA	126	A
3	SA	127	G
3	SA	128	U
3	SA	129	U
3	SA	130	C
3	SA	131	C
3	SA	132	U
3	SA	133	U
3	SA	134	U
3	SA	135	A
3	SA	136	C
3	SA	137	U
3	SA	138	A
3	SA	140	A
3	SA	145	A
3	SA	146	U
3	SA	153	G
3	SA	155	U

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Mol	Chain	Res	Type
3	SA	156	A
3	SA	162	A
3	SA	169	A
3	SA	170	U
3	SA	176	C
3	SA	177	U
3	SA	178	U
3	SA	179	A
3	SA	180	A
3	SA	181	A
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	200	A
3	SA	202	A
3	SA	203	U
3	SA	204	G
3	SA	211	U
3	SA	215	A
3	SA	231	U
3	SA	232	U
3	SA	233	C
3	SA	234	G
3	SA	235	G
3	SA	238	U
3	SA	239	C
3	SA	240	U
3	SA	241	U
3	SA	242	U
3	SA	248	U
3	SA	249	U
3	SA	250	C
3	SA	256	A
3	SA	259	U

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Mol	Chain	Res	Type
3	SA	260	U
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	267	U
3	SA	271	A
3	SA	272	U
3	SA	276	C
3	SA	278	U
3	SA	279	G
3	SA	280	U
3	SA	281	G
3	SA	288	A
3	SA	302	U
3	SA	306	U
3	SA	313	U
3	SA	314	C
3	SA	316	A
3	SA	320	U
3	SA	321	C
3	SA	322	G
3	SA	323	A
3	SA	331	A
3	SA	332	U
3	SA	333	A
3	SA	336	G
3	SA	337	G
3	SA	351	C
3	SA	352	A
3	SA	354	C
3	SA	426	G
3	SA	430	G
3	SA	433	C
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	452	A

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Mol	Chain	Res	Type
3	SA	453	U
3	SA	454	U
3	SA	468	A
3	SA	471	A
3	SA	475	A
3	SA	477	A
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	496	G
3	SA	499	U
3	SA	500	C
3	SA	501	U
3	SA	504	U
3	SA	505	A
3	SA	507	U
3	SA	508	U
3	SA	510	G
3	SA	513	U
3	SA	514	G
3	SA	515	A
3	SA	516	G
3	SA	519	C
3	SA	525	A
3	SA	532	U
3	SA	534	A
3	SA	539	G
3	SA	540	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	544	A
3	SA	545	A
3	SA	548	G
3	SA	551	G
3	SA	552	G
3	SA	563	U

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Mol	Chain	Res	Type
3	SA	564	G
3	SA	565	C
3	SA	570	A
3	SA	572	C
3	SA	573	C
3	SA	574	G
3	SA	575	C
3	SA	579	A
3	SA	580	A
3	SA	582	U
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	601	A
3	SA	602	U
3	SA	603	U
3	SA	623	A
3	SA	624	G
3	SA	635	A
3	SA	638	U
3	SA	648	G
3	SA	649	U
3	SA	658	C
3	SA	667	U
3	SA	670	U
3	SA	674	C
3	SA	686	C
3	SA	687	G
3	SA	690	G
3	SA	694	U
3	SA	695	U
3	SA	696	C
3	SA	697	C
3	SA	698	U
3	SA	699	U
3	SA	700	C
3	SA	702	G
3	SA	744	U
3	SA	746	A

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Mol	Chain	Res	Type
3	SA	747	C
3	SA	748	U
3	SA	749	U
3	SA	750	U
3	SA	751	G
3	SA	752	A
3	SA	754	A
3	SA	755	A
3	SA	756	A
3	SA	757	A
3	SA	758	U
3	SA	759	U
3	SA	760	A
3	SA	763	G
3	SA	765	G
3	SA	766	U
3	SA	771	A
3	SA	772	G
3	SA	773	C
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	787	G
3	SA	789	A
3	SA	790	U
3	SA	791	A
3	SA	792	U
3	SA	794	U
3	SA	795	U
3	SA	796	A
3	SA	797	G
3	SA	798	C
3	SA	802	G
3	SA	803	A
3	SA	804	A

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Mol	Chain	Res	Type
3	SA	811	A
3	SA	812	A
3	SA	813	U
3	SA	815	G
3	SA	816	G
3	SA	820	U
3	SA	821	U
3	SA	822	U
3	SA	827	C
3	SA	828	U
3	SA	842	C
3	SA	850	A
3	SA	858	G
3	SA	859	A
3	SA	860	U
3	SA	862	A
3	SA	863	A
3	SA	864	U
3	SA	865	A
3	SA	873	U
3	SA	875	G
3	SA	876	G
3	SA	881	A
3	SA	898	A
3	SA	906	A
3	SA	912	U
3	SA	913	G
3	SA	914	G
3	SA	921	U
3	SA	928	U
3	SA	929	A
3	SA	931	C
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	1039	A
3	SA	1052	U
3	SA	1053	G

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Mol	Chain	Res	Type
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	1114	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A
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	1136	U
3	SA	1140	G
3	SA	1144	U
3	SA	1145	U
3	SA	1146	G
3	SA	1158	C
3	SA	1164	G
3	SA	1176	G
3	SA	1178	G
3	SA	1470	C
3	SA	1471	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1476	C
3	SA	1483	A
3	SA	1525	A
3	SA	1534	G
3	SA	1535	U
3	SA	1537	C
3	SA	1538	U
3	SA	1539	G

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Mol	Chain	Res	Type
3	SA	1540	G
3	SA	1573	A
3	SA	1574	G
3	SA	1577	A
3	SA	1584	G
3	SA	1590	G
3	SA	1595	U
3	SA	1596	C
3	SA	1600	A
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
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	1633	A
3	SA	1639	C
3	SA	1640	C
3	SA	1651	A
3	SA	1654	G
3	SA	1655	A
3	SA	1656	U
3	SA	1657	U
3	SA	1658	G
3	SA	1662	G
3	SA	1663	G
3	SA	1676	U
3	SA	1679	G
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1689	A
3	SA	1697	G
3	SA	1698	G
3	SA	1700	C
3	SA	1701	A
3	SA	1703	C

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Mol	Chain	Res	Type
3	SA	1704	U
3	SA	1707	A
3	SA	1708	U
3	SA	1709	C
3	SA	1710	U
3	SA	1711	C
3	SA	1712	A
3	SA	1713	G
3	SA	1717	G
3	SA	1718	G
3	SA	1719	A
3	SA	1724	U
3	SA	1725	U
3	SA	1726	G
3	SA	1727	G
3	SA	1728	A
3	SA	1731	A
3	SA	1734	U
3	SA	1736	G
3	SA	1737	G
3	SA	1738	U
3	SA	1742	U
3	SA	1743	U
3	SA	1744	A
3	SA	1746	A
3	SA	1749	A
3	SA	1753	A
3	SA	1754	A
3	SA	1755	A
3	SA	1778	G
3	SA	1790	A
3	SA	1791	A
3	SA	1792	G
3	SA	1793	G
3	SA	1794	A
3	SA	1795	U
3	SA	1796	C
3	SA	1799	U
3	SA	1800	A
3	SA	1801	A
3	SA	1802	A
3	SA	1803	G

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Mol	Chain	Res	Type
3	SA	1804	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	24	U
1	3A	102	U
1	3A	107	C
1	3A	248	G
3	SA	0	U
3	SA	68	A
3	SA	136	C
3	SA	139	C
3	SA	278	U
3	SA	280	U
3	SA	335	U
3	SA	484	C
3	SA	503	G
3	SA	542	A
3	SA	773	C
3	SA	781	U
3	SA	1052	U
3	SA	1063	U
3	SA	1533	C
3	SA	1594	G
3	SA	1754	A
3	SA	1803	G

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	GTP	RJ	1201	56	26,34,34	1.20	1 (3%)	32,54,54	1.70	7 (21%)
57	ADP	RZ	1301	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)

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
55	GTP	RJ	1201	56	-	5/18/38/38	0/3/3/3
57	ADP	RZ	1301	-	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	RJ	1201	GTP	C5-C6	-4.23	1.38	1.47
57	RZ	1301	ADP	C5-C4	2.45	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	RJ	1201	GTP	PA-O3A-PB	-4.49	117.41	132.83
55	RJ	1201	GTP	PB-O3B-PG	-4.12	118.69	132.83
57	RZ	1301	ADP	N3-C2-N1	-3.40	123.36	128.68
55	RJ	1201	GTP	C5-C6-N1	3.36	119.88	113.95
55	RJ	1201	GTP	C8-N7-C5	3.10	108.89	102.99
57	RZ	1301	ADP	C3'-C2'-C1'	3.02	105.52	100.98
55	RJ	1201	GTP	C2-N1-C6	-2.97	119.63	125.10
57	RZ	1301	ADP	C4-C5-N7	-2.93	106.35	109.40
55	RJ	1201	GTP	C3'-C2'-C1'	2.75	105.12	100.98
57	RZ	1301	ADP	PA-O3A-PB	-2.26	125.06	132.83
55	RJ	1201	GTP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	RZ	1301	ADP	C5'-O5'-PA-O2A
57	RZ	1301	ADP	C5'-O5'-PA-O3A
55	RJ	1201	GTP	O4'-C4'-C5'-O5'
55	RJ	1201	GTP	C3'-C4'-C5'-O5'
55	RJ	1201	GTP	PA-O3A-PB-O2B
57	RZ	1301	ADP	O4'-C4'-C5'-O5'
55	RJ	1201	GTP	PG-O3B-PB-O2B
57	RZ	1301	ADP	C3'-C4'-C5'-O5'
55	RJ	1201	GTP	C5'-O5'-PA-O1A

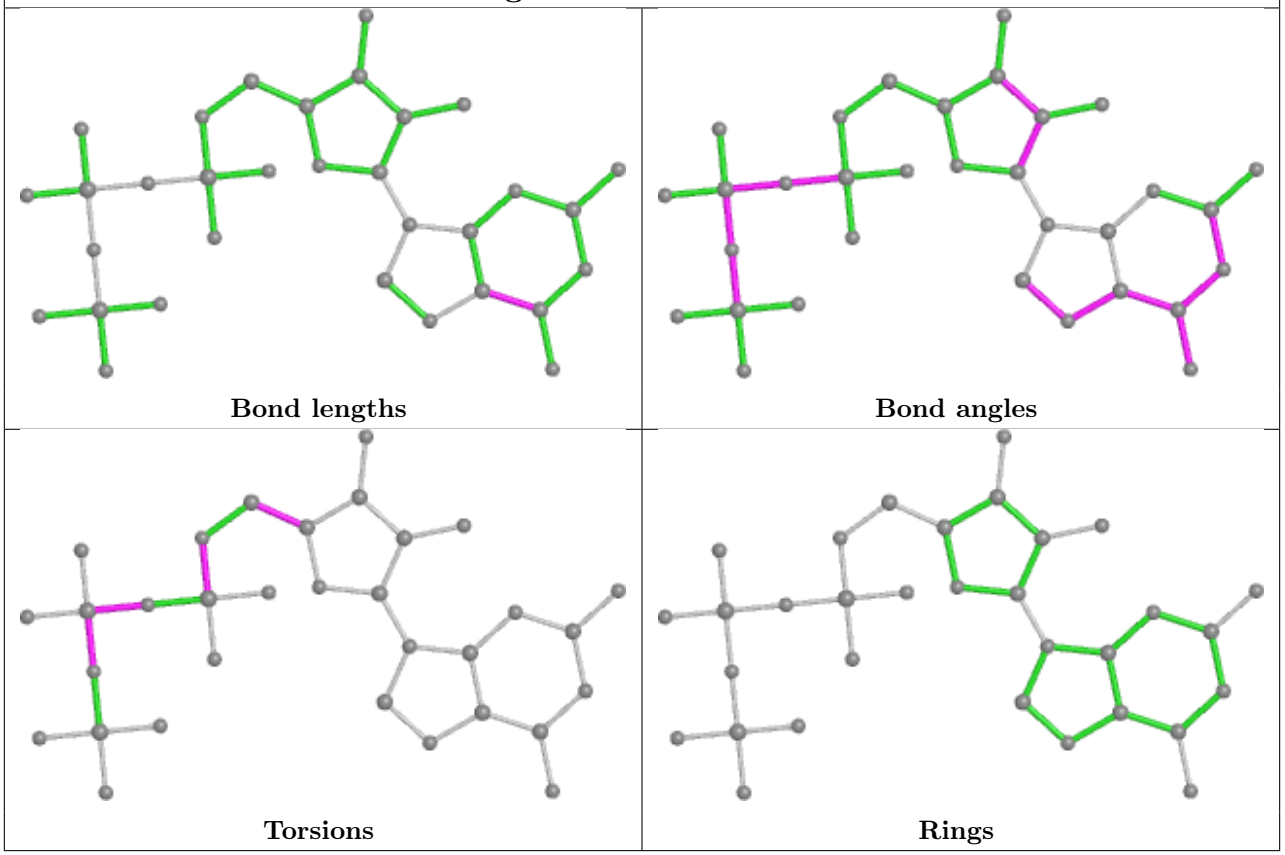
There are no ring outliers.

1 monomer is involved in 1 short contact:

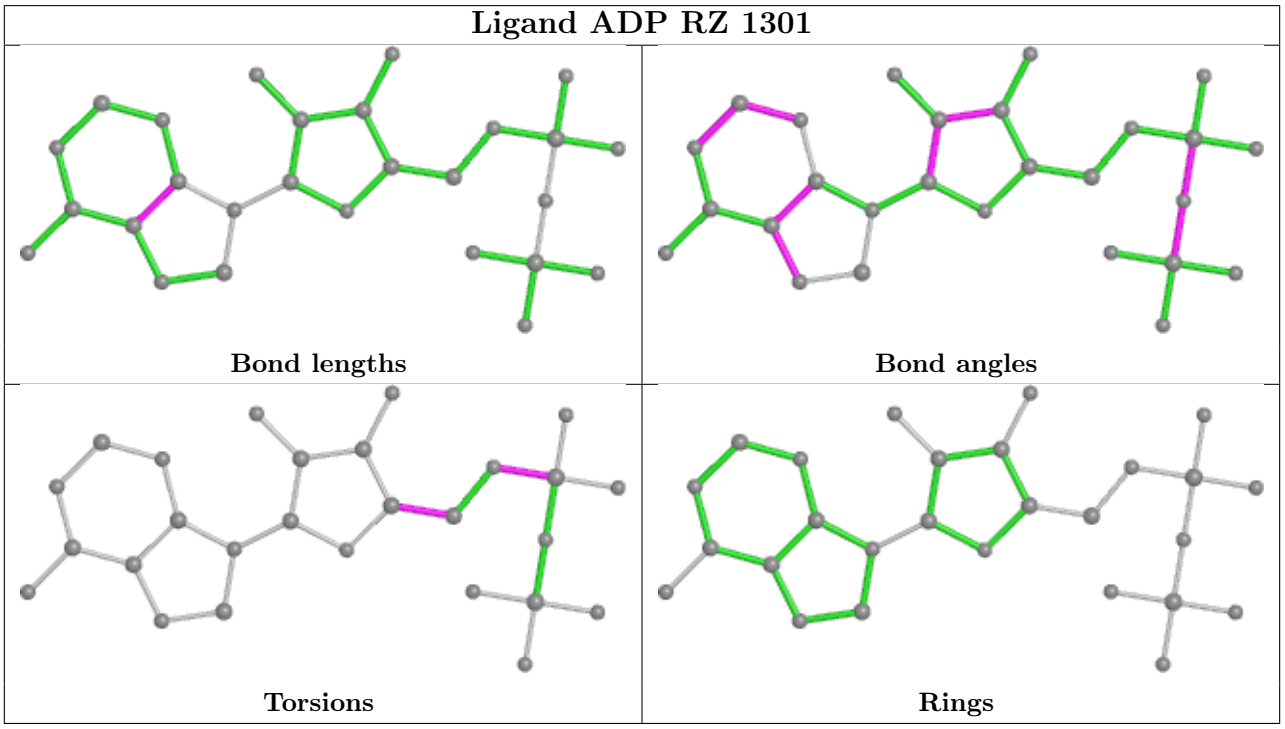
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	RZ	1301	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GTP RJ 1201



Ligand ADP RZ 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

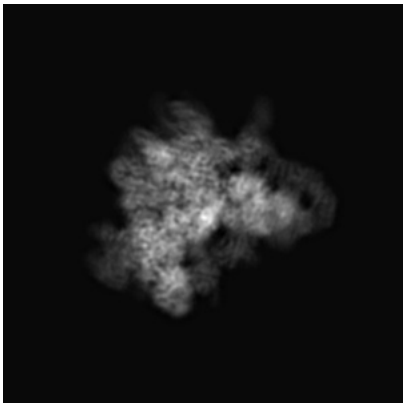
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30585. These allow visual inspection of the internal detail of the map and identification of artifacts.

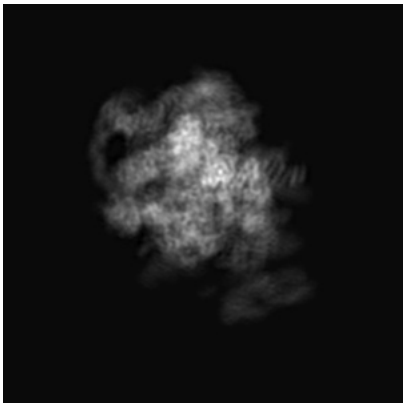
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

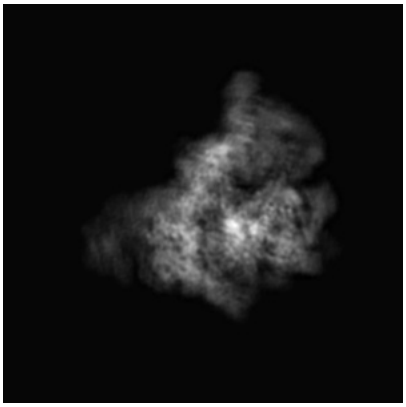
6.1.1 Primary map



X



Y

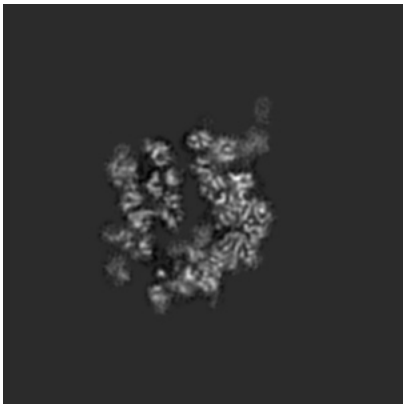


Z

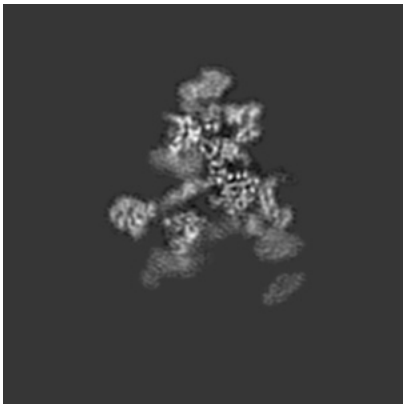
The images above show the map projected in three orthogonal directions.

6.2 Central slices

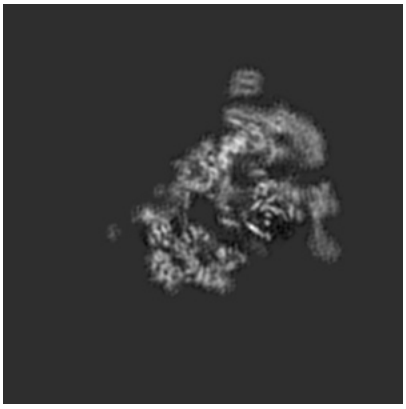
6.2.1 Primary map



X Index: 200



Y Index: 200

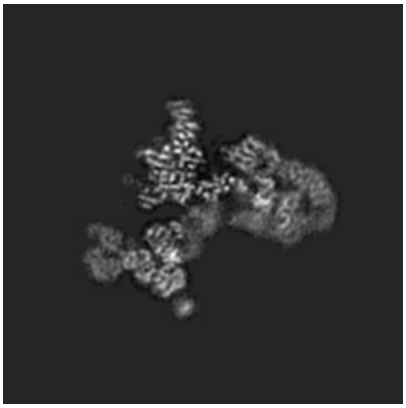


Z Index: 200

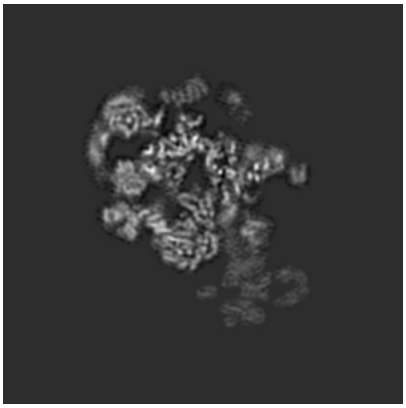
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

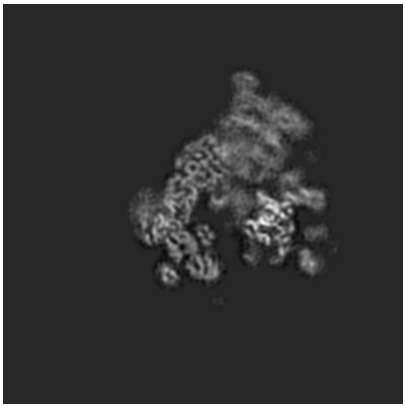
6.3.1 Primary map



X Index: 233



Y Index: 170

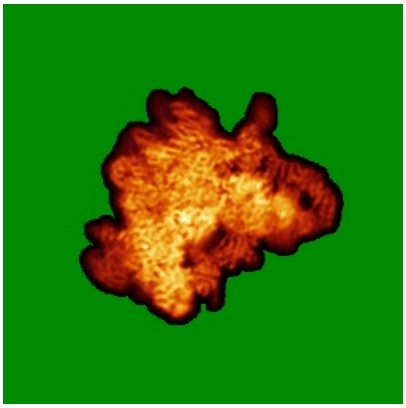


Z Index: 186

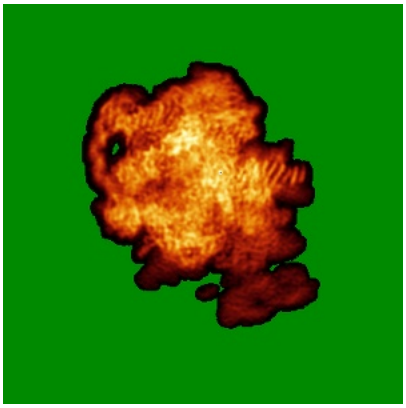
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

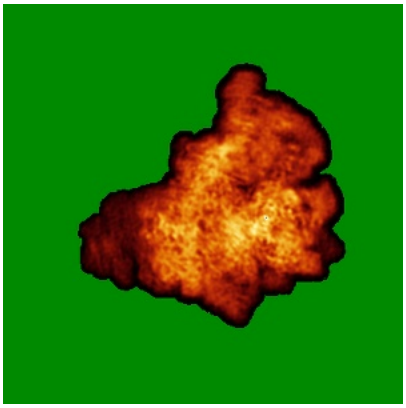
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

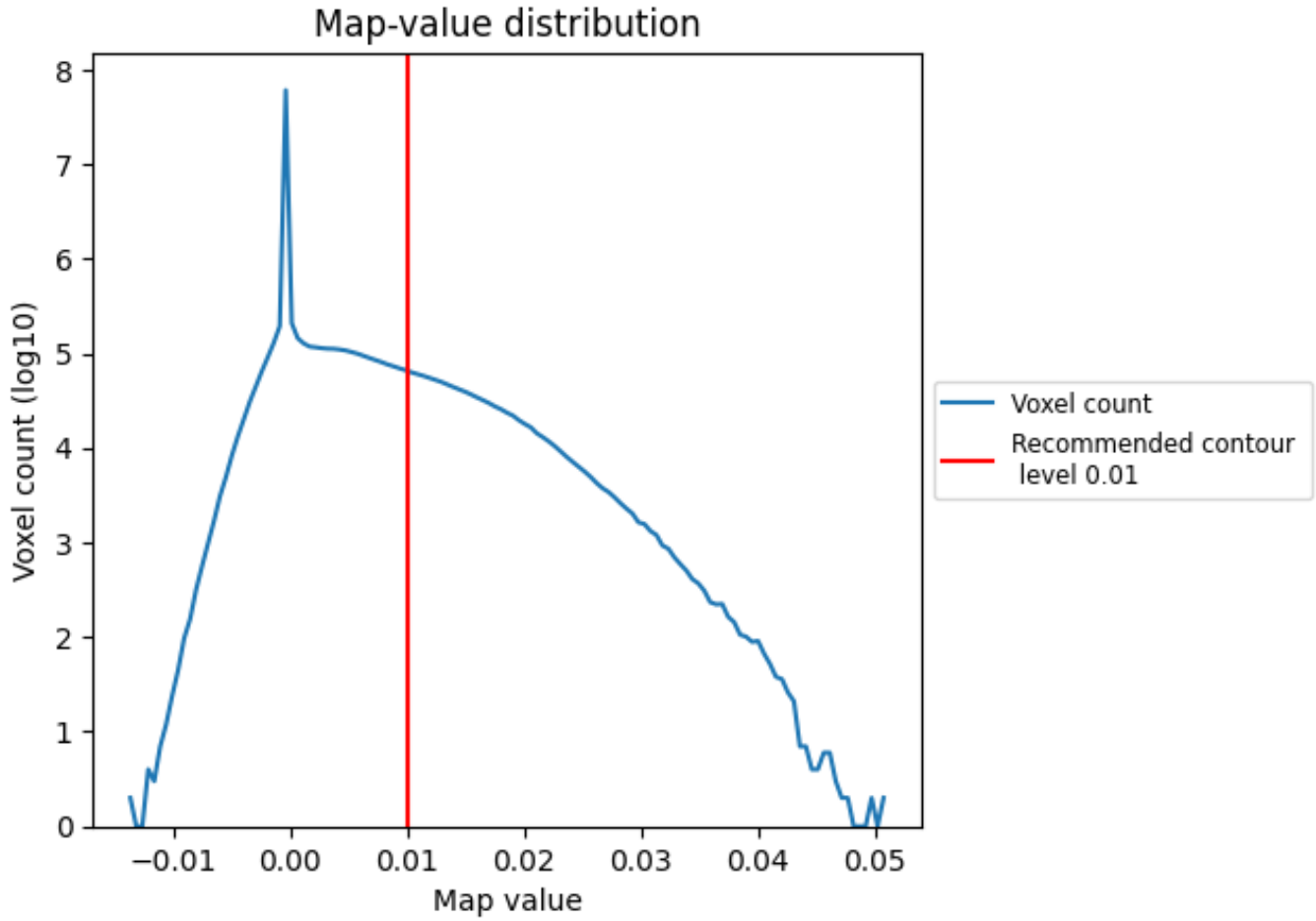
6.6 Mask visualisation (i)

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

7 Map analysis

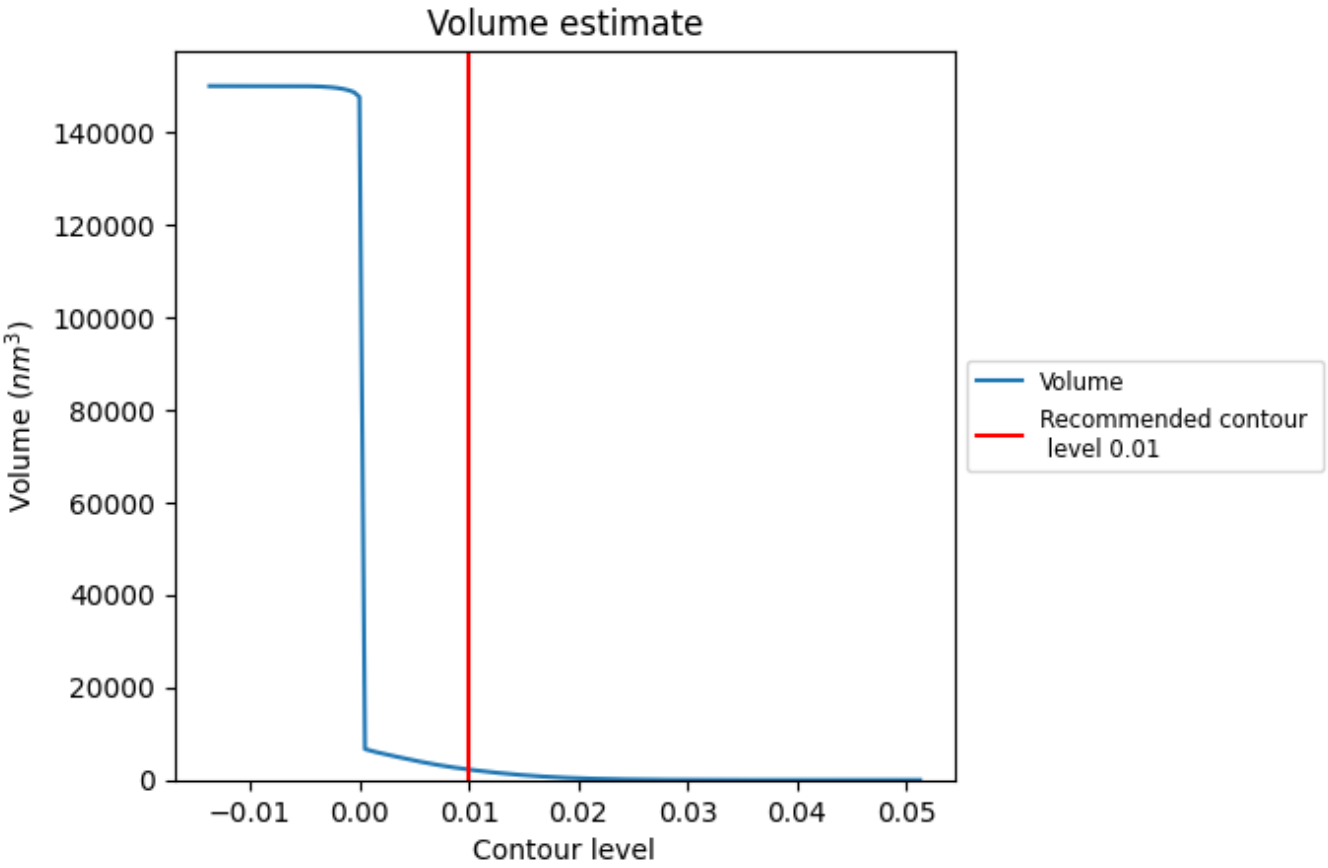
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

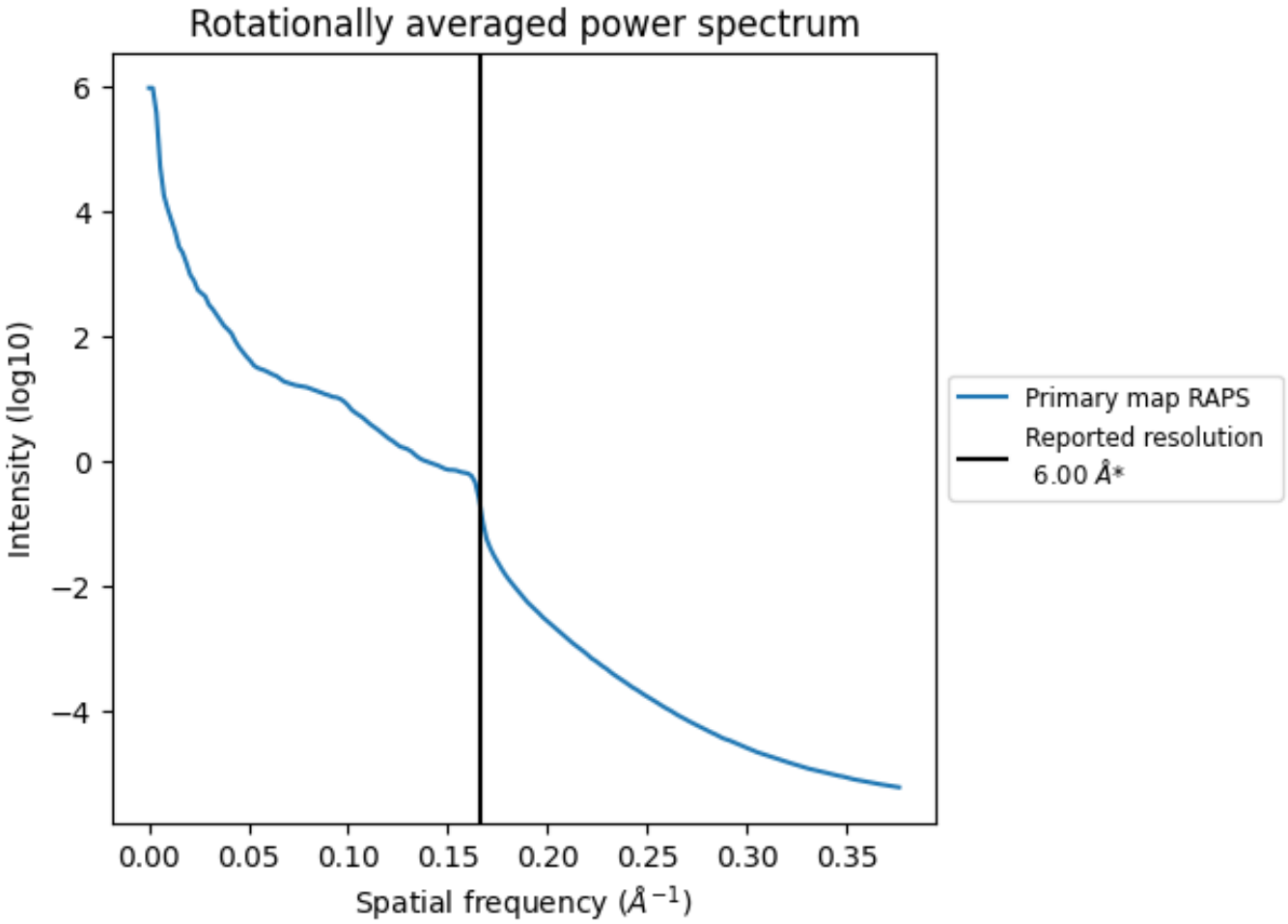
7.2 Volume estimate



The volume at the recommended contour level is 2254 nm^3; this corresponds to an approximate mass of 2036 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 0.167 Å^{-1}

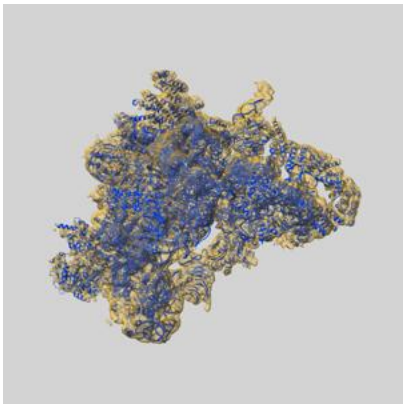
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

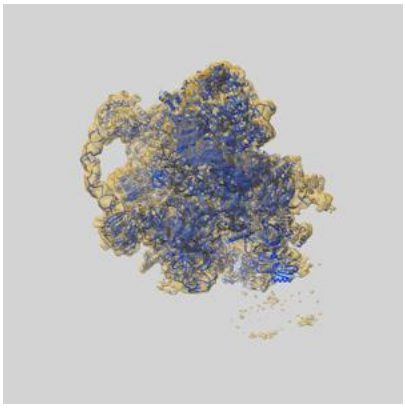
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30585 and PDB model 7D5T. Per-residue inclusion information can be found in section 3 on page 15.

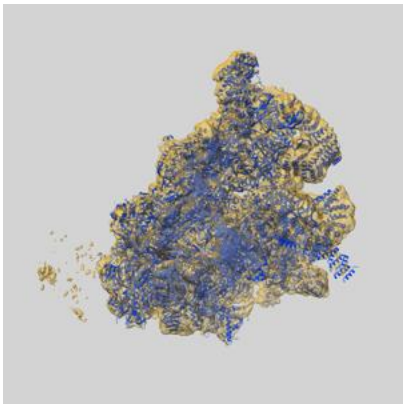
9.1 Map-model overlay



X



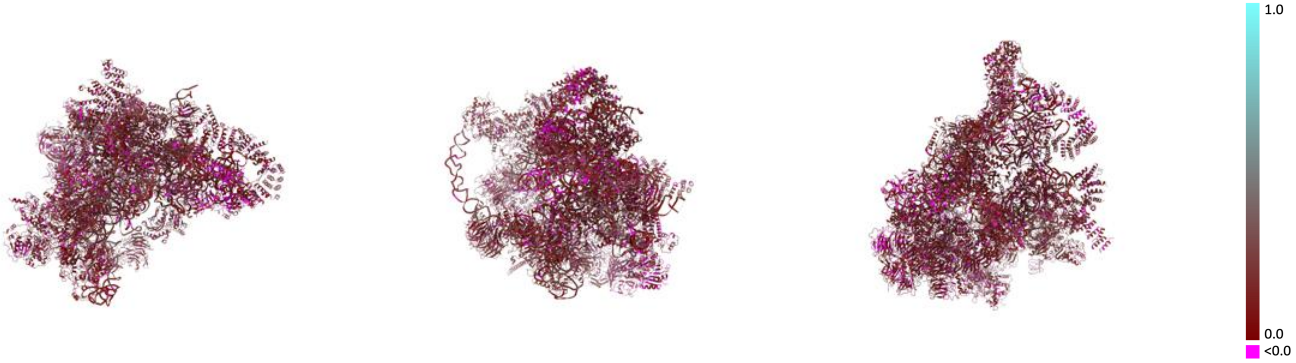
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

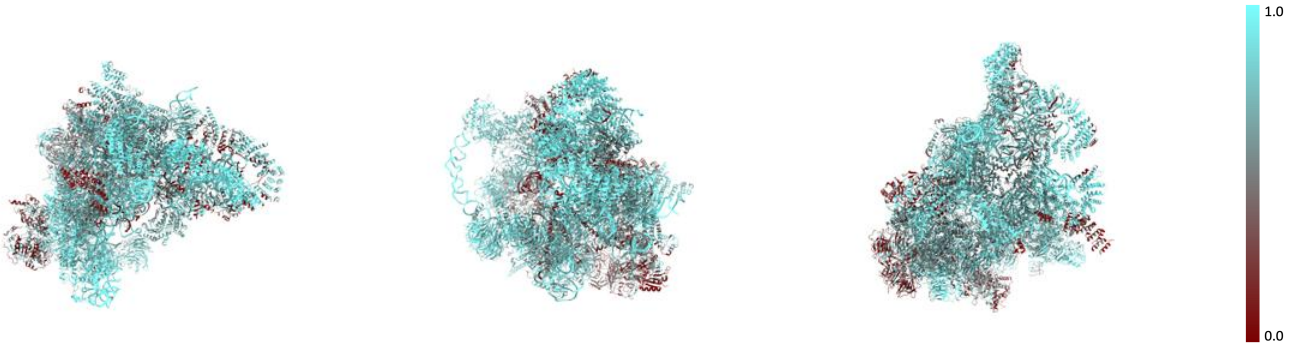
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

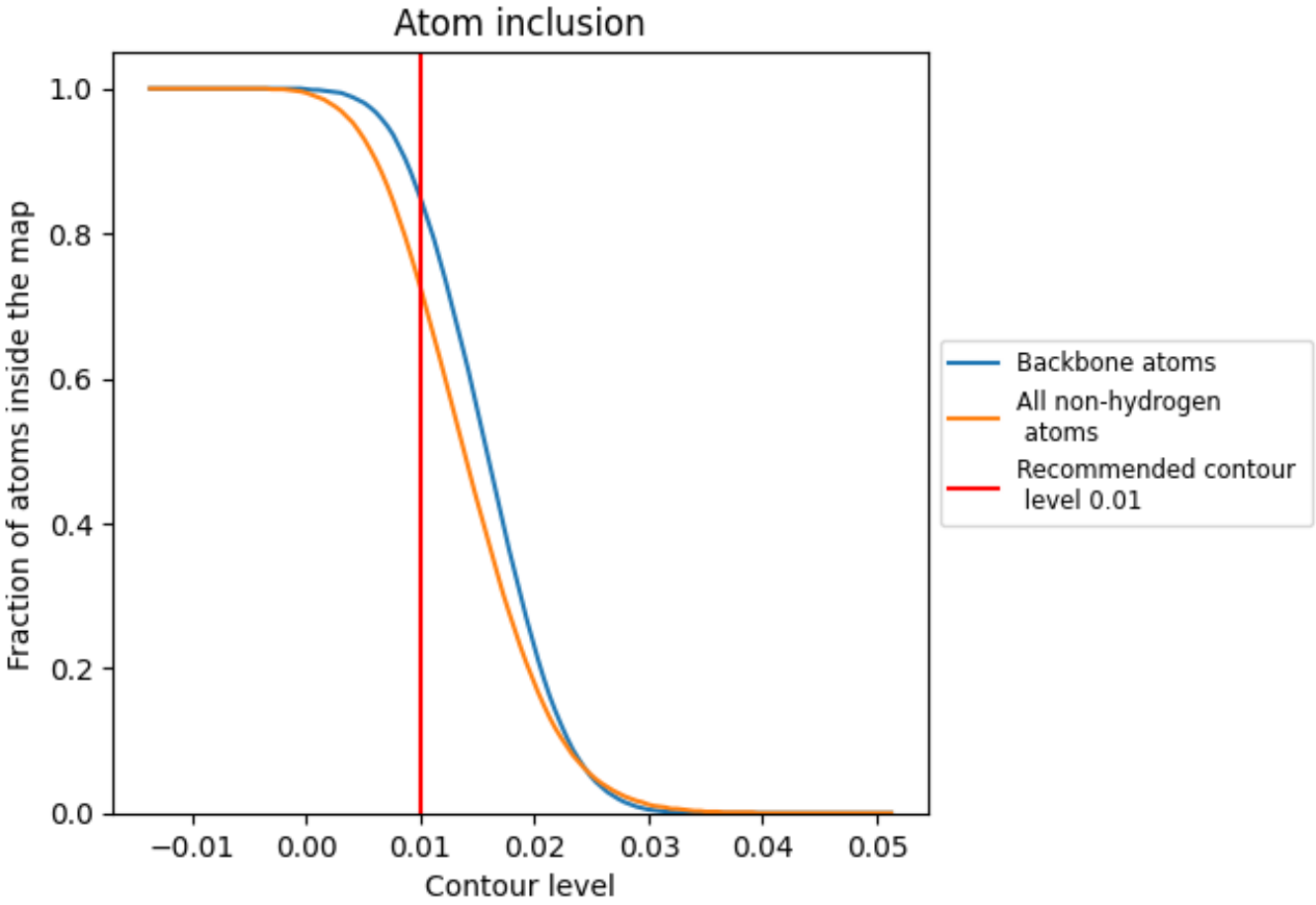
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.1560
3A	0.7930	0.1610
3B	0.6770	0.1630
3C	0.2000	0.0500
3D	0.7370	0.1490
3E	0.6750	0.1330
3F	0.7960	0.1600
3G	0.4540	0.0900
3H	0.6880	0.1680
5A	0.7340	0.1360
5C	0.6900	0.1380
5D	0.3410	0.1110
5E	0.6460	0.1620
5F	0.5990	0.1360
5G	0.5880	0.1350
5H	0.7530	0.1780
5I	0.7610	0.1590
5J	0.4380	0.1360
5K	0.6790	0.1710
A5	0.2450	0.1490
AE	0.5750	0.1560
AG	0.4540	0.1530
B1	0.7400	0.1430
B2	0.8700	0.1600
B3	0.8760	0.1580
B6	0.8120	0.1460
B8	0.4320	0.1260
BE	0.7600	0.1520
RD	0.2370	0.1250
RE	0.8600	0.1660
RF	0.8400	0.1640
RJ	0.7390	0.1570
RK	0.7040	0.1640
RN	0.2980	0.1270
RP	0.8010	0.1550

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Chain	Atom inclusion	Q-score
RQ	0.6120	0.1680
RT	0.6770	0.1700
RZ	0.4480	0.1420
SA	0.8900	0.1880
SC	0.7740	0.1630
SF	0.7130	0.1400
SG	0.7580	0.1730
SH	0.5270	0.0990
SI	0.7200	0.1450
SJ	0.6040	0.0750
SK	0.7280	0.1590
SM	0.3400	0.0870
SO	0.8440	0.1660
SP	0.8360	0.1690
SR	0.7740	0.1600
SX	0.6710	0.1500
SY	0.6180	0.1690
SZ	0.8560	0.1480
Sc	0.7980	0.1870
Sd	0.8110	0.1780
X1	0.4580	0.1770