



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 03:42 pm BST

PDB ID : 6GAW / pdb_00006gaw
EMDB ID : EMD-4368
Title : Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the complete 55S ribosome.
Authors : Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2018-04-13
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

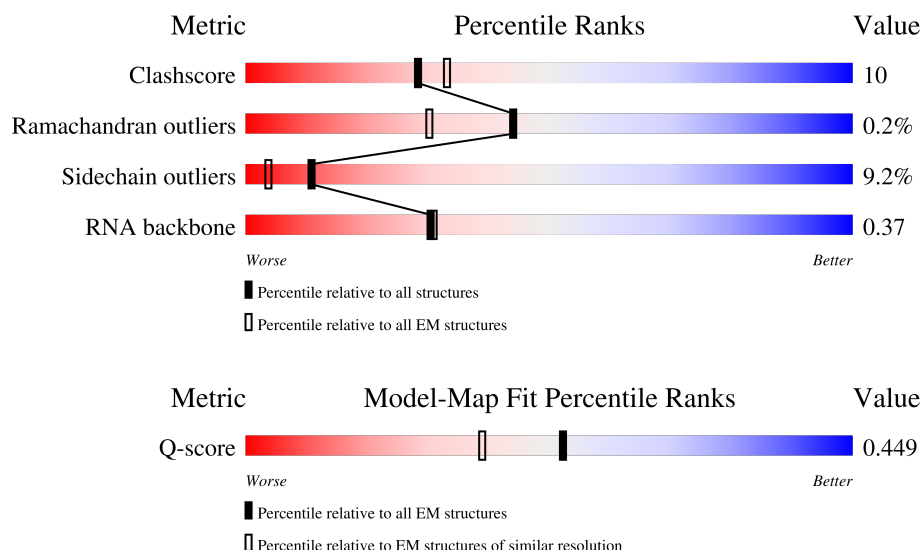
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	BL	198	35% 30% 5% • 65%
1	CL	198	21% 14% 8% • 77%
1	DL	198	14% 8% 5% • 86%

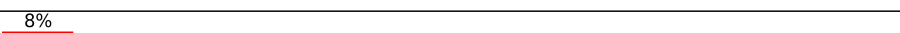
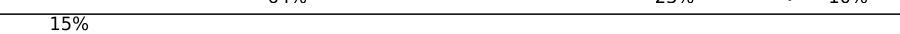
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Mol	Chain	Length	Quality of chain
1	EL	198	
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	
3	B1	256	
4	B2	252	
5	B3	161	
6	B4	126	
7	B5	188	
8	B6	65	
9	B7	95	
10	B8	188	
11	B9	100	
12	BA	1571	
13	BB	73	
14	BC	650	
15	BD	306	
16	BE	348	
17	BF	294	
18	BI	268	
19	BJ	262	
20	BK	192	
21	BN	178	
22	BO	145	

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Mol	Chain	Length	Quality of chain
23	BP	296	
24	BQ	251	
25	BR	169	
26	BS	180	
27	BT	292	
28	BU	149	
29	BV	209	
30	BW	210	
31	BX	150	
32	BY	216	
33	Ba	423	
34	Bb	380	
35	Bc	334	
36	Bd	206	
37	Be	135	
38	Bf	142	
39	Bg	159	
40	Bh	332	
41	Bi	306	
42	Bj	279	
43	Bk	212	
44	Bl	166	
45	Bm	159	
46	Bn	128	
47	Bo	124	

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Mol	Chain	Length	Quality of chain
48	Bp	112	
49	Bq	138	
50	Bt	102	
51	Bu	205	
52	Bv	222	
53	Bw	433	
54	Bx	196	
55	Bz	82	
56	AA	962	
57	AB	289	
58	AC	167	
59	AE	430	
60	AF	124	
61	AG	242	
62	AI	397	
63	AJ	201	
64	AK	196	
65	AL	139	
66	AN	128	
67	AO	239	
68	AP	135	
69	AQ	130	
70	AR	143	
71	AU	87	
72	AV	71	

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Mol	Chain	Length	Quality of chain
73	AX	201	
74	AZ	18	
75	Aa	382	
76	Ab	190	
77	Ac	173	
78	Ad	205	
79	Ae	455	
80	Af	188	
81	Ag	397	
82	Ah	387	
83	Ai	106	
84	Aj	218	
85	Ak	325	
86	Am	118	
87	An	199	
88	Ao	692	
89	Ap	258	

2 Entry composition [i](#)

There are 98 unique types of molecules in this entry. The entry contains 178372 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 protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	CL	45	Total	C	N	O	0	0
			317	203	52	62		
1	DL	27	Total	C	N	O	0	0
			213	137	33	43		
1	EL	28	Total	C	N	O	0	0
			222	143	35	44		
1	FL	27	Total	C	N	O	0	0
			213	137	33	43		
1	GL	27	Total	C	N	O	0	0
			213	137	33	43		
1	HL	26	Total	C	N	O	0	0
			205	131	32	42		
1	BL	70	Total	C	N	O	0	0
			537	346	93	98		

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B0	110	Total	C	N	O	S	0	0
			857	553	156	145	3		

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 5 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 6 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 7 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 8 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 11 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 12 is a RNA chain called 16S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BA	1549	Total	C	N	O	P	0	0
			32950	14798	5993	10610	1549		

- Molecule 13 is a RNA chain called tRNA-Phe, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BB	67	Total	C	N	O	P	0	0
			1427	640	261	459	67		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	71	C	-	insertion	GB 76262549
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 14 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BC	571	Total	C	N	O	S	0	0
			4364	2743	765	839	17		

- Molecule 15 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 16 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 17 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	BI	98	Total	C	N	O		
			805	509	155	141	0	0

- Molecule 19 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BJ	212	Total	C	N	O	S		
			1705	1100	306	290	9	0	0

- Molecule 20 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BK	176	Total	C	N	O	S		
			1303	830	236	235	2	0	0

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BN	177	Total	C	N	O	S		
			1444	926	258	253	7	0	0

- Molecule 22 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BO	115	Total	C	N	O	S		
			896	562	176	154	4	0	0

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BP	288	Total	C	N	O	S		
			2312	1473	430	403	6	0	0

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BQ	222	Total	C	N	O	S		
			1803	1156	331	306	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 26 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 27 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	240	Total	C	N	O	S	0	0
			1954	1253	338	354	9		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 29 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 30 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 31 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BY	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 33 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 36 is a protein called 39S ribosomal protein L40, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Be	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 38 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 39 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 40 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 41 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bi	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L48.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 44 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 45 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 46 is a protein called Mitochondrial ribosomal protein L51.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 47 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bo	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 48 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 49 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bq	68	Total	C	N	O	S	0	0
			542	344	102	95	1		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 51 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 52 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 53 is a protein called mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 54 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 55 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Bz	82	Total	C	N	O	0	0
			410	246	82	82		

- Molecule 56 is a RNA chain called 12S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 57 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 58 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 59 is a protein called Mitochondrial ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 60 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AF	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 61 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 62 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AI	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 63 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AJ	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 64 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 65 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 66 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 67 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 68 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 69 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AQ	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 70 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 71 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 72 is a RNA chain called P-site fMet-tRNA^{Met}, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1390216722
AV	70	C	-	insertion	GB 1390216722
AV	71	A	-	insertion	GB 1390216722

- Molecule 73 is a RNA chain called MT-CO3 mRNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AX	17	Total	C	N	O	P	0	0
			354	161	65	112	16		

- Molecule 74 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 75 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 76 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 77 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 78 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 79 is a protein called mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ae	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 80 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 81 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ag	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

- Molecule 82 is a protein called mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

- Molecule 83 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 84 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 85 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 86 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 87 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 88 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ao	572	Total	C	N	O	S	0	0
			4526	2898	770	834	24		

- Molecule 89 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	B3	1	Total	Mg	0
			1	1	
90	BA	202	Total	Mg	0
			202	202	
90	BB	1	Total	Mg	0
			1	1	
90	BC	2	Total	Mg	0
			2	2	
90	BD	3	Total	Mg	0
			3	3	

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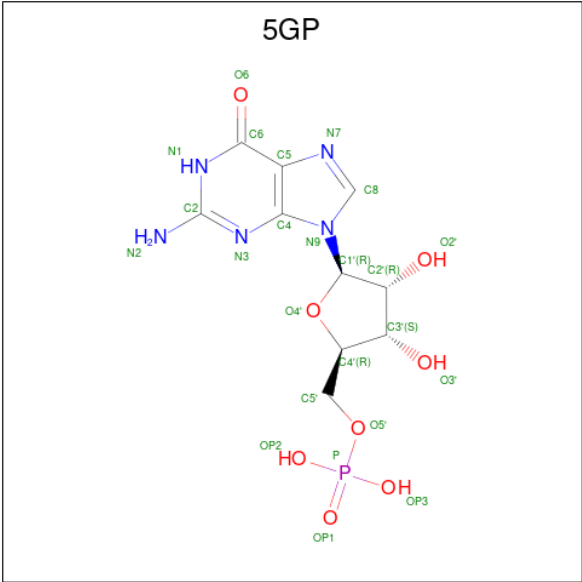
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Mol	Chain	Residues	Atoms		AltConf
90	BE	1	Total 1	Mg 1	0
90	BJ	1	Total 1	Mg 1	0
90	BP	2	Total 2	Mg 2	0
90	Be	1	Total 1	Mg 1	0
90	Bl	1	Total 1	Mg 1	0
90	Bt	2	Total 2	Mg 2	0
90	AA	105	Total 105	Mg 105	0
90	AB	1	Total 1	Mg 1	0
90	AX	1	Total 1	Mg 1	0
90	Ag	1	Total 1	Mg 1	0
90	An	1	Total 1	Mg 1	0

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

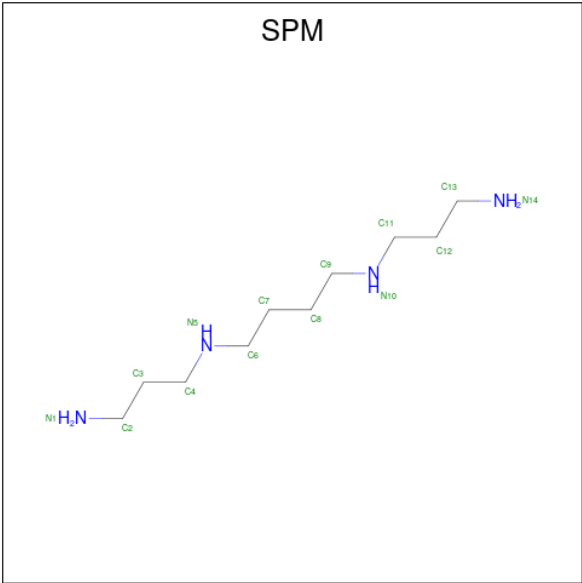
Mol	Chain	Residues	Atoms		AltConf
91	B5	1	Total 1	Zn 1	0
91	B9	1	Total 1	Zn 1	0
91	Bx	1	Total 1	Zn 1	0
91	AR	1	Total 1	Zn 1	0
91	Ac	1	Total 1	Zn 1	0
91	Ap	1	Total 1	Zn 1	0

- Molecule 92 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					AltConf
92	BA	1	Total	C	N	O	P	0
			24	10	5	8	1	
92	BA	1	Total	C	N	O	P	0
			24	10	5	8	1	

- Molecule 93 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



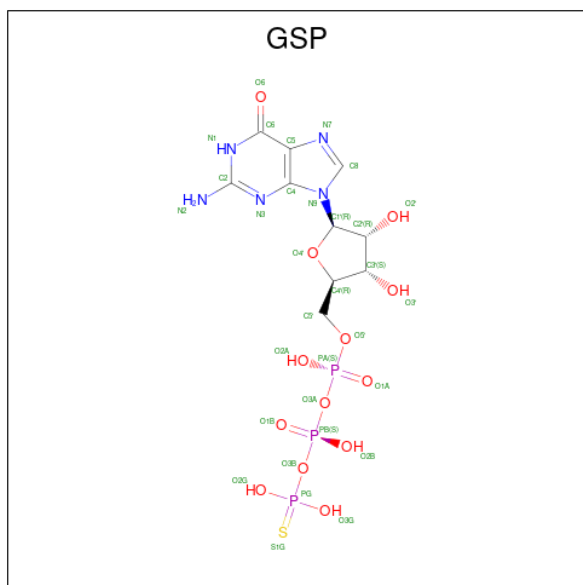
Mol	Chain	Residues	Atoms			AltConf
93	BA	1	Total	C	N	0
			14	10	4	
93	BR	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
93	AA	1	Total	C	N	0
			14	10	4	

- Molecule 94 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

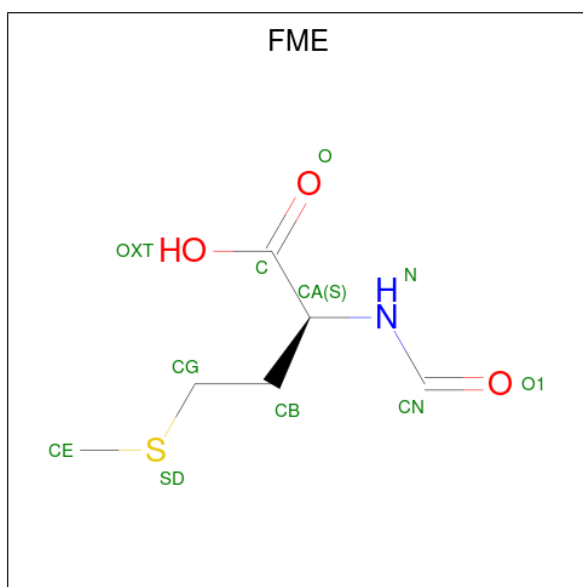


Mol	Chain	Residues	Atoms						AltConf
94	BC	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

- Molecule 95 is SODIUM ION (CCD ID: NA) (formula: Na).

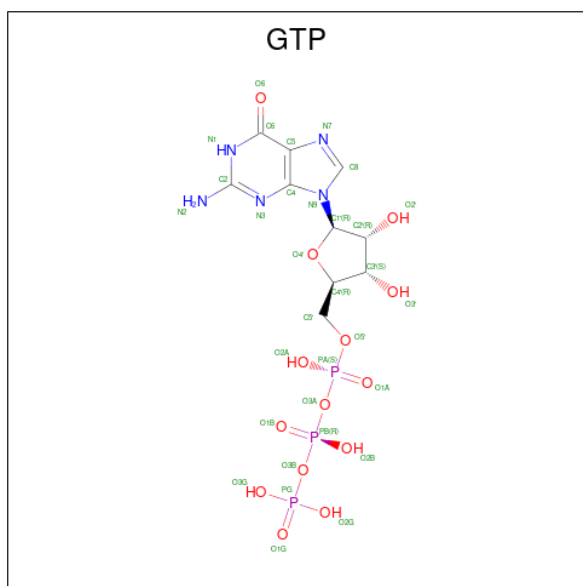
Mol	Chain	Residues	Atoms		AltConf
95	BC	1	Total	Na	0
			1	1	

- Molecule 96 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
96	AV	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 97 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

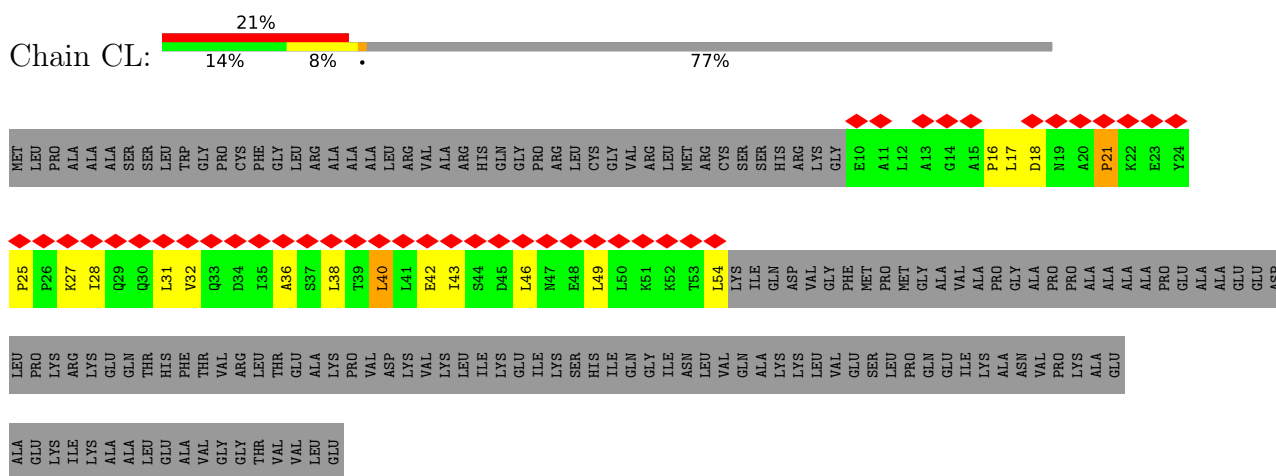
- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	BC	2	Total 2	O 2	0
98	Ag	3	Total 3	O 3	0

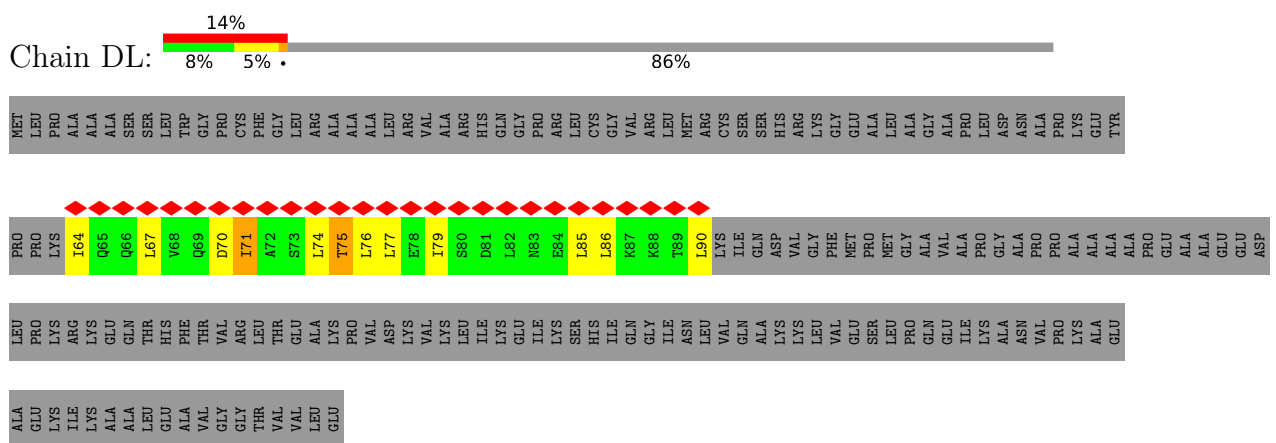
3 Residue-property plots

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

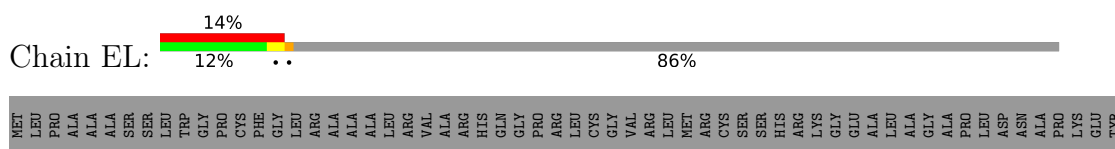
• Molecule 1: Mitochondrial ribosomal protein L12

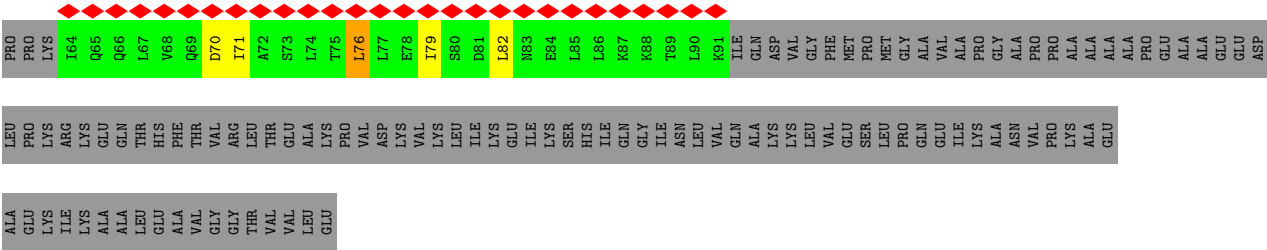


• Molecule 1: Mitochondrial ribosomal protein L12

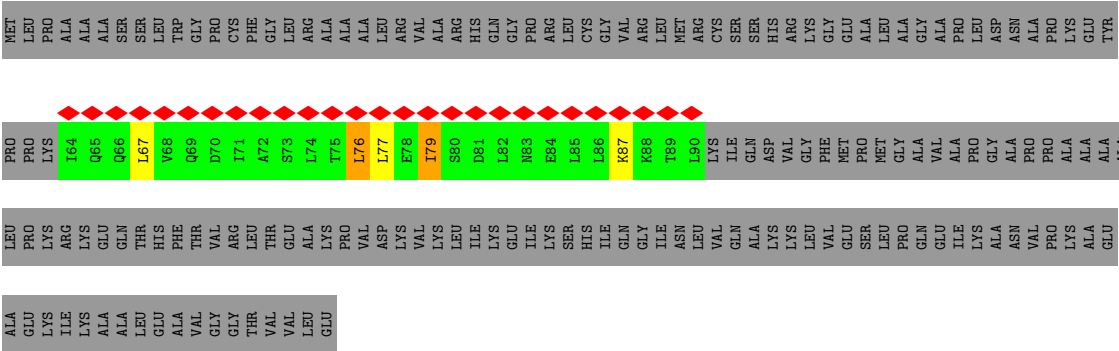


• Molecule 1: Mitochondrial ribosomal protein L12

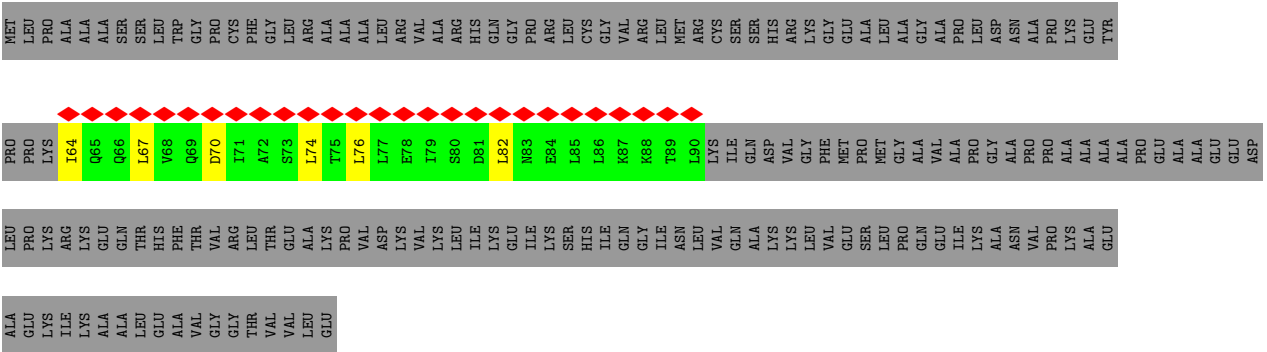




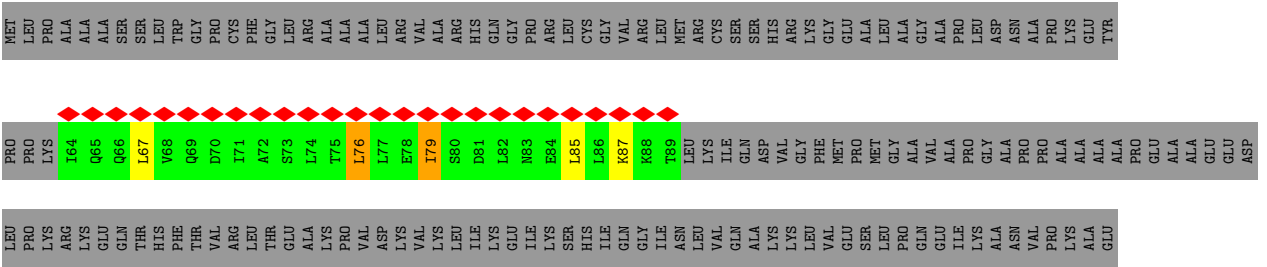
• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



ALA
GLU
LYS
ILE
ALA
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

• Molecule 1: Mitochondrial ribosomal protein L12



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

PRO
PRO
ILE
GLN
LEU
VAL
GLN
THR
H129
F130
T131
V132
R133
L134
T135
A136
E137
K138
P139
V140
D141
K142
V143
K144
L145
I146
K147
E148
I149
K150
S151
H152
I153
Q154
G155
I156
N157
L158
V159
Q160
A161
K162
K163
L164
V165
E166
S167
L168
P169
Q170
E171
I172
K173
A174
N175
V176
P177
K178
A179
E180

A181
E182
K183
I184
K185
A186
A187
L188
E189
A190
V191
G192
T194
V195
V196
L197
E198

• Molecule 2: Mitochondrial ribosomal protein L27



MET
ALA
LEU
ALA
VAL
LEU
ALA
LEU
ARG
THR
ARG
ALA
ALA
VAL
THR
ALA
LEU
SER
PRO
PRO
GLN
ALA
ALA
ALA
LEU
ALA
VAL
ARG
TYR
SER
LYS
LYS
THR
GLY
SER
S39
K40
K45
K49
R50
I53
K54
K55
M56
E57
G58
H59
H62
N65
T69

R74
W75
H76
T100
V117
T118
A119
L120
A124
V125
L126
Y127
K128
V131
S131
V132
V133
V134
P135
T141
L148

• Molecule 3: Mitochondrial ribosomal protein L28



MET
P72
K5
V6
R15
L16
W17
P25
R26
H27
Y28
L29
R30
S31
L32
E33
E34
A35
R36
P40
V41
H42
Y43
H46
R61
D64
P67
P68
V69
P72
S76
Q76
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W85
W86
L87
K96
R100
V101
R102
K103
V104

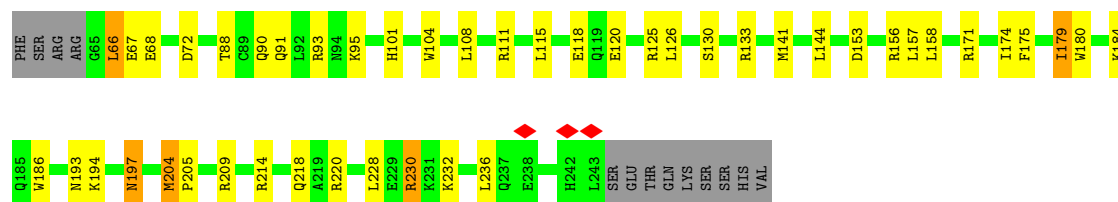
P107
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M129
D133
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T148
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K162
R163
G164
M165
L166
I167
R168
Q172
D173
P174
G175
L176
H177
P178
D179
R184
D189
R190
Y191
K192
T196
P197
E200
A201
E202
W203
V204
G205
I224

Q237
L238
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E245
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ARG
LYS

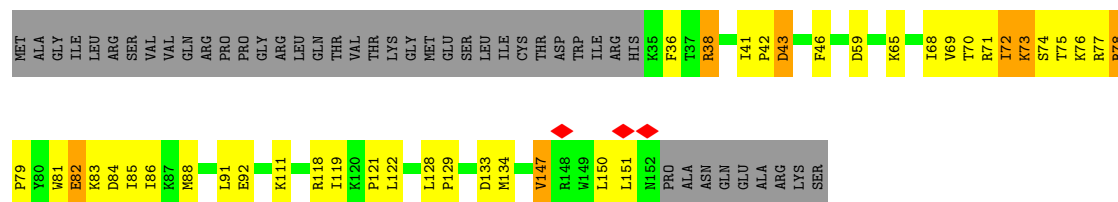
• Molecule 4: Mitochondrial ribosomal protein L47



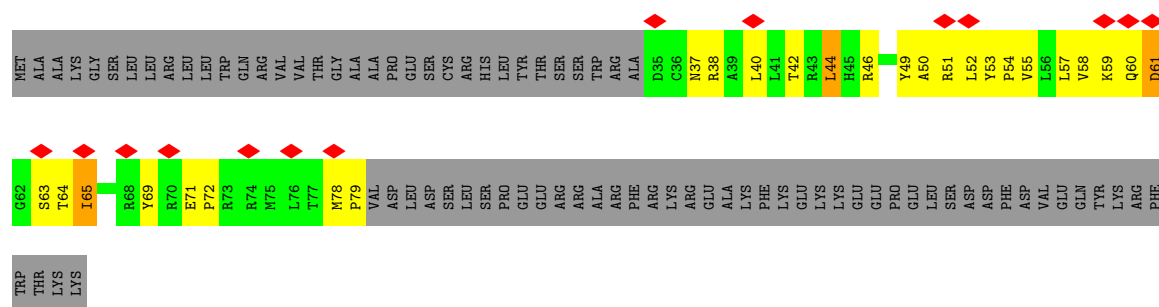
MET
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GLY
LEU
ALA
VAL
PHE
CYS
ARG
ARG
VAL
SER
ALA
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LEU
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CYS
ARG
LEU
LEU
ILE
ARG
PRO
GLN
ALA
PRO
PRO
PRO
SER
THR
SER
CYS
ARG
PHE
SER
PRO
SER
LEU
LEU
LYS
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PHE
GLN
PHE
ARG
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PHE
HIS
THR
THR



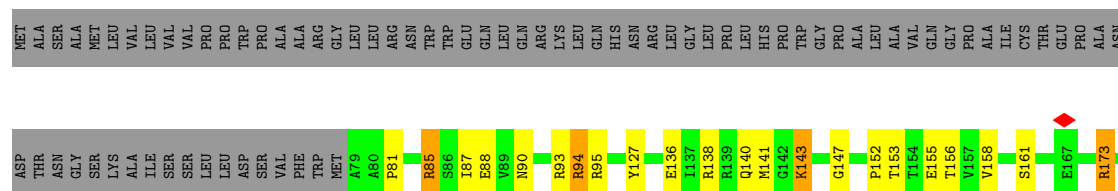
• Molecule 5: uL30m



• Molecule 6: 39S ribosomal protein L55, mitochondrial

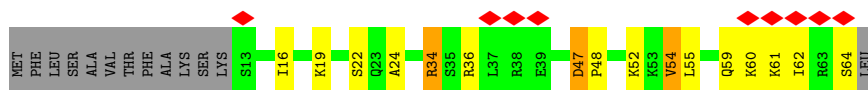


• Molecule 7: bL32m

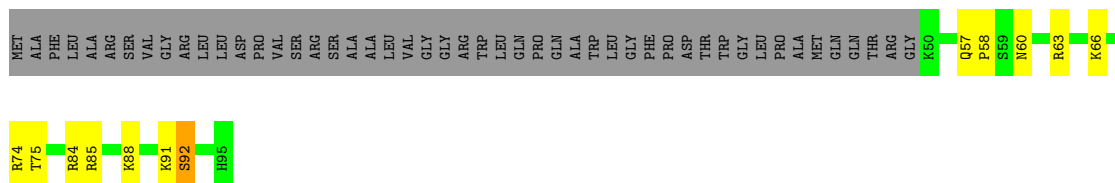
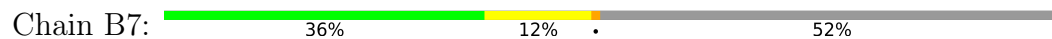


• Molecule 8: bL33m

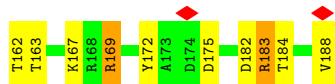
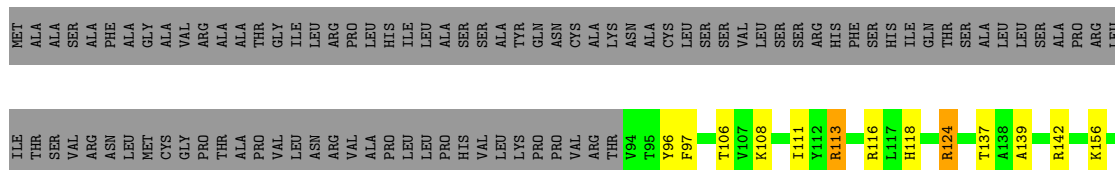




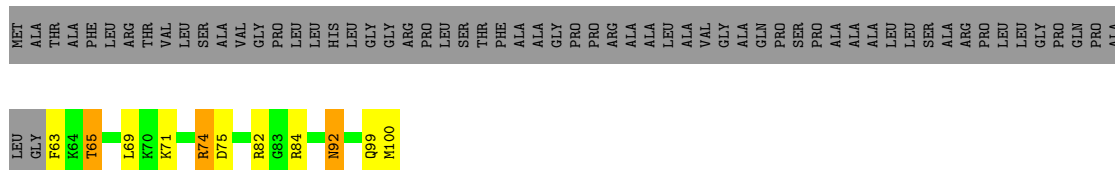
• Molecule 9: Mitochondrial ribosomal protein L34



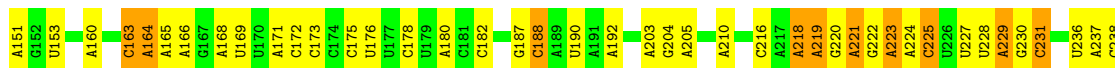
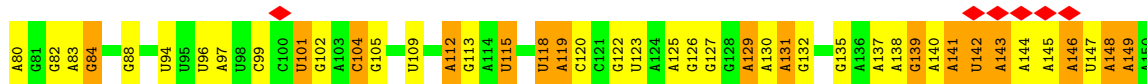
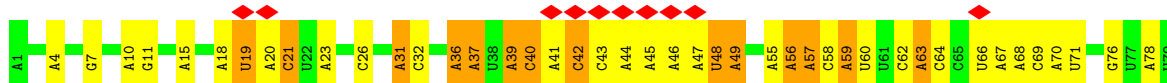
• Molecule 10: Mitochondrial ribosomal protein L35

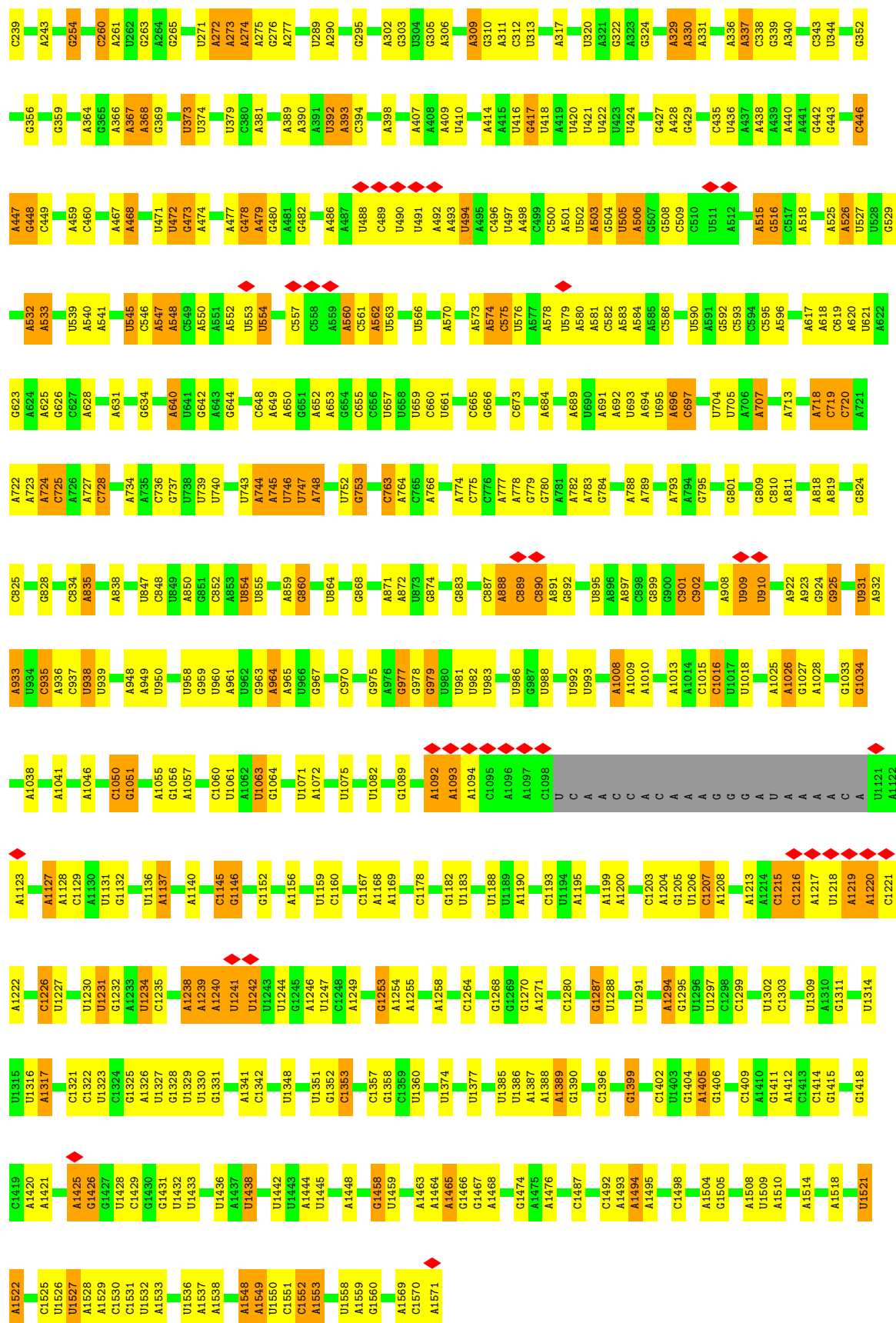


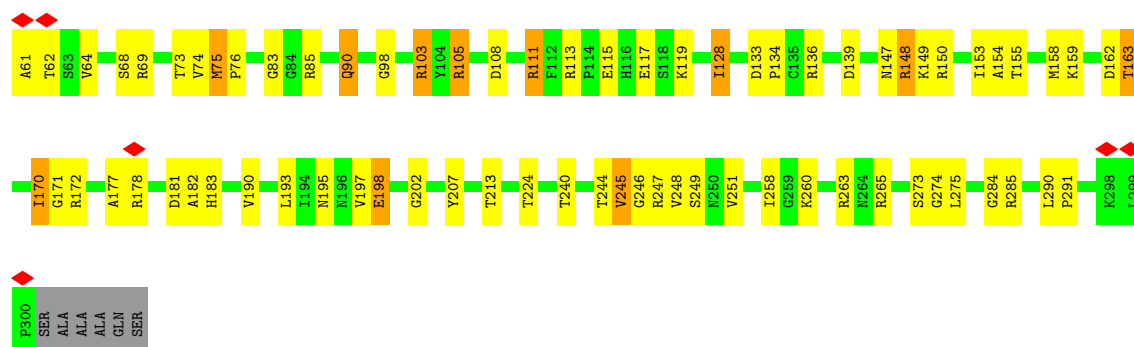
• Molecule 11: Ribosomal protein



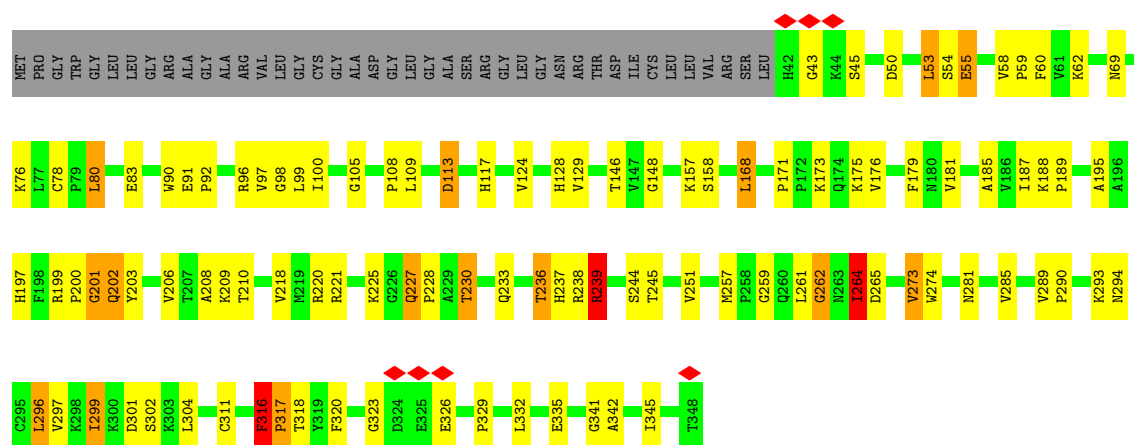
• Molecule 12: 16S ribosomal RNA, mitochondrial



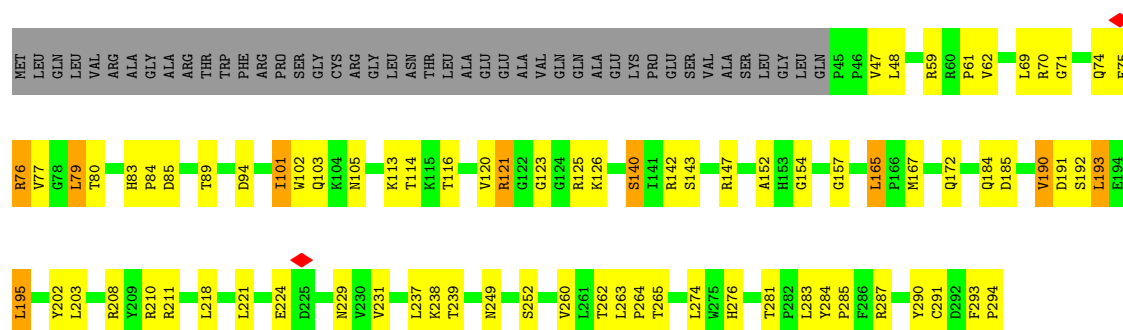




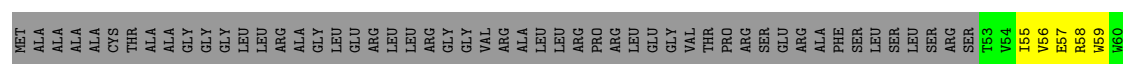
• Molecule 16: ICT1



• Molecule 17: Mitochondrial ribosomal protein L4

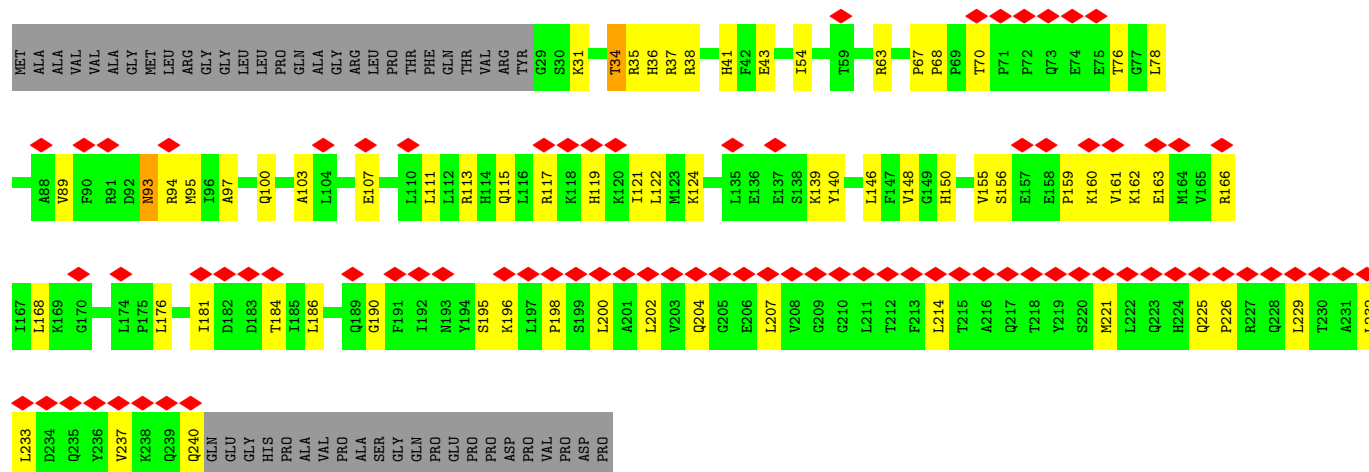


• Molecule 18: Mitochondrial ribosomal protein L9

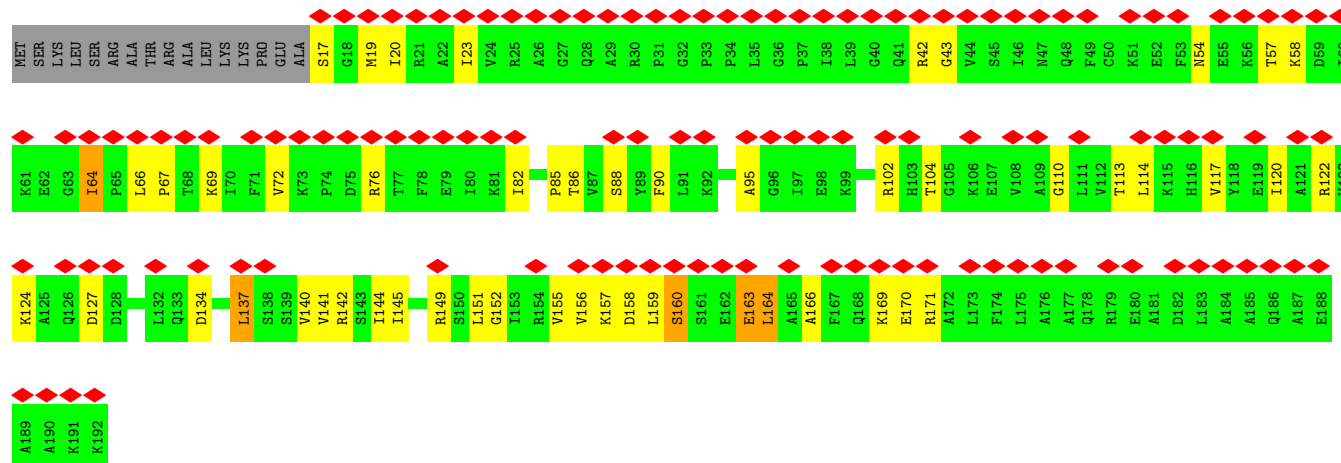




• Molecule 19: Mitochondrial ribosomal protein L10

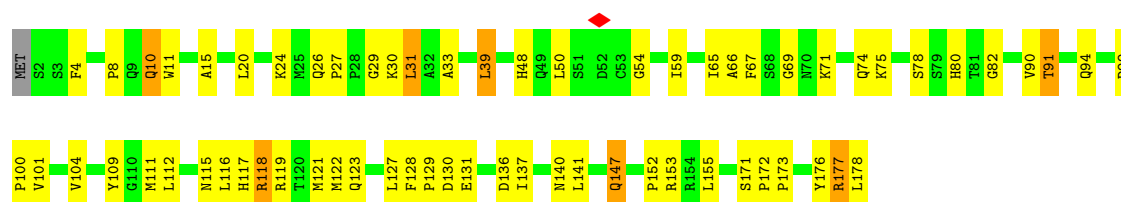


• Molecule 20: Mitochondrial ribosomal protein L11

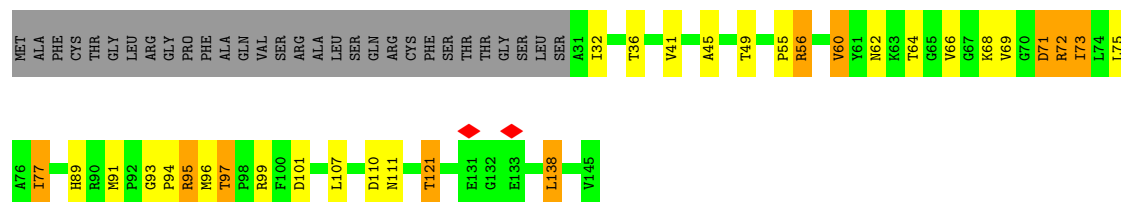


• Molecule 21: 39S ribosomal protein L13, mitochondrial

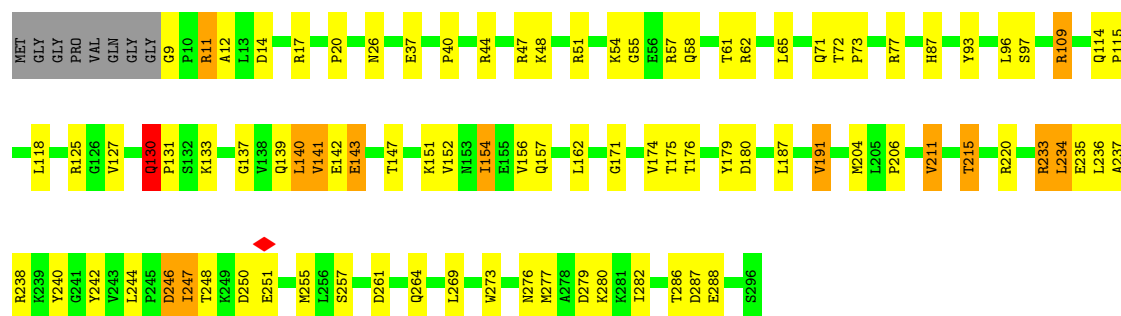




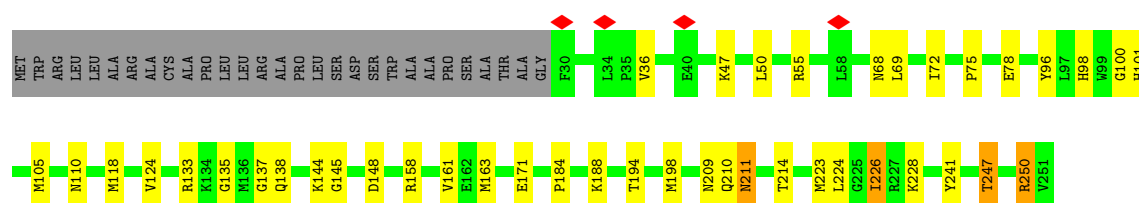
• Molecule 22: uL14m



• Molecule 23: 39S ribosomal protein L15, mitochondrial

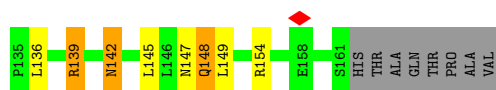


• Molecule 24: 39S ribosomal protein L16, mitochondrial

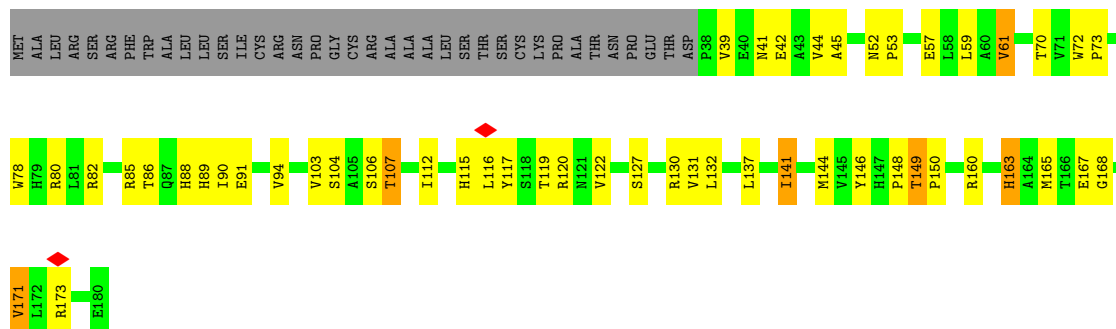


• Molecule 25: 39S ribosomal protein L17, mitochondrial

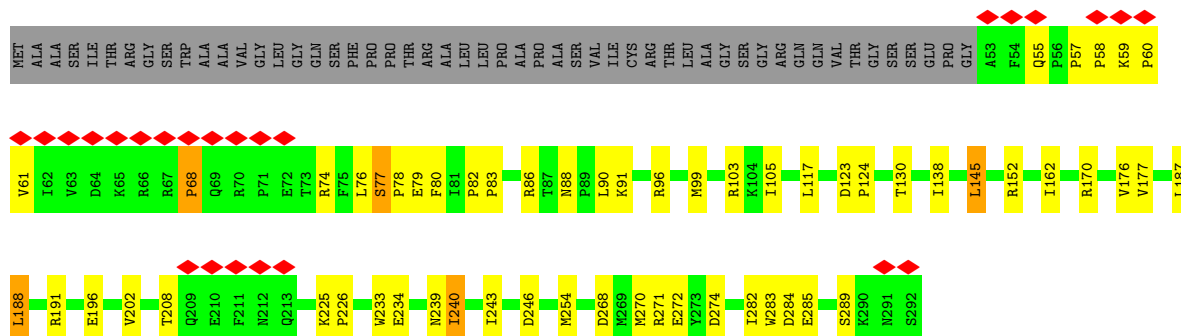




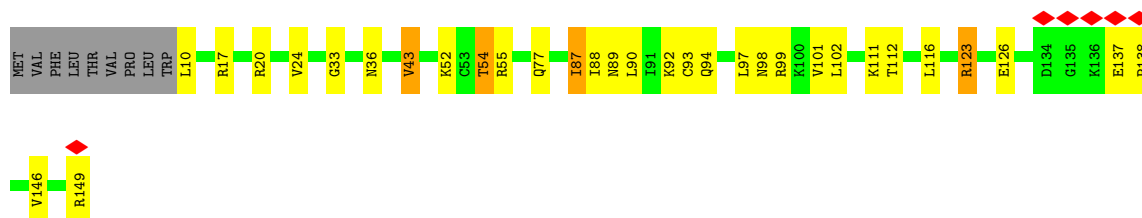
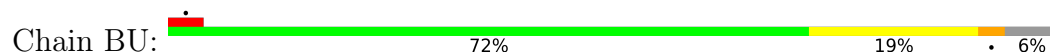
- Molecule 26: Mitochondrial ribosomal protein L18



- Molecule 27: Mitochondrial ribosomal protein L19

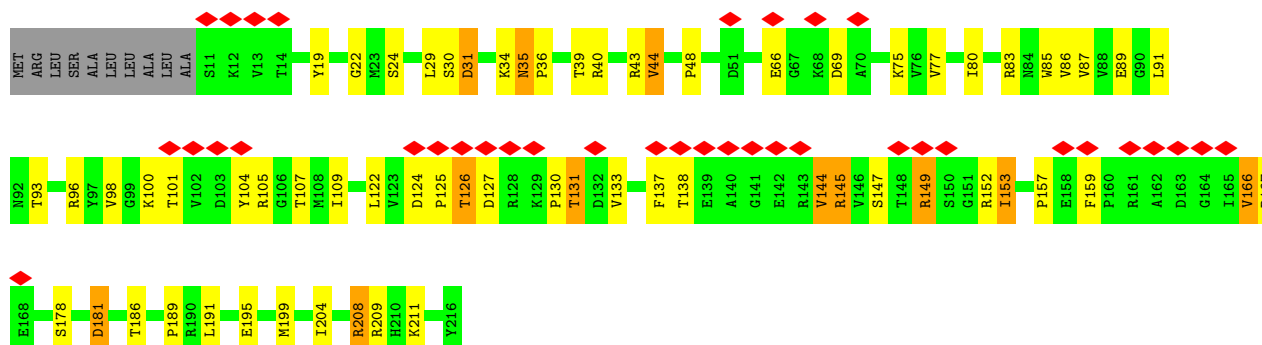
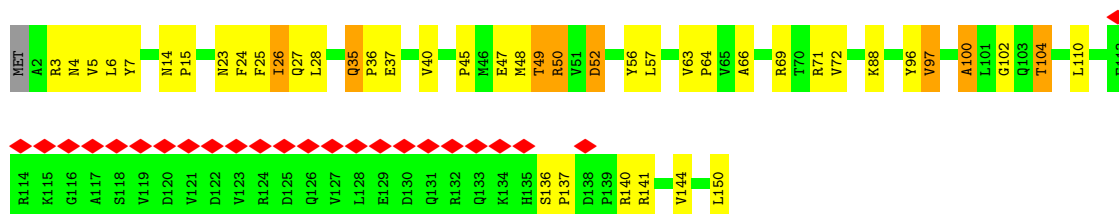
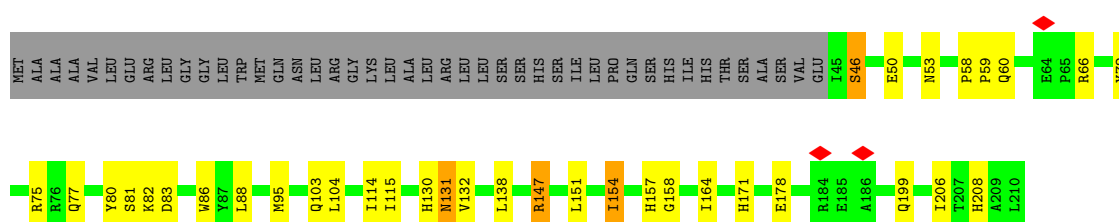
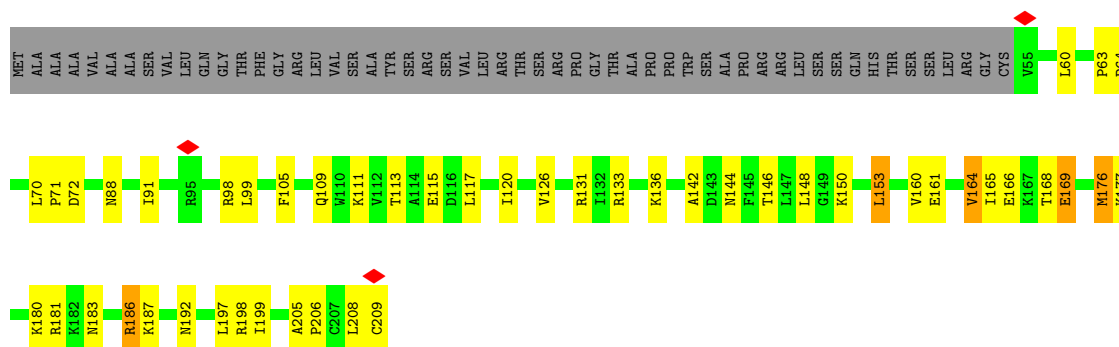


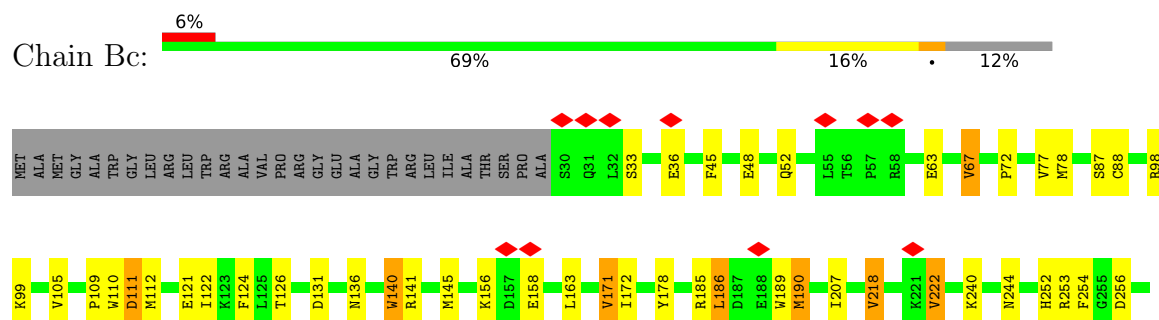
- Molecule 28: Mitochondrial ribosomal protein L20



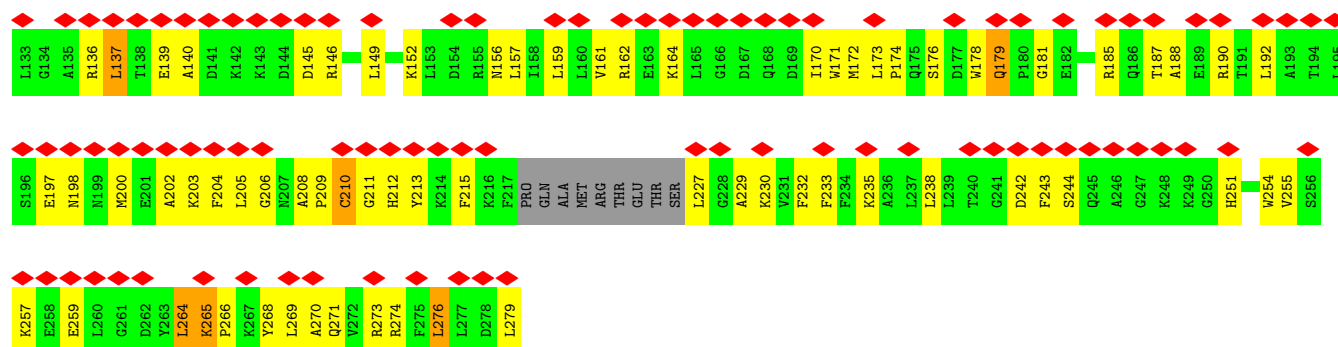
- Molecule 29: Mitochondrial ribosomal protein L21



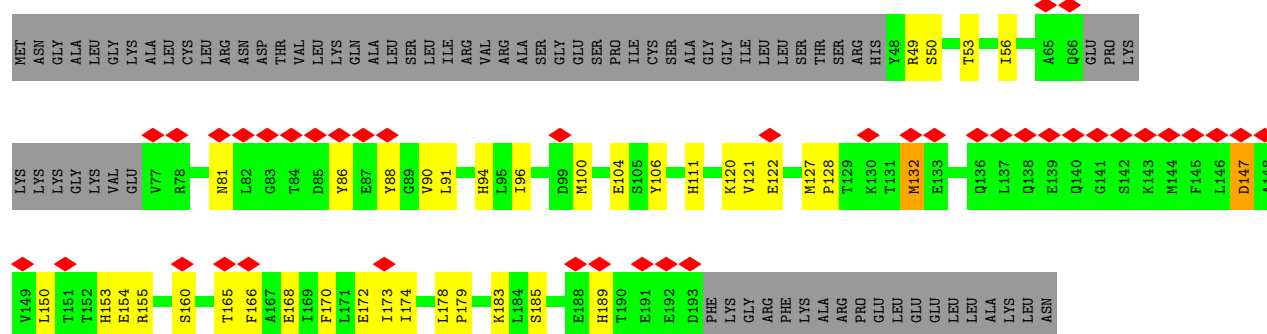




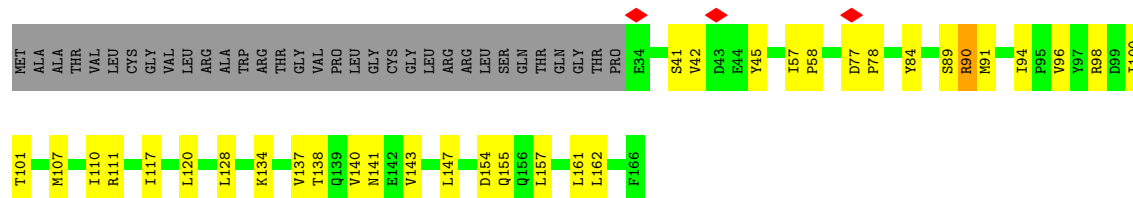




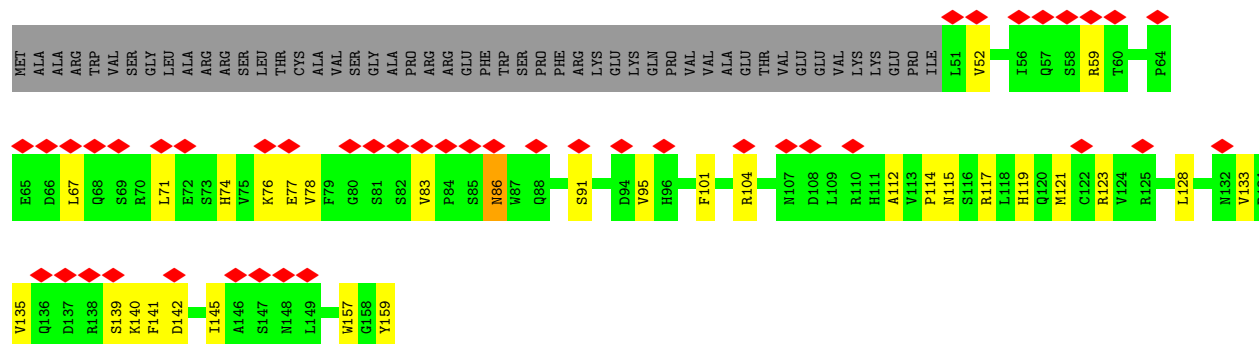
• Molecule 43: Mitochondrial ribosomal protein L48



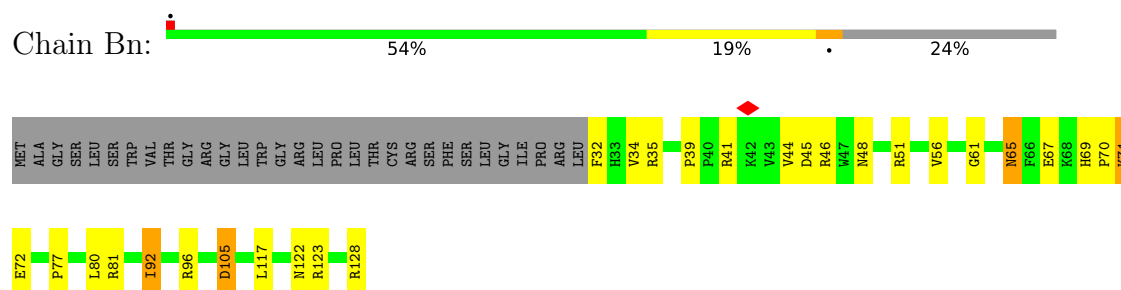
• Molecule 44: 39S ribosomal protein L49, mitochondrial



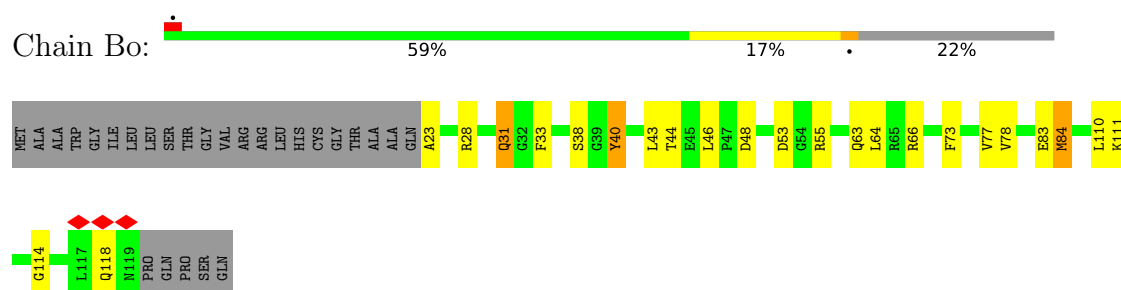
• Molecule 45: mL50



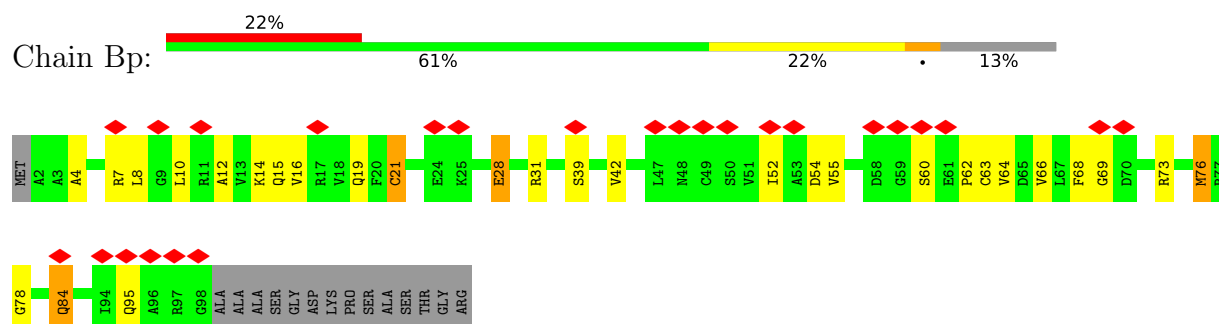
- Molecule 46: Mitochondrial ribosomal protein L51



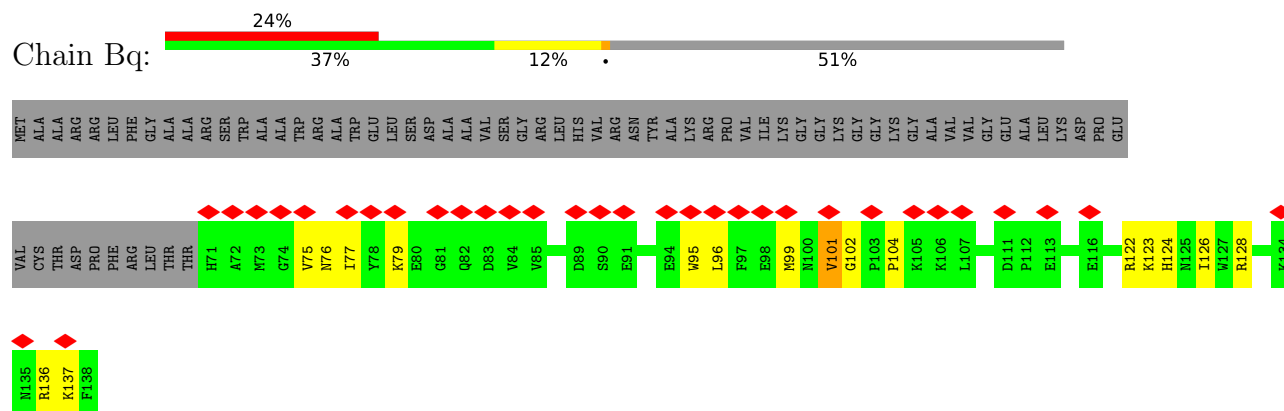
- Molecule 47: 39S ribosomal protein L52, mitochondrial



- Molecule 48: mL53

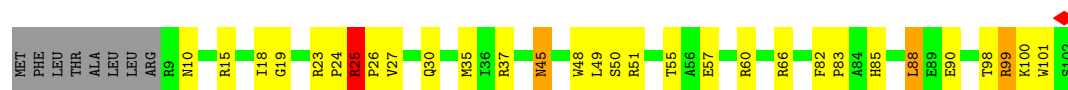


- Molecule 49: mL54

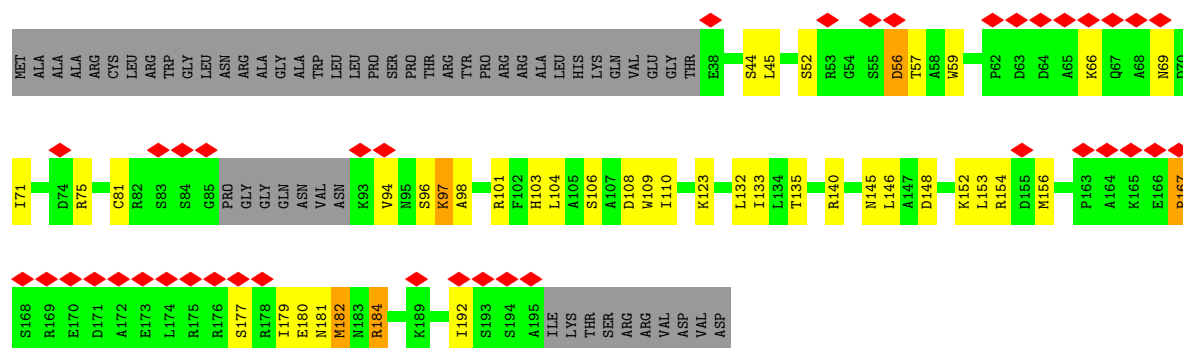


- Molecule 50: Mitochondrial ribosomal protein L57

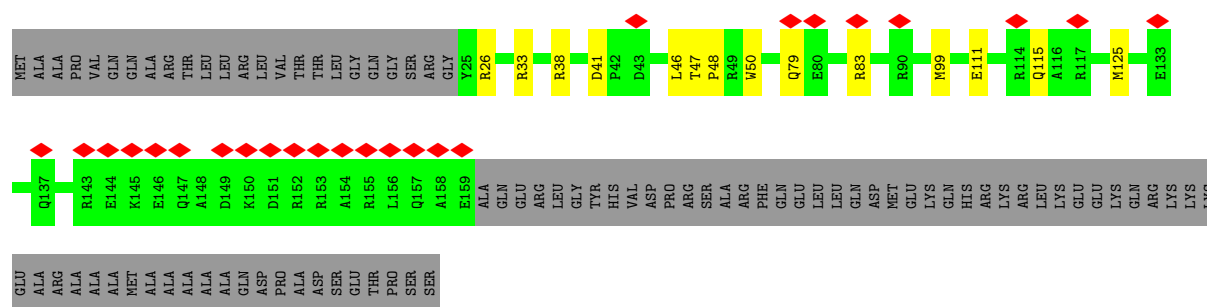




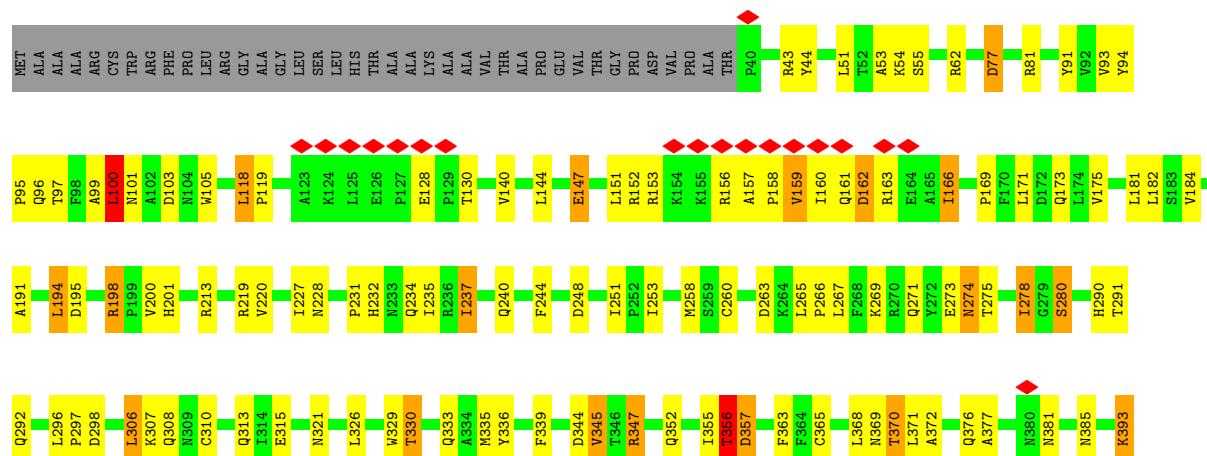
- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 52: mL64

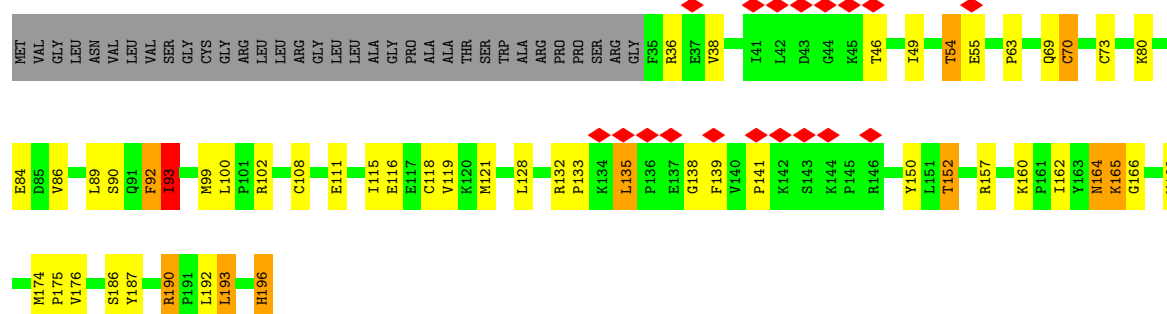


- Molecule 53: mL65

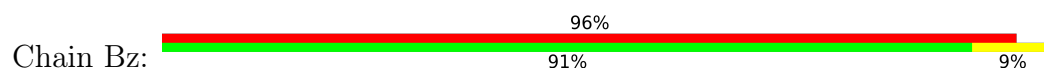




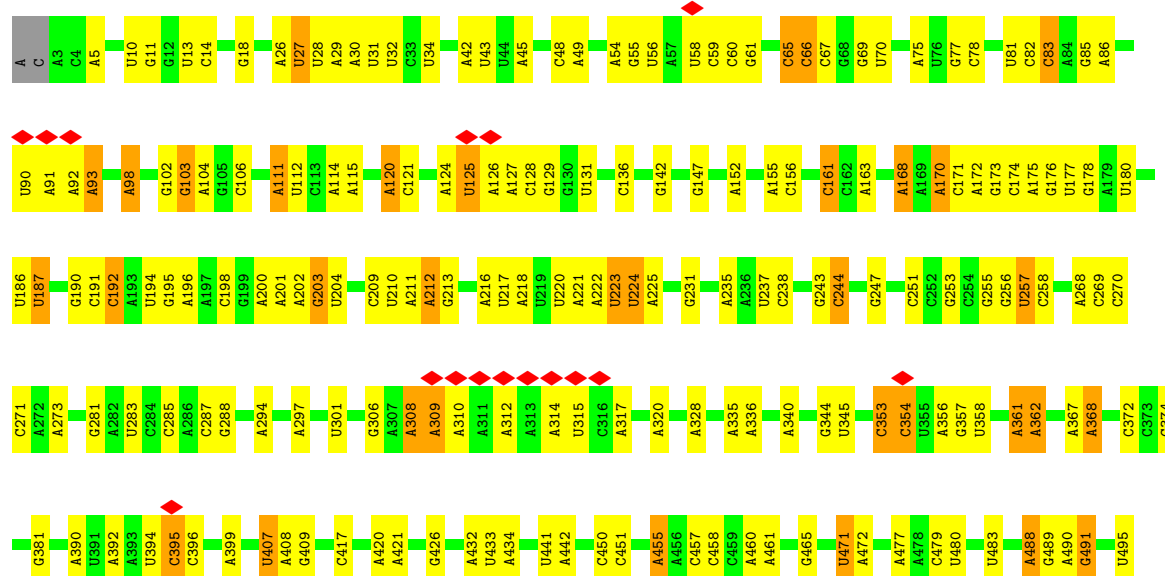
• Molecule 54: Mitochondrial ribosomal protein S18A

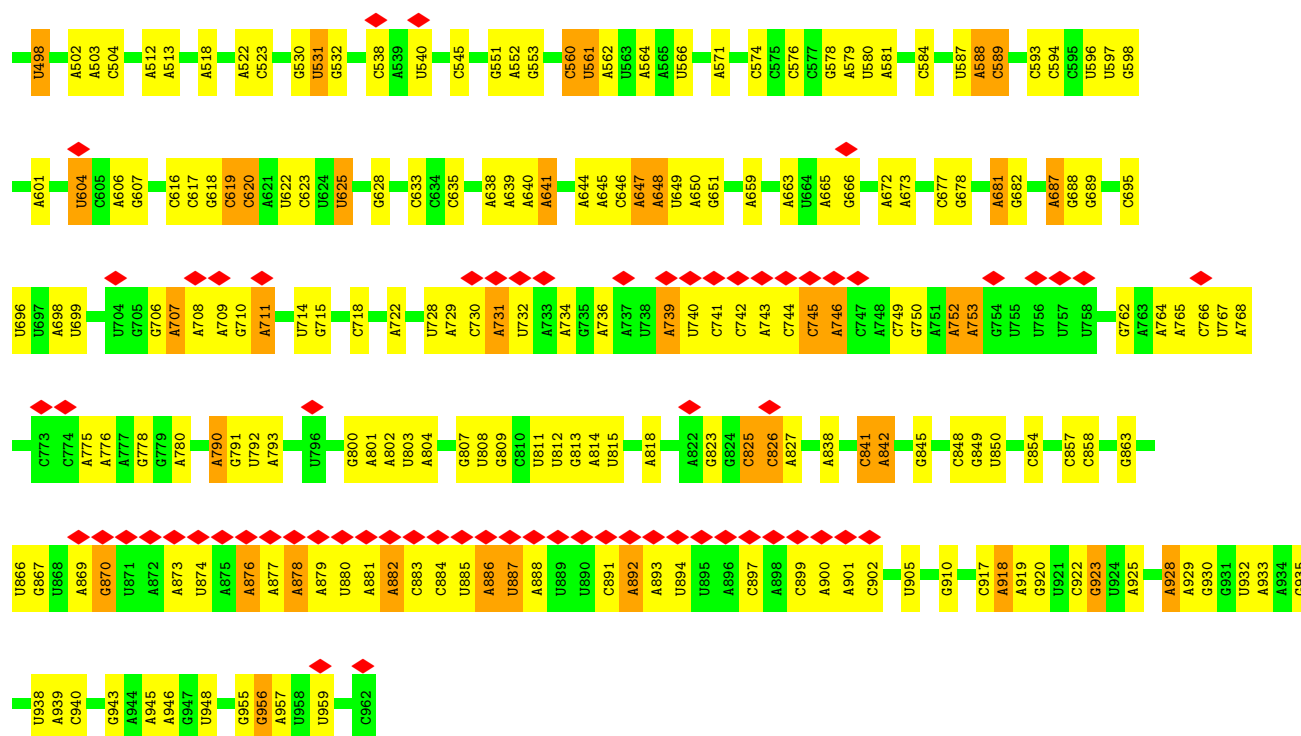


• Molecule 55: unassigned secondary structure elements

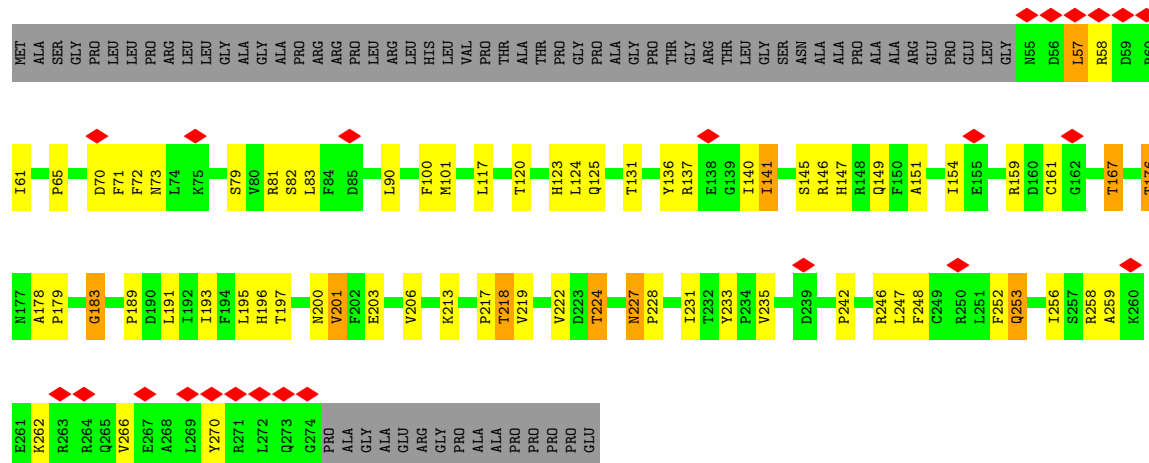


• Molecule 56: 12S ribosomal RNA, mitochondrial

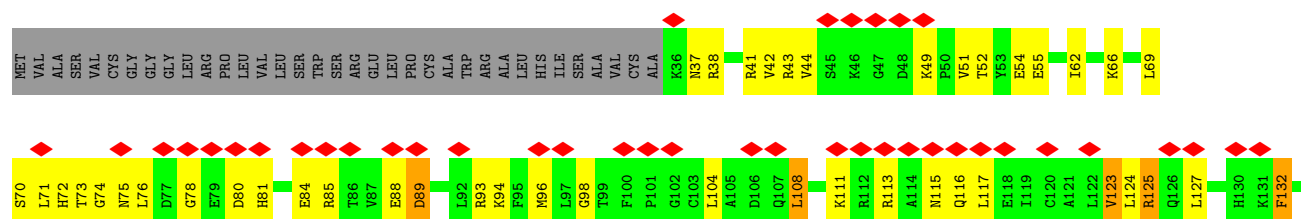


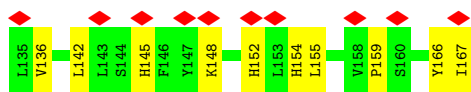


• Molecule 57: Mitochondrial ribosomal protein S2

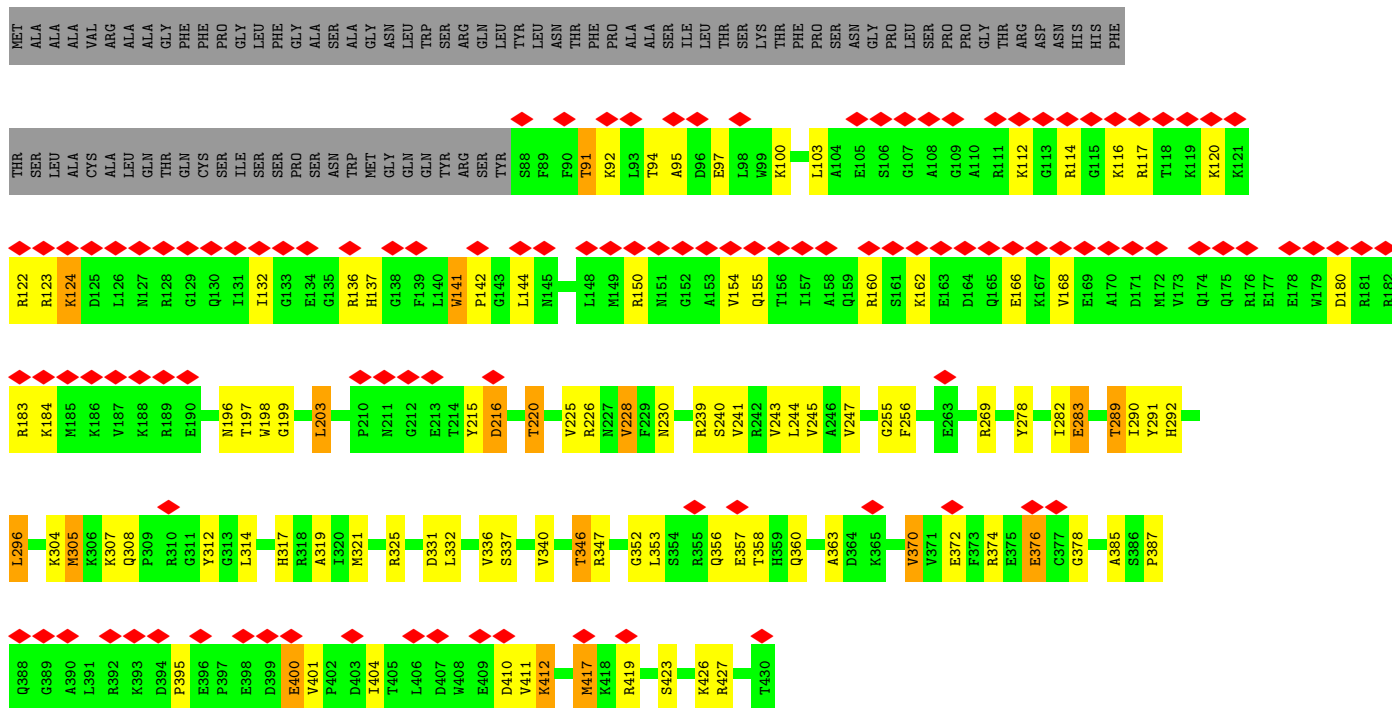


• Molecule 58: Mitochondrial ribosomal protein S24

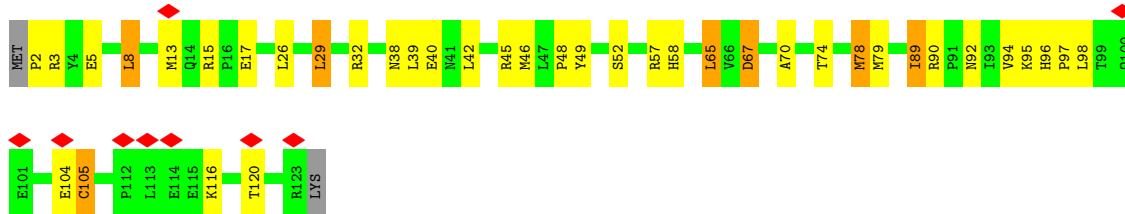




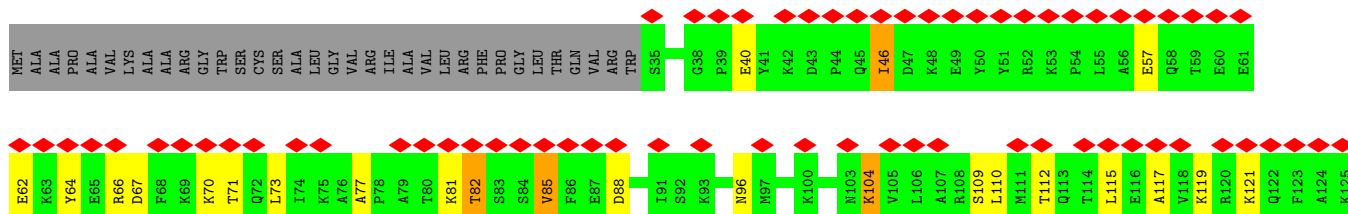
• Molecule 59: Mitochondrial ribosomal protein S5

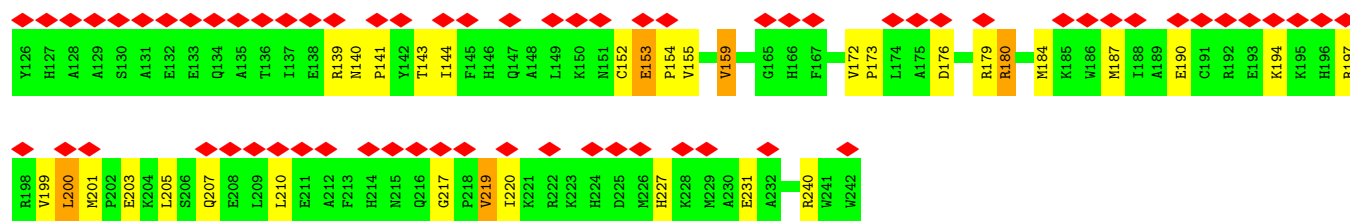


• Molecule 60: Mitochondrial ribosomal protein S6

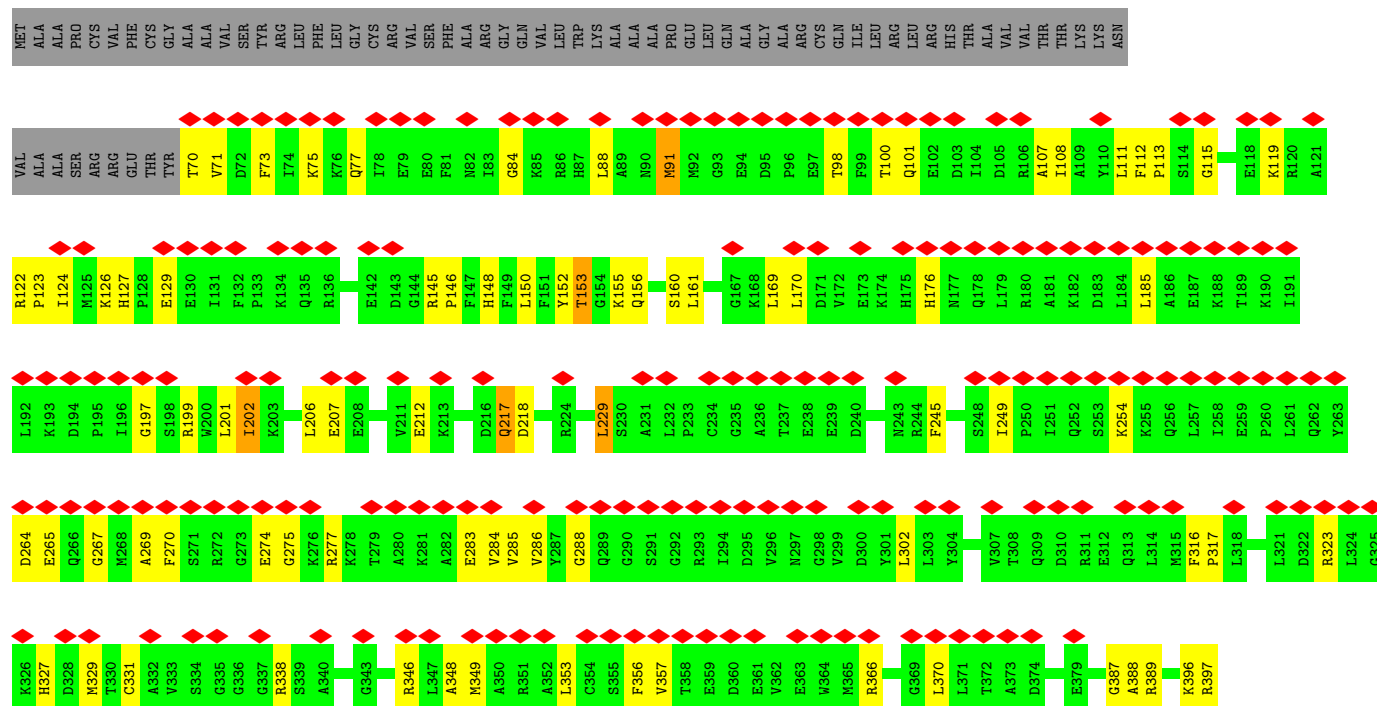


• Molecule 61: Mitochondrial ribosomal protein S7





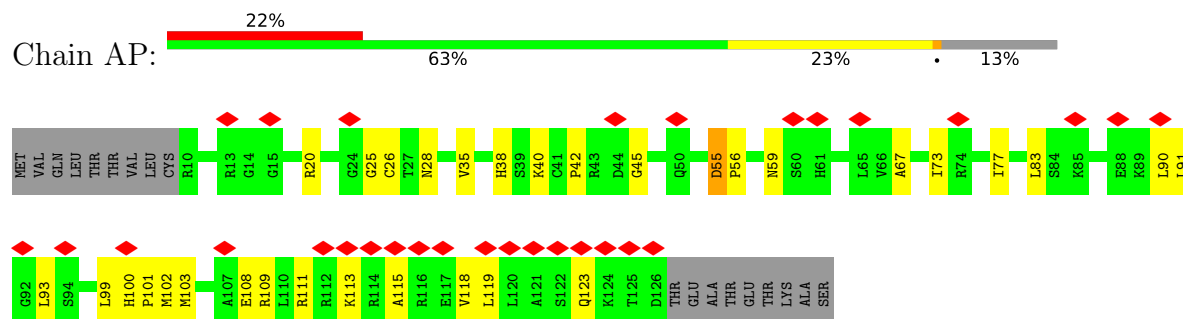
• Molecule 62: 28S ribosomal protein S9, mitochondrial



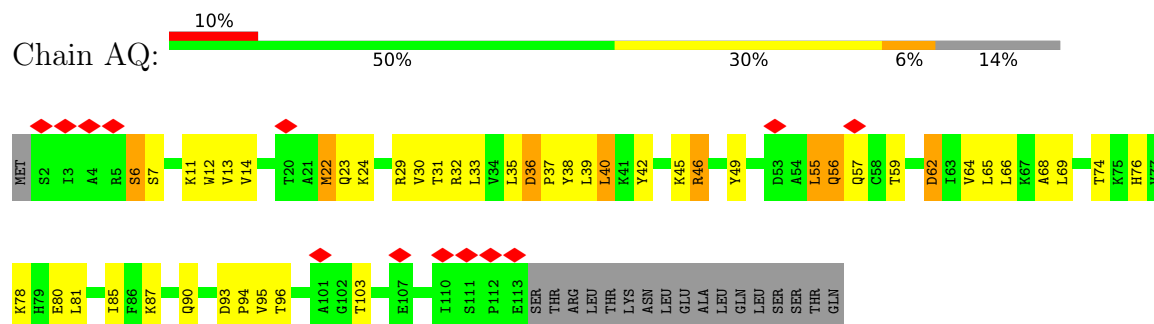
• Molecule 63: Mitochondrial ribosomal protein S10



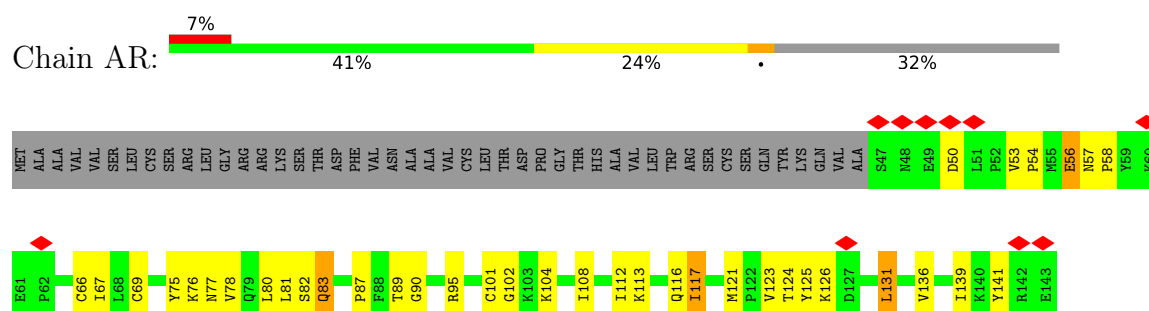
- Molecule 68: bS16m



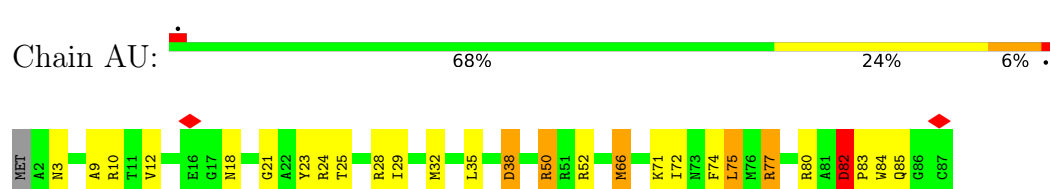
- Molecule 69: uS17m



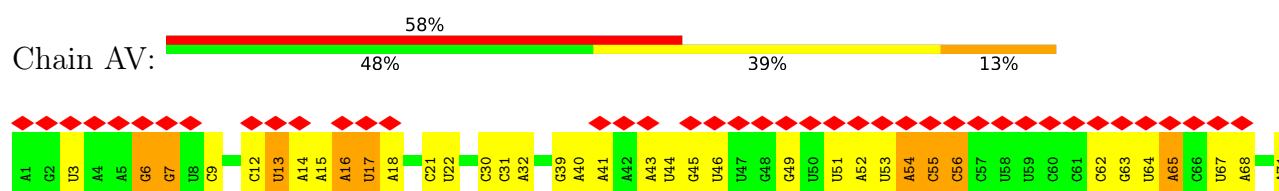
- Molecule 70: Mitochondrial ribosomal protein S18C



- Molecule 71: bS21m

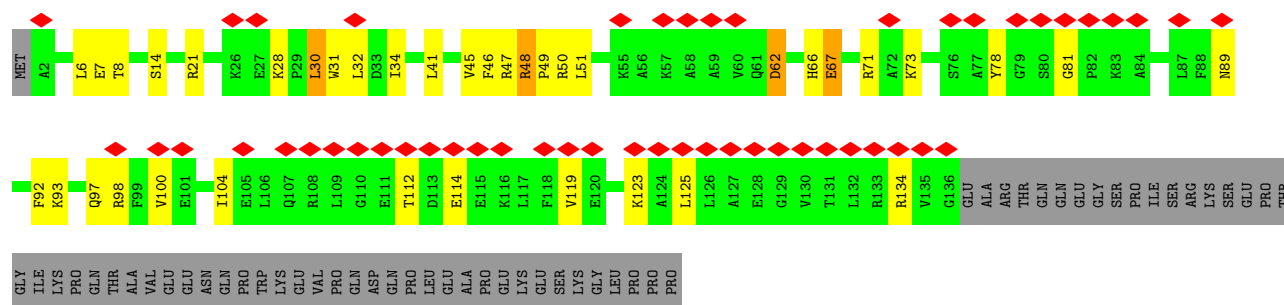


- Molecule 72: P-site fMet-tRNA^{Met}, mitochondrial

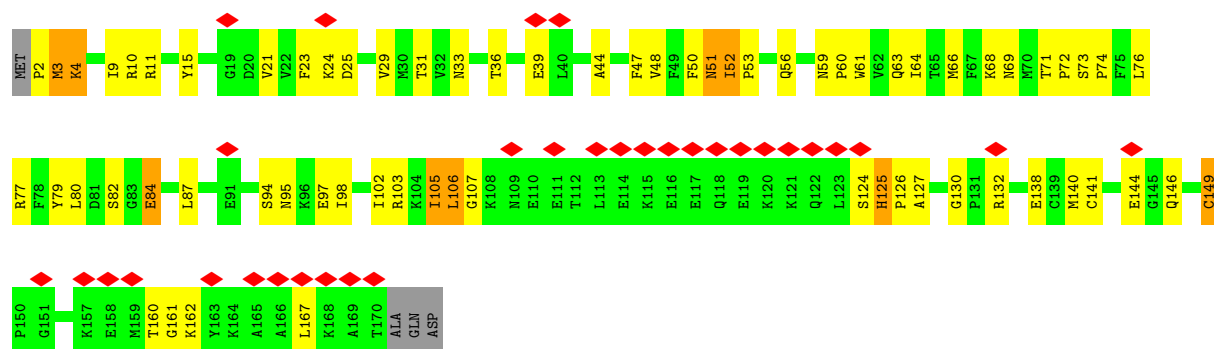


- Molecule 73: MT-CO3 mRNA, mitochondrial

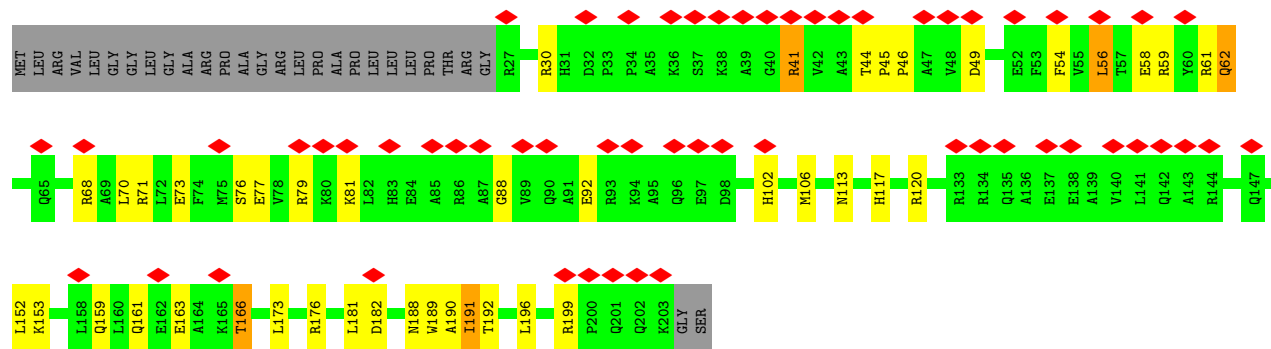




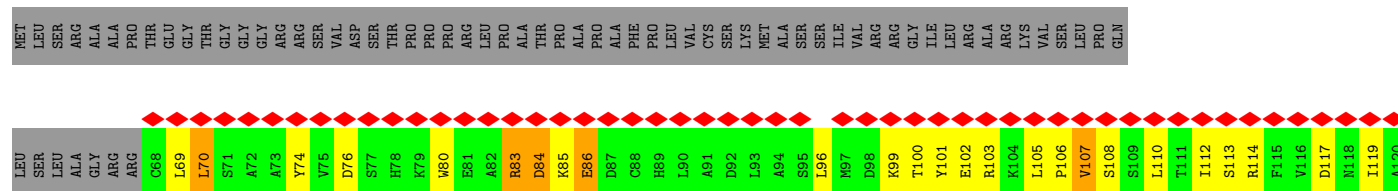
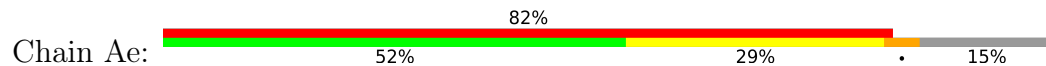
• Molecule 77: Mitochondrial ribosomal protein S25

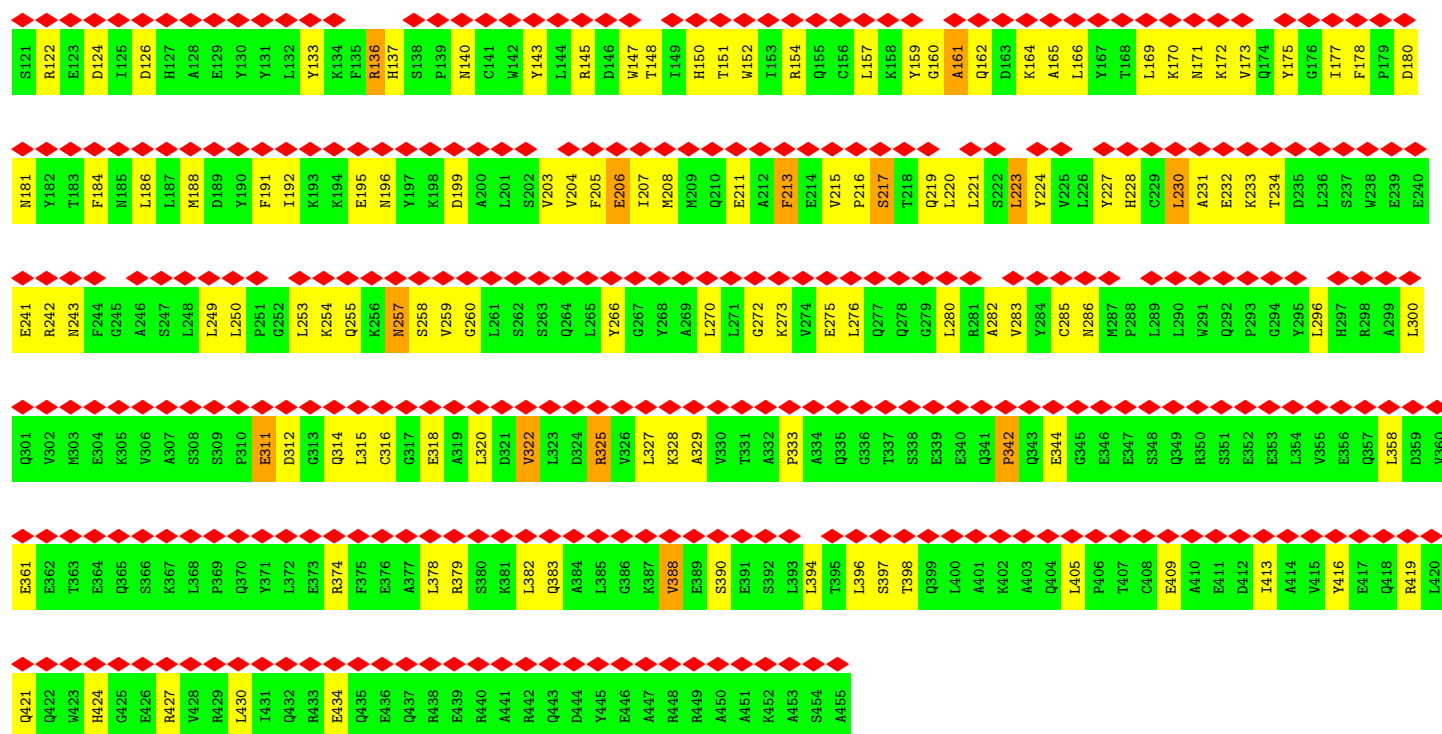


• Molecule 78: Mitochondrial ribosomal protein S26

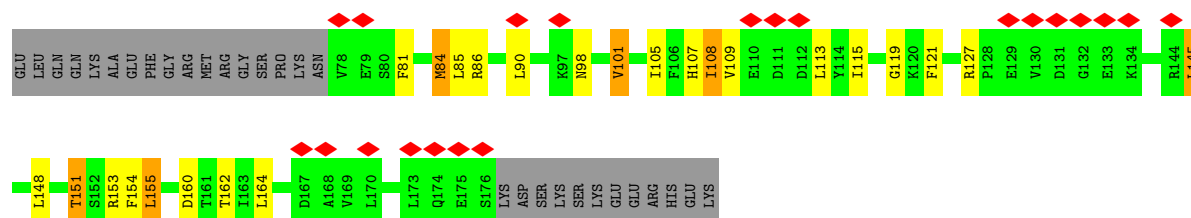
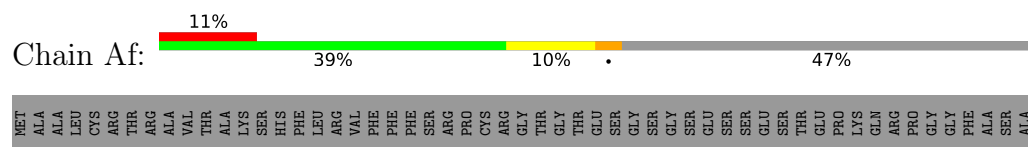


• Molecule 79: mS27

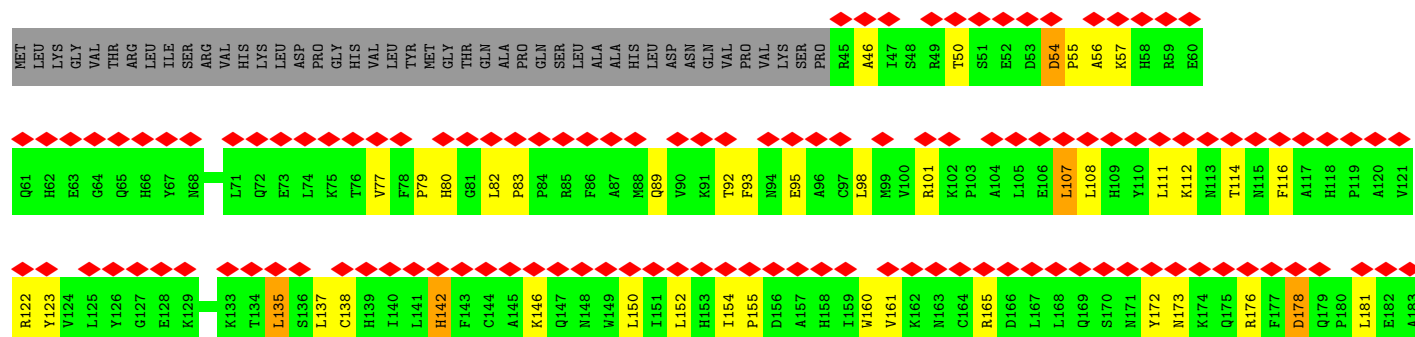
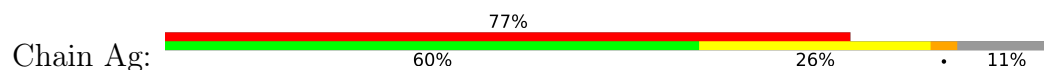


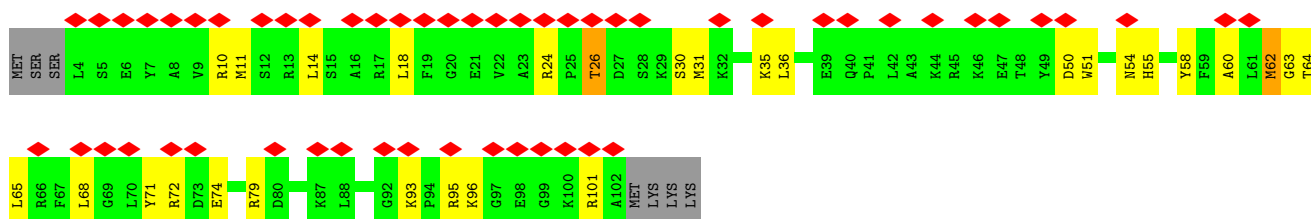


• Molecule 80: 28S ribosomal protein S28, mitochondrial

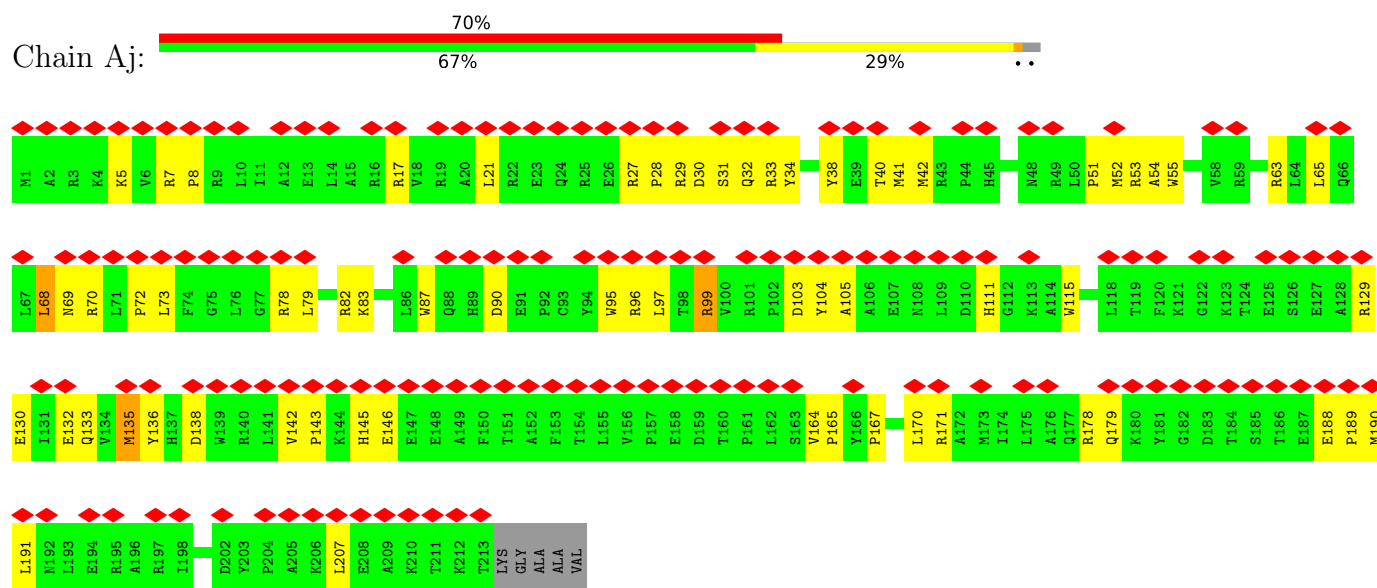


• Molecule 81: Death associated protein 3

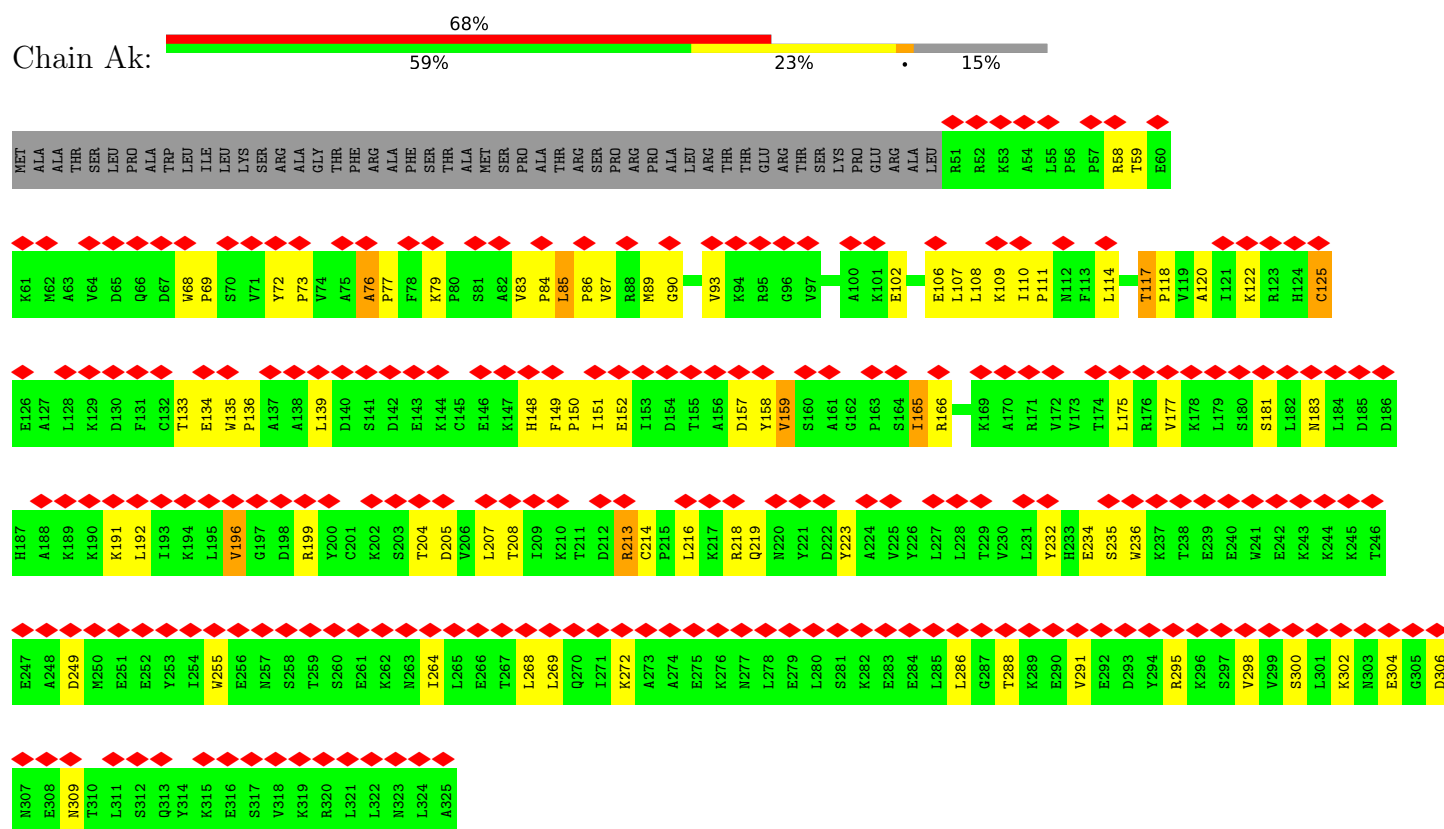




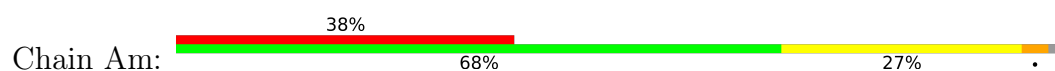
- Molecule 84: 28S ribosomal protein S34, mitochondrial



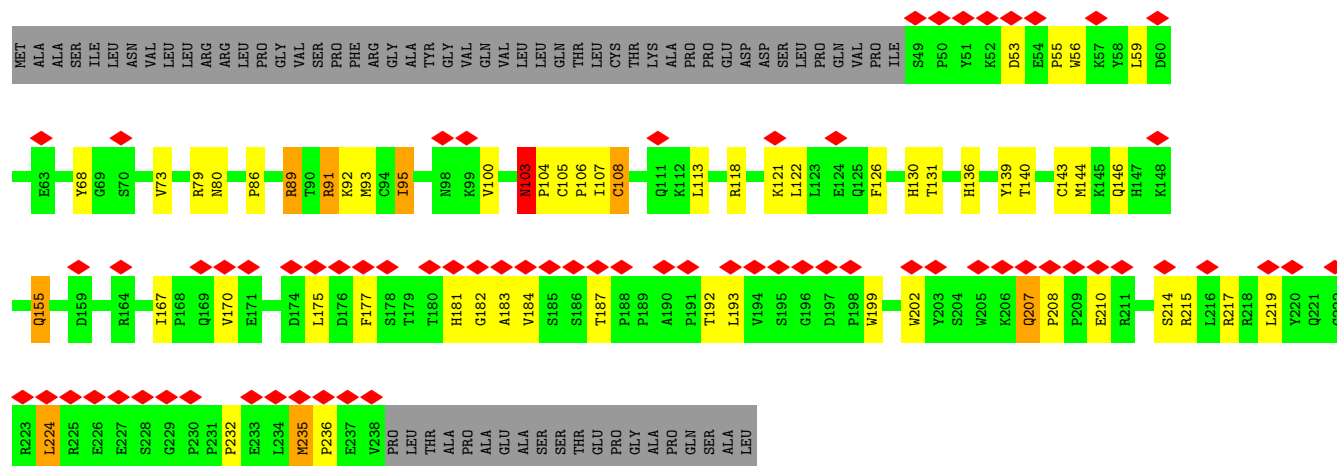
- Molecule 85: 28S ribosomal protein S35, mitochondrial



- Molecule 86: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.453	Depositor
Minimum map value	-0.743	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, GSP, GTP, MG, SPM, NA, ZN, 5GP

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	BL	0.52	0/542	0.81	0/729
1	CL	0.58	0/319	1.10	4/435 (0.9%)
1	DL	0.47	0/212	0.62	0/286
1	EL	0.56	0/221	0.67	0/297
1	FL	0.56	0/212	0.64	0/286
1	GL	0.59	0/212	0.62	0/286
1	HL	0.57	0/204	0.65	0/275
2	B0	0.63	0/880	0.88	1/1189 (0.1%)
3	B1	0.43	0/2093	0.82	0/2835
4	B2	0.51	0/1586	0.82	0/2123
5	B3	0.56	0/993	0.95	2/1341 (0.1%)
6	B4	0.32	0/388	0.96	2/523 (0.4%)
7	B5	0.52	0/917	0.90	4/1227 (0.3%)
8	B6	0.34	0/430	0.89	2/570 (0.4%)
9	B7	0.74	0/395	0.85	0/524
10	B8	0.62	0/853	0.89	0/1136
11	B9	0.53	0/342	0.78	0/450
12	BA	0.39	0/36903	0.44	0/57455
13	BB	0.19	0/1595	0.30	0/2475
14	BC	0.41	0/4432	0.81	4/5989 (0.1%)
15	BD	0.57	0/1898	0.94	5/2555 (0.2%)
16	BE	0.59	0/2493	1.02	14/3387 (0.4%)
17	BF	0.63	0/2069	0.93	5/2816 (0.2%)
18	BI	0.42	0/819	0.86	1/1101 (0.1%)
19	BJ	0.44	0/1742	0.83	2/2358 (0.1%)
20	BK	0.42	0/1323	0.85	1/1785 (0.1%)
21	BN	0.59	0/1487	0.88	5/2017 (0.2%)
22	BO	0.55	0/912	0.89	0/1231
23	BP	0.57	0/2368	0.92	5/3198 (0.2%)
24	BQ	0.50	0/1850	0.84	3/2491 (0.1%)
25	BR	0.59	0/1262	0.83	0/1700
26	BS	0.47	0/1197	0.89	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BT	0.53	0/2002	0.93	7/2708 (0.3%)
28	BU	0.68	0/1179	0.86	0/1578
29	BV	0.60	0/1256	0.96	2/1706 (0.1%)
30	BW	0.60	0/1407	0.88	3/1891 (0.2%)
31	BX	0.53	0/1211	0.94	2/1646 (0.1%)
32	BY	0.38	0/1719	0.90	4/2329 (0.2%)
33	Ba	0.48	0/3267	0.87	1/4455 (0.0%)
34	Bb	0.45	0/3047	0.91	5/4139 (0.1%)
35	Bc	0.41	0/2464	0.85	6/3330 (0.2%)
36	Bd	0.42	0/853	0.94	5/1153 (0.4%)
37	Be	0.47	0/1000	0.97	4/1345 (0.3%)
38	Bf	0.48	0/851	0.92	3/1159 (0.3%)
39	Bg	0.57	0/1191	0.95	4/1614 (0.2%)
40	Bh	0.47	0/2372	0.92	8/3211 (0.2%)
41	Bi	0.41	0/2199	0.89	7/2980 (0.2%)
42	Bj	0.37	0/1811	0.82	0/2436
43	Bk	0.37	0/1108	0.83	0/1499
44	Bl	0.51	0/1135	0.86	0/1549
45	Bm	0.38	0/917	0.78	1/1248 (0.1%)
46	Bn	0.66	0/860	0.91	1/1150 (0.1%)
47	Bo	0.47	0/787	0.84	3/1056 (0.3%)
48	Bp	0.40	0/752	0.86	2/1013 (0.2%)
49	Bq	0.42	0/558	0.83	1/756 (0.1%)
50	Bt	0.60	0/798	1.08	4/1073 (0.4%)
51	Bu	0.36	0/1214	0.78	1/1630 (0.1%)
52	Bv	0.37	0/1157	0.72	0/1560
53	Bw	0.55	0/3206	0.92	7/4354 (0.2%)
54	Bx	0.53	0/1364	0.98	5/1849 (0.3%)
55	Bz	0.44	0/404	0.67	0/556
56	AA	0.27	0/22852	0.37	0/35580
57	AB	0.54	0/1804	0.93	7/2445 (0.3%)
58	AC	0.50	0/1105	0.83	0/1496
59	AE	0.42	0/2785	0.81	4/3735 (0.1%)
60	AF	0.44	0/999	0.90	3/1347 (0.2%)
61	AG	0.53	0/1763	0.87	2/2368 (0.1%)
62	AI	0.48	0/2707	0.79	0/3636
63	AJ	0.55	0/1181	0.89	3/1597 (0.2%)
64	AK	0.46	0/1027	1.02	7/1389 (0.5%)
65	AL	0.38	0/858	0.93	5/1152 (0.4%)
66	AN	0.61	0/874	0.90	2/1171 (0.2%)
67	AO	0.46	0/1473	0.95	7/1970 (0.4%)
68	AP	0.59	0/954	0.94	3/1284 (0.2%)
69	AQ	0.51	0/894	0.93	2/1213 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AR	0.52	0/802	0.92	1/1079 (0.1%)
71	AU	0.46	0/745	0.90	2/993 (0.2%)
72	AV	0.20	0/1673	0.33	0/2602
73	AX	0.24	0/395	0.44	0/612
74	AZ	0.49	0/89	0.79	0/123
75	Aa	0.58	0/2428	0.87	3/3279 (0.1%)
76	Ab	0.49	0/1126	0.90	2/1514 (0.1%)
77	Ac	0.52	1/1399 (0.1%)	0.96	5/1881 (0.3%)
78	Ad	0.54	0/1490	0.88	4/2005 (0.2%)
79	Ae	0.47	0/3171	0.86	7/4292 (0.2%)
80	Af	0.47	0/790	0.83	1/1064 (0.1%)
81	Ag	0.48	0/2945	0.81	2/3984 (0.1%)
82	Ah	0.50	0/1045	0.84	2/1409 (0.1%)
83	Ai	0.46	0/841	0.84	0/1121
84	Aj	0.49	1/1835 (0.1%)	0.85	3/2484 (0.1%)
85	Ak	0.52	0/2268	0.88	8/3069 (0.3%)
86	Am	0.44	0/947	0.90	6/1268 (0.5%)
87	An	0.44	0/650	0.85	0/858
88	Ao	0.47	0/4626	0.84	14/6269 (0.2%)
89	Ap	0.51	0/1616	0.96	6/2195 (0.3%)
All	All	0.45	2/187395 (0.0%)	0.74	257/266151 (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
6	B4	0	1
16	BE	0	1
34	Bb	0	1
46	Bn	0	1
53	Bw	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Aj	167	PRO	CA-C	5.23	1.54	1.51
77	Ac	52	ILE	CA-CB	5.22	1.56	1.54

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bh	284	GLY	CA-C-N	12.87	132.92	120.31
40	Bh	284	GLY	C-N-CA	12.87	132.92	120.31
50	Bt	23	ARG	CA-C-N	11.56	131.15	119.82
50	Bt	23	ARG	C-N-CA	11.56	131.15	119.82
27	BT	68	PRO	N-CA-CB	9.95	113.70	103.25
37	Be	129	TYR	CA-C-N	-9.38	110.12	119.87
37	Be	129	TYR	C-N-CA	-9.38	110.12	119.87
50	Bt	25	ARG	CA-C-N	9.11	129.24	120.31
50	Bt	25	ARG	C-N-CA	9.11	129.24	120.31
64	AK	66	PRO	CA-C-N	9.08	131.19	119.84
64	AK	66	PRO	C-N-CA	9.08	131.19	119.84
69	AQ	36	ASP	CA-C-N	9.00	128.73	119.19
69	AQ	36	ASP	C-N-CA	9.00	128.73	119.19
79	Ae	215	VAL	CA-C-N	-8.76	108.90	119.84
79	Ae	215	VAL	C-N-CA	-8.76	108.90	119.84
32	BY	35	ASN	CA-C-N	8.23	128.85	120.38
32	BY	35	ASN	C-N-CA	8.23	128.85	120.38
6	B4	71	GLU	CA-C-N	8.19	127.85	119.82
6	B4	71	GLU	C-N-CA	8.19	127.85	119.82
15	BD	119	LYS	CA-C-N	7.92	127.56	119.56
15	BD	119	LYS	C-N-CA	7.92	127.56	119.56
8	B6	47	ASP	CA-C-N	7.78	127.44	119.19
8	B6	47	ASP	C-N-CA	7.78	127.44	119.19
14	BC	502	PRO	N-CA-CB	7.76	111.40	103.25
57	AB	227	ASN	CA-C-N	7.67	127.30	119.56
57	AB	227	ASN	C-N-CA	7.67	127.30	119.56
16	BE	345	ILE	N-CA-C	7.66	119.33	109.30
23	BP	9	GLY	CA-C-N	7.39	129.07	119.84
23	BP	9	GLY	C-N-CA	7.39	129.07	119.84
20	BK	160	SER	N-CA-C	7.39	120.03	111.02
57	AB	183	GLY	CA-C-N	7.34	127.69	119.32
57	AB	183	GLY	C-N-CA	7.34	127.69	119.32
85	Ak	83	VAL	CA-C-N	7.34	126.97	119.19
85	Ak	83	VAL	C-N-CA	7.34	126.97	119.19
1	CL	21	PRO	N-CA-CB	7.31	110.92	103.25
67	AO	68	PRO	CA-C-N	7.25	127.84	120.38
67	AO	68	PRO	C-N-CA	7.25	127.84	120.38
88	Ao	642	LEU	CA-C-N	7.20	126.90	119.56
88	Ao	642	LEU	C-N-CA	7.20	126.90	119.56
68	AP	25	GLY	N-CA-C	7.14	120.27	110.56
78	Ad	199	ARG	CA-C-N	7.10	126.73	119.56
78	Ad	199	ARG	C-N-CA	7.10	126.73	119.56
19	BJ	70	THR	CA-C-N	7.08	127.67	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BJ	70	THR	C-N-CA	7.08	127.67	120.38
1	CL	16	PRO	N-CA-CB	7.04	110.77	103.38
41	Bi	89	VAL	CA-C-N	7.04	127.63	120.38
41	Bi	89	VAL	C-N-CA	7.04	127.63	120.38
24	BQ	69	LEU	N-CA-C	-6.99	104.75	113.28
1	CL	17	LEU	N-CA-C	6.98	117.24	108.45
89	Ap	207	GLN	CA-C-N	6.93	124.65	119.66
89	Ap	207	GLN	C-N-CA	6.93	124.65	119.66
60	AF	90	ARG	CA-C-N	6.90	129.20	120.51
60	AF	90	ARG	C-N-CA	6.90	129.20	120.51
63	AJ	126	ILE	N-CA-C	6.90	118.89	106.61
85	Ak	149	PHE	CA-C-N	6.88	126.51	119.56
85	Ak	149	PHE	C-N-CA	6.88	126.51	119.56
16	BE	239	ARG	CA-C-N	6.86	126.54	119.82
16	BE	239	ARG	C-N-CA	6.86	126.54	119.82
39	Bg	117	LYS	CA-C-N	6.85	126.53	119.82
39	Bg	117	LYS	C-N-CA	6.85	126.53	119.82
85	Ak	76	ALA	CA-C-N	6.84	126.52	119.82
85	Ak	76	ALA	C-N-CA	6.84	126.52	119.82
67	AO	194	PRO	CA-C-N	-6.84	113.26	120.03
67	AO	194	PRO	C-N-CA	-6.84	113.26	120.03
35	Bc	263	GLY	CA-C-N	6.80	126.74	120.21
35	Bc	263	GLY	C-N-CA	6.80	126.74	120.21
49	Bq	102	GLY	N-CA-C	6.79	126.19	112.34
88	Ao	203	PRO	N-CA-CB	6.73	110.65	103.52
16	BE	201	GLY	N-CA-C	-6.72	97.24	113.18
51	Bu	167	PRO	N-CA-CB	6.65	110.23	103.25
16	BE	316	PHE	N-CA-C	6.64	121.49	108.21
47	Bo	114	GLY	N-CA-C	6.64	120.67	112.64
65	AL	112	GLY	N-CA-C	6.64	122.19	114.16
38	Bf	80	PRO	N-CA-CB	6.62	110.21	103.25
75	Aa	171	GLU	N-CA-C	6.62	118.15	111.07
16	BE	230	THR	N-CA-C	6.58	121.59	113.50
14	BC	505	PRO	N-CA-CB	6.57	110.08	102.33
79	Ae	342	PRO	N-CA-CB	6.50	110.07	103.25
37	Be	46	GLY	N-CA-C	-6.49	107.36	115.08
2	B0	74	ARG	N-CA-C	-6.42	103.34	112.13
54	Bx	135	LEU	CA-C-N	6.41	126.91	119.47
54	Bx	135	LEU	C-N-CA	6.41	126.91	119.47
1	CL	18	ASP	N-CA-C	6.41	118.80	111.11
38	Bf	78	PRO	N-CA-CB	6.37	109.94	103.25
88	Ao	274	ALA	CA-C-N	6.35	125.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	Ao	274	ALA	C-N-CA	6.35	125.97	119.56
53	Bw	357	ASP	N-CA-C	-6.35	101.08	110.48
7	B5	181	ARG	CA-C-N	6.33	126.30	119.78
7	B5	181	ARG	C-N-CA	6.33	126.30	119.78
48	Bp	21	CYS	CA-C-N	6.33	126.81	119.47
48	Bp	21	CYS	C-N-CA	6.33	126.81	119.47
89	Ap	187	THR	CA-C-N	6.32	126.89	120.38
89	Ap	187	THR	C-N-CA	6.32	126.89	120.38
34	Bb	201	ALA	CA-C-N	6.26	126.45	120.31
34	Bb	201	ALA	C-N-CA	6.26	126.45	120.31
53	Bw	381	ASN	CA-C-N	6.24	127.64	119.84
53	Bw	381	ASN	C-N-CA	6.24	127.64	119.84
38	Bf	90	LEU	N-CA-C	-6.22	105.66	113.18
79	Ae	311	GLU	N-CA-C	6.19	119.28	109.50
66	AN	83	CYS	CA-C-N	6.15	125.83	119.56
66	AN	83	CYS	C-N-CA	6.15	125.83	119.56
15	BD	128	ILE	N-CA-C	6.13	116.77	110.82
71	AU	82	ASP	CA-C-N	6.08	125.48	118.85
71	AU	82	ASP	C-N-CA	6.08	125.48	118.85
27	BT	55	GLN	CA-C-N	6.06	124.08	119.66
27	BT	55	GLN	C-N-CA	6.06	124.08	119.66
30	BW	158	GLY	N-CA-C	-6.05	103.56	111.37
36	Bd	102	PRO	N-CA-C	6.05	118.08	110.70
14	BC	235	THR	CA-C-N	6.04	126.05	119.89
14	BC	235	THR	C-N-CA	6.04	126.05	119.89
79	Ae	217	SER	N-CA-C	-6.01	105.21	112.54
31	BX	100	ALA	N-CA-C	5.99	118.71	111.40
40	Bh	187	PRO	CA-C-N	5.97	126.53	120.38
40	Bh	187	PRO	C-N-CA	5.97	126.53	120.38
16	BE	262	GLY	N-CA-C	5.97	121.89	114.37
75	Aa	228	THR	CA-C-N	5.95	125.89	119.76
75	Aa	228	THR	C-N-CA	5.95	125.89	119.76
65	AL	50	GLY	CA-C-N	5.95	125.65	119.05
65	AL	50	GLY	C-N-CA	5.95	125.65	119.05
89	Ap	103	ASN	CA-C-N	5.94	126.13	120.31
89	Ap	103	ASN	C-N-CA	5.94	126.13	120.31
53	Bw	100	LEU	CA-C-N	-5.94	114.35	123.14
53	Bw	100	LEU	C-N-CA	-5.94	114.35	123.14
57	AB	147	HIS	CA-C-N	-5.92	114.01	122.77
57	AB	147	HIS	C-N-CA	-5.92	114.01	122.77
36	Bd	165	ASP	CA-C-N	5.88	125.59	119.82
36	Bd	165	ASP	C-N-CA	5.88	125.59	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	BF	195	LEU	CA-C-N	5.86	125.56	119.82
17	BF	195	LEU	C-N-CA	5.86	125.56	119.82
54	Bx	164	ASN	N-CA-C	5.86	120.55	113.17
59	AE	378	GLY	CA-C-N	5.84	125.95	119.87
59	AE	378	GLY	C-N-CA	5.84	125.95	119.87
63	AJ	68	GLU	CA-C-N	5.83	127.13	119.84
63	AJ	68	GLU	C-N-CA	5.83	127.13	119.84
46	Bn	123	ARG	N-CA-C	5.83	120.55	113.38
33	Ba	347	THR	N-CA-C	5.82	118.70	108.75
35	Bc	131	ASP	CA-C-N	5.80	125.51	119.82
35	Bc	131	ASP	C-N-CA	5.80	125.51	119.82
84	Aj	167	PRO	O-C-N	5.78	123.97	121.31
64	AK	185	HIS	N-CA-C	-5.74	106.89	112.97
31	BX	102	GLY	N-CA-C	-5.71	107.30	115.64
53	Bw	198	ARG	CA-C-N	5.71	125.64	119.76
53	Bw	198	ARG	C-N-CA	5.71	125.64	119.76
15	BD	284	GLY	N-CA-C	-5.68	102.34	110.46
7	B5	147	GLY	CA-C-N	5.65	124.84	118.97
7	B5	147	GLY	C-N-CA	5.65	124.84	118.97
34	Bb	211	GLY	N-CA-C	-5.64	99.80	113.18
60	AF	105	CYS	N-CA-C	-5.64	101.56	109.96
77	Ac	125	HIS	CA-C-N	5.64	126.01	119.47
77	Ac	125	HIS	C-N-CA	5.64	126.01	119.47
18	BI	106	GLY	N-CA-C	5.63	118.69	110.63
88	Ao	543	HIS	CA-C-N	5.63	126.18	120.38
88	Ao	543	HIS	C-N-CA	5.63	126.18	120.38
85	Ak	214	CYS	CA-C-N	5.62	125.73	119.32
85	Ak	214	CYS	C-N-CA	5.62	125.73	119.32
82	Ah	353	ASN	CA-C-N	5.61	125.14	119.19
82	Ah	353	ASN	C-N-CA	5.61	125.14	119.19
45	Bm	133	VAL	N-CA-C	5.61	113.42	107.76
57	AB	242	PRO	N-CA-C	5.60	117.53	110.70
80	Af	109	VAL	N-CA-C	-5.59	101.02	108.96
16	BE	78	CYS	CA-C-N	5.57	124.92	118.85
16	BE	78	CYS	C-N-CA	5.57	124.92	118.85
64	AK	157	GLY	CA-C-N	5.57	125.18	119.56
64	AK	157	GLY	C-N-CA	5.57	125.18	119.56
54	Bx	63	PRO	CA-C-N	5.55	125.08	119.19
54	Bx	63	PRO	C-N-CA	5.55	125.08	119.19
68	AP	55	ASP	CA-C-N	5.55	125.07	119.19
68	AP	55	ASP	C-N-CA	5.55	125.07	119.19
77	Ac	130	GLY	CA-C-N	5.54	125.47	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	Ac	130	GLY	C-N-CA	5.54	125.47	119.76
86	Am	15	ASN	CA-C-N	5.50	124.69	118.97
86	Am	15	ASN	C-N-CA	5.50	124.69	118.97
27	BT	88	ASN	CA-C-N	5.49	125.84	119.47
27	BT	88	ASN	C-N-CA	5.49	125.84	119.47
30	BW	130	HIS	CA-C-N	-5.48	115.32	123.11
30	BW	130	HIS	C-N-CA	-5.48	115.32	123.11
39	Bg	123	SER	CA-C-N	5.48	125.09	119.56
39	Bg	123	SER	C-N-CA	5.48	125.09	119.56
79	Ae	83	ARG	N-CA-C	5.47	119.12	112.23
21	BN	130	ASP	CA-C-N	-5.46	114.69	122.77
21	BN	130	ASP	C-N-CA	-5.46	114.69	122.77
41	Bi	185	PHE	CA-C-N	-5.42	117.66	122.97
41	Bi	185	PHE	C-N-CA	-5.42	117.66	122.97
47	Bo	46	LEU	CA-C-N	5.39	126.58	119.84
47	Bo	46	LEU	C-N-CA	5.39	126.58	119.84
5	B3	78	ARG	CA-C-N	5.37	125.37	119.89
5	B3	78	ARG	C-N-CA	5.37	125.37	119.89
65	AL	95	ILE	CA-C-N	5.37	125.37	120.21
65	AL	95	ILE	C-N-CA	5.37	125.37	120.21
35	Bc	244	ASN	CA-C-N	5.37	125.44	119.32
35	Bc	244	ASN	C-N-CA	5.37	125.44	119.32
88	Ao	490	PHE	CA-C-N	5.35	125.61	119.83
88	Ao	490	PHE	C-N-CA	5.35	125.61	119.83
23	BP	130	GLN	CA-C-N	5.34	125.15	119.28
23	BP	130	GLN	C-N-CA	5.34	125.15	119.28
27	BT	188	LEU	N-CA-C	-5.32	106.84	113.38
88	Ao	92	ASP	CA-C-N	5.31	124.98	119.56
88	Ao	92	ASP	C-N-CA	5.31	124.98	119.56
67	AO	74	LEU	N-CA-C	5.29	117.12	110.24
79	Ae	86	GLU	N-CA-C	5.29	118.19	111.69
41	Bi	164	VAL	N-CA-C	5.28	115.81	110.05
16	BE	323	GLY	N-CA-C	5.27	119.06	112.73
16	BE	262	GLY	CA-C-N	-5.27	114.67	122.41
16	BE	262	GLY	C-N-CA	-5.27	114.67	122.41
36	Bd	102	PRO	CA-C-N	-5.25	114.31	119.99
36	Bd	102	PRO	C-N-CA	-5.25	114.31	119.99
88	Ao	415	ASP	N-CA-C	5.24	118.46	111.75
34	Bb	252	CYS	CA-C-N	5.23	125.17	119.78
34	Bb	252	CYS	C-N-CA	5.23	125.17	119.78
41	Bi	191	PRO	CA-C-N	5.23	125.52	119.93
41	Bi	191	PRO	C-N-CA	5.23	125.52	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	Aj	136	TYR	CA-C-N	-5.22	115.04	122.77
84	Aj	136	TYR	C-N-CA	-5.22	115.04	122.77
81	Ag	54	ASP	CA-C-N	5.22	125.53	119.47
81	Ag	54	ASP	C-N-CA	5.22	125.53	119.47
21	BN	147	GLN	CA-C-N	5.20	124.81	119.56
21	BN	147	GLN	C-N-CA	5.20	124.81	119.56
21	BN	54	GLY	N-CA-C	-5.18	100.89	113.18
78	Ad	49	ASP	CA-C-N	5.18	124.36	118.97
78	Ad	49	ASP	C-N-CA	5.18	124.36	118.97
17	BF	121	ARG	N-CA-C	5.16	119.43	113.18
77	Ac	144	GLU	N-CA-C	5.16	117.32	111.02
23	BP	191	VAL	CB-CA-C	-5.16	108.88	114.35
59	AE	141	TRP	CA-C-N	5.15	125.19	119.32
59	AE	141	TRP	C-N-CA	5.15	125.19	119.32
32	BY	93	THR	N-CA-C	5.14	117.05	108.99
86	Am	114	LYS	CA-C-N	5.13	124.44	118.85
86	Am	114	LYS	C-N-CA	5.13	124.44	118.85
67	AO	80	VAL	CA-C-N	5.13	125.05	119.76
67	AO	80	VAL	C-N-CA	5.13	125.05	119.76
24	BQ	211	ASN	CA-C-N	5.12	124.73	119.56
24	BQ	211	ASN	C-N-CA	5.12	124.73	119.56
86	Am	18	ARG	CA-C-N	5.11	125.12	119.90
86	Am	18	ARG	C-N-CA	5.11	125.12	119.90
32	BY	126	THR	N-CA-C	5.10	116.53	110.97
16	BE	304	LEU	CA-C-N	5.09	125.12	119.32
16	BE	304	LEU	C-N-CA	5.09	125.12	119.32
17	BF	126	LYS	CA-C-N	5.09	124.88	119.28
17	BF	126	LYS	C-N-CA	5.09	124.88	119.28
29	BV	72	ASP	CA-C-N	5.08	125.37	119.47
29	BV	72	ASP	C-N-CA	5.08	125.37	119.47
27	BT	240	ILE	N-CA-C	5.08	115.08	107.51
37	Be	15	ALA	CB-CA-C	-5.06	109.77	115.79
15	BD	245	VAL	N-CA-C	5.05	115.04	107.51
64	AK	185	HIS	CA-C-N	5.04	131.17	121.54
64	AK	185	HIS	C-N-CA	5.04	131.17	121.54
40	Bh	63	LYS	CA-C-N	5.03	124.47	119.24
40	Bh	63	LYS	C-N-CA	5.03	124.47	119.24
76	Ab	81	GLY	CA-C-N	5.02	124.63	119.56
76	Ab	81	GLY	C-N-CA	5.02	124.63	119.56
61	AG	217	GLY	CA-C-N	5.01	124.67	119.56
61	AG	217	GLY	C-N-CA	5.01	124.67	119.56
40	Bh	184	PHE	CA-C-N	-5.01	114.91	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bh	184	PHE	C-N-CA	-5.01	114.91	119.82
70	AR	90	GLY	N-CA-C	-5.01	108.17	115.63
88	Ao	137	ILE	CA-C-N	5.00	124.61	119.56
88	Ao	137	ILE	C-N-CA	5.00	124.61	119.56

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B4	61	ASP	Peptide
16	BE	316	PHE	Peptide
34	Bb	210	GLU	Peptide
46	Bn	65	ASN	Peptide
53	Bw	356	THR	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	BL	537	0	591	8	0
1	CL	317	0	309	16	0
1	DL	213	0	234	12	0
1	EL	222	0	247	6	0
1	FL	213	0	234	6	0
1	GL	213	0	234	4	0
1	HL	205	0	223	9	0
2	B0	857	0	878	16	0
3	B1	2036	0	2058	41	0
4	B2	1548	0	1583	27	0
5	B3	968	0	1018	32	0
6	B4	381	0	400	18	0
7	B5	902	0	916	22	0
8	B6	425	0	471	11	0
9	B7	387	0	413	10	0
10	B8	833	0	883	20	0
11	B9	335	0	359	11	0
12	BA	32950	0	16673	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	BB	1427	0	726	17	0
14	BC	4364	0	4371	78	0
15	BD	1860	0	1923	43	0
16	BE	2420	0	2418	71	0
17	BF	2011	0	2049	61	0
18	BI	805	0	845	19	0
19	BJ	1705	0	1804	49	0
20	BK	1303	0	1343	41	0
21	BN	1444	0	1437	51	0
22	BO	896	0	946	29	0
23	BP	2312	0	2373	63	0
24	BQ	1803	0	1841	28	0
25	BR	1240	0	1260	27	0
26	BS	1168	0	1159	43	0
27	BT	1954	0	1943	33	0
28	BU	1159	0	1228	27	0
29	BV	1231	0	1278	36	0
30	BW	1374	0	1405	23	0
31	BX	1181	0	1139	29	0
32	BY	1678	0	1683	41	0
33	Ba	3173	0	3153	75	0
34	Bb	2952	0	2840	87	0
35	Bc	2408	0	2415	40	0
36	Bd	832	0	828	44	0
37	Be	972	0	971	23	0
38	Bf	827	0	736	32	0
39	Bg	1167	0	1173	38	0
40	Bh	2319	0	2332	58	0
41	Bi	2138	0	2139	60	0
42	Bj	1775	0	1797	75	0
43	Bk	1087	0	1080	32	0
44	Bl	1097	0	1080	15	0
45	Bm	893	0	878	23	0
46	Bn	837	0	860	23	0
47	Bo	772	0	773	19	0
48	Bp	742	0	749	20	0
49	Bq	542	0	485	19	0
50	Bt	780	0	792	27	0
51	Bu	1198	0	1192	27	0
52	Bv	1131	0	1093	10	0
53	Bw	3126	0	3153	93	0
54	Bx	1325	0	1354	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Bz	410	0	404	6	0
56	AA	20411	0	10345	208	0
57	AB	1762	0	1774	45	0
58	AC	1075	0	1087	33	0
59	AE	2732	0	2774	71	0
60	AF	981	0	1012	26	0
61	AG	1721	0	1747	39	0
62	AI	2650	0	2613	65	0
63	AJ	1155	0	1193	42	0
64	AK	1007	0	1042	26	0
65	AL	840	0	890	22	0
66	AN	858	0	883	44	0
67	AO	1448	0	1536	28	0
68	AP	932	0	951	24	0
69	AQ	875	0	931	40	0
70	AR	784	0	813	32	0
71	AU	734	0	745	25	0
72	AV	1498	0	765	14	0
73	AX	354	0	187	7	0
74	AZ	90	0	89	4	0
75	Aa	2378	0	2392	56	0
76	Ab	1101	0	1118	27	0
77	Ac	1367	0	1385	48	0
78	Ad	1467	0	1466	34	0
79	Ae	3109	0	3029	102	0
80	Af	778	0	791	18	0
81	Ag	2875	0	2886	81	0
82	Ah	1015	0	969	34	0
83	Ai	824	0	842	25	0
84	Aj	1788	0	1799	46	0
85	Ak	2222	0	2270	64	0
86	Am	930	0	959	25	0
87	An	639	0	709	12	0
88	Ao	4526	0	4434	154	0
89	Ap	1564	0	1531	35	0
90	AA	105	0	0	0	0
90	AB	1	0	0	0	0
90	AX	1	0	0	0	0
90	Ag	1	0	0	0	0
90	An	1	0	0	0	0
90	B3	1	0	0	0	0
90	BA	202	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	BB	1	0	0	0	0
90	BC	2	0	0	0	0
90	BD	3	0	0	0	0
90	BE	1	0	0	0	0
90	BJ	1	0	0	0	0
90	BP	2	0	0	0	0
90	Be	1	0	0	0	0
90	Bl	1	0	0	0	0
90	Bt	2	0	0	0	0
91	AR	1	0	0	0	0
91	Ac	1	0	0	0	0
91	Ap	1	0	0	0	0
91	B5	1	0	0	0	0
91	B9	1	0	0	0	0
91	Bx	1	0	0	0	0
92	BA	48	0	24	0	0
93	AA	14	0	26	0	0
93	BA	14	0	26	1	0
93	BR	14	0	26	0	0
94	BC	32	0	12	1	0
95	BC	1	0	0	0	0
96	AV	10	0	10	0	0
97	Ag	32	0	12	2	0
98	Ag	3	0	0	0	0
98	BC	2	0	0	0	0
All	All	178372	0	151265	3127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (3127) 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)
37:Be:25:ARG:HG2	37:Be:25:ARG:HH11	1.04	1.17
62:AI:254:LYS:HB3	62:AI:366:ARG:HH12	1.19	1.07
26:BS:85:ARG:HB3	26:BS:120:ARG:HH12	1.20	1.05
87:An:144:ARG:HG3	87:An:144:ARG:HH11	1.23	1.02
17:BF:287:ARG:HD2	52:Bv:33:ARG:HH12	1.25	1.00
22:BO:72:ARG:HB2	22:BO:72:ARG:HH11	1.25	0.98
69:AQ:6:SER:O	69:AQ:11:LYS:NZ	1.98	0.96
56:AA:255:G:OP1	59:AE:116:LYS:NZ	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Ae:325:ARG:HH12	79:Ae:379:ARG:HH12	1.14	0.93
79:Ae:325:ARG:HH12	79:Ae:379:ARG:NH1	1.66	0.93
37:Be:25:ARG:HG2	37:Be:25:ARG:NH1	1.83	0.91
36:Bd:167:SER:O	42:Bj:203:LYS:NZ	2.04	0.91
37:Be:44:ARG:HH12	53:Bw:157:ALA:HB3	1.36	0.90
71:AU:50:ARG:HH11	71:AU:50:ARG:HG3	1.34	0.89
35:Bc:294:GLN:HE22	35:Bc:320:VAL:H	1.20	0.89
12:BA:49:A:OP1	18:BI:78:ARG:NH1	2.07	0.88
40:Bh:259:ARG:HG3	40:Bh:259:ARG:HH11	1.36	0.88
88:Ao:346:ARG:NH1	88:Ao:381:LEU:HB2	1.89	0.87
77:Ac:71:THR:HG22	77:Ac:73:SER:H	1.38	0.87
7:B5:181:ARG:HH11	7:B5:187:GLN:HG2	1.40	0.87
79:Ae:136:ARG:NH1	79:Ae:173:VAL:O	2.08	0.87
86:Am:11:ALA:HB2	86:Am:19:PRO:HG3	1.55	0.87
35:Bc:186:LEU:HG	35:Bc:189:TRP:HE1	1.39	0.87
75:Aa:221:ARG:NH1	75:Aa:224:ARG:HE	1.74	0.86
79:Ae:181:ASN:OD1	79:Ae:419:ARG:NH1	2.08	0.86
66:AN:125:ARG:HG2	66:AN:125:ARG:HH11	1.40	0.85
12:BA:748:A:OP1	53:Bw:307:LYS:NZ	2.09	0.85
34:Bb:286:ARG:NH1	34:Bb:295:GLN:O	2.10	0.85
77:Ac:51:ASN:ND2	77:Ac:95:ASN:OD1	2.09	0.85
12:BA:889:C:H41	12:BA:1082:U:H4'	1.41	0.85
28:BU:54:THR:HG21	29:BV:176:MET:H	1.40	0.85
39:Bg:17:ASN:HD21	39:Bg:23:VAL:H	1.20	0.84
26:BS:85:ARG:HB3	26:BS:120:ARG:NH1	1.90	0.84
38:Bf:126:ARG:HB2	38:Bf:126:ARG:HH11	1.43	0.84
39:Bg:144:ARG:NH1	40:Bh:260:GLN:OE1	2.09	0.84
75:Aa:198:GLU:OE2	75:Aa:204:ARG:NH1	2.11	0.84
62:AI:254:LYS:HB3	62:AI:366:ARG:NH1	1.93	0.83
88:Ao:346:ARG:NH1	88:Ao:377:TYR:O	2.11	0.83
66:AN:60:ASN:O	66:AN:68:GLN:NE2	2.10	0.83
12:BA:1216:C:H42	26:BS:173:ARG:HH22	1.24	0.83
14:BC:471:LYS:NZ	56:AA:243:G:OP1	2.11	0.83
53:Bw:213:ARG:HB2	53:Bw:213:ARG:HH11	1.44	0.83
56:AA:587:U:H5''	66:AN:33:LYS:NZ	1.94	0.82
53:Bw:97:THR:HG22	53:Bw:99:ALA:H	1.45	0.82
53:Bw:195:ASP:HB2	53:Bw:234:GLN:HB2	1.60	0.81
70:AR:125:TYR:HB3	71:AU:9:ALA:HB2	1.61	0.81
28:BU:112:THR:H	39:Bg:127:GLN:HE22	1.28	0.81
8:B6:59:GLN:HG2	8:B6:60:LYS:HG3	1.62	0.81
24:BQ:50:LEU:H	24:BQ:110:ASN:HD21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BS:86:THR:HG22	26:BS:88:HIS:H	1.45	0.81
2:B0:39:SER:N	12:BA:1156:A:HO2'	1.79	0.81
36:Bd:164:ARG:NH1	43:Bk:88:TYR:HB3	1.96	0.81
20:BK:43:GLY:HA3	20:BK:76:ARG:HH11	1.45	0.80
1:EL:76:LEU:HG	1:HL:79:ILE:HD13	1.63	0.80
10:B8:183:ARG:HH12	34:Bb:354:GLN:HE21	1.30	0.80
33:Ba:207:ASN:HB3	53:Bw:151:LEU:HD11	1.61	0.80
59:AE:197:THR:HG22	59:AE:199:GLY:H	1.45	0.80
57:AB:201:VAL:HG12	86:Am:112:PRO:HG3	1.65	0.79
87:An:144:ARG:HG3	87:An:144:ARG:NH1	1.93	0.79
17:BF:287:ARG:HD2	52:Bv:33:ARG:NH1	1.96	0.79
57:AB:219:VAL:HG22	57:AB:233:TYR:HB2	1.64	0.79
81:Ag:46:ALA:HB3	81:Ag:357:GLN:HG3	1.64	0.79
12:BA:554:U:O2'	54:Bx:102:ARG:NH1	2.15	0.79
12:BA:1287:G:H1	12:BA:1309:U:H3	1.31	0.79
16:BE:96:ARG:NH2	16:BE:197:HIS:O	2.16	0.79
20:BK:159:LEU:O	20:BK:163:GLU:N	2.16	0.79
12:BA:62:C:OP1	18:BI:76:ARG:NH1	2.17	0.78
59:AE:411:VAL:HG21	77:Ac:2:PRO:HD3	1.64	0.78
61:AG:85:VAL:HG22	81:Ag:369:LYS:HD3	1.65	0.78
12:BA:515:A:C8	12:BA:541:A:H4'	2.18	0.78
40:Bh:259:ARG:HH11	40:Bh:259:ARG:CG	1.96	0.78
56:AA:604:U:H1'	83:Ai:95:ARG:HD3	1.66	0.77
20:BK:156:VAL:HG11	20:BK:159:LEU:HD13	1.66	0.77
51:Bu:52:SER:HB2	51:Bu:57:THR:HG21	1.66	0.77
12:BA:69:C:H4'	12:BA:70:A:H5'	1.66	0.77
15:BD:163:THR:HG22	15:BD:178:ARG:HH22	1.49	0.77
66:AN:90:ARG:NH1	66:AN:95:SER:O	2.17	0.77
77:Ac:80:LEU:HD12	77:Ac:84:GLU:HB3	1.65	0.77
33:Ba:144:ARG:O	33:Ba:194:LYS:NZ	2.17	0.77
48:Bp:14:LYS:NZ	48:Bp:69:GLY:HA2	1.99	0.77
23:BP:151:LYS:NZ	23:BP:250:ASP:OD2	2.17	0.77
53:Bw:213:ARG:HB2	53:Bw:213:ARG:NH1	1.99	0.77
17:BF:83:HIS:HD2	17:BF:85:ASP:H	1.32	0.76
81:Ag:312:THR:OG1	97:Ag:500:GTP:O1G	2.01	0.76
12:BA:529:G:H4'	49:Bq:122:ARG:NH1	2.00	0.76
66:AN:53:ARG:HE	82:Ah:364:HIS:HD2	1.30	0.76
5:B3:119:ILE:H	50:Bt:45:ASN:HD21	1.31	0.76
25:BR:25:ARG:NH1	25:BR:51:GLU:OE2	2.16	0.76
78:Ad:58:GLU:OE1	78:Ad:61:ARG:NH1	2.19	0.76
1:FL:87:LYS:HG2	19:BJ:221:MET:HE3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:546:C:O2'	49:Bq:136:ARG:NH2	2.19	0.76
12:BA:1230:U:H5'	12:BA:1231:U:H5'	1.67	0.75
85:Ak:191:LYS:NZ	85:Ak:234:GLU:O	2.16	0.75
12:BA:169:U:OP2	39:Bg:114:ARG:NH2	2.19	0.75
79:Ae:258:SER:HB3	79:Ae:311:GLU:HB3	1.67	0.75
21:BN:80:HIS:HD2	21:BN:82:GLY:H	1.33	0.75
10:B8:183:ARG:NH1	34:Bb:354:GLN:HE21	1.84	0.75
31:BX:35:GLN:HG3	31:BX:36:PRO:HD2	1.69	0.75
41:Bi:186:VAL:HG22	41:Bi:187:GLU:HG3	1.66	0.75
60:AF:57:ARG:HH21	71:AU:3:ASN:HD22	1.33	0.75
5:B3:72:ILE:HD11	5:B3:118:ARG:NH1	2.01	0.75
12:BA:429:G:OP1	23:BP:62:ARG:NH2	2.20	0.74
42:Bj:123:MET:HE3	42:Bj:127:LYS:HZ1	1.52	0.74
56:AA:562:A:O2'	56:AA:708:A:N6	2.19	0.74
9:B7:74:ARG:NH2	12:BA:31:A:O2'	2.20	0.74
26:BS:160:ARG:HH12	34:Bb:126:GLN:HB3	1.52	0.74
12:BA:260:C:H42	12:BA:317:A:H61	1.32	0.74
33:Ba:350:ARG:NH1	33:Ba:384:GLN:O	2.20	0.74
2:B0:76:HIS:CD2	26:BS:70:THR:HG21	2.21	0.74
14:BC:543:GLU:HB3	14:BC:614:LEU:HD11	1.70	0.74
60:AF:58:HIS:CG	60:AF:89:ILE:HD11	2.22	0.74
75:Aa:335:SER:HB2	75:Aa:357:GLU:HG3	1.70	0.74
56:AA:29:A:H2'	56:AA:30:A:C8	2.23	0.74
23:BP:137:GLY:HA3	23:BP:157:GLN:HG3	1.69	0.74
56:AA:841:C:OP2	73:AX:8:A:N6	2.20	0.74
41:Bi:80:CYS:SG	41:Bi:165:THR:OG1	2.46	0.73
57:AB:81:ARG:HA	80:Af:84:MET:HE1	1.70	0.73
85:Ak:166:ARG:HB2	88:Ao:134:GLU:HG3	1.68	0.73
12:BA:58:C:H2'	12:BA:59:A:H5''	1.70	0.73
15:BD:247:ARG:HH12	15:BD:251:VAL:HG11	1.54	0.73
69:AQ:96:THR:HG23	78:Ad:120:ARG:HH11	1.52	0.73
31:BX:140:ARG:NH1	35:Bc:63:GLU:OE2	2.21	0.73
39:Bg:131:HIS:HD2	39:Bg:133:PHE:H	1.35	0.73
77:Ac:23:PHE:H	77:Ac:59:ASN:HD21	1.33	0.73
30:BW:77:GLN:H	30:BW:171:HIS:HD2	1.35	0.73
75:Aa:184:SER:H	75:Aa:192:ARG:HH12	1.36	0.73
4:B2:220:ARG:NH2	46:Bn:105:ASP:OD2	2.21	0.73
40:Bh:105:ARG:HB2	40:Bh:112:LYS:HD2	1.71	0.73
62:AI:150:LEU:O	62:AI:153:THR:OG1	2.05	0.73
33:Ba:333:SER:HB3	33:Ba:363:ASP:HB3	1.70	0.73
40:Bh:105:ARG:HD2	40:Bh:112:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:579:LEU:HD21	88:Ao:599:LEU:HA	1.70	0.73
42:Bj:235:LYS:HZ2	43:Bk:172:GLU:HG2	1.54	0.73
12:BA:142:U:H5''	32:BY:100:LYS:NZ	2.04	0.72
15:BD:73:THR:HG22	15:BD:75:MET:H	1.54	0.72
12:BA:229:A:H4'	12:BA:230:G:H5'	1.71	0.72
26:BS:39:VAL:HG12	26:BS:41:ASN:H	1.54	0.72
17:BF:71:GLY:H	17:BF:74:GLN:HE21	1.37	0.72
62:AI:323:ARG:HH11	62:AI:327:HIS:HE1	1.35	0.72
12:BA:975:G:O2'	12:BA:977:G:OP2	2.06	0.72
36:Bd:143:GLN:HE22	42:Bj:210:CYS:HA	1.55	0.72
65:AL:78:ARG:NH1	65:AL:117:ASP:OD2	2.22	0.72
68:AP:67:ALA:HB1	75:Aa:183:ILE:HD12	1.71	0.72
41:Bi:165:THR:HG23	41:Bi:167:ASN:H	1.54	0.72
78:Ad:166:THR:O	78:Ad:176:ARG:NH2	2.18	0.72
89:Ap:89:ARG:HB2	89:Ap:144:MET:HE3	1.72	0.72
8:B6:59:GLN:HE21	8:B6:60:LYS:HE3	1.53	0.72
28:BU:33:GLY:O	28:BU:36:ASN:ND2	2.23	0.72
88:Ao:544:PRO:HD2	88:Ao:547:LEU:HD12	1.72	0.72
31:BX:45:PRO:HD2	31:BX:48:MET:HE2	1.72	0.71
35:Bc:111:ASP:OD1	35:Bc:111:ASP:N	2.23	0.71
79:Ae:300:LEU:HD13	79:Ae:374:ARG:HD2	1.73	0.71
12:BA:486:A:H61	12:BA:582:C:H42	1.36	0.71
32:BY:122:LEU:HD23	32:BY:133:VAL:HG21	1.72	0.71
48:Bp:14:LYS:HZ1	48:Bp:69:GLY:HA2	1.53	0.71
79:Ae:126:ASP:OD1	79:Ae:164:LYS:NZ	2.23	0.71
56:AA:357:G:H5''	64:AK:91:LYS:HD3	1.72	0.71
61:AG:73:LEU:HG	62:AI:254:LYS:NZ	2.05	0.71
36:Bd:164:ARG:HH12	43:Bk:91:LEU:HD11	1.56	0.71
53:Bw:310:CYS:HB3	53:Bw:313:GLN:HG3	1.72	0.71
20:BK:43:GLY:HA3	20:BK:76:ARG:NH1	2.05	0.71
61:AG:180:ARG:HB3	61:AG:180:ARG:HH11	1.56	0.71
57:AB:57:LEU:HB2	57:AB:270:TYR:HE2	1.55	0.71
79:Ae:157:LEU:HA	79:Ae:161:ALA:HB2	1.71	0.71
12:BA:696:A:H3'	12:BA:697:C:H5''	1.73	0.70
17:BF:76:ARG:NH1	45:Bm:112:ALA:HB2	2.06	0.70
65:AL:70:PRO:HB3	65:AL:117:ASP:HB3	1.72	0.70
75:Aa:221:ARG:HH12	75:Aa:224:ARG:HE	1.37	0.70
88:Ao:485:ILE:HD12	88:Ao:491:PRO:HG3	1.71	0.70
14:BC:397:ARG:HH21	14:BC:422:ARG:HH12	1.38	0.70
58:AC:75:ASN:HD21	66:AN:104:TRP:HE1	1.39	0.70
69:AQ:65:LEU:HB2	69:AQ:85:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:Ap:91:ARG:NH2	89:Ap:103:ASN:O	2.23	0.70
37:Be:44:ARG:NH1	53:Bw:157:ALA:HB3	2.05	0.70
69:AQ:32:ARG:NH2	69:AQ:49:TYR:OH	2.25	0.70
53:Bw:231:PRO:HG2	53:Bw:234:GLN:HE21	1.55	0.70
42:Bj:51:LEU:HD22	42:Bj:192:LEU:HD21	1.73	0.70
56:AA:882:A:H2	56:AA:886:A:H61	1.36	0.70
88:Ao:258:ASN:HD21	88:Ao:288:ASN:HD22	1.40	0.70
79:Ae:318:GLU:OE2	79:Ae:383:GLN:NE2	2.25	0.70
61:AG:64:TYR:HA	61:AG:67:ASP:HB2	1.73	0.70
59:AE:160:ARG:NH1	59:AE:168:VAL:HG21	2.07	0.69
6:B4:38:ARG:NH1	36:Bd:128:GLU:HG2	2.06	0.69
12:BA:888:A:O2'	12:BA:891:A:N6	2.25	0.69
21:BN:140:ASN:HD22	40:Bh:262:GLY:HA2	1.57	0.69
12:BA:515:A:H8	12:BA:541:A:H4'	1.58	0.69
56:AA:201:A:H2'	56:AA:202:A:C8	2.26	0.69
88:Ao:326:MET:HE1	88:Ao:337:THR:HG21	1.72	0.69
48:Bp:73:ARG:HB3	54:Bx:46:THR:HG22	1.75	0.69
61:AG:152:CYS:SG	61:AG:219:VAL:HB	2.33	0.69
88:Ao:267:ARG:HH21	88:Ao:295:TYR:HB2	1.57	0.69
58:AC:125:ARG:HH21	58:AC:159:PRO:HD3	1.58	0.69
79:Ae:154:ARG:HD3	79:Ae:157:LEU:HD12	1.74	0.69
12:BA:1317:A:O2'	24:BQ:137:GLY:HA2	1.92	0.69
75:Aa:119:GLU:HA	89:Ap:131:THR:HG23	1.72	0.69
20:BK:159:LEU:HB3	20:BK:163:GLU:HG2	1.74	0.68
26:BS:130:ARG:NH1	34:Bb:129:ARG:HH11	1.91	0.68
32:BY:19:TYR:OH	32:BY:31:ASP:OD1	2.09	0.68
84:Aj:82:ARG:HG3	84:Aj:138:ASP:HB3	1.75	0.68
56:AA:826:C:H2'	56:AA:827:A:H8	1.58	0.68
24:BQ:124:VAL:HA	24:BQ:158:ARG:HH21	1.58	0.68
58:AC:96:MET:HG3	58:AC:108:LEU:HD21	1.73	0.68
88:Ao:558:ILE:HG23	88:Ao:562:TYR:CE2	2.29	0.68
33:Ba:207:ASN:HD21	33:Ba:229:ARG:HD2	1.56	0.68
38:Bf:122:ARG:HH11	38:Bf:122:ARG:HG3	1.58	0.68
56:AA:587:U:H5''	66:AN:33:LYS:HZ3	1.57	0.68
62:AI:329:MET:HE1	62:AI:349:MET:HG3	1.75	0.68
12:BA:548:A:H5''	49:Bq:126:ILE:HD11	1.75	0.68
79:Ae:100:THR:HG22	79:Ae:103:ARG:HH21	1.58	0.68
84:Aj:27:ARG:HH22	84:Aj:33:ARG:NH1	1.92	0.68
5:B3:46:PHE:O	50:Bt:50:SER:OG	2.11	0.68
19:BJ:119:HIS:CE1	19:BJ:160:LYS:HB2	2.29	0.68
70:AR:116:GLN:HG3	70:AR:121:MET:HE3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:617:PHE:HD2	88:Ao:633:LEU:HD11	1.58	0.68
17:BF:83:HIS:CD2	17:BF:85:ASP:H	2.11	0.68
75:Aa:230:VAL:O	75:Aa:236:ASN:ND2	2.27	0.68
79:Ae:211:GLU:OE2	84:Aj:78:ARG:NH1	2.20	0.68
36:Bd:164:ARG:HH11	43:Bk:88:TYR:HB3	1.58	0.68
70:AR:139:ILE:HD11	71:AU:32:MET:HG2	1.74	0.68
10:B8:172:TYR:HB2	10:B8:175:ASP:HB2	1.76	0.67
24:BQ:118:MET:HE2	24:BQ:163:MET:HE1	1.76	0.67
17:BF:113:LYS:HG3	17:BF:157:GLY:H	1.59	0.67
64:AK:76:ARG:NH1	64:AK:81:LYS:HG2	2.09	0.67
11:B9:65:THR:HG23	11:B9:100:MET:HB3	1.76	0.67
1:BL:134:LEU:HB2	1:BL:172:ILE:HD11	1.76	0.67
25:BR:41:ARG:NH1	25:BR:125:GLU:OE2	2.28	0.67
32:BY:126:THR:HB	32:BY:152:ARG:NH1	2.08	0.67
79:Ae:204:VAL:HG22	79:Ae:221:LEU:HD22	1.76	0.67
12:BA:58:C:C2'	12:BA:59:A:H5''	2.25	0.67
79:Ae:325:ARG:NH1	79:Ae:379:ARG:NH1	2.42	0.67
13:BB:26:C:OP1	34:Bb:59:ARG:NH1	2.24	0.67
14:BC:655:LYS:HZ1	14:BC:674:THR:C	2.02	0.67
42:Bj:187:THR:HG23	42:Bj:190:ARG:HH21	1.60	0.67
56:AA:142:G:OP2	84:Aj:5:LYS:NZ	2.28	0.67
65:AL:32:THR:H	65:AL:35:GLN:HE21	1.42	0.67
19:BJ:148:VAL:HG11	48:Bp:28:GLU:HG2	1.75	0.67
70:AR:77:ASN:HB2	78:Ad:188:ASN:HA	1.75	0.67
75:Aa:303:ILE:HG22	75:Aa:307:LEU:HG	1.77	0.67
35:Bc:190:MET:HE3	35:Bc:291:ARG:HH11	1.60	0.67
50:Bt:24:PRO:HG2	54:Bx:169:TRP:HB2	1.76	0.67
64:AK:150:ARG:HG2	64:AK:175:ILE:HD11	1.77	0.67
81:Ag:264:VAL:HG21	81:Ag:307:LEU:HB3	1.77	0.67
12:BA:137:A:OP1	32:BY:83:ARG:NH1	2.27	0.66
59:AE:103:LEU:HD11	59:AE:123:ARG:HB2	1.77	0.66
11:B9:71:LYS:NZ	12:BA:496:C:OP1	2.19	0.66
32:BY:130:PRO:O	32:BY:149:ARG:NH1	2.29	0.66
59:AE:292:HIS:HE1	59:AE:357:GLU:H	1.44	0.66
63:AJ:92:GLU:HG3	63:AJ:108:VAL:HG11	1.78	0.66
76:Ab:98:ARG:HB3	76:Ab:125:LEU:HD21	1.77	0.66
14:BC:285:LEU:HD13	14:BC:304:LEU:HD11	1.78	0.66
14:BC:721:THR:HG22	14:BC:723:TRP:H	1.60	0.66
27:BT:76:LEU:HD21	27:BT:282:ILE:HD11	1.75	0.66
12:BA:482:G:OP1	47:Bo:23:ALA:N	2.29	0.66
43:Bk:94:HIS:HB2	43:Bk:185:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:346:ARG:HD3	88:Ao:381:LEU:HG	1.77	0.66
12:BA:63:A:H3'	12:BA:64:C:O2	1.95	0.66
12:BA:502:U:H2'	12:BA:503:A:H5''	1.78	0.66
12:BA:1215:C:H42	12:BA:1219:A:H3'	1.60	0.66
88:Ao:427:SER:HB3	88:Ao:463:LYS:HB3	1.78	0.66
41:Bi:88:TYR:OH	41:Bi:108:ARG:NH1	2.29	0.66
6:B4:58:VAL:HG22	6:B4:64:THR:HG22	1.76	0.66
10:B8:156:LYS:NZ	12:BA:427:G:OP2	2.28	0.66
25:BR:118:ARG:HH11	25:BR:118:ARG:HG3	1.60	0.66
61:AG:190:GLU:HG3	61:AG:194:LYS:HD2	1.77	0.66
74:AZ:703:ALA:HA	74:AZ:708:ALA:HB3	1.78	0.66
23:BP:47:ARG:HH11	29:BV:183:ASN:HB2	1.61	0.66
26:BS:115:HIS:HD2	34:Bb:135:VAL:HG22	1.60	0.65
38:Bf:122:ARG:HG3	38:Bf:122:ARG:NH1	2.10	0.65
79:Ae:86:GLU:HG2	79:Ae:114:ARG:HG2	1.78	0.65
3:B1:85:TRP:HD1	3:B1:107:PRO:HD2	1.62	0.65
35:Bc:141:ARG:NH1	35:Bc:263:GLY:HA3	2.11	0.65
47:Bo:63:GLN:HE21	47:Bo:66:ARG:NH1	1.94	0.65
7:B5:127:TYR:OH	25:BR:43:GLU:OE1	2.14	0.65
53:Bw:401:ASP:O	53:Bw:402:ASN:ND2	2.27	0.65
34:Bb:240:ILE:HD13	34:Bb:248:GLY:HA3	1.78	0.65
56:AA:901:A:O3'	87:An:171:ARG:NH1	2.29	0.65
59:AE:283:GLU:OE2	76:Ab:21:ARG:NH1	2.29	0.65
77:Ac:36:THR:H	77:Ac:69:ASN:HD21	1.42	0.65
6:B4:61:ASP:HB3	6:B4:63:SER:H	1.61	0.65
21:BN:8:PRO:HB2	40:Bh:285:PRO:HG2	1.78	0.65
65:AL:78:ARG:HG3	65:AL:118:LEU:HD21	1.79	0.65
79:Ae:312:ASP:HB2	79:Ae:314:GLN:HE21	1.62	0.65
82:Ah:345:LEU:HD11	83:Ai:26:THR:HG21	1.79	0.65
17:BF:249:ASN:ND2	17:BF:252:SER:H	1.95	0.65
33:Ba:387:TRP:HE1	33:Ba:404:ILE:HD11	1.60	0.65
60:AF:58:HIS:CD2	60:AF:89:ILE:HD11	2.31	0.65
12:BA:145:A:H2'	12:BA:146:A:C8	2.32	0.65
12:BA:666:G:H5''	12:BA:779:G:O2'	1.96	0.65
88:Ao:536:MET:SD	88:Ao:581:TYR:OH	2.55	0.65
2:B0:124:ALA:O	34:Bb:51:TYR:OH	2.15	0.65
15:BD:111:ARG:NH1	15:BD:182:ALA:HB2	2.11	0.65
21:BN:15:ALA:HB1	40:Bh:269:VAL:HG21	1.78	0.65
80:Af:113:LEU:HD21	80:Af:127:ARG:HB2	1.79	0.65
32:BY:144:VAL:HG11	32:BY:153:ILE:HD12	1.79	0.65
56:AA:901:A:O2'	87:An:171:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AF:3:ARG:NH1	60:AF:70:ALA:O	2.29	0.65
63:AJ:52:VAL:HG21	88:Ao:479:LYS:HB3	1.78	0.65
7:B5:152:PRO:HG3	7:B5:173:ARG:NH1	2.12	0.64
56:AA:106:C:OP2	69:AQ:45:LYS:NZ	2.30	0.64
56:AA:212:A:H5'	77:Ac:162:LYS:HB2	1.77	0.64
82:Ah:288:ASN:HD21	85:Ak:73:PRO:HG3	1.61	0.64
16:BE:317:PRO:HG2	16:BE:320:PHE:HE2	1.62	0.64
27:BT:233:TRP:HB3	27:BT:240:ILE:HD12	1.79	0.64
79:Ae:224:TYR:HA	79:Ae:227:TYR:HD1	1.63	0.64
12:BA:660:C:O3'	25:BR:81:THR:HG21	1.98	0.64
16:BE:90:TRP:HA	16:BE:316:PHE:HE2	1.63	0.64
39:Bg:73:PRO:HB2	39:Bg:89:ILE:HG13	1.80	0.64
41:Bi:235:GLN:HB2	41:Bi:238:VAL:HG12	1.78	0.64
42:Bj:257:LYS:NZ	42:Bj:273:ARG:HB2	2.12	0.64
68:AP:108:GLU:OE2	78:Ad:59:ARG:NH2	2.30	0.64
75:Aa:184:SER:H	75:Aa:192:ARG:NH1	1.94	0.64
10:B8:97:PHE:H	46:Bn:122:ASN:HD21	1.44	0.64
14:BC:570:VAL:HG13	14:BC:592:LYS:HG3	1.80	0.64
21:BN:80:HIS:CD2	21:BN:82:GLY:H	2.14	0.64
22:BO:72:ARG:HB2	22:BO:72:ARG:NH1	2.07	0.64
22:BO:75:LEU:HD23	22:BO:77:ILE:HD11	1.80	0.64
40:Bh:259:ARG:HB2	40:Bh:271:PHE:HB2	1.78	0.64
77:Ac:105:ILE:HG22	77:Ac:106:LEU:HG	1.79	0.64
1:HL:87:LYS:HG3	19:BJ:232:LEU:HD11	1.79	0.64
5:B3:73:LYS:NZ	12:BA:471:U:OP1	2.30	0.64
51:Bu:75:ARG:NH1	51:Bu:108:ASP:OD1	2.31	0.64
60:AF:105:CYS:HB3	70:AR:69:CYS:SG	2.36	0.64
61:AG:240:ARG:NH2	86:Am:44:THR:O	2.31	0.64
31:BX:140:ARG:HG2	31:BX:140:ARG:HH11	1.62	0.64
25:BR:142:ASN:O	25:BR:148:GLN:NE2	2.31	0.64
56:AA:202:A:C2	78:Ad:46:PRO:HG2	2.32	0.64
88:Ao:446:ASP:O	88:Ao:450:LEU:HG	1.97	0.64
4:B2:175:PHE:O	4:B2:214:ARG:NH2	2.31	0.64
12:BA:1213:A:H2	12:BA:1220:A:H62	1.44	0.64
85:Ak:69:PRO:HB3	85:Ak:120:ALA:HB2	1.80	0.64
7:B5:90:ASN:OD1	7:B5:93:ARG:NH2	2.31	0.63
15:BD:103:ARG:HB2	15:BD:103:ARG:HH11	1.63	0.63
19:BJ:95:MET:HB3	19:BJ:156:SER:HB2	1.80	0.63
34:Bb:308:GLN:NE2	47:Bo:111:LYS:H	1.96	0.63
53:Bw:369:ASN:H	53:Bw:385:ASN:HD22	1.46	0.63
3:B1:196:ILE:HG12	3:B1:197:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B3:75:THR:HB	5:B3:83:LYS:HG2	1.80	0.63
12:BA:477:A:O2'	29:BV:192:ASN:ND2	2.29	0.63
23:BP:14:ASP:OD1	23:BP:17:ARG:NH1	2.31	0.63
36:Bd:136:ILE:HG13	43:Bk:173:ILE:HD11	1.80	0.63
45:Bm:114:PRO:HG2	45:Bm:117:ARG:HG3	1.79	0.63
53:Bw:201:HIS:CD2	53:Bw:228:ASN:HD22	2.16	0.63
81:Ag:173:ASN:O	81:Ag:176:ARG:NH1	2.32	0.63
14:BC:673:LEU:HD23	14:BC:696:LEU:HD23	1.80	0.63
29:BV:136:LYS:NZ	47:Bo:48:ASP:HB3	2.13	0.63
64:AK:175:ILE:HG13	64:AK:176:SER:H	1.62	0.63
33:Ba:108:HIS:HD2	33:Ba:110:ARG:H	1.47	0.63
67:AO:127:GLU:HG2	67:AO:178:VAL:HG11	1.81	0.63
12:BA:143:A:H2'	12:BA:144:A:C8	2.33	0.63
14:BC:392:CYS:HB3	14:BC:423:ASP:HB2	1.79	0.63
20:BK:122:ARG:HB3	20:BK:137:LEU:HD21	1.80	0.63
42:Bj:235:LYS:NZ	43:Bk:172:GLU:HG2	2.12	0.63
60:AF:67:ASP:N	60:AF:67:ASP:OD1	2.31	0.63
61:AG:73:LEU:HG	62:AI:254:LYS:HZ3	1.62	0.63
64:AK:181:THR:H	71:AU:10:ARG:HH12	1.46	0.63
50:Bt:99:ARG:CG	50:Bt:99:ARG:HH11	2.12	0.63
76:Ab:30:LEU:H	76:Ab:30:LEU:HD12	1.63	0.63
1:CL:36:ALA:HB1	1:FL:77:LEU:HG	1.79	0.63
3:B1:144:TYR:O	3:B1:148:THR:OG1	2.14	0.63
12:BA:516:G:O2'	12:BA:533:A:OP2	2.17	0.63
32:BY:29:LEU:HD12	41:Bi:68:PRO:HG3	1.81	0.63
36:Bd:97:LYS:HA	36:Bd:99:ARG:NH1	2.14	0.63
42:Bj:257:LYS:HZ3	42:Bj:273:ARG:HB2	1.64	0.63
12:BA:909:U:H5'	12:BA:910:U:OP2	1.99	0.63
43:Bk:86:TYR:HE1	43:Bk:88:TYR:HD1	1.44	0.63
88:Ao:126:LYS:HA	88:Ao:129:GLN:HG2	1.81	0.63
39:Bg:78:GLU:HG3	39:Bg:84:VAL:HG22	1.80	0.63
23:BP:234:LEU:HB3	51:Bu:66:LYS:NZ	2.14	0.62
53:Bw:244:PHE:HE2	53:Bw:365:CYS:HB3	1.64	0.62
56:AA:825:C:H5''	86:Am:38:ARG:HH12	1.64	0.62
88:Ao:404:MET:SD	88:Ao:437:GLN:HB3	2.39	0.62
88:Ao:551:PHE:HB3	88:Ao:585:LEU:HD13	1.81	0.62
34:Bb:238:THR:HG21	34:Bb:281:PHE:CZ	2.34	0.62
46:Bn:77:PRO:HG2	46:Bn:80:LEU:HB2	1.80	0.62
79:Ae:311:GLU:HA	79:Ae:388:VAL:HG21	1.80	0.62
12:BA:392:U:H2'	12:BA:393:A:H8	1.64	0.62
23:BP:20:PRO:HD3	50:Bt:99:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:465:PHE:HE2	88:Ao:499:LEU:HD21	1.64	0.62
54:Bx:135:LEU:H	54:Bx:139:PHE:HE1	1.46	0.62
88:Ao:443:ASN:HA	88:Ao:447:ASN:HB3	1.81	0.62
46:Bn:69:HIS:HD2	46:Bn:71:LYS:H	1.47	0.62
46:Bn:69:HIS:CD2	46:Bn:71:LYS:HG3	2.34	0.62
79:Ae:100:THR:HG22	79:Ae:103:ARG:NH2	2.14	0.62
81:Ag:383:SER:HB3	81:Ag:393:LEU:HD12	1.80	0.62
33:Ba:193:LEU:HD13	53:Bw:184:VAL:HA	1.80	0.62
53:Bw:393:LYS:HB2	53:Bw:393:LYS:NZ	2.14	0.62
59:AE:160:ARG:HH11	59:AE:168:VAL:HG21	1.65	0.62
84:Aj:82:ARG:HH12	84:Aj:133:GLN:HB2	1.64	0.62
10:B8:113:ARG:NH2	12:BA:84:G:OP2	2.33	0.62
68:AP:102:MET:HE1	78:Ad:56:LEU:HD11	1.82	0.62
3:B1:85:TRP:CD1	3:B1:107:PRO:HD2	2.35	0.62
24:BQ:36:VAL:HG23	49:Bq:128:ARG:HD2	1.81	0.62
41:Bi:126:ARG:HH12	41:Bi:134:ILE:HG12	1.64	0.62
56:AA:956:G:O6	71:AU:50:ARG:NH2	2.32	0.62
59:AE:317:HIS:HD2	59:AE:319:ALA:H	1.48	0.62
74:AZ:695:ALA:HB2	83:Ai:10:ARG:NH1	2.15	0.62
7:B5:161:SER:OG	7:B5:178:GLU:O	2.16	0.62
56:AA:552:A:H2'	56:AA:553:G:C8	2.34	0.62
75:Aa:217:VAL:HG22	75:Aa:226:ILE:HD13	1.81	0.62
81:Ag:161:VAL:HG22	81:Ag:289:ILE:HD11	1.80	0.62
2:B0:100:THR:HG23	34:Bb:73:THR:HA	1.81	0.61
56:AA:471:U:OP2	76:Ab:50:ARG:NH2	2.32	0.61
75:Aa:282:ASP:HA	75:Aa:285:ARG:HG2	1.81	0.61
12:BA:1463:A:H5''	14:BC:266:MET:HE2	1.80	0.61
12:BA:1552:C:H5'	12:BA:1553:A:OP1	2.00	0.61
17:BF:249:ASN:HD21	17:BF:252:SER:H	1.48	0.61
21:BN:109:TYR:HD2	21:BN:122:MET:HE3	1.65	0.61
62:AI:323:ARG:HH11	62:AI:327:HIS:CE1	2.15	0.61
69:AQ:95:VAL:CG1	78:Ad:120:ARG:HH12	2.13	0.61
79:Ae:99:LYS:HE3	79:Ae:103:ARG:HD3	1.82	0.61
1:EL:79:ILE:HD13	1:HL:76:LEU:HG	1.82	0.61
4:B2:232:LYS:NZ	12:BA:10:A:OP1	2.33	0.61
21:BN:74:GLN:HE22	54:Bx:175:PRO:HD2	1.64	0.61
23:BP:51:ARG:NH1	23:BP:57:ARG:O	2.33	0.61
35:Bc:190:MET:HE3	35:Bc:291:ARG:NH1	2.16	0.61
63:AJ:89:ASP:OD1	63:AJ:141:ARG:NH2	2.34	0.61
81:Ag:54:ASP:HB3	81:Ag:57:LYS:HB2	1.82	0.61
84:Aj:132:GLU:HG3	84:Aj:207:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B3:43:ASP:OD1	5:B3:43:ASP:N	2.32	0.61
7:B5:85:ARG:NH1	12:BA:642:G:OP1	2.33	0.61
12:BA:1549:A:H2	38:Bf:104:GLU:HG2	1.65	0.61
63:AJ:128:LYS:HG2	63:AJ:131:ARG:HH21	1.64	0.61
63:AJ:151:SER:HB2	85:Ak:133:THR:HG22	1.81	0.61
16:BE:129:VAL:HG23	16:BE:189:PRO:HA	1.81	0.61
29:BV:131:ARG:NH1	29:BV:161:GLU:OE1	2.28	0.61
14:BC:395:LYS:NZ	56:AA:187:U:OP1	2.27	0.61
21:BN:20:LEU:HB2	21:BN:141:LEU:HD13	1.82	0.61
62:AI:124:ILE:HG23	62:AI:126:LYS:HG3	1.82	0.61
63:AJ:59:THR:HG22	63:AJ:61:PRO:HD3	1.81	0.61
88:Ao:343:LYS:HE2	88:Ao:347:ARG:HH21	1.65	0.61
28:BU:112:THR:H	39:Bg:127:GLN:NE2	1.98	0.61
81:Ag:107:LEU:HD22	81:Ag:342:ILE:HD12	1.81	0.61
88:Ao:539:ALA:HB2	88:Ao:581:TYR:HE1	1.66	0.61
12:BA:392:U:H2'	12:BA:393:A:C8	2.35	0.61
15:BD:111:ARG:HH11	15:BD:182:ALA:HB2	1.65	0.61
32:BY:109:ILE:HD13	41:Bi:76:ILE:HG21	1.83	0.61
64:AK:99:ILE:HD11	64:AK:163:ALA:HB1	1.83	0.61
79:Ae:154:ARG:NH2	79:Ae:416:TYR:OH	2.33	0.61
87:An:173:LEU:HD12	87:An:191:THR:HG23	1.82	0.61
88:Ao:118:LYS:HA	88:Ao:121:ILE:HD12	1.81	0.61
1:DL:90:LEU:HD22	19:BJ:214:LEU:HD13	1.82	0.61
3:B1:156:LYS:NZ	3:B1:205:GLY:O	2.33	0.61
58:AC:148:LYS:NZ	88:Ao:128:PHE:O	2.30	0.61
14:BC:182:VAL:HG12	14:BC:252:THR:HG22	1.82	0.61
30:BW:77:GLN:H	30:BW:171:HIS:CD2	2.18	0.61
33:Ba:153:ARG:HH11	33:Ba:187:LEU:HD22	1.64	0.61
80:Af:155:LEU:HD11	86:Am:27:LEU:HB3	1.82	0.61
12:BA:166:A:H5''	39:Bg:2:THR:HG21	1.83	0.60
15:BD:290:LEU:HD12	15:BD:291:PRO:HD2	1.83	0.60
33:Ba:115:GLU:H	33:Ba:119:GLN:HE21	1.47	0.60
53:Bw:265:LEU:HD23	53:Bw:267:LEU:HG	1.82	0.60
53:Bw:278:ILE:HD11	53:Bw:333:GLN:HG2	1.83	0.60
56:AA:882:A:H5'	79:Ae:108:SER:HB3	1.83	0.60
59:AE:220:THR:HB	59:AE:247:VAL:HG12	1.83	0.60
84:Aj:132:GLU:HG2	84:Aj:133:GLN:HG3	1.83	0.60
67:AO:69:PRO:HD2	67:AO:72:MET:HG3	1.82	0.60
84:Aj:68:LEU:HD21	84:Aj:97:LEU:HD13	1.83	0.60
18:BI:115:LYS:HE3	18:BI:117:SER:HB2	1.83	0.60
42:Bj:162:ARG:HH21	42:Bj:164:LYS:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AB:151:ALA:HA	57:AB:167:THR:HG21	1.82	0.60
72:AV:3:U:H3	72:AV:65:A:H61	1.48	0.60
79:Ae:276:LEU:HD13	79:Ae:328:LYS:HD2	1.82	0.60
85:Ak:196:VAL:HG12	85:Ak:199:ARG:HB2	1.83	0.60
85:Ak:196:VAL:HG11	85:Ak:207:LEU:HD11	1.81	0.60
14:BC:176:LEU:HB3	14:BC:348:LYS:HB3	1.83	0.60
42:Bj:47:LEU:HB3	42:Bj:178:TRP:NE1	2.17	0.60
14:BC:180:SER:OG	14:BC:229:LYS:O	2.19	0.60
26:BS:130:ARG:HH11	34:Bb:129:ARG:NH1	1.98	0.60
40:Bh:121:ASP:N	40:Bh:121:ASP:OD1	2.33	0.60
12:BA:707:A:N1	53:Bw:97:THR:HG23	2.17	0.60
14:BC:188:HIS:HA	14:BC:268:GLN:HB2	1.82	0.60
34:Bb:224:HIS:CD2	34:Bb:227:GLU:H	2.19	0.60
59:AE:370:VAL:HG13	59:AE:385:ALA:HB3	1.83	0.60
61:AG:71:THR:O	62:AI:254:LYS:NZ	2.30	0.60
12:BA:142:U:H5''	32:BY:100:LYS:HZ3	1.66	0.60
12:BA:188:C:H3'	29:BV:181:ARG:NH2	2.17	0.60
17:BF:262:THR:HG22	17:BF:264:PRO:HD2	1.84	0.60
22:BO:99:ARG:HH12	27:BT:191:ARG:NH2	1.99	0.60
24:BQ:209:ASN:HD22	24:BQ:210:GLN:N	1.99	0.60
27:BT:188:LEU:HB3	27:BT:191:ARG:NH1	2.16	0.60
33:Ba:149:ASN:OD1	33:Ba:149:ASN:N	2.32	0.60
35:Bc:156:LYS:HB2	38:Bf:89:ASP:H	1.66	0.60
36:Bd:169:PHE:HB2	36:Bd:170:PRO:HD3	1.84	0.60
57:AB:79:SER:H	57:AB:82:SER:HB3	1.67	0.60
81:Ag:259:VAL:HB	81:Ag:305:ILE:HG22	1.83	0.60
12:BA:164:A:OP1	28:BU:52:LYS:NZ	2.33	0.60
36:Bd:100:GLN:HG2	42:Bj:84:TYR:HA	1.82	0.60
39:Bg:28:ARG:HB3	39:Bg:28:ARG:NH1	2.16	0.60
5:B3:121:PRO:HG3	50:Bt:48:TRP:CH2	2.37	0.60
77:Ac:56:GLN:HB2	77:Ac:64:ILE:HD12	1.81	0.60
12:BA:148:A:H4'	12:BA:149:A:H5''	1.82	0.60
27:BT:96:ARG:NH1	27:BT:285:GLU:OE1	2.35	0.60
30:BW:131:ASN:O	41:Bi:230:ARG:NH2	2.35	0.60
75:Aa:184:SER:O	75:Aa:192:ARG:NH2	2.29	0.60
26:BS:59:LEU:HB3	26:BS:61:VAL:HG23	1.83	0.59
41:Bi:267:PRO:HG2	41:Bi:270:ALA:HB2	1.84	0.59
53:Bw:118:LEU:HG	53:Bw:119:PRO:HD2	1.83	0.59
70:AR:141:TYR:O	71:AU:28:ARG:NH1	2.33	0.59
1:EL:76:LEU:HA	1:EL:79:ILE:HD12	1.83	0.59
3:B1:6:VAL:HB	52:Bv:46:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:1548:A:H3'	12:BA:1549:A:H5'	1.83	0.59
19:BJ:97:ALA:HB1	19:BJ:176:LEU:HD11	1.84	0.59
58:AC:75:ASN:HD21	66:AN:104:TRP:NE1	1.99	0.59
88:Ao:543:HIS:HD2	88:Ao:588:ARG:HG3	1.67	0.59
5:B3:65:LYS:HG2	47:Bo:84:MET:HE3	1.82	0.59
15:BD:258:ILE:HG23	15:BD:263:ARG:HB3	1.83	0.59
16:BE:181:VAL:HG13	16:BE:185:ALA:HB3	1.84	0.59
42:Bj:123:MET:HE3	42:Bj:127:LYS:NZ	2.17	0.59
56:AA:750:G:N1	56:AA:776:A:OP2	2.24	0.59
59:AE:291:TYR:H	59:AE:356:GLN:HE21	1.50	0.59
75:Aa:298:VAL:HA	75:Aa:303:ILE:HD11	1.84	0.59
12:BA:539:U:O4	12:BA:540:A:N6	2.36	0.59
43:Bk:127:MET:HE2	43:Bk:128:PRO:HD2	1.85	0.59
62:AI:302:LEU:HD22	81:Ag:384:ASN:HB3	1.84	0.59
66:AN:58:ARG:HD3	66:AN:72:ASP:HA	1.84	0.59
88:Ao:565:GLN:HB2	88:Ao:572:PRO:HG3	1.85	0.59
14:BC:396:VAL:HG11	14:BC:399:MET:HE2	1.84	0.59
32:BY:131:THR:HG21	32:BY:147:SER:HB3	1.83	0.59
50:Bt:99:ARG:HH11	50:Bt:99:ARG:HB2	1.68	0.59
88:Ao:335:LEU:HD11	88:Ao:370:PRO:HA	1.82	0.59
88:Ao:603:ARG:HD2	88:Ao:636:LEU:HD13	1.85	0.59
29:BV:99:LEU:HD23	29:BV:142:ALA:HB2	1.85	0.59
43:Bk:111:HIS:CE1	43:Bk:121:VAL:HG11	2.37	0.59
56:AA:811:U:H5'	63:AJ:131:ARG:HH12	1.67	0.59
66:AN:91:CYS:SG	66:AN:94:THR:HG22	2.43	0.59
88:Ao:403:VAL:HG12	88:Ao:441:LEU:HD11	1.85	0.59
12:BA:1241:U:H4'	12:BA:1242:U:OP1	2.03	0.59
12:BA:1548:A:H5'	12:BA:1549:A:OP2	2.03	0.59
20:BK:166:ALA:O	20:BK:169:LYS:N	2.35	0.59
27:BT:80:PHE:HB3	27:BT:282:ILE:HD12	1.84	0.59
62:AI:396:LYS:NZ	72:AV:31:C:OP2	2.29	0.59
69:AQ:96:THR:HG23	78:Ad:120:ARG:NH1	2.18	0.59
6:B4:55:VAL:HG21	6:B4:69:TYR:HB3	1.84	0.59
35:Bc:294:GLN:HE22	35:Bc:320:VAL:N	1.97	0.59
56:AA:29:A:H2'	56:AA:30:A:H8	1.66	0.59
58:AC:84:GLU:HB2	58:AC:85:ARG:NH1	2.18	0.59
88:Ao:532:GLU:O	88:Ao:536:MET:HG2	2.03	0.59
13:BB:44:U:H2'	13:BB:45:A:C8	2.37	0.59
21:BN:27:PRO:HG2	21:BN:30:LYS:HB2	1.84	0.59
43:Bk:147:ASP:N	43:Bk:147:ASP:OD1	2.34	0.59
56:AA:136:C:O2	67:AO:198:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Bh:184:PHE:O	40:Bh:186:VAL:HG23	2.03	0.59
56:AA:223:U:O2'	56:AA:224:U:OP1	2.20	0.59
51:Bu:132:LEU:HD21	51:Bu:156:MET:HE1	1.84	0.58
78:Ad:73:GLU:O	78:Ad:76:SER:OG	2.18	0.58
8:B6:16:ILE:HD11	8:B6:61:LYS:HG3	1.85	0.58
12:BA:1216:C:OP2	12:BA:1219:A:N6	2.35	0.58
16:BE:187:ILE:HG22	16:BE:188:LYS:H	1.67	0.58
56:AA:455:A:N7	56:AA:935:G:O2'	2.35	0.58
56:AA:728:U:H2'	56:AA:729:A:H8	1.66	0.58
62:AI:397:ARG:NH2	72:AV:30:C:OP2	2.33	0.58
71:AU:75:LEU:HD11	86:Am:111:PHE:HB2	1.84	0.58
79:Ae:117:ASP:OD2	79:Ae:427:ARG:NH2	2.34	0.58
87:An:144:ARG:HH11	87:An:144:ARG:CG	2.06	0.58
88:Ao:527:ARG:HB3	88:Ao:531:LYS:HZ1	1.68	0.58
26:BS:149:THR:HG22	26:BS:150:PRO:HD2	1.85	0.58
41:Bi:254:ASP:OD2	41:Bi:257:GLY:N	2.36	0.58
67:AO:168:LEU:HD11	67:AO:188:ILE:HG21	1.86	0.58
79:Ae:119:ILE:HG23	79:Ae:124:ASP:HB2	1.84	0.58
1:HL:76:LEU:HA	1:HL:79:ILE:HD12	1.85	0.58
15:BD:177:ALA:HB1	15:BD:245:VAL:HG11	1.85	0.58
34:Bb:308:GLN:HE22	47:Bo:111:LYS:H	1.50	0.58
81:Ag:252:LEU:HB2	81:Ag:254:ILE:HG22	1.85	0.58
82:Ah:335:LYS:O	82:Ah:340:ARG:HG3	2.03	0.58
20:BK:17:SER:N	20:BK:72:VAL:O	2.36	0.58
22:BO:99:ARG:HH12	27:BT:191:ARG:HH21	1.49	0.58
34:Bb:120:GLU:HG2	34:Bb:124:ARG:HE	1.67	0.58
40:Bh:59:ARG:NH1	40:Bh:181:SER:O	2.37	0.58
75:Aa:194:ILE:HG12	75:Aa:211:ARG:NH1	2.19	0.58
5:B3:72:ILE:HD11	5:B3:118:ARG:CZ	2.33	0.58
12:BA:1230:U:H5'	12:BA:1231:U:C5'	2.32	0.58
14:BC:183:VAL:HG22	14:BC:254:ILE:HB	1.86	0.58
65:AL:61:VAL:HG12	65:AL:107:VAL:HG12	1.85	0.58
81:Ag:116:PHE:HB3	81:Ag:302:GLY:HA2	1.86	0.58
17:BF:192:SER:OG	17:BF:193:LEU:N	2.37	0.58
19:BJ:103:ALA:HB3	48:Bp:39:SER:HA	1.85	0.58
26:BS:107:THR:HB	26:BS:119:THR:HG23	1.86	0.58
33:Ba:192:ILE:HD11	33:Ba:199:ALA:HB2	1.84	0.58
39:Bg:35:ARG:HG2	45:Bm:159:TYR:CZ	2.39	0.58
56:AA:441:U:H2'	56:AA:442:A:H8	1.69	0.58
85:Ak:151:ILE:HG12	85:Ak:177:VAL:HG22	1.86	0.58
16:BE:76:LYS:NZ	16:BE:168:LEU:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BP:264:GLN:NE2	23:BP:269:LEU:O	2.33	0.58
44:Bl:77:ASP:HB2	44:Bl:78:PRO:HD3	1.86	0.58
56:AA:90:U:H5'	78:Ad:68:ARG:HH21	1.68	0.58
82:Ah:309:ASN:HD21	85:Ak:158:TYR:H	1.51	0.58
88:Ao:427:SER:HA	88:Ao:467:LEU:HD21	1.86	0.58
14:BC:161:LYS:HB2	14:BC:163:LYS:HE2	1.86	0.58
22:BO:64:THR:HG22	22:BO:66:VAL:H	1.69	0.58
30:BW:66:ARG:NH1	41:Bi:230:ARG:NH1	2.52	0.58
32:BY:98:VAL:HG21	32:BY:109:ILE:HD12	1.86	0.58
56:AA:195:G:H5''	68:AP:20:ARG:HB2	1.85	0.58
75:Aa:230:VAL:HG13	75:Aa:233:LYS:NZ	2.19	0.58
85:Ak:196:VAL:HG12	85:Ak:199:ARG:HD3	1.85	0.58
3:B1:119:LEU:HA	3:B1:168:ARG:NH1	2.18	0.58
11:B9:82:ARG:N	12:BA:1527:U:OP1	2.36	0.58
15:BD:133:ASP:OD2	15:BD:136:ARG:NH1	2.36	0.58
75:Aa:311:ILE:HD13	75:Aa:368:LEU:HD13	1.84	0.58
88:Ao:440:GLY:O	88:Ao:444:THR:OG1	2.22	0.58
79:Ae:147:TRP:O	79:Ae:151:THR:HG23	2.05	0.57
89:Ap:217:ARG:HG2	89:Ap:224:LEU:HD21	1.86	0.57
20:BK:155:VAL:HB	49:Bq:101:VAL:HG13	1.85	0.57
28:BU:97:LEU:HA	29:BV:109:GLN:HE22	1.69	0.57
36:Bd:99:ARG:H	36:Bd:99:ARG:HD3	1.68	0.57
56:AA:213:G:OP1	77:Ac:162:LYS:NZ	2.36	0.57
26:BS:130:ARG:HH11	34:Bb:129:ARG:HH11	1.53	0.57
42:Bj:170:ILE:HG22	42:Bj:172:MET:HB2	1.86	0.57
48:Bp:76:MET:HE3	54:Bx:49:ILE:HD12	1.86	0.57
62:AI:111:LEU:HD22	85:Ak:114:LEU:HD23	1.87	0.57
84:Aj:178:ARG:HH22	84:Aj:189:PRO:HD3	1.69	0.57
88:Ao:558:ILE:HG23	88:Ao:562:TYR:HE2	1.68	0.57
14:BC:562:ASN:OD1	14:BC:589:LYS:NZ	2.36	0.57
30:BW:131:ASN:HD22	41:Bi:278:LYS:HD3	1.69	0.57
36:Bd:151:ARG:HG2	36:Bd:158:HIS:HB3	1.86	0.57
53:Bw:213:ARG:HH11	53:Bw:213:ARG:CB	2.16	0.57
60:AF:32:ARG:HB2	60:AF:78:MET:HE3	1.86	0.57
85:Ak:89:MET:HG2	85:Ak:90:GLY:H	1.69	0.57
12:BA:1092:A:H5'	12:BA:1093:A:OP2	2.04	0.57
14:BC:215:GLN:HE22	14:BC:598:ILE:HA	1.69	0.57
20:BK:64:ILE:HG21	20:BK:90:PHE:HE1	1.69	0.57
53:Bw:128:GLU:O	53:Bw:130:THR:N	2.37	0.57
56:AA:301:U:H5'	67:AO:159:MET:HE3	1.86	0.57
34:Bb:72:ARG:HH11	34:Bb:72:ARG:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Bf:121:HIS:H	38:Bf:121:HIS:CD2	2.22	0.57
40:Bh:278:ARG:HB2	40:Bh:278:ARG:HH11	1.70	0.57
56:AA:884:C:H5'	79:Ae:143:TYR:HE2	1.69	0.57
59:AE:225:VAL:HG23	59:AE:243:VAL:HG12	1.86	0.57
59:AE:308:GLN:HG3	59:AE:312:TYR:CD1	2.39	0.57
62:AI:115:GLY:HA3	63:AJ:84:ASP:HB2	1.87	0.57
79:Ae:106:PRO:HB2	79:Ae:140:ASN:HD21	1.69	0.57
9:B7:66:LYS:NZ	12:BA:254:G:OP1	2.21	0.57
12:BA:1569:A:H4'	16:BE:62:LYS:HG2	1.86	0.57
32:BY:87:VAL:HG11	41:Bi:74:ARG:HH11	1.70	0.57
12:BA:1302:U:OP1	12:BA:1360:U:O2'	2.14	0.57
21:BN:71:LYS:NZ	54:Bx:196:HIS:CD2	2.73	0.57
32:BY:178:SER:OG	32:BY:181:ASP:OD2	2.23	0.57
42:Bj:178:TRP:HB3	42:Bj:187:THR:HG21	1.87	0.57
62:AI:275:GLY:H	62:AI:348:ALA:HB2	1.69	0.57
76:Ab:73:LYS:NZ	76:Ab:114:GLU:HG3	2.19	0.57
85:Ak:165:ILE:H	88:Ao:134:GLU:HB2	1.68	0.57
19:BJ:54:ILE:HD12	24:BQ:211:ASN:HB3	1.87	0.57
23:BP:47:ARG:NH1	29:BV:183:ASN:HB2	2.18	0.57
24:BQ:144:LYS:HG3	24:BQ:145:GLY:H	1.68	0.57
31:BX:37:GLU:HB3	31:BX:104:THR:HG23	1.86	0.57
47:Bo:31:GLN:HB3	47:Bo:33:PHE:CE1	2.39	0.57
56:AA:441:U:H2'	56:AA:442:A:C8	2.40	0.57
16:BE:90:TRP:CH2	16:BE:92:PRO:HA	2.40	0.57
41:Bi:196:GLN:HE22	41:Bi:198:ARG:HE	1.52	0.57
53:Bw:290:HIS:CD2	53:Bw:291:THR:HG23	2.40	0.57
56:AA:344:G:H1	64:AK:121:ASN:HB3	1.70	0.57
88:Ao:423:MET:HE1	88:Ao:463:LYS:HD2	1.86	0.57
14:BC:538:TYR:HA	14:BC:723:TRP:CD1	2.41	0.56
15:BD:128:ILE:HD11	33:Ba:114:LEU:HD21	1.86	0.56
16:BE:197:HIS:CD2	16:BE:318:THR:HG22	2.40	0.56
16:BE:342:ALA:H	27:BT:105:ILE:HD11	1.70	0.56
20:BK:124:LYS:NZ	20:BK:127:ASP:OD2	2.35	0.56
42:Bj:159:LEU:HD23	42:Bj:174:PRO:HG3	1.87	0.56
57:AB:146:ARG:HG3	57:AB:146:ARG:HH11	1.70	0.56
75:Aa:205:LYS:NZ	89:Ap:182:GLY:O	2.37	0.56
48:Bp:15:GLN:HE22	48:Bp:52:ILE:HD12	1.70	0.56
56:AA:752:A:H3'	56:AA:753:A:H5'	1.87	0.56
62:AI:71:VAL:HG12	62:AI:75:LYS:HE3	1.87	0.56
81:Ag:137:LEU:HD11	81:Ag:260:ALA:HB1	1.86	0.56
7:B5:181:ARG:NH1	7:B5:187:GLN:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BI:130:VAL:HB	18:BI:136:ASN:HD21	1.70	0.56
32:BY:133:VAL:HG13	32:BY:145:ARG:HB3	1.88	0.56
57:AB:145:SER:OG	57:AB:196:HIS:ND1	2.29	0.56
57:AB:161:CYS:HB3	57:AB:256:ILE:HG21	1.87	0.56
61:AG:159:VAL:HB	61:AG:172:VAL:HG21	1.86	0.56
81:Ag:365:LEU:HD23	81:Ag:370:ALA:HB1	1.86	0.56
84:Aj:38:TYR:OH	84:Aj:63:ARG:NH2	2.39	0.56
2:B0:118:THR:HG23	34:Bb:52:ARG:HA	1.86	0.56
12:BA:138:A:OP2	32:BY:34:LYS:NZ	2.38	0.56
18:BI:86:THR:HG23	18:BI:89:ARG:NH1	2.20	0.56
29:BV:165:ILE:HD11	29:BV:198:ARG:HB2	1.87	0.56
32:BY:199:MET:HG2	32:BY:204:ILE:HB	1.87	0.56
34:Bb:261:ARG:NH1	34:Bb:341:VAL:HG21	2.20	0.56
66:AN:92:VAL:HG12	66:AN:93:MET:HE3	1.87	0.56
66:AN:125:ARG:HH11	66:AN:125:ARG:CG	2.14	0.56
81:Ag:215:THR:HG23	81:Ag:219:ARG:HG3	1.87	0.56
12:BA:590:U:OP1	47:Bo:66:ARG:NH2	2.38	0.56
12:BA:743:U:H3'	12:BA:744:A:H5''	1.87	0.56
50:Bt:99:ARG:HH11	50:Bt:99:ARG:CB	2.17	0.56
51:Bu:56:ASP:OD1	51:Bu:56:ASP:N	2.36	0.56
67:AO:144:MET:HE3	67:AO:153:HIS:HB2	1.86	0.56
71:AU:66:MET:HE2	86:Am:4:PRO:HD3	1.88	0.56
72:AV:49:G:H1	72:AV:56:C:H42	1.52	0.56
84:Aj:145:HIS:CD2	84:Aj:146:GLU:HG2	2.41	0.56
88:Ao:447:ASN:OD1	88:Ao:447:ASN:N	2.39	0.56
88:Ao:504:ASP:HB2	88:Ao:537:LEU:HD22	1.86	0.56
89:Ap:108:CYS:SG	89:Ap:146:GLN:HG3	2.45	0.56
11:B9:99:GLN:HE21	12:BA:560:A:H2'	1.71	0.56
14:BC:363:PHE:HB3	14:BC:524:VAL:HG13	1.86	0.56
16:BE:96:ARG:NH1	16:BE:301:ASP:OD2	2.39	0.56
17:BF:62:VAL:HG13	45:Bm:119:HIS:HB3	1.87	0.56
19:BJ:41:HIS:CD2	19:BJ:43:GLU:H	2.23	0.56
23:BP:211:VAL:O	23:BP:215:THR:OG1	2.22	0.56
25:BR:41:ARG:NH1	25:BR:134:LEU:HD13	2.21	0.56
30:BW:154:ILE:HG12	41:Bi:52:SER:CB	2.36	0.56
56:AA:209:C:H2'	56:AA:210:U:C6	2.40	0.56
56:AA:928:A:O2'	56:AA:929:A:H5'	2.05	0.56
77:Ac:23:PHE:H	77:Ac:59:ASN:ND2	1.99	0.56
79:Ae:80:TRP:HB2	79:Ae:154:ARG:HH11	1.71	0.56
85:Ak:300:SER:O	85:Ak:304:GLU:HB3	2.05	0.56
12:BA:468:A:C2	50:Bt:18:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:1182:G:H4'	12:BA:1230:U:O2'	2.06	0.56
13:BB:43:C:H2'	13:BB:44:U:H5'	1.87	0.56
14:BC:674:THR:HG22	14:BC:695:SER:O	2.06	0.56
16:BE:113:ASP:N	16:BE:113:ASP:OD1	2.38	0.56
26:BS:130:ARG:NH1	34:Bb:129:ARG:NH1	2.53	0.56
28:BU:98:ASN:H	29:BV:109:GLN:NE2	2.02	0.56
44:Bl:140:VAL:H	50:Bt:85:HIS:CD2	2.23	0.56
56:AA:587:U:H5'	66:AN:33:LYS:HZ1	1.66	0.56
56:AA:826:C:H2'	56:AA:827:A:C8	2.40	0.56
43:Bk:104:GLU:HG2	43:Bk:155:ARG:NH1	2.20	0.56
79:Ae:70:LEU:O	79:Ae:74:TYR:HB2	2.05	0.56
82:Ah:326:LEU:HB2	82:Ah:347:THR:HG23	1.87	0.56
3:B1:197:PRO:HG2	3:B1:200:GLU:HG3	1.88	0.56
5:B3:119:ILE:N	50:Bt:45:ASN:HD21	2.03	0.56
12:BA:1227:U:H5	12:BA:1230:U:O4	1.89	0.56
25:BR:148:GLN:HG3	35:Bc:172:ILE:HG12	1.87	0.56
40:Bh:259:ARG:HG3	40:Bh:259:ARG:NH1	2.11	0.56
53:Bw:393:LYS:HB2	53:Bw:393:LYS:HZ2	1.70	0.56
21:BN:75:LYS:HB2	54:Bx:174:MET:HE1	1.88	0.56
31:BX:71:ARG:NH1	31:BX:96:TYR:OH	2.39	0.56
43:Bk:90:VAL:HB	43:Bk:189:HIS:HB3	1.88	0.56
52:Bv:48:PRO:HB2	52:Bv:50:TRP:CD1	2.40	0.56
56:AA:59:C:C2	84:Aj:54:ALA:HB1	2.41	0.56
59:AE:117:ARG:HG3	73:AX:10:C:H5'	1.88	0.56
70:AR:95:ARG:NH1	70:AR:102:GLY:HA2	2.21	0.56
79:Ae:166:LEU:HD13	79:Ae:199:ASP:HB2	1.87	0.56
12:BA:529:G:H4'	49:Bq:122:ARG:HH12	1.68	0.55
31:BX:50:ARG:NH1	31:BX:69:ARG:HA	2.20	0.55
68:AP:111:ARG:NH2	75:Aa:168:LYS:O	2.39	0.55
1:CL:31:LEU:HD22	1:DL:67:LEU:HD12	1.87	0.55
12:BA:1549:A:C2	38:Bf:104:GLU:HG2	2.40	0.55
32:BY:189:PRO:O	37:Be:93:THR:OG1	2.25	0.55
56:AA:28:U:H2'	56:AA:29:A:C8	2.41	0.55
56:AA:131:U:H1'	69:AQ:23:GLN:HE21	1.69	0.55
68:AP:119:LEU:O	68:AP:123:GLN:HG2	2.06	0.55
79:Ae:80:TRP:HB2	79:Ae:154:ARG:NH1	2.22	0.55
6:B4:51:ARG:HB2	42:Bj:84:TYR:O	2.06	0.55
12:BA:1253:G:O6	23:BP:77:ARG:NH2	2.39	0.55
53:Bw:370:THR:HG22	53:Bw:372:ALA:H	1.71	0.55
58:AC:62:ILE:HG12	58:AC:66:LYS:HE2	1.87	0.55
81:Ag:55:PRO:HD2	81:Ag:146:LYS:NZ	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:539:ALA:HB2	88:Ao:581:TYR:CE1	2.41	0.55
12:BA:203:A:N1	12:BA:356:G:O2'	2.33	0.55
12:BA:725:C:H5	33:Ba:389:LEU:H	1.55	0.55
41:Bi:186:VAL:HG13	41:Bi:219:ARG:HB3	1.87	0.55
59:AE:289:THR:HG21	59:AE:307:LYS:HG3	1.89	0.55
63:AJ:96:VAL:HA	63:AJ:106:ILE:HD11	1.89	0.55
1:GL:76:LEU:HD21	19:BJ:240:GLN:HB2	1.88	0.55
10:B8:183:ARG:NH1	34:Bb:354:GLN:NE2	2.55	0.55
12:BA:874:G:O2'	87:An:199:GLN:OE1	2.22	0.55
23:BP:247:ILE:HD13	51:Bu:59:TRP:HB3	1.87	0.55
56:AA:887:U:H2'	56:AA:888:A:H8	1.72	0.55
89:Ap:136:HIS:CD2	89:Ap:139:TYR:H	2.23	0.55
12:BA:173:C:H1'	38:Bf:126:ARG:HH21	1.70	0.55
14:BC:632:PHE:HB2	14:BC:643:VAL:HB	1.89	0.55
34:Bb:304:TYR:CE2	34:Bb:313:PRO:HD3	2.42	0.55
58:AC:76:LEU:HD22	63:AJ:138:THR:HG23	1.88	0.55
79:Ae:286:ASN:HB3	84:Aj:70:ARG:HH12	1.71	0.55
88:Ao:602:PHE:HD1	88:Ao:609:PRO:HG3	1.71	0.55
3:B1:189:ASP:HA	3:B1:192:LYS:HE3	1.87	0.55
25:BR:67:ASP:OD2	53:Bw:44:TYR:OH	2.22	0.55
53:Bw:274:ASN:OD1	53:Bw:274:ASN:N	2.40	0.55
56:AA:56:U:O2'	56:AA:198:C:O2	2.22	0.55
57:AB:141:ILE:HD13	57:AB:191:LEU:HD23	1.87	0.55
58:AC:132:PHE:HD2	88:Ao:95:LEU:HD21	1.72	0.55
69:AQ:12:TRP:HE3	69:AQ:65:LEU:HD11	1.71	0.55
73:AX:6:C:H2'	73:AX:7:C:H5''	1.89	0.55
1:FL:76:LEU:HA	1:FL:79:ILE:HD12	1.88	0.55
4:B2:204:MET:HB3	4:B2:205:PRO:HD2	1.89	0.55
7:B5:81:PRO:HA	12:BA:1438:U:C2	2.42	0.55
12:BA:1203:C:O2'	23:BP:77:ARG:NH1	2.38	0.55
20:BK:160:SER:HA	20:BK:163:GLU:HB2	1.88	0.55
59:AE:95:ALA:HB2	83:Ai:74:GLU:HB3	1.89	0.55
79:Ae:378:LEU:O	79:Ae:382:LEU:HG	2.07	0.55
88:Ao:160:ARG:HA	88:Ao:163:LEU:HD12	1.89	0.55
21:BN:4:PHE:CD2	40:Bh:285:PRO:HD3	2.42	0.55
21:BN:26:GLN:NE2	21:BN:147:GLN:OE1	2.40	0.55
45:Bm:141:PHE:CE2	45:Bm:145:ILE:HD11	2.42	0.55
53:Bw:77:ASP:OD1	53:Bw:77:ASP:N	2.34	0.55
4:B2:93:ARG:NH1	37:Be:82:THR:O	2.40	0.55
12:BA:122:G:H5'	12:BA:123:U:OP2	2.07	0.55
23:BP:276:ASN:ND2	23:BP:279:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ba:391:VAL:HG13	33:Ba:399:GLU:HB2	1.89	0.55
67:AO:113:MET:O	67:AO:117:LEU:HB2	2.06	0.55
71:AU:83:PRO:HG2	71:AU:84:TRP:CD1	2.42	0.55
88:Ao:285:LEU:HD21	88:Ao:292:ALA:HB2	1.88	0.55
88:Ao:503:LEU:HD22	88:Ao:508:ARG:HB2	1.89	0.55
22:BO:55:PRO:HB3	22:BO:77:ILE:HG23	1.89	0.54
23:BP:97:SER:HB2	23:BP:143:GLU:HB2	1.89	0.54
25:BR:118:ARG:HG3	25:BR:118:ARG:NH1	2.21	0.54
29:BV:136:LYS:HZ2	47:Bo:48:ASP:HB3	1.72	0.54
33:Ba:65:HIS:HD2	33:Ba:66:PHE:O	1.91	0.54
56:AA:800:G:H2'	56:AA:801:A:C8	2.42	0.54
63:AJ:106:ILE:HG22	63:AJ:145:LEU:HB3	1.89	0.54
82:Ah:330:LEU:O	82:Ah:340:ARG:NH2	2.40	0.54
85:Ak:118:PRO:O	85:Ak:122:LYS:HG2	2.07	0.54
14:BC:198:ASP:OD1	14:BC:205:VAL:HG22	2.07	0.54
23:BP:247:ILE:H	23:BP:247:ILE:HD12	1.72	0.54
32:BY:127:ASP:OD1	32:BY:152:ARG:NH1	2.36	0.54
56:AA:209:C:H2'	56:AA:210:U:H6	1.72	0.54
56:AA:728:U:H2'	56:AA:729:A:C8	2.42	0.54
77:Ac:94:SER:HB2	77:Ac:97:GLU:HG3	1.90	0.54
81:Ag:122:ARG:HH11	81:Ag:336:LEU:HD22	1.73	0.54
81:Ag:201:ILE:HG12	81:Ag:255:PHE:HE1	1.72	0.54
89:Ap:59:LEU:HD11	89:Ap:122:LEU:HB2	1.88	0.54
3:B1:119:LEU:HA	3:B1:168:ARG:HH11	1.71	0.54
12:BA:219:A:H5''	44:Bl:91:MET:HE3	1.88	0.54
12:BA:575:C:H5	54:Bx:186:SER:HA	1.71	0.54
17:BF:192:SER:O	17:BF:193:LEU:HB2	2.06	0.54
20:BK:20:ILE:HD11	20:BK:42:ARG:HE	1.71	0.54
34:Bb:373:HIS:O	34:Bb:374:GLU:HG2	2.08	0.54
53:Bw:369:ASN:H	53:Bw:385:ASN:ND2	2.05	0.54
56:AA:792:U:H2'	56:AA:793:A:H8	1.72	0.54
11:B9:69:LEU:HB2	12:BA:560:A:H62	1.71	0.54
21:BN:15:ALA:CB	40:Bh:269:VAL:HG21	2.38	0.54
21:BN:152:PRO:HB3	54:Bx:84:GLU:HG3	1.88	0.54
41:Bi:189:LEU:HB2	41:Bi:217:HIS:HD2	1.73	0.54
53:Bw:156:ARG:NH1	53:Bw:161:GLN:HA	2.23	0.54
56:AA:210:U:H2'	56:AA:211:A:C8	2.42	0.54
62:AI:101:GLN:HE22	62:AI:126:LYS:HA	1.73	0.54
79:Ae:270:LEU:HG	79:Ae:320:LEU:HD21	1.88	0.54
81:Ag:178:ASP:N	81:Ag:178:ASP:OD1	2.40	0.54
88:Ao:574:TRP:CH2	88:Ao:579:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:185:LYS:HD3	1:BL:197:LEU:HG	1.88	0.54
23:BP:12:ALA:HB2	50:Bt:88:LEU:HD21	1.88	0.54
42:Bj:57:PRO:HD3	42:Bj:156:ASN:HB3	1.89	0.54
59:AE:400:GLU:HG2	59:AE:401:VAL:H	1.72	0.54
62:AI:199:ARG:HG2	62:AI:249:ILE:HG23	1.90	0.54
78:Ad:59:ARG:NH1	89:Ap:202:TRP:O	2.40	0.54
33:Ba:351:LEU:HD11	33:Ba:379:ASP:HA	1.89	0.54
56:AA:617:C:H4'	59:AE:100:LYS:HG2	1.90	0.54
56:AA:939:A:H2'	56:AA:940:C:C6	2.43	0.54
77:Ac:76:LEU:HD13	77:Ac:102:ILE:HD11	1.89	0.54
12:BA:811:A:H1'	16:BE:230:THR:CG2	2.38	0.54
20:BK:140:VAL:O	20:BK:144:ILE:HG12	2.07	0.54
38:Bf:134:ARG:HB3	38:Bf:134:ARG:HH11	1.72	0.54
39:Bg:26:LEU:HD21	39:Bg:29:LEU:HD13	1.89	0.54
43:Bk:106:TYR:OH	43:Bk:174:ILE:O	2.26	0.54
59:AE:358:THR:HG22	59:AE:360:GLN:H	1.72	0.54
61:AG:66:ARG:HB3	61:AG:70:LYS:HE3	1.90	0.54
64:AK:195:ARG:HH11	64:AK:195:ARG:HG2	1.72	0.54
84:Aj:171:ARG:NH1	84:Aj:188:GLU:OE2	2.41	0.54
16:BE:108:PRO:HG2	27:BT:145:LEU:HB3	1.89	0.54
16:BE:221:ARG:NH1	16:BE:259:GLY:HA3	2.22	0.54
36:Bd:173:ARG:NH2	42:Bj:56:PRO:HB3	2.22	0.54
39:Bg:44:ARG:NH1	50:Bt:100:LYS:HA	2.23	0.54
39:Bg:93:SER:O	39:Bg:97:ILE:HG12	2.08	0.54
56:AA:168:A:O2'	56:AA:170:A:N1	2.34	0.54
66:AN:52:LEU:O	66:AN:56:SER:OG	2.26	0.54
70:AR:66:CYS:SG	70:AR:104:LYS:HG3	2.48	0.54
70:AR:78:VAL:HG13	70:AR:121:MET:HB2	1.89	0.54
79:Ae:85:LYS:HG3	79:Ae:424:HIS:HE1	1.71	0.54
88:Ao:82:SER:O	88:Ao:487:SER:OG	2.11	0.54
88:Ao:343:LYS:HE2	88:Ao:347:ARG:NH2	2.23	0.54
15:BD:108:ASP:OD1	15:BD:113:ARG:NH1	2.41	0.54
40:Bh:244:GLU:O	40:Bh:248:ARG:HG2	2.08	0.54
42:Bj:185:ARG:NH1	42:Bj:204:PHE:HB3	2.23	0.54
57:AB:57:LEU:HB2	57:AB:270:TYR:CE2	2.40	0.54
57:AB:58:ARG:O	57:AB:61:ILE:HG22	2.08	0.54
60:AF:52:SER:OG	60:AF:57:ARG:HD2	2.08	0.54
66:AN:53:ARG:NE	82:Ah:364:HIS:HD2	2.04	0.54
77:Ac:125:HIS:CD2	77:Ac:127:ALA:H	2.26	0.54
79:Ae:173:VAL:HG13	84:Aj:69:ASN:HB2	1.90	0.54
81:Ag:272:THR:HG23	81:Ag:315:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:25:PRO:HB2	3:B1:27:HIS:CE1	2.43	0.53
3:B1:100:ARG:NH2	18:BI:75:ARG:HE	2.06	0.53
12:BA:937:C:H3'	12:BA:938:U:H5''	1.90	0.53
23:BP:287:ASP:OD1	23:BP:288:GLU:N	2.41	0.53
35:Bc:109:PRO:HB2	35:Bc:264:PRO:HG3	1.91	0.53
41:Bi:165:THR:HG23	41:Bi:167:ASN:N	2.22	0.53
41:Bi:165:THR:HG21	41:Bi:262:HIS:ND1	2.22	0.53
59:AE:154:VAL:HG22	88:Ao:108:LEU:HD21	1.91	0.53
59:AE:289:THR:HG22	59:AE:290:ILE:H	1.73	0.53
82:Ah:296:TRP:HB3	82:Ah:302:LEU:HB2	1.91	0.53
12:BA:129:A:OP1	17:BF:142:ARG:NH2	2.38	0.53
51:Bu:101:ARG:HG2	51:Bu:133:ILE:HG12	1.90	0.53
59:AE:305:MET:HE2	59:AE:332:LEU:HD21	1.90	0.53
59:AE:317:HIS:CD2	59:AE:319:ALA:H	2.26	0.53
75:Aa:287:THR:HG22	75:Aa:289:HIS:H	1.73	0.53
81:Ag:205:GLU:OE2	81:Ag:248:ARG:NH1	2.41	0.53
87:An:163:ARG:HB2	87:An:163:ARG:HH11	1.73	0.53
12:BA:130:A:H2'	12:BA:131:A:O4'	2.08	0.53
27:BT:188:LEU:HB3	27:BT:191:ARG:HH12	1.73	0.53
53:Bw:158:PRO:HB2	53:Bw:160:ILE:HG22	1.91	0.53
62:AI:73:PHE:O	62:AI:77:GLN:HG2	2.07	0.53
70:AR:77:ASN:HD21	70:AR:80:LEU:HB3	1.73	0.53
79:Ae:223:LEU:HD21	79:Ae:398:THR:HA	1.91	0.53
7:B5:140:GLN:HA	7:B5:143:LYS:HE3	1.90	0.53
12:BA:548:A:H5''	49:Bq:126:ILE:CD1	2.38	0.53
12:BA:1458:G:O2'	12:BA:1467:G:O6	2.17	0.53
16:BE:239:ARG:CG	16:BE:239:ARG:HH11	2.21	0.53
29:BV:177:LYS:HD2	29:BV:186:ARG:NH1	2.23	0.53
56:AA:918:A:O2'	56:AA:919:A:H3'	2.09	0.53
62:AI:127:HIS:CD2	62:AI:129:GLU:HG2	2.44	0.53
67:AO:112:LEU:HD23	67:AO:131:VAL:HG13	1.90	0.53
79:Ae:85:LYS:HG3	79:Ae:424:HIS:CE1	2.43	0.53
79:Ae:257:ASN:HD22	79:Ae:260:GLY:H	1.56	0.53
85:Ak:199:ARG:HB3	85:Ak:208:THR:O	2.08	0.53
12:BA:219:A:P	23:BP:109:ARG:HH22	2.31	0.53
33:Ba:361:THR:HG22	33:Ba:363:ASP:H	1.74	0.53
42:Bj:198:ASN:HB2	42:Bj:242:ASP:O	2.08	0.53
53:Bw:292:GLN:HG3	53:Bw:329:TRP:CZ3	2.42	0.53
56:AA:195:G:H2'	56:AA:196:A:C8	2.44	0.53
81:Ag:80:HIS:HB3	81:Ag:155:PRO:HG3	1.89	0.53
84:Aj:30:ASP:HB2	84:Aj:34:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:346:ARG:HH11	88:Ao:381:LEU:HB2	1.70	0.53
88:Ao:608:ILE:HG13	88:Ao:642:LEU:HD21	1.91	0.53
15:BD:170:ILE:HG22	15:BD:171:GLY:H	1.73	0.53
21:BN:90:VAL:HG13	21:BN:94:GLN:HB2	1.90	0.53
40:Bh:105:ARG:CZ	40:Bh:113:GLU:HG3	2.39	0.53
85:Ak:89:MET:HE2	85:Ak:107:LEU:HG	1.91	0.53
14:BC:426:SER:O	14:BC:429:GLU:HB2	2.09	0.53
17:BF:238:LYS:NZ	46:Bn:45:ASP:OD2	2.42	0.53
19:BJ:41:HIS:HD2	19:BJ:43:GLU:H	1.57	0.53
20:BK:149:ARG:HH12	49:Bq:104:PRO:HB3	1.73	0.53
24:BQ:72:ILE:HD11	24:BQ:96:TYR:CZ	2.43	0.53
33:Ba:288:PRO:HD2	33:Ba:324:GLN:NE2	2.24	0.53
43:Bk:111:HIS:HE1	43:Bk:121:VAL:HG11	1.74	0.53
56:AA:891:C:H2'	56:AA:892:A:C8	2.44	0.53
85:Ak:192:LEU:O	85:Ak:196:VAL:HG23	2.09	0.53
2:B0:120:LEU:HD11	2:B0:126:LEU:HD23	1.90	0.53
7:B5:179:ARG:HE	7:B5:182:PRO:HG3	1.74	0.53
12:BA:1294:A:H5'	12:BA:1295:G:OP2	2.09	0.53
16:BE:195:ALA:H	16:BE:281:ASN:HD22	1.56	0.53
20:BK:54:ASN:HB3	20:BK:58:LYS:HE3	1.90	0.53
21:BN:91:THR:HB	21:BN:94:GLN:HE21	1.74	0.53
21:BN:112:LEU:HD13	21:BN:121:MET:HG3	1.91	0.53
25:BR:108:LEU:HD11	25:BR:136:LEU:HD22	1.91	0.53
59:AE:244:LEU:HD21	59:AE:346:THR:HG21	1.91	0.53
62:AI:119:LYS:HA	62:AI:122:ARG:HD2	1.90	0.53
79:Ae:69:LEU:HB2	79:Ae:405:LEU:HD23	1.90	0.53
15:BD:115:GLU:HA	15:BD:148:ARG:HH12	1.74	0.53
35:Bc:141:ARG:HH12	35:Bc:264:PRO:HD2	1.74	0.53
42:Bj:44:PRO:HG2	42:Bj:227:LEU:HA	1.90	0.53
44:Bl:94:ILE:HD11	44:Bl:162:LEU:HG	1.90	0.53
46:Bn:105:ASP:OD1	46:Bn:105:ASP:N	2.24	0.53
62:AI:91:MET:HB2	85:Ak:117:THR:HG21	1.90	0.53
67:AO:195:PRO:HB2	67:AO:196:TYR:CD2	2.44	0.53
76:Ab:67:GLU:OE2	80:Af:86:ARG:NE	2.28	0.53
81:Ag:203:VAL:HG13	81:Ag:245:GLU:HG2	1.89	0.53
4:B2:115:LEU:HB3	31:BX:27:GLN:HG2	1.91	0.53
24:BQ:101:HIS:O	24:BQ:105:MET:HG3	2.08	0.53
34:Bb:96:LYS:HE3	47:Bo:118:GLN:HB2	1.91	0.53
42:Bj:202:ALA:HB2	42:Bj:238:LEU:HD23	1.90	0.53
58:AC:78:GLY:H	63:AJ:81:LYS:NZ	2.07	0.53
59:AE:122:ARG:HB2	59:AE:183:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AE:296:LEU:HD22	59:AE:352:GLY:HA3	1.91	0.53
88:Ao:147:PRO:HG3	88:Ao:160:ARG:HG2	1.91	0.53
16:BE:128:HIS:HD2	16:BE:173:LYS:NZ	2.07	0.52
22:BO:93:GLY:O	22:BO:95:ARG:NH1	2.37	0.52
26:BS:132:LEU:HD23	26:BS:165:MET:HE1	1.91	0.52
40:Bh:259:ARG:CG	40:Bh:259:ARG:NH1	2.65	0.52
63:AJ:136:MET:HE3	66:AN:123:VAL:HG22	1.90	0.52
69:AQ:95:VAL:HG11	78:Ad:120:ARG:HH22	1.74	0.52
81:Ag:173:ASN:HB3	81:Ag:176:ARG:HD2	1.91	0.52
5:B3:78:ARG:NH1	5:B3:82:GLU:OE2	2.42	0.52
12:BA:1399:G:O2'	12:BA:1402:C:OP2	2.22	0.52
16:BE:341:GLY:HA2	27:BT:105:ILE:HD11	1.91	0.52
34:Bb:124:ARG:HH12	36:Bd:115:ALA:CB	2.23	0.52
42:Bj:273:ARG:HA	42:Bj:276:LEU:HB3	1.91	0.52
57:AB:161:CYS:SG	57:AB:253:GLN:HA	2.49	0.52
4:B2:95:LYS:NZ	32:BY:181:ASP:O	2.42	0.52
9:B7:85:ARG:NH1	9:B7:92:SER:O	2.43	0.52
12:BA:407:A:OP2	43:Bk:49:ARG:NH1	2.42	0.52
14:BC:168:ARG:HB2	14:BC:378:ARG:NH2	2.24	0.52
14:BC:289:LYS:HG2	94:BC:901:GSP:C6	2.45	0.52
26:BS:89:HIS:HA	26:BS:119:THR:HG22	1.91	0.52
28:BU:111:LYS:HB2	39:Bg:127:GLN:NE2	2.23	0.52
38:Bf:49:LEU:HD23	38:Bf:60:CYS:HB3	1.90	0.52
56:AA:66:C:O2'	68:AP:40:LYS:O	2.24	0.52
3:B1:16:LEU:HD21	3:B1:29:LEU:HD22	1.91	0.52
7:B5:138:ARG:HB3	12:BA:655:C:C6	2.44	0.52
24:BQ:247:THR:OG1	24:BQ:250:ARG:HG2	2.10	0.52
34:Bb:233:VAL:HG23	34:Bb:298:PHE:CG	2.44	0.52
34:Bb:290:CYS:SG	34:Bb:296:ARG:NH2	2.82	0.52
42:Bj:149:LEU:HD13	42:Bj:254:TRP:CE2	2.44	0.52
69:AQ:62:ASP:N	69:AQ:62:ASP:OD1	2.42	0.52
75:Aa:272:TYR:CD1	75:Aa:293:MET:HB3	2.44	0.52
76:Ab:67:GLU:O	76:Ab:71:ARG:HG3	2.09	0.52
78:Ad:159:GLN:O	78:Ad:163:GLU:HG2	2.09	0.52
88:Ao:342:LEU:O	88:Ao:346:ARG:HG2	2.09	0.52
1:CL:40:LEU:HA	1:CL:43:ILE:HD12	1.92	0.52
7:B5:181:ARG:NH1	7:B5:187:GLN:HG2	2.17	0.52
12:BA:692:A:H2'	12:BA:693:U:H5'	1.91	0.52
12:BA:1238:A:H5'	12:BA:1239:A:OP2	2.10	0.52
27:BT:188:LEU:HD22	27:BT:191:ARG:HH12	1.74	0.52
38:Bf:74:PRO:HD3	40:Bh:256:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bg:34:SER:OG	39:Bg:70:CYS:O	2.26	0.52
45:Bm:77:GLU:HG3	45:Bm:104:ARG:HH11	1.74	0.52
47:Bo:38:SER:O	47:Bo:44:THR:OG1	2.21	0.52
79:Ae:83:ARG:NH2	79:Ae:416:TYR:OH	2.40	0.52
12:BA:527:U:O2'	19:BJ:113:ARG:NH1	2.38	0.52
19:BJ:95:MET:HE2	19:BJ:161:VAL:HG22	1.91	0.52
34:Bb:262:GLY:HA3	34:Bb:342:PHE:HB2	1.92	0.52
41:Bi:170:PRO:O	41:Bi:174:TRP:HB2	2.09	0.52
53:Bw:339:PHE:CD1	53:Bw:345:VAL:HA	2.45	0.52
56:AA:203:G:H2'	56:AA:204:U:C6	2.45	0.52
1:CL:46:LEU:HD21	1:DL:67:LEU:HD23	1.92	0.52
16:BE:55:GLU:H	16:BE:55:GLU:CD	2.18	0.52
17:BF:211:ARG:HD2	45:Bm:59:ARG:NH1	2.24	0.52
1:BL:148:GLU:HG3	1:BL:152:HIS:HD2	1.74	0.52
36:Bd:147:LEU:O	36:Bd:151:ARG:HG3	2.10	0.52
5:B3:134:MET:HE1	47:Bo:78:VAL:HG21	1.91	0.52
16:BE:316:PHE:CG	16:BE:316:PHE:O	2.63	0.52
17:BF:74:GLN:O	17:BF:210:ARG:NH2	2.42	0.52
39:Bg:28:ARG:HB3	39:Bg:28:ARG:HH11	1.75	0.52
56:AA:648:A:OP1	57:AB:200:ASN:ND2	2.43	0.52
63:AJ:179:GLN:O	85:Ak:150:PRO:HD2	2.10	0.52
75:Aa:104:MET:HB3	75:Aa:290:PHE:HE1	1.74	0.52
88:Ao:259:ALA:HA	88:Ao:262:TYR:CE2	2.45	0.52
88:Ao:392:SER:O	88:Ao:396:ILE:HG13	2.10	0.52
88:Ao:469:CYS:SG	88:Ao:470:PHE:N	2.83	0.52
88:Ao:500:LEU:HB3	88:Ao:537:LEU:HD11	1.91	0.52
2:B0:39:SER:N	12:BA:1156:A:O2'	2.41	0.52
12:BA:220:G:H1'	12:BA:231:C:O2'	2.10	0.52
14:BC:179:ARG:NE	14:BC:413:SER:OG	2.41	0.52
35:Bc:67:VAL:HG22	35:Bc:121:GLU:HB2	1.90	0.52
41:Bi:90:PRO:HB2	41:Bi:269:TRP:HH2	1.74	0.52
41:Bi:111:ARG:O	41:Bi:115:ASN:ND2	2.43	0.52
45:Bm:115:ASN:ND2	45:Bm:115:ASN:H	2.07	0.52
59:AE:292:HIS:CE1	59:AE:357:GLU:H	2.26	0.52
62:AI:286:VAL:HB	62:AI:329:MET:HE3	1.90	0.52
78:Ad:189:TRP:HZ3	78:Ad:191:ILE:HG23	1.75	0.52
82:Ah:341:HIS:CG	83:Ai:24:ARG:HD2	2.45	0.52
85:Ak:89:MET:HE3	85:Ak:106:GLU:HB3	1.92	0.52
12:BA:508:G:H4'	20:BK:151:LEU:HD13	1.90	0.52
12:BA:720:C:OP2	15:BD:149:LYS:NZ	2.33	0.52
14:BC:486:TRP:CD1	56:AA:256:G:HO2'	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AG:112:THR:HG23	81:Ag:396:TYR:HB3	1.91	0.52
69:AQ:57:GLN:O	69:AQ:87:LYS:NZ	2.43	0.52
70:AR:116:GLN:HE21	70:AR:123:VAL:HA	1.75	0.52
12:BA:71:U:H3	12:BA:94:U:H3	1.57	0.51
12:BA:1009:A:H2'	12:BA:1010:A:C8	2.45	0.51
12:BA:1145:C:H4'	12:BA:1146:G:O5'	2.09	0.51
14:BC:655:LYS:HZ2	14:BC:673:LEU:C	2.17	0.51
19:BJ:37:ARG:HG3	19:BJ:37:ARG:O	2.10	0.51
22:BO:69:VAL:HG23	22:BO:89:HIS:CE1	2.45	0.51
24:BQ:98:HIS:HD2	24:BQ:100:GLY:H	1.58	0.51
34:Bb:157:LEU:HD13	34:Bb:221:LEU:HD11	1.92	0.51
40:Bh:278:ARG:HB2	40:Bh:278:ARG:NH1	2.25	0.51
41:Bi:288:LYS:HD2	41:Bi:290:TRP:CZ2	2.45	0.51
61:AG:139:ARG:NH2	81:Ag:363:ASN:OD1	2.43	0.51
70:AR:66:CYS:HB3	70:AR:101:CYS:H	1.75	0.51
1:DL:71:ILE:HD13	19:BJ:207:LEU:HD21	1.92	0.51
5:B3:59:ASP:O	50:Bt:51:ARG:NH2	2.42	0.51
12:BA:1008:A:O2'	30:BW:157:HIS:HE1	1.92	0.51
12:BA:1050:C:H2'	12:BA:1327:U:H4'	1.91	0.51
19:BJ:122:LEU:HD21	19:BJ:124:LYS:HE3	1.92	0.51
23:BP:234:LEU:HB3	51:Bu:66:LYS:HZ1	1.75	0.51
33:Ba:347:THR:HG22	33:Ba:349:GLY:H	1.75	0.51
45:Bm:86:ASN:N	45:Bm:86:ASN:OD1	2.41	0.51
53:Bw:244:PHE:CE2	53:Bw:365:CYS:HB3	2.44	0.51
56:AA:287:C:N3	77:Ac:11:ARG:NH2	2.59	0.51
68:AP:28:ASN:ND2	77:Ac:161:GLY:H	2.07	0.51
2:B0:54:LYS:HE2	2:B0:69:THR:HG22	1.92	0.51
6:B4:72:PRO:HG2	42:Bj:87:HIS:CD2	2.46	0.51
10:B8:96:TYR:H	46:Bn:122:ASN:HD22	1.59	0.51
12:BA:1351:U:H2'	12:BA:1353:C:H5''	1.91	0.51
21:BN:4:PHE:CE2	40:Bh:285:PRO:HD3	2.45	0.51
28:BU:146:VAL:HG11	38:Bf:56:ARG:HG2	1.93	0.51
35:Bc:145:MET:HE2	35:Bc:254:PHE:HD1	1.76	0.51
62:AI:254:LYS:HG2	62:AI:366:ARG:HH22	1.75	0.51
69:AQ:24:LYS:H	69:AQ:56:GLN:NE2	2.07	0.51
77:Ac:87:LEU:O	78:Ad:113:ASN:ND2	2.42	0.51
12:BA:925:G:N2	12:BA:964:A:OP2	2.31	0.51
17:BF:123:GLY:O	17:BF:140:SER:HB2	2.10	0.51
34:Bb:47:ARG:HE	43:Bk:120:LYS:HZ1	1.57	0.51
42:Bj:55:ARG:NH2	42:Bj:152:LYS:O	2.40	0.51
42:Bj:116:LEU:N	42:Bj:119:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AE:304:LYS:NZ	59:AE:410:ASP:OD1	2.36	0.51
62:AI:274:GLU:HG2	62:AI:283:GLU:HG2	1.91	0.51
88:Ao:159:GLU:O	88:Ao:163:LEU:HG	2.11	0.51
2:B0:56:MET:H	2:B0:59:HIS:HD2	1.56	0.51
1:BL:134:LEU:HD21	1:BL:145:LEU:HD21	1.92	0.51
29:BV:176:MET:HE2	29:BV:187:LYS:HB2	1.93	0.51
31:BX:7:TYR:CE2	37:Be:37:LYS:HG3	2.46	0.51
38:Bf:74:PRO:HA	40:Bh:256:ARG:HE	1.76	0.51
45:Bm:74:HIS:HA	45:Bm:77:GLU:HG2	1.93	0.51
75:Aa:178:TYR:HB3	75:Aa:180:PHE:CE2	2.45	0.51
81:Ag:154:ILE:HD13	81:Ag:261:VAL:HG22	1.93	0.51
88:Ao:306:LEU:HA	88:Ao:348:PHE:HZ	1.75	0.51
14:BC:183:VAL:HA	14:BC:254:ILE:O	2.10	0.51
30:BW:53:ASN:ND2	30:BW:72:TYR:O	2.43	0.51
35:Bc:300:VAL:HG23	35:Bc:301:HIS:CD2	2.45	0.51
37:Be:88:GLN:O	37:Be:92:GLU:HG2	2.09	0.51
56:AA:28:U:H2'	56:AA:29:A:H8	1.74	0.51
63:AJ:80:VAL:HG23	63:AJ:141:ARG:HB2	1.93	0.51
82:Ah:287:GLN:HG3	88:Ao:448:TRP:CD1	2.46	0.51
88:Ao:301:ILE:HG12	88:Ao:319:ILE:HG23	1.92	0.51
4:B2:209:ARG:HG2	4:B2:209:ARG:HH11	1.76	0.51
12:BA:1522:A:H5''	48:Bp:84:GLN:HE22	1.75	0.51
12:BA:1530:C:H1'	54:Bx:133:PRO:HD2	1.92	0.51
20:BK:66:LEU:HA	20:BK:85:PRO:HA	1.92	0.51
28:BU:98:ASN:H	29:BV:109:GLN:HE22	1.59	0.51
34:Bb:304:TYR:HE2	34:Bb:313:PRO:HD3	1.75	0.51
35:Bc:294:GLN:NE2	35:Bc:320:VAL:H	1.98	0.51
3:B1:43:TYR:HB3	3:B1:67:ILE:HD12	1.93	0.51
28:BU:88:ILE:HG13	28:BU:89:ASN:N	2.24	0.51
29:BV:98:ARG:HH11	29:BV:113:THR:HG21	1.75	0.51
40:Bh:108:LEU:HD12	40:Bh:110:ILE:HD11	1.93	0.51
40:Bh:148:LEU:HD22	40:Bh:305:PHE:HB3	1.93	0.51
41:Bi:293:PHE:CE2	41:Bi:295:GLU:HG2	2.46	0.51
51:Bu:96:SER:O	51:Bu:145:ASN:ND2	2.43	0.51
57:AB:178:ALA:HB3	57:AB:179:PRO:HD3	1.92	0.51
65:AL:96:PRO:O	65:AL:127:ARG:NH1	2.43	0.51
67:AO:144:MET:HE2	67:AO:144:MET:HA	1.91	0.51
76:Ab:93:LYS:HD3	76:Ab:97:GLN:HG2	1.92	0.51
88:Ao:587:LEU:HD12	88:Ao:620:SER:HB2	1.93	0.51
12:BA:113:G:C8	17:BF:121:ARG:HG2	2.46	0.51
12:BA:1092:A:H3'	12:BA:1093:A:H5''	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:559:ASN:HB2	56:AA:180:U:OP1	2.11	0.51
20:BK:86:THR:HG22	20:BK:88:SER:H	1.76	0.51
20:BK:164:LEU:HG	49:Bq:77:ILE:H	1.75	0.51
33:Ba:124:THR:HG23	33:Ba:318:PHE:CG	2.45	0.51
33:Ba:136:VAL:HG22	33:Ba:420:HIS:CD2	2.46	0.51
51:Bu:152:LYS:O	51:Bu:156:MET:HG3	2.11	0.51
53:Bw:240:GLN:OE1	53:Bw:347:ARG:NH1	2.43	0.51
56:AA:640:A:H5''	59:AE:228:VAL:HG11	1.92	0.51
59:AE:122:ARG:HB2	59:AE:183:ARG:HH21	1.76	0.51
59:AE:321:MET:HE2	59:AE:325:ARG:NH2	2.25	0.51
12:BA:574:A:OP1	54:Bx:150:TYR:OH	2.28	0.51
16:BE:195:ALA:H	16:BE:281:ASN:ND2	2.08	0.51
20:BK:142:ARG:HG3	49:Bq:99:MET:HE3	1.93	0.51
25:BR:45:SER:HA	25:BR:121:MET:HE2	1.92	0.51
35:Bc:77:VAL:O	41:Bi:279:THR:HG23	2.11	0.51
54:Bx:190:ARG:HB3	54:Bx:190:ARG:NH1	2.26	0.51
56:AA:26:A:H2'	56:AA:27:U:C6	2.45	0.51
56:AA:635:C:H5'	57:AB:176:THR:HG21	1.92	0.51
56:AA:884:C:H5''	79:Ae:143:TYR:CE2	2.46	0.51
59:AE:132:ILE:HG22	59:AE:144:LEU:HD13	1.93	0.51
74:AZ:703:ALA:HB1	74:AZ:709:ALA:HB2	1.92	0.51
28:BU:92:LYS:HB3	28:BU:123:ARG:NH1	2.26	0.50
56:AA:531:U:H2'	56:AA:532:G:C8	2.45	0.50
56:AA:745:C:H3'	56:AA:746:A:C8	2.46	0.50
62:AI:176:HIS:HE1	62:AI:185:LEU:HD22	1.75	0.50
62:AI:197:GLY:O	62:AI:249:ILE:HG12	2.11	0.50
79:Ae:258:SER:HB2	79:Ae:312:ASP:C	2.35	0.50
82:Ah:341:HIS:CD2	83:Ai:24:ARG:HD2	2.46	0.50
12:BA:447:A:H5''	12:BA:448:G:OP2	2.11	0.50
19:BJ:89:VAL:O	19:BJ:93:ASN:ND2	2.43	0.50
33:Ba:240:ALA:HB2	33:Ba:375:TRP:HH2	1.76	0.50
34:Bb:238:THR:HG21	34:Bb:281:PHE:CE1	2.46	0.50
35:Bc:112:MET:HB2	35:Bc:267:PRO:HB3	1.92	0.50
58:AC:96:MET:HA	58:AC:96:MET:HE2	1.92	0.50
62:AI:207:GLU:HG3	62:AI:212:GLU:O	2.11	0.50
66:AN:70:VAL:O	66:AN:74:GLU:HG2	2.11	0.50
76:Ab:89:ASN:HB3	76:Ab:92:PHE:HB2	1.94	0.50
79:Ae:133:TYR:HB2	79:Ae:175:TYR:CE1	2.46	0.50
81:Ag:77:VAL:HG11	81:Ag:142:HIS:HB2	1.93	0.50
81:Ag:161:VAL:HG21	81:Ag:266:ALA:HB1	1.91	0.50
5:B3:74:SER:HB3	12:BA:472:U:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B4:37:ASN:HD22	6:B4:40:LEU:HD12	1.77	0.50
6:B4:50:ALA:H	36:Bd:94:PHE:HE2	1.60	0.50
12:BA:171:A:OP1	38:Bf:135:LYS:NZ	2.26	0.50
14:BC:298:GLU:O	14:BC:302:LYS:HG2	2.12	0.50
16:BE:197:HIS:NE2	16:BE:318:THR:HG22	2.27	0.50
23:BP:235:GLU:HA	23:BP:238:ARG:HG3	1.93	0.50
28:BU:116:LEU:HD21	29:BV:148:LEU:HD21	1.92	0.50
34:Bb:124:ARG:HH12	36:Bd:115:ALA:HB3	1.76	0.50
42:Bj:198:ASN:HB2	42:Bj:243:PHE:HA	1.94	0.50
53:Bw:101:ASN:O	53:Bw:105:TRP:HD1	1.94	0.50
59:AE:291:TYR:H	59:AE:356:GLN:NE2	2.08	0.50
62:AI:269:ALA:HB1	62:AI:356:PHE:HE2	1.75	0.50
66:AN:60:ASN:HD21	66:AN:62:ILE:HB	1.76	0.50
81:Ag:275:ARG:HE	81:Ag:281:ILE:HG22	1.76	0.50
12:BA:173:C:H1'	38:Bf:126:ARG:NH2	2.26	0.50
12:BA:221:A:H5''	12:BA:222:G:OP2	2.11	0.50
12:BA:1131:U:O2'	18:BI:87:LYS:NZ	2.44	0.50
14:BC:319:GLN:HE22	1:BL:159:VAL:HG23	1.77	0.50
22:BO:95:ARG:HA	22:BO:95:ARG:HH11	1.77	0.50
33:Ba:96:HIS:CD2	33:Ba:97:PRO:HD2	2.47	0.50
33:Ba:229:ARG:HG3	33:Ba:291:LEU:HD23	1.92	0.50
35:Bc:218:VAL:HG12	35:Bc:222:VAL:HG23	1.94	0.50
79:Ae:228:HIS:O	79:Ae:232:GLU:HG3	2.12	0.50
88:Ao:262:TYR:CD1	88:Ao:262:TYR:C	2.88	0.50
88:Ao:559:LYS:HG2	88:Ao:574:TRP:HE1	1.76	0.50
88:Ao:647:GLY:O	88:Ao:651:ARG:HG2	2.12	0.50
2:B0:62:HIS:H	2:B0:65:ASN:ND2	2.10	0.50
11:B9:69:LEU:HB2	12:BA:560:A:N6	2.26	0.50
16:BE:148:GLY:HA3	16:BE:173:LYS:HG3	1.92	0.50
53:Bw:156:ARG:HH11	53:Bw:161:GLN:HA	1.76	0.50
56:AA:390:A:O2'	67:AO:153:HIS:HE1	1.95	0.50
72:AV:15:A:O2'	72:AV:16:A:O4'	2.28	0.50
76:Ab:28:LYS:HG3	76:Ab:32:LEU:HD23	1.94	0.50
85:Ak:216:LEU:HB2	85:Ak:219:GLN:HG3	1.92	0.50
88:Ao:382:PHE:O	88:Ao:386:GLU:HB2	2.10	0.50
88:Ao:469:CYS:SG	88:Ao:498:ASP:HB3	2.51	0.50
10:B8:142:ARG:HB2	10:B8:142:ARG:CZ	2.41	0.50
13:BB:21:C:H1'	34:Bb:143:CYS:HB3	1.92	0.50
14:BC:361:GLU:HB3	14:BC:524:VAL:HG11	1.94	0.50
20:BK:95:ALA:HB1	20:BK:110:GLY:HA3	1.94	0.50
29:BV:148:LEU:HB2	38:Bf:58:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Be:129:TYR:HB3	37:Be:130:PRO:HD3	1.94	0.50
46:Bn:35:ARG:HH12	46:Bn:39:PRO:CA	2.24	0.50
76:Ab:28:LYS:HE3	76:Ab:32:LEU:HD23	1.93	0.50
79:Ae:169:LEU:HD11	79:Ae:184:PHE:HE1	1.77	0.50
88:Ao:308:VAL:HG22	88:Ao:315:LYS:HG3	1.92	0.50
89:Ap:56:TRP:HZ3	89:Ap:118:ARG:HD2	1.76	0.50
25:BR:139:ARG:HH11	25:BR:139:ARG:HG3	1.76	0.50
33:Ba:153:ARG:NH2	53:Bw:191:ALA:HA	2.27	0.50
33:Ba:215:ARG:HH11	33:Ba:215:ARG:HG3	1.77	0.50
40:Bh:79:LEU:HD13	40:Bh:214:PHE:HE2	1.77	0.50
42:Bj:257:LYS:HD3	42:Bj:276:LEU:HD21	1.93	0.50
56:AA:498:U:OP1	87:An:161:ARG:HD3	2.11	0.50
56:AA:677:C:H2'	56:AA:678:G:O4'	2.12	0.50
56:AA:762:G:N1	56:AA:765:A:OP2	2.45	0.50
59:AE:400:GLU:H	59:AE:400:GLU:CD	2.19	0.50
63:AJ:162:ARG:HH12	82:Ah:302:LEU:CD1	2.25	0.50
79:Ae:272:GLY:HA3	79:Ae:296:LEU:HD21	1.94	0.50
81:Ag:55:PRO:HG2	81:Ag:146:LYS:HD2	1.93	0.50
81:Ag:56:ALA:HB1	81:Ag:112:LYS:NZ	2.25	0.50
82:Ah:334:PRO:O	82:Ah:340:ARG:HG2	2.11	0.50
82:Ah:352:LYS:O	82:Ah:354:PRO:HD3	2.12	0.50
1:CL:25:PRO:HD2	1:CL:28:ILE:HD12	1.94	0.50
4:B2:90:GLN:NE2	4:B2:93:ARG:NH1	2.60	0.50
8:B6:24:ALA:HB2	8:B6:54:VAL:HG11	1.94	0.50
12:BA:216:C:OP2	44:Bl:111:ARG:NH2	2.45	0.50
12:BA:745:A:OP2	37:Be:44:ARG:NH2	2.44	0.50
12:BA:748:A:C8	53:Bw:308:GLN:HG2	2.47	0.50
14:BC:179:ARG:HG2	14:BC:180:SER:H	1.77	0.50
17:BF:276:HIS:O	44:Bl:90:ARG:NH2	2.45	0.50
21:BN:91:THR:HB	21:BN:94:GLN:NE2	2.26	0.50
24:BQ:101:HIS:CE1	24:BQ:184:PRO:HG3	2.47	0.50
33:Ba:337:GLU:H	33:Ba:337:GLU:CD	2.19	0.50
42:Bj:209:PRO:HB2	42:Bj:212:HIS:NE2	2.26	0.50
56:AA:174:C:H2'	56:AA:175:A:O4'	2.12	0.50
56:AA:606:A:HO2'	66:AN:28:TYR:HH	1.57	0.50
62:AI:201:LEU:HD21	62:AI:245:PHE:HA	1.94	0.50
66:AN:58:ARG:HB3	66:AN:58:ARG:NH1	2.27	0.50
12:BA:379:U:OP1	23:BP:62:ARG:NH1	2.45	0.50
1:BL:142:LYS:NZ	1:BL:166:GLU:HG2	2.27	0.50
35:Bc:48:GLU:O	35:Bc:52:GLN:HG2	2.12	0.50
41:Bi:88:TYR:CD2	41:Bi:195:VAL:HG11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Bu:177:SER:O	51:Bu:181:ASN:HB2	2.12	0.50
75:Aa:148:LEU:HD21	75:Aa:286:SER:O	2.12	0.50
76:Ab:73:LYS:HZ2	76:Ab:114:GLU:HG3	1.77	0.50
5:B3:79:PRO:HD2	5:B3:82:GLU:OE2	2.12	0.49
10:B8:169:ARG:NH1	10:B8:169:ARG:HG2	2.27	0.49
12:BA:860:G:O5'	15:BD:136:ARG:NH2	2.45	0.49
13:BB:8:U:H5'	13:BB:9:A:OP2	2.12	0.49
15:BD:103:ARG:HH11	15:BD:103:ARG:CB	2.25	0.49
34:Bb:99:ARG:H	34:Bb:99:ARG:HD2	1.77	0.49
35:Bc:207:ILE:HA	35:Bc:269:THR:HG22	1.94	0.49
39:Bg:139:THR:OG1	39:Bg:140:LEU:N	2.45	0.49
41:Bi:150:LEU:HD23	41:Bi:153:ASN:HD22	1.77	0.49
54:Bx:176:VAL:HG21	54:Bx:196:HIS:NE2	2.27	0.49
66:AN:63:LEU:HD13	66:AN:67:LEU:HD13	1.94	0.49
67:AO:109:LYS:O	67:AO:113:MET:HG3	2.12	0.49
70:AR:141:TYR:CD1	71:AU:29:ILE:HD13	2.46	0.49
75:Aa:285:ARG:HH11	75:Aa:285:ARG:CG	2.24	0.49
88:Ao:335:LEU:HB2	88:Ao:368:ILE:HG21	1.93	0.49
1:EL:71:ILE:HG22	1:HL:76:LEU:HD12	1.94	0.49
22:BO:32:ILE:HG23	22:BO:36:THR:OG1	2.12	0.49
31:BX:140:ARG:NH1	31:BX:140:ARG:HG2	2.27	0.49
33:Ba:136:VAL:HG22	33:Ba:420:HIS:HD2	1.77	0.49
34:Bb:265:PHE:CZ	34:Bb:322:ARG:HD2	2.48	0.49
38:Bf:69:TYR:CZ	40:Bh:256:ARG:NH1	2.80	0.49
56:AA:841:C:H1'	73:AX:7:C:N4	2.27	0.49
69:AQ:35:LEU:HD21	69:AQ:40:LEU:HD12	1.93	0.49
81:Ag:209:TRP:HZ3	81:Ag:215:THR:HB	1.76	0.49
88:Ao:353:LYS:NZ	88:Ao:385:HIS:HD2	2.10	0.49
88:Ao:520:LYS:HG3	88:Ao:527:ARG:NH2	2.27	0.49
89:Ap:192:THR:HG21	89:Ap:199:TRP:HA	1.92	0.49
10:B8:169:ARG:HG2	10:B8:169:ARG:HH11	1.76	0.49
12:BA:203:A:H5'	17:BF:152:ALA:CB	2.42	0.49
12:BA:289:U:H2'	12:BA:290:A:C8	2.47	0.49
25:BR:38:ARG:HB2	25:BR:38:ARG:HH11	1.77	0.49
56:AA:202:A:N1	84:Aj:53:ARG:NH2	2.44	0.49
56:AA:308:A:H3'	56:AA:309:A:O4'	2.13	0.49
56:AA:394:U:H4'	56:AA:395:C:H5''	1.94	0.49
57:AB:218:THR:HG22	57:AB:231:ILE:HG23	1.94	0.49
72:AV:16:A:H4'	72:AV:17:U:OP1	2.12	0.49
75:Aa:210:GLU:HG2	75:Aa:213:ARG:NH2	2.27	0.49
81:Ag:333:PHE:HD2	85:Ak:302:LYS:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B0:56:MET:H	2:B0:59:HIS:CD2	2.30	0.49
12:BA:39:A:H4'	12:BA:40:C:OP1	2.12	0.49
12:BA:1537:A:H2'	12:BA:1538:A:O4'	2.12	0.49
14:BC:407:ILE:HD11	14:BC:416:VAL:HG22	1.94	0.49
16:BE:210:THR:OG1	16:BE:262:GLY:O	2.18	0.49
25:BR:92:VAL:C	25:BR:95:PRO:HD2	2.37	0.49
34:Bb:224:HIS:HD2	34:Bb:227:GLU:H	1.59	0.49
42:Bj:53:LEU:HG	42:Bj:238:LEU:HD11	1.94	0.49
59:AE:291:TYR:CZ	59:AE:358:THR:HG23	2.47	0.49
63:AJ:119:THR:OG1	63:AJ:133:GLN:NE2	2.45	0.49
79:Ae:390:SER:HB2	79:Ae:396:LEU:HD12	1.94	0.49
17:BF:284:TYR:HB2	17:BF:285:PRO:HD2	1.94	0.49
23:BP:96:LEU:O	23:BP:140:LEU:HD23	2.12	0.49
23:BP:141:VAL:HG11	34:Bb:377:TYR:CZ	2.48	0.49
24:BQ:188:LYS:NZ	24:BQ:198:MET:HE1	2.28	0.49
30:BW:154:ILE:HG12	41:Bi:52:SER:HB3	1.95	0.49
36:Bd:145:GLU:OE1	42:Bj:274:ARG:NH2	2.42	0.49
43:Bk:81:ASN:HB3	43:Bk:86:TYR:CE2	2.48	0.49
54:Bx:90:SER:HA	54:Bx:93:ILE:HD11	1.94	0.49
56:AA:876:A:H61	84:Aj:17:ARG:HH12	1.59	0.49
63:AJ:162:ARG:HH12	82:Ah:302:LEU:HD12	1.76	0.49
64:AK:177:ILE:HD11	71:AU:23:TYR:HD2	1.77	0.49
75:Aa:327:HIS:CD2	75:Aa:349:LEU:HD11	2.47	0.49
79:Ae:242:ARG:NE	79:Ae:282:ALA:O	2.46	0.49
22:BO:72:ARG:HH11	22:BO:72:ARG:CB	2.11	0.49
22:BO:94:PRO:O	22:BO:97:THR:HB	2.12	0.49
27:BT:117:LEU:HD22	27:BT:176:VAL:HG22	1.94	0.49
31:BX:40:VAL:HB	31:BX:97:VAL:HG22	1.94	0.49
32:BY:191:LEU:HG	37:Be:93:THR:HG21	1.95	0.49
36:Bd:180:PRO:HD3	42:Bj:59:VAL:HG21	1.95	0.49
40:Bh:161:THR:O	40:Bh:192:ARG:NH1	2.42	0.49
41:Bi:90:PRO:HB2	41:Bi:269:TRP:CH2	2.47	0.49
50:Bt:99:ARG:HH11	50:Bt:99:ARG:HG3	1.77	0.49
56:AA:65:C:OP2	78:Ad:30:ARG:HB2	2.12	0.49
56:AA:647:A:C6	71:AU:82:ASP:HB3	2.48	0.49
56:AA:938:U:H2'	56:AA:939:A:C8	2.47	0.49
61:AG:77:ALA:O	62:AI:346:ARG:NH2	2.45	0.49
66:AN:55:ASN:HA	66:AN:58:ARG:HB2	1.95	0.49
1:DL:77:LEU:HD11	19:BJ:186:LEU:HD11	1.94	0.49
5:B3:36:PHE:CE1	24:BQ:228:LYS:HA	2.47	0.49
12:BA:739:U:H2'	12:BA:740:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:745:A:H3'	12:BA:746:U:H5''	1.94	0.49
13:BB:9:A:H5'	13:BB:47:A:H1'	1.95	0.49
22:BO:95:ARG:NH1	22:BO:95:ARG:N	2.60	0.49
26:BS:163:HIS:O	26:BS:167:GLU:HG2	2.12	0.49
33:Ba:213:TRP:HZ3	33:Ba:222:VAL:HG12	1.78	0.49
39:Bg:92:LYS:HB2	39:Bg:97:ILE:HD11	1.95	0.49
57:AB:65:PRO:HG3	57:AB:136:TYR:CE1	2.46	0.49
57:AB:83:LEU:HD23	57:AB:247:LEU:HD21	1.94	0.49
61:AG:119:LYS:HZ1	81:Ag:397:LEU:C	2.20	0.49
66:AN:113:HIS:O	66:AN:117:HIS:HD2	1.96	0.49
68:AP:59:ASN:HD22	77:Ac:146:GLN:HE22	1.60	0.49
84:Aj:30:ASP:HB2	84:Aj:34:TYR:HE1	1.77	0.49
88:Ao:382:PHE:HB3	88:Ao:396:ILE:HD11	1.95	0.49
12:BA:204:G:H2'	23:BP:40:PRO:HG3	1.95	0.49
16:BE:208:ALA:HB3	16:BE:290:PRO:O	2.12	0.49
16:BE:239:ARG:NH1	16:BE:239:ARG:HG2	2.28	0.49
34:Bb:66:ARG:O	34:Bb:75:ARG:NH1	2.42	0.49
36:Bd:171:PHE:HD1	42:Bj:203:LYS:HE2	1.76	0.49
62:AI:349:MET:O	62:AI:353:LEU:HG	2.13	0.49
75:Aa:189:HIS:HB3	75:Aa:215:ILE:HD13	1.95	0.49
88:Ao:386:GLU:HG3	88:Ao:393:SER:HB3	1.94	0.49
17:BF:221:LEU:HD22	17:BF:264:PRO:HB2	1.95	0.49
34:Bb:169:PRO:HA	34:Bb:314:ALA:O	2.12	0.49
36:Bd:147:LEU:HB3	36:Bd:151:ARG:NH1	2.28	0.49
41:Bi:88:TYR:CG	41:Bi:195:VAL:HG11	2.47	0.49
53:Bw:321:ASN:HB3	53:Bw:355:ILE:HD13	1.95	0.49
56:AA:93:A:N3	78:Ad:79:ARG:NH2	2.52	0.49
75:Aa:258:GLU:HG3	75:Aa:259:PRO:HD2	1.94	0.49
82:Ah:284:ARG:HG3	88:Ao:448:TRP:HB3	1.95	0.49
12:BA:276:G:C5	15:BD:260:LYS:HB2	2.48	0.49
12:BA:744:A:OP1	12:BA:744:A:H4'	2.13	0.49
12:BA:1026:A:C6	12:BA:1321:C:H1'	2.48	0.49
17:BF:83:HIS:CD2	17:BF:85:ASP:HB2	2.48	0.49
21:BN:177:ARG:HB2	54:Bx:36:ARG:O	2.12	0.49
23:BP:62:ARG:HG3	46:Bn:128:ARG:HH21	1.78	0.49
27:BT:268:ASP:O	27:BT:270:MET:N	2.46	0.49
33:Ba:280:GLN:HG2	53:Bw:152:ARG:HE	1.77	0.49
56:AA:622:U:H2'	56:AA:623:C:C6	2.48	0.49
56:AA:842:A:H5'	56:AA:845:G:H4'	1.95	0.49
56:AA:876:A:N6	84:Aj:17:ARG:HH12	2.10	0.49
57:AB:193:ILE:HA	57:AB:219:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AP:83:LEU:HD13	68:AP:91:LEU:HD12	1.95	0.49
75:Aa:230:VAL:HG12	75:Aa:236:ASN:HD21	1.78	0.49
81:Ag:101:ARG:HD2	97:Ag:500:GTP:O6	2.13	0.49
85:Ak:255:TRP:CD1	85:Ak:295:ARG:HG2	2.48	0.49
88:Ao:265:MET:HE2	88:Ao:281:LEU:HD11	1.95	0.49
88:Ao:457:ARG:HG2	88:Ao:489:PHE:CZ	2.48	0.49
88:Ao:559:LYS:NZ	88:Ao:582:VAL:HB	2.28	0.49
1:CL:49:LEU:HD12	1:DL:64:ILE:HG21	1.94	0.48
3:B1:163:ARG:NH1	33:Ba:55:LEU:HD11	2.28	0.48
12:BA:509:C:O2'	20:BK:102:ARG:HG3	2.13	0.48
14:BC:660:LYS:HD3	14:BC:670:LYS:NZ	2.28	0.48
17:BF:70:ARG:O	17:BF:202:TYR:OH	2.31	0.48
21:BN:117:HIS:HB3	21:BN:121:MET:HE3	1.94	0.48
23:BP:191:VAL:HG13	23:BP:277:MET:HE1	1.95	0.48
34:Bb:214:TRP:CH2	34:Bb:274:LYS:HE3	2.48	0.48
34:Bb:284:ASP:N	34:Bb:284:ASP:OD1	2.45	0.48
41:Bi:169:PHE:HB3	41:Bi:170:PRO:HD3	1.95	0.48
43:Bk:96:ILE:HG12	43:Bk:154:GLU:HG2	1.94	0.48
56:AA:244:C:H2'	56:AA:256:G:C8	2.48	0.48
56:AA:804:A:C8	66:AN:85:VAL:HG12	2.48	0.48
70:AR:53:VAL:HG21	76:Ab:66:HIS:CE1	2.48	0.48
70:AR:67:ILE:HD13	70:AR:136:VAL:HG11	1.95	0.48
88:Ao:231:THR:O	88:Ao:271:LYS:NZ	2.41	0.48
11:B9:99:GLN:NE2	12:BA:560:A:H2'	2.28	0.48
14:BC:215:GLN:HE22	14:BC:599:ILE:H	1.61	0.48
23:BP:246:ASP:N	23:BP:246:ASP:OD1	2.46	0.48
31:BX:15:PRO:HA	32:BY:208:ARG:HH11	1.78	0.48
35:Bc:281:HIS:CD2	35:Bc:319:MET:HG2	2.48	0.48
44:Bl:110:ILE:HD11	44:Bl:157:LEU:HD13	1.95	0.48
48:Bp:62:PRO:HG2	48:Bp:78:GLY:O	2.13	0.48
79:Ae:152:TRP:HZ3	79:Ae:165:ALA:HA	1.78	0.48
81:Ag:265:ASN:OD1	81:Ag:265:ASN:N	2.30	0.48
88:Ao:580:ASN:HA	88:Ao:613:LEU:HD13	1.94	0.48
3:B1:133:ASP:OD1	18:BI:120:ARG:NH2	2.44	0.48
20:BK:171:ARG:HH22	49:Bq:75:VAL:N	2.11	0.48
22:BO:68:LYS:O	22:BO:71:ASP:HB2	2.14	0.48
33:Ba:367:ASP:O	33:Ba:371:LYS:NZ	2.46	0.48
34:Bb:116:ASN:HB3	34:Bb:118:GLU:HG3	1.95	0.48
56:AA:689:G:H5'	59:AE:91:THR:HG22	1.94	0.48
57:AB:217:PRO:HG3	76:Ab:31:TRP:HB2	1.96	0.48
69:AQ:103:THR:O	77:Ac:72:PRO:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AV:49:G:H1	72:AV:56:C:N4	2.11	0.48
79:Ae:259:VAL:HG11	79:Ae:397:SER:HB3	1.95	0.48
12:BA:1442:U:O2	16:BE:257:MET:HE1	2.13	0.48
14:BC:549:VAL:HG12	65:AL:105:HIS:CD2	2.49	0.48
21:BN:140:ASN:HD22	40:Bh:262:GLY:CA	2.23	0.48
33:Ba:279:PHE:CE1	53:Bw:151:LEU:HD13	2.48	0.48
39:Bg:35:ARG:HB2	50:Bt:101:TRP:HB2	1.94	0.48
53:Bw:163:ARG:HD3	53:Bw:163:ARG:HA	1.67	0.48
77:Ac:29:VAL:HB	77:Ac:79:TYR:HB2	1.94	0.48
79:Ae:136:ARG:HH22	79:Ae:178:PHE:HE1	1.62	0.48
84:Aj:41:MET:HG2	84:Aj:55:TRP:CD1	2.49	0.48
84:Aj:129:ARG:HG2	84:Aj:130:GLU:N	2.28	0.48
85:Ak:268:LEU:O	85:Ak:272:LYS:HG2	2.14	0.48
12:BA:788:A:H3'	25:BR:10:SER:HB2	1.94	0.48
12:BA:1425:A:H3'	12:BA:1426:G:C5'	2.43	0.48
16:BE:69:ASN:OD1	16:BE:171:PRO:HB3	2.12	0.48
36:Bd:106:LEU:HB3	36:Bd:110:GLU:HB2	1.95	0.48
38:Bf:42:ASP:N	38:Bf:42:ASP:OD1	2.45	0.48
39:Bg:37:ALA:O	39:Bg:44:ARG:NH2	2.46	0.48
39:Bg:60:GLY:O	40:Bh:78:ARG:NH1	2.46	0.48
42:Bj:53:LEU:HD11	42:Bj:238:LEU:HD21	1.95	0.48
48:Bp:8:LEU:HD13	48:Bp:95:GLN:HG3	1.95	0.48
56:AA:121:C:OP1	69:AQ:76:HIS:HB2	2.14	0.48
67:AO:126:LEU:HD21	67:AO:170:ASN:HD22	1.77	0.48
79:Ae:266:TYR:CE2	79:Ae:316:CYS:HB3	2.49	0.48
88:Ao:432:LEU:HD23	88:Ao:472:GLU:HG2	1.95	0.48
12:BA:125:A:P	37:Be:17:ARG:HH22	2.35	0.48
12:BA:1240:A:C8	12:BA:1241:U:C5	3.01	0.48
16:BE:60:PHE:HB2	25:BR:154:ARG:NH1	2.27	0.48
16:BE:200:PRO:HA	16:BE:273:VAL:HG22	1.95	0.48
19:BJ:225:GLN:HB2	19:BJ:226:PRO:HD3	1.95	0.48
21:BN:48:HIS:CD2	21:BN:50:LEU:H	2.31	0.48
32:BY:44:VAL:HG11	32:BY:83:ARG:NH2	2.28	0.48
54:Bx:54:THR:HG22	54:Bx:55:GLU:H	1.79	0.48
57:AB:81:ARG:HD2	80:Af:84:MET:HE3	1.94	0.48
63:AJ:118:PHE:CD2	66:AN:101:LYS:NZ	2.81	0.48
64:AK:64:ILE:H	64:AK:64:ILE:HG13	1.39	0.48
86:Am:29:LEU:HD12	86:Am:29:LEU:HA	1.75	0.48
88:Ao:419:PHE:CZ	88:Ao:450:LEU:HD22	2.49	0.48
88:Ao:653:MET:SD	88:Ao:665:ALA:HB1	2.53	0.48
89:Ap:105:CYS:SG	89:Ap:143:CYS:HB3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:100:ARG:HH12	18:BI:75:ARG:HH21	1.60	0.48
10:B8:124:ARG:NH2	12:BA:1204:A:OP1	2.46	0.48
11:B9:92:ASN:OD1	11:B9:92:ASN:N	2.46	0.48
12:BA:438:A:OP2	19:BJ:38:ARG:NH2	2.47	0.48
19:BJ:111:LEU:O	19:BJ:115:GLN:HG2	2.13	0.48
26:BS:171:VAL:HG21	51:Bu:179:ILE:HD13	1.96	0.48
32:BY:105:ARG:HG3	41:Bi:174:TRP:CH2	2.47	0.48
59:AE:395:PRO:HB3	75:Aa:132:GLN:NE2	2.28	0.48
61:AG:121:LYS:NZ	61:AG:207:GLN:HA	2.29	0.48
64:AK:112:ALA:HB3	64:AK:137:ALA:HB2	1.95	0.48
67:AO:155:ARG:O	67:AO:159:MET:HB2	2.13	0.48
69:AQ:33:LEU:HD11	77:Ac:66:MET:HE1	1.96	0.48
78:Ad:54:PHE:CD2	89:Ap:208:PRO:HB3	2.49	0.48
78:Ad:62:GLN:HA	78:Ad:62:GLN:HE21	1.78	0.48
81:Ag:379:LEU:O	81:Ag:383:SER:OG	2.32	0.48
88:Ao:379:ILE:HG12	88:Ao:396:ILE:HG23	1.95	0.48
13:BB:30:G:H1'	36:Bd:122:SER:HB2	1.94	0.48
23:BP:237:ALA:HA	23:BP:242:TYR:CE2	2.49	0.48
38:Bf:114:LYS:HE3	38:Bf:114:LYS:HB2	1.71	0.48
53:Bw:96:GLN:HE21	53:Bw:321:ASN:HD21	1.62	0.48
1:DL:76:LEU:HD21	19:BJ:200:LEU:HA	1.95	0.48
5:B3:68:ILE:HD11	5:B3:122:LEU:HD13	1.96	0.48
12:BA:131:A:H8	12:BA:131:A:OP2	1.96	0.48
12:BA:173:C:O2	38:Bf:126:ARG:NH2	2.47	0.48
19:BJ:93:ASN:CG	19:BJ:155:VAL:HG13	2.39	0.48
19:BJ:162:LYS:NZ	19:BJ:196:LYS:HA	2.28	0.48
21:BN:71:LYS:HZ3	54:Bx:196:HIS:HD2	1.62	0.48
26:BS:72:TRP:CG	26:BS:73:PRO:HA	2.48	0.48
26:BS:115:HIS:CD2	34:Bb:135:VAL:HG22	2.46	0.48
41:Bi:208:ILE:HB	41:Bi:252:LEU:HD12	1.96	0.48
41:Bi:215:ARG:HE	41:Bi:243:LEU:HD11	1.79	0.48
42:Bj:173:LEU:HD23	42:Bj:233:PHE:CE2	2.49	0.48
56:AA:30:A:H2'	56:AA:31:U:C6	2.48	0.48
56:AA:120:A:O2'	69:AQ:22:MET:HE1	2.14	0.48
56:AA:562:A:C2'	56:AA:708:A:H61	2.27	0.48
56:AA:584:C:O2	66:AN:86:ARG:HG2	2.13	0.48
59:AE:216:ASP:OD1	59:AE:216:ASP:N	2.44	0.48
64:AK:175:ILE:HG13	64:AK:176:SER:N	2.28	0.48
73:AX:12:A:HO2'	73:AX:13:U:P	2.36	0.48
88:Ao:559:LYS:NZ	88:Ao:578:SER:O	2.44	0.48
89:Ap:95:ILE:HG22	89:Ap:100:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:145:A:H2'	12:BA:146:A:H8	1.75	0.48
12:BA:175:C:H2'	12:BA:176:U:C6	2.49	0.48
12:BA:1213:A:N1	12:BA:1220:A:N7	2.62	0.48
14:BC:598:ILE:HB	14:BC:601:ARG:HG2	1.96	0.48
23:BP:238:ARG:HH22	51:Bu:69:ASN:HA	1.78	0.48
35:Bc:45:PHE:CD2	35:Bc:253:ARG:NH1	2.82	0.48
58:AC:111:LYS:HB3	63:AJ:166:GLU:HG2	1.95	0.48
59:AE:94:THR:HB	59:AE:97:GLU:HG3	1.96	0.48
79:Ae:358:LEU:HB2	79:Ae:361:GLU:HB2	1.95	0.48
84:Aj:99:ARG:HG3	84:Aj:115:TRP:HB2	1.96	0.48
4:B2:101:HIS:NE2	37:Be:61:PRO:HD3	2.29	0.47
16:BE:45:SER:O	35:Bc:303:ARG:NH2	2.47	0.47
16:BE:293:LYS:O	16:BE:294:ASN:HB2	2.13	0.47
17:BF:287:ARG:CD	52:Bv:33:ARG:HH12	2.12	0.47
29:BV:115:GLU:HG2	39:Bg:19:LEU:HD11	1.95	0.47
36:Bd:151:ARG:HG2	36:Bd:158:HIS:CB	2.44	0.47
53:Bw:158:PRO:C	53:Bw:160:ILE:H	2.22	0.47
56:AA:752:A:H8	56:AA:753:A:H5'	1.78	0.47
56:AA:948:U:H5''	64:AK:196:LEU:HD12	1.96	0.47
64:AK:135:ILE:HD11	64:AK:169:MET:HE2	1.96	0.47
67:AO:134:THR:HG23	67:AO:164:ARG:NH1	2.29	0.47
88:Ao:574:TRP:HH2	88:Ao:579:LEU:HB2	1.77	0.47
1:CL:36:ALA:HA	1:FL:76:LEU:HB3	1.96	0.47
7:B5:88:GLU:OE1	7:B5:88:GLU:N	2.45	0.47
12:BA:734:A:OP2	15:BD:103:ARG:NH1	2.46	0.47
12:BA:811:A:H1'	16:BE:230:THR:HG23	1.96	0.47
12:BA:1216:C:N4	26:BS:173:ARG:HH22	2.02	0.47
19:BJ:146:LEU:HA	48:Bp:31:ARG:HH22	1.79	0.47
30:BW:132:VAL:HG13	30:BW:178:GLU:OE2	2.13	0.47
32:BY:77:VAL:HG21	32:BY:89:GLU:HB3	1.96	0.47
33:Ba:125:LYS:HE3	33:Ba:364:LEU:HA	1.94	0.47
41:Bi:160:LEU:O	41:Bi:164:VAL:HG22	2.14	0.47
56:AA:59:C:H5'	84:Aj:51:PRO:HG3	1.97	0.47
59:AE:124:LYS:HD3	59:AE:183:ARG:NH1	2.29	0.47
67:AO:127:GLU:O	67:AO:131:VAL:HG23	2.13	0.47
81:Ag:332:GLY:O	81:Ag:336:LEU:HB2	2.14	0.47
83:Ai:14:LEU:O	83:Ai:18:LEU:HB2	2.14	0.47
89:Ap:68:TYR:CE2	89:Ap:73:VAL:HG13	2.49	0.47
1:CL:28:ILE:HG21	1:DL:85:LEU:HD12	1.96	0.47
10:B8:169:ARG:HH11	10:B8:169:ARG:CG	2.27	0.47
17:BF:195:LEU:O	17:BF:229:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BK:160:SER:O	20:BK:163:GLU:HB2	2.15	0.47
21:BN:155:LEU:HD13	54:Bx:86:VAL:HG12	1.96	0.47
24:BQ:36:VAL:HG11	49:Bq:124:HIS:HB3	1.95	0.47
50:Bt:99:ARG:HG3	50:Bt:99:ARG:NH1	2.27	0.47
51:Bu:44:SER:OG	51:Bu:45:LEU:N	2.47	0.47
53:Bw:326:LEU:O	53:Bw:330:THR:OG1	2.32	0.47
54:Bx:164:ASN:O	54:Bx:166:GLY:N	2.47	0.47
3:B1:190:ARG:H	3:B1:190:ARG:HG2	1.40	0.47
3:B1:202:GLU:HG3	3:B1:203:TRP:CD1	2.49	0.47
8:B6:16:ILE:HG22	8:B6:34:ARG:O	2.13	0.47
10:B8:142:ARG:NH1	12:BA:1193:C:OP2	2.47	0.47
17:BF:191:ASP:C	17:BF:192:SER:HG	2.23	0.47
40:Bh:227:GLU:HB2	40:Bh:230:GLU:HB2	1.97	0.47
42:Bj:85:SER:HB3	42:Bj:88:GLU:HB2	1.96	0.47
54:Bx:92:PHE:O	54:Bx:93:ILE:HG23	2.14	0.47
56:AA:59:C:N3	84:Aj:54:ALA:HB1	2.29	0.47
57:AB:123:HIS:CE1	76:Ab:41:LEU:HD12	2.50	0.47
57:AB:137:ARG:HD3	76:Ab:34:ILE:HD11	1.95	0.47
60:AF:29:LEU:HD12	60:AF:78:MET:HG2	1.96	0.47
66:AN:101:LYS:HD3	66:AN:101:LYS:HA	1.59	0.47
75:Aa:181:THR:HG23	75:Aa:194:ILE:HD12	1.96	0.47
79:Ae:147:TRP:H	79:Ae:147:TRP:CD1	2.32	0.47
79:Ae:228:HIS:HA	79:Ae:231:ALA:HB3	1.94	0.47
8:B6:54:VAL:HG12	8:B6:55:LEU:H	1.78	0.47
12:BA:1131:U:H2'	12:BA:1132:G:C8	2.49	0.47
23:BP:206:PRO:O	52:Bv:99:MET:HE1	2.14	0.47
46:Bn:65:ASN:O	46:Bn:67:GLU:HG3	2.13	0.47
56:AA:641:A:OP1	59:AE:230:ASN:HB2	2.15	0.47
56:AA:767:U:H2'	56:AA:768:A:C8	2.49	0.47
62:AI:91:MET:SD	85:Ak:85:LEU:HD21	2.55	0.47
71:AU:50:ARG:HG3	71:AU:50:ARG:NH1	2.14	0.47
77:Ac:160:THR:HG22	77:Ac:162:LYS:H	1.79	0.47
88:Ao:375:TYR:O	88:Ao:379:ILE:HG13	2.14	0.47
89:Ap:126:PHE:HE2	89:Ap:140:THR:HG21	1.79	0.47
89:Ap:136:HIS:HD2	89:Ap:139:TYR:H	1.61	0.47
3:B1:163:ARG:HD3	3:B1:205:GLY:H	1.79	0.47
12:BA:1050:C:H5'	12:BA:1051:G:OP1	2.15	0.47
14:BC:255:VAL:HG13	14:BC:281:VAL:HG11	1.96	0.47
20:BK:164:LEU:HD22	20:BK:164:LEU:HA	1.52	0.47
27:BT:152:ARG:HH12	27:BT:191:ARG:HA	1.79	0.47
32:BY:22:GLY:C	32:BY:24:SER:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AN:80:ARG:HE	66:AN:80:ARG:HB2	1.61	0.47
71:AU:21:GLY:HA2	71:AU:24:ARG:HD2	1.97	0.47
86:Am:62:ARG:HG3	86:Am:65:ALA:HB2	1.97	0.47
88:Ao:292:ALA:O	88:Ao:331:VAL:HG21	2.14	0.47
88:Ao:417:MET:HA	88:Ao:420:GLN:HB3	1.96	0.47
89:Ap:235:MET:HA	89:Ap:236:PRO:HD3	1.72	0.47
1:DL:77:LEU:HD12	19:BJ:184:THR:HG21	1.95	0.47
1:EL:79:ILE:CD1	1:HL:76:LEU:HG	2.45	0.47
3:B1:87:LEU:HD23	3:B1:104:VAL:HB	1.96	0.47
3:B1:160:ASP:OD1	3:B1:163:ARG:NH2	2.41	0.47
3:B1:162:LYS:O	3:B1:166:LEU:HB2	2.14	0.47
4:B2:193:ASN:O	4:B2:197:ASN:HB2	2.14	0.47
12:BA:225:C:H5'	23:BP:133:LYS:HE2	1.96	0.47
12:BA:379:U:OP1	23:BP:62:ARG:HD3	2.15	0.47
12:BA:640:A:OP1	30:BW:147:ARG:NH1	2.47	0.47
12:BA:1521:U:H3'	12:BA:1522:A:H5'	1.96	0.47
14:BC:572:TYR:HB3	14:BC:602:LEU:HD11	1.96	0.47
17:BF:114:THR:HG21	17:BF:154:GLY:HA3	1.96	0.47
24:BQ:223:MET:O	24:BQ:226:ILE:HB	2.15	0.47
27:BT:74:ARG:HB3	27:BT:283:TRP:CH2	2.49	0.47
31:BX:66:ALA:HB2	31:BX:100:ALA:HA	1.97	0.47
33:Ba:147:ILE:HG22	33:Ba:148:GLU:H	1.80	0.47
37:Be:73:ASN:OD1	37:Be:74:TYR:N	2.47	0.47
40:Bh:60:ARG:HH11	40:Bh:63:LYS:HB2	1.80	0.47
45:Bm:91:SER:HB2	45:Bm:123:ARG:NH1	2.30	0.47
53:Bw:105:TRP:CE2	53:Bw:258:MET:HE2	2.50	0.47
56:AA:127:A:H2'	56:AA:128:C:C6	2.50	0.47
56:AA:560:C:H42	56:AA:710:G:H1	1.63	0.47
59:AE:376:GLU:HA	75:Aa:118:GLN:NE2	2.30	0.47
62:AI:155:LYS:NZ	62:AI:218:ASP:OD2	2.42	0.47
77:Ac:47:PHE:HA	77:Ac:51:ASN:HD22	1.79	0.47
79:Ae:101:TYR:CZ	79:Ae:107:VAL:HG21	2.49	0.47
79:Ae:177:ILE:HG13	79:Ae:178:PHE:H	1.79	0.47
81:Ag:123:TYR:HE1	81:Ag:340:ILE:HD12	1.79	0.47
82:Ah:284:ARG:HH21	88:Ao:451:ILE:HB	1.79	0.47
82:Ah:301:LYS:HA	88:Ao:137:ILE:HD13	1.97	0.47
85:Ak:136:PRO:HG2	85:Ak:139:LEU:HD12	1.96	0.47
7:B5:141:MET:HE3	7:B5:173:ARG:HH22	1.80	0.47
12:BA:329:A:C2	15:BD:275:LEU:HD13	2.50	0.47
12:BA:494:U:C2	12:BA:560:A:C2	3.03	0.47
12:BA:724:A:H2	12:BA:728:C:H42	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BJ:163:GLU:HG3	19:BJ:166:ARG:NH1	2.29	0.47
25:BR:16:ARG:NH2	25:BR:50:ASP:OD2	2.47	0.47
26:BS:42:GLU:HA	34:Bb:337:MET:HE3	1.97	0.47
31:BX:26:ILE:HD12	31:BX:56:TYR:CE1	2.50	0.47
35:Bc:140:TRP:CE2	35:Bc:171:VAL:HG13	2.49	0.47
38:Bf:126:ARG:HH11	38:Bf:126:ARG:CB	2.20	0.47
41:Bi:89:VAL:HA	41:Bi:90:PRO:HD3	1.65	0.47
56:AA:26:A:H2'	56:AA:27:U:H6	1.79	0.47
56:AA:56:U:OP1	78:Ad:41:ARG:NH2	2.48	0.47
56:AA:128:C:H2'	56:AA:129:G:O4'	2.15	0.47
66:AN:29:TYR:HB3	66:AN:34:MET:HG2	1.97	0.47
79:Ae:188:MET:O	79:Ae:192:ILE:HG13	2.15	0.47
88:Ao:531:LYS:HE3	88:Ao:531:LYS:HB2	1.73	0.47
88:Ao:602:PHE:CD1	88:Ao:609:PRO:HG3	2.50	0.47
8:B6:47:ASP:HA	8:B6:48:PRO:HD3	1.68	0.47
12:BA:320:U:OP1	15:BD:61:ALA:N	2.47	0.47
12:BA:779:G:H5'	53:Bw:219:ARG:HH12	1.80	0.47
21:BN:173:PRO:HG2	21:BN:176:TYR:HB2	1.96	0.47
24:BQ:133:ARG:HG3	24:BQ:148:ASP:OD2	2.15	0.47
33:Ba:160:HIS:HA	33:Ba:164:TRP:HB2	1.96	0.47
34:Bb:159:ARG:NH1	34:Bb:160:ASP:OD1	2.48	0.47
47:Bo:23:ALA:O	47:Bo:28:ARG:NH2	2.47	0.47
59:AE:112:LYS:HB3	59:AE:114:ARG:HG3	1.97	0.47
61:AG:152:CYS:HA	61:AG:220:ILE:HD13	1.97	0.47
63:AJ:115:ILE:HG12	63:AJ:137:ARG:HG2	1.97	0.47
5:B3:71:ARG:HH22	12:BA:473:G:P	2.38	0.47
11:B9:65:THR:CG2	11:B9:100:MET:HB3	2.45	0.47
34:Bb:322:ARG:NH1	51:Bu:180:GLU:OE2	2.48	0.47
36:Bd:102:PRO:HG2	36:Bd:103:PRO:HD3	1.97	0.47
42:Bj:46:ARG:HB3	42:Bj:229:ALA:HB2	1.96	0.47
53:Bw:96:GLN:HE21	53:Bw:321:ASN:ND2	2.13	0.47
56:AA:256:G:H3'	56:AA:257:U:H5'	1.97	0.47
56:AA:283:U:OP1	59:AE:419:ARG:NH1	2.47	0.47
57:AB:154:ILE:HG12	57:AB:195:LEU:HD12	1.96	0.47
69:AQ:93:ASP:OD2	69:AQ:96:THR:OG1	2.33	0.47
71:AU:50:ARG:HH11	71:AU:50:ARG:CG	2.16	0.47
79:Ae:275:GLU:HG3	79:Ae:283:VAL:HG21	1.96	0.47
81:Ag:227:GLN:HE21	81:Ag:231:ARG:NH2	2.13	0.47
12:BA:1199:A:H2'	12:BA:1200:A:O4'	2.16	0.46
14:BC:657:LYS:HZ1	14:BC:713:GLU:CD	2.23	0.46
16:BE:83:GLU:HB2	16:BE:188:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BE:329:PRO:HD2	16:BE:332:LEU:HD21	1.97	0.46
16:BE:335:GLU:H	16:BE:335:GLU:CD	2.23	0.46
17:BF:120:VAL:HG12	17:BF:121:ARG:H	1.80	0.46
31:BX:3:ARG:HB3	31:BX:24:PHE:CE2	2.50	0.46
35:Bc:163:LEU:HB3	35:Bc:178:TYR:HE2	1.80	0.46
51:Bu:108:ASP:OD1	51:Bu:108:ASP:N	2.36	0.46
56:AA:881:A:H4'	79:Ae:103:ARG:HH22	1.80	0.46
56:AA:887:U:H2'	56:AA:888:A:C8	2.51	0.46
61:AG:153:GLU:HG3	61:AG:179:ARG:HB3	1.97	0.46
63:AJ:132:VAL:HG21	66:AN:112:ARG:CZ	2.45	0.46
77:Ac:48:VAL:HA	77:Ac:52:ILE:HG13	1.95	0.46
79:Ae:254:LYS:HB2	79:Ae:260:GLY:HA3	1.96	0.46
85:Ak:148:HIS:O	85:Ak:150:PRO:HD3	2.14	0.46
88:Ao:634:VAL:HG11	88:Ao:652:VAL:HG21	1.96	0.46
4:B2:209:ARG:HG2	4:B2:209:ARG:NH1	2.30	0.46
5:B3:84:ASP:O	5:B3:88:MET:HG2	2.15	0.46
12:BA:935:C:H2'	12:BA:936:A:O4'	2.15	0.46
12:BA:949:A:N3	12:BA:1374:U:H5'	2.31	0.46
23:BP:233:ARG:HD3	23:BP:244:LEU:HD21	1.97	0.46
26:BS:160:ARG:NH1	34:Bb:126:GLN:HB3	2.26	0.46
34:Bb:72:ARG:N	34:Bb:72:ARG:NH1	2.62	0.46
36:Bd:146:ALA:HA	42:Bj:212:HIS:HB2	1.97	0.46
36:Bd:147:LEU:HD21	42:Bj:209:PRO:HD2	1.97	0.46
39:Bg:35:ARG:HD3	45:Bm:157:TRP:CH2	2.50	0.46
40:Bh:141:PHE:CE2	40:Bh:156:LEU:HB3	2.51	0.46
41:Bi:141:ALA:HB1	41:Bi:248:PHE:CZ	2.50	0.46
46:Bn:117:LEU:HD23	46:Bn:117:LEU:HA	1.80	0.46
54:Bx:69:GLN:HB3	54:Bx:70:CYS:SG	2.54	0.46
63:AJ:96:VAL:O	63:AJ:100:LYS:HG2	2.15	0.46
63:AJ:158:GLU:HB2	82:Ah:306:PRO:HD3	1.96	0.46
74:AZ:695:ALA:HB2	83:Ai:10:ARG:HH11	1.79	0.46
75:Aa:279:GLY:HA2	75:Aa:281:TYR:CE1	2.51	0.46
81:Ag:330:LYS:O	81:Ag:334:ASP:HB2	2.15	0.46
82:Ah:309:ASN:O	85:Ak:166:ARG:NH1	2.45	0.46
82:Ah:324:ILE:HD12	85:Ak:213:ARG:HD3	1.97	0.46
6:B4:72:PRO:HG2	42:Bj:87:HIS:CG	2.50	0.46
12:BA:525:A:C2'	12:BA:526:A:H5''	2.45	0.46
12:BA:854:U:HO2'	33:Ba:36:ARG:H	1.62	0.46
12:BA:938:U:OP1	12:BA:938:U:H6	1.98	0.46
12:BA:1494:A:H2'	12:BA:1495:A:C8	2.50	0.46
16:BE:175:LYS:HD2	16:BE:296:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BO:41:VAL:HG13	22:BO:121:THR:HG23	1.97	0.46
41:Bi:168:CYS:HB2	41:Bi:262:HIS:O	2.15	0.46
42:Bj:51:LEU:HD12	42:Bj:188:ALA:HB1	1.96	0.46
42:Bj:162:ARG:HD3	42:Bj:171:TRP:HE3	1.80	0.46
56:AA:561:U:H2'	56:AA:562:A:H5'	1.98	0.46
58:AC:73:THR:HG23	63:AJ:169:ALA:HB2	1.98	0.46
58:AC:94:LYS:NZ	59:AE:92:LYS:HB2	2.30	0.46
60:AF:116:LYS:HG2	76:Ab:51:LEU:HD21	1.96	0.46
68:AP:93:LEU:HG	68:AP:103:MET:HE1	1.97	0.46
70:AR:108:ILE:O	70:AR:112:ILE:HG13	2.15	0.46
77:Ac:141:CYS:HB3	77:Ac:149:CYS:N	2.30	0.46
6:B4:44:LEU:HD23	6:B4:46:ARG:H	1.80	0.46
12:BA:479:A:N1	30:BW:208:HIS:HA	2.30	0.46
12:BA:1464:A:H2'	12:BA:1465:A:C8	2.51	0.46
15:BD:83:GLY:O	15:BD:85:ARG:HG2	2.15	0.46
16:BE:239:ARG:HH11	16:BE:239:ARG:HG2	1.80	0.46
19:BJ:117:ARG:HD3	19:BJ:117:ARG:HA	1.69	0.46
19:BJ:186:LEU:HD22	19:BJ:190:GLY:HA3	1.98	0.46
27:BT:59:LYS:HA	27:BT:60:PRO:HD3	1.80	0.46
33:Ba:240:ALA:HB3	33:Ba:358:GLN:HE22	1.80	0.46
33:Ba:313:MET:HE1	33:Ba:346:GLY:HA3	1.97	0.46
34:Bb:79:GLY:C	34:Bb:81:GLU:H	2.23	0.46
43:Bk:122:GLU:HG2	43:Bk:160:SER:HB2	1.97	0.46
57:AB:203:GLU:HG3	86:Am:114:LYS:NZ	2.30	0.46
66:AN:30:VAL:HG13	66:AN:95:SER:HB2	1.96	0.46
67:AO:113:MET:HG2	67:AO:131:VAL:HG11	1.97	0.46
75:Aa:345:GLU:O	75:Aa:349:LEU:N	2.47	0.46
84:Aj:164:VAL:HG23	84:Aj:191:LEU:HB3	1.98	0.46
85:Ak:89:MET:HG2	85:Ak:90:GLY:N	2.31	0.46
7:B5:138:ARG:HA	7:B5:141:MET:HG2	1.98	0.46
7:B5:181:ARG:HA	7:B5:182:PRO:HD3	1.79	0.46
10:B8:118:HIS:HE1	12:BA:227:U:OP1	1.98	0.46
12:BA:148:A:H2	30:BW:46:SER:HB2	1.80	0.46
12:BA:925:G:O2'	12:BA:963:G:O6	2.30	0.46
14:BC:667:VAL:HG11	14:BC:670:LYS:HE2	1.98	0.46
19:BJ:162:LYS:HG3	19:BJ:195:SER:HB2	1.98	0.46
26:BS:141:ILE:O	26:BS:141:ILE:HG12	2.14	0.46
39:Bg:35:ARG:O	39:Bg:44:ARG:NH1	2.48	0.46
53:Bw:147:GLU:HG3	53:Bw:169:PRO:HG2	1.98	0.46
56:AA:14:C:P	59:AE:226:ARG:HH12	2.38	0.46
56:AA:619:C:H1'	63:AJ:124:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AG:140:ASN:HB3	61:AG:143:THR:HG22	1.98	0.46
63:AJ:170:MET:HE3	63:AJ:172:VAL:HG22	1.98	0.46
85:Ak:291:VAL:O	85:Ak:295:ARG:HG3	2.15	0.46
3:B1:5:LYS:HD2	12:BA:18:A:N7	2.30	0.46
7:B5:90:ASN:O	7:B5:94:ARG:HG2	2.16	0.46
12:BA:78:A:OP1	23:BP:87:HIS:HE1	1.99	0.46
12:BA:187:G:H2'	12:BA:1025:A:N7	2.30	0.46
16:BE:53:LEU:HA	25:BR:147:ASN:HD21	1.81	0.46
17:BF:69:LEU:HD13	17:BF:190:VAL:HG21	1.98	0.46
19:BJ:89:VAL:HG13	19:BJ:93:ASN:HD21	1.80	0.46
20:BK:90:PHE:CD2	20:BK:120:ILE:HG23	2.51	0.46
33:Ba:194:LYS:HB3	33:Ba:195:HIS:HD2	1.80	0.46
36:Bd:121:TRP:CG	42:Bj:70:MET:HE3	2.50	0.46
40:Bh:119:LEU:HA	40:Bh:119:LEU:HD23	1.79	0.46
56:AA:368:A:O2'	71:AU:38:ASP:OD2	2.34	0.46
57:AB:70:ASP:O	57:AB:73:ASN:N	2.30	0.46
57:AB:140:ILE:HB	57:AB:189:PRO:HA	1.97	0.46
67:AO:153:HIS:HA	67:AO:156:PHE:CD2	2.50	0.46
69:AQ:22:MET:HE2	69:AQ:22:MET:HB3	1.75	0.46
69:AQ:35:LEU:HB2	69:AQ:42:TYR:CE1	2.50	0.46
70:AR:56:GLU:H	70:AR:56:GLU:CD	2.21	0.46
70:AR:77:ASN:ND2	70:AR:80:LEU:HB3	2.30	0.46
75:Aa:135:GLU:O	75:Aa:138:LYS:HG2	2.16	0.46
76:Ab:78:TYR:HA	76:Ab:134:ARG:HA	1.96	0.46
3:B1:6:VAL:HG13	12:BA:21:C:H41	1.81	0.46
3:B1:42:HIS:O	18:BI:55:ILE:HA	2.15	0.46
3:B1:72:PRO:O	3:B1:75:SER:HB3	2.15	0.46
5:B3:38:ARG:HB2	12:BA:410:U:OP1	2.16	0.46
5:B3:91:LEU:HD23	5:B3:91:LEU:HA	1.73	0.46
7:B5:94:ARG:NH1	12:BA:644:G:OP2	2.49	0.46
8:B6:62:ILE:HG21	12:BA:1244:U:H4'	1.98	0.46
9:B7:88:LYS:NZ	12:BA:127:G:OP2	2.48	0.46
12:BA:36:A:C4	37:Be:32:LYS:HG3	2.51	0.46
12:BA:477:A:C2'	12:BA:478:G:H5'	2.46	0.46
17:BF:165:LEU:HD12	17:BF:165:LEU:HA	1.70	0.46
17:BF:237:LEU:HD23	17:BF:237:LEU:HA	1.75	0.46
22:BO:45:ALA:O	22:BO:49:THR:HG22	2.16	0.46
33:Ba:293:PHE:CD2	33:Ba:312:LYS:HE2	2.50	0.46
53:Bw:356:THR:HG23	53:Bw:357:ASP:O	2.16	0.46
56:AA:125:U:H2'	56:AA:126:A:O4'	2.16	0.46
56:AA:739:A:H5'	56:AA:740:U:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AE:150:ARG:HB2	59:AE:155:GLN:NE2	2.30	0.46
59:AE:180:ASP:O	59:AE:184:LYS:HG2	2.15	0.46
63:AJ:121:LEU:HB2	66:AN:108:ARG:HE	1.80	0.46
67:AO:76:ASP:HB3	78:Ad:153:LYS:HD2	1.96	0.46
88:Ao:126:LYS:HE3	88:Ao:127:TYR:CE2	2.50	0.46
88:Ao:342:LEU:HD22	88:Ao:356:ALA:HB1	1.97	0.46
88:Ao:412:ASP:HB3	88:Ao:413:PRO:HD2	1.98	0.46
88:Ao:423:MET:HE2	88:Ao:460:TYR:HA	1.97	0.46
12:BA:734:A:OP2	15:BD:105:ARG:NH2	2.49	0.46
18:BI:105:LEU:HD22	18:BI:112:VAL:HG21	1.96	0.46
20:BK:141:VAL:HG12	49:Bq:99:MET:HE1	1.98	0.46
21:BN:177:ARG:NH1	54:Bx:38:VAL:HG11	2.31	0.46
28:BU:149:ARG:HD2	38:Bf:56:ARG:HH21	1.80	0.46
34:Bb:35:MET:HG3	34:Bb:36:PRO:HD2	1.97	0.46
40:Bh:161:THR:HG23	40:Bh:196:PHE:CZ	2.51	0.46
40:Bh:223:MET:HE2	40:Bh:223:MET:HB3	1.89	0.46
54:Bx:99:MET:HE1	54:Bx:119:VAL:HB	1.97	0.46
54:Bx:193:LEU:HD23	54:Bx:193:LEU:HA	1.73	0.46
56:AA:85:G:H2'	56:AA:86:A:C8	2.51	0.46
56:AA:357:G:H21	64:AK:100:GLN:HE22	1.64	0.46
56:AA:825:C:C5'	86:Am:38:ARG:HH12	2.29	0.46
58:AC:70:SER:O	66:AN:121:SER:HB3	2.15	0.46
61:AG:110:LEU:HD22	61:AG:201:MET:HB3	1.98	0.46
62:AI:270:PHE:HD1	62:AI:285:VAL:HG13	1.80	0.46
81:Ag:111:LEU:HA	81:Ag:114:THR:HG23	1.98	0.46
81:Ag:122:ARG:HA	81:Ag:305:ILE:HG13	1.98	0.46
6:B4:37:ASN:HA	6:B4:40:LEU:HD12	1.98	0.46
12:BA:532:A:OP1	49:Bq:123:LYS:HE3	2.16	0.46
13:BB:43:C:C2'	13:BB:44:U:H5'	2.46	0.46
17:BF:61:PRO:HA	17:BF:84:PRO:HD3	1.98	0.46
19:BJ:163:GLU:N	19:BJ:163:GLU:OE1	2.48	0.46
23:BP:156:VAL:O	23:BP:176:THR:HA	2.15	0.46
30:BW:154:ILE:HD13	30:BW:154:ILE:HA	1.77	0.46
33:Ba:174:GLU:HA	33:Ba:296:SER:HB2	1.96	0.46
36:Bd:83:ILE:HB	55:Bz:302:ALA:HB1	1.97	0.46
41:Bi:177:ARG:HG2	41:Bi:177:ARG:HH11	1.81	0.46
51:Bu:75:ARG:HH12	51:Bu:108:ASP:CG	2.23	0.46
53:Bw:182:LEU:HD11	53:Bw:416:VAL:HG22	1.98	0.46
56:AA:103:G:OP1	69:AQ:78:LYS:NZ	2.44	0.46
56:AA:922:C:H2'	56:AA:923:G:O4'	2.15	0.46
59:AE:256:PHE:CZ	59:AE:347:ARG:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AJ:188:ILE:HG12	85:Ak:236:TRP:CE3	2.51	0.46
75:Aa:183:ILE:O	75:Aa:183:ILE:HG12	2.16	0.46
77:Ac:73:SER:HA	77:Ac:74:PRO:HD3	1.81	0.46
77:Ac:77:ARG:HB3	77:Ac:79:TYR:HE1	1.81	0.46
86:Am:13:LEU:HD13	86:Am:13:LEU:HA	1.78	0.46
5:B3:73:LYS:HB3	5:B3:73:LYS:HE2	1.65	0.46
12:BA:623:G:H4'	17:BF:101:ILE:HG13	1.96	0.46
15:BD:213:THR:O	15:BD:248:VAL:HG23	2.17	0.46
16:BE:199:ARG:HD3	16:BE:199:ARG:HA	1.70	0.46
18:BI:59:TRP:CE2	18:BI:81:LYS:HE2	2.51	0.46
19:BJ:100:GLN:OE1	48:Bp:31:ARG:HD3	2.16	0.46
23:BP:11:ARG:HG3	23:BP:12:ALA:N	2.31	0.46
35:Bc:112:MET:HE1	35:Bc:124:PHE:HD1	1.80	0.46
36:Bd:97:LYS:HA	36:Bd:99:ARG:CZ	2.45	0.46
48:Bp:16:VAL:HG22	48:Bp:66:VAL:HG13	1.98	0.46
53:Bw:251:ILE:HG22	53:Bw:253:ILE:H	1.81	0.46
54:Bx:190:ARG:H	54:Bx:190:ARG:HG2	1.54	0.46
56:AA:344:G:N1	64:AK:121:ASN:HB3	2.31	0.46
56:AA:729:A:H2'	56:AA:730:C:O4'	2.16	0.46
56:AA:878:A:H2'	56:AA:879:A:O4'	2.16	0.46
56:AA:884:C:O4'	79:Ae:145:ARG:NH1	2.49	0.46
63:AJ:102:LEU:HG	85:Ak:125:CYS:SG	2.56	0.46
76:Ab:48:ARG:HA	76:Ab:49:PRO:HD3	1.60	0.46
79:Ae:170:LYS:HA	79:Ae:206:GLU:OE2	2.16	0.46
88:Ao:432:LEU:HB2	88:Ao:471:MET:HG2	1.98	0.46
4:B2:157:LEU:HD23	4:B2:157:LEU:HA	1.83	0.45
12:BA:151:A:O5'	12:BA:151:A:H8	1.99	0.45
12:BA:529:G:H4'	49:Bq:122:ARG:HH11	1.80	0.45
12:BA:838:A:H1'	12:BA:933:A:N6	2.30	0.45
12:BA:889:C:N4	12:BA:1082:U:H4'	2.21	0.45
12:BA:1411:G:C2'	12:BA:1412:A:H5'	2.46	0.45
17:BF:167:MET:HB3	17:BF:167:MET:HE2	1.58	0.45
18:BI:109:GLY:HA2	18:BI:140:PHE:CD2	2.51	0.45
20:BK:166:ALA:HB1	20:BK:170:GLU:CD	2.41	0.45
21:BN:71:LYS:HZ1	54:Bx:196:HIS:CD2	2.33	0.45
21:BN:112:LEU:HB2	21:BN:118:ARG:HD2	1.97	0.45
27:BT:76:LEU:HB2	27:BT:283:TRP:HZ3	1.81	0.45
29:BV:168:THR:OG1	29:BV:169:GLU:N	2.49	0.45
33:Ba:117:VAL:O	33:Ba:121:LEU:HG	2.15	0.45
44:Bl:161:LEU:HD23	44:Bl:161:LEU:HA	1.81	0.45
53:Bw:235:ILE:HB	53:Bw:290:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Bz:309:ALA:HB2	55:Bz:402:ALA:HB2	1.98	0.45
56:AA:177:U:H2'	56:AA:178:G:H8	1.81	0.45
57:AB:72:PHE:CE1	57:AB:259:ALA:HA	2.51	0.45
60:AF:38:ASN:HB3	60:AF:67:ASP:OD2	2.15	0.45
65:AL:32:THR:OG1	65:AL:35:GLN:HG3	2.16	0.45
68:AP:100:HIS:HB3	68:AP:103:MET:HG3	1.98	0.45
77:Ac:125:HIS:HA	77:Ac:126:PRO:HD3	1.82	0.45
79:Ae:223:LEU:HD22	79:Ae:223:LEU:HA	1.84	0.45
80:Af:105:ILE:HG21	80:Af:108:ILE:HD11	1.99	0.45
81:Ag:323:LEU:HD13	85:Ak:306:ASP:HB2	1.98	0.45
82:Ah:342:PHE:CE2	82:Ah:343:MET:HE3	2.51	0.45
12:BA:752:U:C2'	12:BA:753:G:H5'	2.46	0.45
12:BA:931:U:H5	12:BA:938:U:O4	1.99	0.45
15:BD:159:LYS:O	15:BD:162:ASP:HB2	2.17	0.45
22:BO:99:ARG:NH1	27:BT:191:ARG:HH21	2.12	0.45
23:BP:180:ASP:HB3	23:BP:204:MET:HB2	1.98	0.45
52:Bv:111:GLU:O	52:Bv:115:GLN:HG2	2.16	0.45
56:AA:251:C:OP1	65:AL:114:ARG:NH1	2.44	0.45
56:AA:361:A:H5'	56:AA:362:A:OP1	2.16	0.45
56:AA:672:A:H2'	56:AA:673:A:O4'	2.16	0.45
56:AA:873:A:H4'	67:AO:225:LYS:NZ	2.31	0.45
58:AC:49:LYS:O	58:AC:166:TYR:HB2	2.16	0.45
62:AI:91:MET:HB3	85:Ak:68:TRP:HB2	1.98	0.45
88:Ao:302:GLU:HA	88:Ao:344:CYS:SG	2.57	0.45
88:Ao:617:PHE:CD2	88:Ao:633:LEU:HD11	2.45	0.45
1:CL:46:LEU:HD11	1:DL:67:LEU:HD22	1.99	0.45
6:B4:79:PRO:HB3	55:Bz:700:ALA:N	2.31	0.45
13:BB:26:C:OP2	26:BS:86:THR:HG23	2.17	0.45
13:BB:35:G:H1'	36:Bd:88:PHE:CZ	2.52	0.45
15:BD:90:GLN:H	15:BD:90:GLN:HG2	1.48	0.45
16:BE:244:SER:OG	16:BE:245:THR:N	2.47	0.45
25:BR:101:ASN:O	25:BR:104:TYR:OH	2.30	0.45
26:BS:57:GLU:HG2	26:BS:78:TRP:CD1	2.50	0.45
31:BX:3:ARG:HG2	31:BX:23:ASN:HB3	1.97	0.45
43:Bk:168:GLU:O	43:Bk:172:GLU:HG3	2.16	0.45
46:Bn:81:ARG:HG2	46:Bn:81:ARG:HH11	1.80	0.45
53:Bw:53:ALA:O	53:Bw:62:ARG:NH2	2.50	0.45
56:AA:285:C:O2'	56:AA:488:A:N1	2.47	0.45
56:AA:730:C:H2'	56:AA:731:A:H4'	1.99	0.45
60:AF:32:ARG:O	60:AF:74:THR:HG21	2.16	0.45
85:Ak:191:LYS:HD3	85:Ak:235:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:119:PHE:CD2	88:Ao:120:ILE:HD13	2.52	0.45
1:CL:38:LEU:HD12	1:CL:46:LEU:HD12	1.99	0.45
1:DL:75:THR:O	1:DL:79:ILE:HG13	2.16	0.45
1:GL:70:ASP:O	1:GL:74:LEU:HG	2.17	0.45
3:B1:238:LEU:HD13	37:Be:102:PHE:HD2	1.81	0.45
6:B4:38:ARG:HH22	36:Bd:129:HIS:HA	1.81	0.45
6:B4:63:SER:HA	36:Bd:179:THR:O	2.16	0.45
8:B6:36:ARG:HH22	8:B6:64:SER:HB3	1.81	0.45
10:B8:137:THR:HG22	10:B8:139:ALA:H	1.81	0.45
12:BA:260:C:OP1	15:BD:98:GLY:N	2.44	0.45
12:BA:901:C:H5'	12:BA:902:C:OP1	2.15	0.45
14:BC:199:LYS:HZ3	14:BC:328:GLY:CA	2.30	0.45
14:BC:490:SER:O	56:AA:919:A:N6	2.46	0.45
14:BC:522:GLY:HA2	14:BC:574:PHE:HB3	1.99	0.45
18:BI:116:LYS:HB3	18:BI:120:ARG:NH1	2.32	0.45
1:BL:148:GLU:HG3	1:BL:152:HIS:CD2	2.52	0.45
27:BT:196:GLU:H	27:BT:196:GLU:CD	2.24	0.45
40:Bh:270:TYR:O	40:Bh:285:PRO:HA	2.16	0.45
43:Bk:122:GLU:CG	43:Bk:160:SER:HB2	2.46	0.45
57:AB:189:PRO:HD3	62:AI:152:TYR:CE1	2.52	0.45
58:AC:145:HIS:CD2	88:Ao:121:ILE:HD13	2.51	0.45
60:AF:89:ILE:HA	60:AF:89:ILE:HD13	1.64	0.45
61:AG:62:GLU:HG2	61:AG:66:ARG:HE	1.81	0.45
69:AQ:69:LEU:HD13	69:AQ:80:GLU:HB2	1.98	0.45
85:Ak:199:ARG:HG2	85:Ak:199:ARG:HH11	1.82	0.45
88:Ao:600:GLY:HA2	88:Ao:603:ARG:NE	2.32	0.45
3:B1:5:LYS:HD3	12:BA:19:U:C4	2.52	0.45
5:B3:81:TRP:O	5:B3:85:ILE:HG12	2.16	0.45
14:BC:179:ARG:HB3	14:BC:347:LEU:HB3	1.97	0.45
23:BP:255:MET:HE3	23:BP:255:MET:HB3	1.79	0.45
29:BV:180:LYS:C	29:BV:181:ARG:HG2	2.42	0.45
33:Ba:96:HIS:CG	33:Ba:97:PRO:HD2	2.51	0.45
45:Bm:157:TRP:NE1	45:Bm:159:TYR:HB2	2.31	0.45
56:AA:200:A:H2'	56:AA:201:A:O4'	2.17	0.45
61:AG:155:VAL:H	61:AG:227:HIS:CE1	2.34	0.45
61:AG:180:ARG:HB3	61:AG:180:ARG:NH1	2.29	0.45
68:AP:67:ALA:HB2	75:Aa:218:TYR:CZ	2.52	0.45
81:Ag:271:THR:HB	81:Ag:281:ILE:O	2.16	0.45
82:Ah:282:THR:HG23	88:Ao:449:LYS:HD3	1.99	0.45
84:Aj:42:MET:HE2	84:Aj:42:MET:HB2	1.87	0.45
88:Ao:559:LYS:HZ3	88:Ao:574:TRP:HZ2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B2:236:LEU:HD13	32:BY:48:PRO:HG3	1.98	0.45
9:B7:74:ARG:HD3	9:B7:74:ARG:HA	1.59	0.45
12:BA:222:G:H1	46:Bn:61:GLY:HA3	1.82	0.45
12:BA:993:U:OP2	16:BE:238:ARG:NH2	2.50	0.45
12:BA:1329:U:O2'	12:BA:1330:U:H5'	2.17	0.45
16:BE:201:GLY:O	16:BE:202:GLN:HB2	2.16	0.45
17:BF:190:VAL:HG13	17:BF:191:ASP:O	2.17	0.45
22:BO:110:ASP:OD1	22:BO:110:ASP:N	2.34	0.45
35:Bc:105:VAL:HB	35:Bc:110:TRP:CD1	2.51	0.45
38:Bf:52:THR:HG22	38:Bf:54:ASP:H	1.81	0.45
41:Bi:177:ARG:HG2	41:Bi:177:ARG:NH1	2.32	0.45
45:Bm:77:GLU:HG3	45:Bm:104:ARG:NH1	2.31	0.45
57:AB:123:HIS:NE2	76:Ab:41:LEU:HD12	2.32	0.45
58:AC:142:LEU:HD21	83:Ai:65:LEU:HD11	1.98	0.45
63:AJ:76:LEU:HD23	63:AJ:145:LEU:HD12	1.97	0.45
72:AV:21:C:N4	72:AV:22:U:O4	2.49	0.45
88:Ao:455:HIS:HA	88:Ao:458:ASN:ND2	2.31	0.45
3:B1:128:THR:HG22	3:B1:129:MET:H	1.81	0.45
12:BA:138:A:C4	12:BA:141:A:H2	2.34	0.45
12:BA:164:A:O2'	12:BA:1016:C:H5	2.00	0.45
12:BA:547:A:H3'	12:BA:548:A:H5'	1.98	0.45
13:BB:29:G:P	36:Bd:133:ARG:HH22	2.39	0.45
16:BE:105:GLY:HA3	27:BT:91:LYS:HD2	1.98	0.45
16:BE:117:HIS:HD2	16:BE:274:TRP:CZ2	2.35	0.45
21:BN:116:LEU:HA	21:BN:116:LEU:HD23	1.71	0.45
23:BP:179:TYR:CE2	23:BP:187:LEU:HD22	2.52	0.45
25:BR:107:MET:O	25:BR:108:LEU:HD23	2.17	0.45
26:BS:61:VAL:HG11	34:Bb:344:PHE:CE2	2.51	0.45
31:BX:72:VAL:O	37:Be:24:LYS:NZ	2.42	0.45
32:BY:75:LYS:HE2	32:BY:159:PHE:HE1	1.81	0.45
35:Bc:33:SER:HB2	35:Bc:36:GLU:HG3	1.99	0.45
36:Bd:146:ALA:HB2	42:Bj:211:GLY:HA2	1.97	0.45
39:Bg:146:ARG:HA	39:Bg:146:ARG:HD3	1.54	0.45
41:Bi:215:ARG:HG3	41:Bi:245:TYR:CE1	2.52	0.45
50:Bt:82:PHE:CG	50:Bt:83:PRO:HD2	2.51	0.45
54:Bx:138:GLY:C	54:Bx:141:PRO:HD2	2.42	0.45
64:AK:179:ASP:OD1	64:AK:181:THR:OG1	2.35	0.45
65:AL:62:VAL:HG21	65:AL:102:LEU:HD22	1.98	0.45
68:AP:118:VAL:HG21	89:Ap:236:PRO:HB2	1.99	0.45
72:AV:54:A:O2'	72:AV:55:C:O5'	2.33	0.45
75:Aa:108:ASP:O	75:Aa:112:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Aa:253:CYS:SG	75:Aa:264:TYR:HA	2.57	0.45
81:Ag:160:TRP:N	81:Ag:160:TRP:CD1	2.85	0.45
88:Ao:294:VAL:HG21	88:Ao:334:ASN:ND2	2.31	0.45
88:Ao:306:LEU:HD21	88:Ao:347:ARG:NH1	2.32	0.45
88:Ao:390:LYS:O	88:Ao:393:SER:OG	2.21	0.45
3:B1:42:HIS:CE1	3:B1:83:GLU:HB2	2.52	0.45
12:BA:337:A:H2'	12:BA:337:A:N3	2.31	0.45
13:BB:24:A:H2'	13:BB:25:G:H8	1.82	0.45
15:BD:75:MET:HB3	15:BD:75:MET:HE2	1.71	0.45
15:BD:147:ASN:OD1	33:Ba:262:THR:HG22	2.17	0.45
23:BP:234:LEU:HD22	51:Bu:66:LYS:HZ2	1.80	0.45
28:BU:137:GLU:HB2	28:BU:138:PRO:HD3	1.99	0.45
29:BV:153:LEU:HD12	29:BV:153:LEU:HA	1.89	0.45
33:Ba:288:PRO:HD2	33:Ba:324:GLN:CD	2.42	0.45
49:Bq:122:ARG:O	49:Bq:126:ILE:HG12	2.16	0.45
53:Bw:278:ILE:HG22	53:Bw:280:SER:H	1.81	0.45
54:Bx:108:CYS:SG	54:Bx:111:GLU:HB2	2.57	0.45
56:AA:111:A:H4'	56:AA:112:U:H5''	1.98	0.45
56:AA:718:C:H1'	56:AA:808:U:O2	2.16	0.45
56:AA:870:G:H8	56:AA:870:G:O5'	2.00	0.45
58:AC:154:HIS:CG	85:Ak:77:PRO:HG3	2.51	0.45
79:Ae:213:PHE:HE2	79:Ae:221:LEU:HD12	1.81	0.45
81:Ag:89:GLN:HE22	81:Ag:359:TYR:HE1	1.65	0.45
81:Ag:328:LEU:HB3	81:Ag:332:GLY:HA3	1.99	0.45
88:Ao:459:PHE:HD2	88:Ao:463:LYS:HE3	1.82	0.45
1:CL:28:ILE:O	1:CL:32:VAL:HG23	2.17	0.45
4:B2:184:LYS:HB3	4:B2:186:TRP:NE1	2.32	0.45
5:B3:133:ASP:HB3	5:B3:147:VAL:HG13	1.98	0.45
7:B5:140:GLN:NE2	7:B5:176:GLU:O	2.44	0.45
10:B8:108:LYS:NZ	12:BA:78:A:OP2	2.49	0.45
12:BA:55:A:C8	12:BA:57:A:OP1	2.70	0.45
12:BA:421:U:H2'	12:BA:422:U:C6	2.52	0.45
12:BA:527:U:HO2'	19:BJ:113:ARG:NH1	2.15	0.45
12:BA:889:C:O2'	12:BA:890:C:OP1	2.32	0.45
12:BA:1530:C:H4'	54:Bx:132:ARG:HD3	1.99	0.45
21:BN:31:LEU:HD12	21:BN:31:LEU:HA	1.77	0.45
24:BQ:47:LYS:HE3	24:BQ:47:LYS:HB2	1.65	0.45
36:Bd:154:SER:HB3	36:Bd:157:LEU:HD12	1.99	0.45
53:Bw:393:LYS:HG3	53:Bw:394:PRO:HD2	1.99	0.45
56:AA:601:A:C6	83:Ai:63:GLY:HA3	2.51	0.45
56:AA:714:U:H2'	56:AA:715:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AE:92:LYS:HE2	83:Ai:79:ARG:NH2	2.31	0.45
65:AL:78:ARG:HH12	65:AL:117:ASP:CG	2.24	0.45
89:Ap:59:LEU:HD13	89:Ap:121:LYS:HB2	1.97	0.45
12:BA:119:A:H5''	12:BA:120:C:OP2	2.17	0.45
12:BA:1127:A:H2'	12:BA:1128:A:C8	2.52	0.45
13:BB:67:A:H2'	13:BB:68:A:O4'	2.16	0.45
14:BC:253:ASP:O	14:BC:282:PRO:HD2	2.16	0.45
14:BC:663:ARG:HH21	14:BC:704:GLN:HG2	1.82	0.45
16:BE:99:LEU:HD13	16:BE:124:VAL:HG21	1.98	0.45
33:Ba:162:ARG:HA	33:Ba:162:ARG:HD2	1.68	0.45
34:Bb:162:PHE:HB2	34:Bb:165:ALA:HB3	1.99	0.45
40:Bh:88:LEU:HD23	40:Bh:88:LEU:HA	1.86	0.45
41:Bi:196:GLN:NE2	41:Bi:198:ARG:HE	2.13	0.45
43:Bk:86:TYR:CE1	43:Bk:88:TYR:HD1	2.31	0.45
48:Bp:4:ALA:HA	48:Bp:7:ARG:NH1	2.32	0.45
50:Bt:18:ILE:HG22	50:Bt:19:GLY:N	2.32	0.45
50:Bt:99:ARG:CG	50:Bt:99:ARG:NH1	2.75	0.45
53:Bw:267:LEU:HA	53:Bw:267:LEU:HD23	1.69	0.45
56:AA:681:A:O4'	59:AE:114:ARG:NH1	2.49	0.45
65:AL:69:LYS:NZ	65:AL:77:ASN:HD22	2.14	0.45
84:Aj:83:LYS:HE2	84:Aj:87:TRP:CE2	2.52	0.45
88:Ao:292:ALA:HB3	88:Ao:297:PHE:CE2	2.52	0.45
88:Ao:543:HIS:CD2	88:Ao:588:ARG:HG3	2.49	0.45
89:Ap:214:SER:HA	89:Ap:217:ARG:NH1	2.31	0.45
12:BA:218:A:C5	34:Bb:379:ILE:HG21	2.52	0.44
12:BA:652:A:H2'	12:BA:653:A:C8	2.52	0.44
17:BF:211:ARG:HD2	45:Bm:59:ARG:CZ	2.47	0.44
19:BJ:139:LYS:HE3	19:BJ:140:TYR:CE2	2.52	0.44
20:BK:114:LEU:HD23	49:Bq:96:LEU:HB3	1.98	0.44
28:BU:94:GLN:HE22	28:BU:146:VAL:N	2.15	0.44
44:Bl:110:ILE:HD12	44:Bl:147:LEU:HD23	1.99	0.44
52:Bv:79:GLN:O	52:Bv:83:ARG:HG3	2.17	0.44
56:AA:175:A:N3	56:AA:187:U:O2'	2.46	0.44
56:AA:407:U:H2'	56:AA:408:A:O4'	2.18	0.44
58:AC:123:VAL:HG21	58:AC:155:LEU:HG	1.99	0.44
66:AN:60:ASN:ND2	66:AN:62:ILE:HB	2.32	0.44
70:AR:113:LYS:HE2	70:AR:113:LYS:HA	1.98	0.44
71:AU:74:PHE:HD2	71:AU:75:LEU:HD23	1.81	0.44
81:Ag:108:LEU:O	81:Ag:112:LYS:HG2	2.17	0.44
84:Aj:90:ASP:CG	89:Ap:215:ARG:HH22	2.26	0.44
85:Ak:150:PRO:HB3	85:Ak:181:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ak:165:ILE:HG13	88:Ao:135:PRO:HD3	1.99	0.44
89:Ap:181:HIS:CD2	89:Ap:183:ALA:H	2.35	0.44
2:B0:125:VAL:HG21	34:Bb:64:GLU:HG3	1.98	0.44
12:BA:138:A:C2	12:BA:141:A:H5''	2.51	0.44
12:BA:505:U:H4'	12:BA:506:A:OP1	2.17	0.44
12:BA:1464:A:H5'	14:BC:188:HIS:HE1	1.82	0.44
17:BF:195:LEU:HD22	17:BF:202:TYR:HE2	1.82	0.44
26:BS:146:TYR:CE2	26:BS:148:PRO:HB3	2.53	0.44
34:Bb:72:ARG:HH11	34:Bb:72:ARG:CA	2.31	0.44
34:Bb:216:LEU:HB3	34:Bb:237:VAL:HG12	2.00	0.44
34:Bb:240:ILE:HG23	34:Bb:244:ARG:O	2.17	0.44
34:Bb:265:PHE:CE2	34:Bb:322:ARG:HD2	2.53	0.44
35:Bc:72:PRO:HB2	41:Bi:293:PHE:CE2	2.52	0.44
42:Bj:179:GLN:HG2	42:Bj:181:GLY:H	1.82	0.44
46:Bn:92:ILE:HD13	46:Bn:92:ILE:HA	1.77	0.44
53:Bw:140:VAL:HG21	53:Bw:412:LEU:HD21	1.99	0.44
61:AG:115:LEU:HD22	61:AG:141:PRO:HB2	1.99	0.44
62:AI:265:GLU:C	62:AI:267:GLY:H	2.25	0.44
66:AN:28:TYR:O	83:Ai:55:HIS:HB3	2.17	0.44
73:AX:8:A:H2	73:AX:9:C:H41	1.65	0.44
75:Aa:228:THR:HA	75:Aa:229:PRO:HD3	1.79	0.44
77:Ac:10:ARG:HA	77:Ac:15:TYR:CD2	2.53	0.44
88:Ao:404:MET:HE2	88:Ao:404:MET:HB3	1.81	0.44
12:BA:1510:A:O3'	54:Bx:160:LYS:NZ	2.49	0.44
14:BC:287:VAL:HG22	14:BC:300:VAL:HG11	1.99	0.44
17:BF:76:ARG:HH12	45:Bm:112:ALA:HB2	1.82	0.44
21:BN:119:ARG:HD3	21:BN:119:ARG:HA	1.87	0.44
21:BN:171:SER:HA	21:BN:172:PRO:HD2	1.91	0.44
23:BP:233:ARG:HG3	23:BP:233:ARG:NH1	2.32	0.44
23:BP:238:ARG:NH2	51:Bu:69:ASN:HA	2.32	0.44
32:BY:87:VAL:HG11	41:Bi:74:ARG:NH1	2.32	0.44
36:Bd:147:LEU:HB3	36:Bd:151:ARG:HH12	1.81	0.44
37:Be:68:LEU:HD12	37:Be:68:LEU:HA	1.91	0.44
42:Bj:185:ARG:HH12	42:Bj:204:PHE:HB3	1.83	0.44
54:Bx:89:LEU:HD11	54:Bx:118:CYS:HB3	1.99	0.44
56:AA:938:U:H2'	56:AA:939:A:H8	1.81	0.44
57:AB:146:ARG:HG3	57:AB:146:ARG:NH1	2.31	0.44
58:AC:69:LEU:HD23	85:Ak:109:LYS:HE2	1.98	0.44
68:AP:73:ILE:O	68:AP:77:ILE:HG13	2.17	0.44
79:Ae:409:GLU:O	79:Ae:413:ILE:HG13	2.17	0.44
81:Ag:93:PHE:C	81:Ag:95:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Ag:209:TRP:HH2	81:Ag:224:VAL:HG13	1.83	0.44
81:Ag:223:GLU:O	81:Ag:227:GLN:HB2	2.17	0.44
88:Ao:116:ALA:O	88:Ao:120:ILE:HG12	2.17	0.44
88:Ao:432:LEU:HD12	88:Ao:435:ALA:HB3	1.99	0.44
88:Ao:442:LEU:HA	88:Ao:450:LEU:HD12	1.99	0.44
2:B0:50:ARG:NH1	12:BA:1200:A:OP1	2.50	0.44
12:BA:343:C:H2'	12:BA:344:U:C6	2.52	0.44
12:BA:620:A:H2'	12:BA:621:U:C6	2.52	0.44
15:BD:207:TYR:CD2	15:BD:207:TYR:N	2.86	0.44
17:BF:75:GLU:OE1	17:BF:76:ARG:NH1	2.50	0.44
1:BL:185:LYS:HB3	1:BL:185:LYS:HE2	1.81	0.44
21:BN:128:PHE:HA	21:BN:129:PRO:HD3	1.79	0.44
22:BO:95:ARG:HH11	22:BO:95:ARG:CA	2.31	0.44
32:BY:195:GLU:OE1	32:BY:195:GLU:N	2.48	0.44
33:Ba:127:GLN:HG3	33:Ba:251:HIS:CE1	2.53	0.44
53:Bw:118:LEU:HD12	53:Bw:118:LEU:HA	1.75	0.44
53:Bw:296:LEU:HD23	53:Bw:296:LEU:HA	1.73	0.44
57:AB:252:PHE:O	57:AB:256:ILE:HG12	2.17	0.44
79:Ae:205:PHE:CZ	79:Ae:243:ASN:HB3	2.53	0.44
83:Ai:60:ALA:O	83:Ai:64:THR:HG23	2.17	0.44
12:BA:37:A:OP1	37:Be:35:GLY:HA2	2.16	0.44
12:BA:112:A:N6	12:BA:115:U:OP2	2.48	0.44
12:BA:660:C:H41	53:Bw:54:LYS:HB3	1.83	0.44
12:BA:739:U:H2'	12:BA:740:U:H6	1.83	0.44
23:BP:26:ASN:OD1	23:BP:26:ASN:N	2.50	0.44
23:BP:142:GLU:CD	23:BP:142:GLU:H	2.26	0.44
28:BU:24:VAL:HG11	28:BU:43:VAL:HG23	2.00	0.44
30:BW:88:LEU:HB3	30:BW:115:ILE:HD12	2.00	0.44
34:Bb:92:LEU:HD23	34:Bb:92:LEU:HA	1.78	0.44
39:Bg:44:ARG:HH12	50:Bt:100:LYS:HA	1.81	0.44
59:AE:120:LYS:HE2	59:AE:122:ARG:HE	1.82	0.44
60:AF:32:ARG:HG3	60:AF:78:MET:HG3	1.99	0.44
61:AG:46:ILE:HG12	62:AI:316:PHE:HZ	1.83	0.44
61:AG:144:ILE:HG21	61:AG:210:LEU:HD23	2.00	0.44
63:AJ:170:MET:HB3	85:Ak:159:VAL:CG1	2.48	0.44
69:AQ:69:LEU:HD12	69:AQ:69:LEU:HA	1.86	0.44
70:AR:50:ASP:HA	80:Af:86:ARG:HH11	1.82	0.44
77:Ac:140:MET:HG2	77:Ac:146:GLN:HG3	1.99	0.44
78:Ad:102:HIS:O	78:Ad:106:MET:HG2	2.17	0.44
12:BA:1521:U:H3'	12:BA:1522:A:C5'	2.47	0.44
14:BC:360:ILE:HG22	14:BC:361:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BF:283:LEU:HD12	17:BF:283:LEU:HA	1.83	0.44
23:BP:114:GLN:HB3	23:BP:115:PRO:HD2	2.00	0.44
23:BP:273:TRP:CE3	23:BP:282:ILE:HG21	2.53	0.44
28:BU:87:ILE:HD13	28:BU:87:ILE:HA	1.85	0.44
29:BV:144:ASN:HD22	38:Bf:63:PRO:HA	1.82	0.44
33:Ba:211:ALA:HB3	33:Ba:222:VAL:HG13	2.00	0.44
35:Bc:99:LYS:O	35:Bc:126:THR:HG23	2.17	0.44
48:Bp:19:GLN:HG2	48:Bp:54:ASP:HB3	1.99	0.44
66:AN:41:ARG:HG2	66:AN:87:ILE:HD13	2.00	0.44
69:AQ:11:LYS:HA	69:AQ:68:ALA:HB2	2.00	0.44
77:Ac:125:HIS:CD2	77:Ac:127:ALA:HB3	2.51	0.44
78:Ad:73:GLU:O	78:Ad:77:GLU:HG3	2.17	0.44
79:Ae:157:LEU:HD23	79:Ae:161:ALA:HB1	2.00	0.44
79:Ae:172:LYS:HG2	79:Ae:178:PHE:CE2	2.52	0.44
79:Ae:188:MET:HG3	79:Ae:221:LEU:HD21	1.99	0.44
79:Ae:241:GLU:HG2	79:Ae:270:LEU:HD22	1.99	0.44
88:Ao:618:LEU:O	88:Ao:622:LYS:HB3	2.18	0.44
12:BA:76:G:O2'	12:BA:88:G:O6	2.34	0.44
18:BI:61:LYS:HB3	18:BI:61:LYS:HE2	1.79	0.44
40:Bh:227:GLU:OE1	40:Bh:302:ARG:HD3	2.17	0.44
50:Bt:25:ARG:HA	50:Bt:26:PRO:HD3	1.89	0.44
56:AA:584:C:H41	56:AA:804:A:H62	1.65	0.44
57:AB:179:PRO:HA	57:AB:183:GLY:O	2.18	0.44
59:AE:372:GLU:HB2	75:Aa:125:TYR:CE2	2.53	0.44
60:AF:5:GLU:OE2	70:AR:76:LYS:NZ	2.50	0.44
61:AG:173:PRO:HB3	86:Am:73:PHE:CZ	2.52	0.44
62:AI:264:ASP:HB2	62:AI:270:PHE:CE2	2.53	0.44
65:AL:45:PRO:HA	65:AL:46:PRO:HD3	1.88	0.44
78:Ad:88:GLY:O	78:Ad:92:GLU:HG2	2.18	0.44
81:Ag:55:PRO:HD2	81:Ag:146:LYS:HZ3	1.82	0.44
81:Ag:386:ASN:HD22	81:Ag:389:GLN:HB2	1.83	0.44
1:HL:79:ILE:H	1:HL:79:ILE:HG13	1.72	0.44
12:BA:1215:C:H3'	12:BA:1219:A:H62	1.83	0.44
12:BA:1508:A:H2	12:BA:1538:A:N7	2.15	0.44
16:BE:91:GLU:HB3	16:BE:92:PRO:HD2	2.00	0.44
26:BS:137:LEU:HD11	26:BS:168:GLY:O	2.17	0.44
30:BW:104:LEU:HD23	30:BW:104:LEU:HA	1.86	0.44
32:BY:105:ARG:H	32:BY:105:ARG:HD3	1.83	0.44
38:Bf:68:PRO:HG2	38:Bf:71:HIS:CG	2.53	0.44
42:Bj:265:LYS:HG3	42:Bj:266:PRO:HD3	2.00	0.44
45:Bm:78:VAL:HG21	45:Bm:101:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Bw:157:ALA:N	53:Bw:158:PRO:HD2	2.32	0.44
62:AI:397:ARG:NH1	72:AV:32:A:OP2	2.51	0.44
63:AJ:72:LEU:HG	85:Ak:135:TRP:CZ3	2.53	0.44
68:AP:55:ASP:HA	68:AP:56:PRO:HD3	1.80	0.44
68:AP:103:MET:HE2	68:AP:103:MET:HB3	1.86	0.44
69:AQ:13:VAL:CG2	69:AQ:66:LEU:HB2	2.48	0.44
69:AQ:36:ASP:HA	69:AQ:37:PRO:HD3	1.65	0.44
71:AU:77:ARG:H	71:AU:77:ARG:HG3	1.51	0.44
77:Ac:60:PRO:HG2	77:Ac:61:TRP:HD1	1.82	0.44
77:Ac:77:ARG:HD3	77:Ac:79:TYR:OH	2.18	0.44
79:Ae:230:LEU:HD22	79:Ae:394:LEU:HD22	2.00	0.44
79:Ae:322:VAL:HG22	79:Ae:325:ARG:CZ	2.48	0.44
81:Ag:55:PRO:HG3	81:Ag:142:HIS:CE1	2.52	0.44
84:Aj:189:PRO:O	84:Aj:190:MET:HE2	2.17	0.44
88:Ao:538:MET:HE3	88:Ao:551:PHE:CD2	2.53	0.44
88:Ao:594:GLU:O	88:Ao:598:MET:HG2	2.18	0.44
1:GL:64:ILE:HD11	1:HL:85:LEU:HD12	2.00	0.44
14:BC:372:THR:HG21	14:BC:425:PRO:HG2	2.00	0.44
21:BN:71:LYS:NZ	54:Bx:196:HIS:HD2	2.15	0.44
22:BO:107:LEU:HD23	22:BO:107:LEU:HA	1.67	0.44
23:BP:47:ARG:O	23:BP:48:LYS:HB2	2.18	0.44
23:BP:151:LYS:HE3	23:BP:171:GLY:O	2.17	0.44
26:BS:104:SER:OG	34:Bb:150:ARG:NH2	2.50	0.44
32:BY:199:MET:HE2	32:BY:199:MET:HB3	1.85	0.44
34:Bb:238:THR:HG22	34:Bb:239:ASN:H	1.83	0.44
35:Bc:78:MET:HE1	35:Bc:88:CYS:HA	2.00	0.44
38:Bf:49:LEU:HD23	38:Bf:49:LEU:HA	1.78	0.44
48:Bp:10:LEU:HD22	48:Bp:42:VAL:HG12	1.99	0.44
53:Bw:91:TYR:CE2	53:Bw:269:LYS:HE3	2.53	0.44
53:Bw:181:LEU:HD23	53:Bw:181:LEU:HA	1.66	0.44
53:Bw:335:MET:HE2	53:Bw:335:MET:HB3	1.81	0.44
58:AC:51:VAL:HG12	58:AC:52:THR:O	2.18	0.44
62:AI:156:GLN:O	62:AI:160:SER:OG	2.22	0.44
66:AN:51:ARG:HG2	66:AN:78:LEU:HD13	1.99	0.44
68:AP:93:LEU:O	75:Aa:197:ARG:NH1	2.51	0.44
70:AR:82:SER:O	70:AR:126:LYS:HD3	2.18	0.44
79:Ae:84:ASP:OD1	79:Ae:84:ASP:N	2.51	0.44
80:Af:101:VAL:HG21	80:Af:145:LEU:HD22	2.00	0.44
80:Af:151:THR:HG23	80:Af:160:ASP:HB3	2.00	0.44
87:An:130:ILE:O	87:An:134:ARG:HG3	2.18	0.44
2:B0:100:THR:HB	2:B0:132:HIS:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BE:90:TRP:HA	16:BE:316:PHE:CE2	2.50	0.43
16:BE:227:GLN:HG2	16:BE:236:THR:O	2.18	0.43
20:BK:23:ILE:HG12	20:BK:67:PRO:HB3	2.00	0.43
22:BO:75:LEU:HD12	22:BO:75:LEU:HA	1.82	0.43
28:BU:94:GLN:HE22	28:BU:146:VAL:H	1.64	0.43
29:BV:209:CYS:C	38:Bf:52:THR:HG23	2.43	0.43
31:BX:141:ARG:HA	31:BX:141:ARG:HD2	1.80	0.43
32:BY:91:LEU:HD23	32:BY:91:LEU:HA	1.59	0.43
42:Bj:271:GLN:O	42:Bj:274:ARG:HB3	2.18	0.43
53:Bw:105:TRP:CD1	53:Bw:265:LEU:HD13	2.53	0.43
56:AA:155:A:H2'	56:AA:156:C:C6	2.53	0.43
56:AA:762:G:N2	56:AA:764:A:H3'	2.33	0.43
56:AA:957:A:P	86:Am:24:ASN:HD21	2.41	0.43
65:AL:69:LYS:HZ3	65:AL:77:ASN:HB3	1.83	0.43
67:AO:105:LEU:HD23	67:AO:105:LEU:HA	1.88	0.43
79:Ae:148:THR:O	79:Ae:151:THR:OG1	2.26	0.43
79:Ae:327:LEU:HA	79:Ae:327:LEU:HD23	1.86	0.43
88:Ao:119:PHE:HD2	88:Ao:120:ILE:HD13	1.82	0.43
3:B1:96:LYS:O	3:B1:96:LYS:HG2	2.18	0.43
11:B9:84:ARG:NH1	11:B9:99:GLN:O	2.51	0.43
12:BA:1386:U:H1'	12:BA:1389:A:N6	2.33	0.43
18:BI:57:GLU:HG2	18:BI:58:ARG:N	2.32	0.43
19:BJ:94:ARG:HB2	19:BJ:159:PRO:HD3	2.00	0.43
28:BU:90:LEU:HD12	28:BU:90:LEU:HA	1.67	0.43
31:BX:3:ARG:HH21	31:BX:4:ASN:HD21	1.67	0.43
31:BX:144:VAL:HG11	41:Bi:233:TYR:CD1	2.53	0.43
32:BY:35:ASN:HA	32:BY:36:PRO:HD2	1.73	0.43
34:Bb:151:LEU:HD23	34:Bb:151:LEU:HA	1.78	0.43
34:Bb:351:HIS:HA	34:Bb:352:PRO:HD3	1.93	0.43
36:Bd:97:LYS:HD2	42:Bj:84:TYR:CZ	2.53	0.43
40:Bh:60:ARG:NH1	40:Bh:63:LYS:HB2	2.33	0.43
51:Bu:182:MET:HB3	51:Bu:182:MET:HE2	1.72	0.43
54:Bx:190:ARG:HB3	54:Bx:190:ARG:HH11	1.83	0.43
56:AA:512:A:H2'	56:AA:513:A:C8	2.53	0.43
56:AA:812:U:H2'	56:AA:813:G:H8	1.83	0.43
56:AA:857:C:H2'	56:AA:858:C:C6	2.53	0.43
58:AC:72:HIS:HD2	58:AC:74:GLY:H	1.66	0.43
59:AE:203:LEU:HA	59:AE:203:LEU:HD12	1.76	0.43
59:AE:314:LEU:HD23	59:AE:314:LEU:HA	1.87	0.43
61:AG:176:ASP:O	61:AG:180:ARG:HG2	2.17	0.43
70:AR:87:PRO:HA	70:AR:126:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ao:397:TYR:CG	88:Ao:434:LEU:HD13	2.54	0.43
1:CL:27:LYS:O	1:CL:31:LEU:HG	2.17	0.43
4:B2:88:THR:HB	4:B2:91:GLN:HG3	2.00	0.43
7:B5:95:ARG:HG2	30:BW:86:TRP:CH2	2.54	0.43
12:BA:142:U:H3'	12:BA:143:A:C5'	2.48	0.43
12:BA:1316:U:H2'	12:BA:1317:A:O4'	2.18	0.43
16:BE:43:GLY:H	35:Bc:98:ARG:HH12	1.66	0.43
16:BE:228:PRO:O	16:BE:233:GLN:HG3	2.19	0.43
17:BF:211:ARG:HB2	45:Bm:59:ARG:NH2	2.33	0.43
26:BS:94:VAL:HG11	26:BS:141:ILE:HD11	2.00	0.43
31:BX:49:THR:HG23	31:BX:52:ASP:OD2	2.17	0.43
33:Ba:212:THR:O	33:Ba:326:ARG:NH1	2.44	0.43
34:Bb:194:THR:HB	34:Bb:197:GLU:OE1	2.18	0.43
41:Bi:102:LYS:HD2	41:Bi:102:LYS:HA	1.57	0.43
46:Bn:35:ARG:NH1	46:Bn:39:PRO:HB3	2.33	0.43
46:Bn:69:HIS:CD2	46:Bn:70:PRO:HD2	2.53	0.43
53:Bw:237:ILE:HD11	53:Bw:290:HIS:HB2	2.00	0.43
56:AA:308:A:H2	77:Ac:68:LYS:NZ	2.17	0.43
56:AA:687:A:H1'	66:AN:109:ILE:HD12	2.00	0.43
62:AI:284:VAL:HG22	62:AI:331:CYS:SG	2.57	0.43
69:AQ:29:ARG:HD3	69:AQ:46:ARG:HD3	2.00	0.43
69:AQ:35:LEU:HB2	69:AQ:42:TYR:CZ	2.53	0.43
79:Ae:266:TYR:CE2	79:Ae:320:LEU:HB2	2.54	0.43
82:Ah:320:PHE:O	82:Ah:324:ILE:HG12	2.18	0.43
88:Ao:314:GLU:O	88:Ao:318:ASN:ND2	2.51	0.43
88:Ao:490:PHE:HA	88:Ao:491:PRO:HD3	1.89	0.43
3:B1:67:ILE:HA	3:B1:68:PRO:HD3	1.89	0.43
3:B1:176:LEU:HD23	3:B1:184:ARG:HG3	2.00	0.43
12:BA:793:A:OP1	16:BE:237:HIS:NE2	2.51	0.43
12:BA:810:C:O2	16:BE:230:THR:HG22	2.18	0.43
13:BB:45:A:H5''	13:BB:46:G:OP2	2.18	0.43
19:BJ:36:HIS:O	19:BJ:37:ARG:HB3	2.17	0.43
21:BN:99:ASP:HA	21:BN:100:PRO:HD3	1.90	0.43
32:BY:209:ARG:HA	32:BY:209:ARG:HD3	1.82	0.43
33:Ba:142:ASP:OD2	33:Ba:144:ARG:HB2	2.19	0.43
33:Ba:207:ASN:OD1	33:Ba:207:ASN:N	2.50	0.43
42:Bj:157:LEU:HD23	42:Bj:254:TRP:HB3	2.00	0.43
51:Bu:153:LEU:HD12	51:Bu:156:MET:HE2	2.01	0.43
56:AA:706:G:H3'	56:AA:707:A:H5''	2.00	0.43
63:AJ:178:GLU:O	85:Ak:151:ILE:HB	2.18	0.43
71:AU:25:THR:O	71:AU:29:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Ac:3:MET:HE2	77:Ac:3:MET:HB3	1.74	0.43
82:Ah:340:ARG:HB3	83:Ai:24:ARG:HH22	1.84	0.43
89:Ap:105:CYS:HB3	89:Ap:106:PRO:HD2	2.00	0.43
2:B0:134:VAL:HA	2:B0:135:PRO:HD3	1.86	0.43
5:B3:71:ARG:NH1	5:B3:92:GLU:O	2.52	0.43
10:B8:96:TYR:H	46:Bn:122:ASN:ND2	2.16	0.43
14:BC:437:GLU:HB2	14:BC:438:PRO:HD3	2.01	0.43
15:BD:133:ASP:OD1	15:BD:134:PRO:HD2	2.18	0.43
15:BD:273:SER:OG	15:BD:274:GLY:N	2.51	0.43
16:BE:227:GLN:CD	16:BE:227:GLN:N	2.77	0.43
22:BO:138:LEU:HD12	22:BO:138:LEU:HA	1.77	0.43
24:BQ:144:LYS:HG3	24:BQ:145:GLY:N	2.34	0.43
26:BS:82:ARG:HG2	26:BS:82:ARG:HH11	1.84	0.43
32:BY:80:ILE:HB	32:BY:85:TRP:HB2	1.99	0.43
34:Bb:72:ARG:HD3	34:Bb:72:ARG:HA	1.73	0.43
36:Bd:168:LEU:HG	42:Bj:205:LEU:O	2.19	0.43
40:Bh:102:GLU:HA	40:Bh:105:ARG:HB3	2.00	0.43
47:Bo:40:TYR:CD1	47:Bo:40:TYR:C	2.97	0.43
53:Bw:93:VAL:HB	53:Bw:227:ILE:HG12	2.01	0.43
54:Bx:99:MET:CE	54:Bx:116:GLU:HA	2.49	0.43
56:AA:48:C:N4	56:AA:172:A:OP2	2.49	0.43
56:AA:598:G:O6	83:Ai:96:LYS:HD3	2.18	0.43
61:AG:117:ALA:O	61:AG:121:LYS:HB2	2.18	0.43
75:Aa:246:HIS:CD2	75:Aa:246:HIS:H	2.36	0.43
75:Aa:307:LEU:HD23	75:Aa:322:LEU:HD23	2.01	0.43
81:Ag:173:ASN:HB2	81:Ag:176:ARG:HB2	2.00	0.43
81:Ag:209:TRP:CZ3	81:Ag:215:THR:HB	2.53	0.43
4:B2:66:LEU:HD12	4:B2:66:LEU:HA	1.68	0.43
4:B2:120:GLU:HG2	31:BX:110:LEU:HD12	1.99	0.43
12:BA:1399:G:H8	12:BA:1404:G:O6	2.01	0.43
15:BD:181:ASP:HB3	15:BD:183:HIS:CE1	2.53	0.43
23:BP:20:PRO:HD3	50:Bt:99:ARG:NH1	2.32	0.43
23:BP:154:ILE:HG22	23:BP:174:VAL:HG13	2.00	0.43
34:Bb:210:GLU:HA	34:Bb:212:SER:H	1.83	0.43
40:Bh:87:LEU:HD23	40:Bh:87:LEU:HA	1.84	0.43
43:Bk:81:ASN:HB3	43:Bk:86:TYR:CZ	2.54	0.43
43:Bk:132:MET:HE1	55:Bz:104:ALA:HB2	2.00	0.43
53:Bw:96:GLN:CD	53:Bw:297:PRO:HD3	2.43	0.43
56:AA:83:C:C4	56:AA:98:A:C6	3.07	0.43
56:AA:202:A:H5'	68:AP:102:MET:CE	2.48	0.43
62:AI:84:GLY:HA3	85:Ak:86:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Ag:82:LEU:HD12	81:Ag:83:PRO:HD2	2.00	0.43
82:Ah:314:ASP:OD1	85:Ak:218:ARG:NH1	2.42	0.43
85:Ak:73:PRO:HB3	88:Ao:78:VAL:HG11	2.00	0.43
89:Ap:155:GLN:NE2	89:Ap:155:GLN:HA	2.34	0.43
7:B5:140:GLN:HE22	7:B5:176:GLU:C	2.25	0.43
27:BT:234:GLU:H	27:BT:234:GLU:HG2	1.29	0.43
30:BW:95:MET:HE1	30:BW:103:GLN:HG3	1.99	0.43
31:BX:7:TYR:HE2	37:Be:37:LYS:HG3	1.84	0.43
35:Bc:186:LEU:HD12	35:Bc:186:LEU:HA	1.90	0.43
41:Bi:180:THR:HB	41:Bi:225:TYR:HB2	1.99	0.43
42:Bj:51:LEU:HD13	42:Bj:192:LEU:HG	2.01	0.43
57:AB:90:LEU:HD13	80:Af:119:GLY:O	2.19	0.43
66:AN:125:ARG:CG	66:AN:125:ARG:NH1	2.77	0.43
69:AQ:94:PRO:HB3	77:Ac:77:ARG:NH2	2.34	0.43
81:Ag:152:LEU:HD21	81:Ag:243:LEU:HD11	2.00	0.43
81:Ag:188:LYS:HE2	81:Ag:229:ILE:HG23	2.01	0.43
88:Ao:442:LEU:HD21	88:Ao:451:ILE:HD11	2.00	0.43
88:Ao:478:LEU:HD21	88:Ao:511:MET:HG3	2.00	0.43
89:Ap:207:GLN:HA	89:Ap:208:PRO:HD3	1.77	0.43
89:Ap:210:GLU:OE2	89:Ap:217:ARG:NH2	2.48	0.43
1:CL:40:LEU:HG	1:FL:79:ILE:HD13	2.01	0.43
22:BO:60:VAL:HG23	22:BO:62:ASN:H	1.83	0.43
41:Bi:277:LEU:HD23	41:Bi:277:LEU:HA	1.86	0.43
42:Bj:146:ARG:NH1	42:Bj:259:GLU:OE2	2.51	0.43
48:Bp:12:ALA:O	48:Bp:68:PHE:HB2	2.18	0.43
56:AA:190:G:H21	56:AA:192:C:N4	2.17	0.43
59:AE:321:MET:HE2	59:AE:325:ARG:HH22	1.83	0.43
62:AI:113:PRO:HD2	85:Ak:111:PRO:O	2.19	0.43
62:AI:288:GLY:HA2	62:AI:327:HIS:CD2	2.54	0.43
65:AL:137:LYS:HA	65:AL:137:LYS:HD3	1.80	0.43
76:Ab:41:LEU:HD23	76:Ab:41:LEU:HA	1.85	0.43
89:Ap:79:ARG:HH12	89:Ap:86:PRO:HB2	1.83	0.43
1:CL:40:LEU:HA	1:CL:43:ILE:HB	2.01	0.43
12:BA:163:C:H42	12:BA:1013:A:H61	1.67	0.43
12:BA:508:G:H4'	20:BK:151:LEU:CD1	2.48	0.43
12:BA:1060:C:H2'	12:BA:1061:U:C6	2.54	0.43
12:BA:1321:C:O2'	12:BA:1322:C:H5'	2.19	0.43
12:BA:1548:A:C2	16:BE:176:VAL:HG21	2.54	0.43
15:BD:128:ILE:HD13	33:Ba:114:LEU:HD11	2.00	0.43
42:Bj:264:LEU:HG	42:Bj:269:LEU:HB3	2.01	0.43
43:Bk:127:MET:HB2	43:Bk:154:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Bo:31:GLN:HB3	47:Bo:33:PHE:CD1	2.54	0.43
53:Bw:103:ASP:OD1	53:Bw:103:ASP:N	2.51	0.43
53:Bw:175:VAL:HG12	53:Bw:194:LEU:HD21	2.01	0.43
56:AA:588:A:H5''	56:AA:589:C:OP2	2.18	0.43
62:Al:88:LEU:HD11	62:Al:107:ALA:HB1	2.01	0.43
68:AP:42:PRO:HG2	68:AP:45:GLY:HA3	2.01	0.43
70:AR:50:ASP:HA	80:Af:86:ARG:NH1	2.34	0.43
71:Au:71:LYS:HA	80:Af:154:PHE:CZ	2.54	0.43
75:Aa:216:GLN:HG3	75:Aa:226:ILE:HG12	2.00	0.43
77:Ac:50:PHE:O	77:Ac:53:PRO:HD2	2.19	0.43
79:Ae:113:SER:HA	79:Ae:148:THR:HG23	2.00	0.43
81:Ag:242:VAL:O	81:Ag:246:LEU:HB2	2.18	0.43
85:Ak:183:ASN:HB3	85:Ak:232:TYR:OH	2.19	0.43
89:Ap:103:ASN:HA	89:Ap:104:PRO:HD3	1.75	0.43
1:CL:42:GLU:O	1:CL:46:LEU:HB2	2.18	0.43
4:B2:194:LYS:HG3	12:BA:42:C:OP1	2.19	0.43
12:BA:175:C:H5''	21:BN:115:ASN:HB2	2.00	0.43
12:BA:573:A:H5'	21:BN:29:GLY:HA3	2.01	0.43
12:BA:581:A:H5''	47:Bo:23:ALA:HB3	2.00	0.43
12:BA:978:G:H2'	12:BA:979:G:H5''	2.01	0.43
14:BC:614:LEU:HD12	14:BC:614:LEU:HA	1.83	0.43
15:BD:75:MET:HA	15:BD:76:PRO:HD3	1.92	0.43
21:BN:10:GLN:HG3	21:BN:11:TRP:N	2.34	0.43
27:BT:74:ARG:HB3	27:BT:283:TRP:CZ2	2.54	0.43
30:BW:58:PRO:HA	30:BW:59:PRO:HD3	1.91	0.43
33:Ba:310:ARG:O	33:Ba:314:ILE:HG12	2.19	0.43
48:Bp:8:LEU:HD23	48:Bp:8:LEU:HA	1.90	0.43
56:AA:353:C:H4'	56:AA:354:C:H5'	2.00	0.43
56:AA:356:A:H2'	56:AA:357:G:C8	2.54	0.43
59:AE:282:ILE:HG23	59:AE:353:LEU:HB3	2.01	0.43
60:AF:94:VAL:HG12	60:AF:95:LYS:O	2.19	0.43
61:AG:199:VAL:HG13	61:AG:203:GLU:CD	2.44	0.43
69:AQ:55:LEU:HD12	69:AQ:57:GLN:HB2	2.00	0.43
77:Ac:47:PHE:HA	77:Ac:51:ASN:ND2	2.33	0.43
81:Ag:123:TYR:CE1	81:Ag:340:ILE:HD12	2.53	0.43
81:Ag:135:LEU:HA	81:Ag:135:LEU:HD12	1.71	0.43
83:Ai:101:ARG:H	83:Ai:101:ARG:HG3	1.51	0.43
84:Aj:73:LEU:HD12	84:Aj:73:LEU:HA	1.91	0.43
88:Ao:468:LEU:O	88:Ao:477:THR:HG22	2.19	0.43
12:BA:43:C:H2'	12:BA:44:A:O4'	2.18	0.42
12:BA:1418:G:N2	12:BA:1421:A:OP2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:519:ILE:HG12	14:BC:549:VAL:HG23	2.01	0.42
16:BE:80:LEU:HD12	16:BE:80:LEU:HA	1.77	0.42
16:BE:264:ILE:HG12	16:BE:265:ASP:H	1.84	0.42
17:BF:231:VAL:HG13	52:Bv:26:ARG:HD2	2.01	0.42
20:BK:19:MET:HE1	20:BK:69:LYS:HB3	2.00	0.42
21:BN:27:PRO:HA	21:BN:66:ALA:O	2.19	0.42
21:BN:178:LEU:HA	21:BN:178:LEU:HD23	1.88	0.42
28:BU:93:CYS:O	29:BV:150:LYS:HE2	2.19	0.42
33:Ba:209:LEU:O	33:Ba:223:HIS:HA	2.19	0.42
43:Bk:166:PHE:O	43:Bk:170:PHE:HB2	2.18	0.42
47:Bo:73:PHE:O	47:Bo:77:VAL:HG23	2.20	0.42
53:Bw:166:ILE:HD13	53:Bw:166:ILE:HA	1.81	0.42
58:AC:113:ARG:O	58:AC:116:GLN:HG2	2.18	0.42
59:AE:162:LYS:O	59:AE:166:GLU:HG2	2.19	0.42
61:AG:119:LYS:NZ	81:Ag:397:LEU:C	2.77	0.42
70:AR:75:TYR:CE1	70:AR:76:LYS:HE2	2.54	0.42
78:Ad:70:LEU:O	78:Ad:73:GLU:HB3	2.18	0.42
79:Ae:110:LEU:HD12	79:Ae:434:GLU:CD	2.44	0.42
82:Ah:343:MET:HE2	82:Ah:343:MET:HA	2.01	0.42
88:Ao:543:HIS:HB3	88:Ao:551:PHE:HE1	1.84	0.42
15:BD:195:ASN:OD1	15:BD:244:THR:HB	2.19	0.42
15:BD:202:GLY:O	33:Ba:30:ALA:N	2.52	0.42
16:BE:202:GLN:HG2	16:BE:203:TYR:H	1.85	0.42
23:BP:54:LYS:HB3	23:BP:55:GLY:H	1.60	0.42
28:BU:116:LEU:HD23	28:BU:116:LEU:HA	1.88	0.42
33:Ba:380:GLN:HB3	33:Ba:410:THR:HG22	2.01	0.42
34:Bb:93:PRO:HA	34:Bb:94:PRO:HD2	1.81	0.42
35:Bc:285:THR:HG22	35:Bc:286:GLN:H	1.84	0.42
47:Bo:83:GLU:OE1	50:Bt:66:ARG:NH1	2.52	0.42
53:Bw:291:THR:HG22	53:Bw:352:GLN:HB2	2.01	0.42
56:AA:114:A:N1	56:AA:136:C:O2'	2.48	0.42
56:AA:876:A:N1	84:Aj:17:ARG:NH1	2.67	0.42
57:AB:131:THR:HG22	57:AB:256:ILE:HD11	2.01	0.42
57:AB:262:LYS:O	57:AB:266:VAL:HG23	2.18	0.42
79:Ae:217:SER:O	79:Ae:221:LEU:N	2.45	0.42
79:Ae:328:LYS:HD3	79:Ae:328:LYS:HA	1.77	0.42
84:Aj:95:TRP:HH2	84:Aj:129:ARG:HD2	1.84	0.42
86:Am:40:LYS:HA	86:Am:40:LYS:HD3	1.80	0.42
88:Ao:574:TRP:HA	88:Ao:575:PRO:HD3	1.82	0.42
3:B1:83:GLU:OE2	3:B1:107:PRO:HB3	2.19	0.42
3:B1:102:ARG:NH1	12:BA:48:U:C5	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:48:U:O2'	12:BA:49:A:H4'	2.19	0.42
12:BA:139:G:C6	41:Bi:72:LEU:HD22	2.54	0.42
12:BA:416:U:H2'	12:BA:417:G:C8	2.54	0.42
12:BA:753:G:OP1	37:Be:24:LYS:HE2	2.19	0.42
12:BA:788:A:C2	25:BR:17:ARG:NH1	2.87	0.42
14:BC:519:ILE:HG12	14:BC:549:VAL:CG2	2.49	0.42
24:BQ:247:THR:HG1	24:BQ:250:ARG:HG2	1.83	0.42
27:BT:268:ASP:HB3	27:BT:271:ARG:HB2	2.01	0.42
31:BX:136:SER:HA	31:BX:137:PRO:HD3	1.90	0.42
34:Bb:197:GLU:OE1	34:Bb:197:GLU:N	2.52	0.42
34:Bb:266:HIS:N	34:Bb:266:HIS:CD2	2.87	0.42
53:Bw:159:VAL:O	53:Bw:161:GLN:HG2	2.19	0.42
56:AA:420:A:OP1	64:AK:192:LYS:HG2	2.19	0.42
58:AC:93:ARG:NH1	58:AC:108:LEU:O	2.52	0.42
61:AG:180:ARG:O	61:AG:184:MET:HG3	2.20	0.42
62:AI:108:ILE:HG23	62:AI:112:PHE:HD2	1.83	0.42
64:AK:100:GLN:HE21	64:AK:108:PRO:HB3	1.84	0.42
81:Ag:211:LYS:HE3	81:Ag:212:ARG:HE	1.84	0.42
85:Ak:58:ARG:NH2	88:Ao:91:ASP:OD2	2.53	0.42
85:Ak:72:TYR:CE2	85:Ak:76:ALA:HB3	2.54	0.42
88:Ao:419:PHE:CE2	88:Ao:450:LEU:HD13	2.55	0.42
3:B1:165:MET:HE2	3:B1:165:MET:HB3	1.91	0.42
9:B7:84:ARG:NH1	12:BA:126:G:OP1	2.52	0.42
11:B9:74:ARG:NH1	12:BA:545:U:O2'	2.51	0.42
12:BA:373:U:H1'	12:BA:1146:G:O2'	2.18	0.42
12:BA:582:C:OP2	47:Bo:23:ALA:HB2	2.19	0.42
12:BA:1207:C:H5'	12:BA:1208:A:OP2	2.19	0.42
14:BC:282:PRO:HG2	14:BC:345:LEU:HD11	2.01	0.42
17:BF:290:TYR:HB2	17:BF:293:PHE:HB3	2.00	0.42
30:BW:154:ILE:HD11	41:Bi:47:GLN:HE21	1.84	0.42
31:BX:3:ARG:O	31:BX:5:VAL:HG23	2.19	0.42
36:Bd:150:LEU:HD12	42:Bj:232:PHE:CE2	2.55	0.42
38:Bf:138:PRO:HA	38:Bf:139:PRO:HD3	1.92	0.42
56:AA:91:A:H2'	56:AA:92:A:O4'	2.20	0.42
56:AA:308:A:H3'	56:AA:309:A:C5'	2.49	0.42
56:AA:736:A:O2'	81:Ag:165:ARG:NH2	2.52	0.42
57:AB:100:PHE:CZ	76:Ab:47:ARG:HB3	2.53	0.42
63:AJ:121:LEU:HB2	66:AN:108:ARG:NE	2.35	0.42
63:AJ:151:SER:O	63:AJ:155:VAL:HG23	2.20	0.42
65:AL:33:LEU:HD23	65:AL:33:LEU:HA	1.85	0.42
65:AL:37:HIS:HD2	69:AQ:36:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Aa:150:MET:HE3	75:Aa:288:ARG:O	2.19	0.42
77:Ac:24:LYS:HG3	77:Ac:107:GLY:O	2.20	0.42
77:Ac:44:ALA:O	77:Ac:47:PHE:HB3	2.20	0.42
79:Ae:233:LYS:O	79:Ae:234:THR:OG1	2.35	0.42
81:Ag:284:GLU:OE2	81:Ag:293:ARG:NH1	2.51	0.42
83:Ai:54:ASN:O	83:Ai:58:TYR:HD2	2.02	0.42
84:Aj:31:SER:HA	84:Aj:111:HIS:CD2	2.55	0.42
85:Ak:306:ASP:OD1	85:Ak:306:ASP:N	2.52	0.42
88:Ao:417:MET:HG3	88:Ao:456:ARG:NH1	2.34	0.42
4:B2:111:ARG:HD3	31:BX:25:PHE:CE1	2.55	0.42
4:B2:130:SER:OG	4:B2:133:ARG:HD2	2.19	0.42
5:B3:78:ARG:HH21	24:BQ:228:LYS:HD3	1.84	0.42
12:BA:273:A:O2'	12:BA:274:A:H5''	2.19	0.42
12:BA:659:U:H5''	53:Bw:55:SER:HB2	2.02	0.42
14:BC:381:LEU:HB3	14:BC:410:ALA:HB3	2.01	0.42
17:BF:262:THR:O	17:BF:265:THR:HB	2.20	0.42
20:BK:104:THR:HG23	20:BK:152:GLY:HA2	2.00	0.42
25:BR:110:ILE:HD12	25:BR:110:ILE:HA	1.84	0.42
27:BT:82:PRO:HA	27:BT:83:PRO:HD3	1.89	0.42
29:BV:164:VAL:HA	29:BV:197:LEU:HD23	2.01	0.42
33:Ba:295:GLU:HB3	33:Ba:303:ARG:HG2	2.01	0.42
39:Bg:6:THR:HG22	39:Bg:7:ALA:H	1.84	0.42
40:Bh:59:ARG:HA	40:Bh:184:PHE:CD1	2.54	0.42
42:Bj:46:ARG:HB3	42:Bj:229:ALA:CB	2.49	0.42
42:Bj:161:VAL:HA	42:Bj:251:HIS:O	2.18	0.42
57:AB:73:ASN:O	57:AB:258:ARG:NH1	2.52	0.42
58:AC:98:GLY:HA3	83:Ai:71:TYR:CE1	2.54	0.42
61:AG:154:PRO:O	61:AG:179:ARG:HD2	2.20	0.42
62:AI:389:ARG:HA	62:AI:389:ARG:HD3	1.81	0.42
67:AO:69:PRO:HA	67:AO:70:PRO:HD3	1.87	0.42
84:Aj:28:PRO:HB3	84:Aj:32:GLN:HE21	1.85	0.42
85:Ak:110:ILE:HD13	85:Ak:110:ILE:HA	1.82	0.42
12:BA:435:C:H2'	12:BA:436:U:C6	2.55	0.42
12:BA:477:A:H2'	12:BA:478:G:H5'	2.01	0.42
12:BA:626:G:O4'	17:BF:154:GLY:HA2	2.19	0.42
12:BA:1425:A:H5''	12:BA:1425:A:N3	2.34	0.42
15:BD:68:SER:CB	33:Ba:38:THR:HG21	2.49	0.42
21:BN:39:LEU:HD12	21:BN:39:LEU:HA	1.86	0.42
21:BN:117:HIS:O	21:BN:121:MET:HG2	2.19	0.42
21:BN:137:ILE:HA	21:BN:140:ASN:OD1	2.19	0.42
21:BN:140:ASN:HA	40:Bh:262:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BQ:135:GLY:O	24:BQ:138:GLN:HG2	2.19	0.42
26:BS:90:ILE:HD11	26:BS:120:ARG:HH11	1.85	0.42
33:Ba:215:ARG:HG3	33:Ba:215:ARG:NH1	2.35	0.42
34:Bb:187:VAL:HG13	34:Bb:319:PHE:HB3	2.01	0.42
50:Bt:25:ARG:O	50:Bt:25:ARG:HG2	2.13	0.42
56:AA:358:U:H4'	64:AK:89:HIS:CD2	2.55	0.42
57:AB:117:LEU:HA	57:AB:120:THR:HB	2.02	0.42
60:AF:42:LEU:HD21	60:AF:65:LEU:HD22	2.00	0.42
62:AI:387:GLY:O	62:AI:388:ALA:HB3	2.20	0.42
65:AL:69:LYS:HA	65:AL:70:PRO:HD3	1.84	0.42
65:AL:104:GLU:C	65:AL:105:HIS:CG	2.98	0.42
81:Ag:111:LEU:HD23	81:Ag:114:THR:HG21	2.01	0.42
82:Ah:353:ASN:HA	82:Ah:354:PRO:HD3	1.89	0.42
83:Ai:26:THR:HG22	83:Ai:30:SER:HB2	2.00	0.42
88:Ao:266:ILE:HG12	88:Ao:278:ALA:HB1	2.02	0.42
9:B7:91:LYS:HB2	12:BA:118:U:H5''	2.01	0.42
10:B8:116:ARG:NE	10:B8:167:LYS:HG2	2.35	0.42
12:BA:442:G:OP1	24:BQ:144:LYS:HE3	2.19	0.42
12:BA:562:A:H3'	12:BA:562:A:N3	2.35	0.42
12:BA:574:A:H2'	54:Bx:192:LEU:HD22	2.02	0.42
12:BA:1215:C:N4	12:BA:1219:A:H3'	2.30	0.42
15:BD:154:ALA:O	15:BD:249:SER:OG	2.19	0.42
19:BJ:198:PRO:HB3	19:BJ:202:LEU:HD12	2.01	0.42
23:BP:220:ARG:NH2	23:BP:236:LEU:HD22	2.35	0.42
27:BT:145:LEU:HD12	27:BT:145:LEU:HA	1.77	0.42
28:BU:17:ARG:HA	28:BU:20:ARG:HG3	2.02	0.42
29:BV:63:PRO:HG3	54:Bx:187:TYR:CE2	2.55	0.42
29:BV:99:LEU:O	29:BV:113:THR:HG23	2.20	0.42
33:Ba:387:TRP:NE1	33:Ba:399:GLU:OE1	2.53	0.42
37:Be:118:GLU:HA	37:Be:119:PRO:HD3	1.87	0.42
39:Bg:73:PRO:HD2	39:Bg:90:HIS:HB2	2.02	0.42
40:Bh:105:ARG:HH11	40:Bh:116:LEU:HD23	1.85	0.42
41:Bi:293:PHE:HE2	41:Bi:295:GLU:HG2	1.84	0.42
44:Bl:162:LEU:HD23	44:Bl:162:LEU:HA	1.88	0.42
46:Bn:46:ARG:HA	46:Bn:51:ARG:HD2	2.02	0.42
46:Bn:69:HIS:O	46:Bn:72:GLU:HG2	2.20	0.42
60:AF:97:PRO:HG3	70:AR:76:LYS:NZ	2.33	0.42
62:AI:123:PRO:HG3	85:Ak:89:MET:SD	2.60	0.42
70:AR:131:LEU:HD13	70:AR:131:LEU:HA	1.90	0.42
76:Ab:48:ARG:HH11	76:Ab:48:ARG:CG	2.33	0.42
77:Ac:132:ARG:HG2	77:Ac:138:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Af:81:PHE:HA	80:Af:84:MET:SD	2.60	0.42
80:Af:90:LEU:HD23	80:Af:90:LEU:HA	1.89	0.42
81:Ag:92:THR:HG21	81:Ag:364:TRP:CZ3	2.55	0.42
81:Ag:122:ARG:HG2	81:Ag:305:ILE:HD11	2.01	0.42
88:Ao:518:ASP:HB3	88:Ao:522:TYR:CE1	2.55	0.42
5:B3:36:PHE:HE2	5:B3:79:PRO:HG3	1.85	0.42
8:B6:19:LYS:HB2	8:B6:62:ILE:HD11	2.02	0.42
9:B7:57:GLN:HA	9:B7:58:PRO:HD3	1.81	0.42
12:BA:272:A:H3'	12:BA:273:A:H5''	2.01	0.42
16:BE:58:VAL:HB	16:BE:59:PRO:HD3	2.01	0.42
16:BE:98:GLY:HA3	16:BE:179:PHE:CE1	2.55	0.42
16:BE:157:LYS:HD3	16:BE:157:LYS:HA	1.56	0.42
16:BE:206:VAL:HG22	16:BE:299:ILE:HG23	2.02	0.42
20:BK:66:LEU:HD13	20:BK:82:ILE:HG23	2.00	0.42
26:BS:52:ASN:HD22	26:BS:53:PRO:HD2	1.83	0.42
29:BV:60:LEU:HB2	54:Bx:80:LYS:O	2.19	0.42
31:BX:3:ARG:HB3	31:BX:24:PHE:HE2	1.85	0.42
31:BX:150:LEU:HD13	41:Bi:240:ARG:HG2	2.00	0.42
33:Ba:153:ARG:NH1	33:Ba:187:LEU:HD22	2.34	0.42
34:Bb:94:PRO:HA	34:Bb:95:PRO:HD3	1.89	0.42
42:Bj:197:GLU:O	42:Bj:244:SER:HB3	2.19	0.42
48:Bp:21:CYS:SG	48:Bp:60:SER:N	2.93	0.42
53:Bw:339:PHE:HB3	53:Bw:344:ASP:O	2.20	0.42
53:Bw:368:LEU:HD21	53:Bw:371:LEU:HD13	2.02	0.42
57:AB:124:LEU:HD22	57:AB:248:PHE:HE1	1.85	0.42
58:AC:37:ASN:O	58:AC:43:ARG:NH2	2.52	0.42
58:AC:89:ASP:O	58:AC:93:ARG:HG2	2.20	0.42
59:AE:141:TRP:HA	59:AE:142:PRO:HD3	1.90	0.42
63:AJ:158:GLU:HG2	88:Ao:70:ILE:HG21	2.02	0.42
75:Aa:348:HIS:HA	75:Aa:351:LYS:HD2	2.02	0.42
79:Ae:178:PHE:CG	84:Aj:72:PRO:HA	2.55	0.42
80:Af:107:HIS:C	80:Af:108:ILE:HG12	2.44	0.42
82:Ah:324:ILE:HG13	85:Ak:223:TYR:CD1	2.55	0.42
88:Ao:372:LEU:O	88:Ao:418:PHE:HB2	2.20	0.42
88:Ao:457:ARG:HG2	88:Ao:489:PHE:CE1	2.54	0.42
1:GL:67:LEU:HD22	1:HL:67:LEU:HD12	2.01	0.42
12:BA:230:G:H2'	12:BA:231:C:C6	2.55	0.42
12:BA:443:G:O6	19:BJ:31:LYS:NZ	2.32	0.42
12:BA:811:A:O5'	12:BA:811:A:H8	2.03	0.42
16:BE:264:ILE:HG12	16:BE:265:ASP:N	2.34	0.42
19:BJ:34:THR:OG1	19:BJ:35:ARG:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BN:33:ALA:HA	21:BN:111:MET:HE1	2.02	0.42
28:BU:99:ARG:HG3	28:BU:99:ARG:HH11	1.85	0.42
29:BV:88:ASN:ND2	29:BV:208:LEU:HB3	2.34	0.42
32:BY:145:ARG:HH12	32:BY:157:PRO:HD3	1.85	0.42
33:Ba:373:LEU:HD12	33:Ba:373:LEU:HA	1.72	0.42
34:Bb:185:MET:HE1	51:Bu:184:ARG:HD2	2.02	0.42
35:Bc:111:ASP:OD2	35:Bc:252:HIS:HE1	2.02	0.42
40:Bh:301:LEU:HA	40:Bh:301:LEU:HD12	1.75	0.42
42:Bj:137:LEU:HD23	42:Bj:140:ALA:HB3	2.01	0.42
42:Bj:208:ALA:HA	42:Bj:209:PRO:HD3	1.81	0.42
42:Bj:266:PRO:O	42:Bj:270:ALA:HB2	2.20	0.42
46:Bn:128:ARG:HD3	46:Bn:128:ARG:HA	1.67	0.42
53:Bw:94:TYR:HA	53:Bw:95:PRO:HD3	1.91	0.42
53:Bw:352:GLN:HB3	53:Bw:418:PHE:CD2	2.55	0.42
53:Bw:363:PHE:HB3	53:Bw:418:PHE:CZ	2.55	0.42
56:AA:60:C:H4'	84:Aj:34:TYR:HE2	1.85	0.42
56:AA:81:U:O2'	69:AQ:7:SER:O	2.28	0.42
56:AA:881:A:H4'	79:Ae:103:ARG:NH2	2.35	0.42
58:AC:42:VAL:HG21	58:AC:55:GLU:HB3	2.00	0.42
62:AI:316:PHE:CD1	62:AI:370:LEU:HD21	2.55	0.42
64:AK:123:LYS:H	64:AK:123:LYS:HG2	1.59	0.42
72:AV:6:G:H2'	72:AV:7:G:H5'	2.00	0.42
72:AV:40:A:H2'	72:AV:41:A:C8	2.55	0.42
79:Ae:191:PHE:HE2	79:Ae:203:VAL:HG21	1.84	0.42
82:Ah:352:LYS:HG2	85:Ak:213:ARG:HH21	1.85	0.42
85:Ak:59:THR:HG23	85:Ak:84:PRO:HA	2.02	0.42
9:B7:74:ARG:HH22	12:BA:31:A:HO2'	1.63	0.42
12:BA:367:A:H1'	12:BA:368:A:C2	2.55	0.42
12:BA:379:U:P	23:BP:62:ARG:HH11	2.43	0.42
14:BC:199:LYS:NZ	14:BC:328:GLY:HA3	2.35	0.42
18:BI:55:ILE:O	18:BI:83:VAL:HG22	2.19	0.42
19:BJ:161:VAL:HG21	19:BJ:181:ILE:HD13	2.02	0.42
21:BN:111:MET:HE2	21:BN:111:MET:HB3	1.84	0.42
24:BQ:78:GLU:OE2	24:BQ:158:ARG:NH1	2.53	0.42
26:BS:61:VAL:HG13	34:Bb:346:ARG:HH22	1.85	0.42
32:BY:211:LYS:HD2	33:Ba:82:TRP:CD1	2.55	0.42
34:Bb:251:THR:HG23	34:Bb:285:THR:HA	2.02	0.42
35:Bc:240:LYS:HD2	35:Bc:240:LYS:HA	1.89	0.42
39:Bg:15:LEU:HD12	39:Bg:15:LEU:HA	1.87	0.42
39:Bg:35:ARG:HD3	45:Bm:157:TRP:HH2	1.85	0.42
40:Bh:231:MET:H	40:Bh:231:MET:HG2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Bi:138:PRO:HB2	41:Bi:192:PRO:HG2	2.02	0.42
42:Bj:120:LEU:HB3	42:Bj:124:TRP:CH2	2.54	0.42
43:Bk:178:LEU:HA	43:Bk:179:PRO:HD3	1.85	0.42
46:Bn:69:HIS:CD2	46:Bn:71:LYS:H	2.31	0.42
56:AA:69:G:H2'	56:AA:70:U:O4'	2.19	0.42
56:AA:161:C:OP1	56:AA:163:A:N6	2.53	0.42
56:AA:882:A:H1'	79:Ae:106:PRO:HG2	2.02	0.42
72:AV:12:C:H2'	72:AV:13:U:O4'	2.20	0.42
79:Ae:195:GLU:HB3	79:Ae:196:ASN:H	1.65	0.42
86:Am:95:GLU:OE2	86:Am:101:PRO:HD3	2.19	0.42
89:Ap:55:PRO:HD2	89:Ap:56:TRP:CE3	2.55	0.42
5:B3:46:PHE:CZ	5:B3:111:LYS:HG2	2.56	0.41
6:B4:53:TYR:HA	6:B4:54:PRO:HD3	1.90	0.41
13:BB:69:C:H3'	13:BB:70:A:H5''	2.02	0.41
14:BC:574:PHE:O	14:BC:576:VAL:HG13	2.19	0.41
19:BJ:233:LEU:O	19:BJ:237:VAL:HG23	2.20	0.41
23:BP:130:GLN:HA	23:BP:131:PRO:HD3	1.86	0.41
26:BS:117:TYR:OH	34:Bb:120:GLU:OE1	2.22	0.41
29:BV:166:GLU:CD	39:Bg:108:SER:HB2	2.45	0.41
33:Ba:67:MET:HE3	33:Ba:68:PRO:HD2	2.01	0.41
33:Ba:107:PHE:HB2	33:Ba:265:LEU:HD22	2.02	0.41
34:Bb:238:THR:HG21	34:Bb:281:PHE:HZ	1.81	0.41
35:Bc:158:GLU:HB3	35:Bc:185:ARG:NH2	2.35	0.41
40:Bh:60:ARG:HG2	40:Bh:177:GLN:HE21	1.84	0.41
40:Bh:191:LEU:HD23	40:Bh:191:LEU:HA	1.74	0.41
41:Bi:202:LEU:HD13	41:Bi:205:GLN:NE2	2.35	0.41
49:Bq:76:ASN:H	49:Bq:79:LYS:CB	2.33	0.41
53:Bw:420:LEU:HD12	53:Bw:420:LEU:HA	1.85	0.41
56:AA:220:U:H2'	56:AA:221:A:C8	2.54	0.41
56:AA:372:C:H1'	86:Am:4:PRO:HG3	2.02	0.41
56:AA:409:G:N2	56:AA:451:C:H1'	2.36	0.41
59:AE:308:GLN:HG3	59:AE:312:TYR:CE1	2.53	0.41
61:AG:200:LEU:HD22	61:AG:200:LEU:HA	1.85	0.41
62:AI:275:GLY:N	62:AI:348:ALA:HB2	2.35	0.41
67:AO:116:VAL:HG22	67:AO:185:GLU:HB3	2.01	0.41
69:AQ:38:TYR:HD2	69:AQ:39:LEU:HD12	1.85	0.41
79:Ae:119:ILE:HG23	79:Ae:124:ASP:CB	2.48	0.41
85:Ak:89:MET:HE2	85:Ak:89:MET:HB3	1.84	0.41
88:Ao:434:LEU:O	88:Ao:438:VAL:HG23	2.20	0.41
88:Ao:582:VAL:HG11	88:Ao:598:MET:HG3	2.02	0.41
3:B1:42:HIS:O	18:BI:55:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B4:59:LYS:HE2	6:B4:65:ILE:HD11	2.02	0.41
10:B8:188:VAL:HG11	12:BA:424:U:H4'	2.02	0.41
12:BA:130:A:C6	12:BA:131:A:C2	3.08	0.41
12:BA:889:C:HO2'	12:BA:890:C:P	2.43	0.41
12:BA:1226:C:H3'	12:BA:1227:U:O2	2.21	0.41
14:BC:197:LEU:HA	14:BC:197:LEU:HD23	1.80	0.41
15:BD:195:ASN:ND2	15:BD:246:GLY:O	2.53	0.41
17:BF:167:MET:HE1	17:BF:276:HIS:CE1	2.55	0.41
17:BF:184:GLN:O	17:BF:185:ASP:HB2	2.20	0.41
24:BQ:250:ARG:HA	24:BQ:250:ARG:HD2	1.79	0.41
25:BR:41:ARG:HB2	25:BR:125:GLU:HG3	2.02	0.41
36:Bd:142:ALA:HA	42:Bj:274:ARG:HH21	1.85	0.41
40:Bh:258:THR:HG22	40:Bh:259:ARG:HG2	2.01	0.41
42:Bj:116:LEU:HG	42:Bj:117:ALA:H	1.85	0.41
50:Bt:18:ILE:HD13	50:Bt:18:ILE:HG21	1.85	0.41
51:Bu:98:ALA:HB3	51:Bu:145:ASN:HB3	2.02	0.41
53:Bw:198:ARG:CB	53:Bw:198:ARG:HH11	2.33	0.41
53:Bw:306:LEU:HD23	53:Bw:306:LEU:HA	1.77	0.41
57:AB:65:PRO:HB3	57:AB:71:PHE:CE2	2.56	0.41
58:AC:81:HIS:O	58:AC:85:ARG:HG2	2.20	0.41
59:AE:289:THR:HG23	59:AE:331:ASP:O	2.20	0.41
61:AG:81:LYS:HB2	61:AG:81:LYS:HE3	1.83	0.41
64:AK:64:ILE:HG22	71:AU:12:VAL:HG13	2.02	0.41
77:Ac:94:SER:O	77:Ac:98:ILE:HG13	2.19	0.41
79:Ae:216:PRO:HB2	79:Ae:219:GLN:CD	2.45	0.41
80:Af:98:ASN:N	80:Af:145:LEU:O	2.53	0.41
81:Ag:216:GLU:O	81:Ag:219:ARG:HG2	2.20	0.41
2:B0:76:HIS:HE1	2:B0:128:LYS:HD2	1.85	0.41
4:B2:125:ARG:HH11	4:B2:125:ARG:HG3	1.84	0.41
4:B2:156:ARG:HB2	37:Be:128:LEU:HB3	2.02	0.41
12:BA:373:U:H2'	12:BA:1063:U:C2	2.56	0.41
12:BA:505:U:OP1	20:BK:86:THR:HA	2.20	0.41
12:BA:763:C:O3'	93:BA:3205:SPM:H131	2.20	0.41
14:BC:410:ALA:HB2	14:BC:416:VAL:HG21	2.02	0.41
20:BK:90:PHE:HD2	20:BK:120:ILE:HG23	1.84	0.41
21:BN:69:GLY:HA2	54:Bx:152:THR:HA	2.03	0.41
23:BP:118:LEU:HD12	23:BP:118:LEU:HA	1.82	0.41
26:BS:91:GLU:HG3	26:BS:106:SER:HB3	2.02	0.41
34:Bb:27:ARG:HA	34:Bb:27:ARG:HD2	1.80	0.41
34:Bb:261:ARG:HA	34:Bb:323:TRP:CG	2.56	0.41
39:Bg:131:HIS:HB2	39:Bg:132:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Bx:164:ASN:O	54:Bx:165:LYS:C	2.61	0.41
56:AA:268:A:H2'	56:AA:269:C:H6	1.84	0.41
56:AA:522:A:H2'	56:AA:523:C:O4'	2.19	0.41
59:AE:427:ARG:HH11	59:AE:427:ARG:HG2	1.85	0.41
60:AF:26:LEU:HD23	60:AF:26:LEU:HA	1.85	0.41
62:AI:145:ARG:HA	62:AI:146:PRO:HD3	1.94	0.41
63:AJ:158:GLU:HG2	88:Ao:70:ILE:HD12	2.02	0.41
64:AK:184:PRO:C	64:AK:186:ASN:H	2.28	0.41
65:AL:33:LEU:HD22	69:AQ:39:LEU:HD23	2.02	0.41
68:AP:109:ARG:O	68:AP:113:LYS:HG3	2.20	0.41
69:AQ:93:ASP:HA	69:AQ:94:PRO:HD2	1.94	0.41
78:Ad:152:LEU:HD23	78:Ad:152:LEU:HA	1.82	0.41
79:Ae:137:HIS:O	84:Aj:104:TYR:HB2	2.20	0.41
79:Ae:172:LYS:HB3	79:Ae:173:VAL:H	1.61	0.41
84:Aj:7:ARG:HA	84:Aj:8:PRO:HD3	1.77	0.41
4:B2:179:ILE:HG12	4:B2:180:TRP:N	2.35	0.41
7:B5:155:GLU:OE2	25:BR:96:ARG:NH1	2.53	0.41
12:BA:130:A:OP1	17:BF:147:ARG:NH2	2.53	0.41
12:BA:1487:C:H1'	22:BO:95:ARG:NH2	2.35	0.41
15:BD:197:VAL:HG12	15:BD:198:GLU:O	2.20	0.41
20:BK:67:PRO:HD2	20:BK:85:PRO:HA	2.01	0.41
24:BQ:209:ASN:HD22	24:BQ:209:ASN:C	2.28	0.41
27:BT:96:ARG:HH11	27:BT:285:GLU:CD	2.28	0.41
34:Bb:184:LEU:HD12	34:Bb:184:LEU:HA	1.91	0.41
40:Bh:45:LEU:HA	40:Bh:45:LEU:HD12	1.74	0.41
40:Bh:284:GLY:HA2	40:Bh:285:PRO:HD3	1.82	0.41
42:Bj:162:ARG:HD3	42:Bj:171:TRP:CE3	2.55	0.41
55:Bz:702:ALA:HA	55:Bz:705:ALA:HB3	2.02	0.41
56:AA:56:U:P	78:Ad:41:ARG:HH22	2.43	0.41
59:AE:412:LYS:HG2	59:AE:417:MET:HB2	2.01	0.41
61:AG:82:THR:HA	62:AI:316:PHE:CD2	2.55	0.41
64:AK:181:THR:H	71:AU:10:ARG:NH1	2.14	0.41
67:AO:229:ARG:HD3	67:AO:229:ARG:HA	1.93	0.41
69:AQ:22:MET:H	69:AQ:22:MET:HG2	1.59	0.41
81:Ag:333:PHE:CD2	85:Ak:302:LYS:HE2	2.54	0.41
86:Am:6:LEU:HD12	86:Am:6:LEU:HA	1.70	0.41
89:Ap:202:TRP:CD1	89:Ap:202:TRP:H	2.38	0.41
12:BA:236:U:H5'	23:BP:37:GLU:HB3	2.02	0.41
14:BC:188:HIS:CD2	14:BC:268:GLN:H	2.39	0.41
14:BC:397:ARG:O	14:BC:398:LEU:HD23	2.20	0.41
14:BC:397:ARG:NH2	14:BC:422:ARG:HH12	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:401:ASP:OD1	14:BC:402:GLU:N	2.52	0.41
16:BE:296:LEU:HD12	16:BE:296:LEU:HA	1.95	0.41
19:BJ:168:LEU:HD13	19:BJ:176:LEU:HB2	2.02	0.41
22:BO:56:ARG:HH11	22:BO:56:ARG:CG	2.33	0.41
28:BU:102:LEU:HD23	28:BU:102:LEU:HA	1.72	0.41
33:Ba:34:GLY:HA3	33:Ba:39:ARG:HE	1.86	0.41
33:Ba:173:ARG:HA	33:Ba:176:TYR:CD2	2.56	0.41
41:Bi:271:PRO:HA	41:Bi:272:PRO:HD3	1.99	0.41
51:Bu:97:LYS:HE2	51:Bu:97:LYS:HB2	1.89	0.41
53:Bw:278:ILE:HB	53:Bw:336:TYR:CE2	2.55	0.41
53:Bw:372:ALA:HB1	53:Bw:377:ALA:HB1	2.02	0.41
54:Bx:192:LEU:HD23	54:Bx:192:LEU:HA	1.88	0.41
62:AI:91:MET:H	62:AI:91:MET:HG2	1.62	0.41
62:AI:123:PRO:N	85:Ak:89:MET:HG3	2.35	0.41
64:AK:85:ILE:HD12	64:AK:175:ILE:HD13	2.01	0.41
65:AL:127:ARG:HD2	65:AL:127:ARG:HA	1.87	0.41
69:AQ:55:LEU:H	69:AQ:55:LEU:HG	1.58	0.41
75:Aa:150:MET:HE2	75:Aa:150:MET:HB3	1.84	0.41
76:Ab:62:ASP:OD1	76:Ab:62:ASP:N	2.52	0.41
80:Af:105:ILE:HG12	80:Af:115:ILE:HG12	2.02	0.41
84:Aj:135:MET:SD	84:Aj:135:MET:N	2.79	0.41
3:B1:40:PRO:HB3	3:B1:43:TYR:CZ	2.54	0.41
12:BA:104:C:H41	17:BF:105:ASN:ND2	2.18	0.41
12:BA:446:C:H1'	12:BA:1280:C:O2'	2.21	0.41
12:BA:801:G:H4'	22:BO:36:THR:HG22	2.02	0.41
12:BA:1060:C:H5''	12:BA:1152:G:O2'	2.20	0.41
12:BA:1414:C:H2'	12:BA:1415:G:C8	2.56	0.41
19:BJ:67:PRO:HA	19:BJ:68:PRO:HD3	1.94	0.41
20:BK:164:LEU:HD21	49:Bq:76:ASN:HA	2.03	0.41
21:BN:59:ILE:HB	21:BN:127:LEU:HD23	2.02	0.41
21:BN:155:LEU:HB2	54:Bx:86:VAL:HG11	2.02	0.41
24:BQ:75:PRO:HB3	24:BQ:241:TYR:CZ	2.55	0.41
27:BT:77:SER:HA	27:BT:78:PRO:HD3	1.90	0.41
56:AA:374:C:OP2	86:Am:9:ARG:NH2	2.46	0.41
56:AA:460:A:H4'	56:AA:461:A:OP2	2.19	0.41
59:AE:426:LYS:HD2	89:Ap:136:HIS:CG	2.56	0.41
60:AF:2:PRO:HB2	60:AF:96:HIS:CD2	2.56	0.41
60:AF:8:LEU:HD23	60:AF:8:LEU:HA	1.93	0.41
62:AI:217:GLN:H	62:AI:217:GLN:HG2	1.59	0.41
68:AP:115:ALA:HB2	89:Ap:232:PRO:HG2	2.03	0.41
69:AQ:96:THR:HG22	78:Ad:117:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:AR:117:ILE:HD13	70:AR:117:ILE:HA	1.92	0.41
75:Aa:128:MET:HB3	75:Aa:132:GLN:HB2	2.03	0.41
77:Ac:21:VAL:HG22	77:Ac:103:ARG:HB2	2.02	0.41
81:Ag:56:ALA:C	81:Ag:112:LYS:HZ1	2.29	0.41
83:Ai:62:MET:CE	83:Ai:65:LEU:HD12	2.50	0.41
84:Aj:29:ARG:HG2	84:Aj:105:ALA:HB3	2.03	0.41
12:BA:71:U:OP2	46:Bn:96:ARG:NH2	2.54	0.41
12:BA:138:A:C5	12:BA:141:A:H2	2.38	0.41
12:BA:302:A:H2'	12:BA:303:G:O4'	2.21	0.41
12:BA:1033:G:H2'	12:BA:1034:G:O4'	2.21	0.41
12:BA:1159:U:H2'	12:BA:1160:C:H6	1.85	0.41
14:BC:180:SER:HA	14:BC:181:PRO:HD3	1.85	0.41
16:BE:221:ARG:HA	16:BE:261:LEU:HD22	2.03	0.41
19:BJ:117:ARG:HG3	20:BK:134:ASP:HB3	2.03	0.41
26:BS:144:MET:HE2	26:BS:144:MET:HB3	1.97	0.41
34:Bb:124:ARG:HH22	36:Bd:116:LEU:HA	1.85	0.41
36:Bd:143:GLN:NE2	42:Bj:210:CYS:O	2.53	0.41
39:Bg:35:ARG:HG3	39:Bg:36:ASP:N	2.35	0.41
40:Bh:186:VAL:HA	40:Bh:187:PRO:HD2	1.89	0.41
50:Bt:15:ARG:HD3	50:Bt:18:ILE:HD12	2.03	0.41
56:AA:26:A:OP1	56:AA:218:A:H4'	2.21	0.41
56:AA:607:G:O6	83:Ai:93:LYS:HE2	2.20	0.41
56:AA:881:A:H1'	79:Ae:105:LEU:HD13	2.02	0.41
57:AB:227:ASN:HA	57:AB:228:PRO:HD2	1.91	0.41
59:AE:198:TRP:HB2	59:AE:225:VAL:CG1	2.50	0.41
64:AK:77:TRP:HB3	64:AK:148:HIS:CD2	2.55	0.41
66:AN:62:ILE:HG21	82:Ah:341:HIS:HB3	2.03	0.41
66:AN:103:ARG:HB3	66:AN:104:TRP:CE3	2.56	0.41
67:AO:210:LEU:HB2	87:An:189:TRP:CZ2	2.56	0.41
68:AP:100:HIS:HA	68:AP:101:PRO:HD2	1.89	0.41
76:Ab:8:THR:HG23	76:Ab:46:PHE:HD2	1.85	0.41
77:Ac:167:LEU:HD23	77:Ac:167:LEU:HA	1.91	0.41
88:Ao:80:ARG:NH2	88:Ao:488:VAL:HG22	2.36	0.41
88:Ao:260:HIS:O	88:Ao:263:CYS:HB3	2.20	0.41
1:EL:70:ASP:HB2	1:FL:67:LEU:HD21	2.03	0.41
12:BA:223:A:H5'	17:BF:285:PRO:HD3	2.02	0.41
12:BA:330:A:N3	12:BA:330:A:H2'	2.35	0.41
12:BA:718:A:H5''	12:BA:719:C:OP2	2.20	0.41
12:BA:1404:G:H4'	12:BA:1405:A:C8	2.56	0.41
14:BC:424:LEU:HD23	14:BC:424:LEU:HA	1.82	0.41
16:BE:100:ILE:HD13	16:BE:175:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BE:209:LYS:HA	16:BE:264:ILE:O	2.20	0.41
23:BP:72:THR:HA	23:BP:73:PRO:HD3	1.84	0.41
25:BR:145:LEU:HB2	35:Bc:136:ASN:OD1	2.20	0.41
26:BS:116:LEU:HA	26:BS:116:LEU:HD12	1.76	0.41
27:BT:99:MET:H	27:BT:99:MET:HG2	1.73	0.41
30:BW:138:LEU:HD23	30:BW:178:GLU:HA	2.03	0.41
31:BX:63:VAL:HA	31:BX:64:PRO:HD3	1.83	0.41
32:BY:124:ASP:HA	32:BY:125:PRO:HD3	1.90	0.41
33:Ba:309:LEU:O	33:Ba:313:MET:HG2	2.20	0.41
38:Bf:84:ILE:HA	38:Bf:92:LEU:CB	2.51	0.41
41:Bi:270:ALA:HA	41:Bi:271:PRO:HD3	1.97	0.41
42:Bj:56:PRO:HA	42:Bj:57:PRO:HD2	1.96	0.41
43:Bk:100:MET:HG2	43:Bk:153:HIS:CD2	2.55	0.41
45:Bm:139:SER:OG	45:Bm:140:LYS:N	2.54	0.41
56:AA:633:C:OP1	59:AE:269:ARG:NH1	2.54	0.41
62:AI:169:LEU:HD13	62:AI:229:LEU:HA	2.01	0.41
62:AI:316:PHE:HB3	62:AI:317:PRO:HD3	2.03	0.41
63:AJ:52:VAL:HG13	88:Ao:479:LYS:HD3	2.02	0.41
69:AQ:14:VAL:H	77:Ac:63:GLN:HE22	1.69	0.41
70:AR:53:VAL:HA	70:AR:54:PRO:HD3	1.88	0.41
76:Ab:119:VAL:O	76:Ab:123:LYS:HG2	2.19	0.41
77:Ac:82:SER:OG	77:Ac:84:GLU:HB2	2.20	0.41
79:Ae:80:TRP:HE3	79:Ae:83:ARG:HD2	1.86	0.41
79:Ae:96:LEU:O	79:Ae:100:THR:HG23	2.20	0.41
79:Ae:273:LYS:HE2	79:Ae:273:LYS:HB3	1.86	0.41
81:Ag:201:ILE:O	81:Ag:220:PRO:HA	2.21	0.41
84:Aj:142:VAL:HA	84:Aj:143:PRO:HD3	1.90	0.41
88:Ao:67:LYS:HE3	88:Ao:67:LYS:HB2	1.87	0.41
1:DL:70:ASP:O	1:DL:74:LEU:HG	2.20	0.41
4:B2:104:TRP:CH2	4:B2:141:MET:HE2	2.56	0.41
5:B3:41:ILE:HA	5:B3:42:PRO:HD2	1.90	0.41
12:BA:479:A:H8	12:BA:479:A:OP1	2.04	0.41
12:BA:720:C:OP1	12:BA:720:C:H6	2.04	0.41
13:BB:28:A:H2'	13:BB:29:G:H5''	2.03	0.41
14:BC:184:THR:HG23	14:BC:233:LEU:HB2	2.02	0.41
17:BF:48:LEU:HD22	45:Bm:95:VAL:HG12	2.02	0.41
17:BF:101:ILE:HA	17:BF:101:ILE:HD12	1.80	0.41
17:BF:293:PHE:HA	17:BF:294:PRO:HD3	1.94	0.41
22:BO:95:ARG:HH11	22:BO:95:ARG:N	2.17	0.41
26:BS:106:SER:O	26:BS:112:ILE:HD12	2.21	0.41
27:BT:57:PRO:HA	27:BT:58:PRO:HD3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:225:LYS:HB3	27:BT:226:PRO:HD2	2.02	0.41
29:BV:70:LEU:HA	29:BV:71:PRO:HD3	1.82	0.41
29:BV:105:PHE:HE2	29:BV:120:ILE:HG12	1.86	0.41
29:BV:205:ALA:HA	29:BV:206:PRO:HD3	1.90	0.41
32:BY:166:VAL:HA	32:BY:167:PRO:HD3	1.85	0.41
33:Ba:42:GLU:H	33:Ba:42:GLU:HG3	1.61	0.41
34:Bb:79:GLY:C	34:Bb:81:GLU:N	2.78	0.41
34:Bb:238:THR:HG22	34:Bb:239:ASN:N	2.36	0.41
36:Bd:174:GLN:HE22	43:Bk:183:LYS:HE2	1.85	0.41
39:Bg:21:ARG:HH21	40:Bh:214:PHE:HA	1.86	0.41
39:Bg:89:ILE:HB	39:Bg:97:ILE:HD12	2.03	0.41
40:Bh:56:PRO:HA	40:Bh:57:PRO:HD3	1.88	0.41
41:Bi:122:ILE:CG2	41:Bi:126:ARG:HH11	2.34	0.41
41:Bi:165:THR:CG2	41:Bi:262:HIS:HA	2.51	0.41
44:Bl:57:ILE:HA	44:Bl:58:PRO:HD2	1.90	0.41
44:Bl:84:TYR:CE1	44:Bl:120:LEU:HD13	2.56	0.41
44:Bl:96:VAL:HG22	44:Bl:110:ILE:HG12	2.01	0.41
51:Bu:71:ILE:HD11	51:Bu:154:ARG:HG3	2.02	0.41
53:Bw:105:TRP:CG	53:Bw:265:LEU:HD13	2.55	0.41
53:Bw:144:LEU:HD23	53:Bw:144:LEU:HA	1.89	0.41
53:Bw:263:ASP:O	53:Bw:266:PRO:HA	2.21	0.41
53:Bw:273:GLU:O	53:Bw:273:GLU:HG3	2.21	0.41
56:AA:13:U:OP1	59:AE:226:ARG:HD3	2.20	0.41
56:AA:551:G:H21	56:AA:778:G:H4'	1.86	0.41
56:AA:790:A:N1	56:AA:818:A:H5''	2.36	0.41
56:AA:814:A:H2'	56:AA:815:U:C6	2.55	0.41
59:AE:363:ALA:O	59:AE:387:PRO:HB3	2.20	0.41
60:AF:2:PRO:HG2	60:AF:98:LEU:HB2	2.02	0.41
60:AF:48:PRO:HB2	60:AF:49:TYR:CD2	2.56	0.41
61:AG:231:GLU:OE1	86:Am:57:LYS:HB2	2.21	0.41
62:AI:202:ILE:H	62:AI:202:ILE:HG13	1.65	0.41
63:AJ:136:MET:HE2	63:AJ:136:MET:HB3	1.87	0.41
70:AR:57:ASN:HA	70:AR:58:PRO:HD3	1.77	0.41
71:AU:72:ILE:HD12	86:Am:104:LEU:HD22	2.01	0.41
75:Aa:237:LEU:HD23	75:Aa:237:LEU:HA	1.94	0.41
75:Aa:334:GLN:H	75:Aa:334:GLN:HG2	1.63	0.41
79:Ae:110:LEU:HD11	79:Ae:430:LEU:HB3	2.02	0.41
79:Ae:203:VAL:O	79:Ae:207:ILE:HG13	2.21	0.41
79:Ae:329:ALA:O	79:Ae:333:PRO:HD2	2.20	0.41
82:Ah:298:LYS:HG3	88:Ao:68:VAL:HG11	2.02	0.41
85:Ak:286:LEU:HD23	85:Ak:291:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Am:104:LEU:HD23	86:Am:104:LEU:HA	1.81	0.41
88:Ao:401:ASN:HA	88:Ao:404:MET:SD	2.61	0.41
12:BA:573:A:N6	54:Bx:196:HIS:HB3	2.35	0.41
12:BA:659:U:OP2	53:Bw:55:SER:HB2	2.21	0.41
12:BA:746:U:O2'	12:BA:747:U:OP2	2.28	0.41
14:BC:485:LEU:O	14:BC:489:ARG:HB2	2.21	0.41
15:BD:248:VAL:HG12	15:BD:249:SER:H	1.85	0.41
16:BE:54:SER:H	25:BR:147:ASN:ND2	2.18	0.41
23:BP:280:LYS:HD3	44:Bl:45:TYR:CE2	2.56	0.41
27:BT:99:MET:O	27:BT:103:ARG:HG3	2.21	0.41
29:BV:63:PRO:HA	29:BV:64:PRO:HD3	1.86	0.41
29:BV:146:THR:OG1	38:Bf:62:HIS:HE1	2.04	0.41
33:Ba:313:MET:HE2	33:Ba:313:MET:HB3	1.76	0.41
38:Bf:56:ARG:CB	38:Bf:56:ARG:HH11	2.34	0.41
42:Bj:192:LEU:HB3	42:Bj:200:MET:SD	2.61	0.41
51:Bu:103:HIS:HD2	51:Bu:106:SER:H	1.68	0.41
53:Bw:171:LEU:HD23	53:Bw:232:HIS:CD2	2.56	0.41
56:AA:220:U:H2'	56:AA:221:A:H8	1.86	0.41
57:AB:149:GLN:HG3	71:AU:84:TRP:CZ2	2.56	0.41
62:AI:201:LEU:HD11	62:AI:245:PHE:HD1	1.86	0.41
63:AJ:148:LEU:HD23	63:AJ:148:LEU:HA	1.86	0.41
67:AO:171:LEU:HD23	67:AO:171:LEU:HA	1.86	0.41
67:AO:178:VAL:O	67:AO:182:ILE:HG12	2.21	0.41
77:Ac:4:LYS:O	77:Ac:11:ARG:NH1	2.54	0.41
80:Af:121:PHE:HE2	80:Af:164:LEU:HD22	1.86	0.41
81:Ag:79:PRO:HG2	81:Ag:193:ALA:HA	2.03	0.41
82:Ah:348:CYS:O	82:Ah:351:SER:HB3	2.21	0.41
83:Ai:64:THR:O	83:Ai:68:LEU:HG	2.20	0.41
85:Ak:166:ARG:HD3	85:Ak:166:ARG:HA	1.86	0.41
88:Ao:305:ALA:O	88:Ao:308:VAL:HG23	2.21	0.41
3:B1:173:ASP:HA	3:B1:174:PRO:HD3	1.84	0.40
5:B3:128:LEU:HA	5:B3:129:PRO:HD3	1.88	0.40
9:B7:60:ASN:OD1	9:B7:63:ARG:NH1	2.53	0.40
12:BA:379:U:P	23:BP:62:ARG:NH1	2.94	0.40
14:BC:257:LEU:HD11	14:BC:269:THR:HG23	2.02	0.40
15:BD:139:ASP:H	15:BD:249:SER:HB2	1.86	0.40
17:BF:218:LEU:HD23	17:BF:260:VAL:HB	2.03	0.40
27:BT:123:ASP:HA	27:BT:124:PRO:HD3	1.93	0.40
30:BW:82:LYS:HE3	30:BW:83:ASP:OD1	2.20	0.40
30:BW:114:ILE:H	30:BW:114:ILE:HG12	1.66	0.40
35:Bc:313:LEU:HD12	35:Bc:313:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Bh:213:LEU:HD23	40:Bh:213:LEU:HA	1.90	0.40
43:Bk:155:ARG:HA	43:Bk:155:ARG:HD3	1.78	0.40
44:Bl:134:LYS:HE3	44:Bl:134:LYS:HB2	1.96	0.40
51:Bu:75:ARG:HH11	51:Bu:109:TRP:HE3	1.67	0.40
53:Bw:162:ASP:OD1	53:Bw:162:ASP:N	2.55	0.40
56:AA:27:U:H2'	56:AA:28:U:C6	2.56	0.40
56:AA:866:U:H2'	56:AA:867:G:C8	2.56	0.40
61:AG:96:ASN:OD1	61:AG:104:LYS:HE3	2.21	0.40
72:AV:39:G:H2'	72:AV:40:A:C8	2.56	0.40
75:Aa:299:ASN:HD21	75:Aa:329:LEU:HD13	1.85	0.40
81:Ag:325:GLN:HB3	85:Ak:306:ASP:OD1	2.20	0.40
83:Ai:35:LYS:HD2	83:Ai:35:LYS:HA	1.88	0.40
86:Am:66:CYS:HB2	86:Am:69:GLU:OE1	2.21	0.40
87:An:174:LYS:HG3	87:An:177:TRP:CZ2	2.56	0.40
88:Ao:129:GLN:NE2	88:Ao:144:TYR:OH	2.46	0.40
12:BA:178:C:H1'	28:BU:55:ARG:NH2	2.37	0.40
12:BA:1234:U:H2'	12:BA:1235:C:O4'	2.21	0.40
14:BC:310:VAL:HB	14:BC:316:GLY:HA3	2.02	0.40
23:BP:93:TYR:HB3	23:BP:139:GLN:HB3	2.02	0.40
26:BS:127:SER:O	26:BS:131:VAL:HG23	2.22	0.40
33:Ba:90:LEU:HA	33:Ba:90:LEU:HD23	1.87	0.40
33:Ba:329:TYR:HB3	33:Ba:334:LYS:NZ	2.36	0.40
39:Bg:27:GLN:O	39:Bg:61:VAL:HA	2.21	0.40
40:Bh:245:LEU:HA	40:Bh:245:LEU:HD23	1.84	0.40
41:Bi:288:LYS:H	41:Bi:288:LYS:HG2	1.60	0.40
42:Bj:176:SER:HB3	42:Bj:187:THR:HG22	2.03	0.40
56:AA:663:A:H1'	66:AN:127:MET:HE2	2.03	0.40
58:AC:125:ARG:NH1	88:Ao:94:TYR:HB2	2.35	0.40
59:AE:255:GLY:HA3	59:AE:278:TYR:O	2.21	0.40
60:AF:15:ARG:NH2	78:Ad:182:ASP:OD1	2.47	0.40
62:AI:170:LEU:HD23	62:AI:170:LEU:HA	1.94	0.40
63:AJ:68:GLU:HA	63:AJ:69:PRO:HD3	1.72	0.40
68:AP:38:HIS:HD2	68:AP:40:LYS:H	1.67	0.40
75:Aa:167:ASP:OD2	75:Aa:197:ARG:NH2	2.55	0.40
75:Aa:316:VAL:HG21	75:Aa:371:TYR:CE2	2.57	0.40
77:Ac:141:CYS:HB3	77:Ac:149:CYS:H	1.86	0.40
78:Ad:44:THR:HA	78:Ad:45:PRO:HD3	1.90	0.40
81:Ag:160:TRP:CE3	81:Ag:288:LEU:HB3	2.56	0.40
81:Ag:254:ILE:HG23	81:Ag:255:PHE:HD1	1.86	0.40
83:Ai:62:MET:HE2	83:Ai:62:MET:HA	2.03	0.40
84:Aj:79:LEU:HD21	84:Aj:96:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Aj:165:PRO:HA	84:Aj:190:MET:HE1	2.03	0.40
89:Ap:92:LYS:HA	89:Ap:144:MET:HB2	2.03	0.40
1:CL:54:LEU:HD13	19:BJ:204:GLN:HB3	2.03	0.40
6:B4:60:GLN:HB3	55:Bz:702:ALA:HB1	2.03	0.40
8:B6:52:LYS:HG3	52:Bv:125:MET:HE2	2.02	0.40
12:BA:274:A:H1'	12:BA:309:A:O2'	2.21	0.40
12:BA:435:C:H2'	12:BA:436:U:H6	1.86	0.40
12:BA:835:A:H5''	12:BA:1431:G:H4'	2.02	0.40
12:BA:1136:U:H2'	12:BA:1137:A:O4'	2.22	0.40
17:BF:211:ARG:HB2	45:Bm:59:ARG:HH22	1.86	0.40
22:BO:73:ILE:HD13	22:BO:73:ILE:HG21	1.81	0.40
33:Ba:328:LEU:HB2	33:Ba:329:TYR:CE1	2.56	0.40
39:Bg:65:VAL:HG12	39:Bg:67:PRO:HD3	2.03	0.40
56:AA:270:C:H2'	56:AA:271:C:C6	2.56	0.40
56:AA:619:C:H5'	56:AA:620:C:OP2	2.21	0.40
56:AA:625:U:H5	56:AA:659:A:OP1	2.04	0.40
56:AA:848:C:H2'	56:AA:849:G:C8	2.55	0.40
58:AC:132:PHE:O	58:AC:136:VAL:HG23	2.22	0.40
60:AF:79:MET:HE1	60:AF:92:ASN:HA	2.03	0.40
61:AG:172:VAL:HA	61:AG:173:PRO:HD2	1.85	0.40
62:AI:148:HIS:CE1	62:AI:150:LEU:HB2	2.57	0.40
67:AO:144:MET:HE1	67:AO:150:ASP:HB3	2.02	0.40
75:Aa:141:VAL:O	75:Aa:145:LYS:HG2	2.21	0.40
78:Ad:181:LEU:HD23	78:Ad:181:LEU:HA	1.82	0.40
79:Ae:74:TYR:HB3	79:Ae:76:ASP:OD1	2.22	0.40
81:Ag:323:LEU:HA	81:Ag:324:PRO:HD3	1.88	0.40
84:Aj:83:LYS:HE2	84:Aj:87:TRP:CZ2	2.55	0.40
88:Ao:527:ARG:O	88:Ao:531:LYS:HB2	2.21	0.40
3:B1:100:ARG:NH1	18:BI:75:ARG:HH21	2.18	0.40
5:B3:76:LYS:O	5:B3:77:ARG:HB2	2.22	0.40
5:B3:84:ASP:HB3	5:B3:88:MET:HE3	2.04	0.40
12:BA:160:A:N6	38:Bf:119:THR:HG21	2.36	0.40
12:BA:1238:A:H3'	12:BA:1239:A:H5''	2.03	0.40
13:BB:43:C:OP2	26:BS:122:VAL:HG23	2.22	0.40
14:BC:322:PRO:O	14:BC:330:ASN:HB2	2.22	0.40
14:BC:524:VAL:O	14:BC:527:SER:OG	2.36	0.40
17:BF:102:TRP:HB2	17:BF:165:LEU:HD22	2.02	0.40
17:BF:103:GLN:HE22	17:BF:249:ASN:HB2	1.86	0.40
17:BF:274:LEU:HD23	17:BF:274:LEU:HA	1.78	0.40
19:BJ:107:GLU:H	19:BJ:107:GLU:HG3	1.67	0.40
20:BK:159:LEU:CB	20:BK:163:GLU:HG2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BY:101:THR:HG22	32:BY:104:TYR:HB3	2.02	0.40
34:Bb:66:ARG:HA	34:Bb:75:ARG:CZ	2.51	0.40
42:Bj:215:PHE:O	42:Bj:229:ALA:HB3	2.21	0.40
42:Bj:264:LEU:HD12	42:Bj:264:LEU:HA	1.89	0.40
45:Bm:76:LYS:HG2	45:Bm:83:VAL:HG23	2.03	0.40
48:Bp:63:CYS:SG	48:Bp:64:VAL:N	2.94	0.40
56:AA:235:A:H1'	89:Ap:80:ASN:HB3	2.04	0.40
56:AA:490:A:H2'	56:AA:491:G:O4'	2.22	0.40
56:AA:561:U:H1'	56:AA:711:A:H62	1.86	0.40
56:AA:647:A:H3'	56:AA:648:A:H5'	2.03	0.40
56:AA:801:A:H2	56:AA:809:G:H22	1.70	0.40
57:AB:101:MET:HG3	57:AB:224:THR:O	2.22	0.40
59:AE:122:ARG:NH1	73:AX:13:U:O2'	2.54	0.40
70:AR:81:LEU:HD13	70:AR:112:ILE:HA	2.02	0.40
78:Ad:77:GLU:O	78:Ad:81:LYS:HG3	2.22	0.40
86:Am:112:PRO:HG2	86:Am:114:LYS:HE2	2.03	0.40
88:Ao:336:GLN:HA	88:Ao:339:ASN:HB3	2.02	0.40
4:B2:104:TRP:CZ3	4:B2:141:MET:HE2	2.57	0.40
4:B2:230:ARG:NH2	12:BA:101:U:O2'	2.55	0.40
6:B4:40:LEU:HD23	6:B4:40:LEU:HA	1.97	0.40
12:BA:56:A:N3	12:BA:56:A:H2'	2.35	0.40
12:BA:164:A:P	28:BU:52:LYS:NZ	2.94	0.40
16:BE:225:LYS:HE2	16:BE:225:LYS:HB3	1.74	0.40
17:BF:79:LEU:HD22	17:BF:79:LEU:HA	1.77	0.40
19:BJ:119:HIS:CD2	19:BJ:163:GLU:HG2	2.56	0.40
23:BP:162:LEU:HD13	23:BP:240:TYR:CE1	2.57	0.40
34:Bb:67:LYS:HA	34:Bb:68:PRO:HD3	1.85	0.40
34:Bb:71:TRP:C	34:Bb:72:ARG:NH1	2.80	0.40
40:Bh:51:LEU:HD22	40:Bh:51:LEU:HA	1.88	0.40
42:Bj:185:ARG:NH1	42:Bj:206:GLY:O	2.54	0.40
42:Bj:213:TYR:HB3	42:Bj:268:TYR:HD1	1.86	0.40
43:Bk:96:ILE:HG23	43:Bk:154:GLU:HG2	2.04	0.40
56:AA:687:A:H2'	56:AA:688:G:O4'	2.22	0.40
58:AC:85:ARG:NH1	58:AC:88:GLU:OE1	2.54	0.40
60:AF:104:GLU:N	60:AF:104:GLU:OE1	2.54	0.40
65:AL:55:ARG:HH11	65:AL:55:ARG:CG	2.35	0.40
66:AN:105:ARG:HG2	83:Ai:51:TRP:CZ3	2.56	0.40
70:AR:83:GLN:HE22	78:Ad:190:ALA:HB1	1.87	0.40
76:Ab:100:VAL:O	76:Ab:104:ILE:HG13	2.22	0.40
79:Ae:160:GLY:C	79:Ae:162:GLN:H	2.30	0.40
84:Aj:178:ARG:NH2	84:Aj:189:PRO:HD3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Am:100:PRO:HA	86:Am:101:PRO:HD3	1.93	0.40
88:Ao:542:GLN:O	88:Ao:544:PRO:HD3	2.21	0.40
88:Ao:582:VAL:O	88:Ao:586:PHE:HB2	2.22	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	
1	BL	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
1	CL	43/198 (22%)	41 (95%)	1 (2%)	1 (2%)	5	29
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	25 (96%)	1 (4%)	0	100	100
1	FL	25/198 (13%)	25 (100%)	0	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	104 (96%)	4 (4%)	0	100	100
3	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
4	B2	177/252 (70%)	172 (97%)	5 (3%)	0	100	100
5	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
6	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
7	B5	108/188 (57%)	106 (98%)	2 (2%)	0	100	100
8	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
10	B8	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	B9	36/100 (36%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BC	569/650 (88%)	548 (96%)	20 (4%)	1 (0%)	43	73
15	BD	238/306 (78%)	226 (95%)	12 (5%)	0	100	100
16	BE	305/348 (88%)	284 (93%)	18 (6%)	3 (1%)	12	45
17	BF	248/294 (84%)	237 (96%)	11 (4%)	0	100	100
18	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
19	BJ	210/262 (80%)	202 (96%)	8 (4%)	0	100	100
20	BK	174/192 (91%)	166 (95%)	7 (4%)	1 (1%)	21	56
21	BN	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
22	BO	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
23	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
24	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
25	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
26	BS	141/180 (78%)	131 (93%)	9 (6%)	1 (1%)	18	52
27	BT	238/292 (82%)	229 (96%)	8 (3%)	1 (0%)	30	62
28	BU	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
29	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
30	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
31	BX	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
32	BY	204/216 (94%)	193 (95%)	11 (5%)	0	100	100
33	Ba	391/423 (92%)	377 (96%)	14 (4%)	0	100	100
34	Bb	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
35	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
36	Bd	97/206 (47%)	89 (92%)	7 (7%)	1 (1%)	12	45
37	Be	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
38	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	33
39	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
40	Bh	287/332 (86%)	276 (96%)	11 (4%)	0	100	100
41	Bi	258/306 (84%)	248 (96%)	10 (4%)	0	100	100
42	Bj	211/279 (76%)	199 (94%)	12 (6%)	0	100	100
43	Bk	132/212 (62%)	126 (96%)	6 (4%)	0	100	100
44	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Bm	107/159 (67%)	104 (97%)	3 (3%)	0	100	100
46	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
47	Bo	95/124 (77%)	91 (96%)	4 (4%)	0	100	100
48	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
49	Bq	66/138 (48%)	64 (97%)	1 (2%)	1 (2%)	8	37
50	Bt	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
51	Bu	147/205 (72%)	136 (92%)	10 (7%)	1 (1%)	18	52
52	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
53	Bw	385/433 (89%)	365 (95%)	18 (5%)	2 (0%)	24	59
54	Bx	160/196 (82%)	156 (98%)	3 (2%)	1 (1%)	21	56
55	Bz	70/82 (85%)	70 (100%)	0	0	100	100
57	AB	218/289 (75%)	213 (98%)	5 (2%)	0	100	100
58	AC	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
59	AE	341/430 (79%)	327 (96%)	14 (4%)	0	100	100
60	AF	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
61	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
62	AI	326/397 (82%)	313 (96%)	13 (4%)	0	100	100
63	AJ	138/201 (69%)	129 (94%)	7 (5%)	2 (1%)	9	39
64	AK	135/196 (69%)	129 (96%)	5 (4%)	1 (1%)	18	52
65	AL	107/139 (77%)	105 (98%)	2 (2%)	0	100	100
66	AN	99/128 (77%)	99 (100%)	0	0	100	100
67	AO	173/239 (72%)	167 (96%)	6 (4%)	0	100	100
68	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
69	AQ	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
70	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
71	AU	84/87 (97%)	84 (100%)	0	0	100	100
74	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
75	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100	100
76	Ab	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
77	Ac	167/173 (96%)	157 (94%)	9 (5%)	1 (1%)	21	56
78	Ad	175/205 (85%)	170 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	Ae	386/455 (85%)	350 (91%)	32 (8%)	4 (1%)	12	45
80	Af	97/188 (52%)	92 (95%)	5 (5%)	0	100	100
81	Ag	351/397 (88%)	338 (96%)	13 (4%)	0	100	100
82	Ah	118/387 (30%)	116 (98%)	2 (2%)	0	100	100
83	Ai	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
84	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
85	Ak	273/325 (84%)	265 (97%)	8 (3%)	0	100	100
86	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
87	An	70/199 (35%)	68 (97%)	2 (3%)	0	100	100
88	Ao	564/692 (82%)	532 (94%)	32 (6%)	0	100	100
89	Ap	188/258 (73%)	182 (97%)	6 (3%)	0	100	100
All	All	14839/20063 (74%)	14258 (96%)	557 (4%)	24 (0%)	44	73

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CL	21	PRO
14	BC	502	PRO
27	BT	68	PRO
38	Bf	78	PRO
38	Bf	80	PRO
51	Bu	167	PRO
16	BE	202	GLN
53	Bw	159	VAL
54	Bx	93	ILE
63	AJ	179	GLN
63	AJ	185	ARG
16	BE	317	PRO
79	Ae	285	CYS
20	BK	157	LYS
49	Bq	101	VAL
53	Bw	100	LEU
77	Ac	105	ILE
79	Ae	161	ALA
79	Ae	342	PRO
79	Ae	344	GLU
16	BE	264	ILE
64	AK	186	ASN

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Mol	Chain	Res	Type
36	Bd	170	PRO
26	BS	45	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BL	59/157 (38%)	58 (98%)	1 (2%)	53	75
1	CL	30/157 (19%)	29 (97%)	1 (3%)	33	65
1	DL	26/157 (17%)	23 (88%)	3 (12%)	5	24
1	EL	27/157 (17%)	25 (93%)	2 (7%)	13	43
1	FL	26/157 (17%)	24 (92%)	2 (8%)	12	41
1	GL	26/157 (17%)	25 (96%)	1 (4%)	29	62
1	HL	25/157 (16%)	23 (92%)	2 (8%)	11	40
2	B0	90/115 (78%)	80 (89%)	10 (11%)	6	25
3	B1	219/229 (96%)	192 (88%)	27 (12%)	4	22
4	B2	164/228 (72%)	146 (89%)	18 (11%)	6	26
5	B3	110/147 (75%)	99 (90%)	11 (10%)	7	30
6	B4	42/114 (37%)	35 (83%)	7 (17%)	2	11
7	B5	99/163 (61%)	89 (90%)	10 (10%)	7	30
8	B6	49/60 (82%)	46 (94%)	3 (6%)	17	49
9	B7	41/78 (53%)	39 (95%)	2 (5%)	22	55
10	B8	87/162 (54%)	77 (88%)	10 (12%)	5	24
11	B9	36/77 (47%)	31 (86%)	5 (14%)	3	17
14	BC	464/553 (84%)	447 (96%)	17 (4%)	30	63
15	BD	193/248 (78%)	168 (87%)	25 (13%)	4	20
16	BE	263/290 (91%)	237 (90%)	26 (10%)	7	31
17	BF	217/251 (86%)	193 (89%)	24 (11%)	6	25
18	BI	88/228 (39%)	83 (94%)	5 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	BJ	192/230 (84%)	184 (96%)	8 (4%)	26	60
20	BK	129/151 (85%)	120 (93%)	9 (7%)	14	45
21	BN	156/157 (99%)	140 (90%)	16 (10%)	7	28
22	BO	99/123 (80%)	85 (86%)	14 (14%)	3	17
23	BP	245/249 (98%)	217 (89%)	28 (11%)	5	24
24	BQ	190/210 (90%)	180 (95%)	10 (5%)	20	53
25	BR	132/143 (92%)	118 (89%)	14 (11%)	6	27
26	BS	123/153 (80%)	114 (93%)	9 (7%)	13	43
27	BT	212/258 (82%)	190 (90%)	22 (10%)	7	28
28	BU	118/127 (93%)	110 (93%)	8 (7%)	14	46
29	BV	136/178 (76%)	124 (91%)	12 (9%)	9	35
30	BW	144/180 (80%)	131 (91%)	13 (9%)	9	34
31	BX	116/134 (87%)	103 (89%)	13 (11%)	6	25
32	BY	185/192 (96%)	163 (88%)	22 (12%)	5	23
33	Ba	348/365 (95%)	310 (89%)	38 (11%)	6	26
34	Bb	310/328 (94%)	273 (88%)	37 (12%)	5	23
35	Bc	271/299 (91%)	255 (94%)	16 (6%)	18	50
36	Bd	92/181 (51%)	85 (92%)	7 (8%)	12	42
37	Be	100/108 (93%)	85 (85%)	15 (15%)	3	15
38	Bf	80/133 (60%)	68 (85%)	12 (15%)	3	15
39	Bg	128/136 (94%)	110 (86%)	18 (14%)	3	17
40	Bh	251/284 (88%)	223 (89%)	28 (11%)	6	25
41	Bi	236/275 (86%)	220 (93%)	16 (7%)	14	46
42	Bj	190/242 (78%)	173 (91%)	17 (9%)	9	34
43	Bk	119/181 (66%)	112 (94%)	7 (6%)	18	50
44	Bl	122/147 (83%)	106 (87%)	16 (13%)	4	19
45	Bm	103/145 (71%)	95 (92%)	8 (8%)	11	41
46	Bn	88/113 (78%)	79 (90%)	9 (10%)	7	29
47	Bo	77/97 (79%)	69 (90%)	8 (10%)	7	28
48	Bp	79/88 (90%)	75 (95%)	4 (5%)	21	54
49	Bq	50/114 (44%)	48 (96%)	2 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Bt	75/82 (92%)	60 (80%)	15 (20%)	1	7
51	Bu	126/177 (71%)	112 (89%)	14 (11%)	6	25
52	Bv	115/183 (63%)	112 (97%)	3 (3%)	40	69
53	Bw	340/373 (91%)	299 (88%)	41 (12%)	5	22
54	Bx	149/173 (86%)	133 (89%)	16 (11%)	6	27
57	AB	187/233 (80%)	171 (91%)	16 (9%)	10	36
58	AC	115/142 (81%)	97 (84%)	18 (16%)	2	13
59	AE	282/351 (80%)	252 (89%)	30 (11%)	6	27
60	AF	107/109 (98%)	94 (88%)	13 (12%)	5	22
61	AG	181/205 (88%)	165 (91%)	16 (9%)	9	35
62	AI	273/333 (82%)	260 (95%)	13 (5%)	23	56
63	AJ	130/181 (72%)	114 (88%)	16 (12%)	4	22
64	AK	103/151 (68%)	94 (91%)	9 (9%)	9	36
65	AL	92/116 (79%)	87 (95%)	5 (5%)	20	53
66	AN	92/114 (81%)	77 (84%)	15 (16%)	2	12
67	AO	159/205 (78%)	146 (92%)	13 (8%)	10	39
68	AP	97/113 (86%)	93 (96%)	4 (4%)	27	60
69	AQ	97/114 (85%)	83 (86%)	14 (14%)	3	16
70	AR	89/127 (70%)	83 (93%)	6 (7%)	15	47
71	AU	77/78 (99%)	66 (86%)	11 (14%)	3	16
75	Aa	258/330 (78%)	230 (89%)	28 (11%)	6	26
76	Ab	113/162 (70%)	104 (92%)	9 (8%)	11	40
77	Ac	152/155 (98%)	140 (92%)	12 (8%)	11	40
78	Ad	149/168 (89%)	139 (93%)	10 (7%)	15	47
79	Ae	325/393 (83%)	296 (91%)	29 (9%)	9	34
80	Af	86/160 (54%)	76 (88%)	10 (12%)	5	24
81	Ag	312/350 (89%)	290 (93%)	22 (7%)	13	44
82	Ah	109/346 (32%)	102 (94%)	7 (6%)	16	48
83	Ai	86/93 (92%)	79 (92%)	7 (8%)	11	39
84	Aj	188/190 (99%)	178 (95%)	10 (5%)	20	53
85	Ak	249/289 (86%)	225 (90%)	24 (10%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	Am	100/102 (98%)	88 (88%)	12 (12%)	5	23
87	An	66/174 (38%)	59 (89%)	7 (11%)	6	27
88	Ao	478/604 (79%)	455 (95%)	23 (5%)	23	56
89	Ap	170/225 (76%)	150 (88%)	20 (12%)	5	23
All	All	12929/17064 (76%)	11743 (91%)	1186 (9%)	11	33

All (1186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CL	40	LEU
1	DL	71	ILE
1	DL	75	THR
1	DL	86	LEU
1	EL	76	LEU
1	EL	82	LEU
1	FL	76	LEU
1	FL	79	ILE
1	GL	82	LEU
1	HL	76	LEU
1	HL	79	ILE
2	B0	45	LYS
2	B0	49	LYS
2	B0	50	ARG
2	B0	53	ILE
2	B0	57	GLU
2	B0	117	VAL
2	B0	118	THR
2	B0	126	LEU
2	B0	131	VAL
2	B0	141	THR
3	B1	6	VAL
3	B1	31	SER
3	B1	32	LEU
3	B1	46	HIS
3	B1	61	ARG
3	B1	64	ASP
3	B1	69	VAL
3	B1	75	SER
3	B1	77	LEU
3	B1	79	LEU
3	B1	101	VAL

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Mol	Chain	Res	Type
3	B1	104	VAL
3	B1	112	ARG
3	B1	120	ASP
3	B1	126	THR
3	B1	128	THR
3	B1	148	THR
3	B1	152	ASP
3	B1	155	SER
3	B1	161	LEU
3	B1	172	GLN
3	B1	177	HIS
3	B1	179	ASP
3	B1	190	ARG
3	B1	204	VAL
3	B1	224	ILE
3	B1	238	LEU
4	B2	66	LEU
4	B2	67	GLU
4	B2	68	GLU
4	B2	72	ASP
4	B2	108	LEU
4	B2	118	GLU
4	B2	126	LEU
4	B2	144	LEU
4	B2	153	ASP
4	B2	158	LEU
4	B2	171	ARG
4	B2	174	ILE
4	B2	179	ILE
4	B2	197	ASN
4	B2	204	MET
4	B2	218	GLN
4	B2	228	LEU
4	B2	230	ARG
5	B3	38	ARG
5	B3	43	ASP
5	B3	69	VAL
5	B3	70	THR
5	B3	72	ILE
5	B3	73	LYS
5	B3	82	GLU
5	B3	86	ILE

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Mol	Chain	Res	Type
5	B3	147	VAL
5	B3	150	LEU
5	B3	151	LEU
6	B4	42	THR
6	B4	44	LEU
6	B4	49	TYR
6	B4	52	LEU
6	B4	57	LEU
6	B4	65	ILE
6	B4	78	MET
7	B5	85	ARG
7	B5	87	ILE
7	B5	94	ARG
7	B5	136	GLU
7	B5	143	LYS
7	B5	153	THR
7	B5	156	THR
7	B5	158	VAL
7	B5	173	ARG
7	B5	186	THR
8	B6	22	SER
8	B6	34	ARG
8	B6	54	VAL
9	B7	75	THR
9	B7	92	SER
10	B8	106	THR
10	B8	111	ILE
10	B8	113	ARG
10	B8	124	ARG
10	B8	162	THR
10	B8	163	THR
10	B8	169	ARG
10	B8	182	ASP
10	B8	183	ARG
10	B8	184	THR
11	B9	63	PHE
11	B9	65	THR
11	B9	74	ARG
11	B9	75	ASP
11	B9	92	ASN
14	BC	163	LYS
14	BC	184	THR

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Mol	Chain	Res	Type
14	BC	226	SER
14	BC	251	VAL
14	BC	253	ASP
14	BC	283	ILE
14	BC	330	ASN
14	BC	392	CYS
14	BC	471	LYS
14	BC	472	GLU
14	BC	484	LEU
14	BC	494	PHE
14	BC	520	ILE
14	BC	524	VAL
14	BC	537	THR
14	BC	570	VAL
14	BC	679	HIS
15	BD	62	THR
15	BD	64	VAL
15	BD	69	ARG
15	BD	74	VAL
15	BD	75	MET
15	BD	90	GLN
15	BD	103	ARG
15	BD	105	ARG
15	BD	111	ARG
15	BD	117	GLU
15	BD	148	ARG
15	BD	150	ARG
15	BD	153	ILE
15	BD	155	THR
15	BD	158	MET
15	BD	163	THR
15	BD	170	ILE
15	BD	172	ARG
15	BD	190	VAL
15	BD	193	LEU
15	BD	198	GLU
15	BD	224	THR
15	BD	240	THR
15	BD	265	ARG
15	BD	285	ARG
16	BE	50	ASP
16	BE	53	LEU

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Mol	Chain	Res	Type
16	BE	55	GLU
16	BE	80	LEU
16	BE	97	VAL
16	BE	109	LEU
16	BE	113	ASP
16	BE	146	THR
16	BE	158	SER
16	BE	168	LEU
16	BE	218	VAL
16	BE	220	ARG
16	BE	227	GLN
16	BE	236	THR
16	BE	239	ARG
16	BE	251	VAL
16	BE	264	ILE
16	BE	273	VAL
16	BE	285	VAL
16	BE	289	VAL
16	BE	296	LEU
16	BE	297	VAL
16	BE	299	ILE
16	BE	302	SER
16	BE	311	CYS
16	BE	326	GLU
17	BF	47	VAL
17	BF	59	ARG
17	BF	76	ARG
17	BF	77	VAL
17	BF	79	LEU
17	BF	80	THR
17	BF	89	THR
17	BF	94	ASP
17	BF	101	ILE
17	BF	116	THR
17	BF	125	ARG
17	BF	140	SER
17	BF	143	SER
17	BF	165	LEU
17	BF	172	GLN
17	BF	190	VAL
17	BF	193	LEU
17	BF	203	LEU

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Mol	Chain	Res	Type
17	BF	208	ARG
17	BF	224	GLU
17	BF	239	THR
17	BF	263	LEU
17	BF	281	THR
17	BF	291	CYS
18	BI	56	VAL
18	BI	75	ARG
18	BI	76	ARG
18	BI	99	THR
18	BI	130	VAL
19	BJ	34	THR
19	BJ	63	ARG
19	BJ	76	THR
19	BJ	78	LEU
19	BJ	93	ASN
19	BJ	121	ILE
19	BJ	150	HIS
19	BJ	229	LEU
20	BK	57	THR
20	BK	64	ILE
20	BK	113	THR
20	BK	117	VAL
20	BK	137	LEU
20	BK	145	ILE
20	BK	158	ASP
20	BK	163	GLU
20	BK	164	LEU
1	BL	159	VAL
21	BN	10	GLN
21	BN	24	LYS
21	BN	31	LEU
21	BN	39	LEU
21	BN	65	ILE
21	BN	67	PHE
21	BN	78	SER
21	BN	91	THR
21	BN	101	VAL
21	BN	104	VAL
21	BN	118	ARG
21	BN	123	GLN
21	BN	131	GLU

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Mol	Chain	Res	Type
21	BN	136	ASP
21	BN	153	ARG
21	BN	177	ARG
22	BO	56	ARG
22	BO	60	VAL
22	BO	71	ASP
22	BO	72	ARG
22	BO	73	ILE
22	BO	77	ILE
22	BO	91	MET
22	BO	95	ARG
22	BO	96	MET
22	BO	97	THR
22	BO	101	ASP
22	BO	111	ASN
22	BO	121	THR
22	BO	138	LEU
23	BP	11	ARG
23	BP	44	ARG
23	BP	58	GLN
23	BP	61	THR
23	BP	65	LEU
23	BP	71	GLN
23	BP	109	ARG
23	BP	125	ARG
23	BP	127	VAL
23	BP	130	GLN
23	BP	140	LEU
23	BP	141	VAL
23	BP	143	GLU
23	BP	147	THR
23	BP	152	VAL
23	BP	154	ILE
23	BP	175	THR
23	BP	211	VAL
23	BP	215	THR
23	BP	233	ARG
23	BP	234	LEU
23	BP	246	ASP
23	BP	247	ILE
23	BP	248	THR
23	BP	251	GLU

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Mol	Chain	Res	Type
23	BP	257	SER
23	BP	261	ASP
23	BP	286	THR
24	BQ	55	ARG
24	BQ	68	ASN
24	BQ	161	VAL
24	BQ	171	GLU
24	BQ	194	THR
24	BQ	214	THR
24	BQ	224	LEU
24	BQ	226	ILE
24	BQ	247	THR
24	BQ	250	ARG
25	BR	24	SER
25	BR	30	GLN
25	BR	38	ARG
25	BR	67	ASP
25	BR	84	ASP
25	BR	93	LEU
25	BR	98	GLN
25	BR	110	ILE
25	BR	118	ARG
25	BR	134	LEU
25	BR	139	ARG
25	BR	142	ASN
25	BR	148	GLN
25	BR	149	LEU
26	BS	44	VAL
26	BS	61	VAL
26	BS	80	ARG
26	BS	103	VAL
26	BS	107	THR
26	BS	141	ILE
26	BS	149	THR
26	BS	163	HIS
26	BS	171	VAL
27	BT	61	VAL
27	BT	77	SER
27	BT	79	GLU
27	BT	86	ARG
27	BT	90	LEU
27	BT	130	THR

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Mol	Chain	Res	Type
27	BT	138	ILE
27	BT	145	LEU
27	BT	162	ILE
27	BT	170	ARG
27	BT	177	VAL
27	BT	187	LEU
27	BT	202	VAL
27	BT	208	THR
27	BT	239	ASN
27	BT	243	ILE
27	BT	246	ASP
27	BT	254	MET
27	BT	272	GLU
27	BT	274	ASP
27	BT	284	ASP
27	BT	289	SER
28	BU	10	LEU
28	BU	43	VAL
28	BU	54	THR
28	BU	77	GLN
28	BU	87	ILE
28	BU	101	VAL
28	BU	123	ARG
28	BU	126	GLU
29	BV	91	ILE
29	BV	111	LYS
29	BV	117	LEU
29	BV	126	VAL
29	BV	133	ARG
29	BV	153	LEU
29	BV	160	VAL
29	BV	164	VAL
29	BV	169	GLU
29	BV	176	MET
29	BV	186	ARG
29	BV	199	ILE
30	BW	46	SER
30	BW	50	GLU
30	BW	60	GLN
30	BW	75	ARG
30	BW	80	TYR
30	BW	81	SER

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Mol	Chain	Res	Type
30	BW	131	ASN
30	BW	147	ARG
30	BW	151	LEU
30	BW	154	ILE
30	BW	164	ILE
30	BW	199	GLN
30	BW	206	ILE
31	BX	6	LEU
31	BX	14	ASN
31	BX	26	ILE
31	BX	28	LEU
31	BX	35	GLN
31	BX	47	GLU
31	BX	49	THR
31	BX	50	ARG
31	BX	52	ASP
31	BX	57	LEU
31	BX	88	LYS
31	BX	97	VAL
31	BX	104	THR
32	BY	30	SER
32	BY	31	ASP
32	BY	39	THR
32	BY	40	ARG
32	BY	43	ARG
32	BY	44	VAL
32	BY	66	GLU
32	BY	69	ASP
32	BY	86	VAL
32	BY	96	ARG
32	BY	107	THR
32	BY	131	THR
32	BY	137	PHE
32	BY	138	THR
32	BY	144	VAL
32	BY	145	ARG
32	BY	149	ARG
32	BY	153	ILE
32	BY	166	VAL
32	BY	181	ASP
32	BY	186	THR
32	BY	208	ARG

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Mol	Chain	Res	Type
33	Ba	42	GLU
33	Ba	47	ASP
33	Ba	49	VAL
33	Ba	58	ILE
33	Ba	63	LYS
33	Ba	67	MET
33	Ba	113	LEU
33	Ba	137	LEU
33	Ba	147	ILE
33	Ba	149	ASN
33	Ba	163	LEU
33	Ba	167	THR
33	Ba	175	THR
33	Ba	189	LYS
33	Ba	191	GLN
33	Ba	193	LEU
33	Ba	195	HIS
33	Ba	202	ILE
33	Ba	207	ASN
33	Ba	222	VAL
33	Ba	234	ASP
33	Ba	256	PHE
33	Ba	262	THR
33	Ba	270	VAL
33	Ba	294	LEU
33	Ba	322	LEU
33	Ba	324	GLN
33	Ba	335	VAL
33	Ba	337	GLU
33	Ba	345	VAL
33	Ba	347	THR
33	Ba	348	ASP
33	Ba	373	LEU
33	Ba	381	LEU
33	Ba	391	VAL
33	Ba	396	VAL
33	Ba	398	VAL
33	Ba	415	LEU
34	Bb	32	LEU
34	Bb	35	MET
34	Bb	40	ILE
34	Bb	50	LYS

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Mol	Chain	Res	Type
34	Bb	51	TYR
34	Bb	52	ARG
34	Bb	53	SER
34	Bb	72	ARG
34	Bb	88	VAL
34	Bb	90	ILE
34	Bb	99	ARG
34	Bb	118	GLU
34	Bb	120	GLU
34	Bb	130	ILE
34	Bb	135	VAL
34	Bb	173	LEU
34	Bb	179	VAL
34	Bb	210	GLU
34	Bb	222	ASP
34	Bb	229	ASP
34	Bb	233	VAL
34	Bb	237	VAL
34	Bb	238	THR
34	Bb	245	VAL
34	Bb	246	THR
34	Bb	261	ARG
34	Bb	267	ARG
34	Bb	272	LEU
34	Bb	276	ASP
34	Bb	281	PHE
34	Bb	284	ASP
34	Bb	288	SER
34	Bb	324	ASP
34	Bb	343	GLU
34	Bb	356	ARG
34	Bb	360	ARG
34	Bb	376	THR
35	Bc	67	VAL
35	Bc	87	SER
35	Bc	111	ASP
35	Bc	122	ILE
35	Bc	140	TRP
35	Bc	171	VAL
35	Bc	186	LEU
35	Bc	190	MET
35	Bc	218	VAL

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Mol	Chain	Res	Type
35	Bc	222	VAL
35	Bc	256	ASP
35	Bc	260	VAL
35	Bc	280	VAL
35	Bc	285	THR
35	Bc	297	SER
35	Bc	319	MET
36	Bd	89	ILE
36	Bd	98	GLU
36	Bd	106	LEU
36	Bd	132	GLU
36	Bd	136	ILE
36	Bd	150	LEU
36	Bd	168	LEU
37	Be	17	ARG
37	Be	23	SER
37	Be	25	ARG
37	Be	28	ARG
37	Be	29	THR
37	Be	31	CYS
37	Be	50	GLN
37	Be	60	VAL
37	Be	66	PHE
37	Be	68	LEU
37	Be	78	GLU
37	Be	106	THR
37	Be	111	HIS
37	Be	122	GLU
37	Be	127	GLN
38	Bf	42	ASP
38	Bf	56	ARG
38	Bf	58	ILE
38	Bf	59	VAL
38	Bf	60	CYS
38	Bf	67	ILE
38	Bf	70	GLU
38	Bf	75	ILE
38	Bf	114	LYS
38	Bf	122	ARG
38	Bf	126	ARG
38	Bf	134	ARG
39	Bg	2	THR

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Mol	Chain	Res	Type
39	Bg	6	THR
39	Bg	14	VAL
39	Bg	15	LEU
39	Bg	30	SER
39	Bg	33	LEU
39	Bg	47	VAL
39	Bg	52	THR
39	Bg	61	VAL
39	Bg	68	ARG
39	Bg	80	LEU
39	Bg	91	CYS
39	Bg	93	SER
39	Bg	112	VAL
39	Bg	125	SER
39	Bg	126	ILE
39	Bg	127	GLN
39	Bg	148	VAL
40	Bh	45	LEU
40	Bh	47	ARG
40	Bh	51	LEU
40	Bh	52	ARG
40	Bh	78	ARG
40	Bh	82	THR
40	Bh	98	ILE
40	Bh	110	ILE
40	Bh	121	ASP
40	Bh	148	LEU
40	Bh	154	THR
40	Bh	177	GLN
40	Bh	178	LEU
40	Bh	191	LEU
40	Bh	192	ARG
40	Bh	216	ARG
40	Bh	227	GLU
40	Bh	231	MET
40	Bh	233	THR
40	Bh	254	GLU
40	Bh	259	ARG
40	Bh	263	SER
40	Bh	264	THR
40	Bh	265	THR
40	Bh	267	LEU

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Mol	Chain	Res	Type
40	Bh	289	VAL
40	Bh	301	LEU
40	Bh	307	PHE
41	Bi	57	VAL
41	Bi	74	ARG
41	Bi	76	ILE
41	Bi	85	PHE
41	Bi	112	LEU
41	Bi	165	THR
41	Bi	176	ILE
41	Bi	181	VAL
41	Bi	186	VAL
41	Bi	196	GLN
41	Bi	221	THR
41	Bi	238	VAL
41	Bi	242	VAL
41	Bi	244	GLU
41	Bi	246	VAL
41	Bi	281	MET
42	Bj	51	LEU
42	Bj	55	ARG
42	Bj	60	THR
42	Bj	64	THR
42	Bj	119	ASP
42	Bj	136	ARG
42	Bj	137	LEU
42	Bj	139	GLU
42	Bj	145	ASP
42	Bj	179	GLN
42	Bj	210	CYS
42	Bj	230	LYS
42	Bj	255	VAL
42	Bj	264	LEU
42	Bj	265	LYS
42	Bj	276	LEU
42	Bj	279	LEU
43	Bk	50	SER
43	Bk	53	THR
43	Bk	56	ILE
43	Bk	132	MET
43	Bk	147	ASP
43	Bk	150	LEU

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Mol	Chain	Res	Type
43	Bk	165	THR
44	Bl	41	SER
44	Bl	42	VAL
44	Bl	89	SER
44	Bl	90	ARG
44	Bl	98	ARG
44	Bl	100	ILE
44	Bl	101	THR
44	Bl	107	MET
44	Bl	117	ILE
44	Bl	128	LEU
44	Bl	137	VAL
44	Bl	138	THR
44	Bl	141	ASN
44	Bl	143	VAL
44	Bl	154	ASP
44	Bl	155	GLN
45	Bm	52	VAL
45	Bm	67	LEU
45	Bm	71	LEU
45	Bm	86	ASN
45	Bm	121	MET
45	Bm	128	LEU
45	Bm	135	VAL
45	Bm	142	ASP
46	Bn	32	PHE
46	Bn	34	VAL
46	Bn	41	ARG
46	Bn	44	VAL
46	Bn	48	ASN
46	Bn	56	VAL
46	Bn	71	LYS
46	Bn	92	ILE
46	Bn	105	ASP
47	Bo	31	GLN
47	Bo	40	TYR
47	Bo	43	LEU
47	Bo	53	ASP
47	Bo	55	ARG
47	Bo	64	LEU
47	Bo	84	MET
47	Bo	110	LEU

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Mol	Chain	Res	Type
48	Bp	28	GLU
48	Bp	55	VAL
48	Bp	76	MET
48	Bp	84	GLN
49	Bq	95	TRP
49	Bq	137	LYS
50	Bt	10	ASN
50	Bt	25	ARG
50	Bt	27	VAL
50	Bt	30	GLN
50	Bt	35	MET
50	Bt	37	ARG
50	Bt	45	ASN
50	Bt	49	LEU
50	Bt	55	THR
50	Bt	57	GLU
50	Bt	60	ARG
50	Bt	88	LEU
50	Bt	90	GLU
50	Bt	98	THR
50	Bt	99	ARG
51	Bu	56	ASP
51	Bu	81	CYS
51	Bu	94	VAL
51	Bu	97	LYS
51	Bu	104	LEU
51	Bu	110	ILE
51	Bu	123	LYS
51	Bu	135	THR
51	Bu	140	ARG
51	Bu	146	LEU
51	Bu	148	ASP
51	Bu	182	MET
51	Bu	184	ARG
51	Bu	192	ILE
52	Bv	38	ARG
52	Bv	41	ASP
52	Bv	47	THR
53	Bw	43	ARG
53	Bw	51	LEU
53	Bw	77	ASP
53	Bw	81	ARG

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Mol	Chain	Res	Type
53	Bw	100	LEU
53	Bw	118	LEU
53	Bw	147	GLU
53	Bw	153	ARG
53	Bw	162	ASP
53	Bw	166	ILE
53	Bw	173	GLN
53	Bw	194	LEU
53	Bw	200	VAL
53	Bw	220	VAL
53	Bw	237	ILE
53	Bw	248	ASP
53	Bw	260	CYS
53	Bw	271	GLN
53	Bw	274	ASN
53	Bw	275	THR
53	Bw	278	ILE
53	Bw	280	SER
53	Bw	298	ASP
53	Bw	306	LEU
53	Bw	315	GLU
53	Bw	330	THR
53	Bw	345	VAL
53	Bw	347	ARG
53	Bw	356	THR
53	Bw	370	THR
53	Bw	376	GLN
53	Bw	393	LYS
53	Bw	395	LEU
53	Bw	399	ILE
53	Bw	402	ASN
53	Bw	405	LYS
53	Bw	410	ASP
53	Bw	414	GLN
53	Bw	415	LEU
53	Bw	420	LEU
53	Bw	421	ASN
54	Bx	54	THR
54	Bx	70	CYS
54	Bx	73	CYS
54	Bx	92	PHE
54	Bx	93	ILE

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Mol	Chain	Res	Type
54	Bx	100	LEU
54	Bx	115	ILE
54	Bx	121	MET
54	Bx	128	LEU
54	Bx	152	THR
54	Bx	157	ARG
54	Bx	162	ILE
54	Bx	165	LYS
54	Bx	190	ARG
54	Bx	193	LEU
54	Bx	196	HIS
57	AB	57	LEU
57	AB	125	GLN
57	AB	141	ILE
57	AB	159	ARG
57	AB	167	THR
57	AB	176	THR
57	AB	197	THR
57	AB	201	VAL
57	AB	206	VAL
57	AB	213	LYS
57	AB	218	THR
57	AB	222	VAL
57	AB	224	THR
57	AB	235	VAL
57	AB	246	ARG
57	AB	253	GLN
58	AC	38	ARG
58	AC	41	ARG
58	AC	44	VAL
58	AC	54	GLU
58	AC	71	LEU
58	AC	80	ASP
58	AC	89	ASP
58	AC	104	LEU
58	AC	108	LEU
58	AC	115	ASN
58	AC	117	LEU
58	AC	123	VAL
58	AC	124	LEU
58	AC	125	ARG
58	AC	127	LEU

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Mol	Chain	Res	Type
58	AC	132	PHE
58	AC	152	HIS
58	AC	167	ILE
59	AE	91	THR
59	AE	124	LYS
59	AE	136	ARG
59	AE	137	HIS
59	AE	196	ASN
59	AE	203	LEU
59	AE	215	TYR
59	AE	216	ASP
59	AE	220	THR
59	AE	228	VAL
59	AE	239	ARG
59	AE	240	SER
59	AE	241	VAL
59	AE	245	VAL
59	AE	283	GLU
59	AE	289	THR
59	AE	296	LEU
59	AE	305	MET
59	AE	336	VAL
59	AE	337	SER
59	AE	340	VAL
59	AE	346	THR
59	AE	370	VAL
59	AE	374	ARG
59	AE	376	GLU
59	AE	400	GLU
59	AE	404	ILE
59	AE	412	LYS
59	AE	417	MET
59	AE	423	SER
60	AF	8	LEU
60	AF	13	MET
60	AF	17	GLU
60	AF	29	LEU
60	AF	39	LEU
60	AF	40	GLU
60	AF	45	ARG
60	AF	46	MET
60	AF	65	LEU

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Mol	Chain	Res	Type
60	AF	67	ASP
60	AF	78	MET
60	AF	89	ILE
60	AF	120	THR
61	AG	40	GLU
61	AG	46	ILE
61	AG	57	GLU
61	AG	82	THR
61	AG	85	VAL
61	AG	88	ASP
61	AG	104	LYS
61	AG	109	SER
61	AG	153	GLU
61	AG	159	VAL
61	AG	180	ARG
61	AG	187	MET
61	AG	197	ARG
61	AG	200	LEU
61	AG	205	LEU
61	AG	219	VAL
62	AI	70	THR
62	AI	91	MET
62	AI	98	THR
62	AI	100	THR
62	AI	153	THR
62	AI	161	LEU
62	AI	202	ILE
62	AI	206	LEU
62	AI	217	GLN
62	AI	229	LEU
62	AI	277	ARG
62	AI	338	ARG
62	AI	357	VAL
63	AJ	52	VAL
63	AJ	64	THR
63	AJ	80	VAL
63	AJ	92	GLU
63	AJ	126	ILE
63	AJ	133	GLN
63	AJ	136	MET
63	AJ	145	LEU
63	AJ	148	LEU

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Mol	Chain	Res	Type
63	AJ	158	GLU
63	AJ	166	GLU
63	AJ	168	VAL
63	AJ	172	VAL
63	AJ	174	LYS
63	AJ	175	THR
63	AJ	184	ILE
64	AK	64	ILE
64	AK	68	ILE
64	AK	83	GLU
64	AK	85	ILE
64	AK	121	ASN
64	AK	147	THR
64	AK	153	VAL
64	AK	161	LEU
64	AK	177	ILE
65	AL	55	ARG
65	AL	67	ILE
65	AL	95	ILE
65	AL	101	SER
65	AL	102	LEU
66	AN	30	VAL
66	AN	34	MET
66	AN	35	LEU
66	AN	43	MET
66	AN	56	SER
66	AN	58	ARG
66	AN	80	ARG
66	AN	81	ASP
66	AN	92	VAL
66	AN	93	MET
66	AN	94	THR
66	AN	101	LYS
66	AN	102	ARG
66	AN	106	LEU
66	AN	125	ARG
67	AO	72	MET
67	AO	73	LEU
67	AO	74	LEU
67	AO	80	VAL
67	AO	83	ILE
67	AO	122	ASP

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Mol	Chain	Res	Type
67	AO	127	GLU
67	AO	130	ILE
67	AO	158	LEU
67	AO	159	MET
67	AO	167	MET
67	AO	198	ARG
67	AO	208	LYS
68	AP	26	CYS
68	AP	35	VAL
68	AP	90	LEU
68	AP	99	LEU
69	AQ	6	SER
69	AQ	22	MET
69	AQ	30	VAL
69	AQ	31	THR
69	AQ	40	LEU
69	AQ	46	ARG
69	AQ	55	LEU
69	AQ	56	GLN
69	AQ	59	THR
69	AQ	62	ASP
69	AQ	64	VAL
69	AQ	74	THR
69	AQ	81	LEU
69	AQ	90	GLN
70	AR	56	GLU
70	AR	83	GLN
70	AR	89	THR
70	AR	117	ILE
70	AR	124	THR
70	AR	131	LEU
71	AU	18	ASN
71	AU	35	LEU
71	AU	38	ASP
71	AU	50	ARG
71	AU	52	ARG
71	AU	66	MET
71	AU	75	LEU
71	AU	77	ARG
71	AU	80	ARG
71	AU	82	ASP
71	AU	85	GLN

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Mol	Chain	Res	Type
75	Aa	117	LEU
75	Aa	118	GLN
75	Aa	126	LYS
75	Aa	129	THR
75	Aa	147	ARG
75	Aa	150	MET
75	Aa	163	VAL
75	Aa	167	ASP
75	Aa	177	LYS
75	Aa	183	ILE
75	Aa	195	VAL
75	Aa	197	ARG
75	Aa	202	THR
75	Aa	204	ARG
75	Aa	214	MET
75	Aa	221	ARG
75	Aa	222	GLU
75	Aa	240	MET
75	Aa	276	ASP
75	Aa	284	LEU
75	Aa	285	ARG
75	Aa	293	MET
75	Aa	295	TRP
75	Aa	325	LEU
75	Aa	329	LEU
75	Aa	337	GLN
75	Aa	347	LEU
75	Aa	356	THR
76	Ab	6	LEU
76	Ab	7	GLU
76	Ab	14	SER
76	Ab	30	LEU
76	Ab	45	VAL
76	Ab	48	ARG
76	Ab	62	ASP
76	Ab	67	GLU
76	Ab	112	THR
77	Ac	3	MET
77	Ac	4	LYS
77	Ac	9	ILE
77	Ac	25	ASP
77	Ac	31	THR

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Mol	Chain	Res	Type
77	Ac	33	ASN
77	Ac	39	GLU
77	Ac	51	ASN
77	Ac	84	GLU
77	Ac	106	LEU
77	Ac	124	SER
77	Ac	149	CYS
78	Ad	41	ARG
78	Ad	56	LEU
78	Ad	62	GLN
78	Ad	71	ARG
78	Ad	161	GLN
78	Ad	166	THR
78	Ad	173	LEU
78	Ad	191	ILE
78	Ad	192	THR
78	Ad	196	LEU
79	Ae	70	LEU
79	Ae	84	ASP
79	Ae	102	GLU
79	Ae	107	VAL
79	Ae	112	ILE
79	Ae	122	ARG
79	Ae	136	ARG
79	Ae	150	HIS
79	Ae	159	TYR
79	Ae	171	ASN
79	Ae	180	ASP
79	Ae	186	LEU
79	Ae	206	GLU
79	Ae	208	MET
79	Ae	213	PHE
79	Ae	220	LEU
79	Ae	223	LEU
79	Ae	230	LEU
79	Ae	249	LEU
79	Ae	250	LEU
79	Ae	253	LEU
79	Ae	255	GLN
79	Ae	257	ASN
79	Ae	280	LEU
79	Ae	315	LEU

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Mol	Chain	Res	Type
79	Ae	322	VAL
79	Ae	325	ARG
79	Ae	388	VAL
79	Ae	421	GLN
80	Af	84	MET
80	Af	85	LEU
80	Af	101	VAL
80	Af	108	ILE
80	Af	145	LEU
80	Af	148	LEU
80	Af	151	THR
80	Af	153	ARG
80	Af	155	LEU
80	Af	162	THR
81	Ag	50	THR
81	Ag	98	LEU
81	Ag	107	LEU
81	Ag	135	LEU
81	Ag	138	CYS
81	Ag	142	HIS
81	Ag	150	LEU
81	Ag	172	TYR
81	Ag	178	ASP
81	Ag	181	LEU
81	Ag	194	ASN
81	Ag	243	LEU
81	Ag	246	LEU
81	Ag	264	VAL
81	Ag	265	ASN
81	Ag	296	VAL
81	Ag	305	ILE
81	Ag	334	ASP
81	Ag	336	LEU
81	Ag	337	ASP
81	Ag	372	THR
81	Ag	397	LEU
82	Ah	302	LEU
82	Ah	308	ASN
82	Ah	328	LYS
82	Ah	343	MET
82	Ah	359	LYS
82	Ah	369	ARG

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Mol	Chain	Res	Type
82	Ah	384	ILE
83	Ai	11	MET
83	Ai	26	THR
83	Ai	31	MET
83	Ai	36	LEU
83	Ai	50	ASP
83	Ai	62	MET
83	Ai	72	ARG
84	Aj	21	LEU
84	Aj	40	THR
84	Aj	52	MET
84	Aj	65	LEU
84	Aj	68	LEU
84	Aj	99	ARG
84	Aj	103	ASP
84	Aj	135	MET
84	Aj	170	LEU
84	Aj	179	GLN
85	Ak	79	LYS
85	Ak	85	LEU
85	Ak	87	VAL
85	Ak	93	VAL
85	Ak	102	GLU
85	Ak	108	LEU
85	Ak	117	THR
85	Ak	125	CYS
85	Ak	134	GLU
85	Ak	152	GLU
85	Ak	157	ASP
85	Ak	159	VAL
85	Ak	165	ILE
85	Ak	175	LEU
85	Ak	196	VAL
85	Ak	204	THR
85	Ak	205	ASP
85	Ak	213	ARG
85	Ak	249	ASP
85	Ak	264	ILE
85	Ak	269	LEU
85	Ak	288	THR
85	Ak	298	VAL
85	Ak	309	ASN

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Mol	Chain	Res	Type
86	Am	6	LEU
86	Am	13	LEU
86	Am	17	ARG
86	Am	25	LYS
86	Am	29	LEU
86	Am	33	VAL
86	Am	48	GLU
86	Am	49	MET
86	Am	53	MET
86	Am	63	ASP
86	Am	72	ASP
86	Am	113	ASN
87	An	130	ILE
87	An	144	ARG
87	An	145	LYS
87	An	158	ARG
87	An	163	ARG
87	An	164	GLN
87	An	199	GLN
88	Ao	71	LEU
88	Ao	137	ILE
88	Ao	243	THR
88	Ao	256	GLU
88	Ao	262	TYR
88	Ao	285	LEU
88	Ao	296	THR
88	Ao	387	SER
88	Ao	414	ASP
88	Ao	416	ASP
88	Ao	423	MET
88	Ao	441	LEU
88	Ao	442	LEU
88	Ao	446	ASP
88	Ao	447	ASN
88	Ao	488	VAL
88	Ao	538	MET
88	Ao	582	VAL
88	Ao	608	ILE
88	Ao	614	LEU
88	Ao	645	CYS
88	Ao	652	VAL
88	Ao	661	GLU

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Mol	Chain	Res	Type
89	Ap	53	ASP
89	Ap	89	ARG
89	Ap	91	ARG
89	Ap	93	MET
89	Ap	95	ILE
89	Ap	103	ASN
89	Ap	107	ILE
89	Ap	108	CYS
89	Ap	113	LEU
89	Ap	130	HIS
89	Ap	155	GLN
89	Ap	167	ILE
89	Ap	170	VAL
89	Ap	175	LEU
89	Ap	177	PHE
89	Ap	184	VAL
89	Ap	193	LEU
89	Ap	219	LEU
89	Ap	224	LEU
89	Ap	235	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (312) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	41	ASN
2	B0	59	HIS
2	B0	76	HIS
3	B1	27	HIS
3	B1	42	HIS
3	B1	172	GLN
4	B2	75	ASN
4	B2	90	GLN
4	B2	97	ASN
5	B3	67	HIS
6	B4	37	ASN
6	B4	47	GLN
7	B5	170	GLN
8	B6	59	GLN
9	B7	65	HIS
10	B8	118	HIS
10	B8	170	ASN
14	BC	188	HIS

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Mol	Chain	Res	Type
14	BC	215	GLN
14	BC	268	GLN
14	BC	319	GLN
14	BC	330	ASN
15	BD	183	HIS
16	BE	57	ASN
16	BE	72	GLN
16	BE	128	HIS
16	BE	154	HIS
16	BE	156	HIS
16	BE	197	HIS
16	BE	202	GLN
16	BE	281	ASN
16	BE	292	HIS
17	BF	74	GLN
17	BF	83	HIS
17	BF	103	GLN
17	BF	105	ASN
17	BF	172	GLN
17	BF	201	GLN
17	BF	249	ASN
18	BI	88	HIS
18	BI	121	ASN
18	BI	136	ASN
19	BJ	41	HIS
19	BJ	45	GLN
19	BJ	73	GLN
19	BJ	93	ASN
19	BJ	115	GLN
19	BJ	119	HIS
19	BJ	217	GLN
20	BK	54	ASN
20	BK	84	GLN
20	BK	103	HIS
1	BL	152	HIS
21	BN	40	GLN
21	BN	48	HIS
21	BN	49	GLN
21	BN	74	GLN
21	BN	80	HIS
21	BN	94	GLN
21	BN	140	ASN

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Mol	Chain	Res	Type
22	BO	80	GLN
22	BO	89	HIS
23	BP	84	ASN
23	BP	87	HIS
23	BP	94	GLN
23	BP	170	ASN
24	BQ	98	HIS
24	BQ	110	ASN
24	BQ	138	GLN
24	BQ	209	ASN
25	BR	27	HIS
25	BR	30	GLN
25	BR	98	GLN
25	BR	112	ASN
25	BR	147	ASN
25	BR	151	GLN
26	BS	52	ASN
26	BS	79	HIS
26	BS	115	HIS
26	BS	147	HIS
27	BT	153	ASN
27	BT	258	GLN
28	BU	77	GLN
28	BU	79	HIS
28	BU	94	GLN
29	BV	79	HIS
29	BV	104	HIS
29	BV	108	HIS
29	BV	109	GLN
29	BV	122	ASN
29	BV	144	ASN
30	BW	131	ASN
30	BW	157	HIS
30	BW	171	HIS
30	BW	199	GLN
30	BW	203	ASN
30	BW	208	HIS
31	BX	4	ASN
31	BX	27	GLN
32	BY	35	ASN
32	BY	78	GLN
32	BY	84	ASN

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Mol	Chain	Res	Type
32	BY	210	HIS
33	Ba	65	HIS
33	Ba	108	HIS
33	Ba	119	GLN
33	Ba	156	ASN
33	Ba	195	HIS
33	Ba	207	ASN
33	Ba	223	HIS
33	Ba	251	HIS
33	Ba	266	GLN
33	Ba	274	ASN
33	Ba	289	HIS
33	Ba	358	GLN
33	Ba	360	ASN
33	Ba	385	HIS
33	Ba	420	HIS
34	Bb	224	HIS
34	Bb	239	ASN
34	Bb	275	GLN
34	Bb	295	GLN
34	Bb	308	GLN
34	Bb	354	GLN
34	Bb	361	GLN
35	Bc	252	HIS
35	Bc	274	GLN
35	Bc	294	GLN
35	Bc	301	HIS
36	Bd	143	GLN
38	Bf	44	ASN
38	Bf	62	HIS
38	Bf	121	HIS
39	Bg	17	ASN
39	Bg	120	HIS
39	Bg	127	GLN
39	Bg	131	HIS
39	Bg	135	ASN
40	Bh	94	ASN
40	Bh	118	ASN
40	Bh	177	GLN
40	Bh	236	ASN
41	Bi	47	GLN
41	Bi	115	ASN

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Mol	Chain	Res	Type
41	Bi	196	GLN
41	Bi	207	ASN
42	Bj	76	GLN
42	Bj	87	HIS
43	Bk	111	HIS
44	Bl	46	HIS
44	Bl	92	HIS
44	Bl	141	ASN
45	Bm	115	ASN
46	Bn	33	HIS
46	Bn	69	HIS
46	Bn	120	HIS
46	Bn	122	ASN
47	Bo	31	GLN
47	Bo	63	GLN
48	Bp	15	GLN
48	Bp	84	GLN
48	Bp	93	HIS
49	Bq	129	HIS
50	Bt	30	GLN
50	Bt	34	ASN
50	Bt	45	ASN
50	Bt	85	HIS
51	Bu	145	ASN
52	Bv	107	GLN
53	Bw	67	GLN
53	Bw	71	HIS
53	Bw	96	GLN
53	Bw	104	ASN
53	Bw	107	GLN
53	Bw	201	HIS
53	Bw	234	GLN
53	Bw	271	GLN
53	Bw	290	HIS
53	Bw	385	ASN
54	Bx	112	HIS
54	Bx	164	ASN
54	Bx	184	ASN
54	Bx	196	HIS
57	AB	68	HIS
57	AB	152	HIS
58	AC	60	HIS

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Mol	Chain	Res	Type
58	AC	75	ASN
58	AC	115	ASN
58	AC	145	HIS
58	AC	154	HIS
59	AE	196	ASN
59	AE	292	HIS
59	AE	317	HIS
59	AE	356	GLN
59	AE	360	GLN
59	AE	361	GLN
59	AE	369	HIS
60	AF	41	ASN
61	AG	146	HIS
61	AG	196	HIS
61	AG	233	ASN
61	AG	238	HIS
62	AI	87	HIS
62	AI	101	GLN
62	AI	127	HIS
62	AI	176	HIS
62	AI	177	ASN
62	AI	221	GLN
62	AI	327	HIS
62	AI	367	GLN
63	AJ	109	HIS
63	AJ	133	GLN
64	AK	89	HIS
64	AK	95	ASN
64	AK	100	GLN
65	AL	35	GLN
65	AL	37	HIS
65	AL	77	ASN
65	AL	100	HIS
65	AL	105	HIS
65	AL	106	HIS
66	AN	60	ASN
66	AN	117	HIS
67	AO	84	HIS
67	AO	119	ASN
67	AO	153	HIS
67	AO	170	ASN
68	AP	28	ASN

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Mol	Chain	Res	Type
68	AP	75	HIS
69	AQ	23	GLN
69	AQ	56	GLN
69	AQ	57	GLN
69	AQ	76	HIS
70	AR	77	ASN
70	AR	79	GLN
70	AR	116	GLN
71	AU	3	ASN
75	Aa	132	GLN
75	Aa	243	GLN
75	Aa	245	GLN
75	Aa	246	HIS
75	Aa	299	ASN
75	Aa	327	HIS
75	Aa	337	GLN
75	Aa	348	HIS
77	Ac	37	HIS
77	Ac	51	ASN
77	Ac	56	GLN
77	Ac	59	ASN
77	Ac	63	GLN
77	Ac	69	ASN
77	Ac	95	ASN
77	Ac	125	HIS
77	Ac	146	GLN
78	Ad	62	GLN
78	Ad	117	HIS
78	Ad	161	GLN
79	Ae	140	ASN
79	Ae	185	ASN
79	Ae	196	ASN
79	Ae	257	ASN
79	Ae	301	GLN
79	Ae	314	GLN
79	Ae	404	GLN
79	Ae	421	GLN
79	Ae	422	GLN
79	Ae	424	HIS
80	Af	87	HIS
80	Af	98	ASN
81	Ag	58	HIS

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Mol	Chain	Res	Type
81	Ag	89	GLN
81	Ag	118	HIS
81	Ag	139	HIS
81	Ag	142	HIS
81	Ag	147	GLN
81	Ag	153	HIS
81	Ag	227	GLN
81	Ag	301	GLN
81	Ag	325	GLN
81	Ag	386	ASN
82	Ah	288	ASN
82	Ah	309	ASN
82	Ah	323	HIS
82	Ah	364	HIS
83	Ai	55	HIS
83	Ai	75	HIS
84	Aj	32	GLN
84	Aj	111	HIS
85	Ak	263	ASN
85	Ak	303	ASN
86	Am	15	ASN
86	Am	24	ASN
86	Am	32	HIS
86	Am	109	HIS
86	Am	113	ASN
87	An	140	HIS
87	An	164	GLN
87	An	166	GLN
88	Ao	129	GLN
88	Ao	258	ASN
88	Ao	318	ASN
88	Ao	329	GLN
88	Ao	385	HIS
88	Ao	455	HIS
88	Ao	543	HIS
89	Ap	81	HIS
89	Ap	103	ASN
89	Ap	136	HIS
89	Ap	147	HIS
89	Ap	155	GLN
89	Ap	181	HIS
89	Ap	221	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	BA	1547/1571 (98%)	471 (30%)	7 (0%)
13	BB	64/73 (87%)	24 (37%)	0
56	AA	959/962 (99%)	237 (24%)	3 (0%)
72	AV	70/71 (98%)	25 (35%)	0
73	AX	16/201 (7%)	10 (62%)	1 (6%)
All	All	2656/2878 (92%)	767 (28%)	11 (0%)

All (767) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	BA	4	A
12	BA	7	G
12	BA	11	G
12	BA	15	A
12	BA	19	U
12	BA	20	A
12	BA	21	C
12	BA	23	A
12	BA	26	C
12	BA	31	A
12	BA	32	C
12	BA	36	A
12	BA	37	A
12	BA	39	A
12	BA	40	C
12	BA	41	A
12	BA	42	C
12	BA	45	A
12	BA	46	A
12	BA	47	A
12	BA	48	U
12	BA	49	A
12	BA	56	A
12	BA	57	A
12	BA	59	A
12	BA	60	U
12	BA	63	A
12	BA	66	U
12	BA	67	A
12	BA	68	A
12	BA	80	A

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Mol	Chain	Res	Type
12	BA	82	G
12	BA	83	A
12	BA	84	G
12	BA	96	U
12	BA	97	A
12	BA	99	C
12	BA	101	U
12	BA	102	G
12	BA	104	C
12	BA	105	G
12	BA	109	U
12	BA	112	A
12	BA	115	U
12	BA	118	U
12	BA	119	A
12	BA	129	A
12	BA	131	A
12	BA	132	G
12	BA	135	G
12	BA	139	G
12	BA	140	A
12	BA	141	A
12	BA	142	U
12	BA	143	A
12	BA	146	A
12	BA	147	U
12	BA	148	A
12	BA	149	A
12	BA	153	U
12	BA	163	C
12	BA	164	A
12	BA	165	A
12	BA	168	A
12	BA	172	C
12	BA	180	A
12	BA	182	C
12	BA	188	C
12	BA	190	U
12	BA	192	A
12	BA	205	A
12	BA	210	A
12	BA	218	A

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Mol	Chain	Res	Type
12	BA	219	A
12	BA	221	A
12	BA	223	A
12	BA	224	A
12	BA	225	C
12	BA	228	U
12	BA	229	A
12	BA	231	C
12	BA	237	A
12	BA	238	C
12	BA	239	C
12	BA	243	A
12	BA	254	G
12	BA	260	C
12	BA	261	A
12	BA	263	G
12	BA	265	G
12	BA	271	U
12	BA	272	A
12	BA	273	A
12	BA	274	A
12	BA	275	A
12	BA	277	A
12	BA	295	G
12	BA	305	G
12	BA	306	A
12	BA	309	A
12	BA	310	G
12	BA	311	A
12	BA	312	C
12	BA	313	U
12	BA	322	G
12	BA	324	G
12	BA	329	A
12	BA	330	A
12	BA	331	A
12	BA	336	A
12	BA	337	A
12	BA	338	C
12	BA	339	G
12	BA	340	A
12	BA	352	G

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Mol	Chain	Res	Type
12	BA	359	G
12	BA	364	A
12	BA	366	A
12	BA	367	A
12	BA	368	A
12	BA	369	G
12	BA	373	U
12	BA	374	U
12	BA	381	A
12	BA	389	A
12	BA	390	A
12	BA	392	U
12	BA	393	A
12	BA	394	C
12	BA	398	A
12	BA	409	A
12	BA	414	A
12	BA	417	G
12	BA	418	U
12	BA	420	U
12	BA	428	A
12	BA	440	A
12	BA	446	C
12	BA	447	A
12	BA	448	G
12	BA	449	C
12	BA	459	A
12	BA	460	C
12	BA	467	A
12	BA	468	A
12	BA	472	U
12	BA	473	G
12	BA	474	A
12	BA	478	G
12	BA	479	A
12	BA	480	G
12	BA	488	U
12	BA	489	C
12	BA	490	U
12	BA	491	U
12	BA	492	A
12	BA	493	A

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Mol	Chain	Res	Type
12	BA	494	U
12	BA	497	U
12	BA	498	A
12	BA	500	C
12	BA	501	A
12	BA	503	A
12	BA	504	G
12	BA	505	U
12	BA	506	A
12	BA	515	A
12	BA	516	G
12	BA	518	A
12	BA	526	A
12	BA	532	A
12	BA	533	A
12	BA	545	U
12	BA	547	A
12	BA	548	A
12	BA	550	A
12	BA	552	A
12	BA	553	U
12	BA	554	U
12	BA	557	C
12	BA	560	A
12	BA	561	C
12	BA	562	A
12	BA	563	U
12	BA	566	U
12	BA	570	A
12	BA	574	A
12	BA	575	C
12	BA	576	U
12	BA	578	A
12	BA	579	U
12	BA	580	A
12	BA	583	A
12	BA	584	A
12	BA	586	C
12	BA	592	G
12	BA	593	C
12	BA	595	C
12	BA	596	A

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Mol	Chain	Res	Type
12	BA	617	A
12	BA	618	A
12	BA	619	C
12	BA	625	A
12	BA	628	A
12	BA	631	A
12	BA	634	G
12	BA	640	A
12	BA	648	C
12	BA	649	A
12	BA	650	A
12	BA	657	U
12	BA	661	U
12	BA	665	C
12	BA	673	C
12	BA	684	A
12	BA	689	A
12	BA	691	A
12	BA	694	A
12	BA	695	U
12	BA	696	A
12	BA	697	C
12	BA	704	U
12	BA	705	U
12	BA	707	A
12	BA	713	A
12	BA	718	A
12	BA	719	C
12	BA	720	C
12	BA	722	A
12	BA	723	A
12	BA	724	A
12	BA	725	C
12	BA	727	A
12	BA	728	C
12	BA	736	C
12	BA	737	G
12	BA	744	A
12	BA	745	A
12	BA	746	U
12	BA	747	U
12	BA	748	A

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Mol	Chain	Res	Type
12	BA	753	G
12	BA	763	C
12	BA	764	A
12	BA	766	A
12	BA	774	A
12	BA	775	C
12	BA	777	A
12	BA	778	A
12	BA	780	G
12	BA	782	A
12	BA	783	A
12	BA	784	G
12	BA	789	A
12	BA	795	G
12	BA	809	G
12	BA	818	A
12	BA	819	A
12	BA	824	G
12	BA	825	C
12	BA	828	G
12	BA	834	C
12	BA	835	A
12	BA	847	U
12	BA	848	C
12	BA	850	A
12	BA	852	C
12	BA	854	U
12	BA	855	U
12	BA	859	A
12	BA	860	G
12	BA	864	U
12	BA	868	G
12	BA	871	A
12	BA	872	A
12	BA	883	G
12	BA	887	C
12	BA	888	A
12	BA	889	C
12	BA	890	C
12	BA	892	G
12	BA	895	U
12	BA	897	A

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Mol	Chain	Res	Type
12	BA	899	G
12	BA	901	C
12	BA	902	C
12	BA	908	A
12	BA	909	U
12	BA	910	U
12	BA	922	A
12	BA	923	A
12	BA	924	G
12	BA	925	G
12	BA	931	U
12	BA	932	A
12	BA	933	A
12	BA	935	C
12	BA	938	U
12	BA	939	U
12	BA	948	A
12	BA	950	U
12	BA	958	U
12	BA	959	G
12	BA	960	U
12	BA	961	A
12	BA	964	A
12	BA	965	A
12	BA	967	G
12	BA	970	C
12	BA	977	G
12	BA	979	G
12	BA	981	U
12	BA	982	U
12	BA	983	U
12	BA	986	U
12	BA	988	U
12	BA	992	U
12	BA	1008	A
12	BA	1015	C
12	BA	1016	C
12	BA	1018	U
12	BA	1026	A
12	BA	1027	G
12	BA	1028	A
12	BA	1034	G

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Mol	Chain	Res	Type
12	BA	1038	A
12	BA	1041	A
12	BA	1046	A
12	BA	1050	C
12	BA	1051	G
12	BA	1055	A
12	BA	1056	G
12	BA	1057	A
12	BA	1063	U
12	BA	1064	G
12	BA	1071	U
12	BA	1072	A
12	BA	1075	U
12	BA	1089	G
12	BA	1092	A
12	BA	1093	A
12	BA	1094	A
12	BA	1123	A
12	BA	1127	A
12	BA	1129	C
12	BA	1137	A
12	BA	1140	A
12	BA	1145	C
12	BA	1146	G
12	BA	1167	C
12	BA	1168	A
12	BA	1169	A
12	BA	1178	C
12	BA	1183	U
12	BA	1188	U
12	BA	1190	A
12	BA	1195	A
12	BA	1205	G
12	BA	1206	U
12	BA	1207	C
12	BA	1215	C
12	BA	1216	C
12	BA	1217	A
12	BA	1218	U
12	BA	1219	A
12	BA	1220	A
12	BA	1221	C

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Mol	Chain	Res	Type
12	BA	1222	A
12	BA	1226	C
12	BA	1231	U
12	BA	1232	G
12	BA	1234	U
12	BA	1238	A
12	BA	1239	A
12	BA	1240	A
12	BA	1241	U
12	BA	1242	U
12	BA	1246	A
12	BA	1247	U
12	BA	1249	A
12	BA	1253	G
12	BA	1254	A
12	BA	1255	A
12	BA	1258	A
12	BA	1264	C
12	BA	1268	G
12	BA	1270	G
12	BA	1271	A
12	BA	1287	G
12	BA	1288	U
12	BA	1291	U
12	BA	1294	A
12	BA	1297	U
12	BA	1299	C
12	BA	1303	C
12	BA	1311	G
12	BA	1314	U
12	BA	1317	A
12	BA	1323	U
12	BA	1325	G
12	BA	1326	A
12	BA	1328	G
12	BA	1331	G
12	BA	1341	A
12	BA	1342	C
12	BA	1348	U
12	BA	1352	G
12	BA	1353	C
12	BA	1357	C

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Mol	Chain	Res	Type
12	BA	1358	G
12	BA	1377	U
12	BA	1385	U
12	BA	1387	A
12	BA	1388	A
12	BA	1389	A
12	BA	1390	G
12	BA	1396	C
12	BA	1399	G
12	BA	1405	A
12	BA	1406	G
12	BA	1409	C
12	BA	1420	A
12	BA	1425	A
12	BA	1426	G
12	BA	1428	U
12	BA	1429	C
12	BA	1432	U
12	BA	1433	U
12	BA	1436	U
12	BA	1438	U
12	BA	1444	A
12	BA	1445	U
12	BA	1448	A
12	BA	1458	G
12	BA	1459	U
12	BA	1465	A
12	BA	1466	G
12	BA	1468	A
12	BA	1474	G
12	BA	1476	A
12	BA	1492	C
12	BA	1493	A
12	BA	1494	A
12	BA	1498	C
12	BA	1504	A
12	BA	1505	G
12	BA	1509	U
12	BA	1514	A
12	BA	1518	A
12	BA	1521	U
12	BA	1522	A

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Mol	Chain	Res	Type
12	BA	1525	C
12	BA	1526	U
12	BA	1527	U
12	BA	1528	A
12	BA	1529	A
12	BA	1531	C
12	BA	1532	U
12	BA	1533	A
12	BA	1536	U
12	BA	1548	A
12	BA	1549	A
12	BA	1550	U
12	BA	1551	C
12	BA	1552	C
12	BA	1553	A
12	BA	1558	U
12	BA	1559	A
12	BA	1560	G
12	BA	1570	C
12	BA	1571	A
13	BB	3	U
13	BB	5	A
13	BB	7	G
13	BB	8	U
13	BB	9	A
13	BB	13	U
13	BB	21	C
13	BB	23	A
13	BB	24	A
13	BB	25	G
13	BB	29	G
13	BB	30	G
13	BB	34	U
13	BB	35	G
13	BB	43	C
13	BB	44	U
13	BB	45	A
13	BB	46	G
13	BB	47	A
13	BB	48	U
13	BB	55	C
13	BB	67	A

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Mol	Chain	Res	Type
13	BB	69	C
13	BB	70	A
56	AA	5	A
56	AA	10	U
56	AA	11	G
56	AA	18	G
56	AA	27	U
56	AA	32	U
56	AA	34	U
56	AA	42	A
56	AA	43	U
56	AA	45	A
56	AA	49	A
56	AA	54	A
56	AA	55	G
56	AA	58	U
56	AA	61	G
56	AA	65	C
56	AA	66	C
56	AA	67	C
56	AA	75	A
56	AA	77	G
56	AA	78	C
56	AA	82	C
56	AA	83	C
56	AA	93	A
56	AA	98	A
56	AA	102	G
56	AA	103	G
56	AA	104	A
56	AA	111	A
56	AA	115	A
56	AA	120	A
56	AA	124	A
56	AA	125	U
56	AA	147	G
56	AA	152	A
56	AA	161	C
56	AA	168	A
56	AA	170	A
56	AA	171	C
56	AA	173	G

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Mol	Chain	Res	Type
56	AA	176	G
56	AA	186	U
56	AA	187	U
56	AA	191	C
56	AA	192	C
56	AA	194	U
56	AA	203	G
56	AA	212	A
56	AA	216	A
56	AA	217	U
56	AA	222	A
56	AA	223	U
56	AA	224	U
56	AA	225	A
56	AA	231	G
56	AA	237	U
56	AA	238	C
56	AA	244	C
56	AA	247	G
56	AA	253	G
56	AA	257	U
56	AA	258	C
56	AA	273	A
56	AA	281	G
56	AA	288	G
56	AA	294	A
56	AA	297	A
56	AA	306	G
56	AA	308	A
56	AA	309	A
56	AA	310	A
56	AA	312	A
56	AA	314	A
56	AA	315	U
56	AA	317	A
56	AA	320	A
56	AA	328	A
56	AA	335	A
56	AA	336	A
56	AA	340	A
56	AA	345	U
56	AA	353	C

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Mol	Chain	Res	Type
56	AA	354	C
56	AA	361	A
56	AA	362	A
56	AA	367	A
56	AA	368	A
56	AA	381	G
56	AA	392	A
56	AA	395	C
56	AA	396	C
56	AA	399	A
56	AA	407	U
56	AA	417	C
56	AA	421	A
56	AA	426	G
56	AA	432	A
56	AA	433	U
56	AA	434	A
56	AA	450	C
56	AA	455	A
56	AA	457	C
56	AA	458	C
56	AA	465	G
56	AA	471	U
56	AA	472	A
56	AA	477	A
56	AA	479	C
56	AA	480	U
56	AA	483	U
56	AA	488	A
56	AA	489	G
56	AA	491	G
56	AA	495	U
56	AA	498	U
56	AA	502	A
56	AA	503	A
56	AA	504	C
56	AA	518	A
56	AA	530	G
56	AA	531	U
56	AA	538	C
56	AA	540	U
56	AA	545	C

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Mol	Chain	Res	Type
56	AA	560	C
56	AA	561	U
56	AA	564	A
56	AA	566	U
56	AA	571	A
56	AA	574	C
56	AA	576	C
56	AA	578	G
56	AA	579	A
56	AA	580	U
56	AA	581	A
56	AA	588	A
56	AA	589	C
56	AA	593	C
56	AA	594	C
56	AA	596	U
56	AA	597	U
56	AA	604	U
56	AA	616	C
56	AA	618	G
56	AA	619	C
56	AA	620	C
56	AA	625	U
56	AA	628	G
56	AA	638	A
56	AA	639	A
56	AA	641	A
56	AA	644	A
56	AA	645	A
56	AA	646	C
56	AA	647	A
56	AA	648	A
56	AA	649	U
56	AA	650	A
56	AA	651	G
56	AA	665	A
56	AA	666	G
56	AA	681	A
56	AA	682	G
56	AA	687	A
56	AA	695	C
56	AA	696	U

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Mol	Chain	Res	Type
56	AA	698	A
56	AA	699	U
56	AA	707	A
56	AA	709	A
56	AA	711	A
56	AA	722	A
56	AA	731	A
56	AA	732	U
56	AA	734	A
56	AA	739	A
56	AA	741	C
56	AA	742	C
56	AA	743	A
56	AA	744	C
56	AA	745	C
56	AA	746	A
56	AA	749	C
56	AA	752	A
56	AA	753	A
56	AA	766	C
56	AA	775	A
56	AA	780	A
56	AA	790	A
56	AA	791	G
56	AA	802	A
56	AA	803	U
56	AA	807	G
56	AA	823	G
56	AA	825	C
56	AA	826	C
56	AA	838	A
56	AA	841	C
56	AA	842	A
56	AA	850	U
56	AA	854	C
56	AA	863	G
56	AA	869	A
56	AA	870	G
56	AA	874	U
56	AA	876	A
56	AA	877	A
56	AA	878	A

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Mol	Chain	Res	Type
56	AA	880	U
56	AA	883	C
56	AA	885	U
56	AA	886	A
56	AA	887	U
56	AA	892	A
56	AA	893	A
56	AA	894	U
56	AA	897	C
56	AA	899	C
56	AA	900	A
56	AA	902	C
56	AA	905	U
56	AA	910	G
56	AA	917	C
56	AA	918	A
56	AA	920	G
56	AA	923	G
56	AA	925	A
56	AA	928	A
56	AA	930	G
56	AA	932	U
56	AA	933	A
56	AA	943	G
56	AA	945	A
56	AA	946	A
56	AA	955	G
56	AA	956	G
56	AA	959	U
72	AV	6	G
72	AV	7	G
72	AV	9	C
72	AV	13	U
72	AV	14	A
72	AV	16	A
72	AV	17	U
72	AV	18	A
72	AV	43	A
72	AV	44	U
72	AV	45	G
72	AV	46	U
72	AV	51	U

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Mol	Chain	Res	Type
72	AV	52	A
72	AV	53	U
72	AV	54	A
72	AV	55	C
72	AV	56	C
72	AV	62	C
72	AV	63	G
72	AV	64	U
72	AV	65	A
72	AV	67	U
72	AV	68	A
72	AV	71	A
73	AX	3	G
73	AX	4	A
73	AX	7	C
73	AX	8	A
73	AX	9	C
73	AX	10	C
73	AX	11	A
73	AX	13	U
73	AX	14	C
73	AX	15	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	BA	48	U
12	BA	101	U
12	BA	1145	C
12	BA	1219	A
12	BA	1220	A
12	BA	1240	A
12	BA	1241	U
56	AA	395	C
56	AA	743	A
56	AA	882	A
73	AX	12	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 341 ligands modelled in this entry, 333 are monoatomic - leaving 8 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
96	FME	AV	101	72	8,9,10	0.97	0	7,9,11	0.80	0
92	5GP	BA	3204	-	26,26,26	0.90	1 (3%)	40,40,40	1.84	9 (22%)
93	SPM	AA	3001	-	13,13,13	0.43	0	12,12,12	0.77	0
92	5GP	BA	3203	-	26,26,26	0.99	1 (3%)	40,40,40	2.20	10 (25%)
93	SPM	BR	201	-	13,13,13	0.39	0	12,12,12	0.80	0
97	GTP	Ag	500	90	30,34,34	0.77	1 (3%)	46,54,54	1.69	12 (26%)
94	GSP	BC	901	90	30,34,34	1.90	2 (6%)	41,54,54	1.78	9 (21%)
93	SPM	BA	3205	-	13,13,13	0.23	0	12,12,12	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	FME	AV	101	72	-	4/7/9/11	-
92	5GP	BA	3204	-	-	5/10/26/26	0/3/3/3
93	SPM	AA	3001	-	-	7/11/11/11	-
92	5GP	BA	3203	-	-	5/10/26/26	0/3/3/3
93	SPM	BR	201	-	-	8/11/11/11	-
97	GTP	Ag	500	90	-	6/22/38/38	0/3/3/3
94	GSP	BC	901	90	-	0/21/38/38	0/3/3/3
93	SPM	BA	3205	-	-	4/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	BC	901	GSP	PG-S1G	-9.31	1.70	1.90
92	BA	3203	5GP	C6-N1	-2.70	1.33	1.38
94	BC	901	GSP	C2-N3	2.40	1.38	1.33
92	BA	3204	5GP	C6-N1	-2.35	1.34	1.38
97	Ag	500	GTP	C2-N3	2.25	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	BA	3203	5GP	C5-C4-N3	-7.88	115.68	128.46
92	BA	3204	5GP	C5-C4-N3	-6.47	117.96	128.46
92	BA	3203	5GP	C2-N3-C4	5.63	122.34	112.30
94	BC	901	GSP	C5-C4-N3	-5.36	119.76	128.46
92	BA	3203	5GP	N9-C4-N3	5.17	136.32	125.94
97	Ag	500	GTP	C2-N3-C4	4.86	120.96	112.30
97	Ag	500	GTP	C5-C4-N3	-4.77	120.72	128.46
94	BC	901	GSP	C2-N3-C4	4.69	120.66	112.30
92	BA	3204	5GP	C2-N3-C4	4.61	120.51	112.30
92	BA	3204	5GP	N9-C4-N3	3.78	133.53	125.94
94	BC	901	GSP	N9-C4-N3	3.41	132.79	125.94
92	BA	3203	5GP	C2-N1-C6	-3.14	119.37	125.10
92	BA	3203	5GP	C5-C6-N1	3.05	120.92	113.19
97	Ag	500	GTP	N9-C4-N3	2.92	131.81	125.94
92	BA	3204	5GP	C2-N1-C6	-2.82	119.95	125.10
92	BA	3203	5GP	C4-C5-N7	-2.77	106.33	110.72
94	BC	901	GSP	C2-N1-C6	-2.76	120.06	125.10
94	BC	901	GSP	PA-O3A-PB	-2.75	123.40	132.83
92	BA	3203	5GP	C8-N7-C5	2.65	109.04	104.24
92	BA	3204	5GP	C5-C6-N1	2.59	119.77	113.19
94	BC	901	GSP	C8-N7-C5	2.57	108.89	104.24
97	Ag	500	GTP	C5-C6-N1	2.55	119.66	113.19
94	BC	901	GSP	C5-C6-N1	2.49	119.51	113.19
97	Ag	500	GTP	C2-N1-C6	-2.44	120.64	125.10
92	BA	3204	5GP	C4-C5-N7	-2.42	106.89	110.72
94	BC	901	GSP	N9-C8-N7	-2.39	108.88	113.39
92	BA	3204	5GP	O6-C6-C5	-2.39	120.26	126.60
97	Ag	500	GTP	O6-C6-C5	-2.38	120.28	126.60
92	BA	3203	5GP	C1'-N9-C8	-2.35	120.00	126.70
94	BC	901	GSP	O6-C6-C5	-2.35	120.37	126.60
97	Ag	500	GTP	PA-O3A-PB	-2.26	125.08	132.83
97	Ag	500	GTP	C8-N7-C5	2.25	108.31	104.24
97	Ag	500	GTP	N1-C2-N3	-2.24	119.14	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	Ag	500	GTP	O2G-PG-O3B	2.24	112.13	104.64
97	Ag	500	GTP	N9-C8-N7	-2.23	109.19	113.39
92	BA	3203	5GP	C1'-N9-C4	2.13	132.83	126.50
92	BA	3203	5GP	N9-C8-N7	-2.09	109.46	113.39
92	BA	3204	5GP	OP3-P-O5'	-2.06	101.24	106.73
97	Ag	500	GTP	N2-C2-N1	2.06	121.10	116.71
92	BA	3204	5GP	C8-N7-C5	2.01	107.88	104.24

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	BA	3203	5GP	C5'-O5'-P-OP3
92	BA	3203	5GP	C5'-O5'-P-OP2
92	BA	3204	5GP	C5'-O5'-P-OP1
92	BA	3204	5GP	C5'-O5'-P-OP2
96	AV	101	FME	C-CA-CB-CG
96	AV	101	FME	CA-CB-CG-SD
97	Ag	500	GTP	C5'-O5'-PA-O3A
97	Ag	500	GTP	C5'-O5'-PA-O1A
92	BA	3204	5GP	O4'-C4'-C5'-O5'
92	BA	3204	5GP	C3'-C4'-C5'-O5'
97	Ag	500	GTP	O4'-C4'-C5'-O5'
93	BR	201	SPM	C2-C3-C4-N5
93	BR	201	SPM	N5-C6-C7-C8
93	AA	3001	SPM	C7-C8-C9-N10
93	BA	3205	SPM	C7-C8-C9-N10
93	AA	3001	SPM	C8-C9-N10-C11
93	AA	3001	SPM	C12-C11-N10-C9
93	BA	3205	SPM	C7-C6-N5-C4
93	BR	201	SPM	C8-C9-N10-C11
93	AA	3001	SPM	C2-C3-C4-N5
96	AV	101	FME	N-CA-CB-CG
96	AV	101	FME	CB-CG-SD-CE
93	BR	201	SPM	N1-C2-C3-C4
93	BA	3205	SPM	C2-C3-C4-N5
93	BA	3205	SPM	C6-C7-C8-C9
92	BA	3203	5GP	C5'-O5'-P-OP1
93	BR	201	SPM	C6-C7-C8-C9
97	Ag	500	GTP	C3'-C4'-C5'-O5'
92	BA	3203	5GP	C4'-C5'-O5'-P
97	Ag	500	GTP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
93	BR	201	SPM	N10-C11-C12-C13
93	AA	3001	SPM	N1-C2-C3-C4
93	AA	3001	SPM	C6-C7-C8-C9
92	BA	3204	5GP	C5'-O5'-P-OP3
93	BR	201	SPM	C12-C11-N10-C9
97	Ag	500	GTP	PA-O3A-PB-O1B
93	AA	3001	SPM	C3-C4-N5-C6
93	BR	201	SPM	C7-C8-C9-N10
92	BA	3203	5GP	O4'-C4'-C5'-O5'

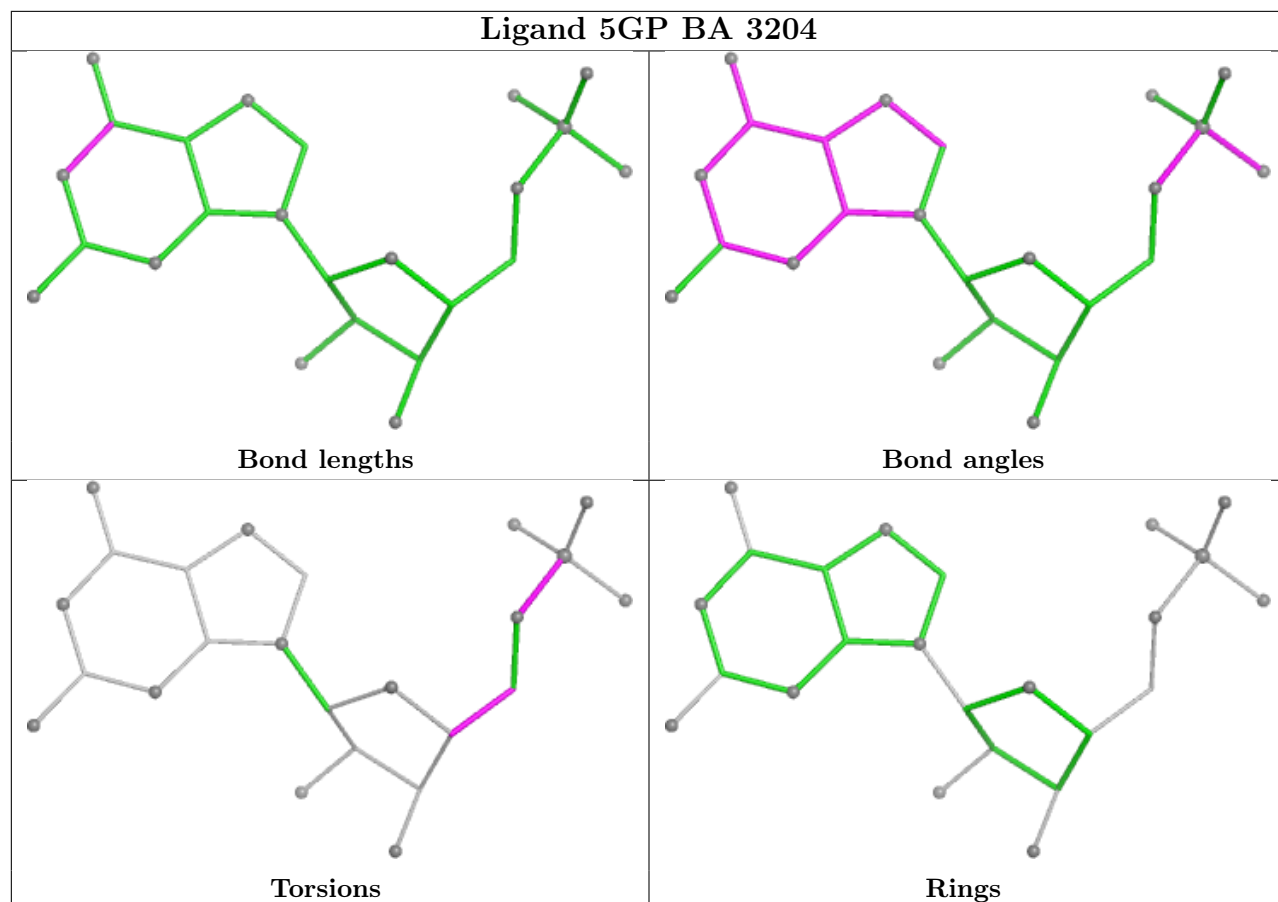
There are no ring outliers.

3 monomers are involved in 4 short contacts:

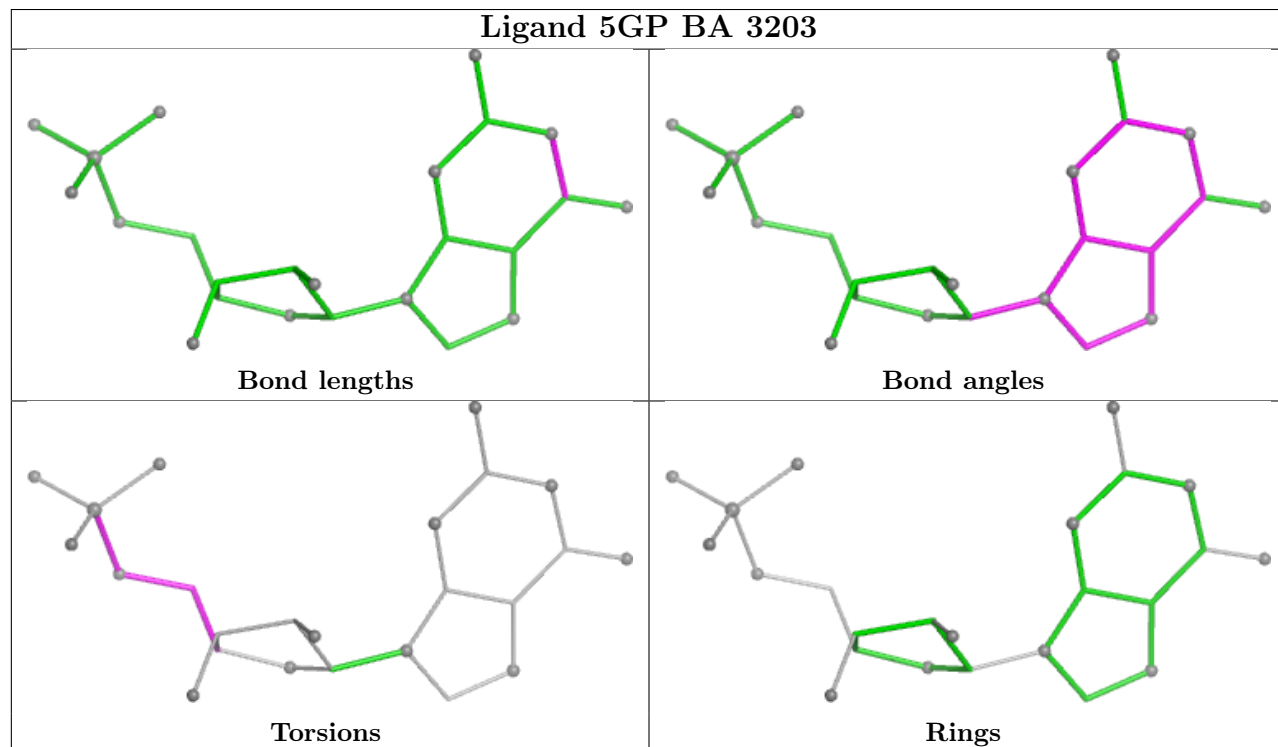
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	Ag	500	GTP	2	0
94	BC	901	GSP	1	0
93	BA	3205	SPM	1	0

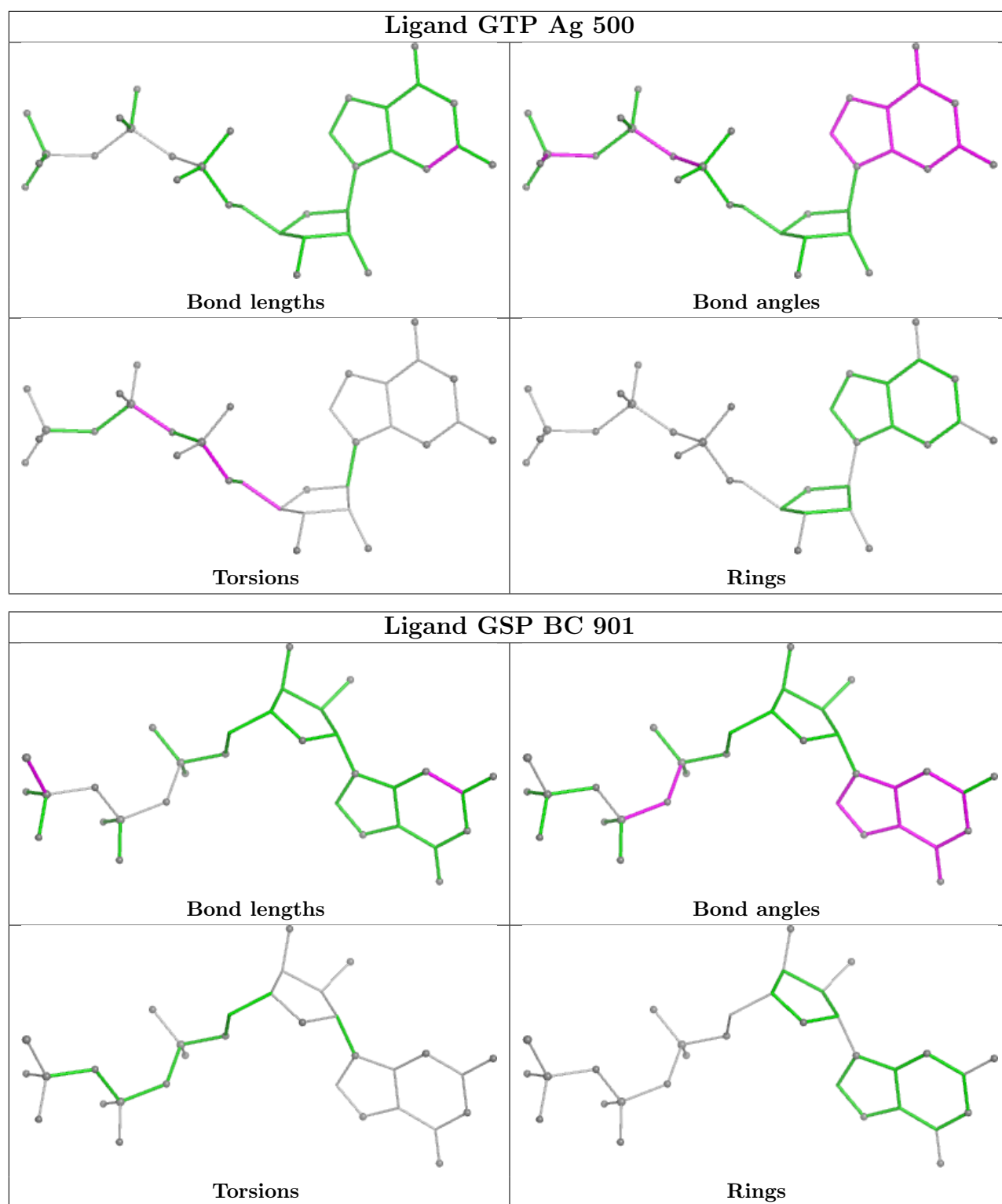
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 5GP BA 3204



Ligand 5GP BA 3203





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Bz	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	710:ALA	C	1001:ALA	N	59.86
1	Bz	415:ALA	C	601:ALA	N	51.54
1	Bz	106:ALA	C	301:ALA	N	30.13
1	Bz	615:ALA	C	700:ALA	N	17.90
1	Bz	315:ALA	C	399:ALA	N	16.24

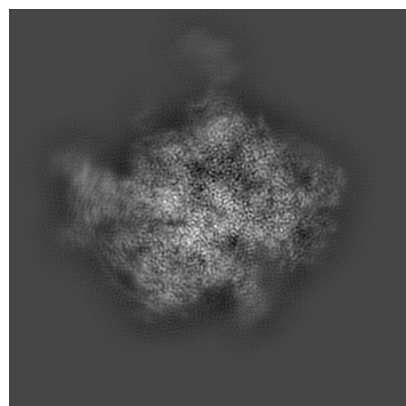
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4368. These allow visual inspection of the internal detail of the map and identification of artifacts.

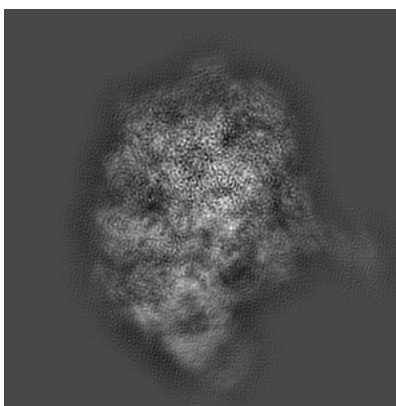
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

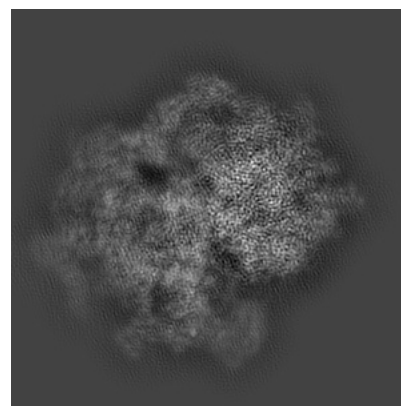
6.1.1 Primary map



X

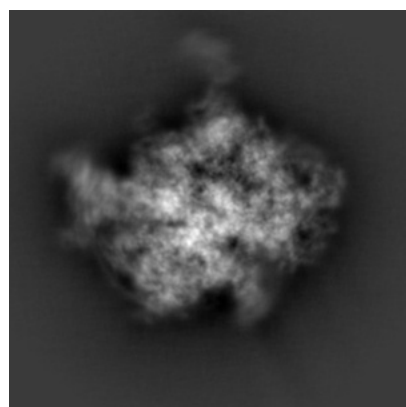


Y

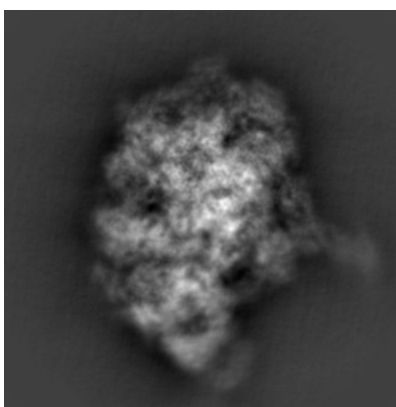


Z

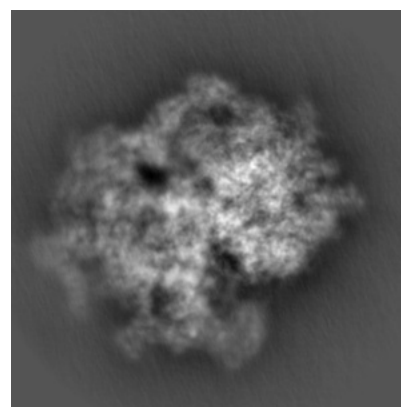
6.1.2 Raw map



X



Y

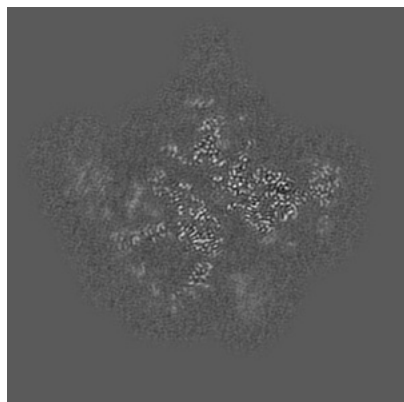


Z

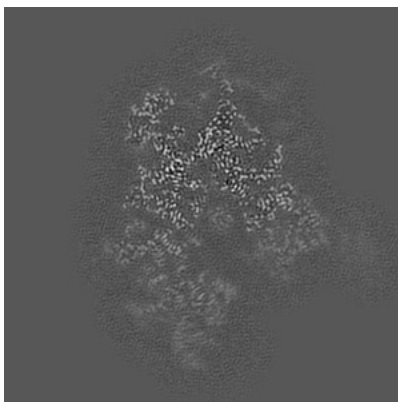
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

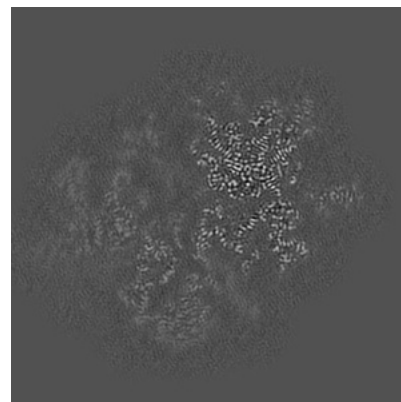
6.2.1 Primary map



X Index: 140

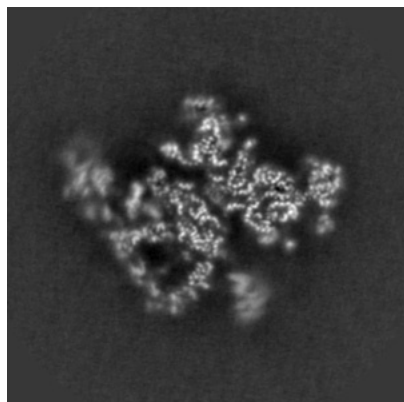


Y Index: 140

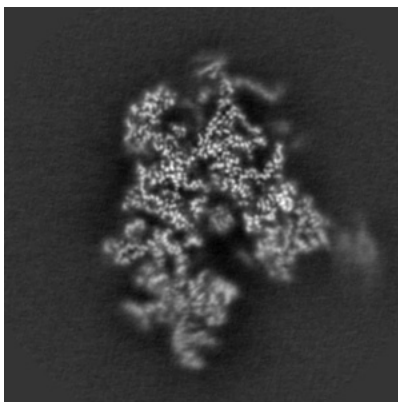


Z Index: 140

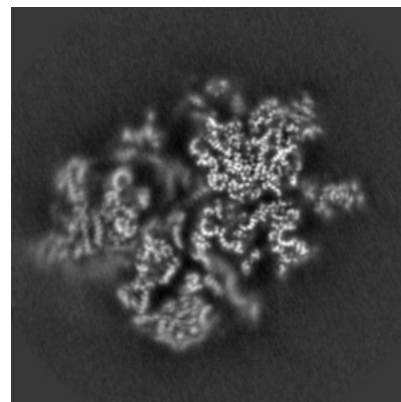
6.2.2 Raw map



X Index: 140



Y Index: 140

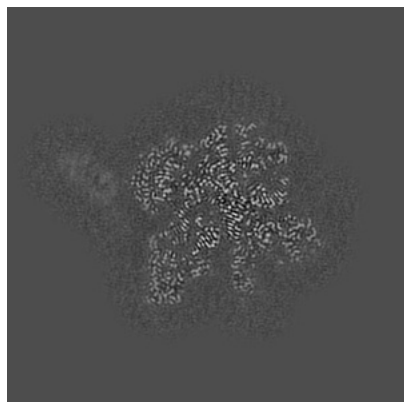


Z Index: 140

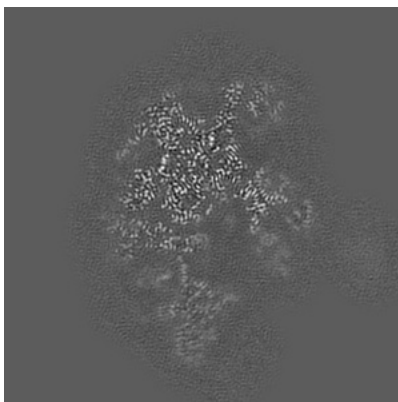
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

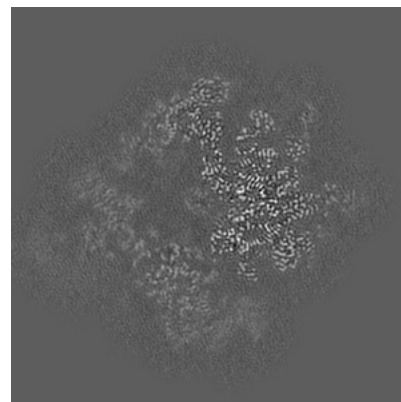
6.3.1 Primary map



X Index: 166

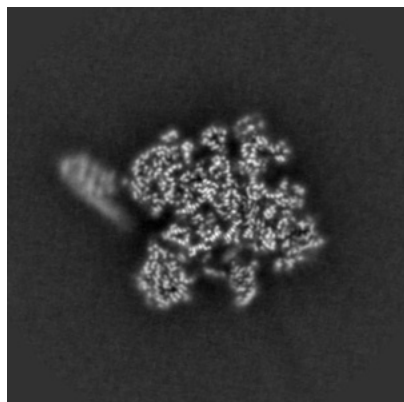


Y Index: 133

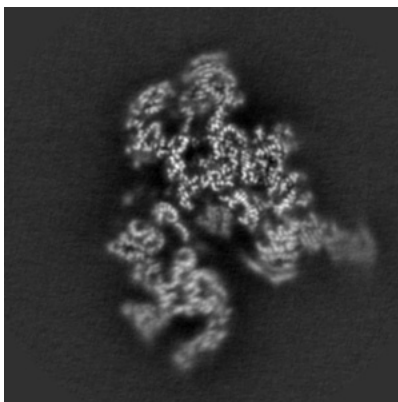


Z Index: 151

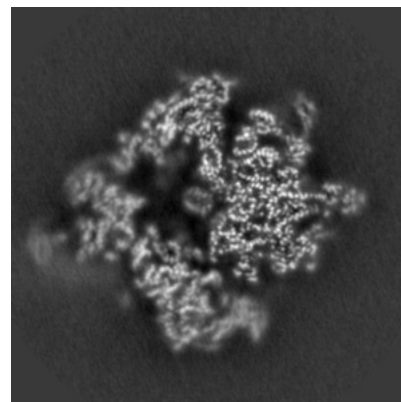
6.3.2 Raw map



X Index: 169



Y Index: 147

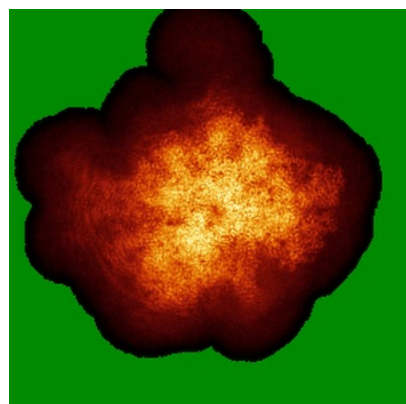


Z Index: 150

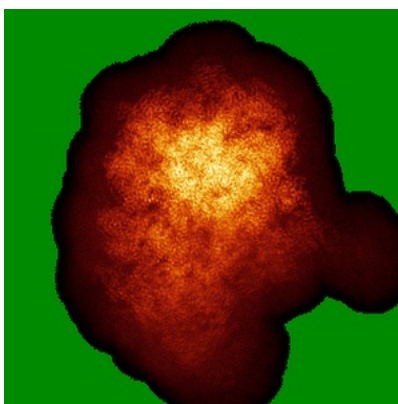
The images above show the largest variance slices of the map in three orthogonal directions.

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

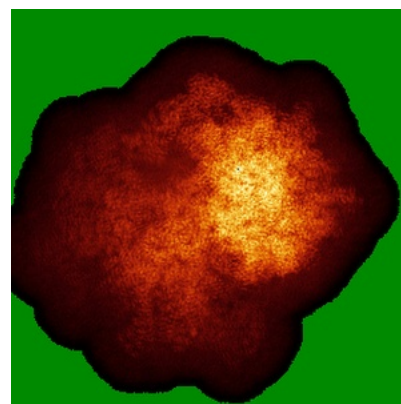
6.4.1 Primary map



X

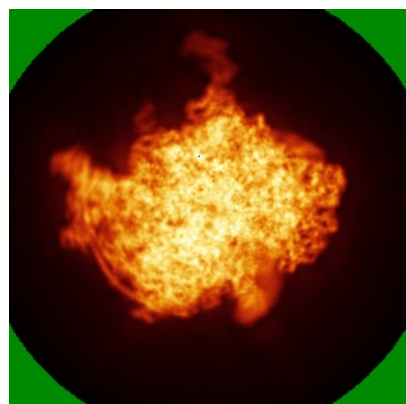


Y

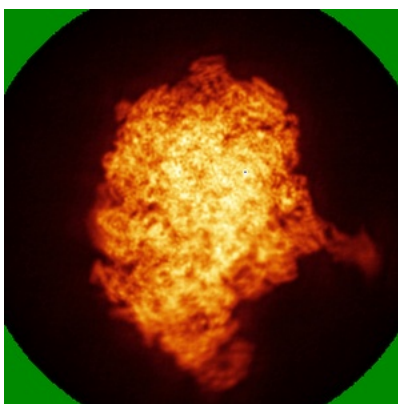


Z

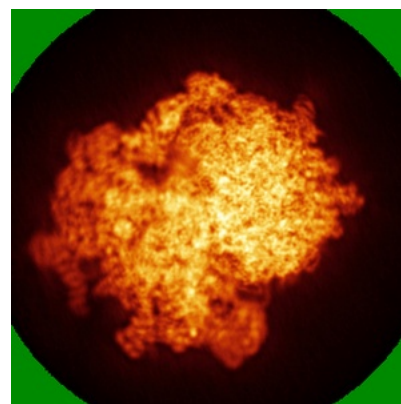
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

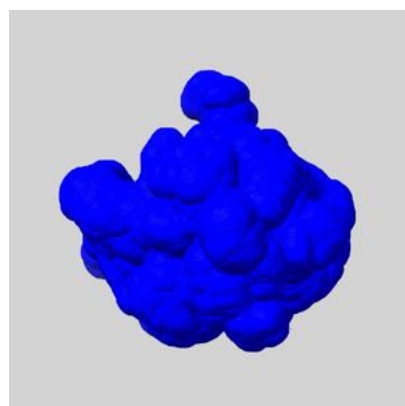
6.6 Mask visualisation [i](#)

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

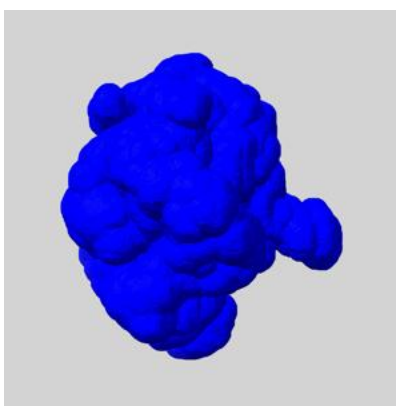
A mask typically either:

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

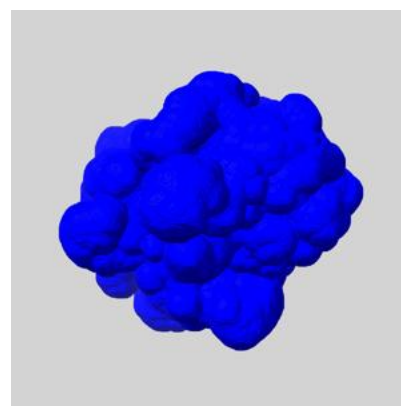
6.6.1 emd_4368_msk_1.map [i](#)



X



Y

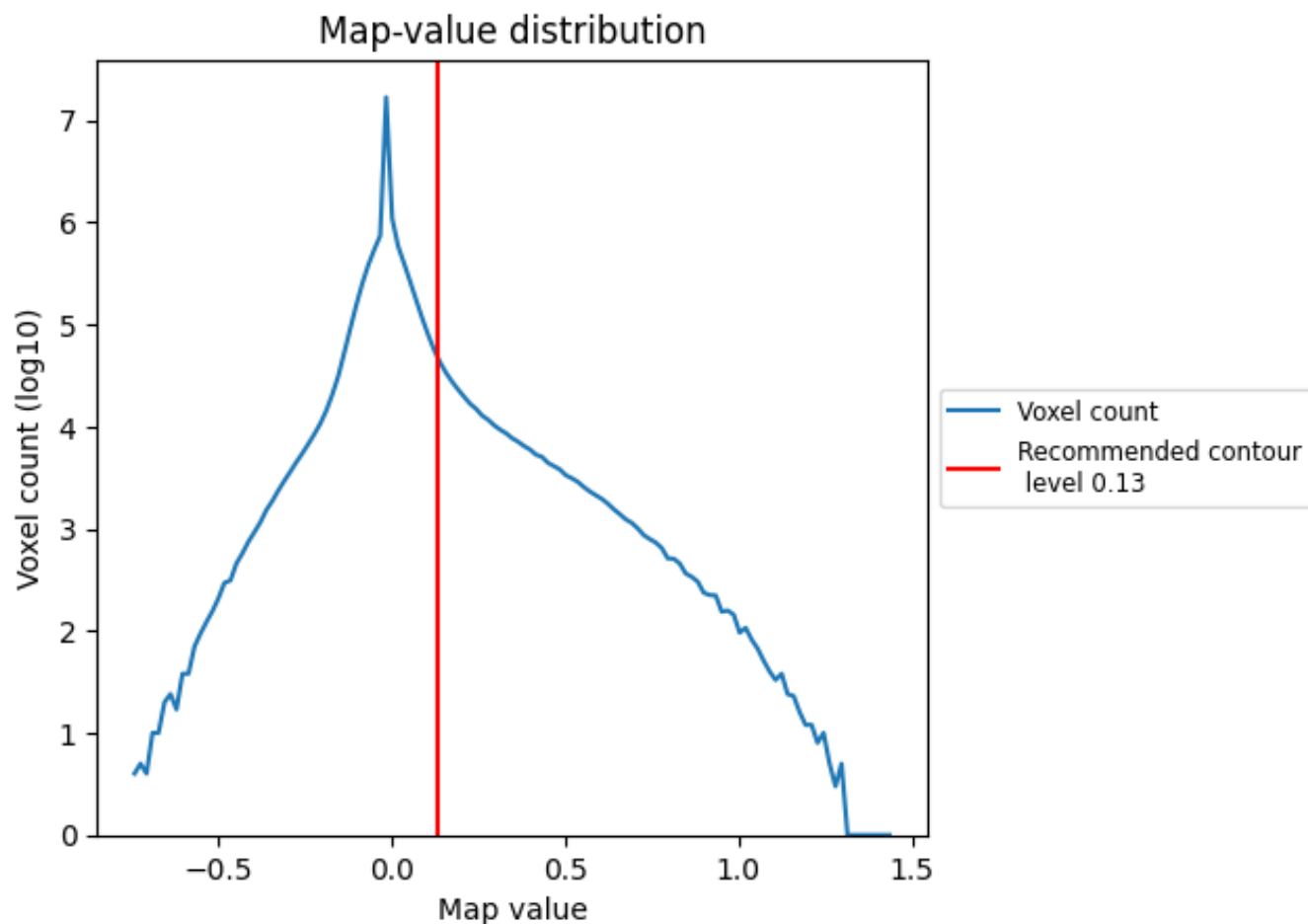


Z

7 Map analysis [i](#)

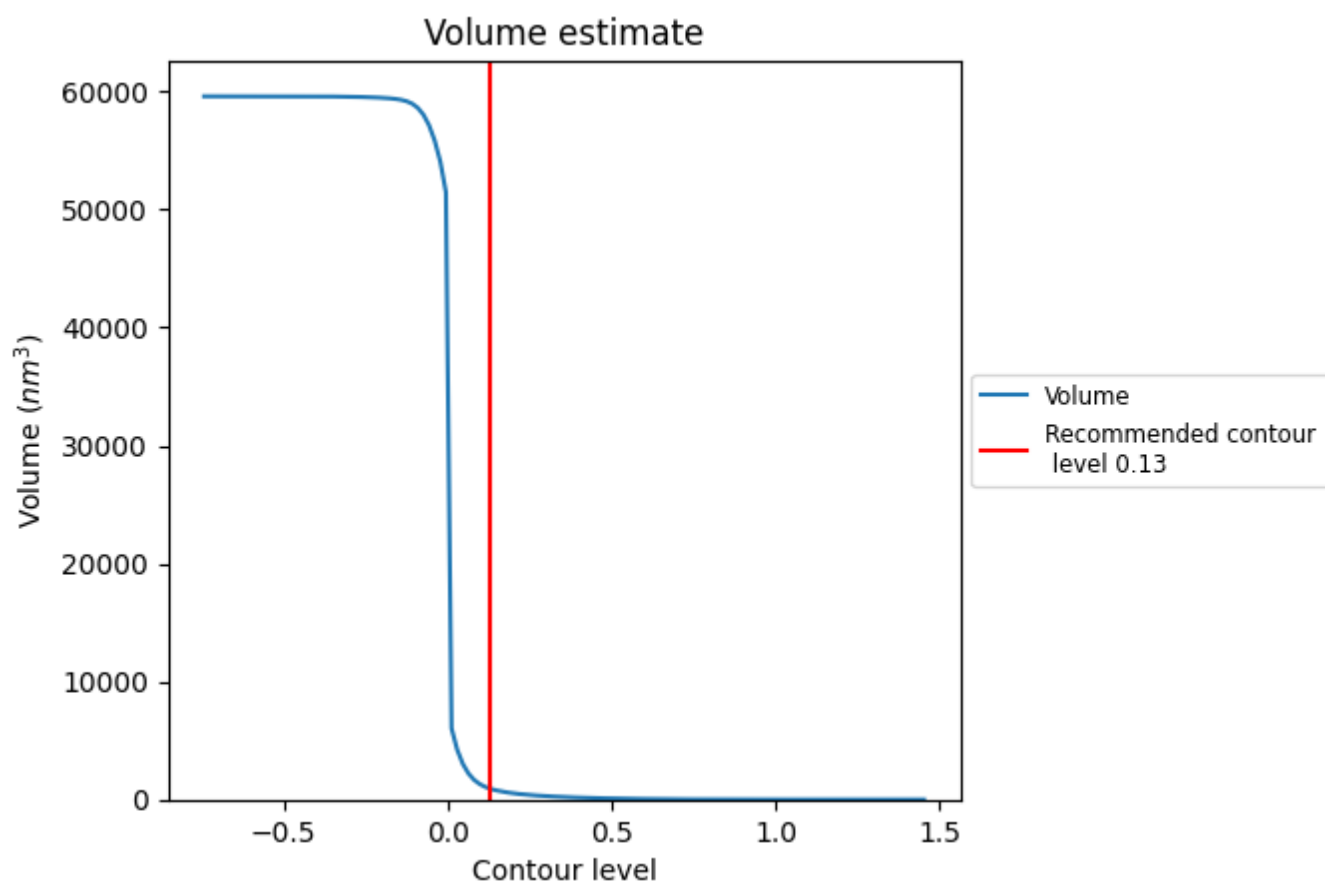
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

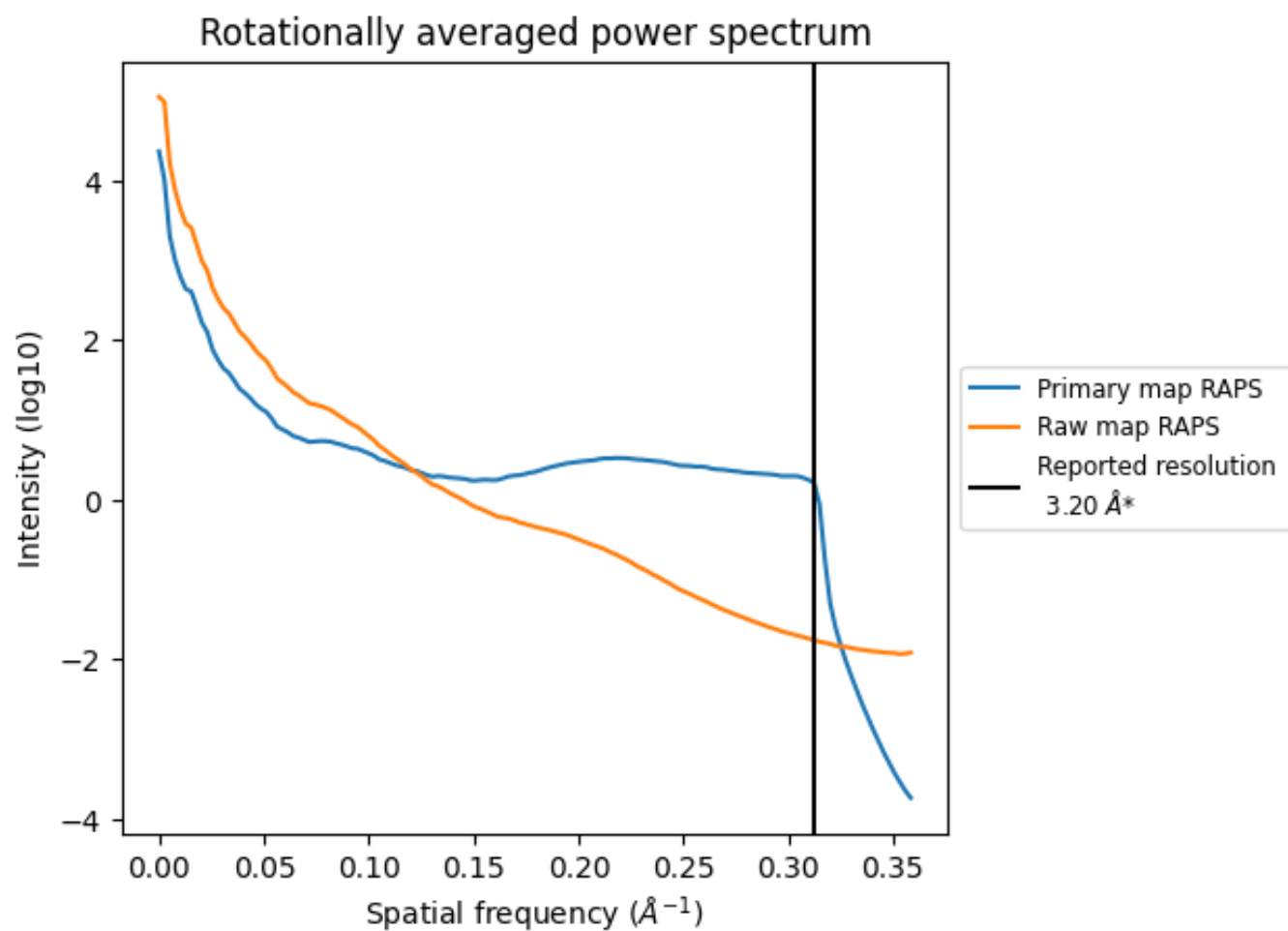
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920 nm^3 ; this corresponds to an approximate mass of 831 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

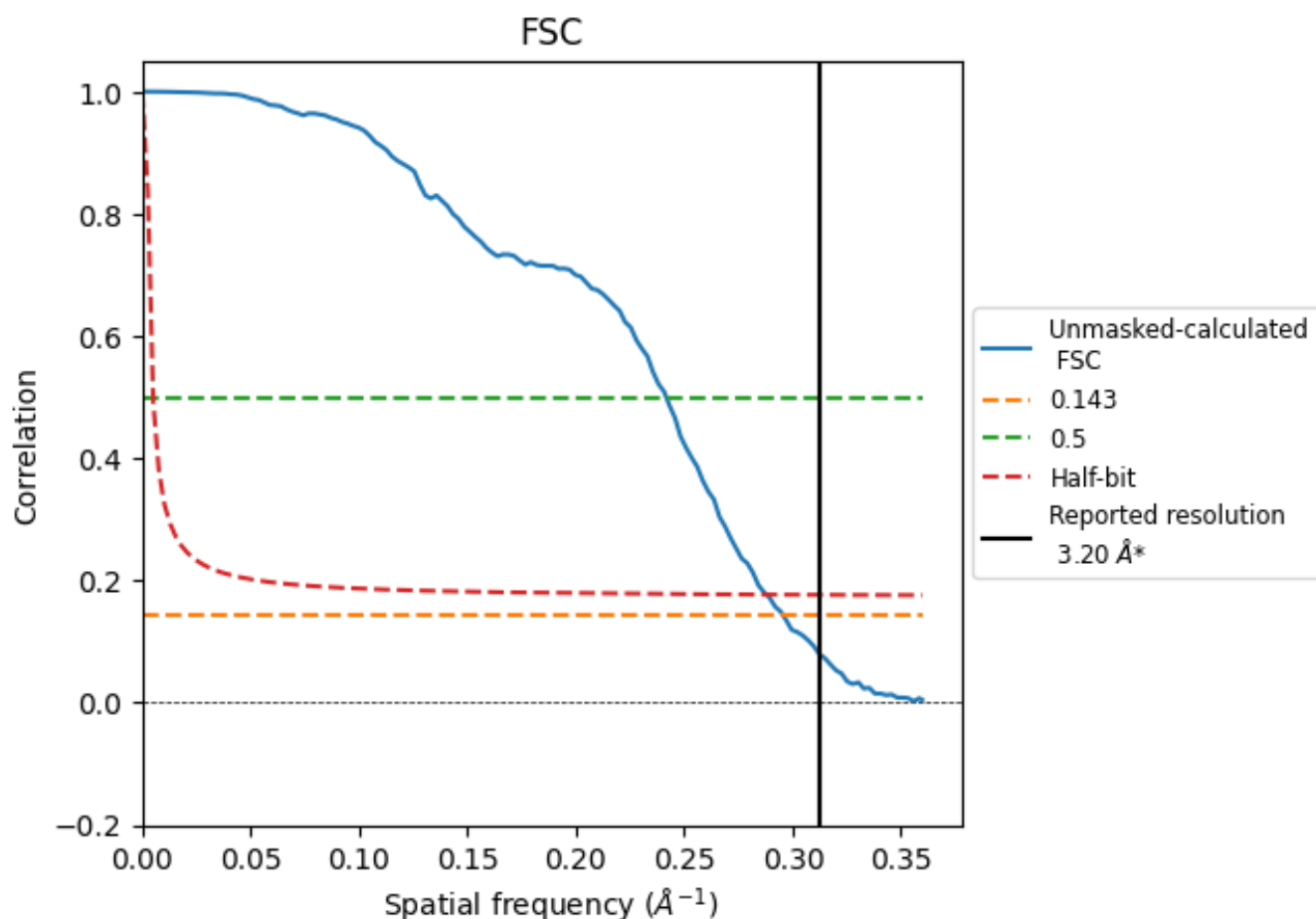


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

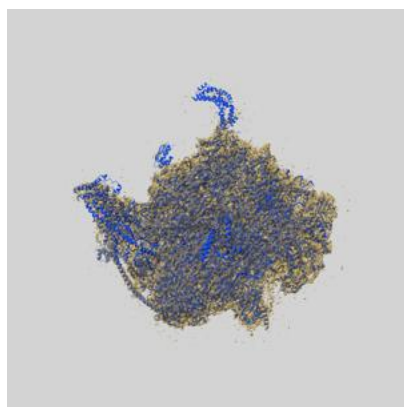
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	4.14	3.47

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

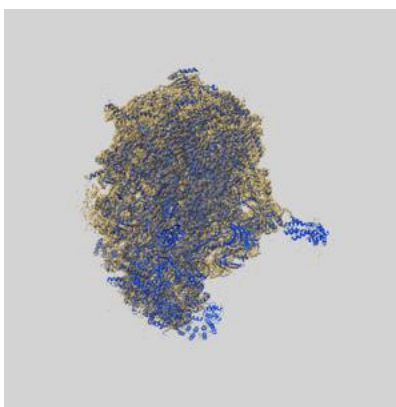
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4368 and PDB model 6GAW. Per-residue inclusion information can be found in section [3](#) on page [26](#).

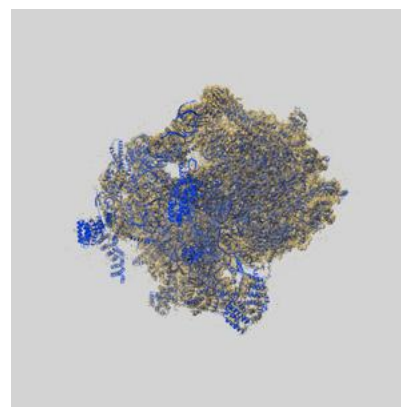
9.1 Map-model overlay [i](#)



X



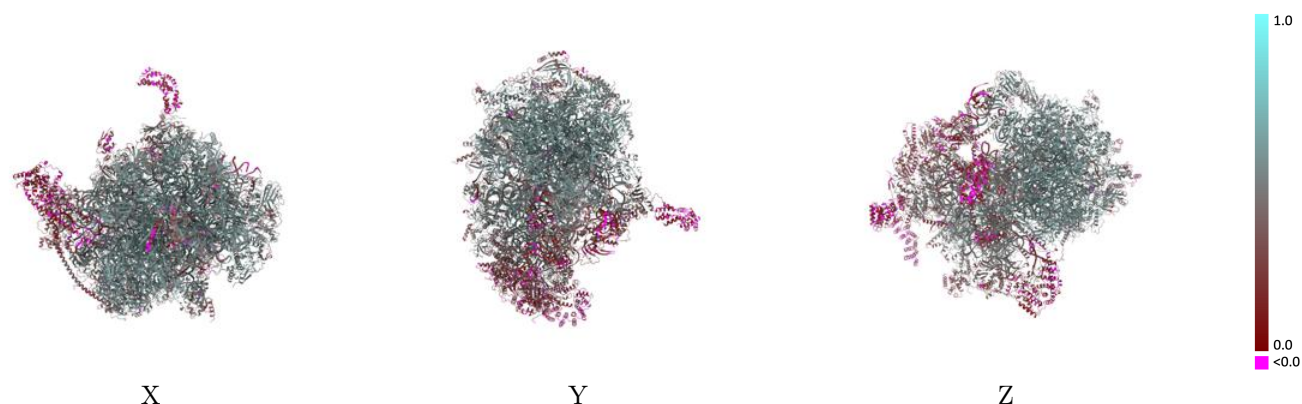
Y



Z

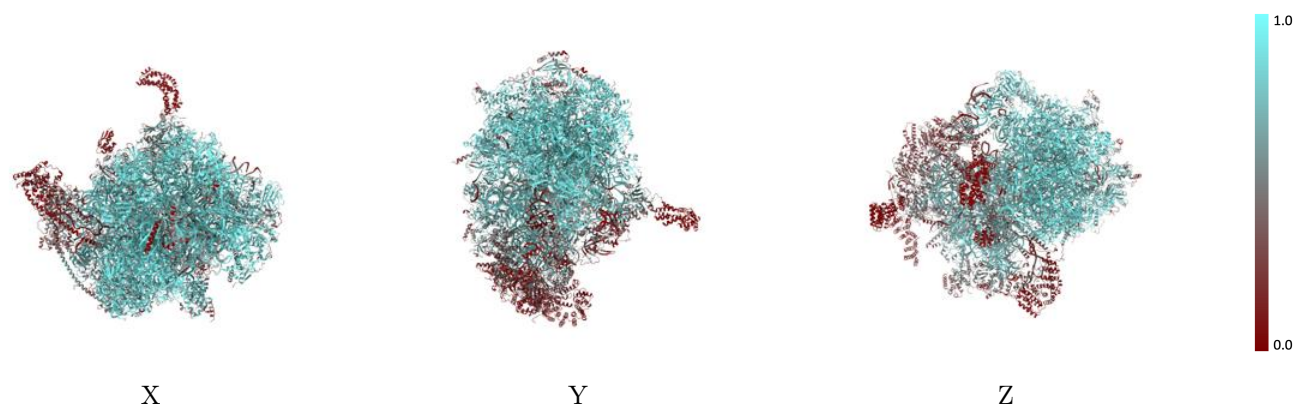
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



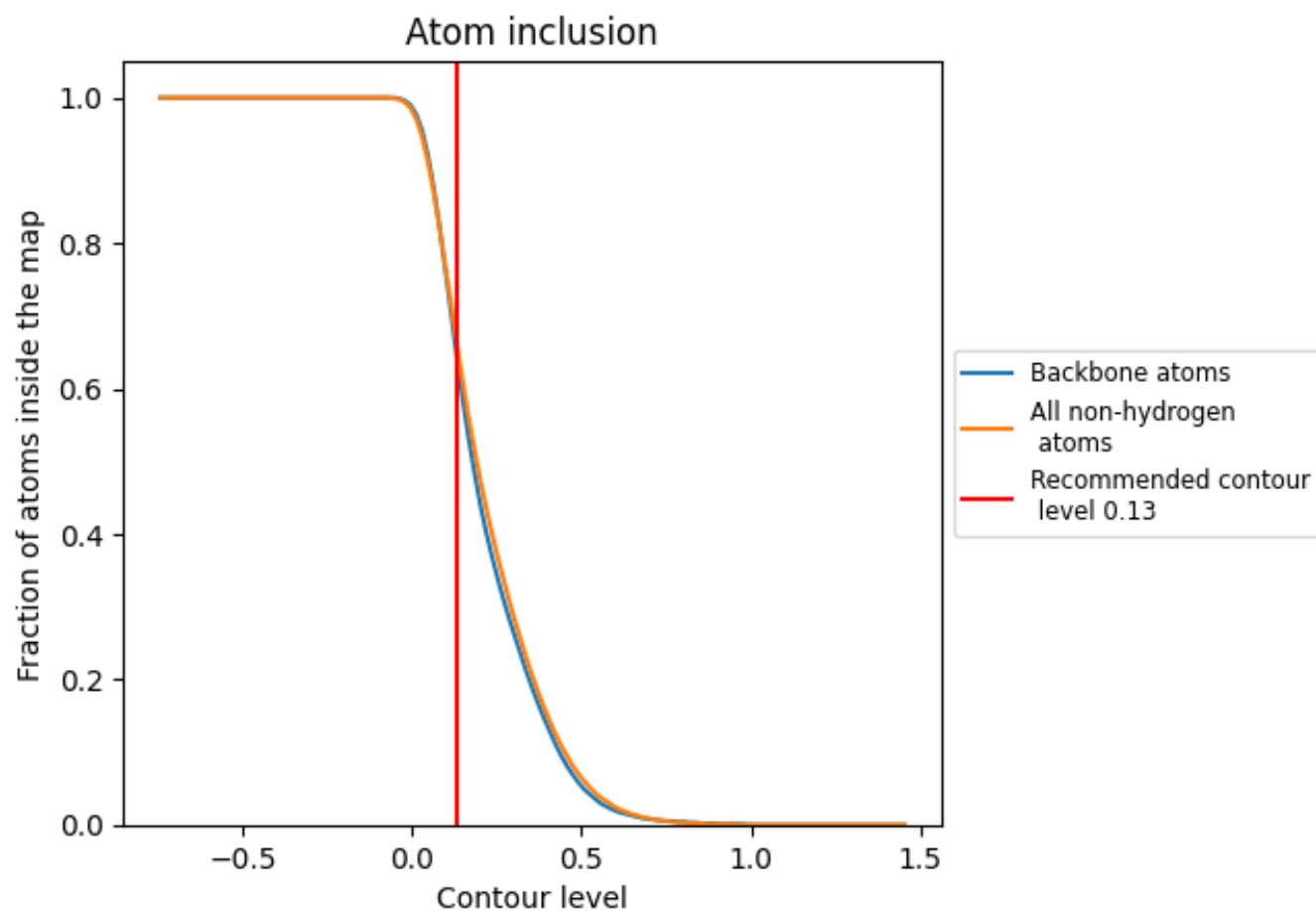
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 67% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4490
AA	 0.7870	 0.4730
AB	 0.6540	 0.4630
AC	 0.4770	 0.4340
AE	 0.5570	 0.4420
AF	 0.7110	 0.5020
AG	 0.3320	 0.3290
AI	 0.3990	 0.3330
AJ	 0.3240	 0.3080
AK	 0.6590	 0.4780
AL	 0.7300	 0.5200
AN	 0.5280	 0.4060
AO	 0.6030	 0.4290
AP	 0.5490	 0.3920
AQ	 0.6390	 0.4540
AR	 0.7050	 0.4800
AU	 0.7460	 0.5060
AV	 0.4010	 0.3030
AX	 0.1800	 0.1870
AZ	 0.2440	 0.2290
Aa	 0.3800	 0.3060
Ab	 0.5330	 0.4040
Ac	 0.6080	 0.4360
Ad	 0.5070	 0.3310
Ae	 0.1270	 0.1240
Af	 0.5810	 0.4450
Ag	 0.2040	 0.2230
Ah	 0.2320	 0.2310
Ai	 0.3800	 0.3240
Aj	 0.2890	 0.2510
Ak	 0.2460	 0.2530
Am	 0.4920	 0.3980
An	 0.6950	 0.5050
Ao	 0.0670	 0.1060
Ap	 0.5180	 0.3850



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Chain	Atom inclusion	Q-score
B0	 0.8910	 0.5710
B1	 0.7650	 0.4980
B2	 0.8300	 0.5390
B3	 0.8500	 0.5500
B4	 0.5550	 0.3310
B5	 0.8400	 0.5470
B6	 0.6390	 0.4760
B7	 0.9270	 0.6030
B8	 0.9030	 0.5850
B9	 0.8940	 0.5710
BA	 0.9150	 0.5630
BB	 0.5430	 0.2790
BC	 0.4340	 0.3750
BD	 0.8540	 0.5590
BE	 0.8520	 0.5520
BF	 0.8700	 0.5600
BI	 0.6740	 0.4570
BJ	 0.4640	 0.3340
BK	 0.2670	 0.2110
BL	 0.0240	 0.1230
BN	 0.8940	 0.5730
BO	 0.8230	 0.5420
BP	 0.8570	 0.5520
BQ	 0.8270	 0.5420
BR	 0.8690	 0.5640
BS	 0.8160	 0.5240
BT	 0.7610	 0.5120
BU	 0.8770	 0.5630
BV	 0.8390	 0.5520
BW	 0.8640	 0.5650
BX	 0.7950	 0.5120
BY	 0.6430	 0.4670
Ba	 0.8290	 0.5310
Bb	 0.7840	 0.4880
Bc	 0.7520	 0.4910
Bd	 0.4750	 0.2810
Be	 0.7600	 0.4980
Bf	 0.7460	 0.4730
Bg	 0.8780	 0.5640
Bh	 0.7960	 0.5070
Bi	 0.5650	 0.4090
Bj	 0.3400	 0.2220

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Chain	Atom inclusion	Q-score
Bk	 0.5230	 0.3700
Bl	 0.8450	 0.5460
Bm	 0.4910	 0.4160
Bn	 0.8980	 0.5730
Bo	 0.7870	 0.5200
Bp	 0.5690	 0.3840
Bq	 0.4930	 0.3500
Bt	 0.8730	 0.5670
Bu	 0.6080	 0.4020
Bv	 0.6450	 0.4400
Bw	 0.8210	 0.5270
Bx	 0.7890	 0.5160
Bz	 0.0780	 0.0740
CL	 0.0950	 0.1430
DL	 0.0380	 0.0930
EL	 0.0000	 0.0630
FL	 0.0050	 -0.0030
GL	 0.0000	 0.0290
HL	 0.0000	 0.0450