



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:12 AM UTC

PDB ID : 6VLZ / pdb_00006vlz
EMDB ID : EMD-21233
Title : Structure of the human mitochondrial ribosome-EF-G1 complex (ClassI)
Authors : Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on : 2020-01-27
Resolution : 2.97 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:

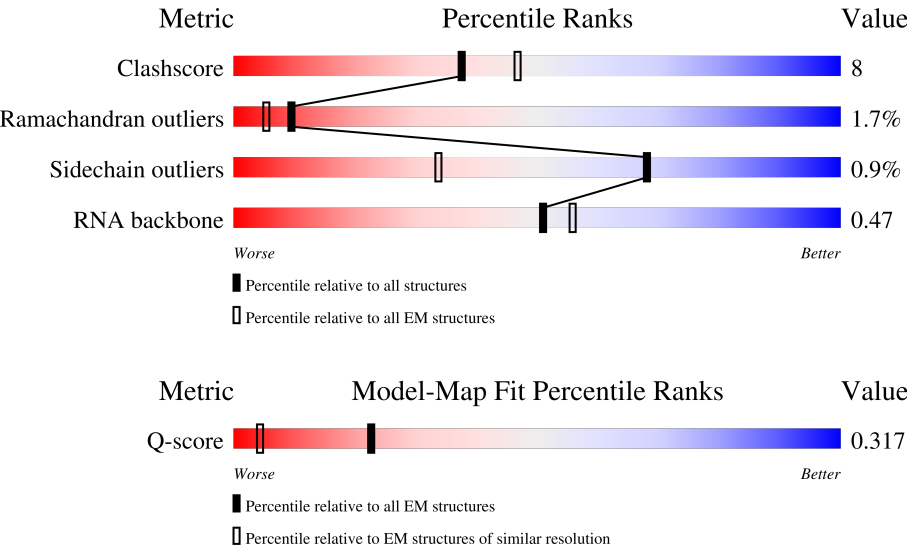
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	AA	954	
2	AB	296	
3	AC	167	

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Mol	Chain	Length	Quality of chain
4	AE	125	
5	AI	194	
6	AJ	138	
7	AK	128	
8	AM	137	
9	AN	130	
10	AO	258	
11	AP	142	
12	AQ	87	
13	AT	173	
14	AW	187	
15	AX	398	
16	A2	118	
17	AH	201	
18	AL	257	
19	AR	360	
20	AS	190	
21	AU	205	
22	AV	414	
23	AY	395	
24	AZ	106	
25	A1	323	
26	A0	218	
27	A3	199	
28	A4	689	

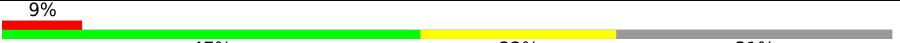
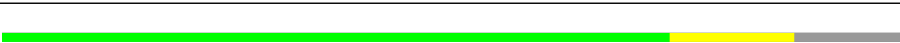
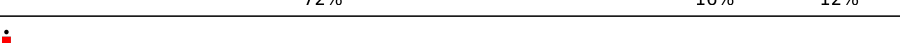
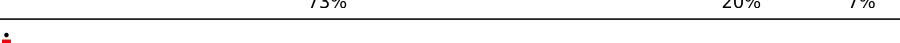
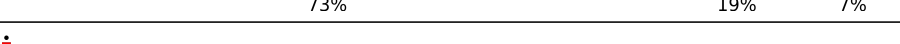
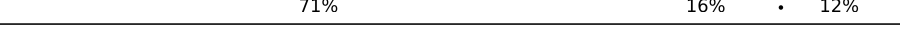
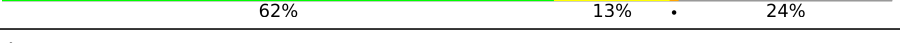
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Mol	Chain	Length	Quality of chain
29	AD	430	
30	AF	242	
31	AG	396	
32	A	1559	
33	B	73	
34	D	305	
35	F	311	
36	H	267	
37	K	178	
38	L	145	
39	M	296	
40	O	175	
41	R	149	
42	S	205	
43	T	212	
44	W	148	
45	X	256	
46	Y	250	
47	Z	161	
48	0	188	
49	1	65	
50	2	92	
51	3	188	
52	4	103	
53	8	206	

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Mol	Chain	Length	Quality of chain
54	b	155	
55	e	279	
56	g	166	
57	i	128	
58	j	123	
59	m	128	
60	o	102	
61	q	222	
62	r	196	
63	J	192	
64	I	261	
65	N	251	
66	P	179	
67	U	153	
68	V	216	
69	E	348	
70	5	423	
71	6	380	
72	7	338	
73	9	137	
74	a	142	
75	c	332	
76	d	306	
77	f	194	
78	h	158	

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Mol	Chain	Length	Quality of chain
79	k	112	
80	l	138	
81	p	206	
82	s	439	
83	Q	292	
84	TA	198	
84	TB	198	
84	TC	198	
85	u	65	
86	v	751	
87	A5	11	
88	A7	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	Y5P	A5	1	-	-	X	-
88	P5P	A7	1	-	-	X	-
92	GCP	v	802	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 174849 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 12s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	944	Total	C	N	O	P	0	0
			20030	8980	3612	6494	944		

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	220	Total	C	N	O	S	0	0
			1787	1141	324	312	10		

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 5 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AI	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 6 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AJ	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 7 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AK	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 8 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AM	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 9 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AN	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 10 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AO	190	Total	C	N	O	S	0	0
			1570	998	291	274	7		

- Molecule 11 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AP	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 12 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AQ	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	conflict	UNP P82921

- Molecule 13 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 14 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AW	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 15 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AX	353	Total	C	N	O	S	0	0
			2860	1828	503	518	11		

- Molecule 16 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A2	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 17 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AH	122	Total	C	N	O	S	0	0
			1014	656	172	183	3		

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AL	174	Total	C	N	O	S	0	0
			1451	924	271	249	7		

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	292	Total	C	N	O	S	0	0
			2388	1521	410	449	8		

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	177	Total	C	N	O	S	0	0
			1499	922	305	268	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	367	Total	C	N	O	S	0	0
			3009	1931	502	564	12		

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AY	120	Total	C	N	O	S	0	0
			1016	657	167	190	2		

- Molecule 24 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AZ	99	Total	C	N	O	S	0	0
			833	531	152	146	4		

- Molecule 25 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A1	275	Total	C	N	O	S	0	0
			2231	1414	380	426	11		

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A0	214	Total	C	N	O	S	0	0
			1781	1125	341	310	5		

- Molecule 27 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A3	72	Total	C	N	O	S	0	0
			639	409	137	92	1		

- Molecule 28 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A4	549	Total	C	N	O	S	0	0
			3010	1841	573	593	3		

- Molecule 29 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 30 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AF	208	Total	C	N	O	S	0	0
			1724	1103	312	298	11		

- Molecule 31 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AG	315	Total	C	N	O	S	0	0
			2587	1640	462	471	14		

- Molecule 32 is a RNA chain called 16s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	1527	Total	C	N	O	P	0	0
			32395	14536	5844	10488	1527		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	C	conflict	GB 1616239084

- Molecule 33 is a RNA chain called tRNAval.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 34 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	239	Total	C	N	O	S	0	0
			1866	1162	377	318	9		

- Molecule 35 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 36 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	98	Total	C	N	O		0	0
			806	510	156	140			

- Molecule 37 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 38 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 40 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 41 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 42 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 43 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 44 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 45 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	148	ALA	THR	conflict	UNP Q13084
X	149	SER	PRO	conflict	UNP Q13084
X	150	GLY	LYS	conflict	UNP Q13084

- Molecule 46 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 47 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 48 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 49 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 50 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 51 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 52 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 53 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 54 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 55 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 56 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	g	132	Total	C	N	O	S	0	0
			1096	709	191	194	2		

- Molecule 57 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 58 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	j	93	Total	C	N	O	S	0	0
			740	460	143	135	2		

- Molecule 59 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 60 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 61 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	q	168	Total	C	N	O	S	0	0
			1294	801	255	233	5		

- Molecule 62 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 63 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 64 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	I	179	Total	C	N	O	S	0	0
			1435	925	258	242	10		

- Molecule 65 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 66 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	P	143	Total	C	N	O	S	0	0
			1165	729	223	208	5		

- Molecule 67 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	U	152	Total	C	N	O	S	0	0
			1224	774	233	214	3		

- Molecule 68 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V	206	Total	C	N	O	S	0	0
			1682	1071	299	304	8		

- Molecule 69 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	E	306	Total	C	N	O	S	0	0
			2410	1547	419	433	11		

- Molecule 70 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 71 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 72 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	7	297	Total	C	N	O	S	0	0
			2410	1540	409	443	18		

- Molecule 73 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 74 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a	108	Total	C	N	O	S	0	0
			896	560	162	169	5		

- Molecule 75 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	c	289	Total	C	N	O	S	0	0
			2322	1483	400	430	9		

- Molecule 76 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	257	Total	C	N	O	S	0	0
			2075	1326	363	372	14		

- Molecule 77 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	f	146	Total	C	N	O	S	0	0
			1126	714	186	222	4		

- Molecule 78 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	h	110	Total	C	N	O	S	0	0
			894	568	156	167	3		

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l	72	Total	C	N	O	S	0	0
			619	394	112	111	2		

- Molecule 81 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	p	152	Total	C	N	O	S	0	0
			1227	762	232	229	4		

- Molecule 82 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	s	393	Total	C	N	O	S	0	0
			3178	2036	565	563	14		

- Molecule 83 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Q	240	Total	C	N	O	S	0	0
			1995	1280	354	352	9		

- Molecule 84 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	TA	45	Total	C	N	O	0	0
			345	222	54	69		
84	TB	27	Total	C	N	O	0	0
			213	137	33	43		
84	TC	71	Total	C	N	O	0	0
			352	210	71	71		

- Molecule 85 is a protein called P-site finger.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	u	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 86 is a protein called Elongation factor G, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	v	712	Total	C	N	O	S	0	0
			5546	3494	957	1062	33		

- Molecule 87 is a DNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	A5	11	Total	C	N	O	P	0	0
			213	104	32	66	11		

- Molecule 88 is a DNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	A7	62	Total	C	N	O	P	0	0
			1197	586	180	370	61		

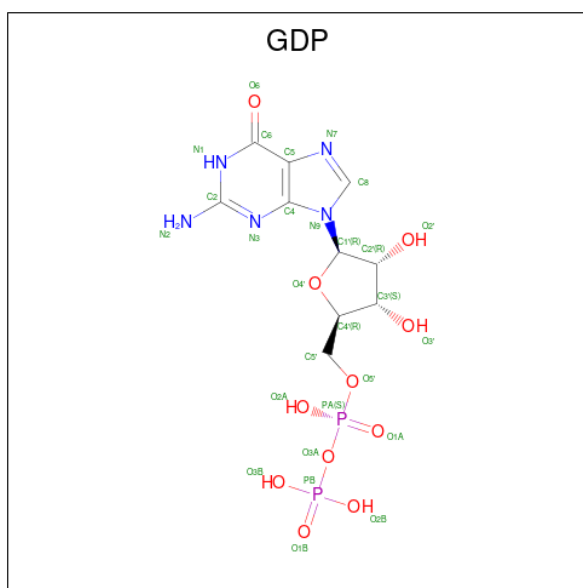
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	26	Total	Mg	0
			26	26	
89	A2	1	Total	Mg	0
			1	1	
89	AH	1	Total	Mg	0
			1	1	
89	A	97	Total	Mg	0
			97	97	
89	D	1	Total	Mg	0
			1	1	
89	W	1	Total	Mg	0
			1	1	
89	g	1	Total	Mg	0
			1	1	
89	E	1	Total	Mg	0
			1	1	
89	v	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

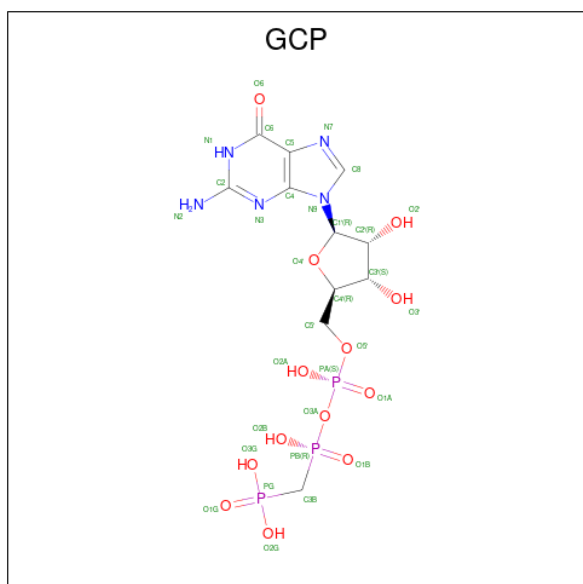
Mol	Chain	Residues	Atoms		AltConf
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
91	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 92 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

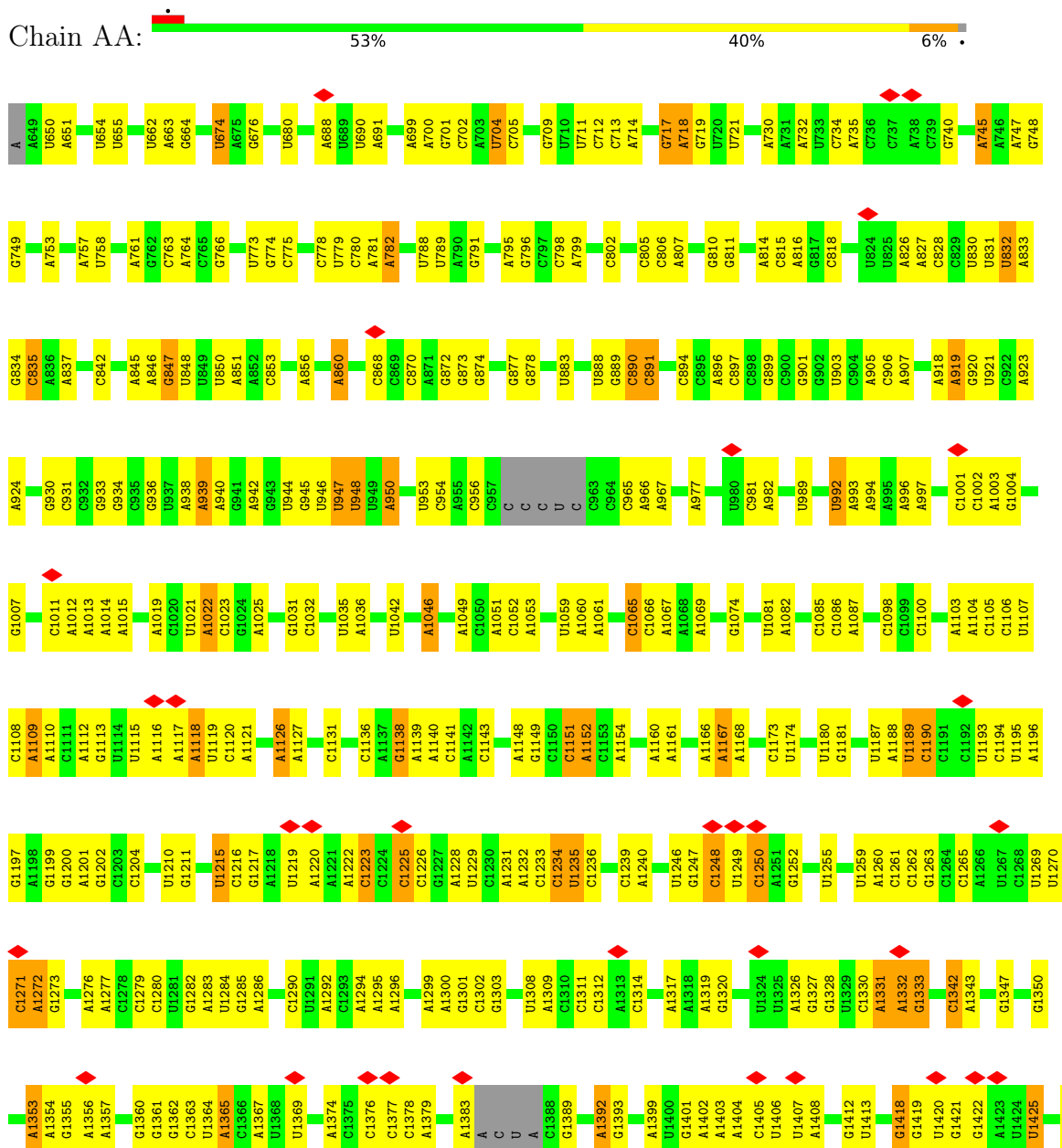


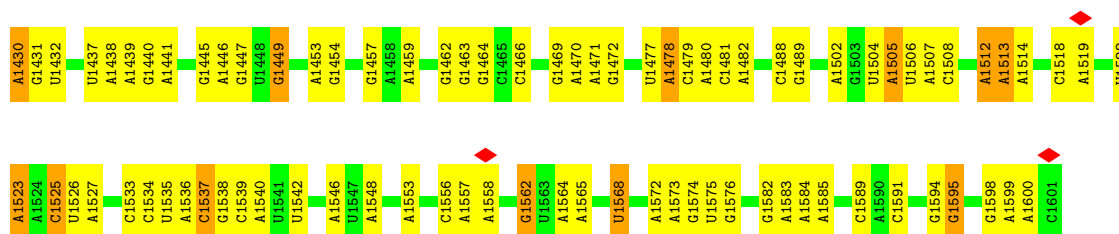
Mol	Chain	Residues	Atoms					AltConf
92	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

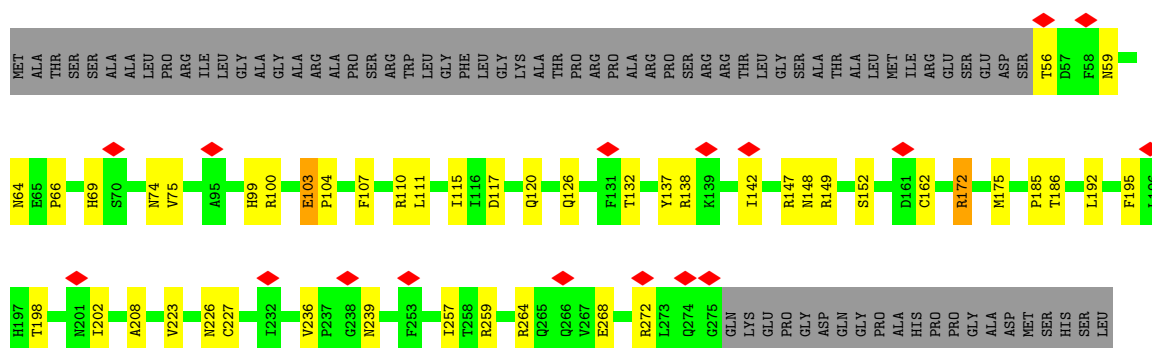
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 12s rRNA

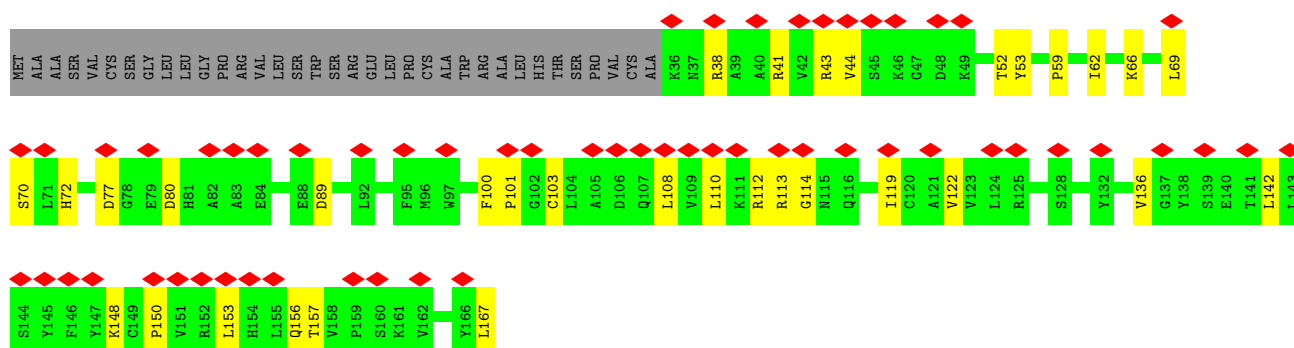




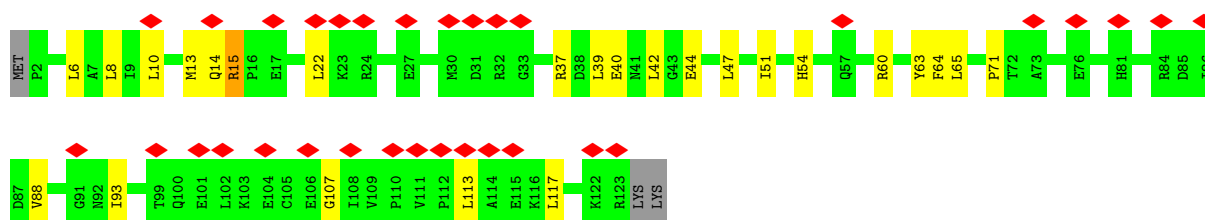
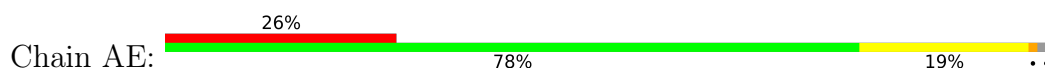
• Molecule 2: 28S ribosomal protein S2, mitochondrial



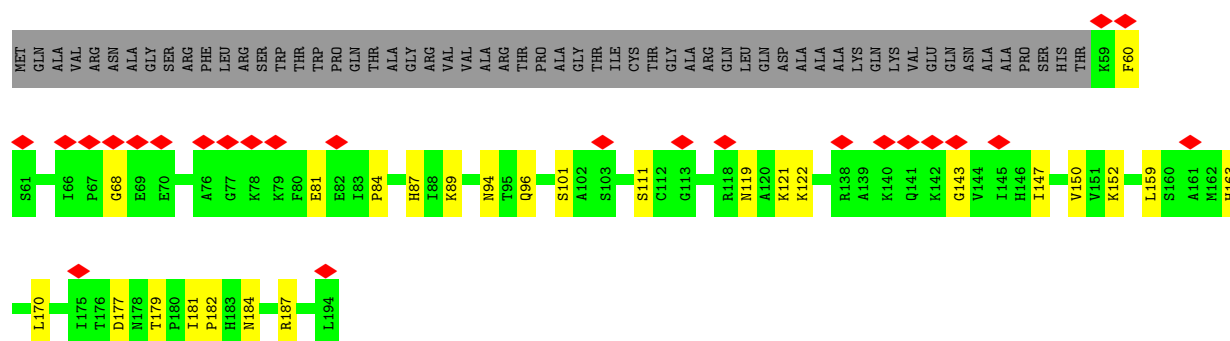
• Molecule 3: 28S ribosomal protein S24, mitochondrial



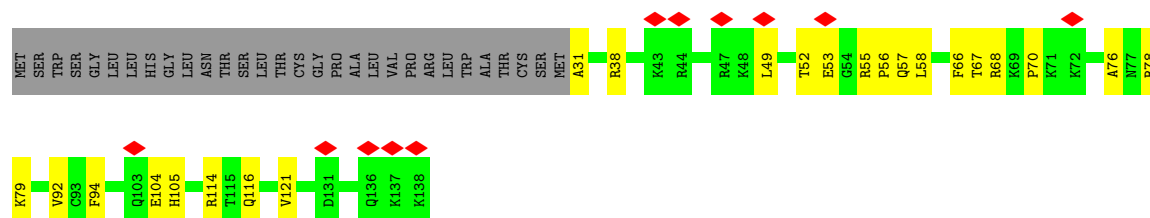
• Molecule 4: 28S ribosomal protein S6, mitochondrial



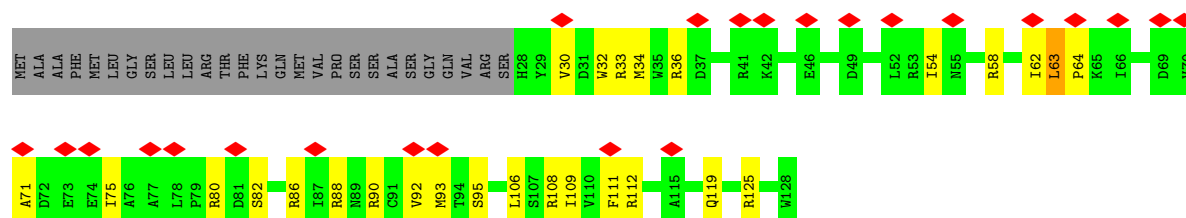
• Molecule 5: 28S ribosomal protein S11, mitochondrial



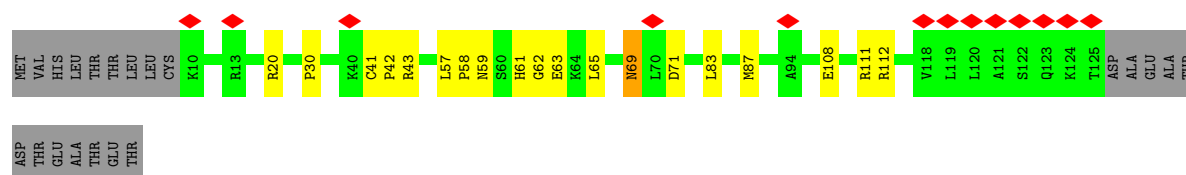
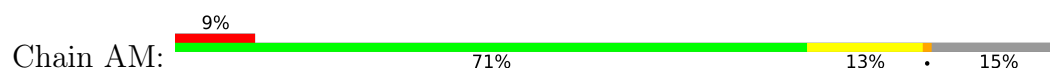
- Molecule 6: 28S ribosomal protein S12, mitochondrial



- Molecule 7: 28S ribosomal protein S14, mitochondrial

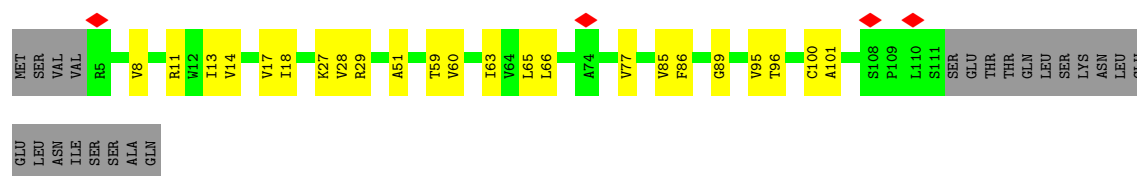


- Molecule 8: 28S ribosomal protein S16, mitochondrial

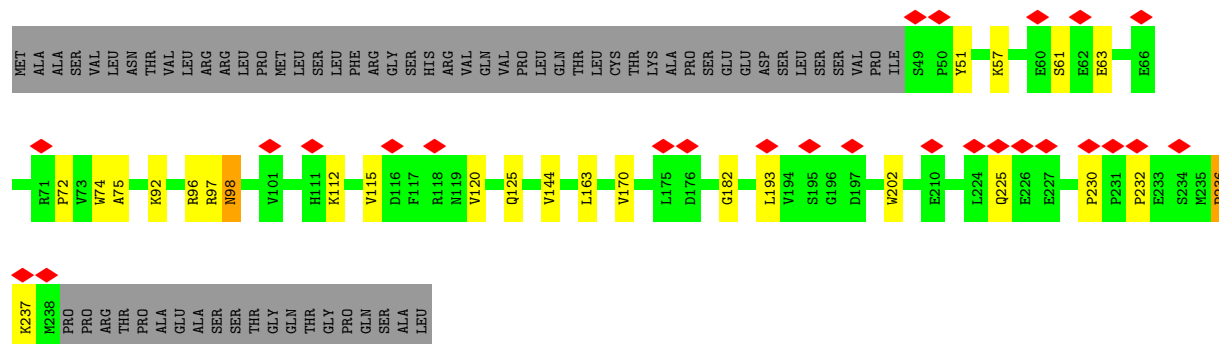


- Molecule 9: 28S ribosomal protein S17, mitochondrial

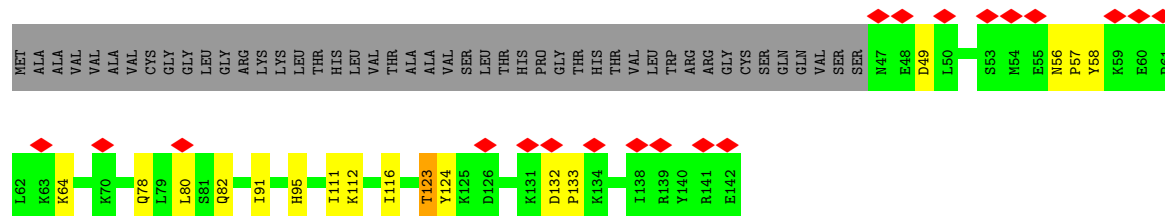




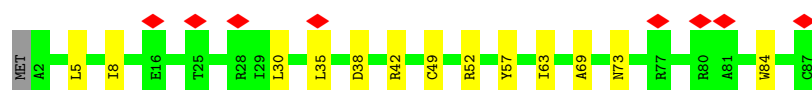
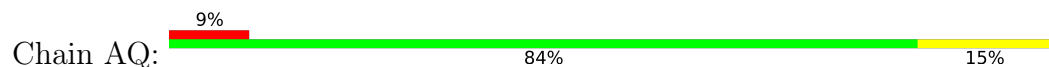
- Molecule 10: 28S ribosomal protein S18b, mitochondrial



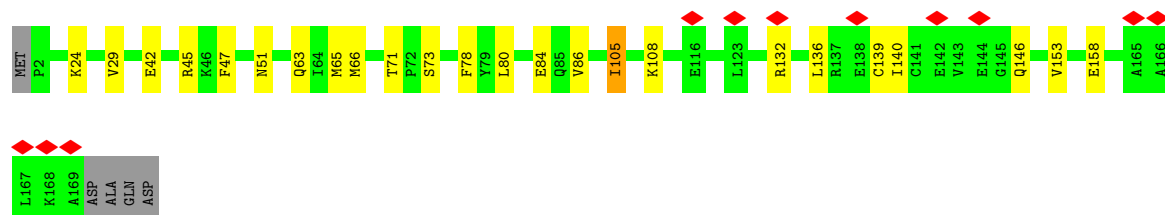
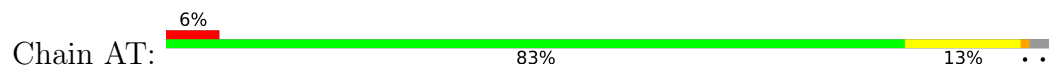
- Molecule 11: 28S ribosomal protein S18c, mitochondrial

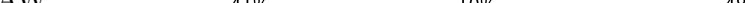


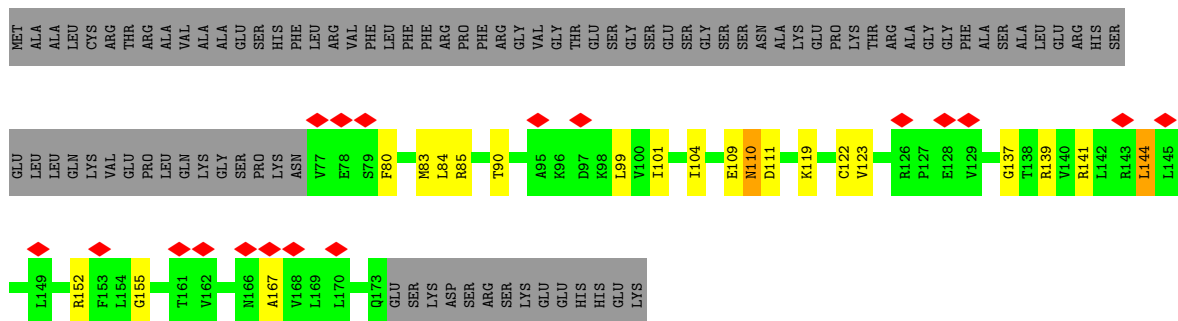
- Molecule 12: 28S ribosomal protein S21, mitochondrial

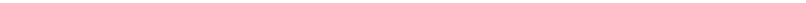


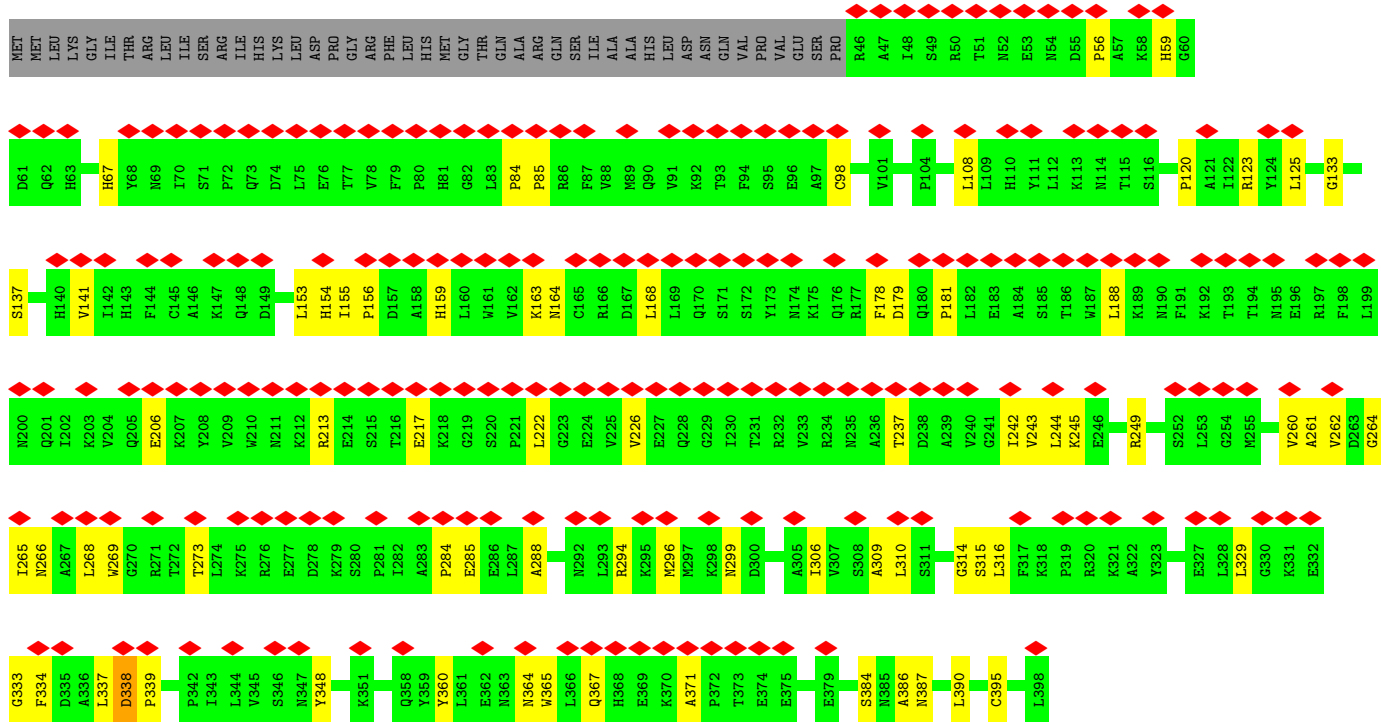
- Molecule 13: 28S ribosomal protein S25, mitochondrial

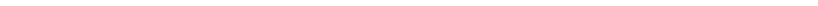


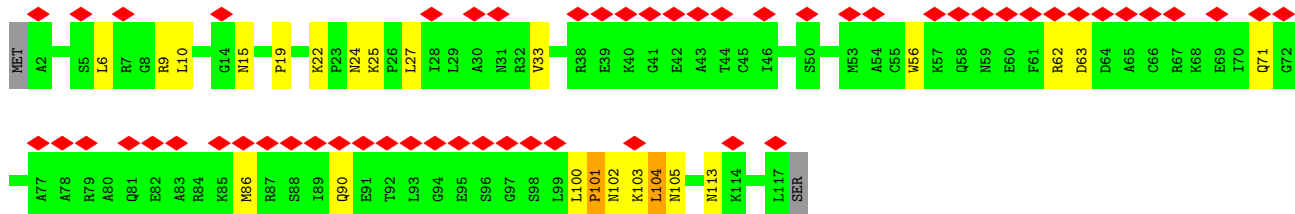
- Chain AW: 



- Chain AX: 

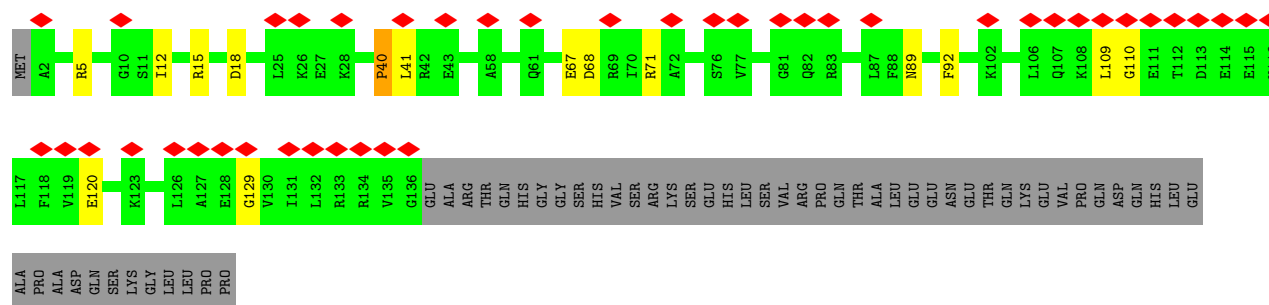


- Chain A2:  47% 79% 18% ..

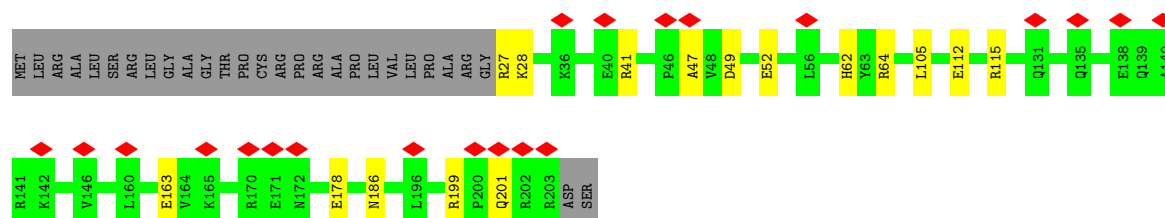
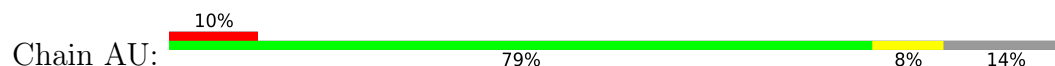


-
- | Response | Percentage |
|--------------------------------|------------|
| Current government is the best | 34% |
| Best government | 49% |
| Don't know | 9% |
| Worse government | 39% |

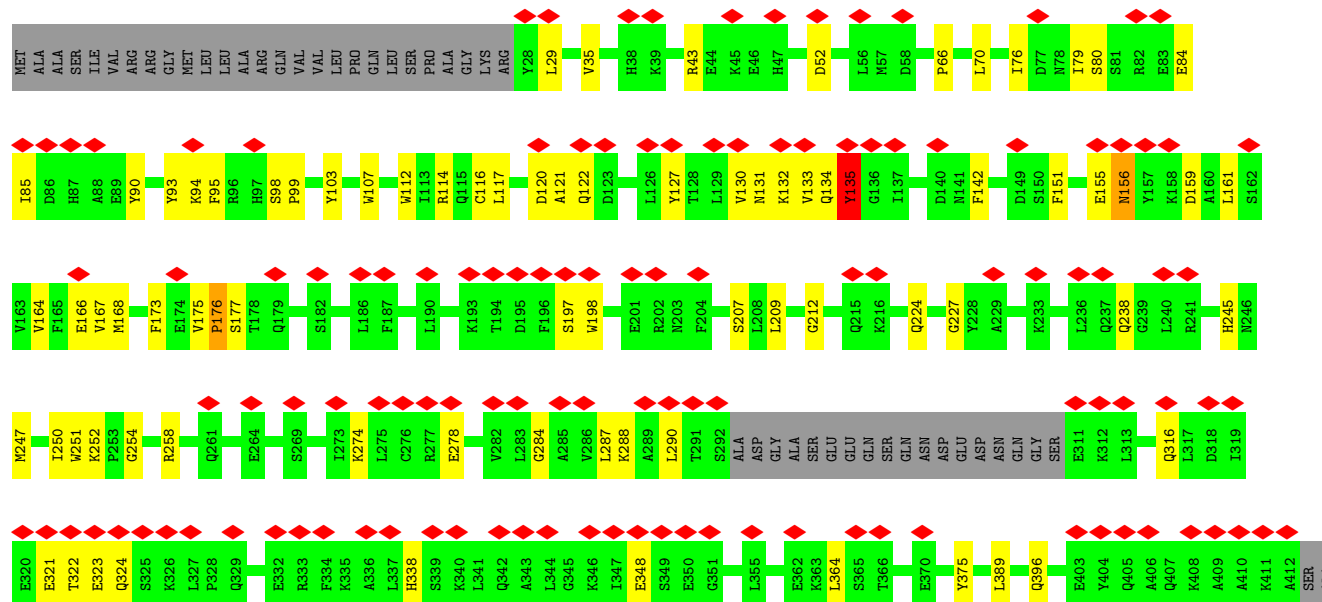




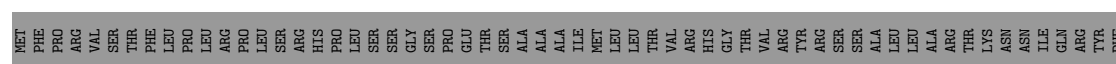
- Molecule 21: 28S ribosomal protein S26, mitochondrial

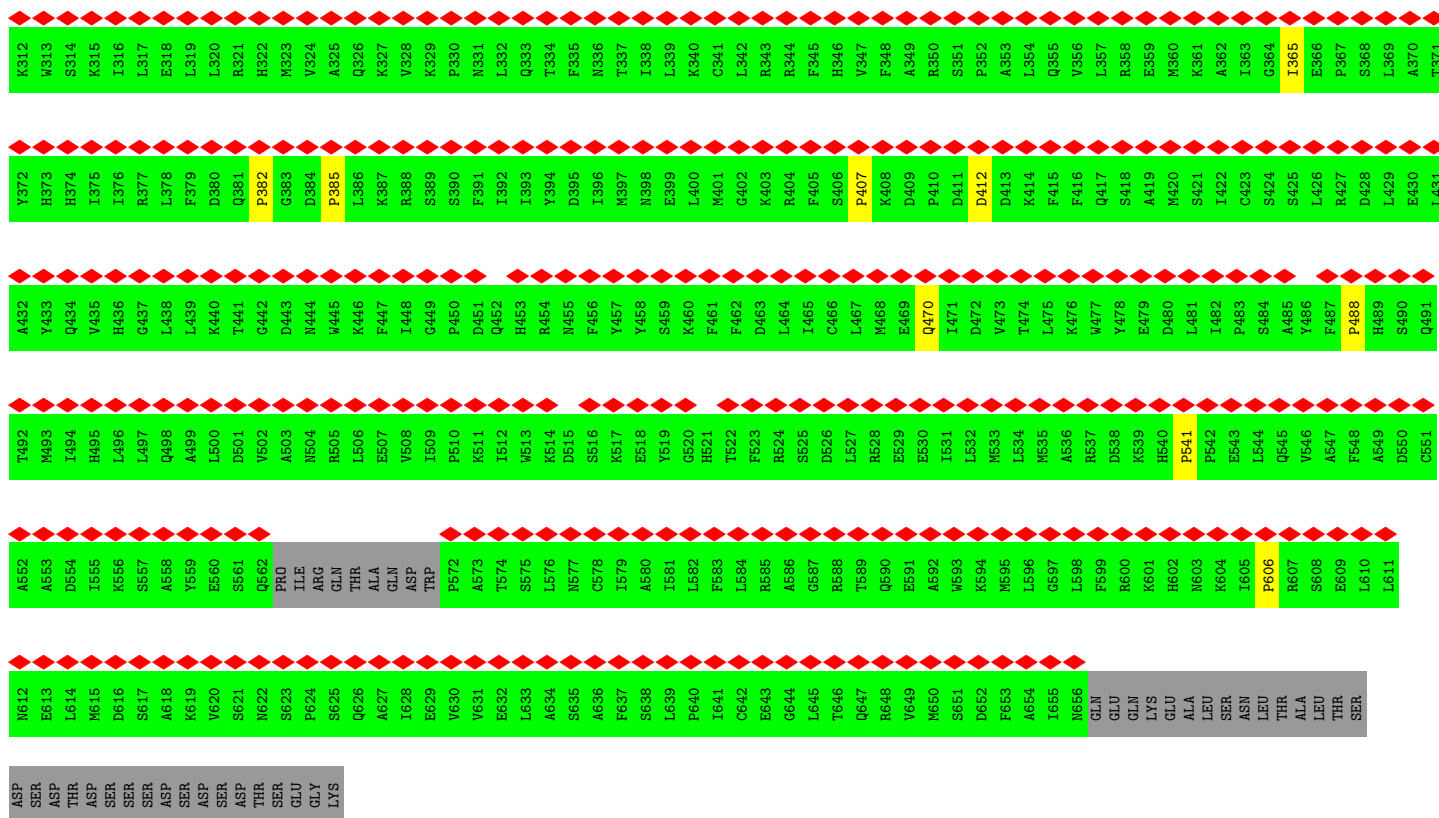


- Molecule 22: 28S ribosomal protein S27, mitochondrial

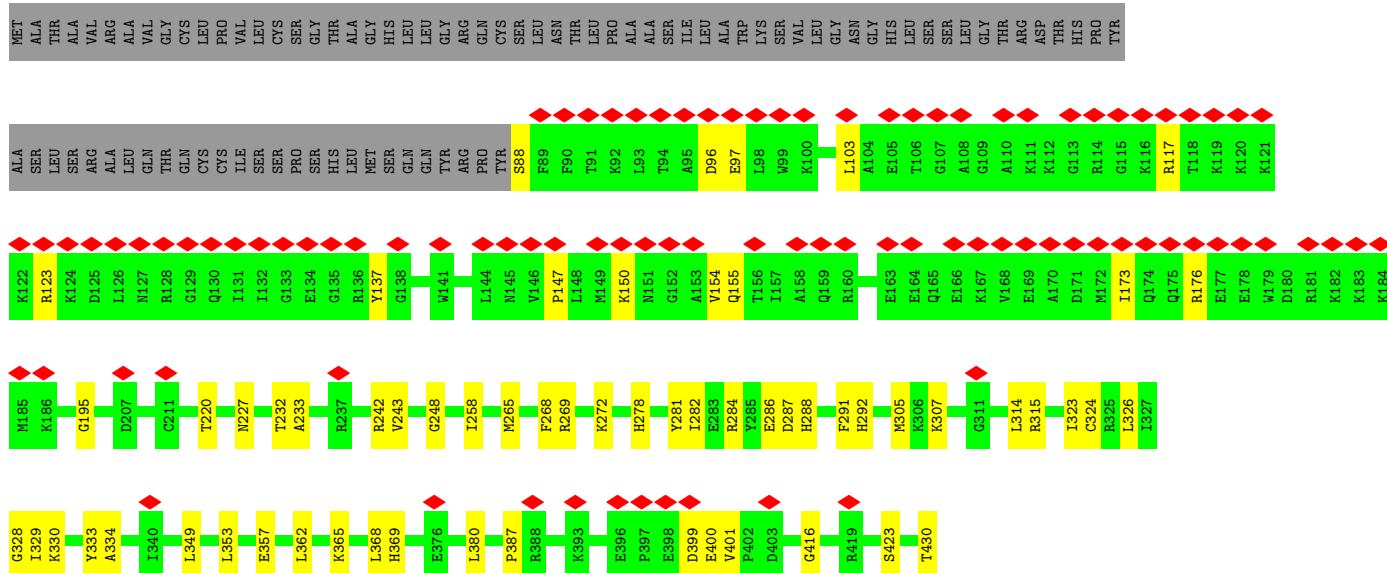


- Molecule 23: 28S ribosomal protein S31, mitochondrial

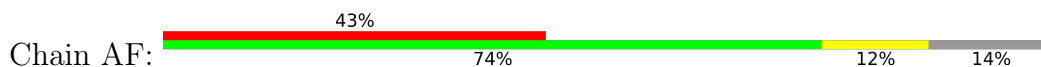




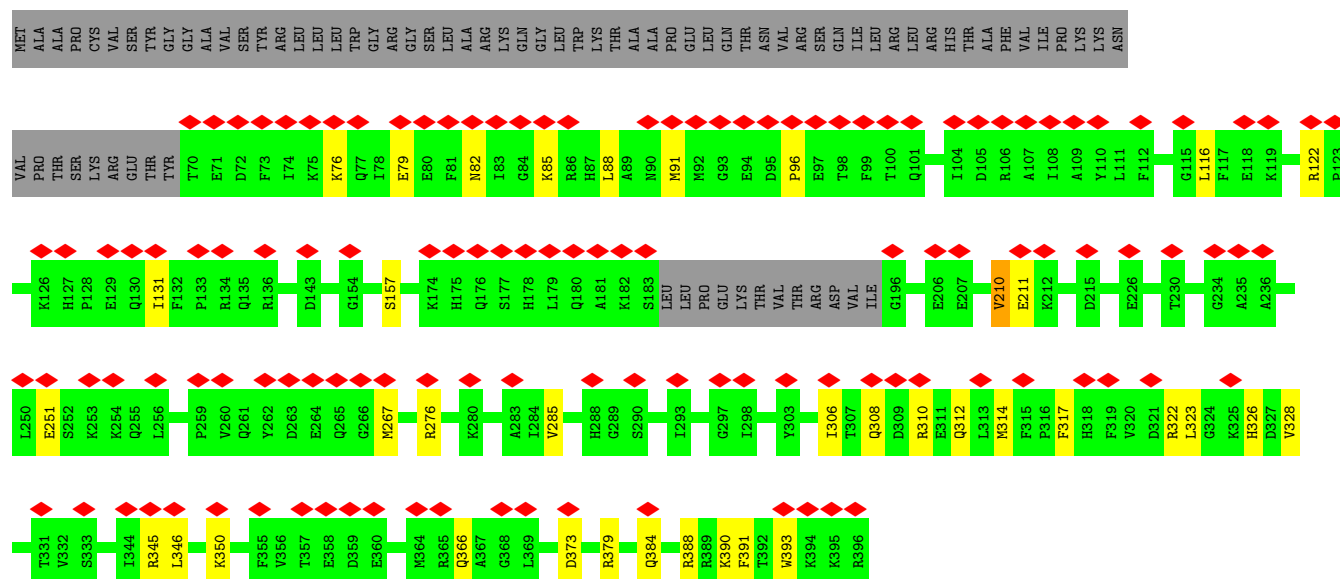
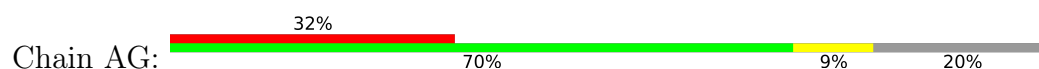
- Molecule 29: 28S ribosomal protein S5, mitochondrial



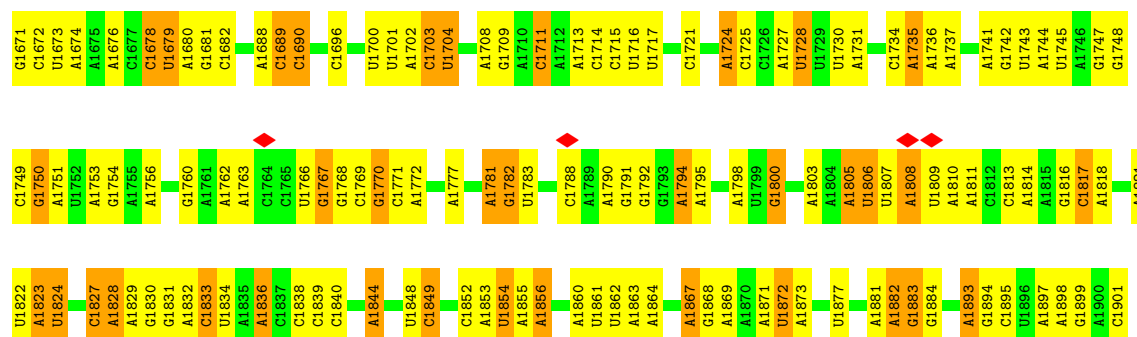
- Molecule 30: 28S ribosomal protein S7, mitochondrial



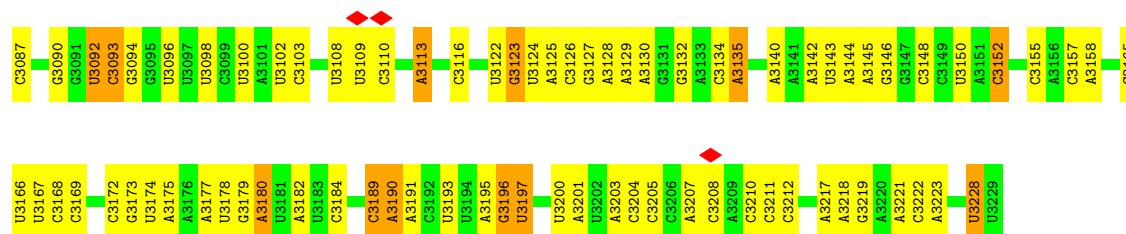
- Molecule 31: 28S ribosomal protein S9, mitochondrial



- Molecule 32: 16s rRNA



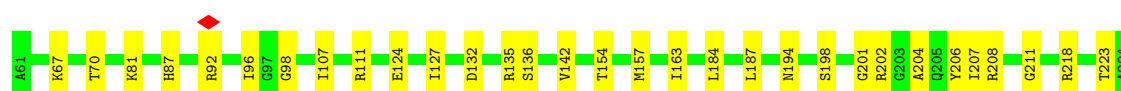
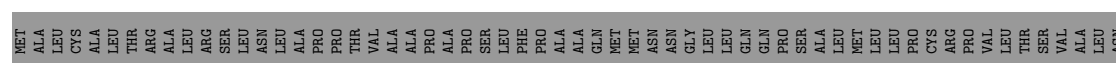
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A3003	A1907	A2085	A2171	A2236	A2313	C2393	C2484	C2584	G2654	U2749	C2836	A2926	A3003
G3004	C2001	A2086	A2172	A2237	A2314	A2394	C2489	G2585	U2655	U2750	U2841	C2927	G3004
A3005	A1908	U2087	G2173	A2241	A2315	A2395	C2493	U2586	C2656	A2753	C2842	C2928	A3005
U3006	G2002	U2088	G2174	A2244	U2316	C2396	C2493	U2587	U2657	A2754	U2843	U2929	U3006
G3007	A2003	C2092	A2178	U2244	G2317	U2404	C2493	C2588	C2658	A2755	G2844	U2930	G3007
G3010	G2004	U2093	A2179	A2245	A2318	C2405	A2503	A2590	U2660	A2756	U2844	A2931	G3010
A3011	C2005	G2094	A2180	A2246	A2319	A2406	A2504	A2591	U2661	C2756	C2847	G2932	A3011
U3012	A1912	C2095	A2181	A2250	A2320	U2407	A2505	G2592	U2662	A2757	A2848	U2933	U3012
G3013	C1915	U2096	G2182	A2251	A2321	U2407	U2506	G2593	U2663	G2758	G2849	A2935	G3013
G3016	G1916	C2097	C2183	A2252	C2322	C2414	U2507	U2594	U2664	U2759	A2853	U2936	G3016
G3022	A1917	G2098	A2184	U2253	U2325	C2415	A2508	C2597	A2672	C	U2854	A2937	G3022
U3024	G1918	G2099	C2187	U2254	G2331	U2421	U2509	A2598	G2673	C	U2854	A2938	U3024
G3027	U1924	G2011	C2188	U2255	C2332	U2422	U2510	C2602	U2674	U	G2860	C2939	G3027
G3031	A1925	G2015	C2189	U2256	U2333	A2425	G2511	A2601	G2675	A	U2864	C2942	G3031
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U3042	A1935	G2023	U2194	U2261	G2338	C2433	A2523	U2607	C2689	C	C2869	C2947	U3042
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U3052	A1938	A2027	G2197	U2264	G2341	U2436	A2526	C2612	G2693	C	C2872	U2950	A3052
A3053	G1939	G2028	A2198	U2265	U2350	U2437	U2527	C2613	U2694	A	U2873	A2951	A3053
G3054	A1941	A2031	A2199	U2266	U2351	U2438	A2528	C2614	C2695	C	U2874	U2952	G3054
C3060	G1942	G2040	G2201	U2267	U2352	U2439	A2529	U2615	C2696	C	U2875	U2953	C3060
G3063	A1943	C2043	G2202	U2268	U2353	U2440	U2530	U2616	C2697	C	U2876	U2954	G3063
U3066	G1944	C2036	U2205	U2269	U2354	U2441	A2531	U2617	U2698	C	U2877	U2955	U3066
G3068	A1951	U2037	A2208	U2270	U2355	U2442	A2532	U2618	G2699	C	C2878	U2956	G3068
A3069	U1952	U2038	G2209	U2271	U2356	U2443	A2533	U2619	U2706	C	U2879	U2957	A3069
G3070	A1953	A2039	C2210	U2272	U2357	U2444	A2534	U2620	A2707	C	A2880	U2958	G3070
U3071	U1954	G2040	C2211	U2273	U2358	U2445	A2535	U2621	U2708	C	C2881	U2959	U3071
C3073	G1955	C2043	C2212	U2274	U2359	U2446	A2536	U2622	U2709	C	U2882	U2960	C3073
A3074	G1956	C2043	C2213	U2275	U2360	U2447	A2537	U2623	U2710	C	U2883	U2961	A3074
C3077	U1957	A2060	C2214	U2276	U2361	U2448	A2538	U2624	A2711	C	C2884	U2962	C3077
G3078	G1958	C2065	A2215	U2277	U2362	U2449	A2539	U2625	C2712	C	C2885	U2963	G3078
U3079	G1959	A2060	A2142	U2278	U2363	U2450	A2540	U2626	C2713	C	U2886	U2964	U3079
U3081	U1965	C2066	A2143	U2279	U2364	U2451	A2541	U2627	C2714	C	C2887	U2965	U3081
G3082	G1966	A2060	A2144	U2280	U2365	U2452	A2542	U2628	A2715	C	U2888	U2966	G3082
A3085	U1967	C2065	A2145	U2281	U2366	U2453	A2543	U2629	U2716	C	U2889	U2967	A3085
U3086	G1968	A2065	A2146	U2282	U2367	U2454	A2544	U2630	U2717	C	C2890	U2968	U3086
C3077	U1979	C2066	A2147	U2283	U2368	U2455	A2545	U2631	U2718	C	U2891	U2969	C3077
G3078	A1980	C2067	A2148	U2284	U2369	U2456	A2546	U2632	U2719	C	C2892	U2970	G3078
G3079	G1981	C2068	A2149	U2285	U2370	U2457	A2547	U2633	U2720	C	U2893	U2971	G3079
U3081	G1982	U2069	A2150	U2286	U2371	U2458	A2548	U2634	U2721	C	U2894	U2972	U3081
G3082	G1983	C2070	A2151	U2287	U2372	U2459	A2549	U2635	U2722	C	U2895	U2973	G3082
A3085	U1984	C2071	A2152	U2288	U2373	U2460	A2550	U2636	U2723	C	U2896	U2974	A3085
U3086	G1985	C2072	A2153	U2289	U2374	U2461	A2551	U2637	U2724	C	U2897	U2975	U3086
C3077	G1986	C2073	A2154	U2290	U2375	U2462	A2552	U2638	U2725	C	U2898	U2976	C3077
G3078	U1987	C2074	A2155	U2291	U2376	U2463	A2553	U2639	U2726	C	U2899	U2977	G3078
G3079	C2075	C2075	A2156	U2292	U2377	U2464	A2554	U2640	U2727	C	U2900	U2978	G3079
G3080	C2076	C2076	A2157	U2293	U2378	U2465	A2555	U2641	U2728	C	U2901	U2979	G3080
A3081	C2077	C2077	A2158	U2294	U2379	U2466	A2556	U2642	U2729	C	U2902	U2980	A3081
G3082	C2078	C2078	A2159	U2295	U2380	U2467	A2557	U2643	U2730	C	U2903	U2981	G3082
A3085	C2079	C2079	A2160	U2296	C2381	U2468	A2558	U2644	U2731	C	U2904	U2982	A3085
U3086	U2080	U2080	A2161	U2297	A2382	U2469	A2559	U2645	U2732	C	U2905	U2983	U3086
G2082	G2082	G2082	A2162	U2298	U2383	U2470	A2560	U2646	U2733	C	U2906	U2984	G2082
			A2163	U2299	U2384	U2471	A2561	U2647	U2734	C	U2907	U2985	
			A2164	U2300	U2385	U2472	A2562	U2648	U2735	C	U2908	U2986	
			A2165	U2301	U2386	U2473	A2563	U2649	U2736	C	U2909	U2987	
			A2166	U2302	U2387	U2474	A2564	U2650	U2737	C	U2910	U2988	
			A2167	U2303	U2388	U2475	A2565	U2651	U2738	C	U2911	U2989	
			A2168	U2304	U2389	U2476	A2566	U2652	U2739	C	U2912	U2990	
			A2169	U2305	U2390	U2477	A2567	U2653	U2740	C	U2913	U2991	
			A2170	U2306	U2391	U2478	A2568	U2654	U2741	C	U2914	U2992	
			A2171	U2307	U2392	U2479	A2569	U2655	U2742	C	U2915	U2993	
			A2172	U2308	U2393	U2480	A2570	U2656	U2743	C	U2916	U2994	
			A2173	U2309	U2394	U2481	A2571	U2657	U2744	C	U2917	U2995	
			A2174	U2310	U2395	U2482	A2572	U2658	U2745	C	U2918	U2996	
			A2175	U2311	U2396	U2483	A2573	U2659	U2746	C	U2919	U2997	
			A2176	U2312	U2397	U2484	A2574	U2660	U2747	C	U2920	U2998	
			A2177	U2313	U2398	U2485	A2575	U2661	U2748	C	U2921	U2999	
			A2178	U2314	U2399	U2486	A2576	U2662	U2749	C	U2922		
			A2179	U2315	U2400	U2487	A2577	U2663	U2750	C	U2923		
			A2180	U2316	U2401	U2488	A2578	U2664	U2751	C	U2924		
			A2181	U2317	U2402	U2489	A2579	U2665	U2752	C	U2925		
			A2182	U2318	U2403	U2490	A2580	U2666	U2753	C	U2926		
			A2183	U2319	U2404	U2491	A2581	U2667	U2754	C	U2927		
			A2184	U2320	U2405	U2492	A2582	U2668	U2755	C	U2928		
			A2185	U2321	U2406	U2493	A2583	U2669	U2756	C	U2929		
			A2186	U2322	U2407	U2494	A2584	U2670	U2757	C	U2930		
			A2187	U2323	U2408	U2495	A2585	U2671	U2758	C	U2931		
			A2188	U2324	U2409	U2496	A2586	U2672	U2759	C	U2932		
			A2189	U2325	U2410	U2497	A2587	U2673	U2760	C	U2933		
			A2190	U2326	U2411	U2498	A2588	U2674	U2761	C	U2934		
			A2191	U2327	U2412	U2499	A2589	U2675	U2762	C	U2935		
			A2192	U2328	U2413	U2500	A2590	U2676	U2763	C	U2936		
			A2193	U2329	U2414	U2501	A2591	U2677	U2764	C	U2937		
			A2194	U2330	U2415	U2502	A2592	U2678	U2765	C	U2938		
			A2195	U2331	U2416	U2503	A2593	U2679	U2766	C	U2939		
			A2196	U2332	U2417	U2504	A2594	U2680	U2767	C	U2940		
			A2197	U2333	U2418	U2505	A2595	U2681	U2768	C	U2941		
			A2198	U2334	U2419	U2506	A2596	U2682	U2769	C	U2942		
			A2199	U2335	U2420	U2507	A2597	U2683	U2770	C	U2943		
			A2200	U2336	U2421	U2508	A2598	U2684	U2771	C	U2944		
			A2201	U2337	U2422	U2509	A2599	U2685	U2772	C	U2945		
			A2202	U2338	U2423	U2510	A2600	U2686	U2773	C</			



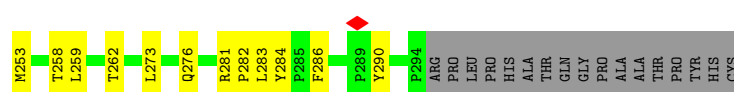
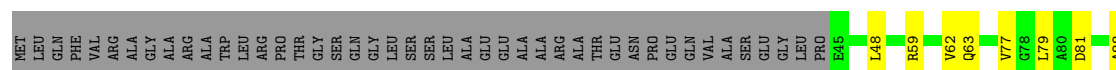
• Molecule 33: tRNAval



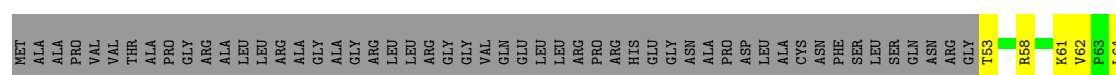
• Molecule 34: 39S ribosomal protein L2, mitochondrial



• Molecule 35: 39S ribosomal protein L4, mitochondrial



• Molecule 36: 39S ribosomal protein L9, mitochondrial

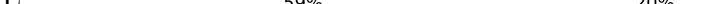


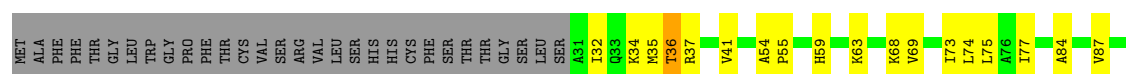
- Molecule 37: 39S ribosomal protein L13, mitochondrial

Chain K: 84% 15% .



- Molecule 38: 39S ribosomal protein L14, mitochondrial

Chain L:  59% 20% 21%



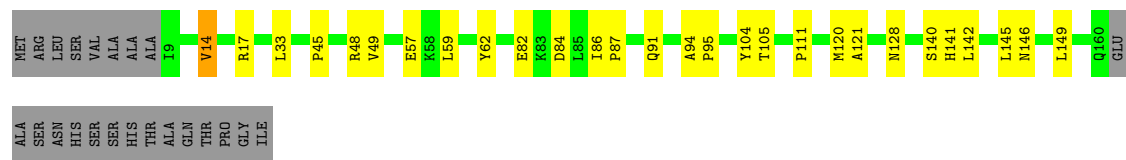
- Molecule 39: 39S ribosomal protein L15, mitochondrial

Chain M: 76% 21% .



- Molecule 40: 39S ribosomal protein L17, mitochondrial

Chain O: 71% 15% • 13%

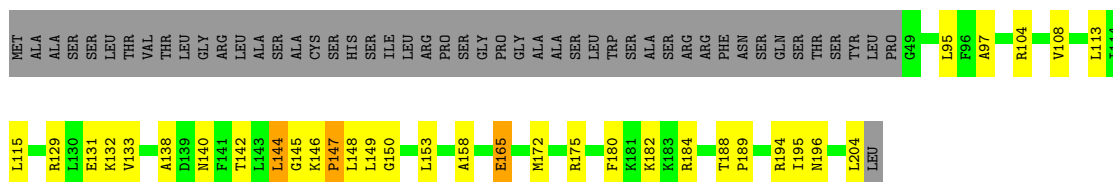


- Molecule 41: 39S ribosomal protein L20, mitochondrial

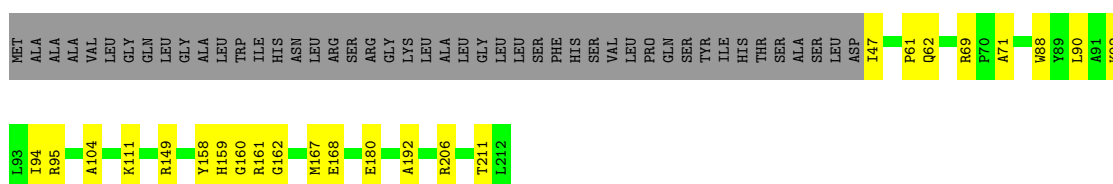
Chain R: 79% 13% • 6%



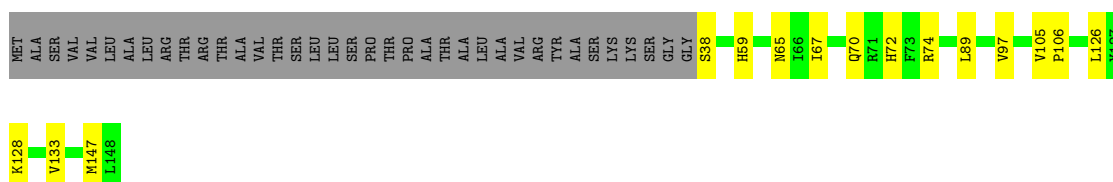
- Molecule 42: 39S ribosomal protein L21, mitochondrial



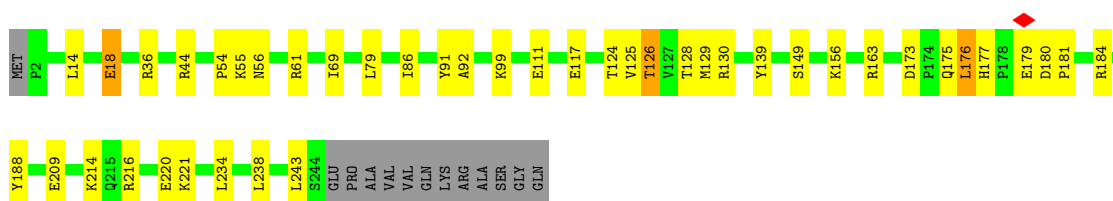
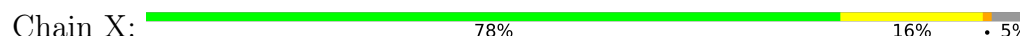
- Molecule 43: 39S ribosomal protein L22, mitochondrial



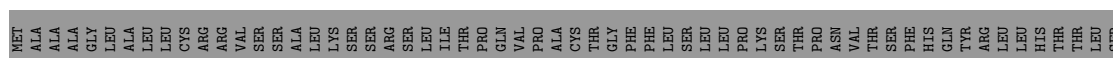
- Molecule 44: 39S ribosomal protein L27, mitochondrial

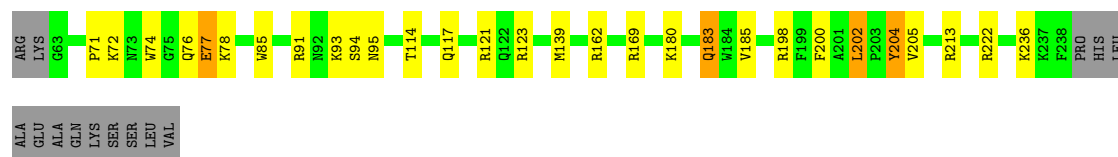


- Molecule 45: 39S ribosomal protein L28, mitochondrial



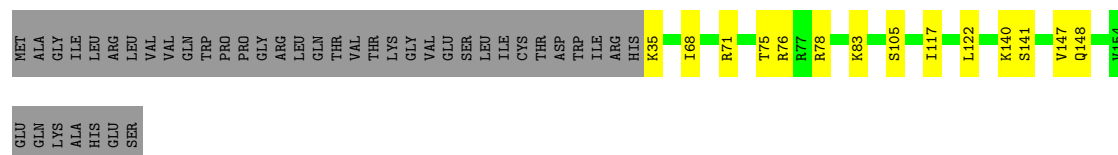
- Molecule 46: 39S ribosomal protein L47, mitochondrial





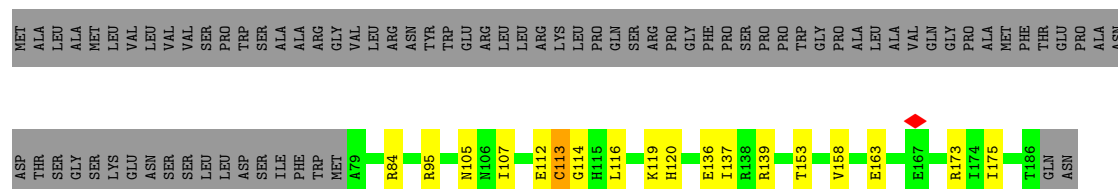
- Molecule 47: 39S ribosomal protein L30, mitochondrial

Chain Z: 66% 9% 25%



- Molecule 48: 39S ribosomal protein L32, mitochondrial

Chain 0: 48% 9% 43%



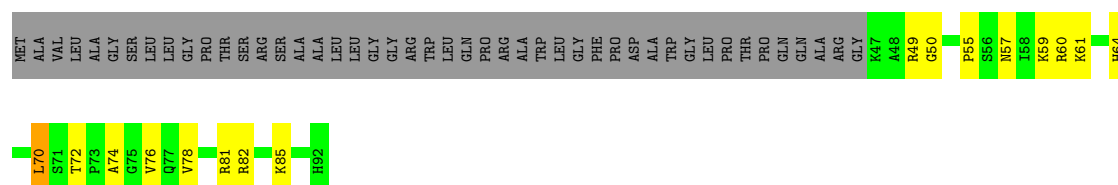
- Molecule 49: 39S ribosomal protein L33, mitochondrial

Chain 1: 58% 22% 20%



- Molecule 50: 39S ribosomal protein L34, mitochondrial

Chain 2: 33% 16% 50%

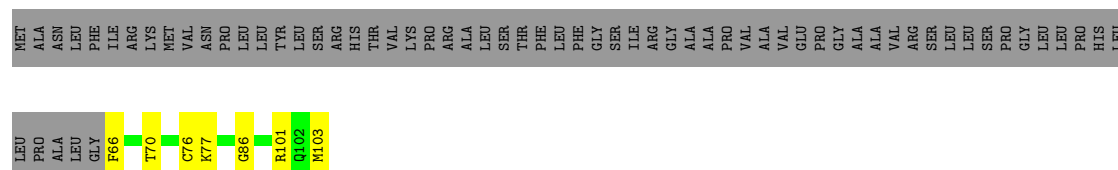


- Molecule 51: 39S ribosomal protein L35, mitochondrial

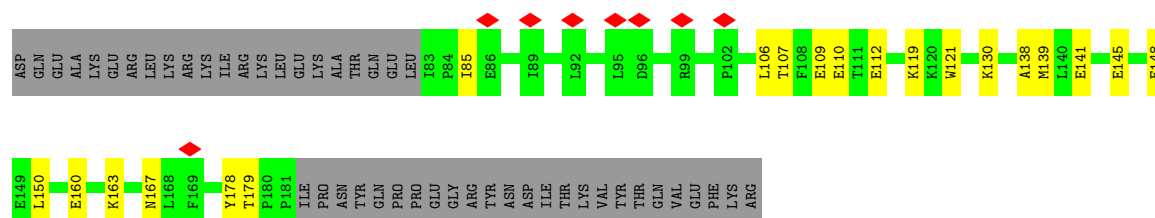
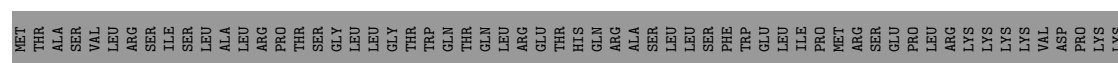
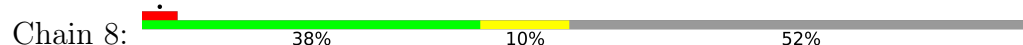
Chain 3: 36% 15% 49%



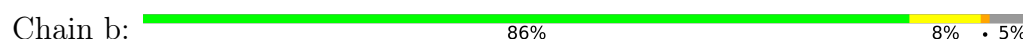
- Molecule 52: 39S ribosomal protein L36, mitochondrial



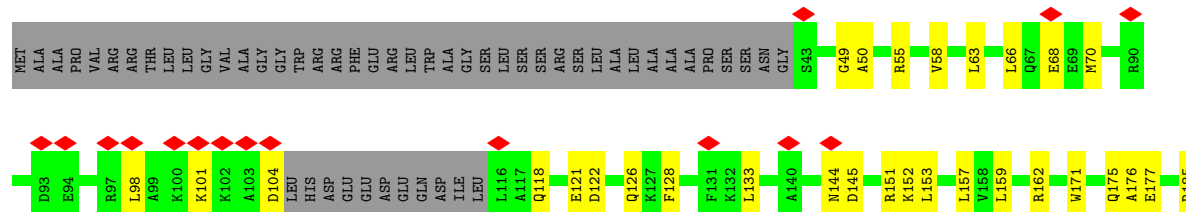
- Molecule 53: 39S ribosomal protein L40, mitochondrial

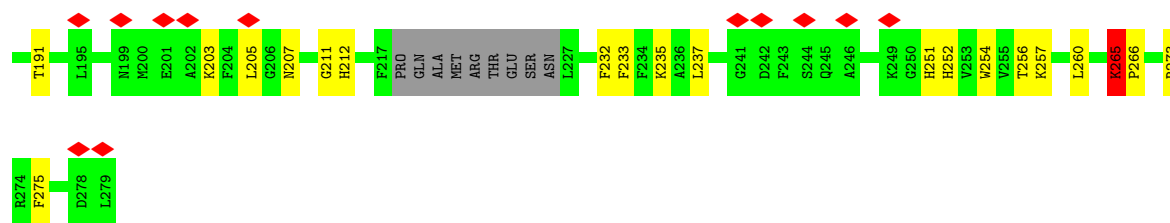


- Molecule 54: 39S ribosomal protein L43, mitochondrial

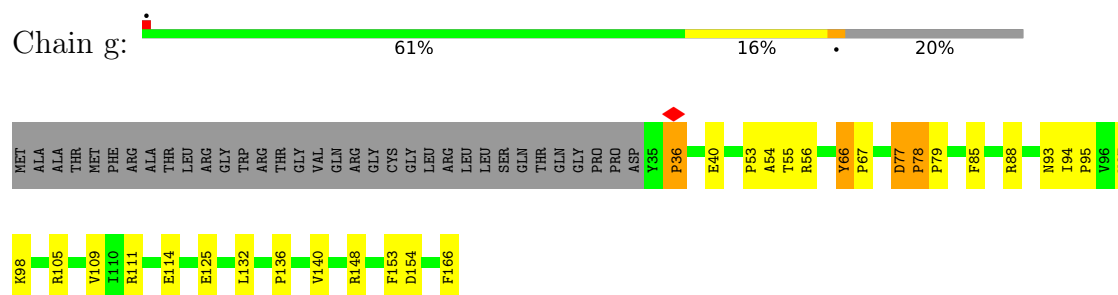


- Molecule 55: 39S ribosomal protein L46, mitochondrial

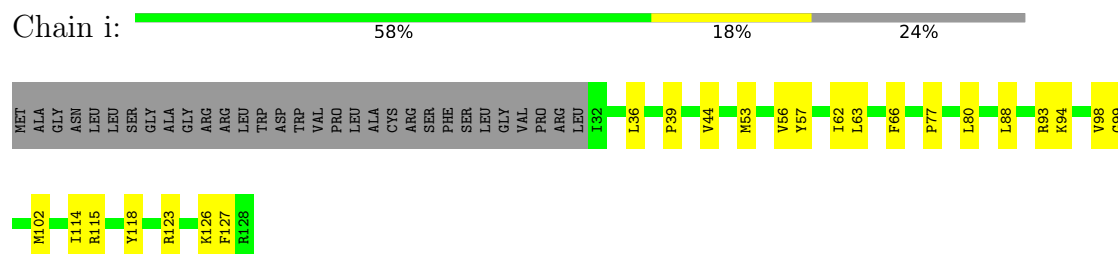




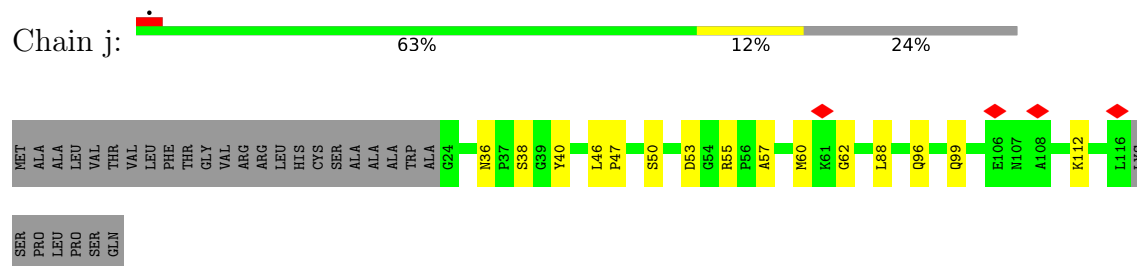
- Molecule 56: 39S ribosomal protein L49, mitochondrial



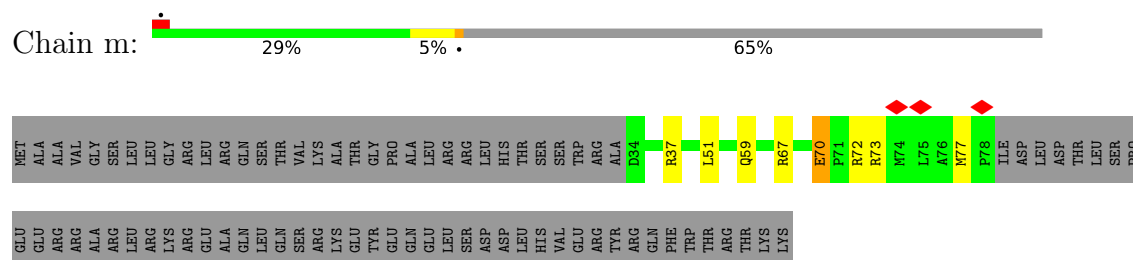
- Molecule 57: 39S ribosomal protein L51, mitochondrial



- Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



- Molecule 59: 39S ribosomal protein L55, mitochondrial



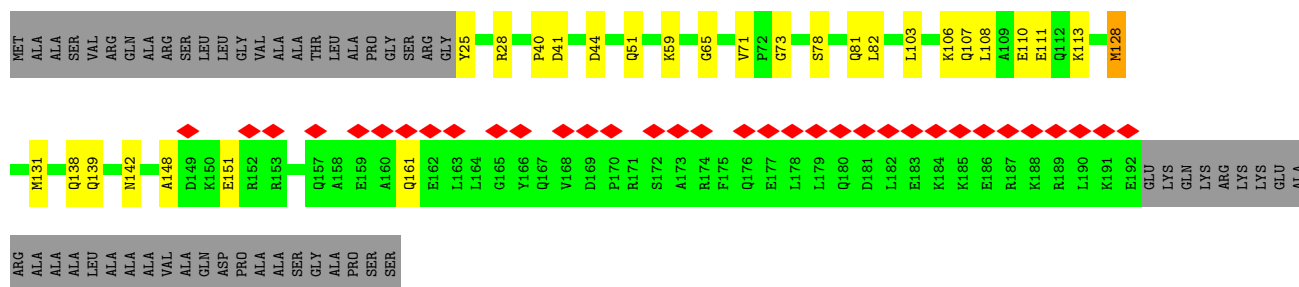
- Molecule 60: Ribosomal protein 63, mitochondrial

Chain o: 



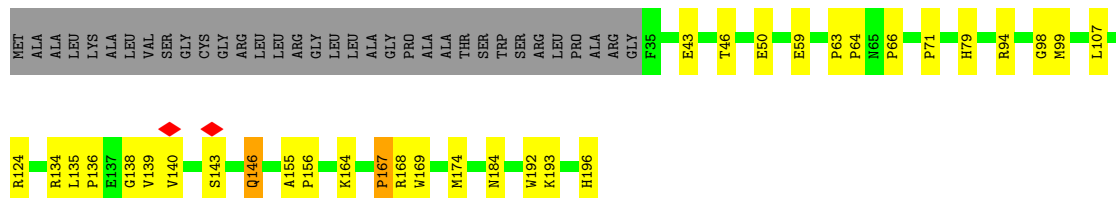
- Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q: 



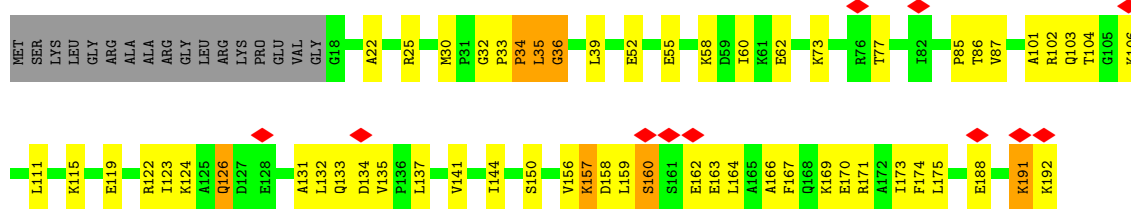
- Molecule 62: 39S ribosomal protein S18a, mitochondrial

Chain r: 



- Molecule 63: 39S ribosomal protein L11, mitochondrial

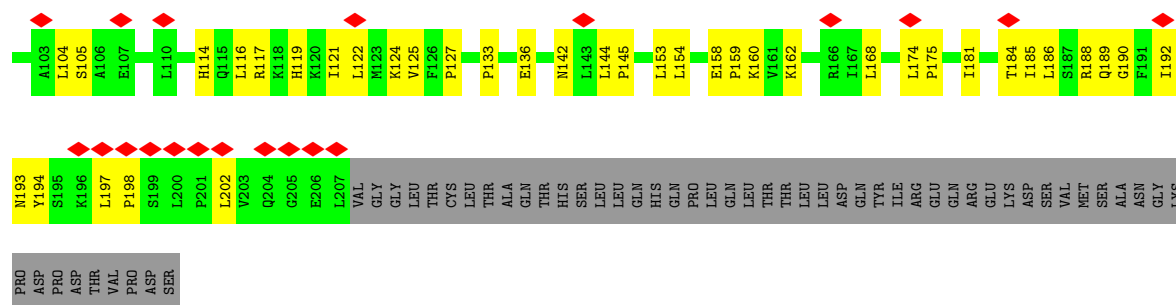
Chain J: 



- Molecule 64: 39S ribosomal protein L10, mitochondrial

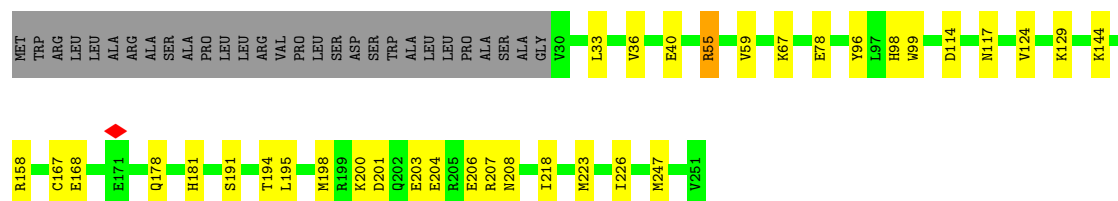
Chain I: 





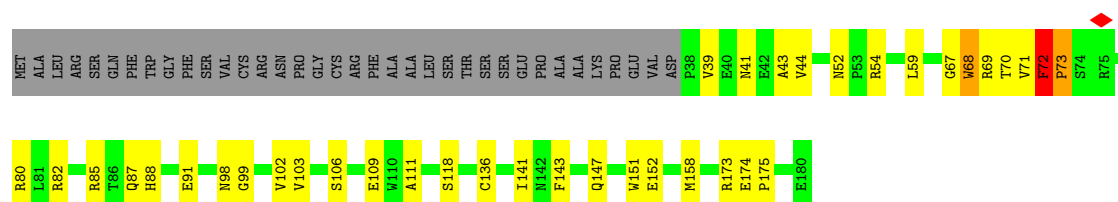
- Molecule 65: 39S ribosomal protein L16, mitochondrial

Chain N: 75% 14% 12%



- Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain P: 59% 20% 20%



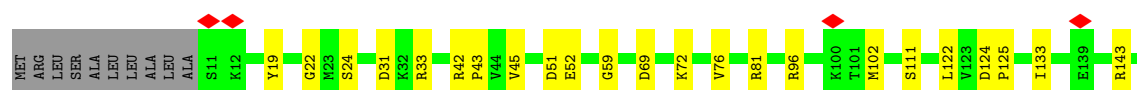
- Molecule 67: 39S ribosomal protein L23, mitochondrial

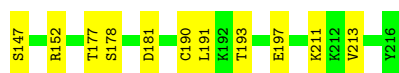
Chain U: 6% 76% 24%



- Molecule 68: 39S ribosomal protein L24, mitochondrial

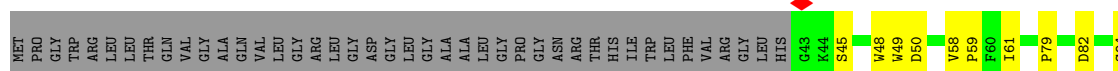
Chain V: 80% 16% 5%





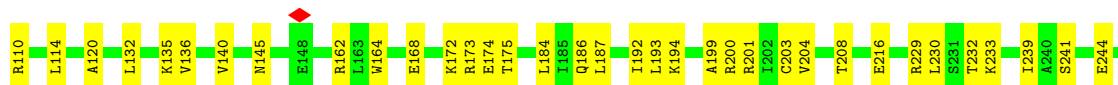
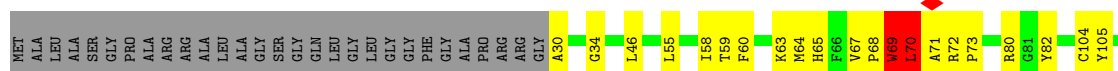
- Molecule 69: 39S ribosomal protein L3, mitochondrial

Chain E: 72% 16% 12%



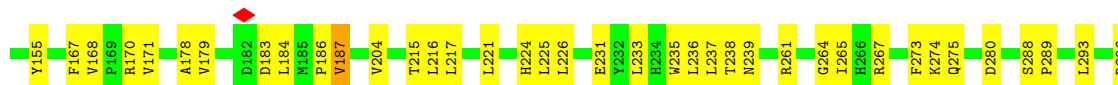
- Molecule 70: 39S ribosomal protein L37, mitochondrial

Chain 5: 73% 20% 7%



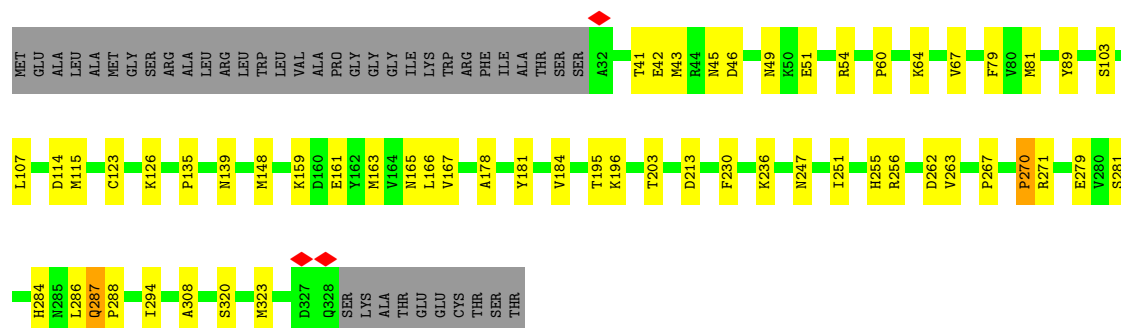
- Molecule 71: 39S ribosomal protein L38, mitochondrial

Chain 6: 73% 19% 7%



- Molecule 72: 39S ribosomal protein L39, mitochondrial

Chain 7: 71% 16% 12%



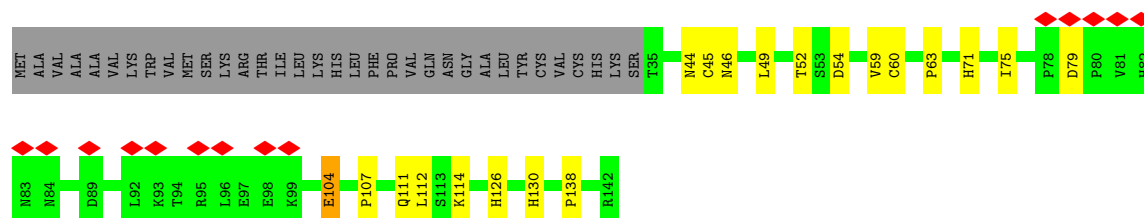
- Molecule 73: 39S ribosomal protein L41, mitochondrial

Chain 9: 78% 12% 9%



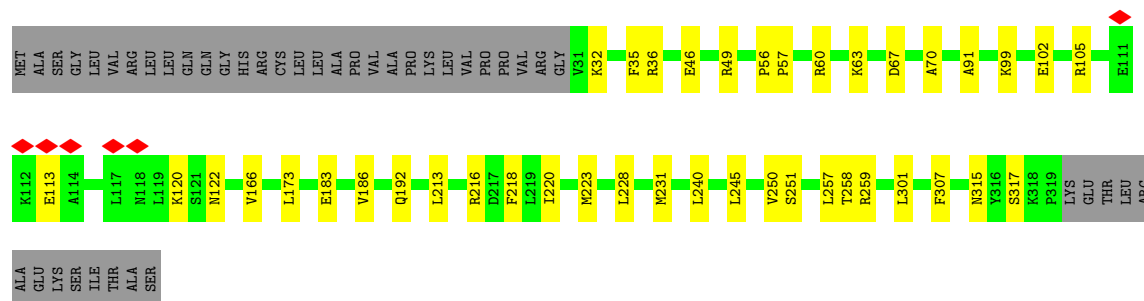
- Molecule 74: 39S ribosomal protein L42, mitochondrial

Chain a: 10% 62% 13% 24%



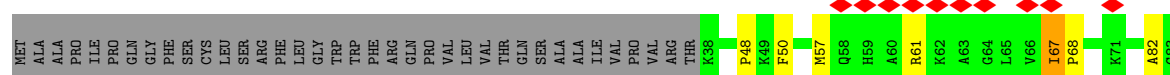
- Molecule 75: 39S ribosomal protein L44, mitochondrial

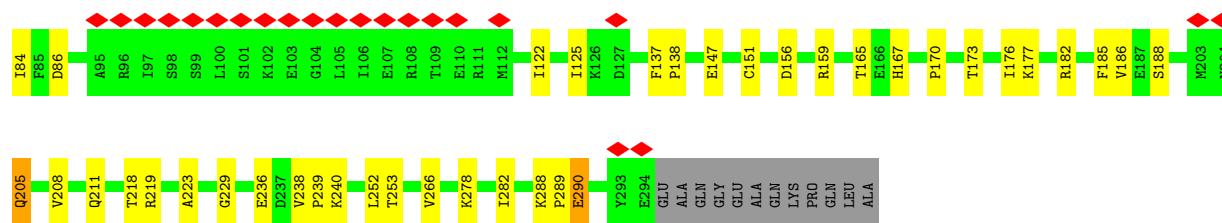
Chain c: 75% 12% 13%



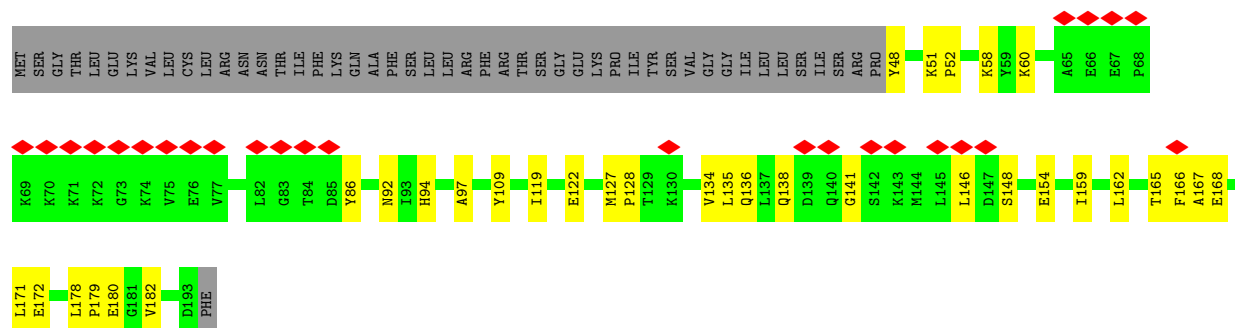
- Molecule 76: 39S ribosomal protein L45, mitochondrial

Chain d: 10% 69% 14% 16%

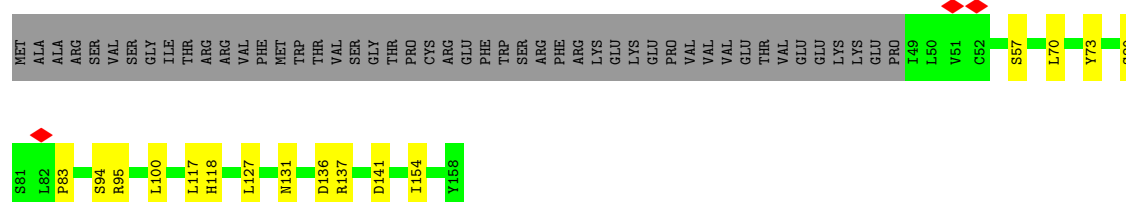




- Molecule 77: 39S ribosomal protein L48, mitochondrial



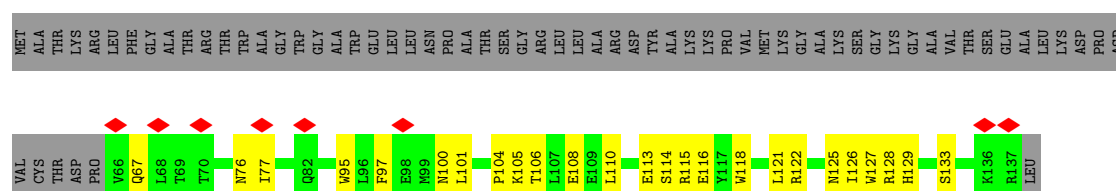
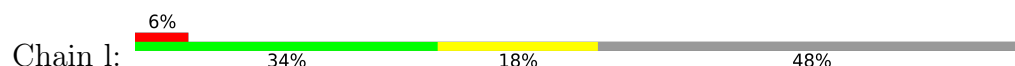
- Molecule 78: 39S ribosomal protein L50, mitochondrial



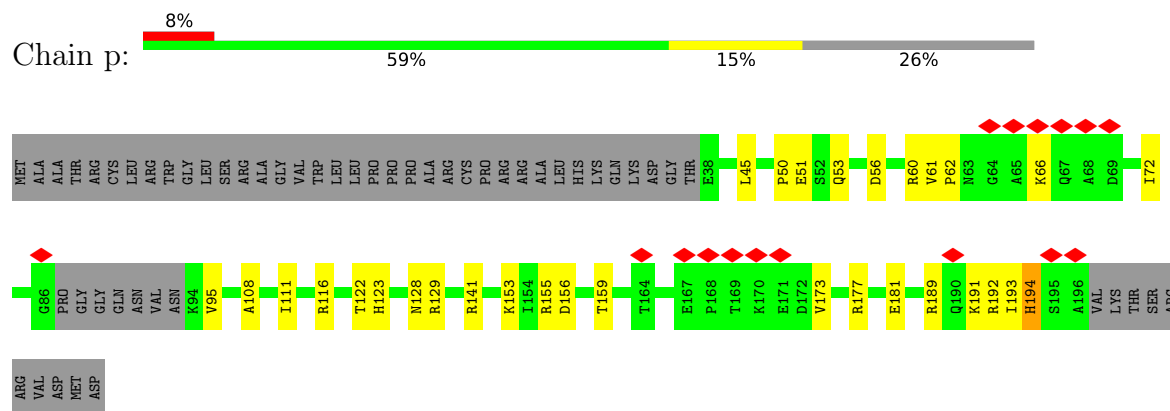
- Molecule 79: 39S ribosomal protein L53, mitochondrial



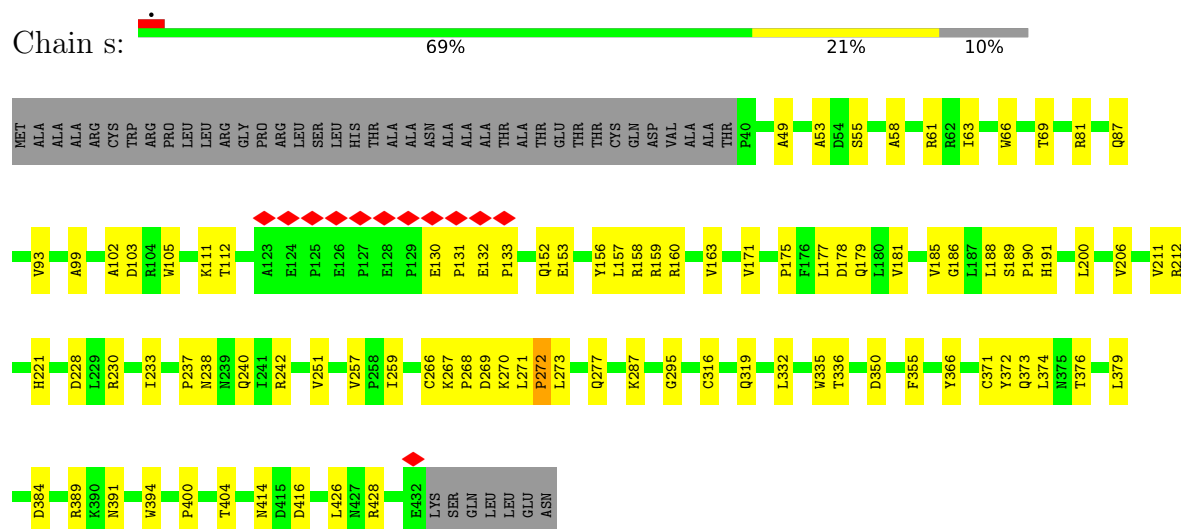
- Molecule 80: 39S ribosomal protein L54, mitochondrial



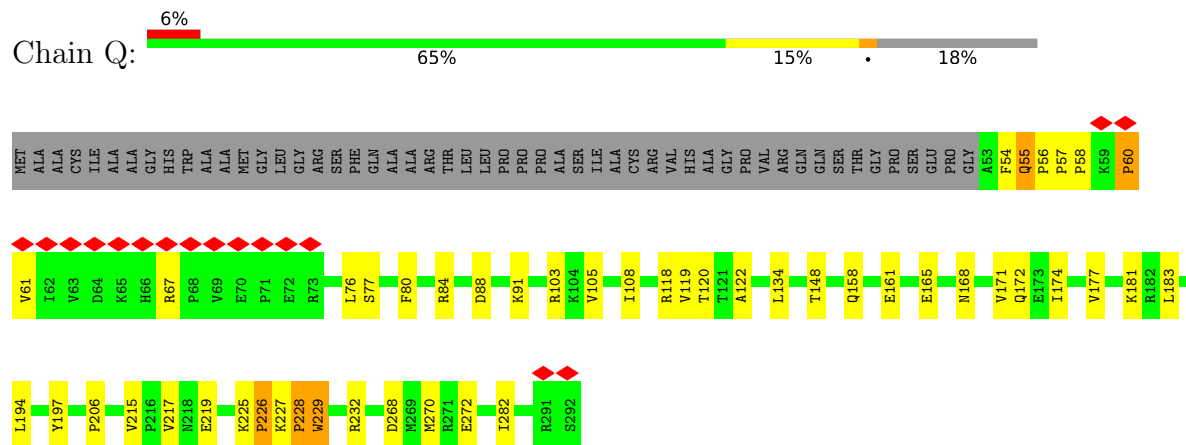
- Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 82: 39S ribosomal protein S30, mitochondrial

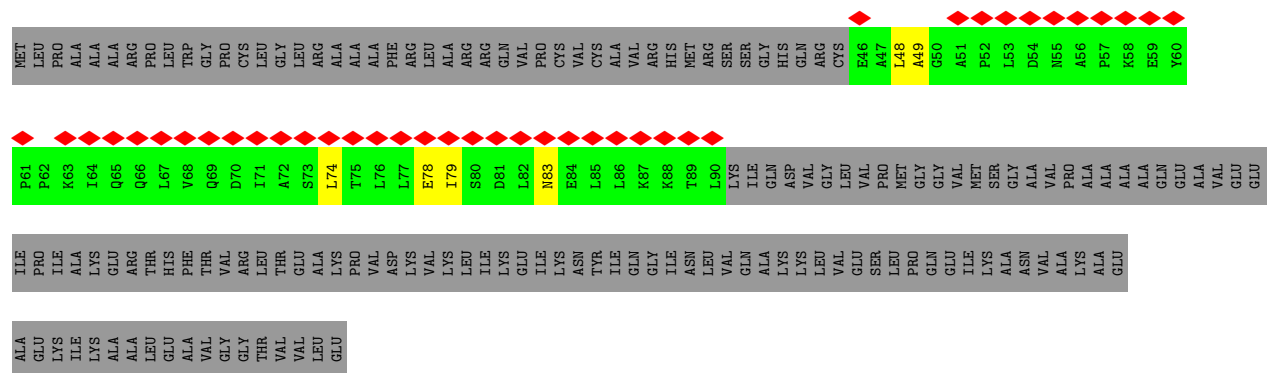


- Molecule 83: 39S ribosomal protein L19, mitochondrial

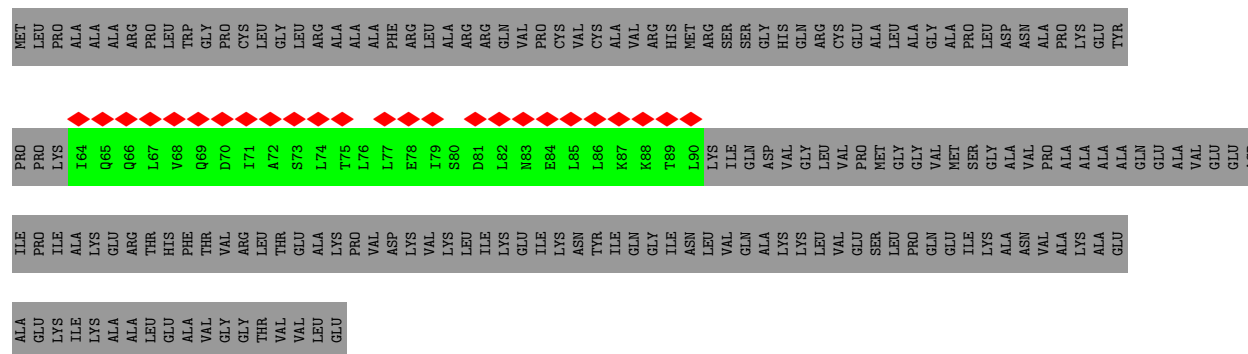


- Molecule 84: 39S ribosomal protein L12, mitochondrial

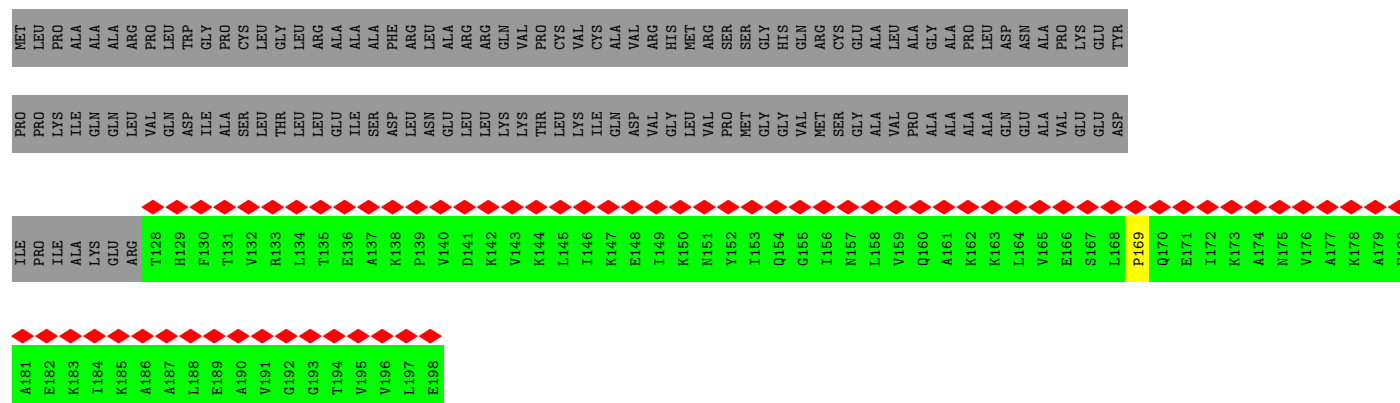




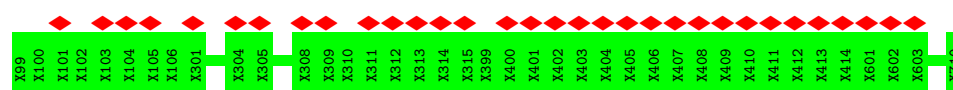
- Molecule 84: 39S ribosomal protein L12, mitochondrial



- Molecule 84: 39S ribosomal protein L12, mitochondrial



- Molecule 85: P-site finger



Chain v: 10% 68% 24% 5%



Y5P61	◆
Y5P62	◆
Y5P63	◆
Y5P64	◆
Y5P65	◆
Y5P66	◆
Y5P67	◆
Y5P68	◆
Y5P69	◆
Y5P70	◆
471	◆

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99804	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 ($e^-/\text{\AA}^2$)	69.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.725	Depositor
Minimum map value	-1.810	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.267	Depositor
Map size ($\text{\AA}$)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, Y5P, P5P, GDP, GCP

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	AA	0.06	0/22406	0.16	0/34881
2	AB	0.07	0/1830	0.23	0/2477
3	AC	0.07	0/1112	0.24	0/1505
4	AE	0.09	0/989	0.37	0/1335
5	AI	0.08	0/1031	0.34	0/1390
6	AJ	0.09	0/854	0.27	0/1148
7	AK	0.09	0/879	0.29	0/1182
8	AM	0.08	0/941	0.25	0/1265
9	AN	0.07	0/864	0.22	0/1169
10	AO	0.08	0/1624	0.22	0/2209
11	AP	0.07	0/791	0.21	0/1062
12	AQ	0.09	0/752	0.27	0/1001
13	AT	0.08	0/1402	0.21	0/1883
14	AW	0.08	0/778	0.27	0/1048
15	AX	0.08	0/2932	0.22	0/3968
16	A2	0.09	0/939	0.27	0/1256
17	AH	0.07	0/1037	0.21	0/1403
18	AL	0.09	0/1475	0.24	0/1970
19	AR	0.07	0/2435	0.21	0/3288
20	AS	0.09	0/1138	0.24	0/1533
21	AU	0.10	0/1521	0.26	0/2039
22	AV	0.08	0/3071	0.22	0/4147
23	AY	0.10	0/1046	0.34	0/1410
24	AZ	0.07	0/851	0.22	0/1133
25	A1	0.08	0/2277	0.24	0/3079
26	A0	0.08	0/1827	0.26	0/2473
27	A3	0.10	0/650	0.31	0/855
28	A4	0.06	0/3028	0.16	0/4197
29	AD	0.07	0/2783	0.23	0/3724
30	AF	0.09	0/1765	0.27	0/2369
31	AG	0.07	0/2642	0.23	0/3538
32	A	0.07	0/36246	0.18	0/56422

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B	0.06	0/1328	0.15	0/2056
34	D	0.08	0/1904	0.25	0/2561
35	F	0.08	0/2071	0.26	0/2817
36	H	0.10	0/820	0.29	0/1102
37	K	0.07	0/1495	0.24	0/2029
38	L	0.07	0/904	0.24	0/1218
39	M	0.09	0/2359	0.27	0/3185
40	O	0.10	0/1269	0.29	0/1708
41	R	0.10	0/1174	0.44	2/1572 (0.1%)
42	S	0.10	0/1276	0.40	3/1729 (0.2%)
43	T	0.07	0/1402	0.24	0/1886
44	W	0.07	0/893	0.22	0/1204
45	X	0.07	0/2081	0.23	0/2812
46	Y	0.08	0/1552	0.25	0/2079
47	Z	0.07	0/1003	0.23	0/1354
48	0	0.08	0/895	0.26	0/1201
49	1	0.07	0/438	0.26	0/583
50	2	0.08	0/382	0.27	0/507
51	3	0.08	0/852	0.24	0/1136
52	4	0.09	0/350	0.30	0/461
53	8	0.09	0/855	0.24	0/1152
54	b	0.08	0/1202	0.26	0/1626
55	e	0.08	0/1797	0.25	0/2422
56	g	0.12	0/1132	0.30	0/1543
57	i	0.09	0/849	0.27	0/1135
58	j	0.08	0/755	0.25	0/1016
59	m	0.09	0/379	0.28	0/510
60	o	0.11	0/818	0.36	0/1097
61	q	0.10	0/1325	0.33	0/1799
62	r	0.09	0/1362	0.25	0/1846
63	J	0.27	1/1348 (0.1%)	0.38	0/1813
64	I	0.09	0/1467	0.28	0/1984
65	N	0.08	0/1833	0.25	0/2468
66	P	0.15	0/1191	0.38	0/1611
67	U	0.10	0/1254	0.27	0/1700
68	V	0.09	0/1727	0.25	0/2341
69	E	0.07	0/2479	0.20	0/3360
70	5	0.17	1/3305 (0.0%)	0.31	0/4502
71	6	0.08	0/3043	0.24	0/4140
72	7	0.07	0/2467	0.22	0/3337
73	9	0.08	0/1025	0.24	0/1379
74	a	0.08	0/923	0.22	0/1254
75	c	0.08	0/2371	0.23	0/3205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.09	0/2132	0.25	0/2887
77	f	0.06	0/1144	0.21	0/1551
78	h	0.08	0/917	0.24	0/1249
79	k	0.10	0/754	0.27	0/1017
80	l	0.08	0/636	0.23	0/860
81	p	0.09	0/1246	0.25	0/1675
82	s	0.09	0/3262	0.29	0/4435
83	Q	0.11	0/2044	0.27	0/2757
84	TA	0.12	0/349	0.39	0/475
84	TB	0.06	0/212	0.16	0/286
84	TC	0.07	0/351	0.27	0/488
86	v	0.14	0/5647	0.34	0/7623
All	All	0.09	2/181965 (0.0%)	0.24	5/258102 (0.0%)

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
41	R	0	1
42	S	0	1
56	g	0	1
66	P	0	1
82	s	0	1
86	v	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	J	188	GLU	C-N	8.15	1.45	1.34
70	5	69	TRP	NE1-CE2	-5.47	1.31	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S	144	LEU	CA-C-N	-6.20	109.27	121.41
42	S	144	LEU	C-N-CA	-6.20	109.27	121.41
42	S	145	GLY	N-CA-C	5.96	127.31	113.18
41	R	136	LYS	CA-C-N	5.65	135.58	121.80
41	R	136	LYS	C-N-CA	5.65	135.58	121.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	P	72	PHE	Peptide
41	R	134	ASP	Peptide
42	S	144	LEU	Peptide
56	g	79	PRO	Peptide
82	s	160	ARG	Peptide
86	v	338	LYS	Peptide

5.2 Too-close contacts

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	AA	20030	0	10171	256	0
2	AB	1787	0	1779	27	0
3	AC	1082	0	1088	25	0
4	AE	972	0	1001	13	0
5	AI	1011	0	1052	14	0
6	AJ	838	0	887	17	0
7	AK	861	0	885	23	0
8	AM	920	0	951	13	0
9	AN	846	0	908	14	0
10	AO	1570	0	1534	18	0
11	AP	774	0	803	11	0
12	AQ	740	0	754	12	0
13	AT	1371	0	1396	14	0
14	AW	766	0	785	13	0
15	AX	2860	0	2856	43	0
16	A2	925	0	964	15	0
17	AH	1014	0	1036	20	0
18	AL	1451	0	1543	15	0
19	AR	2388	0	2410	28	0
20	AS	1111	0	1115	7	0
21	AU	1499	0	1512	13	0
22	AV	3009	0	3006	51	0
23	AY	1016	0	962	17	0
24	AZ	833	0	853	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A1	2231	0	2261	28	0
26	A0	1781	0	1791	20	0
27	A3	639	0	715	5	0
28	A4	3010	0	1760	14	0
29	AD	2731	0	2802	48	0
30	AF	1724	0	1765	17	0
31	AG	2587	0	2572	24	0
32	A	32395	0	16450	525	0
33	B	1191	0	607	12	0
34	D	1866	0	1927	30	0
35	F	2013	0	2044	35	0
36	H	806	0	849	18	0
37	K	1451	0	1448	15	0
38	L	889	0	941	18	0
39	M	2305	0	2378	44	0
40	O	1245	0	1283	17	0
41	R	1153	0	1214	16	0
42	S	1251	0	1322	27	0
43	T	1368	0	1410	16	0
44	W	871	0	897	12	0
45	X	2027	0	2040	30	0
46	Y	1517	0	1561	27	0
47	Z	978	0	1030	10	0
48	0	880	0	904	11	0
49	1	433	0	475	20	0
50	2	376	0	406	13	0
51	3	831	0	883	20	0
52	4	342	0	362	6	0
53	8	836	0	844	17	0
54	b	1178	0	1180	10	0
55	e	1762	0	1767	33	0
56	g	1096	0	1081	22	0
57	i	827	0	857	17	0
58	j	740	0	741	9	0
59	m	372	0	387	5	0
60	o	797	0	804	14	0
61	q	1294	0	1178	20	0
62	r	1322	0	1350	22	0
63	J	1330	0	1405	129	0
64	I	1435	0	1519	81	0
65	N	1786	0	1817	33	0
66	P	1165	0	1162	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	U	1224	0	1191	26	0
68	V	1682	0	1692	24	0
69	E	2410	0	2418	37	0
70	5	3210	0	3206	111	0
71	6	2948	0	2841	53	0
72	7	2410	0	2415	32	0
73	9	997	0	987	12	0
74	a	896	0	847	15	0
75	c	2322	0	2338	23	0
76	d	2075	0	2037	30	0
77	f	1126	0	1106	24	0
78	h	894	0	881	9	0
79	k	743	0	758	13	0
80	l	619	0	611	47	0
81	p	1227	0	1239	23	0
82	s	3178	0	3124	65	0
83	Q	1995	0	2036	37	0
84	TA	345	0	364	5	0
84	TB	213	0	234	0	0
84	TC	352	0	169	0	0
85	u	325	0	76	0	0
86	v	5546	0	5505	142	0
87	A5	213	0	122	14	0
88	A7	1197	0	690	33	0
89	A	97	0	0	0	0
89	A2	1	0	0	0	0
89	AA	26	0	0	0	0
89	AH	1	0	0	0	0
89	D	1	0	0	0	0
89	E	1	0	0	0	0
89	W	1	0	0	0	0
89	g	1	0	0	0	0
89	v	1	0	0	0	0
90	0	1	0	0	0	0
90	4	1	0	0	0	0
90	AB	1	0	0	0	0
90	AO	1	0	0	0	0
90	AP	1	0	0	0	0
90	AT	1	0	0	0	0
90	r	1	0	0	0	0
91	AX	28	0	9	0	0
92	v	32	0	14	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	174849	0	147350	2370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2370) 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)
70:5:60:PHE:CD1	70:5:71:ALA:HB1	1.25	1.65
63:J:171:ARG:HA	63:J:174:PHE:CE2	1.29	1.65
70:5:68:PRO:HG2	70:5:69:TRP:CE3	1.24	1.63
63:J:132:LEU:HG	64:I:114:HIS:CG	1.40	1.52
45:X:156:LYS:NZ	70:5:70:LEU:HD23	1.25	1.47
86:v:59:LYS:CG	92:v:802:GCP:O1B	1.65	1.43
70:5:68:PRO:HG2	70:5:69:TRP:CZ3	1.54	1.41
86:v:301:LEU:HD22	92:v:802:GCP:C2	1.51	1.41
63:J:174:PHE:CE1	63:J:175:LEU:CD2	2.11	1.34
70:5:68:PRO:CG	70:5:69:TRP:CZ3	2.14	1.31
63:J:132:LEU:CB	64:I:114:HIS:HB2	1.63	1.29
49:1:61:LYS:HG3	88:A7:1:P5P:C5'	1.64	1.27
63:J:174:PHE:CE1	63:J:175:LEU:HD22	1.69	1.27
70:5:60:PHE:HE1	70:5:71:ALA:C	1.41	1.26
32:A:3110:C:H42	32:A:3203:A:N6	1.33	1.25
63:J:111:LEU:HD13	63:J:170:GLU:OE2	1.23	1.25
70:5:60:PHE:CD1	70:5:71:ALA:CB	2.19	1.25
70:5:68:PRO:CG	70:5:69:TRP:CE3	2.20	1.24
63:J:132:LEU:HG	64:I:114:HIS:CD2	1.73	1.22
63:J:171:ARG:CA	63:J:174:PHE:CE2	2.25	1.20
86:v:301:LEU:CD2	92:v:802:GCP:N3	2.06	1.19
49:1:61:LYS:O	88:A7:1:P5P:H4'	1.42	1.18
86:v:301:LEU:HD21	92:v:802:GCP:N3	1.59	1.17
63:J:132:LEU:HB3	64:I:114:HIS:HB2	1.25	1.17
70:5:67:VAL:HG23	70:5:71:ALA:HB3	1.16	1.13
63:J:134:ASP:OD2	64:I:122:LEU:HD11	1.49	1.12
29:AD:147:PRO:HG3	87:A5:10:Y5P:HA	1.30	1.11
32:A:2170:G:O2'	63:J:87:VAL:HG21	1.51	1.11
63:J:132:LEU:CG	64:I:114:HIS:CG	2.33	1.11
63:J:159:LEU:HB3	63:J:162:GLU:HB3	1.28	1.10
86:v:78:GLU:HG3	92:v:802:GCP:H3'	1.27	1.10
45:X:156:LYS:NZ	70:5:70:LEU:CD2	2.13	1.09
70:5:60:PHE:HD1	70:5:71:ALA:CB	1.58	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:5:60:PHE:CE1	70:5:71:ALA:C	2.29	1.09
86:v:301:LEU:CD2	92:v:802:GCP:C2	2.30	1.09
29:AD:227:ASN:HD21	87:A5:1:Y5P:H4	1.12	1.09
49:1:40:LYS:NZ	88:A7:60:Y5P:OP1	1.82	1.09
45:X:156:LYS:HZ2	70:5:70:LEU:CD2	1.63	1.08
32:A:3110:C:N4	32:A:3203:A:H61	1.50	1.08
64:I:81:LEU:HB3	80:l:115:ARG:HH12	1.18	1.08
49:1:61:LYS:CG	88:A7:1:P5P:H5'1	1.85	1.07
63:J:171:ARG:NH2	80:l:76:ASN:O	1.88	1.06
70:5:68:PRO:HG3	70:5:69:TRP:HZ3	1.18	1.04
63:J:132:LEU:HG	64:I:114:HIS:CB	1.86	1.04
86:v:58:GLY:CA	92:v:802:GCP:O2A	2.05	1.04
70:5:67:VAL:CG2	70:5:71:ALA:HB3	1.89	1.03
70:5:60:PHE:HE1	70:5:71:ALA:O	1.39	1.02
70:5:60:PHE:CE1	70:5:71:ALA:O	2.13	1.02
70:5:67:VAL:HG23	70:5:71:ALA:CB	1.90	1.02
63:J:167:PHE:O	63:J:171:ARG:HD3	1.60	1.02
63:J:171:ARG:HA	63:J:174:PHE:CD2	1.95	1.01
63:J:159:LEU:HD13	63:J:162:GLU:HG2	1.40	1.01
70:5:203:CYS:O	82:s:179:GLN:NE2	1.94	1.00
70:5:67:VAL:CG2	70:5:71:ALA:CB	2.39	0.99
86:v:301:LEU:CD2	92:v:802:GCP:C4	2.41	0.99
32:A:1721:C:H42	32:A:1730:U:H3	1.00	0.99
63:J:174:PHE:CE1	63:J:175:LEU:HD23	1.99	0.98
29:AD:227:ASN:ND2	87:A5:1:Y5P:H4	1.77	0.98
63:J:132:LEU:CG	64:I:114:HIS:CB	2.42	0.98
70:5:68:PRO:CG	70:5:69:TRP:HZ3	1.63	0.97
1:AA:1197:G:H1	1:AA:1425:U:H3	1.04	0.97
86:v:175:LYS:HA	92:v:802:GCP:O6	1.64	0.97
63:J:132:LEU:C	64:I:117:ARG:HE	1.71	0.97
63:J:174:PHE:HE1	63:J:175:LEU:CD2	1.64	0.96
86:v:58:GLY:HA2	92:v:802:GCP:O2A	1.64	0.96
86:v:59:LYS:HG2	92:v:802:GCP:O1B	0.78	0.95
32:A:3125:A:N6	32:A:3132:G:H21	1.65	0.94
32:A:2174:G:N2	63:J:102:ARG:O	2.02	0.93
86:v:301:LEU:HD21	92:v:802:GCP:C4	1.99	0.92
32:A:3010:G:H1	32:A:3027:U:H3	1.09	0.92
63:J:132:LEU:CB	64:I:114:HIS:CB	2.48	0.92
70:5:279:PHE:HA	82:s:156:TYR:CE2	2.05	0.91
70:5:279:PHE:HA	82:s:156:TYR:HE2	1.31	0.91
63:J:111:LEU:CD1	63:J:170:GLU:OE2	2.17	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3013:G:H1	32:A:3024:U:H3	1.20	0.90
32:A:3110:C:H42	32:A:3203:A:H61	0.91	0.90
49:1:61:LYS:HG3	88:A7:1:P5P:H5'1	0.92	0.89
63:J:174:PHE:HE1	63:J:175:LEU:HD22	1.23	0.89
63:J:167:PHE:O	63:J:171:ARG:CD	2.21	0.89
63:J:133:GLN:N	64:I:117:ARG:NE	2.21	0.89
63:J:171:ARG:HA	63:J:174:PHE:HE2	1.10	0.89
32:A:2549:C:H42	32:A:2565:A:H62	1.18	0.88
29:AD:117:ARG:HD2	87:A5:1:Y5P:HB	1.53	0.88
45:X:156:LYS:HZ3	70:5:70:LEU:HD23	1.39	0.88
63:J:132:LEU:HA	64:I:114:HIS:ND1	1.89	0.87
32:A:1724:A:H61	32:A:2040:G:N2	1.73	0.87
70:5:204:VAL:HG13	82:s:152:GLN:HE21	1.39	0.87
32:A:3110:C:N4	32:A:3203:A:N6	2.14	0.86
49:1:61:LYS:O	88:A7:1:P5P:C4'	2.22	0.86
32:A:3049:U:H3	32:A:3053:A:H62	1.20	0.86
70:5:69:TRP:H	70:5:69:TRP:HE3	1.18	0.86
32:A:3125:A:H62	32:A:3132:G:N2	1.73	0.86
86:v:78:GLU:HG3	92:v:802:GCP:C3'	2.06	0.86
1:AA:1430:A:H5'	30:AF:35:SER:HB3	1.58	0.85
49:1:40:LYS:CE	88:A7:60:Y5P:OP1	2.23	0.85
32:A:2187:C:C4	63:J:103:GLN:OE1	2.30	0.85
63:J:170:GLU:O	63:J:174:PHE:CD2	2.30	0.84
63:J:156:VAL:O	63:J:157:LYS:O	1.95	0.84
70:5:60:PHE:CE1	70:5:71:ALA:HB1	2.10	0.83
86:v:301:LEU:HD22	92:v:802:GCP:N1	1.93	0.83
86:v:59:LYS:HD2	92:v:802:GCP:O2G	1.77	0.83
64:I:78:LEU:HD11	80:l:118:TRP:CE3	2.14	0.83
32:A:1721:C:N4	32:A:1730:U:H3	1.77	0.83
32:A:2549:C:N4	32:A:2565:A:H62	1.76	0.83
45:X:156:LYS:HZ3	70:5:70:LEU:CD2	1.91	0.82
32:A:2170:G:O2'	63:J:87:VAL:CG2	2.27	0.82
32:A:3033:U:H5''	32:A:3034:U:H5'	1.61	0.82
32:A:2171:U:OP1	63:J:86:THR:OG1	1.96	0.82
63:J:132:LEU:CG	64:I:114:HIS:HB2	2.06	0.81
32:A:3179:G:H21	32:A:3190:A:N6	1.78	0.81
64:I:81:LEU:HB2	80:l:115:ARG:HH22	1.46	0.81
32:A:2200:A:O2'	80:l:133:SER:O	1.97	0.81
70:5:68:PRO:HG3	70:5:69:TRP:CZ3	1.97	0.81
70:5:69:TRP:HE3	70:5:69:TRP:N	1.79	0.81
32:A:3125:A:N6	32:A:3132:G:N2	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2203:G:N2	32:A:2208:A:H62	1.78	0.80
32:A:2939:C:H42	32:A:2991:U:H3	1.27	0.80
1:AA:735:A:N6	1:AA:740:G:N1	2.29	0.80
64:I:81:LEU:HB3	80:I:115:ARG:NH1	1.96	0.80
70:5:68:PRO:HG2	70:5:69:TRP:HE3	0.97	0.79
32:A:2213:A:O2'	80:I:129:HIS:CD2	2.35	0.79
86:v:122:PRO:O	92:v:802:GCP:O2G	2.01	0.79
32:A:2613:U:H3	32:A:2619:A:H61	1.30	0.78
64:I:81:LEU:CB	80:I:115:ARG:HH12	1.95	0.78
63:J:132:LEU:CA	64:I:114:HIS:HB2	2.13	0.78
63:J:159:LEU:HD13	63:J:162:GLU:CG	2.14	0.78
32:A:2203:G:H21	32:A:2208:A:N6	1.81	0.78
32:A:1724:A:N6	32:A:2040:G:N2	2.32	0.77
70:5:278:GLY:HA2	82:s:158:ARG:HG3	1.65	0.77
33:B:1607:U:H3	33:B:1664:G:H1	1.31	0.77
63:J:174:PHE:CD1	63:J:175:LEU:HD22	2.19	0.77
39:M:140:LEU:HB2	39:M:156:VAL:HG11	1.67	0.77
32:A:2374:A:H62	82:s:272:PRO:HB2	1.49	0.77
86:v:59:LYS:HG2	92:v:802:GCP:PB	2.19	0.77
86:v:319:ASN:O	86:v:322:GLU:N	2.14	0.77
22:AV:131:ASN:HB3	22:AV:135:TYR:HB2	1.68	0.76
32:A:3179:G:N2	32:A:3190:A:H62	1.83	0.76
32:A:1711:C:OP2	70:5:72:ARG:NH2	2.18	0.76
63:J:159:LEU:O	63:J:163:GLU:CG	2.33	0.76
22:AV:93:TYR:HB2	83:Q:54:PHE:HB2	1.66	0.76
32:A:2909:G:H1'	88:A7:69:Y5P:H4A	1.68	0.76
86:v:319:ASN:HB2	86:v:320:PRO:HD2	1.68	0.76
6:AJ:105:HIS:H	86:v:489:LYS:HZ3	1.32	0.75
46:Y:200:PHE:CB	70:5:68:PRO:HG3	2.17	0.75
61:q:78:SER:H	61:q:81:GLN:HE21	1.35	0.75
88:A7:59:Y5P:H4A	88:A7:60:Y5P:H4	1.68	0.75
32:A:2549:C:H42	32:A:2565:A:N6	1.85	0.74
46:Y:200:PHE:HB2	70:5:68:PRO:HG3	1.68	0.74
63:J:132:LEU:CG	64:I:114:HIS:CD2	2.62	0.74
32:A:1724:A:N6	32:A:2040:G:H21	1.85	0.74
70:5:192:ILE:HG21	82:s:186:GLY:O	1.88	0.73
88:A7:61:Y5P:H4A	88:A7:62:Y5P:H4	1.70	0.73
22:AV:151:PHE:HA	22:AV:156:ASN:HD22	1.53	0.73
32:A:3110:C:N3	32:A:3203:A:N1	2.37	0.72
48:0:113:CYS:SG	48:0:114:GLY:N	2.62	0.72
63:J:134:ASP:OD2	64:I:122:LEU:CD1	2.32	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D:111:ARG:HH22	34:D:163:ILE:HD12	1.53	0.72
63:J:164:LEU:CD2	80:l:77:ILE:O	2.37	0.72
32:A:2203:G:H21	32:A:2208:A:H62	1.34	0.72
32:A:2187:C:C5	63:J:103:GLN:OE1	2.44	0.71
63:J:132:LEU:HA	64:I:114:HIS:CG	2.26	0.71
63:J:132:LEU:HA	64:I:114:HIS:HD1	1.55	0.71
83:Q:225:LYS:O	83:Q:229:TRP:NE1	2.18	0.71
54:b:49:ARG:HG3	54:b:50:GLU:HG3	1.72	0.71
63:J:164:LEU:HD22	80:l:77:ILE:HB	1.72	0.71
1:AA:780:C:N3	18:AL:196:ARG:NH2	2.39	0.70
63:J:170:GLU:O	63:J:174:PHE:HD2	1.73	0.70
32:A:2472:A:N3	32:A:2474:C:N4	2.38	0.70
70:5:193:LEU:HA	82:s:190:PRO:HG3	1.72	0.70
1:AA:947:U:O2	1:AA:1046:A:N7	2.23	0.70
86:v:45:LYS:HB3	86:v:114:VAL:HG22	1.74	0.70
8:AM:69:ASN:ND2	8:AM:71:ASP:OD1	2.25	0.70
66:P:72:PHE:HZ	71:6:54:PHE:HE2	1.39	0.70
86:v:58:GLY:N	92:v:802:GCP:O2A	2.23	0.70
70:5:69:TRP:CE3	70:5:69:TRP:N	2.58	0.70
76:d:165:THR:HG23	76:d:167:HIS:H	1.57	0.70
86:v:78:GLU:CG	92:v:802:GCP:H3'	2.15	0.70
70:5:60:PHE:CE1	70:5:71:ALA:CB	2.73	0.70
82:s:99:ALA:HB1	82:s:271:LEU:HD23	1.74	0.69
32:A:2174:G:O2'	63:J:101:ALA:O	2.10	0.69
70:5:69:TRP:O	70:5:70:LEU:C	2.32	0.69
32:A:2085:A:H2'	32:A:2086:A:H8	1.57	0.69
66:P:72:PHE:CD2	66:P:73:PRO:HD2	2.27	0.69
63:J:133:GLN:N	64:I:117:ARG:HE	1.83	0.69
65:N:36:VAL:HG12	80:l:128:ARG:HD2	1.74	0.69
86:v:353:PHE:HA	86:v:376:GLY:HA3	1.74	0.69
43:T:71:ALA:H	43:T:180:GLU:HG2	1.58	0.69
32:A:1783:U:H3	32:A:1794:A:H62	1.40	0.69
32:A:2339:G:H21	32:A:2427:C:H5'	1.56	0.69
3:AC:38:ARG:HB3	3:AC:43:ARG:HH21	1.58	0.69
32:A:3082:G:N2	32:A:3085:A:OP2	2.26	0.69
46:Y:114:THR:HG22	67:U:28:LEU:H	1.59	0.68
63:J:158:ASP:OD2	80:l:97:PHE:CE1	2.46	0.68
19:AR:175:ARG:HE	19:AR:181:LEU:HD13	1.59	0.68
86:v:40:VAL:HG22	86:v:41:ILE:HG13	1.73	0.68
32:A:2188:A:C2	63:J:104:THR:HB	2.28	0.68
32:A:2222:U:H5'	32:A:2223:A:H5'	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:s:332:LEU:HD13	82:s:372:TYR:HB2	1.75	0.68
86:v:335:SER:O	86:v:337:GLU:N	2.27	0.68
22:AV:80:SER:H	22:AV:84:GLU:HG3	1.59	0.68
51:3:172:TYR:HB2	51:3:175:ASP:HB2	1.76	0.68
1:AA:1269:U:OP1	1:AA:1271:C:N4	2.27	0.68
39:M:276:ASN:HD21	61:q:65:GLY:HA2	1.58	0.68
84:TA:74:LEU:HD11	84:TA:79:ILE:HG13	1.76	0.68
86:v:526:ARG:HE	86:v:605:SER:HB2	1.60	0.67
32:A:1834:U:H3	43:T:206:ARG:HA	1.58	0.67
1:AA:1110:A:H61	1:AA:1131:C:H42	1.42	0.67
49:1:40:LYS:HE2	88:A7:60:Y5P:OP1	1.94	0.67
63:J:132:LEU:C	64:I:117:ARG:NE	2.48	0.67
29:AD:147:PRO:CG	87:A5:10:Y5P:HA	2.16	0.67
51:3:147:PHE:HB2	71:6:363:LEU:HB2	1.75	0.67
63:J:170:GLU:HA	63:J:173:ILE:HG12	1.76	0.67
78:h:127:LEU:O	78:h:131:ASN:ND2	2.28	0.67
92:v:802:GCP:O2B	92:v:802:GCP:O3G	2.13	0.67
65:N:33:LEU:HD22	80:l:125:ASN:HD22	1.60	0.67
86:v:723:CYS:HG	86:v:727:THR:HG1	1.41	0.67
70:5:68:PRO:CG	70:5:69:TRP:HE3	1.81	0.67
75:c:216:ARG:HG3	75:c:220:ILE:HD12	1.76	0.67
47:Z:78:ARG:O	47:Z:83:LYS:NZ	2.28	0.66
86:v:319:ASN:O	86:v:321:SER:N	2.28	0.66
32:A:1838:C:H4'	37:K:116:LEU:HD12	1.76	0.66
86:v:598:PRO:HG3	86:v:638:LEU:HD23	1.78	0.66
1:AA:1200:G:O6	1:AA:1365:A:N1	2.28	0.66
14:AW:104:ILE:HB	14:AW:137:GLY:H	1.60	0.66
30:AF:214:HIS:O	30:AF:216:GLN:NE2	2.29	0.66
86:v:42:PRO:HD2	86:v:46:ILE:HD11	1.78	0.66
32:A:3122:U:H4'	32:A:3123:G:H4'	1.78	0.66
86:v:163:LYS:HB3	86:v:290:ARG:HH21	1.61	0.66
1:AA:860:A:N7	1:AA:919:A:O2'	2.28	0.66
1:AA:1151:C:OP2	1:AA:1152:A:N6	2.29	0.66
32:A:3049:U:H3	32:A:3053:A:N6	1.94	0.66
36:H:62:VAL:HG22	36:H:64:LEU:H	1.60	0.66
32:A:2998:U:H5''	69:E:225:LYS:HB2	1.78	0.66
1:AA:1265:C:H5'	17:AH:122:GLN:HE21	1.61	0.66
86:v:346:SER:HB2	86:v:349:ASN:HD21	1.61	0.66
32:A:2232:A:H1'	32:A:3002:G:H21	1.59	0.65
63:J:25:ARG:NH1	80:l:67:GLN:OE1	2.28	0.65
64:I:78:LEU:CD1	80:l:118:TRP:CE3	2.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2503:A:H1'	32:A:3094:G:H21	1.61	0.65
65:N:33:LEU:HB3	80:l:125:ASN:ND2	2.10	0.65
21:AU:64:ARG:HB3	26:A0:198:MET:HE3	1.77	0.65
23:AY:313:PHE:O	23:AY:315:ILE:N	2.30	0.65
32:A:2554:A:N3	34:D:285:LYS:NZ	2.44	0.65
51:3:126:LYS:HE3	51:3:148:VAL:HG21	1.78	0.65
71:6:184:LEU:HG	71:6:186:PRO:HD3	1.79	0.65
63:J:33:PRO:O	63:J:35:LEU:N	2.30	0.65
32:A:1674:A:N7	43:T:47:ILE:N	2.44	0.65
32:A:2350:A:H61	32:A:2360:U:H2'	1.62	0.65
57:i:94:LYS:NZ	57:i:102:MET:SD	2.70	0.65
64:l:47:LEU:HD22	65:N:226:ILE:HG12	1.77	0.65
65:N:124:VAL:HG12	65:N:158:ARG:HE	1.62	0.65
1:AA:713:C:H5''	8:AM:42:PRO:HG3	1.77	0.64
70:5:193:LEU:CA	82:s:190:PRO:HG3	2.27	0.64
86:v:333:ASP:H	86:v:439:LEU:HD22	1.61	0.64
32:A:3179:G:H21	32:A:3190:A:H62	1.42	0.64
63:J:22:ALA:HB1	63:J:35:LEU:HD21	1.79	0.64
1:AA:1430:A:N6	1:AA:1459:A:OP2	2.25	0.64
32:A:2753:A:H2'	32:A:2754:A:H8	1.63	0.64
57:i:99:GLY:HA2	57:i:102:MET:HE2	1.80	0.64
86:v:704:ARG:NH1	86:v:704:ARG:O	2.31	0.64
82:s:63:ILE:HA	82:s:66:TRP:HD1	1.62	0.64
1:AA:806:C:N4	1:AA:1512:A:O2'	2.31	0.63
2:AB:223:VAL:HG23	2:AB:227:CYS:HB2	1.79	0.63
77:f:134:VAL:HB	77:f:148:SER:HB2	1.79	0.63
1:AA:1314:C:O2	30:AF:36:ARG:HA	1.98	0.63
37:K:37:ILE:HG23	37:K:42:LEU:HB2	1.79	0.63
32:A:1867:A:H62	32:A:2295:C:H5	1.47	0.63
15:AX:387:ASN:HD22	15:AX:390:LEU:H	1.45	0.63
22:AV:212:GLY:O	22:AV:224:GLN:NE2	2.31	0.63
32:A:2155:A:N6	62:r:169:TRP:O	2.31	0.63
32:A:2307:U:H1'	48:0:84:ARG:HG3	1.78	0.63
32:A:3049:U:O4	32:A:3053:A:N7	2.31	0.63
86:v:288:LEU:HD21	86:v:318:PRO:HG3	1.80	0.63
1:AA:730:A:N6	1:AA:745:A:N7	2.45	0.63
29:AD:147:PRO:HD3	87:A5:10:Y5P:HB2	1.81	0.63
32:A:1744:A:H62	32:A:1754:G:H21	1.46	0.63
32:A:2658:U:OP1	69:E:225:LYS:NZ	2.32	0.63
1:AA:1263:G:OP2	3:AC:38:ARG:NH1	2.32	0.63
18:AL:215:GLU:HG3	27:A3:186:PRO:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AD:248:GLY:HA3	29:AD:326:LEU:HB3	1.80	0.63
63:J:158:ASP:OD2	80:I:97:PHE:HE1	1.82	0.63
71:6:261:ARG:HD3	71:6:341:VAL:HG12	1.81	0.62
32:A:1924:U:H5''	34:D:81:LYS:HB2	1.80	0.62
65:N:218:ILE:HG23	65:N:223:MET:HB2	1.80	0.62
42:S:140:ASN:HD22	74:a:63:PRO:HA	1.64	0.62
63:J:132:LEU:CA	64:I:117:ARG:HE	2.12	0.62
81:p:111:ILE:O	81:p:116:ARG:NH2	2.32	0.62
82:s:242:ARG:HA	82:s:295:GLY:HA2	1.81	0.62
63:J:35:LEU:HD12	63:J:39:LEU:HD11	1.82	0.62
63:J:174:PHE:CZ	63:J:175:LEU:HD23	2.35	0.62
32:A:2625:C:O2'	32:A:2627:G:OP1	2.18	0.62
41:R:83:TYR:OH	41:R:99:ARG:NH1	2.33	0.62
1:AA:735:A:N6	1:AA:740:G:H1	1.98	0.62
29:AD:117:ARG:CD	87:A5:1:Y5P:HB	2.25	0.62
32:A:2363:A:OP2	32:A:2432:A:N6	2.32	0.62
35:F:89:THR:HG22	35:F:179:THR:HG21	1.82	0.62
46:Y:121:ARG:NH1	67:U:30:ARG:O	2.32	0.62
49:1:54:VAL:HA	61:q:128:MET:HE2	1.82	0.62
59:m:59:GLN:NE2	59:m:77:MET:O	2.33	0.62
32:A:2373:A:OP1	67:U:50:ARG:NH2	2.33	0.62
34:D:70:THR:HG22	70:5:34:GLY:HA2	1.82	0.62
82:s:177:LEU:HD23	82:s:238:ASN:HD22	1.65	0.62
86:v:175:LYS:HB3	92:v:802:GCP:C6	2.30	0.62
40:O:140:SER:O	40:O:146:ASN:ND2	2.32	0.61
81:p:192:ARG:HG3	81:p:193:ILE:HG22	1.81	0.61
84:TA:74:LEU:HD13	84:TA:78:GLU:HB3	1.82	0.61
1:AA:832:U:H2'	1:AA:833:A:H8	1.65	0.61
32:A:2962:C:H42	32:A:3016:G:H22	1.48	0.61
32:A:2971:A:OP1	65:N:98:HIS:NE2	2.32	0.61
1:AA:1361:G:H2'	1:AA:1362:G:H8	1.63	0.61
32:A:3010:G:N2	32:A:3027:U:O2	2.31	0.61
55:e:58:VAL:HB	55:e:153:LEU:HB2	1.81	0.61
8:AM:112:ARG:NH1	10:AO:230:PRO:O	2.33	0.61
15:AX:154:HIS:HA	15:AX:261:ALA:HB3	1.83	0.61
32:A:2388:A:H61	34:D:127:ILE:HG21	1.65	0.61
70:5:201:ARG:HG2	70:5:232:THR:HG22	1.82	0.61
86:v:43:ASN:ND2	86:v:413:TYR:OH	2.33	0.61
1:AA:702:C:O2	1:AA:842:C:O2'	2.18	0.61
13:AT:78:PHE:HB2	13:AT:86:VAL:HB	1.83	0.61
32:A:1811:A:H61	75:c:49:ARG:HH21	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3063:G:O2'	32:A:3066:C:OP2	2.18	0.61
86:v:101:THR:HG23	86:v:122:PRO:HA	1.82	0.61
1:AA:1342:C:H2'	24:AZ:101:ARG:HE	1.66	0.61
32:A:2143:G:H2'	32:A:2144:A:H8	1.65	0.61
63:J:174:PHE:CD1	63:J:175:LEU:N	2.69	0.61
86:v:255:GLU:O	86:v:259:ASN:ND2	2.30	0.61
8:AM:20:ARG:NH1	8:AM:41:CYS:SG	2.74	0.61
65:N:191:SER:H	65:N:194:THR:HG1	1.48	0.61
1:AA:1216:C:H2'	1:AA:1217:G:H8	1.63	0.61
32:A:1852:C:O2'	32:A:1854:U:OP2	2.18	0.61
63:J:171:ARG:CA	63:J:174:PHE:CD2	2.73	0.61
82:s:237:PRO:HG2	82:s:240:GLN:HE21	1.65	0.61
63:J:167:PHE:HB3	63:J:171:ARG:CZ	2.31	0.61
1:AA:1235:U:H5''	7:AK:33:ARG:HH21	1.66	0.60
1:AA:1508:C:N3	1:AA:1542:U:O4	2.34	0.60
32:A:1881:A:OP2	56:g:111:ARG:NH2	2.31	0.60
48:0:119:LYS:O	48:0:120:HIS:ND1	2.34	0.60
86:v:383:THR:OG1	86:v:394:ARG:NH1	2.34	0.60
32:A:3128:A:H8	86:v:704:ARG:HH21	1.48	0.60
86:v:221:ARG:HE	86:v:235:TYR:HB3	1.66	0.60
32:A:2472:A:H1'	32:A:2474:C:H41	1.67	0.60
32:A:3000:A:H2'	32:A:3001:G:H8	1.66	0.60
44:W:105:VAL:O	66:P:71:VAL:HG12	2.02	0.60
86:v:47:ARG:NH2	86:v:314:LEU:O	2.34	0.60
32:A:2588:C:H42	32:A:2592:G:H22	1.48	0.60
71:6:330:ILE:O	71:6:334:LEU:HB2	2.01	0.60
28:A4:81:ASP:HB3	28:A4:84:ALA:HB2	1.83	0.60
47:Z:147:VAL:HG13	47:Z:148:GLN:HG3	1.84	0.60
75:c:60:ARG:HD2	75:c:63:LYS:HD2	1.82	0.60
32:A:2112:A:H1'	32:A:2943:G:H21	1.65	0.60
86:v:472:ARG:HH11	86:v:475:ARG:HH11	1.48	0.60
63:J:55:GLU:HA	63:J:58:LYS:HE2	1.84	0.60
1:AA:1052:C:H5''	18:AL:149:LYS:HD2	1.83	0.60
39:M:91:ARG:NH2	39:M:209:GLU:OE2	2.33	0.60
60:o:22:ARG:HH21	64:I:39:VAL:HG13	1.67	0.60
63:J:171:ARG:HH22	80:l:76:ASN:C	2.02	0.60
69:E:227:GLN:NE2	69:E:236:THR:O	2.34	0.60
29:AD:242:ARG:HD2	29:AD:258:ILE:HD11	1.84	0.60
63:J:174:PHE:CD1	63:J:174:PHE:C	2.79	0.60
79:k:10:LEU:O	79:k:46:ASN:ND2	2.35	0.60
26:A0:78:ARG:NH2	26:A0:142:VAL:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D:96:ILE:O	34:D:269:ARG:NH1	2.35	0.60
49:I:61:LYS:O	88:A7:1:P5P:C5'	2.49	0.60
63:J:164:LEU:HD21	80:I:77:ILE:O	2.00	0.60
72:7:107:LEU:HB3	72:7:126:LYS:HB3	1.84	0.60
1:AA:1439:A:H2'	1:AA:1440:G:H8	1.66	0.59
1:AA:1504:U:H4'	32:A:2612:C:H4'	1.83	0.59
2:AB:198:THR:OG1	2:AB:227:CYS:SG	2.60	0.59
10:AO:225:GLN:HB2	21:AU:47:ALA:HB1	1.83	0.59
32:A:2196:A:O2'	32:A:2213:A:N1	2.34	0.59
32:A:2376:A:O2'	73:9:28:ARG:NH2	2.34	0.59
39:M:182:ARG:HE	39:M:201:PRO:HG3	1.67	0.59
1:AA:1317:A:H4'	31:AG:379:ARG:HH21	1.66	0.59
1:AA:1504:U:O4	1:AA:1505:A:N6	2.35	0.59
40:O:141:HIS:HD2	40:O:146:ASN:HB3	1.67	0.59
1:AA:1116:A:N6	2:AB:100:ARG:O	2.30	0.59
11:AP:80:LEU:HD12	11:AP:111:ILE:HG13	1.84	0.59
32:A:1955:G:N2	32:A:1960:A:H61	2.00	0.59
32:A:2028:G:H4'	32:A:2047:U:H4'	1.84	0.59
65:N:167:CYS:SG	65:N:168:GLU:N	2.76	0.59
86:v:548:GLN:HB3	86:v:625:SER:HB3	1.84	0.59
1:AA:1103:A:O2'	1:AA:1574:G:N2	2.33	0.59
1:AA:1431:G:OP2	30:AF:36:ARG:HB2	2.01	0.59
22:AV:250:ILE:HG22	22:AV:252:LYS:H	1.66	0.59
40:O:33:LEU:HD21	40:O:59:LEU:HD22	1.83	0.59
76:d:67:ILE:H	76:d:68:PRO:CD	2.15	0.59
76:d:182:ARG:HB2	76:d:223:ALA:HB3	1.85	0.59
1:AA:1525:C:H41	22:AV:103:TYR:HA	1.67	0.59
34:D:136:SER:O	34:D:249:ASN:ND2	2.35	0.59
48:O:112:GLU:O	48:O:114:GLY:N	2.36	0.59
55:e:49:GLY:HA2	55:e:232:PHE:H	1.66	0.59
61:q:41:ASP:HB3	61:q:44:ASP:HB2	1.83	0.59
81:p:108:ALA:O	81:p:116:ARG:NH2	2.33	0.59
32:A:3113:A:OP1	32:A:3167:U:O2'	2.20	0.59
64:I:142:ASN:ND2	84:TA:49:ALA:O	2.35	0.59
64:I:189:GLN:O	64:I:193:ASN:ND2	2.35	0.59
1:AA:805:C:N4	1:AA:1513:A:OP2	2.34	0.59
1:AA:1568:U:O4'	1:AA:1595:G:N2	2.35	0.59
29:AD:323:ILE:HD11	29:AD:349:LEU:HD23	1.85	0.59
29:AD:362:LEU:HA	29:AD:365:LYS:HG2	1.85	0.59
70:5:201:ARG:HB3	70:5:230:LEU:HD11	1.85	0.59
88:A7:63:Y5P:H4A	88:A7:64:Y5P:H4	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1148:A:N6	1:AA:1149:G:O6	2.35	0.59
1:AA:1248:C:H5''	7:AK:32:TRP:HZ2	1.68	0.59
12:AQ:69:ALA:O	12:AQ:73:ASN:ND2	2.33	0.59
32:A:2508:C:H2'	32:A:2509:A:C8	2.38	0.59
32:A:2520:C:O2	32:A:2528:G:N2	2.31	0.59
70:5:174:GLU:HG3	70:5:296:LYS:HB3	1.84	0.59
19:AR:82:MET:HE3	19:AR:288:GLN:HE22	1.67	0.59
26:A0:135:MET:SD	26:A0:135:MET:N	2.73	0.59
53:8:160:GLU:O	55:e:207:ASN:ND2	2.35	0.59
86:v:175:LYS:CA	92:v:802:GCP:O6	2.48	0.58
86:v:679:ASP:HB2	86:v:686:THR:HB	1.85	0.58
13:AT:139:CYS:SG	13:AT:140:ILE:N	2.76	0.58
22:AV:29:LEU:HB2	22:AV:364:LEU:HD21	1.85	0.58
32:A:2917:G:O6	39:M:77:ARG:NH2	2.35	0.58
40:O:104:TYR:HD1	40:O:105:THR:HG23	1.68	0.58
58:j:53:ASP:OD2	58:j:55:ARG:NH2	2.37	0.58
7:AK:108:ARG:HH12	17:AH:124:VAL:HA	1.68	0.58
15:AX:244:LEU:HB3	15:AX:296:MET:HE3	1.85	0.58
19:AR:221:GLN:OE1	19:AR:223:ARG:NH2	2.35	0.58
57:i:77:PRO:HD2	57:i:80:LEU:HD11	1.85	0.58
1:AA:1053:A:N1	1:AA:1100:C:O2'	2.35	0.58
25:A1:55:PRO:HB3	28:A4:93:PRO:HG3	1.84	0.58
25:A1:66:TRP:HE1	25:A1:112:LEU:HB3	1.69	0.58
32:A:1882:A:OP1	56:g:93:ASN:ND2	2.35	0.58
32:A:1911:C:H2'	32:A:1912:A:H8	1.67	0.58
32:A:1951:C:H2'	32:A:1952:U:C6	2.39	0.58
32:A:2466:A:H2'	32:A:2467:A:C8	2.38	0.58
49:1:20:MET:HB3	49:1:56:PHE:HB3	1.85	0.58
69:E:346:THR:HG22	83:Q:172:GLN:HE22	1.69	0.58
82:s:159:ARG:NH2	82:s:171:VAL:O	2.36	0.58
86:v:397:ARG:NH1	86:v:406:MET:SD	2.73	0.58
32:A:3174:U:N3	32:A:3196:G:O6	2.37	0.58
46:Y:72:LYS:O	46:Y:76:GLN:NE2	2.36	0.58
64:I:95:MET:HE3	64:I:159:PRO:HB3	1.85	0.58
2:AB:268:GLU:OE1	2:AB:272:ARG:NH2	2.37	0.58
32:A:1795:A:H5'	35:F:147:ARG:HH12	1.67	0.58
32:A:2366:G:H2'	32:A:2367:A:H8	1.68	0.58
64:I:77:GLY:HA3	80:l:118:TRP:HZ2	1.68	0.58
79:k:65:ASP:HA	79:k:75:ILE:HA	1.86	0.58
86:v:319:ASN:O	86:v:322:GLU:HG3	2.02	0.58
15:AX:108:LEU:HD23	15:AX:141:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:94:LYS:HB2	83:Q:57:PRO:HG3	1.83	0.58
27:A3:174:ARG:HA	27:A3:177:TRP:CE2	2.39	0.58
39:M:284:LYS:HB2	56:g:40:GLU:HB3	1.86	0.58
72:7:115:MET:HB3	72:7:270:PRO:HB3	1.86	0.58
82:s:49:ALA:O	82:s:61:ARG:NH1	2.37	0.58
32:A:1999:A:H4'	50:2:49:ARG:HE	1.69	0.58
46:Y:198:ARG:NH2	50:2:70:LEU:O	2.37	0.58
61:q:71:VAL:HG22	61:q:73:GLY:H	1.67	0.58
65:N:33:LEU:HB3	80:l:125:ASN:HD21	1.69	0.58
86:v:142:VAL:HA	86:v:169:PHE:HB2	1.86	0.58
86:v:663:GLN:HB3	86:v:706:CYS:HB3	1.85	0.58
1:AA:704:U:OP1	1:AA:845:A:N6	2.32	0.58
11:AP:82:GLN:NE2	11:AP:133:PRO:O	2.35	0.58
69:E:343:PRO:HA	83:Q:105:VAL:HG21	1.85	0.58
70:5:216:GLU:OE2	70:5:367:ASN:ND2	2.36	0.58
86:v:356:LEU:HD22	86:v:441:MET:HE3	1.86	0.58
1:AA:735:A:C6	1:AA:740:G:N1	2.72	0.58
1:AA:1294:A:OP2	2:AB:147:ARG:NH2	2.37	0.58
3:AC:44:VAL:HG13	3:AC:167:LEU:HD21	1.84	0.58
32:A:2048:U:O4	32:A:2092:C:N3	2.36	0.58
1:AA:888:U:H3	1:AA:905:A:H62	1.51	0.57
9:AN:100:CYS:SG	9:AN:101:ALA:N	2.77	0.57
25:A1:211:ARG:NH1	25:A1:221:TYR:OH	2.37	0.57
32:A:2274:A:OP1	75:c:36:ARG:NH1	2.36	0.57
56:g:94:ILE:HD12	56:g:95:PRO:HD2	1.85	0.57
56:g:109:VAL:HG22	56:g:148:ARG:HG2	1.86	0.57
58:j:60:MET:N	58:j:60:MET:SD	2.76	0.57
68:V:122:LEU:HD23	68:V:133:ILE:HG13	1.86	0.57
69:E:277:ASN:HB3	69:E:282:ILE:H	1.69	0.57
3:AC:80:ASP:OD2	24:AZ:46:LYS:NZ	2.34	0.57
23:AY:326:SER:O	25:A1:217:GLN:NE2	2.37	0.57
63:J:156:VAL:HG21	63:J:159:LEU:HD12	1.86	0.57
32:A:1813:C:H41	57:i:36:LEU:HD21	1.69	0.57
32:A:2174:G:HO2'	63:J:101:ALA:C	2.13	0.57
33:B:1628:C:H2'	33:B:1629:A:H8	1.69	0.57
63:J:102:ARG:HG3	63:J:103:GLN:HG2	1.87	0.57
66:P:102:VAL:HG23	66:P:103:VAL:HG12	1.87	0.57
1:AA:1585:A:H62	27:A3:141:HIS:HE1	1.52	0.57
2:AB:75:VAL:O	2:AB:126:GLN:NE2	2.38	0.57
2:AB:110:ARG:NH2	20:AS:68:ASP:OD1	2.37	0.57
16:A2:62:ARG:HE	16:A2:63:ASP:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AH:117:ARG:HG2	17:AH:135:GLU:HG2	1.85	0.57
69:E:294:ASN:HD21	83:Q:88:ASP:HB2	1.69	0.57
66:P:43:ALA:HB1	71:6:226:LEU:HD13	1.87	0.57
22:AV:247:MET:N	22:AV:247:MET:SD	2.78	0.57
32:A:2209:G:H3'	32:A:2210:C:H5''	1.87	0.57
32:A:3108:U:O2	69:E:266:ARG:NH2	2.37	0.57
32:A:2325:U:OP2	82:s:55:SER:OG	2.22	0.57
63:J:85:PRO:O	63:J:124:LYS:NZ	2.38	0.57
1:AA:701:G:O6	26:A0:48:ARG:NH2	2.38	0.57
26:A0:88:GLN:NE2	26:A0:202:ASP:OD2	2.38	0.57
64:I:76:ILE:HD12	64:I:78:LEU:HD13	1.86	0.57
70:5:204:VAL:HG13	82:s:152:GLN:NE2	2.16	0.57
7:AK:34:MET:SD	29:AD:88:SER:OG	2.62	0.57
30:AF:74:ILE:HG13	31:AG:366:GLN:HA	1.87	0.57
32:A:2213:A:H4'	80:l:129:HIS:NE2	2.20	0.57
40:O:49:VAL:HG21	40:O:121:ALA:HB3	1.87	0.57
30:AF:176:ASP:OD1	30:AF:179:ARG:NH2	2.38	0.57
32:A:1821:A:OP2	48:0:95:ARG:NH1	2.37	0.57
1:AA:853:C:H4'	8:AM:43:ARG:HH12	1.70	0.56
22:AV:274:LYS:HD3	22:AV:348:GLU:HB3	1.87	0.56
23:AY:346:PRO:HD2	23:AY:392:ILE:HD12	1.87	0.56
31:AG:312:GLN:OE1	31:AG:345:ARG:NH1	2.38	0.56
32:A:2536:G:H2'	32:A:2537:G:H8	1.70	0.56
57:i:53:MET:HE3	57:i:56:VAL:HG21	1.87	0.56
15:AX:222:LEU:HD11	15:AX:243:VAL:HG13	1.87	0.56
16:A2:101:PRO:O	16:A2:105:ASN:ND2	2.39	0.56
25:A1:250:GLU:HA	25:A1:301:ASN:HD21	1.68	0.56
32:A:2110:A:OP2	65:N:67:LYS:NZ	2.39	0.56
32:A:2819:G:H21	44:W:38:SER:HB3	1.69	0.56
32:A:3031:G:H2'	32:A:3032:G:C8	2.40	0.56
1:AA:934:G:O6	6:AJ:31:ALA:N	2.38	0.56
1:AA:1086:C:H2'	1:AA:1087:A:C8	2.40	0.56
1:AA:1086:C:H2'	1:AA:1087:A:H8	1.69	0.56
2:AB:99:HIS:HB2	2:AB:226:ASN:HA	1.87	0.56
2:AB:149:ARG:NH2	12:AQ:84:TRP:O	2.38	0.56
2:AB:239:ASN:OD1	14:AW:119:LYS:NZ	2.38	0.56
7:AK:54:ILE:HG21	7:AK:75:ILE:HB	1.88	0.56
15:AX:120:PRO:HB2	15:AX:299:ASN:HB2	1.87	0.56
29:AD:232:THR:OG1	29:AD:233:ALA:N	2.37	0.56
32:A:1849:C:OP2	39:M:53:HIS:NE2	2.39	0.56
32:A:1952:U:H2'	32:A:1953:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2103:A:N3	47:Z:35:LYS:N	2.53	0.56
32:A:2214:A:C4'	80:l:126:ILE:HD11	2.35	0.56
32:A:2290:A:H1'	35:F:108:ARG:HH12	1.70	0.56
42:S:142:THR:OG1	74:a:60:CYS:SG	2.63	0.56
46:Y:93:LYS:NZ	68:V:181:ASP:O	2.38	0.56
55:e:235:LYS:NZ	77:f:172:GLU:OE1	2.37	0.56
56:g:105:ARG:HH12	60:o:83:PRO:HD3	1.69	0.56
63:J:171:ARG:HG3	63:J:174:PHE:HE2	1.70	0.56
72:7:135:PRO:O	72:7:139:ASN:ND2	2.38	0.56
79:k:63:CYS:HA	79:k:77:ARG:HA	1.87	0.56
86:v:132:GLU:HG3	86:v:136:ARG:HE	1.69	0.56
1:AA:704:U:O2'	26:A0:82:ARG:NH2	2.38	0.56
1:AA:1350:G:OP1	7:AK:80:ARG:NH2	2.39	0.56
3:AC:148:LYS:HB3	28:A4:137:ILE:HD12	1.86	0.56
26:A0:93:CYS:HB3	26:A0:121:LYS:H	1.69	0.56
32:A:1864:A:OP2	41:R:17:ARG:NH1	2.39	0.56
86:v:58:GLY:C	92:v:802:GCP:O2A	2.48	0.56
1:AA:1233:C:N3	1:AA:1403:A:N6	2.53	0.56
29:AD:265:MET:HE1	87:A5:4:Y5P:H4	1.87	0.56
32:A:2214:A:O2'	80:l:122:ARG:HD3	2.06	0.56
63:J:132:LEU:HD23	64:I:114:HIS:HB3	1.87	0.56
15:AX:125:LEU:HD11	15:AX:310:LEU:HB2	1.88	0.56
15:AX:266:ASN:ND2	15:AX:315:SER:OG	2.39	0.56
32:A:1916:G:N2	32:A:1998:U:OP2	2.34	0.56
71:6:184:LEU:HD13	81:p:191:LYS:HD3	1.87	0.56
82:s:371:CYS:HB2	82:s:394:TRP:HB2	1.86	0.56
5:AI:184:ASN:OD1	12:AQ:42:ARG:NH1	2.39	0.56
20:AS:12:ILE:HG22	20:AS:15:ARG:HH21	1.71	0.56
32:A:1682:C:OP1	46:Y:222:ARG:NH1	2.36	0.56
32:A:2083:U:O4	32:A:2084:A:N6	2.38	0.56
32:A:2257:C:OP1	58:j:62:GLY:N	2.39	0.56
38:L:99:ARG:HB3	83:Q:161:GLU:HB2	1.86	0.56
41:R:47:ILE:HG12	42:S:172:MET:HE1	1.86	0.56
45:X:36:ARG:NH2	45:X:149:SER:OG	2.37	0.56
63:J:111:LEU:HD13	63:J:170:GLU:CD	2.23	0.56
86:v:191:ARG:NH2	86:v:252:GLU:OE2	2.39	0.56
32:A:1756:A:O2'	45:X:61:ARG:NH2	2.38	0.56
71:6:184:LEU:HD22	81:p:191:LYS:HB2	1.87	0.56
32:A:2188:A:C2	63:J:104:THR:CB	2.88	0.56
50:2:78:VAL:HG22	50:2:81:ARG:HH21	1.71	0.56
68:V:124:ASP:OD2	68:V:152:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:E:209:LYS:NZ	69:E:263:ASN:OD1	2.34	0.56
69:E:218:VAL:HB	69:E:258:PRO:HG3	1.87	0.56
88:A7:70:Y5P:H4A	88:A7:71:P5P:C6	2.35	0.56
9:AN:18:ILE:HD11	9:AN:29:ARG:HB3	1.87	0.56
32:A:2277:U:H2'	32:A:2278:A:H8	1.71	0.56
32:A:2395:A:OP2	70:5:300:ARG:NH2	2.39	0.56
47:Z:68:ILE:HD11	47:Z:122:LEU:HD13	1.88	0.56
22:AV:198:TRP:NE1	22:AV:238:GLN:OE1	2.39	0.55
32:A:1911:C:H2'	32:A:1912:A:C8	2.40	0.55
1:AA:1235:U:H4'	7:AK:90:ARG:HH21	1.71	0.55
11:AP:49:ASP:OD1	14:AW:85:ARG:NH1	2.39	0.55
43:T:90:LEU:HD21	43:T:111:LYS:HD2	1.87	0.55
1:AA:1572:A:H2'	1:AA:1573:A:H8	1.71	0.55
6:AJ:55:ARG:HD3	6:AJ:58:LEU:HD21	1.88	0.55
32:A:1725:C:O2	32:A:2921:A:N6	2.40	0.55
32:A:2171:U:OP1	63:J:86:THR:CB	2.53	0.55
41:R:94:GLN:HB3	42:S:147:PRO:HD3	1.89	0.55
70:5:69:TRP:O	70:5:71:ALA:N	2.38	0.55
72:7:159:LYS:HG2	72:7:161:GLU:H	1.72	0.55
77:f:136:GLN:HB2	77:f:146:LEU:HB2	1.88	0.55
1:AA:890:C:H4'	1:AA:891:C:H5	1.70	0.55
1:AA:894:C:H41	6:AJ:78:ARG:HH22	1.54	0.55
1:AA:997:A:H4'	1:AA:1074:G:H4'	1.88	0.55
13:AT:132:ARG:NH1	13:AT:136:LEU:O	2.39	0.55
19:AR:219:TYR:O	19:AR:256:ARG:NH2	2.38	0.55
32:A:1979:U:H2'	32:A:1980:A:H8	1.70	0.55
32:A:2442:U:OP1	82:s:81:ARG:NH2	2.39	0.55
45:X:181:PRO:HB3	45:X:184:ARG:HH11	1.71	0.55
68:V:52:GLU:HB3	68:V:143:ARG:HH22	1.71	0.55
83:Q:225:LYS:HB3	83:Q:226:PRO:HD2	1.87	0.55
32:A:2214:A:O4'	80:l:126:ILE:HD11	2.07	0.55
32:A:2466:A:H2'	32:A:2467:A:H8	1.72	0.55
55:e:55:ARG:HD3	55:e:157:LEU:HD13	1.87	0.55
72:7:41:THR:O	72:7:45:ASN:ND2	2.39	0.55
86:v:555:VAL:HB	86:v:610:VAL:HB	1.87	0.55
60:o:31:ALA:HB1	64:I:46:LYS:HE3	1.89	0.55
63:J:159:LEU:O	63:J:163:GLU:CB	2.54	0.55
1:AA:1276:A:N6	1:AA:1299:A:O2'	2.40	0.55
1:AA:1506:U:H2'	1:AA:1507:A:H8	1.72	0.55
1:AA:1537:C:OP2	1:AA:1538:G:N2	2.40	0.55
14:AW:80:PHE:HA	14:AW:83:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AX:153:LEU:HD23	15:AX:260:VAL:HG22	1.89	0.55
18:AL:80:GLY:HA2	18:AL:83:LYS:HD3	1.89	0.55
45:X:128:THR:OG1	45:X:129:MET:N	2.35	0.55
49:1:17:LEU:HB3	49:1:63:ARG:HB3	1.89	0.55
1:AA:1252:G:H5'	7:AK:30:VAL:HG23	1.88	0.55
1:AA:1598:G:OP1	12:AQ:57:TYR:OH	2.24	0.55
7:AK:90:ARG:NH1	7:AK:95:SER:O	2.40	0.55
32:A:1798:A:N3	68:V:42:ARG:NH2	2.54	0.55
32:A:1834:U:OP2	54:b:116:ARG:NH1	2.39	0.55
32:A:2178:A:N6	86:v:675:ILE:O	2.40	0.55
32:A:2868:C:O2'	39:M:77:ARG:NH1	2.40	0.55
51:3:183:ARG:NH1	71:6:355:LYS:O	2.40	0.55
66:P:109:GLU:HG2	66:P:111:ALA:H	1.70	0.55
69:E:105:GLY:HA3	83:Q:91:LYS:HD2	1.89	0.55
1:AA:1271:C:O2'	1:AA:1272:A:O4'	2.24	0.55
4:AE:117:LEU:HD13	16:A2:10:LEU:HD12	1.89	0.55
66:P:68:TRP:O	66:P:70:THR:N	2.38	0.55
82:s:271:LEU:O	82:s:273:LEU:N	2.40	0.55
1:AA:773:U:H2'	1:AA:774:G:H8	1.72	0.55
1:AA:1464:G:H21	1:AA:1466:C:H42	1.55	0.55
5:AI:89:LYS:HA	5:AI:152:LYS:HB3	1.89	0.55
17:AH:88:LEU:HG	17:AH:141:ARG:HD2	1.88	0.55
19:AR:202:ARG:NH1	19:AR:234:GLN:O	2.40	0.55
22:AV:43:ARG:NH2	22:AV:375:TYR:OH	2.40	0.55
31:AG:384:GLN:HG2	31:AG:390:LYS:HD3	1.88	0.55
32:A:3011:A:O2'	32:A:3173:G:N2	2.32	0.55
35:F:230:ILE:HG13	35:F:242:LEU:HD11	1.87	0.55
77:f:127:MET:SD	77:f:127:MET:N	2.80	0.55
84:TA:79:ILE:O	84:TA:83:ASN:ND2	2.35	0.55
1:AA:989:U:OP1	5:AI:94:ASN:ND2	2.39	0.54
23:AY:331:HIS:O	23:AY:369:LYS:NZ	2.39	0.54
28:A4:137:ILE:HG22	28:A4:139:CYS:H	1.72	0.54
32:A:2367:A:N3	46:Y:123:ARG:NH1	2.50	0.54
33:B:1611:G:O6	33:B:1644:G:N2	2.33	0.54
34:D:204:ALA:O	34:D:208:ARG:NH1	2.39	0.54
46:Y:121:ARG:HH22	67:U:32:GLY:HA2	1.73	0.54
73:9:53:ILE:HG22	73:9:55:GLU:H	1.72	0.54
86:v:59:LYS:HG3	92:v:802:GCP:O1B	1.94	0.54
32:A:1994:A:O2'	32:A:1995:A:OP2	2.23	0.54
32:A:2962:C:H42	32:A:3016:G:N2	2.04	0.54
32:A:3126:C:N4	32:A:3127:G:O6	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:E:182:THR:OG1	69:E:183:ASP:N	2.36	0.54
75:c:173:LEU:HD21	75:c:218:PHE:HE1	1.70	0.54
86:v:465:LYS:HB2	86:v:512:TYR:HE1	1.72	0.54
12:AQ:38:ASP:OD1	12:AQ:42:ARG:NH2	2.40	0.54
19:AR:209:ILE:HA	19:AR:214:ASN:HD22	1.71	0.54
32:A:2017:U:OP1	39:M:54:LYS:NZ	2.40	0.54
32:A:3189:C:HO2'	62:r:155:ALA:H	1.51	0.54
66:P:72:PHE:CZ	71:6:54:PHE:HE2	2.24	0.54
1:AA:1222:A:OP2	31:AG:393:TRP:NE1	2.35	0.54
3:AC:70:SER:HA	3:AC:110:LEU:HB2	1.89	0.54
3:AC:100:PHE:HB3	3:AC:103:CYS:HB2	1.90	0.54
5:AI:159:LEU:O	5:AI:163:HIS:ND1	2.37	0.54
14:AW:101:ILE:HD11	14:AW:139:ARG:HB3	1.90	0.54
15:AX:360:TYR:HB3	15:AX:365:TRP:HB3	1.89	0.54
32:A:2020:U:O4	39:M:58:GLN:NE2	2.40	0.54
53:8:85:ILE:HB	77:f:128:PRO:HG3	1.88	0.54
61:q:139:GLN:HA	61:q:142:ASN:HD21	1.72	0.54
67:U:68:VAL:HG22	67:U:97:VAL:HG12	1.88	0.54
1:AA:1556:C:H2'	1:AA:1557:A:H8	1.73	0.54
29:AD:287:ASP:O	29:AD:330:LYS:NZ	2.39	0.54
32:A:1745:U:O4	51:3:108:LYS:NZ	2.39	0.54
32:A:3007:C:N4	32:A:3054:G:N7	2.55	0.54
34:D:211:GLY:H	34:D:247:VAL:HB	1.71	0.54
46:Y:95:ASN:ND2	68:V:197:GLU:OE1	2.40	0.54
77:f:178:LEU:HD12	77:f:179:PRO:HD2	1.90	0.54
86:v:313:VAL:O	86:v:317:LEU:HB2	2.08	0.54
1:AA:700:A:N6	1:AA:709:G:O2'	2.40	0.54
32:A:2383:U:O4	32:A:2384:A:N6	2.40	0.54
42:S:150:GLY:H	42:S:153:LEU:HD12	1.73	0.54
63:J:171:ARG:CA	63:J:174:PHE:HE2	1.96	0.54
70:5:204:VAL:HA	82:s:152:GLN:HE22	1.72	0.54
82:s:191:HIS:O	82:s:428:ARG:NH2	2.40	0.54
23:AY:360:LYS:NZ	24:AZ:21:GLU:OE2	2.40	0.54
32:A:1731:A:H61	57:i:115:ARG:HG2	1.73	0.54
32:A:1884:G:H1'	32:A:1895:C:H1'	1.90	0.54
32:A:2900:C:N3	88:A7:71:P5P:H2	2.21	0.54
32:A:3032:G:N2	32:A:3052:A:N3	2.46	0.54
32:A:3127:G:O2'	86:v:704:ARG:NH2	2.41	0.54
68:V:190:CYS:SG	68:V:191:LEU:N	2.78	0.54
73:9:27:PRO:O	73:9:31:ARG:NE	2.37	0.54
1:AA:705:C:N4	26:A0:57:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1141:C:O2'	1:AA:1553:A:O2'	2.25	0.54
1:AA:1228:A:H4'	1:AA:1229:U:H5''	1.89	0.54
3:AC:77:ASP:N	3:AC:77:ASP:OD1	2.39	0.54
17:AH:102:LEU:O	25:A1:127:LYS:NZ	2.40	0.54
32:A:1907:A:N3	32:A:2930:U:O2'	2.38	0.54
64:I:133:PRO:HA	64:I:136:GLU:HG2	1.90	0.54
1:AA:1115:U:O2	1:AA:1118:A:N6	2.41	0.54
32:A:2370:A:OP1	67:U:41:GLN:NE2	2.41	0.54
32:A:2469:A:H2'	32:A:2470:G:C8	2.43	0.54
76:d:170:PRO:HA	76:d:173:THR:HG22	1.90	0.54
86:v:59:LYS:CG	92:v:802:GCP:PB	2.86	0.54
29:AD:265:MET:HE1	87:A5:4:Y5P:C4	2.38	0.54
32:A:2507:A:O2'	32:A:2508:C:OP1	2.25	0.54
32:A:3157:C:O2'	83:Q:84:ARG:O	2.23	0.54
32:A:3190:A:H4'	62:r:124:ARG:HH21	1.72	0.54
50:2:70:LEU:HD22	50:2:76:VAL:HG22	1.90	0.54
55:e:157:LEU:HG	55:e:256:THR:HG22	1.90	0.54
25:A1:86:ARG:HD2	31:AG:131:ILE:HD13	1.89	0.53
25:A1:149:ILE:HA	25:A1:175:VAL:HG22	1.90	0.53
30:AF:57:GLU:OE1	30:AF:59:THR:N	2.33	0.53
32:A:1783:U:O4	32:A:1794:A:N7	2.41	0.53
35:F:222:THR:O	35:F:224:GLU:N	2.35	0.53
46:Y:200:PHE:HB3	70:5:68:PRO:HD3	1.90	0.53
62:r:71:PRO:HD2	62:r:107:LEU:HD23	1.90	0.53
63:J:30:MET:N	63:J:30:MET:SD	2.81	0.53
63:J:167:PHE:O	63:J:171:ARG:HD2	2.06	0.53
8:AM:59:ASN:ND2	8:AM:63:GLU:O	2.42	0.53
32:A:1903:C:H41	39:M:58:GLN:HG2	1.73	0.53
55:e:265:LYS:H	55:e:266:PRO:HD2	1.73	0.53
61:q:103:LEU:HA	61:q:106:LYS:HZ3	1.73	0.53
66:P:91:GLU:HG3	66:P:106:SER:HB3	1.89	0.53
77:f:138:GLN:OE1	77:f:141:GLY:N	2.40	0.53
2:AB:103:GLU:H	2:AB:104:PRO:HD2	1.72	0.53
31:AG:79:GLU:HA	31:AG:82:ASN:ND2	2.24	0.53
32:A:2145:G:N1	32:A:2256:U:O4	2.40	0.53
32:A:2900:C:C2	88:A7:71:P5P:H2	2.43	0.53
32:A:3148:C:O2'	69:E:106:MET:SD	2.66	0.53
51:3:183:ARG:NH2	71:6:356:ARG:O	2.39	0.53
64:I:81:LEU:HD12	80:l:115:ARG:NH2	2.23	0.53
64:I:125:VAL:HG12	64:I:153:LEU:H	1.72	0.53
64:I:189:GLN:HA	64:I:192:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:s:105:TRP:HZ3	82:s:268:PRO:HA	1.73	0.53
1:AA:996:A:H3'	1:AA:997:A:H8	1.72	0.53
1:AA:1239:C:H2'	1:AA:1240:A:H8	1.72	0.53
19:AR:335:GLU:HB3	19:AR:337:GLN:HE22	1.73	0.53
30:AF:119:LYS:HE3	30:AF:123:PHE:HE2	1.73	0.53
32:A:2289:G:H2'	32:A:2290:A:C8	2.44	0.53
56:g:54:ALA:O	56:g:56:ARG:N	2.41	0.53
82:s:212:ARG:HD3	82:s:379:LEU:HB3	1.89	0.53
82:s:266:CYS:SG	82:s:267:LYS:N	2.81	0.53
15:AX:364:ASN:O	15:AX:367:GLN:NE2	2.42	0.53
32:A:2461:A:OP1	69:E:238:ARG:N	2.42	0.53
32:A:2933:G:N2	32:A:2936:U:O2	2.37	0.53
56:g:154:ASP:OD1	56:g:154:ASP:N	2.37	0.53
63:J:159:LEU:CB	63:J:162:GLU:HB3	2.20	0.53
70:5:104:CYS:SG	70:5:105:TYR:N	2.81	0.53
86:v:553:ILE:HB	86:v:612:GLN:HB2	1.89	0.53
1:AA:1098:C:H4'	1:AA:1151:C:H2'	1.90	0.53
9:AN:17:VAL:HG22	9:AN:28:VAL:HG22	1.90	0.53
32:A:3174:U:H2'	32:A:3175:A:C8	2.42	0.53
41:R:29:ARG:NH2	41:R:36:ASN:O	2.41	0.53
62:r:135:LEU:HD11	62:r:139:VAL:HG13	1.91	0.53
63:J:156:VAL:O	63:J:157:LYS:C	2.51	0.53
4:AE:15:ARG:NH1	21:AU:178:GLU:OE1	2.42	0.53
32:A:2111:C:OP1	64:I:35:ARG:NH1	2.40	0.53
33:B:1637:C:OP1	71:6:52:ARG:NH1	2.41	0.53
39:M:73:PRO:HD2	39:M:76:ILE:HD12	1.91	0.53
1:AA:749:G:H1'	9:AN:8:VAL:HA	1.91	0.53
28:A4:130:LYS:HE2	28:A4:132:ILE:HD11	1.91	0.53
32:A:1679:U:H4'	68:V:43:PRO:HD2	1.91	0.53
32:A:2213:A:O2'	80:l:129:HIS:HD2	1.91	0.53
32:A:2938:A:OP1	32:A:2984:A:N6	2.42	0.53
32:A:3196:G:H4'	32:A:3197:U:O5'	2.09	0.53
64:I:186:LEU:HG	64:I:190:GLY:HA3	1.90	0.53
25:A1:258:SER:HA	25:A1:261:ASN:HD21	1.73	0.53
26:A0:68:LEU:HD11	26:A0:75:GLY:HA3	1.91	0.53
32:A:1834:U:H4'	74:a:138:PRO:HB2	1.89	0.53
32:A:1936:A:OP1	32:A:1938:A:N6	2.42	0.53
32:A:1966:G:H2'	32:A:1967:U:C6	2.44	0.53
35:F:62:VAL:HG13	78:h:118:HIS:HB2	1.89	0.53
70:5:377:ASP:OD1	70:5:380:GLN:NE2	2.42	0.53
71:6:332:HIS:HD2	81:p:129:ARG:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:7:165:ASN:HB2	72:7:184:VAL:HB	1.91	0.53
32:A:1749:C:OP2	32:A:2899:C:O2'	2.25	0.53
32:A:1953:A:N6	32:A:1965:A:H61	2.07	0.53
38:L:69:VAL:HG12	38:L:127:LEU:HD21	1.90	0.53
64:I:119:HIS:O	64:I:160:LYS:NZ	2.39	0.53
1:AA:1361:G:H2'	1:AA:1362:G:C8	2.43	0.52
32:A:2144:A:H1'	42:S:188:THR:HG21	1.92	0.52
32:A:2155:A:O2'	32:A:2156:A:O4'	2.24	0.52
35:F:276:GLN:HE21	57:i:62:ILE:HG23	1.73	0.52
39:M:169:LYS:NZ	39:M:241:GLY:O	2.32	0.52
52:4:76:CYS:SG	52:4:77:LYS:N	2.81	0.52
63:J:159:LEU:O	63:J:163:GLU:HG3	2.09	0.52
82:s:87:GLN:O	82:s:277:GLN:NE2	2.42	0.52
82:s:267:LYS:HD2	82:s:270:LYS:HZ1	1.75	0.52
86:v:319:ASN:C	86:v:321:SER:N	2.66	0.52
22:AV:79:ILE:HG23	22:AV:84:GLU:HB2	1.91	0.52
32:A:2805:A:H2	45:X:99:LYS:HE3	1.74	0.52
58:j:36:ASN:ND2	58:j:38:SER:OG	2.35	0.52
3:AC:101:PRO:HG3	24:AZ:72:ARG:HD3	1.91	0.52
32:A:1868:G:OP2	32:A:1868:G:N2	2.39	0.52
32:A:2134:A:H4'	32:A:2135:A:H5'	1.91	0.52
35:F:234:THR:O	61:q:25:TYR:N	2.42	0.52
63:J:137:LEU:HB2	80:l:95:TRP:HH2	1.74	0.52
69:E:334:ASP:OD1	69:E:335:GLU:N	2.43	0.52
86:v:78:GLU:OE2	92:v:802:GCP:O1A	2.27	0.52
32:A:1782:G:N2	32:A:1794:A:OP2	2.42	0.52
32:A:3189:C:C6	52:4:86:GLY:HA2	2.45	0.52
37:K:26:GLN:HE22	37:K:149:ARG:H	1.57	0.52
39:M:78:ILE:O	51:3:113:ARG:NH1	2.38	0.52
70:5:192:ILE:HG23	82:s:190:PRO:HD3	1.92	0.52
75:c:213:LEU:HD22	75:c:216:ARG:HH21	1.74	0.52
86:v:675:ILE:HG22	86:v:689:ALA:HA	1.90	0.52
1:AA:734:C:H2'	1:AA:735:A:C8	2.45	0.52
1:AA:735:A:N1	1:AA:740:G:C2	2.78	0.52
2:AB:172:ARG:H	2:AB:175:MET:HE3	1.74	0.52
32:A:1673:U:C4	32:A:1674:A:H1'	2.44	0.52
32:A:2160:A:N6	52:4:70:THR:O	2.42	0.52
32:A:2187:C:N4	63:J:103:GLN:HA	2.24	0.52
63:J:191:LYS:HA	63:J:191:LYS:HE3	1.92	0.52
86:v:49:ILE:HA	86:v:140:GLY:HA3	1.91	0.52
1:AA:891:C:H5''	6:AJ:76:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AT:42:GLU:OE1	13:AT:45:ARG:NH2	2.43	0.52
22:AV:70:LEU:HD11	22:AV:389:LEU:HB3	1.90	0.52
22:AV:250:ILE:HD11	26:A0:146:GLU:HG3	1.90	0.52
32:A:2016:C:O2	32:A:2931:A:O2'	2.27	0.52
32:A:2292:G:H5'	35:F:154:GLY:HA2	1.91	0.52
32:A:2365:U:H2'	32:A:2366:G:C8	2.44	0.52
63:J:132:LEU:HA	64:I:114:HIS:CB	2.39	0.52
64:I:181:ILE:O	64:I:184:THR:OG1	2.22	0.52
70:5:132:LEU:HD21	70:5:377:ASP:HB2	1.91	0.52
86:v:53:ALA:HB2	86:v:144:VAL:HB	1.92	0.52
8:AM:83:LEU:HD22	8:AM:87:MET:HG2	1.90	0.52
21:AU:112:GLU:OE1	21:AU:115:ARG:NH2	2.43	0.52
32:A:2027:A:O2'	32:A:2048:U:OP1	2.27	0.52
32:A:2370:A:OP2	67:U:71:ARG:NH2	2.43	0.52
35:F:103:GLN:HE22	35:F:251:HIS:H	1.57	0.52
37:K:20:LEU:HD22	37:K:141:LEU:HD13	1.91	0.52
61:q:138:GLN:O	61:q:142:ASN:ND2	2.43	0.52
63:J:192:LYS:OXT	63:J:192:LYS:HD2	2.10	0.52
79:k:49:CYS:SG	79:k:50:SER:N	2.83	0.52
1:AA:662:U:O2'	1:AA:939:A:N6	2.42	0.52
19:AR:323:GLU:O	19:AR:327:LEU:N	2.37	0.52
56:g:77:ASP:HB2	56:g:78:PRO:HD2	1.92	0.52
2:AB:64:ASN:OD1	2:AB:138:ARG:NH2	2.42	0.52
14:AW:110:ASN:ND2	14:AW:111:ASP:OD1	2.42	0.52
16:A2:19:PRO:HG2	16:A2:22:LYS:HE2	1.91	0.52
32:A:2373:A:H1'	32:A:2374:A:H8	1.75	0.52
32:A:2661:U:H2'	32:A:2662:A:H8	1.75	0.52
38:L:68:LYS:NZ	38:L:91:MET:SD	2.82	0.52
72:7:213:ASP:OD2	72:7:271:ARG:NH1	2.43	0.52
83:Q:227:LYS:N	83:Q:228:PRO:HD3	2.24	0.52
32:A:2085:A:H2'	32:A:2086:A:C8	2.43	0.52
32:A:2244:U:OP2	41:R:82:LYS:NZ	2.39	0.52
49:1:61:LYS:HG3	88:A7:1:P5P:H5'2	1.76	0.52
71:6:217:LEU:HD13	71:6:236:LEU:HD13	1.90	0.52
72:7:79:PHE:HB3	72:7:81:MET:HE2	1.91	0.52
1:AA:860:A:N1	1:AA:920:G:O6	2.43	0.51
1:AA:981:C:O3'	34:D:218:ARG:NH1	2.43	0.51
42:S:165:GLU:HA	42:S:189:PRO:HA	1.91	0.51
45:X:214:LYS:HB2	70:5:58:ILE:HD13	1.91	0.51
54:b:78:GLU:HG2	54:b:84:VAL:HG22	1.91	0.51
55:e:122:ASP:O	55:e:126:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AG:285:VAL:HA	31:AG:328:VAL:HG12	1.92	0.51
32:A:2654:U:H2'	32:A:2655:G:H5''	1.91	0.51
38:L:34:LYS:HE2	38:L:59:HIS:HA	1.92	0.51
53:8:179:THR:HG21	55:e:133:LEU:HB2	1.93	0.51
55:e:159:LEU:HD11	55:e:252:HIS:HB2	1.91	0.51
64:I:40:MET:HB3	64:I:44:ARG:HD3	1.91	0.51
65:N:114:ASP:OD2	65:N:117:ASN:ND2	2.43	0.51
1:AA:773:U:H2'	1:AA:774:G:C8	2.46	0.51
1:AA:919:A:OP2	10:AO:96:ARG:NH1	2.43	0.51
1:AA:944:U:H2'	1:AA:945:G:C8	2.46	0.51
32:A:1744:A:H62	32:A:1754:G:N2	2.08	0.51
32:A:2508:C:H2'	32:A:2509:A:H8	1.75	0.51
65:N:33:LEU:O	80:l:121:LEU:HD21	2.10	0.51
1:AA:674:U:O2	6:AJ:57:GLN:NE2	2.42	0.51
13:AT:105:ILE:HA	21:AU:105:LEU:HD13	1.91	0.51
19:AR:295:ASP:O	19:AR:299:ASN:ND2	2.31	0.51
29:AD:324:CYS:HB2	29:AD:329:ILE:HB	1.92	0.51
31:AG:267:MET:N	31:AG:267:MET:SD	2.84	0.51
47:Z:75:THR:HB	47:Z:83:LYS:HG2	1.92	0.51
69:E:218:VAL:HG23	69:E:222:TRP:HD1	1.75	0.51
86:v:175:LYS:HA	92:v:802:GCP:C6	2.38	0.51
32:A:2277:U:H2'	32:A:2278:A:C8	2.46	0.51
32:A:2472:A:OP2	32:A:2653:C:N4	2.44	0.51
32:A:2691:U:H2'	32:A:2692:G:C8	2.46	0.51
39:M:95:PRO:HB2	71:6:380:TYR:HB3	1.92	0.51
65:N:40:GLU:N	65:N:40:GLU:OE1	2.44	0.51
68:V:22:GLY:O	68:V:24:SER:N	2.42	0.51
22:AV:254:GLY:O	22:AV:258:ARG:NH1	2.44	0.51
29:AD:147:PRO:HD3	87:A5:10:Y5P:C5'	2.40	0.51
32:A:1767:G:H2'	32:A:1768:G:C8	2.46	0.51
32:A:1794:A:OP1	35:F:142:ARG:NH2	2.41	0.51
32:A:1861:U:H3	32:A:2304:G:H1	1.57	0.51
32:A:2065:A:OP1	77:f:48:TYR:N	2.43	0.51
39:M:155:GLU:OE2	39:M:179:TYR:OH	2.29	0.51
45:X:216:ARG:HH12	70:5:63:LYS:N	2.09	0.51
53:8:121:TRP:HB2	55:e:70:MET:HE3	1.91	0.51
67:U:132:GLU:OE2	67:U:136:GLN:NE2	2.43	0.51
79:k:10:LEU:HD22	79:k:42:VAL:HG22	1.93	0.51
86:v:299:SER:H	86:v:304:LYS:HB2	1.76	0.51
1:AA:1277:A:H5''	29:AD:269:ARG:HH22	1.75	0.51
1:AA:1282:G:N2	1:AA:1286:A:OP2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:K:20:LEU:HB2	37:K:141:LEU:HD22	1.92	0.51
70:5:173:ARG:NH1	70:5:348:ASP:O	2.41	0.51
80:l:100:ASN:OD1	80:l:101:LEU:N	2.43	0.51
81:p:51:GLU:OE1	81:p:51:GLU:N	2.44	0.51
10:AO:120:VAL:HG23	10:AO:163:LEU:HD23	1.93	0.51
19:AR:103:TYR:OH	29:AD:307:LYS:NZ	2.43	0.51
22:AV:164:VAL:HA	22:AV:167:VAL:HG22	1.93	0.51
32:A:1742:G:O2'	32:A:1754:G:O6	2.28	0.51
32:A:1883:G:N7	35:F:281:ARG:NH1	2.59	0.51
32:A:2257:C:H2'	32:A:2258:A:C4	2.46	0.51
32:A:2942:C:H2'	32:A:2943:G:C8	2.46	0.51
32:A:3179:G:H2'	32:A:3180:A:C8	2.46	0.51
51:3:137:THR:HG23	51:3:140:ARG:H	1.75	0.51
2:AB:117:ASP:HB3	2:AB:120:GLN:HE22	1.76	0.51
26:A0:62:SER:OG	26:A0:66:GLN:OE1	2.27	0.51
32:A:1800:G:H22	32:A:1803:A:H5'	1.74	0.51
32:A:1930:C:O2'	32:A:1944:C:N4	2.44	0.51
63:J:132:LEU:CB	64:I:114:HIS:CG	2.90	0.51
72:7:287:GLN:H	72:7:288:PRO:HD2	1.75	0.51
86:v:736:LEU:HD11	86:v:743:PRO:HG3	1.93	0.51
1:AA:655:U:O4	1:AA:1168:A:N6	2.44	0.51
1:AA:992:U:O2'	1:AA:994:A:OP2	2.24	0.51
1:AA:1098:C:O2'	1:AA:1152:A:OP1	2.29	0.51
13:AT:158:GLU:OE1	13:AT:158:GLU:N	2.43	0.51
16:A2:100:LEU:HD11	16:A2:103:LYS:HD3	1.93	0.51
22:AV:90:TYR:HB3	83:Q:57:PRO:HB3	1.93	0.51
32:A:3063:G:OP1	32:A:3063:G:N2	2.44	0.51
44:W:97:VAL:HG22	44:W:133:VAL:HG22	1.91	0.51
67:U:153:LEU:HD21	76:d:240:LYS:HD3	1.93	0.51
72:7:49:ASN:OD1	72:7:256:ARG:NH1	2.43	0.51
1:AA:1303:G:H4'	1:AA:1320:G:H4'	1.92	0.50
3:AC:41:ARG:HH21	3:AC:59:PRO:HD2	1.77	0.50
32:A:2138:U:O2'	32:A:2151:A:N3	2.37	0.50
32:A:2466:A:H5''	83:Q:232:ARG:HE	1.75	0.50
53:8:107:THR:HG23	53:8:110:GLU:H	1.76	0.50
60:o:15:ARG:HG2	60:o:18:ILE:HG12	1.93	0.50
63:J:156:VAL:HG21	63:J:159:LEU:CD1	2.40	0.50
71:6:322:ARG:NH1	81:p:181:GLU:OE1	2.44	0.50
83:Q:148:THR:HG22	83:Q:165:GLU:HG2	1.93	0.50
86:v:47:ARG:HB2	86:v:116:ILE:HG13	1.91	0.50
86:v:671:ARG:NE	86:v:702:GLU:OE2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1743:U:H2'	32:A:1744:A:C8	2.46	0.50
32:A:2860:G:O2'	44:W:65:ASN:OD1	2.27	0.50
83:Q:76:LEU:HD21	83:Q:282:ILE:HD11	1.93	0.50
83:Q:268:ASP:O	83:Q:270:MET:N	2.44	0.50
1:AA:877:G:H5'	1:AA:906:C:H2'	1.93	0.50
1:AA:1277:A:OP1	29:AD:269:ARG:NH2	2.44	0.50
32:A:2232:A:O2'	32:A:3002:G:N3	2.43	0.50
32:A:2519:G:C5	34:D:228:LEU:HD13	2.46	0.50
42:S:146:LYS:O	42:S:148:LEU:N	2.45	0.50
44:W:67:ILE:N	44:W:89:LEU:O	2.43	0.50
64:I:77:GLY:HA3	80:I:118:TRP:CZ2	2.47	0.50
68:V:147:SER:HB3	68:V:152:ARG:H	1.75	0.50
76:d:48:PRO:HB2	76:d:50:PHE:HD1	1.77	0.50
86:v:557:GLU:HB2	86:v:608:ARG:HD2	1.93	0.50
15:AX:242:ILE:HA	15:AX:245:LYS:HE2	1.93	0.50
15:AX:348:TYR:H	15:AX:386:ALA:HB1	1.76	0.50
34:D:198:SER:HB3	34:D:206:TYR:HE2	1.76	0.50
64:I:92:ASP:OD1	64:I:93:ASN:N	2.44	0.50
7:AK:92:VAL:HG23	7:AK:93:MET:HG3	1.93	0.50
15:AX:262:VAL:HG21	15:AX:268:LEU:HD11	1.94	0.50
25:A1:164:ARG:HG3	28:A4:134:GLU:HG3	1.93	0.50
32:A:1814:A:N3	32:A:1862:U:O2'	2.42	0.50
32:A:2406:A:O2'	70:5:110:ARG:NH1	2.44	0.50
86:v:560:ASP:N	86:v:560:ASP:OD1	2.45	0.50
1:AA:944:U:H2'	1:AA:945:G:H8	1.76	0.50
1:AA:1399:A:H2	1:AA:1445:G:H4'	1.75	0.50
6:AJ:92:VAL:HG13	6:AJ:121:VAL:HG12	1.93	0.50
19:AR:162:SER:H	19:AR:170:ARG:HH12	1.59	0.50
19:AR:219:TYR:OH	19:AR:249:THR:OG1	2.29	0.50
31:AG:276:ARG:HE	31:AG:373:ASP:HB3	1.77	0.50
32:A:2982:C:N4	32:A:2983:G:O6	2.45	0.50
37:K:168:ARG:HB3	62:r:59:GLU:HA	1.93	0.50
40:O:62:TYR:OH	83:Q:272:GLU:OE1	2.27	0.50
43:T:62:GLN:HG3	76:d:229:GLY:HA3	1.94	0.50
56:g:125:GLU:HG3	56:g:136:PRO:HD2	1.92	0.50
64:I:119:HIS:CE1	64:I:160:LYS:HD2	2.46	0.50
65:N:33:LEU:HD22	80:I:125:ASN:ND2	2.25	0.50
68:V:33:ARG:NH2	76:d:61:ARG:O	2.45	0.50
72:7:64:LYS:NZ	76:d:278:LYS:O	2.44	0.50
82:s:63:ILE:HA	82:s:66:TRP:CD1	2.45	0.50
82:s:178:ASP:HA	82:s:181:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1261:C:H2'	1:AA:1262:C:C6	2.46	0.50
1:AA:1401:G:N2	1:AA:1404:A:OP2	2.44	0.50
2:AB:115:ILE:HG21	14:AW:84:LEU:HD13	1.93	0.50
3:AC:69:LEU:HD23	25:A1:107:LYS:HE2	1.94	0.50
22:AV:66:PRO:HB3	22:AV:99:PRO:HD2	1.93	0.50
32:A:1965:A:H2'	32:A:1966:G:C8	2.46	0.50
32:A:2860:G:OP2	71:6:368:ARG:NH1	2.45	0.50
38:L:98:PRO:HG3	38:L:124:PRO:HB3	1.93	0.50
46:Y:117:GLN:HG2	67:U:29:VAL:HG22	1.93	0.50
51:3:132:LYS:O	51:3:136:LYS:NZ	2.35	0.50
70:5:230:LEU:HD23	70:5:289:HIS:HD2	1.77	0.50
72:7:89:TYR:HB2	72:7:115:MET:HG3	1.93	0.50
74:a:104:GLU:HG2	74:a:107:PRO:HD2	1.93	0.50
86:v:332:GLU:HG3	86:v:439:LEU:HD13	1.93	0.50
1:AA:1438:A:H2'	1:AA:1439:A:C8	2.46	0.50
10:AO:92:LYS:HA	10:AO:144:VAL:HG12	1.92	0.50
22:AV:168:MET:HG3	22:AV:207:SER:HA	1.93	0.50
25:A1:257:SER:O	25:A1:261:ASN:ND2	2.44	0.50
32:A:2598:A:N6	32:A:2625:C:O5'	2.44	0.50
35:F:282:PRO:O	35:F:284:TYR:N	2.44	0.50
36:H:84:GLU:OE1	45:X:44:ARG:NH2	2.44	0.50
39:M:264:GLN:HE22	39:M:270:ALA:HA	1.75	0.50
44:W:147:MET:HE3	71:6:338:ARG:HB2	1.92	0.50
45:X:209:GLU:OE2	70:5:69:TRP:NE1	2.44	0.50
66:P:143:PHE:HB3	66:P:174:GLU:HG2	1.94	0.50
76:d:57:MET:SD	76:d:57:MET:N	2.85	0.50
82:s:112:THR:HG22	82:s:391:ASN:HB2	1.93	0.50
86:v:680:GLY:HA2	86:v:685:PHE:HA	1.92	0.50
3:AC:69:LEU:HD12	7:AK:119:GLN:HG2	1.94	0.50
17:AH:180:LEU:HD22	17:AH:184:ILE:HD13	1.94	0.50
22:AV:130:VAL:HA	22:AV:166:GLU:HG3	1.94	0.50
22:AV:131:ASN:ND2	22:AV:134:GLN:HB3	2.27	0.50
29:AD:103:LEU:HD21	29:AD:123:ARG:HB2	1.94	0.50
32:A:1741:A:H4'	32:A:1742:G:H4'	1.94	0.50
32:A:1800:G:H2'	32:A:1805:A:H61	1.77	0.50
32:A:2661:U:OP2	69:E:238:ARG:NH2	2.45	0.50
63:J:34:PRO:O	63:J:36:GLY:N	2.41	0.50
83:Q:119:VAL:HG22	83:Q:174:ILE:HG23	1.94	0.50
1:AA:826:A:H61	6:AJ:56:PRO:HD2	1.77	0.49
2:AB:132:THR:HG22	2:AB:192:LEU:HD21	1.94	0.49
22:AV:287:LEU:HD23	22:AV:290:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3143:U:H2'	32:A:3144:A:C8	2.46	0.49
39:M:273:TRP:HE1	39:M:284:LYS:HG2	1.76	0.49
41:R:94:GLN:OE1	42:S:146:LYS:HE2	2.12	0.49
51:3:116:ARG:NH2	51:3:159:ASP:OD1	2.45	0.49
68:V:51:ASP:OD1	68:V:81:ARG:NH2	2.41	0.49
86:v:207:LEU:O	86:v:209:GLY:N	2.45	0.49
86:v:332:GLU:N	86:v:338:LYS:O	2.31	0.49
1:AA:1204:C:O2'	1:AA:1225:C:N4	2.45	0.49
15:AX:181:PRO:HA	15:AX:237:THR:HB	1.93	0.49
25:A1:245:GLU:HA	25:A1:248:MET:HE3	1.93	0.49
26:A0:129:ARG:NH2	26:A0:204:PRO:O	2.44	0.49
31:AG:306:ILE:HG22	31:AG:308:GLN:H	1.77	0.49
32:A:1881:A:H62	56:g:111:ARG:HD3	1.77	0.49
43:T:149:ARG:NH1	43:T:168:GLU:OE2	2.38	0.49
45:X:69:ILE:HG22	45:X:86:ILE:HG12	1.92	0.49
49:1:55:LEU:HD12	61:q:131:MET:HE2	1.94	0.49
72:7:286:LEU:HD23	72:7:286:LEU:H	1.77	0.49
78:h:137:ARG:NH2	78:h:141:ASP:O	2.45	0.49
81:p:156:ASP:HA	81:p:159:THR:HG22	1.94	0.49
1:AA:663:A:H2'	1:AA:664:G:H8	1.77	0.49
1:AA:1032:C:H1'	11:AP:116:ILE:HG21	1.94	0.49
1:AA:1194:C:H5''	30:AF:185:LYS:HD2	1.94	0.49
1:AA:1195:U:H2'	1:AA:1196:A:H8	1.77	0.49
26:A0:133:HIS:HB2	26:A0:139:TRP:HZ2	1.78	0.49
32:A:1860:A:H2'	32:A:1861:U:C6	2.47	0.49
32:A:2025:C:OP2	42:S:182:LYS:NZ	2.35	0.49
32:A:2841:U:H5'	65:N:144:LYS:HD3	1.93	0.49
33:B:1622:A:H2'	33:B:1623:G:C8	2.46	0.49
34:D:107:ILE:HG13	34:D:135:ARG:HH12	1.77	0.49
83:Q:77:SER:HB3	83:Q:80:PHE:HD2	1.77	0.49
86:v:197:ASN:OD1	86:v:198:ALA:N	2.45	0.49
1:AA:1226:C:OP1	17:AH:128:LYS:NZ	2.36	0.49
5:AI:87:HIS:HA	5:AI:150:VAL:HB	1.94	0.49
15:AX:299:ASN:ND2	15:AX:338:ASP:OD1	2.46	0.49
32:A:1728:U:H3	32:A:1750:G:H1	1.59	0.49
32:A:2822:C:O2'	32:A:2915:C:OP2	2.29	0.49
32:A:2908:U:OP1	51:3:133:LEU:N	2.43	0.49
39:M:233:ARG:HH12	39:M:244:LEU:HD21	1.78	0.49
42:S:204:LEU:HD11	74:a:59:VAL:HG21	1.94	0.49
46:Y:169:ARG:HH21	70:5:64:MET:HB2	1.77	0.49
65:N:203:GLU:HA	65:N:206:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:s:251:VAL:O	82:s:373:GLN:NE2	2.42	0.49
86:v:205:MET:HG3	86:v:242:LEU:HD21	1.94	0.49
86:v:658:ASN:ND2	86:v:683:ASP:O	2.45	0.49
1:AA:735:A:C6	1:AA:740:G:C2	3.00	0.49
1:AA:1365:A:O2'	1:AA:1418:G:N2	2.45	0.49
32:A:2302:U:H2'	32:A:2303:A:C8	2.47	0.49
53:8:150:LEU:HB2	55:e:212:HIS:HE1	1.77	0.49
63:J:60:ILE:HG22	63:J:62:GLU:H	1.78	0.49
63:J:132:LEU:CA	64:I:114:HIS:CB	2.84	0.49
64:I:168:LEU:HB2	64:I:174:LEU:HD23	1.93	0.49
66:P:44:VAL:HA	71:6:225:LEU:HB3	1.95	0.49
70:5:351:VAL:HG12	70:5:381:LEU:HG	1.93	0.49
81:p:56:ASP:OD2	81:p:60:ARG:NH2	2.45	0.49
86:v:216:ASP:HB3	86:v:218:ILE:HG22	1.94	0.49
1:AA:802:C:O3'	1:AA:816:A:N6	2.45	0.49
1:AA:940:A:H2	1:AA:1136:C:H1'	1.78	0.49
1:AA:950:A:OP1	9:AN:29:ARG:NH1	2.46	0.49
29:AD:117:ARG:HD2	87:A5:1:Y5P:C3'	2.34	0.49
32:A:3066:C:O2'	69:E:233:GLN:OE1	2.24	0.49
64:I:194:TYR:HA	64:I:197:LEU:HD23	1.95	0.49
83:Q:54:PHE:O	83:Q:55:GLN:NE2	2.44	0.49
86:v:657:PRO:HA	86:v:684:TYR:HB3	1.95	0.49
1:AA:1347:G:OP1	7:AK:36:ARG:NH1	2.45	0.49
4:AE:22:LEU:HD22	4:AE:39:LEU:HD11	1.94	0.49
9:AN:14:VAL:HG12	13:AT:29:VAL:HG21	1.94	0.49
42:S:129:ARG:NH1	42:S:131:GLU:OE2	2.46	0.49
50:2:57:ASN:ND2	73:9:25:ARG:O	2.45	0.49
53:8:178:TYR:CZ	77:f:180:GLU:HG2	2.48	0.49
67:U:80:ARG:NH1	67:U:84:ASN:OD1	2.46	0.49
70:5:241:SER:N	70:5:244:GLU:OE2	2.40	0.49
77:f:165:THR:O	77:f:168:GLU:HG3	2.12	0.49
83:Q:168:ASN:HB3	83:Q:171:VAL:HG23	1.93	0.49
1:AA:1197:G:N2	1:AA:1425:U:O2	2.38	0.49
2:AB:142:ILE:HG22	2:AB:192:LEU:HD23	1.94	0.49
21:AU:186:ASN:O	21:AU:199:ARG:NH2	2.46	0.49
28:A4:136:HIS:HE1	28:A4:141:MET:HE3	1.77	0.49
29:AD:220:THR:HG21	29:AD:272:LYS:HG2	1.94	0.49
32:A:1808:A:OP2	76:d:177:LYS:NZ	2.45	0.49
32:A:2193:U:H1'	63:J:133:GLN:NE2	2.27	0.49
32:A:2952:U:O2'	52:4:70:THR:OG1	2.30	0.49
53:8:167:ASN:HD22	55:e:185:ARG:HH22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:N:204:GLU:OE2	65:N:208:ASN:ND2	2.46	0.49
66:P:67:GLY:O	66:P:69:ARG:N	2.46	0.49
72:7:166:LEU:HD22	72:7:181:TYR:HE2	1.77	0.49
74:a:45:CYS:SG	74:a:46:ASN:N	2.86	0.49
83:Q:177:VAL:HA	83:Q:206:PRO:HB3	1.95	0.49
1:AA:1235:U:O2	7:AK:88:ARG:NH2	2.46	0.49
32:A:2538:C:H2'	32:A:2539:A:O4'	2.13	0.49
32:A:2571:G:H1	32:A:2586:U:H3	1.61	0.49
32:A:2864:U:H5'	32:A:2865:C:H4'	1.95	0.49
32:A:3116:C:H42	32:A:3140:A:H61	1.59	0.49
32:A:3143:U:H2'	32:A:3144:A:H8	1.77	0.49
39:M:176:THR:HB	39:M:221:GLY:HA2	1.95	0.49
65:N:247:MET:N	65:N:247:MET:SD	2.86	0.49
86:v:331:LYS:HA	86:v:339:THR:HA	1.95	0.49
1:AA:1139:A:H2'	1:AA:1140:A:C8	2.47	0.49
28:A4:137:ILE:HB	28:A4:140:LEU:HD23	1.95	0.49
30:AF:168:TYR:HB3	30:AF:236:LEU:HD13	1.94	0.49
31:AG:116:LEU:O	31:AG:122:ARG:NH2	2.42	0.49
32:A:2235:C:O2'	62:r:164:LYS:O	2.28	0.49
32:A:2317:G:H2'	32:A:2318:A:H8	1.76	0.49
32:A:2453:G:O6	32:A:2672:A:N6	2.45	0.49
39:M:36:PRO:HB2	39:M:38:ARG:HH22	1.78	0.49
69:E:79:PRO:HG3	69:E:192:PRO:HD2	1.94	0.49
69:E:134:SER:OG	69:E:137:ASN:ND2	2.46	0.49
72:7:42:GLU:HA	72:7:45:ASN:HD21	1.76	0.49
82:s:228:ASP:O	82:s:230:ARG:NH1	2.46	0.49
83:Q:55:GLN:HG3	83:Q:56:PRO:HD2	1.95	0.49
86:v:386:ASN:OD1	86:v:387:THR:N	2.46	0.49
3:AC:52:THR:OG1	3:AC:53:TYR:N	2.35	0.48
9:AN:63:ILE:HD12	9:AN:86:PHE:HB2	1.95	0.48
15:AX:188:LEU:HD22	15:AX:226:VAL:HG13	1.95	0.48
22:AV:274:LYS:NZ	22:AV:278:GLU:OE2	2.38	0.48
32:A:2927:C:H4'	32:A:3074:A:H4'	1.94	0.48
1:AA:1439:A:H2'	1:AA:1440:G:C8	2.46	0.48
15:AX:133:GLY:O	15:AX:137:SER:OG	2.27	0.48
16:A2:10:LEU:O	16:A2:15:ASN:ND2	2.46	0.48
22:AV:212:GLY:HA3	22:AV:224:GLN:HG3	1.95	0.48
34:D:194:ASN:HD22	34:D:247:VAL:HG22	1.78	0.48
38:L:32:ILE:HG23	38:L:36:THR:HG21	1.95	0.48
56:g:77:ASP:OD1	56:g:77:ASP:N	2.32	0.48
66:P:69:ARG:HA	66:P:69:ARG:HE	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:c:223:MET:HE3	75:c:231:MET:HE1	1.93	0.48
86:v:68:TYR:HD2	86:v:72:ARG:O	1.96	0.48
1:AA:674:U:O2'	6:AJ:57:GLN:OE1	2.28	0.48
1:AA:1437:U:H2'	1:AA:1438:A:H8	1.78	0.48
9:AN:95:VAL:HG12	9:AN:96:THR:HG23	1.95	0.48
11:AP:91:ILE:HD12	11:AP:111:ILE:HD13	1.95	0.48
29:AD:227:ASN:ND2	87:A5:1:Y5P:C4	2.65	0.48
32:A:1747:G:O2'	32:A:1750:G:O6	2.27	0.48
32:A:1783:U:H3	32:A:1794:A:N6	2.09	0.48
32:A:1915:C:H2'	32:A:1916:G:C8	2.48	0.48
32:A:2267:U:H2'	32:A:2268:G:C8	2.48	0.48
32:A:2559:U:H4'	32:A:2560:G:O5'	2.13	0.48
32:A:3152:C:O4'	38:L:95:ARG:NH1	2.46	0.48
32:A:3193:U:H4'	62:r:138:GLY:HA3	1.94	0.48
35:F:63:GLN:HA	35:F:81:ASP:HA	1.95	0.48
38:L:37:ARG:HD2	38:L:54:ALA:HB3	1.95	0.48
39:M:44:ARG:HG3	39:M:45:ARG:HG3	1.95	0.48
53:8:106:LEU:HD22	53:8:110:GLU:HG2	1.95	0.48
55:e:162:ARG:HB3	55:e:251:HIS:HB2	1.95	0.48
56:g:66:TYR:N	56:g:67:PRO:HD2	2.28	0.48
65:N:96:TYR:OH	65:N:129:LYS:NZ	2.46	0.48
75:c:102:GLU:HA	75:c:105:ARG:HG2	1.94	0.48
83:Q:120:THR:HG23	83:Q:172:GLN:HB2	1.94	0.48
86:v:425:CYS:SG	86:v:426:ALA:N	2.86	0.48
86:v:654:VAL:HB	86:v:687:LEU:HB3	1.95	0.48
2:AB:111:LEU:HD21	11:AP:58:TYR:HD2	1.77	0.48
25:A1:214:LEU:O	25:A1:218:ASN:ND2	2.46	0.48
32:A:1951:C:H2'	32:A:1952:U:H6	1.78	0.48
32:A:2536:G:H2'	32:A:2537:G:C8	2.48	0.48
58:j:88:LEU:HD11	60:o:53:TYR:HE2	1.78	0.48
59:m:37:ARG:HH21	77:f:109:TYR:HE1	1.61	0.48
62:r:79:HIS:HB3	62:r:184:ASN:HA	1.95	0.48
70:5:204:VAL:HG11	70:5:279:PHE:HZ	1.78	0.48
82:s:316:CYS:HB3	82:s:319:GLN:HB2	1.94	0.48
86:v:61:THR:O	86:v:65:ARG:HG2	2.13	0.48
14:AW:99:LEU:HD11	14:AW:141:ARG:HE	1.78	0.48
15:AX:265:ILE:HB	15:AX:269:TRP:HZ3	1.79	0.48
32:A:1737:A:N6	32:A:1760:G:H21	2.10	0.48
32:A:2039:A:H62	32:A:2729:U:H1'	1.78	0.48
32:A:2190:C:OP1	80:l:127:TRP:CH2	2.66	0.48
32:A:2255:C:H2'	32:A:2256:U:H5	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:N:78:GLU:HG2	65:N:158:ARG:HH12	1.78	0.48
70:5:244:GLU:O	70:5:248:THR:OG1	2.30	0.48
32:A:2126:U:O4	47:Z:76:ARG:NH1	2.36	0.48
35:F:126:LYS:NZ	35:F:128:TRP:O	2.46	0.48
86:v:159:ASN:HA	86:v:162:MET:HE3	1.94	0.48
1:AA:1332:A:H3'	1:AA:1333:G:H8	1.79	0.48
3:AC:108:LEU:HD11	3:AC:119:ILE:HB	1.96	0.48
13:AT:80:LEU:HD12	13:AT:84:GLU:HB2	1.95	0.48
32:A:2314:C:H2'	32:A:2315:A:C5	2.49	0.48
32:A:2795:U:O2	36:H:87:LYS:NZ	2.45	0.48
32:A:2919:A:H4'	88:A7:71:P5P:O3'	2.13	0.48
46:Y:91:ARG:NH1	73:9:83:GLU:OE1	2.46	0.48
77:f:135:LEU:HD23	77:f:135:LEU:H	1.78	0.48
1:AA:982:A:N6	1:AA:1007:G:O6	2.46	0.48
1:AA:1402:A:O3'	7:AK:58:ARG:NH2	2.47	0.48
19:AR:87:LEU:HD11	19:AR:119:VAL:HG22	1.95	0.48
32:A:2081:U:H2'	32:A:2082:G:C8	2.49	0.48
32:A:3179:G:N2	32:A:3190:A:N6	2.44	0.48
66:P:39:VAL:HG12	66:P:41:ASN:H	1.79	0.48
82:s:93:VAL:HB	82:s:233:ILE:HG12	1.96	0.48
83:Q:165:GLU:HB2	83:Q:168:ASN:HB2	1.94	0.48
1:AA:1225:C:OP2	1:AA:1360:G:N2	2.34	0.48
5:AI:119:ASN:O	5:AI:121:LYS:N	2.41	0.48
32:A:2173:G:H2'	32:A:2174:G:H8	1.79	0.48
32:A:2995:G:O2'	32:A:3042:U:OP1	2.31	0.48
35:F:253:MET:HE3	35:F:259:LEU:HD22	1.96	0.48
49:1:17:LEU:HD11	49:1:31:ASN:HB3	1.96	0.48
63:J:33:PRO:HB2	63:J:34:PRO:HD2	1.95	0.48
68:V:96:ARG:NE	68:V:111:SER:OG	2.47	0.48
1:AA:1556:C:H2'	1:AA:1557:A:C8	2.48	0.48
13:AT:47:PHE:HD1	13:AT:51:ASN:HD22	1.60	0.48
24:AZ:85:LEU:HD23	24:AZ:88:LEU:HD21	1.96	0.48
32:A:2187:C:C2	63:J:106:LYS:NZ	2.82	0.48
32:A:3000:A:H2'	32:A:3001:G:C8	2.48	0.48
32:A:3080:G:H2'	32:A:3081:A:H8	1.79	0.48
53:8:139:MET:HG2	55:e:275:PHE:HA	1.95	0.48
70:5:145:ASN:HA	70:5:194:LYS:HE2	1.95	0.48
80:l:114:SER:OG	80:l:116:GLU:OE1	2.32	0.48
1:AA:1195:U:H2'	1:AA:1196:A:C8	2.48	0.47
1:AA:1231:A:O2'	1:AA:1236:C:N4	2.46	0.47
1:AA:1591:C:H5''	12:AQ:49:CYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:84:PRO:HB3	5:AI:101:SER:HA	1.96	0.47
29:AD:315:ARG:HB2	29:AD:333:TYR:HD1	1.78	0.47
30:AF:186:TRP:HH2	30:AF:226:LEU:HD13	1.79	0.47
31:AG:317:PHE:HB3	31:AG:323:LEU:HD23	1.96	0.47
32:A:2298:A:H61	35:F:145:LEU:HD22	1.77	0.47
32:A:2395:A:H1'	70:5:385:HIS:HB2	1.96	0.47
71:6:239:ASN:ND2	71:6:280:ASP:OD1	2.40	0.47
82:s:111:LYS:NZ	82:s:384:ASP:OD1	2.45	0.47
86:v:250:ARG:HH21	86:v:274:PRO:HB2	1.78	0.47
1:AA:1441:A:N1	1:AA:1449:G:O6	2.47	0.47
32:A:1676:A:C4	57:i:36:LEU:HD23	2.49	0.47
32:A:1954:U:H5'	32:A:2462:A:H4'	1.96	0.47
38:L:41:VAL:HG11	38:L:104:ASN:HD22	1.79	0.47
58:j:50:SER:HA	58:j:57:ALA:HB2	1.96	0.47
60:o:35:MET:HG2	60:o:38:ARG:HH21	1.80	0.47
62:r:63:PRO:HG2	62:r:66:PRO:HG3	1.95	0.47
77:f:48:TYR:HB3	77:f:51:LYS:HG2	1.96	0.47
82:s:66:TRP:HA	82:s:69:THR:HG22	1.95	0.47
1:AA:918:A:H3'	10:AO:96:ARG:HH12	1.79	0.47
23:AY:327:GLU:O	23:AY:331:HIS:ND1	2.41	0.47
32:A:1703:C:O2'	32:A:1704:U:OP2	2.26	0.47
32:A:1790:A:OP1	50:2:82:ARG:NH2	2.47	0.47
35:F:102:TRP:HE1	35:F:164:MET:HA	1.79	0.47
35:F:182:LEU:HD13	35:F:187:LEU:HD23	1.94	0.47
36:H:70:LYS:HB2	36:H:72:ARG:HH12	1.79	0.47
36:H:119:GLY:HA2	36:H:123:LEU:HD12	1.96	0.47
39:M:216:ASP:OD1	39:M:217:ALA:N	2.46	0.47
62:r:50:GLU:OE2	79:k:77:ARG:NH1	2.47	0.47
68:V:19:TYR:OH	68:V:31:ASP:OD2	2.33	0.47
68:V:69:ASP:HB2	68:V:72:LYS:HD2	1.96	0.47
70:5:60:PHE:CD1	70:5:71:ALA:CA	2.95	0.47
71:6:147:HIS:HA	71:6:150:ARG:HG2	1.97	0.47
19:AR:69:THR:HG22	19:AR:71:MET:H	1.78	0.47
32:A:1770:G:O3'	41:R:11:ARG:NH1	2.48	0.47
36:H:119:GLY:HA2	36:H:123:LEU:HB2	1.97	0.47
56:g:85:PHE:N	56:g:114:GLU:O	2.47	0.47
63:J:171:ARG:HD2	63:J:171:ARG:N	2.28	0.47
71:6:274:LYS:N	71:6:312:THR:O	2.47	0.47
82:s:257:VAL:HG22	82:s:259:ILE:H	1.80	0.47
82:s:267:LYS:HG2	82:s:269:ASP:H	1.78	0.47
1:AA:944:U:O2'	1:AA:1025:A:N3	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A2:102:ASN:HA	16:A2:105:ASN:HD21	1.79	0.47
25:A1:78:PRO:HB3	25:A1:99:LYS:HB2	1.97	0.47
25:A1:286:THR:HB	25:A1:289:ILE:HG22	1.96	0.47
32:A:1829:A:H2'	32:A:1830:G:C8	2.50	0.47
32:A:1833:C:O5'	54:b:116:ARG:NH1	2.48	0.47
32:A:2439:U:H2'	32:A:2440:G:H8	1.79	0.47
32:A:2521:A:N6	34:D:202:ARG:O	2.43	0.47
62:r:174:MET:N	62:r:174:MET:SD	2.88	0.47
70:5:63:LYS:HD2	70:5:67:VAL:HG11	1.96	0.47
82:s:366:TYR:HA	82:s:400:PRO:HA	1.96	0.47
86:v:53:ALA:HB3	86:v:59:LYS:HB3	1.97	0.47
1:AA:1432:U:H4'	31:AG:388:ARG:HG3	1.95	0.47
3:AC:122:VAL:HG12	3:AC:156:GLN:HB3	1.96	0.47
23:AY:383:LYS:HD3	23:AY:386:ILE:HD12	1.96	0.47
29:AD:117:ARG:CD	87:A5:1:Y5P:C3'	2.91	0.47
32:A:1863:A:H2'	32:A:1864:A:H8	1.80	0.47
32:A:2962:C:N4	32:A:3016:G:H22	2.11	0.47
32:A:2989:G:O2'	32:A:2990:A:OP2	2.30	0.47
44:W:106:PRO:O	66:P:72:PHE:HE1	1.97	0.47
63:J:160:SER:O	63:J:163:GLU:HG3	2.15	0.47
1:AA:835:C:N4	1:AA:851:A:OP2	2.41	0.47
1:AA:1138:G:H2'	1:AA:1139:A:C8	2.50	0.47
1:AA:1438:A:H2'	1:AA:1439:A:H8	1.78	0.47
9:AN:18:ILE:HB	9:AN:27:LYS:HE3	1.97	0.47
15:AX:163:LYS:HG3	15:AX:164:ASN:HD22	1.80	0.47
15:AX:273:THR:HG23	15:AX:316:LEU:HD13	1.97	0.47
29:AD:173:ILE:O	29:AD:176:ARG:HG3	2.14	0.47
32:A:2527:A:O4'	34:D:67:LYS:NZ	2.42	0.47
32:A:2899:C:H5'	51:3:113:ARG:HH22	1.78	0.47
32:A:2948:C:H2'	32:A:2949:C:C6	2.50	0.47
35:F:48:LEU:HD11	78:h:95:ARG:HB2	1.97	0.47
41:R:114:LYS:NZ	74:a:45:CYS:O	2.38	0.47
55:e:177:GLU:OE1	55:e:177:GLU:N	2.47	0.47
57:i:63:LEU:HD23	57:i:63:LEU:H	1.80	0.47
64:I:198:PRO:HB2	64:I:202:LEU:HD11	1.97	0.47
66:P:59:LEU:HD11	71:6:264:GLY:HA2	1.97	0.47
66:P:80:ARG:HH12	66:P:82:ARG:HD3	1.80	0.47
70:5:60:PHE:CD1	70:5:67:VAL:HG22	2.50	0.47
71:6:265:ILE:HD12	71:6:322:ARG:HG2	1.96	0.47
76:d:84:ILE:HA	76:d:211:GLN:HE22	1.80	0.47
82:s:99:ALA:HB3	82:s:102:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:s:270:LYS:HD3	82:s:270:LYS:HA	1.65	0.47
86:v:67:LEU:HD11	86:v:72:ARG:HD3	1.97	0.47
86:v:201:MET:HA	86:v:217:LEU:HD11	1.96	0.47
25:A1:169:ARG:O	25:A1:218:ASN:ND2	2.47	0.47
32:A:1673:U:O2	32:A:1816:G:C6	2.68	0.47
32:A:1828:A:H4'	32:A:1829:A:H8	1.79	0.47
58:j:46:LEU:HD12	58:j:47:PRO:HD2	1.96	0.47
60:o:55:THR:O	60:o:57:GLU:N	2.43	0.47
68:V:178:SER:OG	68:V:181:ASP:OD2	2.28	0.47
70:5:186:GLN:HE22	82:s:185:VAL:HG23	1.80	0.47
71:6:187:VAL:HG23	71:6:319:PHE:HB3	1.97	0.47
72:7:67:VAL:HG13	72:7:79:PHE:HB2	1.96	0.47
76:d:67:ILE:H	76:d:68:PRO:HD2	1.79	0.47
83:Q:181:LYS:HB2	83:Q:217:VAL:HG22	1.96	0.47
2:AB:66:PRO:HA	2:AB:69:HIS:HD2	1.79	0.47
19:AR:155:LYS:HB3	19:AR:177:PRO:HD3	1.97	0.47
31:AG:76:LYS:O	31:AG:79:GLU:HG3	2.15	0.47
37:K:171:THR:HG22	62:r:59:GLU:H	1.80	0.47
46:Y:183:GLN:HE21	68:V:213:VAL:HG21	1.80	0.47
50:2:57:ASN:OD1	50:2:60:ARG:NH2	2.40	0.47
55:e:63:LEU:HD21	55:e:68:GLU:HB2	1.96	0.47
63:J:159:LEU:O	63:J:163:GLU:HB3	2.14	0.47
86:v:91:SER:HA	86:v:95:GLU:HB2	1.97	0.47
86:v:436:ASN:CG	86:v:439:LEU:HG	2.40	0.47
86:v:655:VAL:HG22	86:v:686:THR:HG23	1.97	0.47
11:AP:78:GLN:NE2	11:AP:132:ASP:OD1	2.45	0.47
32:A:1868:G:H21	32:A:1868:G:P	2.38	0.47
41:R:15:THR:HG22	75:c:32:LYS:HB3	1.97	0.47
41:R:146:VAL:CG2	42:S:146:LYS:HD3	2.45	0.47
62:r:43:GLU:O	62:r:46:THR:OG1	2.30	0.47
65:N:33:LEU:CB	80:l:125:ASN:ND2	2.78	0.47
65:N:55:ARG:HG2	65:N:99:TRP:CG	2.50	0.47
69:E:48:TRP:HD1	69:E:50:ASP:H	1.63	0.47
1:AA:1106:C:O2'	1:AA:1108:C:OP2	2.31	0.46
2:AB:107:PHE:HB2	2:AB:117:ASP:HB2	1.97	0.46
17:AH:175:THR:OG1	25:A1:150:GLU:OE1	2.32	0.46
18:AL:71:LEU:HD21	18:AL:76:GLN:HA	1.97	0.46
32:A:2715:A:O2'	69:E:245:THR:O	2.25	0.46
32:A:3134:C:H5''	32:A:3135:A:H8	1.79	0.46
60:o:12:ILE:HG21	60:o:16:GLN:HB3	1.97	0.46
71:6:293:LEU:HD11	71:6:335:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:d:67:ILE:HG22	76:d:68:PRO:HD3	1.97	0.46
82:s:336:THR:HB	82:s:374:LEU:HD22	1.96	0.46
86:v:147:ALA:O	86:v:149:GLY:N	2.48	0.46
1:AA:1239:C:H2'	1:AA:1240:A:C8	2.51	0.46
1:AA:1453:A:H2'	1:AA:1454:G:H8	1.80	0.46
15:AX:284:PRO:HB2	15:AX:294:ARG:HH21	1.79	0.46
15:AX:329:LEU:HB3	15:AX:333:GLY:HA3	1.98	0.46
30:AF:79:ALA:HB1	31:AG:308:GLN:HE21	1.80	0.46
32:A:1769:C:O2'	32:A:2276:C:O2	2.30	0.46
32:A:2117:U:O2'	32:A:2836:C:O2	2.27	0.46
32:A:2214:A:H5'	80:l:126:ILE:HD11	1.97	0.46
36:H:58:ARG:HH11	36:H:77:HIS:HB3	1.79	0.46
39:M:226:PRO:HD3	81:p:45:LEU:HD11	1.97	0.46
58:j:96:GLN:O	58:j:99:GLN:HG3	2.15	0.46
59:m:70:GLU:O	59:m:72:ARG:N	2.45	0.46
63:J:73:LYS:HD2	63:J:77:THR:HB	1.97	0.46
63:J:171:ARG:HG3	63:J:174:PHE:CE2	2.48	0.46
72:7:262:ASP:OD1	72:7:263:VAL:N	2.46	0.46
8:AM:30:PRO:HD2	8:AM:57:LEU:HD11	1.98	0.46
19:AR:213:GLU:O	19:AR:216:ARG:HG3	2.16	0.46
24:AZ:67:PHE:HB3	29:AD:137:TYR:HE1	1.80	0.46
32:A:2068:C:OP2	77:f:58:LYS:NZ	2.39	0.46
32:A:3144:A:H2'	32:A:3145:A:H8	1.80	0.46
34:D:142:VAL:HG11	34:D:163:ILE:HD11	1.97	0.46
46:Y:185:VAL:HG22	67:U:9:LEU:HD21	1.97	0.46
70:5:140:VAL:HB	70:5:416:ALA:HB2	1.96	0.46
70:5:164:TRP:HD1	82:s:287:LYS:HD2	1.80	0.46
86:v:319:ASN:C	86:v:321:SER:H	2.23	0.46
1:AA:1431:G:O2'	1:AA:1457:G:O6	2.30	0.46
6:AJ:67:THR:HG22	6:AJ:79:LYS:HA	1.97	0.46
12:AQ:5:LEU:HD12	12:AQ:8:ILE:HD12	1.98	0.46
14:AW:144:LEU:H	14:AW:167:ALA:HB1	1.81	0.46
16:A2:33:VAL:HG21	16:A2:104:LEU:HD13	1.96	0.46
32:A:1754:G:H5''	51:3:100:ARG:CZ	2.45	0.46
32:A:1848:U:H5''	39:M:53:HIS:CE1	2.50	0.46
32:A:1925:A:H2'	32:A:1926:A:C8	2.49	0.46
32:A:1955:G:N2	32:A:1960:A:N6	2.63	0.46
32:A:2075:U:O2'	32:A:2833:A:N7	2.40	0.46
35:F:175:LYS:HG2	35:F:273:LEU:HD13	1.98	0.46
39:M:208:GLU:OE2	61:q:106:LYS:NZ	2.42	0.46
49:1:65:LEU:HD23	49:1:65:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:81:LEU:HD11	80:l:113:GLU:C	2.40	0.46
68:V:59:GLY:H	68:V:76:VAL:HG13	1.80	0.46
70:5:172:LYS:O	70:5:175:THR:HG22	2.16	0.46
71:6:31:PRO:HA	77:f:52:PRO:HB3	1.97	0.46
1:AA:1562:G:O2'	1:AA:1583:A:N1	2.34	0.46
20:AS:18:ASP:HB3	29:AD:281:TYR:CG	2.51	0.46
31:AG:88:LEU:HA	31:AG:91:MET:HG2	1.97	0.46
51:3:110:VAL:HG13	51:3:158:LEU:HD22	1.97	0.46
57:i:57:TYR:OH	61:q:28:ARG:O	2.25	0.46
63:J:159:LEU:O	63:J:163:GLU:HG2	2.11	0.46
66:P:44:VAL:HG13	71:6:225:LEU:HD13	1.98	0.46
70:5:184:LEU:HD22	70:5:411:PHE:HE1	1.81	0.46
70:5:208:THR:OG1	82:s:158:ARG:HB3	2.15	0.46
86:v:101:THR:HG22	92:v:802:GCP:O3G	2.15	0.46
86:v:559:LEU:HD12	86:v:606:GLY:HA2	1.96	0.46
17:AH:179:GLN:NE2	25:A1:146:HIS:O	2.48	0.46
32:A:2601:A:N7	32:A:3077:C:O2'	2.43	0.46
32:A:2909:G:C2	88:A7:70:Y5P:H4	2.50	0.46
35:F:186:ASP:HB3	35:F:258:THR:HA	1.98	0.46
63:J:132:LEU:CA	64:I:114:HIS:CG	2.95	0.46
63:J:132:LEU:CD2	64:I:114:HIS:CB	2.93	0.46
70:5:67:VAL:CG2	70:5:71:ALA:HB2	2.41	0.46
76:d:208:VAL:HG22	76:d:253:THR:HG23	1.98	0.46
86:v:152:GLN:N	86:v:155:THR:OG1	2.46	0.46
86:v:335:SER:C	86:v:337:GLU:H	2.23	0.46
86:v:436:ASN:O	86:v:439:LEU:HD11	2.16	0.46
1:AA:1012:A:N6	1:AA:1065:C:H42	2.14	0.46
1:AA:1066:C:H2'	1:AA:1067:A:C8	2.51	0.46
4:AE:42:LEU:HB2	4:AE:63:TYR:HB2	1.96	0.46
15:AX:365:TRP:NE1	15:AX:395:CYS:O	2.44	0.46
18:AL:72:LEU:HD11	18:AL:75:TYR:HD2	1.80	0.46
19:AR:143:ALA:HB3	19:AR:181:LEU:HB3	1.97	0.46
24:AZ:40:LEU:HD12	24:AZ:41:PRO:HD2	1.96	0.46
24:AZ:65:LEU:HD13	24:AZ:70:LEU:HD22	1.98	0.46
35:F:63:GLN:HG2	35:F:81:ASP:HB3	1.98	0.46
37:K:52:ASP:O	43:T:206:ARG:NH1	2.48	0.46
45:X:180:ASP:N	45:X:180:ASP:OD1	2.49	0.46
76:d:151:CYS:HB2	76:d:156:ASP:HB3	1.97	0.46
86:v:146:CYS:HA	86:v:173:ILE:HG23	1.98	0.46
88:A7:64:Y5P:H4A	88:A7:65:Y5P:C2	2.46	0.46
1:AA:1260:A:N6	1:AA:1330:C:O2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1505:A:N1	1:AA:1546:A:N6	2.64	0.46
1:AA:1589:C:OP1	5:AI:187:ARG:NH1	2.49	0.46
23:AY:334:LEU:HB2	23:AY:355:THR:HG23	1.97	0.46
26:A0:129:ARG:HD2	26:A0:206:LYS:HD3	1.98	0.46
32:A:1742:G:H2'	51:3:105:LYS:HA	1.97	0.46
32:A:1827:C:O4'	32:A:2698:G:N2	2.49	0.46
32:A:2212:C:H2'	32:A:2213:A:C8	2.51	0.46
32:A:2366:G:H2'	32:A:2367:A:C8	2.48	0.46
32:A:2472:A:N6	32:A:2481:A:N1	2.56	0.46
36:H:131:TYR:HB3	45:X:139:TYR:HD1	1.81	0.46
76:d:147:GLU:OE1	76:d:159:ARG:NH2	2.48	0.46
83:Q:103:ARG:HE	83:Q:108:ILE:HD12	1.80	0.46
1:AA:1477:U:H2'	1:AA:1479:C:H41	1.81	0.46
3:AC:157:THR:HG23	28:A4:92:ASP:HB2	1.98	0.46
29:AD:399:ASP:OD1	29:AD:399:ASP:N	2.46	0.46
32:A:1737:A:H62	32:A:1760:G:H21	1.64	0.46
32:A:1816:G:H2'	32:A:1817:C:C6	2.51	0.46
32:A:1980:A:OP2	50:2:59:LYS:NZ	2.47	0.46
32:A:2317:G:H2'	32:A:2318:A:C8	2.50	0.46
32:A:2395:A:H2'	32:A:2396:C:H5''	1.97	0.46
44:W:106:PRO:O	66:P:72:PHE:CE1	2.69	0.46
86:v:548:GLN:HE21	86:v:625:SER:HB3	1.81	0.46
15:AX:285:GLU:OE2	15:AX:294:ARG:NH1	2.49	0.46
29:AD:265:MET:CE	87:A5:4:Y5P:H4	2.45	0.46
32:A:2740:A:H2'	32:A:2741:A:H8	1.80	0.46
55:e:176:ALA:HA	55:e:191:THR:HG21	1.98	0.46
65:N:198:MET:HA	65:N:201:ASP:OD2	2.17	0.46
1:AA:888:U:O4	1:AA:905:A:N7	2.49	0.45
1:AA:1173:C:H2'	1:AA:1174:U:C6	2.50	0.45
8:AM:61:HIS:HE1	19:AR:191:ARG:HH12	1.64	0.45
15:AX:56:PRO:HA	15:AX:59:HIS:HD2	1.81	0.45
17:AH:172:VAL:HB	25:A1:155:ASP:HB2	1.99	0.45
21:AU:49:ASP:HB3	21:AU:52:GLU:HB3	1.97	0.45
31:AG:322:ARG:HD3	31:AG:326:HIS:CE1	2.51	0.45
32:A:1737:A:O2'	57:i:93:ARG:NH2	2.40	0.45
32:A:2318:A:H2'	32:A:2319:A:C8	2.52	0.45
32:A:2661:U:H2'	32:A:2662:A:C8	2.51	0.45
35:F:116:THR:HG23	35:F:118:ALA:H	1.80	0.45
39:M:141:VAL:HG12	39:M:143:GLU:H	1.81	0.45
39:M:179:TYR:HB3	39:M:183:SER:HB2	1.97	0.45
40:O:94:ALA:HB3	40:O:95:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S:133:VAL:HG23	42:S:149:LEU:HB2	1.98	0.45
63:J:191:LYS:HE3	63:J:192:LYS:N	2.31	0.45
64:I:188:ARG:NH1	79:k:53:ALA:O	2.46	0.45
67:U:99:LEU:HD13	67:U:103:GLN:HB2	1.98	0.45
86:v:175:LYS:HB3	92:v:802:GCP:C5	2.46	0.45
1:AA:757:A:H4'	1:AA:758:U:H5''	1.97	0.45
1:AA:778:C:H2'	1:AA:779:U:C6	2.52	0.45
6:AJ:52:THR:O	6:AJ:53:GLU:HG3	2.17	0.45
32:A:1955:G:H21	32:A:1960:A:N6	2.15	0.45
32:A:2024:C:OP1	42:S:182:LYS:HA	2.16	0.45
34:D:132:ASP:OD2	34:D:135:ARG:NH1	2.49	0.45
34:D:225:ILE:HA	34:D:235:GLN:HA	1.98	0.45
66:P:72:PHE:HB2	66:P:73:PRO:CD	2.46	0.45
66:P:73:PRO:HA	66:P:147:GLN:CD	2.41	0.45
71:6:155:TYR:O	71:6:267:ARG:NH1	2.36	0.45
72:7:247:ASN:HD21	72:7:251:ILE:H	1.63	0.45
74:a:111:GLN:HA	74:a:114:LYS:HG2	1.98	0.45
76:d:288:LYS:O	76:d:290:GLU:N	2.50	0.45
1:AA:1019:A:N7	11:AP:95:HIS:NE2	2.64	0.45
22:AV:175:VAL:O	22:AV:177:SER:N	2.49	0.45
32:A:1877:U:H1'	39:M:33:SER:HB2	1.98	0.45
32:A:1979:U:H2'	32:A:1980:A:C8	2.50	0.45
32:A:2003:A:OP2	32:A:2734:A:O2'	2.33	0.45
32:A:2032:G:H2'	32:A:2033:A:H8	1.79	0.45
45:X:156:LYS:HZ2	70:5:70:LEU:HD23	0.66	0.45
70:5:67:VAL:HB	70:5:68:PRO:HD2	1.97	0.45
77:f:119:ILE:HD13	77:f:166:PHE:HE2	1.80	0.45
80:l:106:THR:OG1	80:l:108:GLU:OE1	2.27	0.45
82:s:153:GLU:HA	82:s:157:LEU:HD12	1.98	0.45
83:Q:183:LEU:HD21	83:Q:219:GLU:HG2	1.97	0.45
1:AA:810:G:H2'	1:AA:811:G:H8	1.82	0.45
1:AA:860:A:C2	1:AA:920:G:O6	2.69	0.45
1:AA:1488:C:H2'	1:AA:1489:G:C8	2.50	0.45
7:AK:112:ARG:HH11	17:AH:132:VAL:HG21	1.81	0.45
12:AQ:63:ILE:HD13	16:A2:6:LEU:HD11	1.97	0.45
17:AH:187:PRO:HG2	25:A1:231:HIS:NE2	2.32	0.45
22:AV:316:GLN:NE2	22:AV:323:GLU:OE1	2.49	0.45
29:AD:284:ARG:HH11	29:AD:328:GLY:HA3	1.82	0.45
32:A:1724:A:N6	32:A:2040:G:C2	2.80	0.45
32:A:1753:A:OP1	57:i:118:TYR:OH	2.32	0.45
32:A:2579:C:C5	32:A:2580:U:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3190:A:H2'	32:A:3191:A:C8	2.51	0.45
35:F:59:ARG:NH1	35:F:88:ALA:O	2.48	0.45
35:F:184:GLN:HE22	39:M:22:VAL:HG23	1.82	0.45
40:O:45:PRO:HA	40:O:120:MET:HA	1.97	0.45
42:S:194:ARG:HD3	54:b:18:GLY:HA3	1.98	0.45
86:v:442:GLU:HG3	86:v:444:ILE:HG22	1.97	0.45
15:AX:179:ASP:HB3	15:AX:288:ALA:HB3	1.98	0.45
19:AR:214:ASN:HA	19:AR:217:THR:HG22	1.99	0.45
22:AV:114:ARG:HD3	22:AV:117:LEU:HD21	1.97	0.45
22:AV:168:MET:HA	22:AV:173:PHE:HE1	1.82	0.45
24:AZ:53:PRO:O	24:AZ:55:HIS:ND1	2.43	0.45
32:A:1852:C:O2'	32:A:1856:A:N6	2.50	0.45
32:A:2018:G:H2'	32:A:2019:G:C8	2.52	0.45
33:B:1624:C:OP1	71:6:59:ARG:NH1	2.45	0.45
33:B:1642:G:H4'	53:8:119:LYS:HE3	1.99	0.45
36:H:87:LYS:HG3	36:H:88:HIS:CD2	2.51	0.45
39:M:165:ALA:O	39:M:169:LYS:HG2	2.16	0.45
86:v:162:MET:HE3	86:v:162:MET:HB3	1.83	0.45
2:AB:162:CYS:HB3	2:AB:257:ILE:HG21	1.97	0.45
32:A:1830:G:H2'	32:A:1831:G:H8	1.80	0.45
32:A:2018:G:H2'	32:A:2019:G:H8	1.81	0.45
32:A:2256:U:H2'	32:A:2257:C:C6	2.51	0.45
32:A:3092:U:H2'	32:A:3093:C:C6	2.51	0.45
32:A:3146:G:N2	69:E:268:GLU:OE2	2.49	0.45
36:H:58:ARG:HD3	36:H:77:HIS:HB3	1.98	0.45
55:e:98:LEU:HD23	55:e:101:LYS:HZ1	1.81	0.45
55:e:162:ARG:HH11	55:e:171:TRP:HB2	1.81	0.45
63:J:132:LEU:HB3	64:I:114:HIS:CB	2.18	0.45
70:5:277:THR:HB	70:5:323:ALA:HB1	1.97	0.45
71:6:374:GLU:HB2	81:p:141:ARG:HH12	1.81	0.45
72:7:51:GLU:OE2	72:7:54:ARG:NH2	2.46	0.45
1:AA:847:G:H2'	1:AA:848:U:C6	2.51	0.45
1:AA:1219:U:O2'	1:AA:1223:C:N3	2.45	0.45
1:AA:1478:A:N6	1:AA:1565:A:O2'	2.50	0.45
32:A:1770:G:H2'	32:A:1771:C:C6	2.52	0.45
32:A:1899:G:H21	39:M:35:LYS:HD3	1.80	0.45
32:A:2362:A:N6	32:A:2432:A:O4'	2.50	0.45
32:A:2710:C:H2'	32:A:2711:A:H8	1.82	0.45
37:K:58:VAL:HG22	37:K:126:HIS:HB2	1.99	0.45
41:R:137:GLU:HB3	41:R:138:PRO:HD3	1.98	0.45
46:Y:200:PHE:HB3	70:5:68:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:1:35:ASN:OD1	49:1:36:ARG:N	2.50	0.45
71:6:45:LEU:O	71:6:50:LYS:NZ	2.39	0.45
72:7:43:MET:HA	72:7:46:ASP:OD2	2.16	0.45
81:p:128:ASN:OD1	81:p:129:ARG:N	2.43	0.45
86:v:679:ASP:N	86:v:686:THR:O	2.43	0.45
18:AL:138:TYR:HB2	18:AL:155:LEU:HD13	1.97	0.45
19:AR:107:THR:HG22	29:AD:368:LEU:HD22	1.99	0.45
32:A:1828:A:H4'	32:A:1829:A:C8	2.52	0.45
32:A:2069:U:O2'	32:A:2070:C:O4'	2.30	0.45
32:A:2245:A:H4'	32:A:2246:A:OP1	2.17	0.45
33:B:1607:U:O2'	33:B:1608:G:OP1	2.32	0.45
34:D:201:GLY:O	70:5:30:ALA:N	2.50	0.45
37:K:134:PRO:HD2	37:K:137:ILE:HD12	1.99	0.45
53:8:163:LYS:HA	77:f:86:TYR:HB2	1.97	0.45
66:P:73:PRO:HA	66:P:147:GLN:OE1	2.17	0.45
67:U:19:VAL:HB	73:9:136:LEU:HD23	1.98	0.45
72:7:203:THR:HG21	72:7:279:GLU:HG2	1.98	0.45
88:A7:12:Y5P:H4A	88:A7:13:Y5P:H4	1.99	0.45
1:AA:1166:A:H62	6:AJ:114:ARG:HH12	1.65	0.45
1:AA:1308:U:H2'	1:AA:1309:A:C8	2.52	0.45
7:AK:106:LEU:HD11	7:AK:111:PHE:HB2	1.99	0.45
9:AN:51:ALA:HB2	9:AN:66:LEU:HD22	1.99	0.45
10:AO:182:GLY:O	19:AR:183:LYS:NZ	2.41	0.45
16:A2:10:LEU:HD11	16:A2:27:LEU:HD12	1.99	0.45
32:A:1824:U:OP2	32:A:2706:A:O2'	2.35	0.45
32:A:1862:U:H2'	32:A:1863:A:H8	1.82	0.45
32:A:1942:C:H2'	32:A:1943:A:O4'	2.16	0.45
32:A:2171:U:OP1	63:J:86:THR:HA	2.17	0.45
32:A:2263:C:H4'	42:S:175:ARG:HH12	1.82	0.45
32:A:3079:G:N1	32:A:3090:G:O6	2.50	0.45
36:H:133:SER:OG	36:H:136:ASN:OD1	2.29	0.45
43:T:192:ALA:HB1	74:a:112:LEU:HD21	1.98	0.45
63:J:133:GLN:N	64:I:117:ARG:CZ	2.78	0.45
66:P:41:ASN:HB3	71:6:293:LEU:HD13	1.97	0.45
70:5:344:SER:HB3	70:5:355:LEU:HD23	1.98	0.45
75:c:315:ASN:HD21	75:c:317:SER:HB2	1.82	0.45
1:AA:1201:A:H2'	1:AA:1202:G:C8	2.52	0.45
1:AA:1332:A:H3'	1:AA:1333:G:C8	2.51	0.45
3:AC:150:PRO:HB3	23:AY:309:LYS:HD3	1.98	0.45
32:A:2489:C:N4	32:A:2647:G:O6	2.50	0.45
32:A:3205:C:OP1	69:E:177:LYS:NZ	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:149:LEU:HD22	69:E:61:ILE:HD11	1.99	0.45
82:s:414:ASN:ND2	82:s:416:ASP:OD1	2.51	0.45
86:v:310:LEU:HA	86:v:313:VAL:HG22	1.98	0.45
1:AA:1469:G:H2'	1:AA:1470:A:H8	1.82	0.44
15:AX:168:LEU:HD21	15:AX:178:PHE:HB3	1.98	0.44
22:AV:197:SER:OG	22:AV:198:TRP:N	2.50	0.44
32:A:2216:A:H5''	64:I:127:PRO:HB3	1.99	0.44
49:1:61:LYS:HE3	88:A7:1:P5P:O5'	2.17	0.44
62:r:94:ARG:HD2	62:r:98:GLY:HA3	1.99	0.44
69:E:58:VAL:HB	69:E:59:PRO:HD3	1.99	0.44
70:5:200:ARG:HD3	70:5:233:LYS:HB2	1.99	0.44
71:6:233:LEU:O	71:6:296:ARG:NH1	2.46	0.44
77:f:97:ALA:HB2	77:f:182:VAL:HA	1.99	0.44
1:AA:763:C:H42	18:AL:206:LYS:HE2	1.82	0.44
1:AA:877:G:H2'	1:AA:878:G:C8	2.52	0.44
1:AA:1060:A:H2'	1:AA:1061:A:H8	1.82	0.44
1:AA:1112:A:H2'	1:AA:1113:G:C8	2.52	0.44
5:AI:179:THR:HG21	12:AQ:35:LEU:HD21	1.99	0.44
10:AO:193:LEU:HD23	10:AO:193:LEU:H	1.81	0.44
15:AX:334:PHE:HA	15:AX:337:LEU:HG	1.98	0.44
32:A:1678:C:HO2'	32:A:1679:U:H6	1.65	0.44
32:A:1696:C:OP2	46:Y:180:LYS:NZ	2.37	0.44
32:A:2108:G:O2'	32:A:2111:C:N4	2.35	0.44
32:A:2665:U:OP2	40:O:17:ARG:NH1	2.50	0.44
35:F:126:LYS:HZ1	35:F:130:GLN:N	2.16	0.44
53:8:150:LEU:HB2	55:e:212:HIS:CE1	2.51	0.44
54:b:54:PHE:HD2	54:b:63:ILE:HD11	1.82	0.44
66:P:85:ARG:HD2	66:P:158:MET:HE3	1.99	0.44
66:P:136:CYS:HB2	66:P:141:ILE:HG23	1.98	0.44
70:5:60:PHE:CE1	70:5:71:ALA:CA	2.98	0.44
1:AA:701:G:H2'	1:AA:702:C:C6	2.52	0.44
2:AB:195:PHE:HZ	2:AB:208:ALA:HB3	1.82	0.44
10:AO:202:TRP:CG	21:AU:62:HIS:HD1	2.35	0.44
22:AV:251:TRP:HH2	26:A0:142:VAL:HG12	1.83	0.44
32:A:2524:A:N1	34:D:92:ARG:HD3	2.32	0.44
62:r:167:PRO:HB2	62:r:168:ARG:H	1.61	0.44
68:V:102:MET:SD	68:V:102:MET:N	2.80	0.44
71:6:90:ILE:HG13	71:6:167:PHE:HB3	1.99	0.44
74:a:52:THR:HG22	74:a:54:ASP:H	1.82	0.44
86:v:59:LYS:N	92:v:802:GCP:O2A	2.51	0.44
1:AA:873:G:H2'	1:AA:874:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:939:A:OP1	27:A3:132:LYS:NZ	2.50	0.44
7:AK:63:LEU:HD12	7:AK:64:PRO:HD2	1.98	0.44
32:A:2004:G:H2'	32:A:2005:C:C6	2.52	0.44
32:A:2160:A:H2	32:A:2226:U:H5''	1.83	0.44
32:A:2740:A:N3	32:A:2921:A:O2'	2.40	0.44
32:A:2939:C:N4	32:A:2991:U:H3	2.06	0.44
32:A:3041:U:H4'	32:A:3042:U:OP1	2.16	0.44
42:S:115:LEU:HB3	54:b:118:PRO:HB2	1.99	0.44
46:Y:202:LEU:HB3	46:Y:204:TYR:CE2	2.52	0.44
63:J:131:ALA:O	64:I:114:HIS:CE1	2.71	0.44
69:E:99:LEU:HD11	69:E:197:HIS:HB3	1.98	0.44
70:5:136:VAL:HG11	70:5:417:LEU:HD23	1.99	0.44
70:5:168:GLU:OE1	70:5:168:GLU:N	2.49	0.44
71:6:46:GLU:OE1	71:6:46:GLU:N	2.47	0.44
71:6:216:LEU:HB3	71:6:237:LEU:HD23	1.98	0.44
72:7:166:LEU:HB2	72:7:236:LYS:HE2	1.99	0.44
82:s:53:ALA:HB3	82:s:58:ALA:HB2	1.99	0.44
86:v:138:LEU:HD22	86:v:372:ARG:HH11	1.82	0.44
86:v:214:ILE:HD11	86:v:308:PRO:HG2	1.98	0.44
1:AA:1035:U:H2'	1:AA:1036:A:H8	1.83	0.44
1:AA:1392:A:H5''	1:AA:1393:G:C8	2.52	0.44
8:AM:108:GLU:HG2	10:AO:232:PRO:HG2	1.99	0.44
22:AV:76:ILE:HD13	22:AV:112:TRP:HB2	1.99	0.44
29:AD:400:GLU:HG2	29:AD:401:VAL:HG22	2.00	0.44
32:A:1744:A:N6	32:A:1754:G:H21	2.14	0.44
32:A:2369:A:O2'	32:A:2370:A:O4'	2.26	0.44
32:A:2603:C:H4'	32:A:3090:G:H1'	2.00	0.44
38:L:73:ILE:O	38:L:84:ALA:N	2.51	0.44
43:T:92:LYS:HA	43:T:95:ARG:HG2	1.98	0.44
70:5:60:PHE:CG	70:5:67:VAL:HG22	2.52	0.44
71:6:273:PHE:HA	71:6:313:PRO:HA	2.00	0.44
88:A7:21:Y5P:H4A	88:A7:22:Y5P:H4	2.00	0.44
1:AA:1225:C:O2'	1:AA:1449:G:O2'	2.25	0.44
1:AA:1234:C:H5''	1:AA:1235:U:H5	1.83	0.44
1:AA:1412:G:N2	1:AA:1413:U:O4	2.51	0.44
9:AN:13:ILE:HG23	9:AN:66:LEU:HB2	1.98	0.44
17:AH:161:GLN:HB3	23:AY:313:PHE:CE2	2.53	0.44
32:A:1830:G:H2'	32:A:1831:G:C8	2.52	0.44
32:A:2212:C:H2'	32:A:2213:A:H8	1.82	0.44
32:A:2233:U:N3	32:A:2688:C:OP1	2.39	0.44
38:L:55:PRO:HB2	38:L:75:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:b:141:ARG:H	74:a:71:HIS:HA	1.83	0.44
59:m:51:LEU:HB3	59:m:67:ARG:HB3	2.00	0.44
61:q:108:LEU:O	61:q:111:GLU:HG3	2.18	0.44
67:U:35:GLN:NE2	82:s:270:LYS:HD2	2.32	0.44
71:6:66:GLN:HG2	71:6:75:ARG:HH22	1.83	0.44
83:Q:194:LEU:HD12	83:Q:197:TYR:HE2	1.83	0.44
1:AA:705:C:H2'	26:A0:136:TYR:CZ	2.53	0.44
1:AA:774:G:H2'	1:AA:775:C:C6	2.52	0.44
1:AA:810:G:H2'	1:AA:811:G:C8	2.52	0.44
1:AA:1216:C:H2'	1:AA:1217:G:C8	2.49	0.44
10:AO:96:ARG:O	10:AO:98:ASN:N	2.51	0.44
34:D:225:ILE:HG13	34:D:235:GLN:HB3	1.99	0.44
38:L:129:LYS:HE3	38:L:130:ARG:HH12	1.83	0.44
43:T:161:ARG:HG2	43:T:162:GLY:H	1.83	0.44
48:0:137:ILE:HD13	48:0:158:VAL:HG11	2.00	0.44
67:U:48:MET:HE2	67:U:53:LEU:HA	1.99	0.44
69:E:210:THR:OG1	69:E:262:GLY:O	2.34	0.44
75:c:258:THR:HG22	75:c:259:ARG:HG3	1.99	0.44
86:v:171:THR:O	86:v:296:PHE:N	2.50	0.44
86:v:472:ARG:NH1	86:v:475:ARG:HH11	2.14	0.44
1:AA:700:A:H2'	21:AU:28:LYS:HD2	2.00	0.44
20:AS:5:ARG:HB2	29:AD:278:HIS:CD2	2.53	0.44
29:AD:96:ASP:OD1	29:AD:97:GLU:N	2.51	0.44
31:AG:314:MET:HE3	31:AG:314:MET:HB3	1.91	0.44
32:A:1981:G:H2'	32:A:1982:G:H8	1.83	0.44
32:A:2586:U:H2'	32:A:2587:G:C8	2.52	0.44
33:B:1663:C:H2'	33:B:1664:G:H8	1.83	0.44
37:K:153:LYS:HE2	37:K:158:TYR:HA	1.99	0.44
40:O:82:GLU:O	40:O:84:ASP:N	2.41	0.44
45:X:234:LEU:HD23	45:X:238:LEU:HD23	1.99	0.44
47:Z:71:ARG:HA	47:Z:117:ILE:HG22	1.99	0.44
64:I:105:SER:N	79:k:40:GLU:OE2	2.48	0.44
71:6:183:ASP:HB3	81:p:189:ARG:HB3	1.99	0.44
1:AA:1248:C:O2'	1:AA:1250:C:OP1	2.36	0.44
15:AX:155:ILE:HD12	15:AX:262:VAL:HB	1.99	0.44
15:AX:206:GLU:HB2	15:AX:249:ARG:HH12	1.82	0.44
32:A:2065:A:C8	44:W:74:ARG:HG3	2.53	0.44
32:A:2123:C:OP1	47:Z:76:ARG:NH2	2.50	0.44
32:A:2959:G:H21	32:A:2965:A:H62	1.66	0.44
41:R:119:LEU:HD23	74:a:49:LEU:HD13	2.00	0.44
63:J:141:VAL:HA	63:J:144:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:185:ILE:HD11	84:TA:48:LEU:HD13	2.00	0.44
65:N:195:LEU:HA	65:N:198:MET:HG2	2.00	0.44
75:c:240:LEU:HD23	75:c:301:LEU:HD21	2.00	0.44
1:AA:923:A:H2'	1:AA:924:A:C8	2.53	0.43
10:AO:63:GLU:OE1	10:AO:112:LYS:NZ	2.43	0.43
19:AR:78:ILE:HD12	19:AR:303:LEU:HD13	2.00	0.43
22:AV:120:ASP:O	22:AV:122:GLN:N	2.51	0.43
32:A:1721:C:O2'	57:i:123:ARG:NH2	2.51	0.43
32:A:2371:U:O2	32:A:2422:U:H5''	2.18	0.43
32:A:2606:U:H4'	32:A:2607:U:H3'	1.99	0.43
32:A:3144:A:H2'	32:A:3145:A:C8	2.53	0.43
64:I:175:PRO:HB3	79:k:53:ALA:HB1	2.00	0.43
67:U:27:GLN:HB2	67:U:43:ARG:HB3	2.00	0.43
86:v:357:ALA:HB2	86:v:371:VAL:HG22	2.00	0.43
1:AA:815:C:O2	1:AA:818:C:N4	2.40	0.43
1:AA:1479:C:H2'	1:AA:1480:A:C8	2.52	0.43
1:AA:1523:A:N6	22:AV:396:GLN:OE1	2.50	0.43
14:AW:155:GLY:O	16:A2:113:ASN:ND2	2.41	0.43
17:AH:109:HIS:NE2	17:AH:142:CYS:SG	2.91	0.43
25:A1:237:GLU:OE1	25:A1:239:TRP:NE1	2.44	0.43
29:AD:305:MET:HA	29:AD:334:ALA:HA	2.00	0.43
32:A:1805:A:O2'	32:A:1806:U:OP1	2.31	0.43
32:A:2236:C:OP1	60:o:9:ARG:N	2.51	0.43
75:c:91:ALA:O	75:c:122:ASN:ND2	2.51	0.43
79:k:65:ASP:OD1	79:k:65:ASP:N	2.51	0.43
86:v:332:GLU:O	86:v:337:GLU:HA	2.18	0.43
88:A7:47:Y5P:H4A	88:A7:48:P5P:N7	2.33	0.43
1:AA:1085:C:H2'	1:AA:1086:C:C6	2.53	0.43
2:AB:148:ASN:O	2:AB:152:SER:OG	2.36	0.43
32:A:1862:U:H2'	32:A:1863:A:C8	2.54	0.43
32:A:2311:U:H2'	32:A:2312:A:H8	1.82	0.43
40:O:86:ILE:HB	40:O:87:PRO:HD3	1.99	0.43
45:X:79:LEU:HB2	45:X:125:VAL:HG11	2.01	0.43
51:3:180:TYR:HD1	71:6:366:LEU:HD12	1.83	0.43
63:J:52:GLU:O	63:J:55:GLU:HG3	2.18	0.43
71:6:178:ALA:HA	81:p:194:HIS:CD2	2.53	0.43
76:d:86:ASP:OD1	76:d:86:ASP:N	2.51	0.43
76:d:218:THR:OG1	76:d:219:ARG:N	2.50	0.43
86:v:657:PRO:HD2	86:v:707:THR:OG1	2.18	0.43
88:A7:64:Y5P:H4A	88:A7:65:Y5P:N3	2.33	0.43
1:AA:1399:A:O3'	24:AZ:32:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1584:A:OP1	27:A3:141:HIS:NE2	2.35	0.43
23:AY:313:PHE:O	23:AY:315:ILE:HG13	2.18	0.43
24:AZ:32:LYS:HA	24:AZ:35:LYS:HG2	2.00	0.43
26:A0:213:ALA:O	26:A0:215:GLY:N	2.52	0.43
32:A:2954:C:O2'	65:N:178:GLN:NE2	2.50	0.43
66:P:98:ASN:OD1	66:P:99:GLY:N	2.51	0.43
86:v:270:GLU:C	86:v:271:GLU:HG3	2.43	0.43
16:A2:6:LEU:HA	16:A2:9:ARG:HD3	2.00	0.43
21:AU:186:ASN:HB2	21:AU:201:GLN:HE21	1.82	0.43
22:AV:127:TYR:O	22:AV:131:ASN:HB2	2.18	0.43
30:AF:70:LYS:NZ	31:AG:251:GLU:OE1	2.39	0.43
32:A:1792:G:OP2	50:2:85:LYS:NZ	2.44	0.43
32:A:3078:C:N4	32:A:3079:G:O6	2.52	0.43
34:D:154:THR:HG22	34:D:157:MET:HE3	2.01	0.43
56:g:140:VAL:H	60:o:85:HIS:CD2	2.36	0.43
65:N:33:LEU:CB	80:l:125:ASN:HD21	2.32	0.43
68:V:51:ASP:HA	68:V:81:ARG:HH22	1.84	0.43
69:E:221:ARG:HG3	69:E:261:MET:HG3	2.00	0.43
72:7:178:ALA:HB2	72:7:320:SER:HB2	1.99	0.43
77:f:94:HIS:ND1	77:f:154:GLU:OE2	2.45	0.43
79:k:39:SER:OG	79:k:40:GLU:N	2.50	0.43
86:v:214:ILE:HG12	86:v:225:PHE:HE2	1.84	0.43
1:AA:936:G:H4'	1:AA:1107:U:H2'	2.01	0.43
1:AA:1035:U:H2'	1:AA:1036:A:C8	2.53	0.43
1:AA:1104:A:OP2	1:AA:1591:C:O2'	2.37	0.43
1:AA:1235:U:H5''	7:AK:33:ARG:HD3	2.00	0.43
1:AA:1302:C:N4	1:AA:1303:G:O6	2.52	0.43
4:AE:10:LEU:HB3	4:AE:13:MET:SD	2.59	0.43
14:AW:90:THR:O	20:AS:71:ARG:NH1	2.52	0.43
22:AV:209:LEU:HD23	22:AV:224:GLN:HA	2.00	0.43
32:A:2321:A:OP2	32:A:2322:C:N4	2.51	0.43
32:A:3002:G:H2'	32:A:3003:A:C8	2.53	0.43
39:M:30:ASN:OD1	60:o:86:ARG:NH2	2.49	0.43
53:8:145:GLU:O	53:8:148:GLU:HG3	2.19	0.43
70:5:60:PHE:HD1	70:5:71:ALA:HB1	0.69	0.43
75:c:46:GLU:HG2	75:c:49:ARG:HH12	1.82	0.43
75:c:105:ARG:NH1	75:c:113:GLU:OE2	2.50	0.43
1:AA:735:A:N6	1:AA:740:G:C6	2.70	0.43
1:AA:747:A:H2'	1:AA:748:G:C8	2.54	0.43
1:AA:832:U:H2'	1:AA:833:A:C8	2.51	0.43
1:AA:1201:A:H2'	1:AA:1202:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1591:C:OP1	12:AQ:52:ARG:NH2	2.50	0.43
19:AR:157:VAL:HG13	19:AR:174:VAL:HG22	2.01	0.43
22:AV:284:GLY:O	22:AV:288:LYS:HG2	2.18	0.43
32:A:1788:C:O2	50:2:64:HIS:NE2	2.32	0.43
32:A:1881:A:N7	56:g:111:ARG:NE	2.66	0.43
32:A:2620:G:H2'	32:A:2621:G:H8	1.83	0.43
32:A:2642:C:H2'	32:A:2643:G:C8	2.53	0.43
32:A:2909:G:N3	88:A7:69:Y5P:H4A	2.34	0.43
32:A:3102:U:H2'	32:A:3103:C:H6	1.84	0.43
39:M:164:ILE:HG12	39:M:174:VAL:HG11	1.99	0.43
42:S:158:ALA:HA	42:S:195:ILE:HA	2.01	0.43
55:e:66:LEU:HD23	55:e:66:LEU:H	1.83	0.43
63:J:171:ARG:CG	63:J:174:PHE:HE2	2.32	0.43
66:P:175:PRO:HG3	81:p:177:ARG:HD3	2.01	0.43
70:5:239:ILE:HG12	70:5:341:VAL:HG21	2.01	0.43
88:A7:20:P5P:C6	88:A7:21:Y5P:H4	2.48	0.43
1:AA:989:U:OP2	5:AI:122:LYS:NZ	2.45	0.43
1:AA:1279:C:H2'	1:AA:1280:C:H6	1.84	0.43
1:AA:1308:U:H2'	1:AA:1309:A:H8	1.83	0.43
3:AC:136:VAL:HG22	3:AC:153:LEU:HD22	2.01	0.43
22:AV:209:LEU:HG	22:AV:227:GLY:HA3	2.00	0.43
29:AD:314:LEU:HD12	29:AD:430:THR:HG21	2.00	0.43
32:A:1690:C:N3	46:Y:213:ARG:NE	2.57	0.43
32:A:1792:G:O2'	35:F:125:ARG:NH2	2.52	0.43
32:A:2366:G:H5''	67:U:79:ARG:HH21	1.84	0.43
32:A:3178:U:O2'	62:r:134:ARG:NH1	2.52	0.43
32:A:3222:C:H2'	32:A:3223:A:O4'	2.19	0.43
39:M:273:TRP:NE1	39:M:284:LYS:HG2	2.33	0.43
42:S:97:ALA:N	42:S:108:VAL:O	2.47	0.43
63:J:131:ALA:O	64:I:114:HIS:ND1	2.51	0.43
63:J:132:LEU:CD2	64:I:114:HIS:HB3	2.48	0.43
63:J:174:PHE:CZ	63:J:175:LEU:CD2	2.87	0.43
68:V:177:THR:HG22	73:9:74:VAL:HA	2.01	0.43
68:V:211:LYS:HE3	70:5:82:TYR:CD1	2.54	0.43
70:5:162:ARG:NH1	70:5:383:TYR:OH	2.52	0.43
75:c:166:VAL:HG21	75:c:192:GLN:HG3	2.01	0.43
78:h:73:TYR:HE1	78:h:100:LEU:HG	1.84	0.43
81:p:122:THR:HG23	81:p:123:HIS:CD2	2.54	0.43
83:Q:60:PRO:HB2	83:Q:61:VAL:H	1.64	0.43
86:v:70:THR:HG21	86:v:109:THR:HB	2.01	0.43
86:v:539:HIS:N	86:v:550:GLY:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1437:U:H2'	1:AA:1438:A:C8	2.54	0.43
1:AA:1506:U:H2'	1:AA:1507:A:C8	2.51	0.43
4:AE:8:LEU:HB3	4:AE:64:PHE:HB2	1.99	0.43
6:AJ:104:GLU:HB3	86:v:489:LYS:NZ	2.34	0.43
18:AL:175:ASP:O	18:AL:178:GLU:HG3	2.19	0.43
22:AV:322:THR:HG22	22:AV:324:GLN:H	1.83	0.43
25:A1:252:ILE:O	25:A1:256:SER:OG	2.34	0.43
29:AD:369:HIS:HA	29:AD:387:PRO:HD3	2.01	0.43
32:A:2272:C:N3	32:A:2273:A:N6	2.67	0.43
46:Y:139:MET:HE1	67:U:25:PHE:HE1	1.84	0.43
64:I:81:LEU:CB	80:l:115:ARG:NH1	2.71	0.43
70:5:283:TYR:OH	82:s:152:GLN:HG3	2.19	0.43
83:Q:122:ALA:HB2	83:Q:172:GLN:HE21	1.84	0.43
1:AA:1031:G:H4'	11:AP:112:LYS:HE2	2.00	0.43
1:AA:1059:U:O4	1:AA:1060:A:N6	2.52	0.43
2:AB:74:ASN:O	2:AB:259:ARG:NH1	2.52	0.43
8:AM:58:PRO:HB3	19:AR:154:THR:HG21	2.00	0.43
15:AX:390:LEU:HD13	31:AG:310:ARG:HH12	1.84	0.43
19:AR:91:PHE:HB2	29:AD:380:LEU:HD22	2.00	0.43
22:AV:142:PHE:HE1	22:AV:176:PRO:HG2	1.84	0.43
25:A1:86:ARG:HG2	25:A1:98:ALA:HA	2.00	0.43
28:A4:72:GLN:HA	28:A4:76:SER:HB2	2.01	0.43
29:AD:292:HIS:HE1	29:AD:357:GLU:H	1.66	0.43
31:AG:85:LYS:NZ	31:AG:96:PRO:O	2.52	0.43
32:A:1822:U:O2	32:A:2707:A:O2'	2.30	0.43
32:A:2079:C:H42	60:o:60:ARG:NH2	2.17	0.43
32:A:2533:A:H2'	32:A:2534:G:C8	2.54	0.43
32:A:3032:G:H2'	32:A:3033:U:O4'	2.19	0.43
32:A:3122:U:H5'	32:A:3124:U:H6	1.84	0.43
34:D:187:LEU:HD21	34:D:244:VAL:HG22	2.00	0.43
38:L:55:PRO:HB3	38:L:77:ILE:HG12	2.01	0.43
40:O:145:LEU:HD11	72:7:308:ALA:HB2	2.01	0.43
41:R:148:TYR:CE1	42:S:147:PRO:HG2	2.53	0.43
55:e:118:GLN:O	55:e:121:GLU:HG3	2.19	0.43
67:U:26:ILE:HG22	67:U:44:ILE:HG22	2.00	0.43
78:h:70:LEU:HA	78:h:73:TYR:CD2	2.54	0.43
82:s:295:GLY:HA3	82:s:335:TRP:HZ2	1.83	0.43
1:AA:717:G:H4'	1:AA:718:A:O5'	2.19	0.42
1:AA:1126:A:H2'	1:AA:1127:A:C8	2.53	0.42
1:AA:1210:U:H2'	1:AA:1211:G:C8	2.53	0.42
1:AA:1261:C:H2'	1:AA:1262:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1332:A:C8	7:AK:109:ILE:HG21	2.52	0.42
4:AE:44:GLU:OE1	4:AE:60:ARG:NE	2.52	0.42
15:AX:153:LEU:HB3	15:AX:260:VAL:HA	2.00	0.42
16:A2:24:ASN:OD1	16:A2:25:LYS:N	2.51	0.42
16:A2:56:TRP:NE1	16:A2:63:ASP:OD1	2.51	0.42
21:AU:41:ARG:O	26:A0:49:ARG:NH2	2.52	0.42
22:AV:95:PHE:O	22:AV:98:SER:OG	2.33	0.42
22:AV:159:ASP:N	22:AV:159:ASP:OD1	2.50	0.42
32:A:1861:U:O4	32:A:2304:G:O6	2.37	0.42
32:A:2425:A:C6	82:s:221:HIS:HA	2.54	0.42
32:A:2943:G:H2'	32:A:2944:C:C6	2.54	0.42
32:A:2955:U:OP2	32:A:2963:A:N6	2.52	0.42
32:A:3196:G:H1'	32:A:3197:U:OP2	2.19	0.42
33:B:1642:G:H2'	33:B:1643:A:C8	2.54	0.42
51:3:118:HIS:CD2	51:3:169:ARG:HB2	2.54	0.42
53:8:138:ALA:O	53:8:141:GLU:HG3	2.18	0.42
54:b:45:GLU:O	54:b:49:ARG:HG2	2.18	0.42
69:E:102:LEU:HD21	69:E:294:ASN:HA	2.01	0.42
70:5:63:LYS:HB2	70:5:65:HIS:CE1	2.54	0.42
76:d:219:ARG:NH1	76:d:239:PRO:O	2.48	0.42
80:l:105:LYS:HB3	80:l:110:LEU:HD21	2.01	0.42
1:AA:945:G:H2'	1:AA:946:U:C6	2.54	0.42
19:AR:224:HIS:HD2	19:AR:261:LEU:HD11	1.84	0.42
22:AV:245:HIS:N	22:AV:247:MET:SD	2.92	0.42
32:A:1689:C:H2'	32:A:1690:C:C5	2.54	0.42
32:A:2087:U:H2'	32:A:2088:U:C6	2.54	0.42
32:A:2439:U:H2'	32:A:2440:G:C8	2.54	0.42
32:A:2507:A:HO2'	32:A:2508:C:P	2.40	0.42
32:A:2622:G:H2'	32:A:2623:A:C8	2.54	0.42
32:A:3041:U:H3'	32:A:3043:C:H5	1.84	0.42
32:A:3219:G:O2'	32:A:3221:A:OP2	2.25	0.42
33:B:1625:A:N7	66:P:87:GLN:NE2	2.59	0.42
36:H:138:LYS:O	36:H:141:GLU:HG3	2.19	0.42
39:M:117:ASP:OD1	39:M:117:ASP:N	2.52	0.42
39:M:212:PRO:HD3	61:q:103:LEU:HD13	2.00	0.42
56:g:88:ARG:NH2	56:g:166:PHE:O	2.52	0.42
64:I:97:ALA:HB3	64:I:154:LEU:HD12	2.01	0.42
70:5:192:ILE:HD11	70:5:199:ALA:HB2	2.00	0.42
71:6:235:TRP:CE2	71:6:237:LEU:HD21	2.55	0.42
2:AB:56:THR:HG22	2:AB:59:ASN:H	1.83	0.42
3:AC:113:ARG:NH2	17:AH:161:GLN:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AO:74:TRP:HE1	10:AO:125:GLN:HB3	1.83	0.42
17:AH:183:HIS:HB2	17:AH:187:PRO:HB3	2.01	0.42
32:A:1688:A:H2'	32:A:1689:C:H4'	2.01	0.42
32:A:1907:A:H2'	32:A:1908:A:C8	2.54	0.42
32:A:2080:U:H5	47:Z:105:SER:HB3	1.85	0.42
32:A:2420:U:O2'	73:9:23:SER:OG	2.28	0.42
32:A:3108:U:H3	69:E:264:ILE:HG21	1.83	0.42
32:A:3228:U:OP2	69:E:49:TRP:NE1	2.50	0.42
35:F:281:ARG:HG3	39:M:125:ARG:HD3	2.02	0.42
37:K:22:ASP:OD1	37:K:23:GLY:N	2.52	0.42
37:K:51:SER:O	43:T:206:ARG:NH1	2.53	0.42
56:g:77:ASP:O	56:g:78:PRO:C	2.61	0.42
71:6:215:THR:HG22	71:6:238:THR:HA	2.01	0.42
1:AA:947:U:O2'	1:AA:948:U:OP1	2.29	0.42
1:AA:1180:U:H2'	1:AA:1181:G:H8	1.84	0.42
1:AA:1216:C:H1'	1:AA:1331:A:N6	2.33	0.42
1:AA:1591:C:H5'	12:AQ:52:ARG:HH22	1.84	0.42
8:AM:65:LEU:HD12	13:AT:146:GLN:HE22	1.84	0.42
30:AF:178:ARG:HA	30:AF:178:ARG:HD2	1.85	0.42
32:A:1830:G:H4'	41:R:53:CYS:HB2	2.00	0.42
32:A:2017:U:H2'	32:A:2018:G:H8	1.84	0.42
32:A:2307:U:H2'	32:A:2308:A:O4'	2.19	0.42
32:A:2597:C:H2'	32:A:2598:A:C8	2.55	0.42
32:A:2673:G:H2'	32:A:2674:U:H6	1.84	0.42
32:A:2935:A:H3'	32:A:2936:U:H2'	2.00	0.42
32:A:3123:G:N2	32:A:3132:G:OP2	2.50	0.42
37:K:27:PRO:HD3	37:K:149:ARG:HD2	2.00	0.42
39:M:238:ARG:NH2	81:p:66:LYS:O	2.52	0.42
40:O:57:GLU:HA	40:O:104:TYR:HE1	1.84	0.42
42:S:132:LYS:HA	42:S:148:LEU:HD13	2.01	0.42
62:r:94:ARG:NE	62:r:99:MET:O	2.52	0.42
76:d:137:PHE:N	76:d:138:PRO:HD2	2.34	0.42
76:d:205:GLN:HE21	76:d:205:GLN:HB2	1.68	0.42
82:s:211:VAL:HG22	82:s:230:ARG:HG3	2.01	0.42
1:AA:699:A:H4'	1:AA:850:U:H4'	2.01	0.42
1:AA:1194:C:H2'	1:AA:1195:U:C6	2.54	0.42
5:AI:96:GLN:HG2	5:AI:111:SER:HB3	2.01	0.42
5:AI:177:ASP:OD1	5:AI:177:ASP:N	2.53	0.42
30:AF:62:GLU:HG2	30:AF:66:ARG:HE	1.84	0.42
32:A:2804:A:H2'	32:A:2805:A:C8	2.54	0.42
42:S:175:ARG:HB2	42:S:180:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Y:71:PRO:HA	46:Y:74:TRP:CE2	2.55	0.42
67:U:46:MET:HE1	67:U:72:VAL:HG13	2.01	0.42
69:E:233:GLN:HB2	69:E:237:HIS:HE1	1.85	0.42
70:5:63:LYS:HD2	70:5:67:VAL:CG1	2.49	0.42
71:6:261:ARG:HG2	71:6:323:TRP:CE2	2.54	0.42
73:9:131:TYR:HB3	73:9:132:PRO:HD3	2.01	0.42
75:c:99:LYS:O	75:c:102:GLU:HG3	2.18	0.42
86:v:402:HIS:HB2	86:v:405:MET:O	2.20	0.42
1:AA:1441:A:H2	1:AA:1449:G:H1	1.66	0.42
6:AJ:116:GLN:OE1	6:AJ:116:GLN:N	2.52	0.42
7:AK:106:LEU:HD21	7:AK:111:PHE:HB2	2.02	0.42
9:AN:14:VAL:HA	9:AN:65:LEU:HA	2.01	0.42
15:AX:123:ARG:HG2	15:AX:306:ILE:HD11	2.01	0.42
17:AH:161:GLN:HG2	17:AH:170:MET:HE1	2.01	0.42
32:A:1893:A:O2'	56:g:98:LYS:O	2.29	0.42
32:A:2048:U:O2'	32:A:2267:U:O2'	2.28	0.42
32:A:2470:G:O2'	38:L:35:MET:O	2.38	0.42
35:F:286:PHE:HA	35:F:290:TYR:CE1	2.54	0.42
45:X:176:LEU:HG	45:X:177:HIS:CD2	2.54	0.42
50:2:72:THR:HG22	50:2:74:ALA:H	1.85	0.42
63:J:166:ALA:HA	63:J:169:LYS:HE3	2.01	0.42
70:5:59:THR:OG1	70:5:60:PHE:N	2.52	0.42
70:5:201:ARG:HD3	70:5:230:LEU:HD21	2.01	0.42
70:5:204:VAL:HB	70:5:229:ARG:HG3	2.01	0.42
71:6:221:LEU:HB2	71:6:267:ARG:HG3	2.00	0.42
2:AB:137:TYR:O	2:AB:264:ARG:NH1	2.52	0.42
13:AT:66:MET:N	13:AT:66:MET:SD	2.93	0.42
15:AX:213:ARG:NH2	55:e:104:ASP:O	2.49	0.42
17:AH:162:ARG:CZ	23:AY:313:PHE:CD1	3.02	0.42
32:A:1771:C:H2'	32:A:1772:A:C8	2.54	0.42
32:A:2080:U:OP1	60:o:67:ARG:NH1	2.53	0.42
32:A:2174:G:H1'	63:J:101:ALA:O	2.19	0.42
32:A:2311:U:H2'	32:A:2312:A:C8	2.55	0.42
32:A:2909:G:C2	88:A7:70:Y5P:N3	2.87	0.42
32:A:2944:C:H2'	32:A:2945:A:O4'	2.19	0.42
32:A:2989:G:H5''	32:A:2990:A:H5'	2.02	0.42
44:W:70:GLN:NE2	44:W:74:ARG:HB3	2.34	0.42
63:J:191:LYS:HE3	63:J:191:LYS:CA	2.49	0.42
64:I:114:HIS:HA	64:I:117:ARG:HG2	2.02	0.42
75:c:56:PRO:HA	75:c:57:PRO:HD3	1.95	0.42
82:s:103:ASP:N	82:s:103:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:v:78:GLU:HG3	92:v:802:GCP:C2'	2.49	0.42
1:AA:1002:C:H2'	1:AA:1003:A:C8	2.54	0.42
1:AA:1052:C:H2'	1:AA:1053:A:O4'	2.20	0.42
1:AA:1052:C:H4'	18:AL:149:LYS:HB3	2.00	0.42
1:AA:1232:A:H5''	1:AA:1353:A:H61	1.83	0.42
1:AA:1319:A:OP1	7:AK:125:ARG:NH1	2.53	0.42
3:AC:62:ILE:HA	3:AC:66:LYS:HB3	2.01	0.42
10:AO:170:VAL:HG11	19:AR:233:ALA:HB2	2.01	0.42
13:AT:24:LYS:HA	13:AT:108:LYS:HE3	2.01	0.42
25:A1:66:TRP:HZ2	25:A1:112:LEU:HD13	1.84	0.42
28:A4:119:PHE:O	28:A4:123:SER:OG	2.35	0.42
29:AD:150:LYS:HB2	29:AD:155:GLN:HE21	1.85	0.42
32:A:2067:C:H4'	77:f:60:LYS:HD2	2.01	0.42
32:A:2145:G:N3	42:S:104:ARG:NH1	2.67	0.42
32:A:2537:G:H2'	32:A:2538:C:C6	2.55	0.42
32:A:2550:A:N6	32:A:2590:A:N1	2.67	0.42
36:H:79:VAL:HG11	45:X:91:TYR:CZ	2.55	0.42
45:X:117:GLU:O	45:X:175:GLN:NE2	2.47	0.42
47:Z:140:LYS:HG2	47:Z:141:SER:H	1.84	0.42
55:e:50:ALA:HA	55:e:175:GLN:HA	2.02	0.42
55:e:144:ASN:OD1	55:e:145:ASP:N	2.53	0.42
63:J:115:LYS:HG3	63:J:158:ASP:OD1	2.20	0.42
64:I:162:LYS:HE2	64:I:162:LYS:HB2	1.92	0.42
64:I:190:GLY:HA2	64:I:193:ASN:HD21	1.84	0.42
65:N:204:GLU:OE1	65:N:207:ARG:NH2	2.51	0.42
69:E:274:TRP:HE1	69:E:286:ASN:HB2	1.84	0.42
70:5:135:LYS:HZ1	70:5:239:ILE:HA	1.84	0.42
76:d:208:VAL:HG23	76:d:252:LEU:HB2	2.02	0.42
82:s:355:PHE:HB2	82:s:374:LEU:HB3	2.01	0.42
1:AA:896:A:H2'	1:AA:897:C:C6	2.55	0.42
1:AA:1430:A:H8	1:AA:1430:A:OP1	2.02	0.42
33:B:1609:U:O2	33:B:1616:A:N6	2.53	0.42
34:D:235:GLN:NE2	34:D:294:SER:OG	2.51	0.42
42:S:113:LEU:HD21	42:S:194:ARG:HH11	1.85	0.42
43:T:104:ALA:HB1	48:0:107:ILE:HG21	2.02	0.42
46:Y:236:LYS:HE3	46:Y:236:LYS:HB3	1.92	0.42
53:8:109:GLU:O	53:8:112:GLU:HG3	2.20	0.42
53:8:130:LYS:HE3	53:8:130:LYS:HB3	1.91	0.42
62:r:146:GLN:HE21	62:r:146:GLN:HB2	1.67	0.42
63:J:119:GLU:HA	63:J:122:ARG:HG2	2.01	0.42
65:N:200:LYS:O	65:N:203:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:P:87:GLN:HG3	66:P:88:HIS:CD2	2.54	0.42
68:V:52:GLU:OE1	68:V:52:GLU:N	2.52	0.42
88:A7:70:Y5P:H4A	88:A7:71:P5P:C5	2.49	0.42
1:AA:1440:G:H2'	1:AA:1441:A:H8	1.85	0.42
3:AC:89:ASP:OD1	3:AC:112:ARG:NH2	2.40	0.42
22:AV:131:ASN:O	22:AV:133:VAL:N	2.53	0.42
32:A:1827:C:O2'	32:A:1844:A:OP1	2.30	0.42
37:K:21:LEU:HB3	37:K:59:ILE:HG12	2.01	0.42
38:L:87:VAL:HG21	38:L:106:VAL:HG23	2.01	0.42
46:Y:85:TRP:HH2	73:9:70:LEU:HD11	1.84	0.42
51:3:150:CYS:HB2	51:3:154:GLN:HE21	1.84	0.42
52:4:66:PHE:HB3	52:4:101:ARG:HB2	2.01	0.42
57:i:88:LEU:HD11	57:i:114:ILE:HG23	2.02	0.42
61:q:40:PRO:HG3	61:q:51:GLN:HB3	2.01	0.42
64:I:50:VAL:HG13	64:I:51:THR:HG23	2.02	0.42
73:9:45:THR:OG1	73:9:46:SER:N	2.52	0.42
86:v:527:GLU:HB3	86:v:645:ILE:HG12	2.00	0.42
9:AN:59:THR:OG1	9:AN:60:VAL:N	2.53	0.41
15:AX:67:HIS:HB3	15:AX:98:CYS:HB3	2.01	0.41
23:AY:364:LEU:HD22	23:AY:368:GLN:HG2	2.02	0.41
31:AG:346:LEU:HG	31:AG:350:LYS:HE2	2.01	0.41
32:A:2267:U:H2'	32:A:2268:G:H8	1.85	0.41
32:A:2901:A:H2'	32:A:2902:A:H8	1.85	0.41
32:A:2951:A:O2'	52:4:103:MET:SD	2.78	0.41
32:A:3195:A:OP2	32:A:3196:G:O2'	2.28	0.41
46:Y:202:LEU:HB3	46:Y:204:TYR:HE2	1.85	0.41
48:O:105:ASN:O	69:E:45:SER:OG	2.33	0.41
54:b:65:VAL:HB	78:h:154:ILE:HG22	2.01	0.41
64:I:81:LEU:HB2	80:l:115:ARG:NH2	2.24	0.41
72:7:184:VAL:HG22	72:7:294:ILE:HG22	2.02	0.41
75:c:228:LEU:HD22	75:c:307:PHE:HB3	2.02	0.41
82:s:266:CYS:SG	82:s:270:LYS:HG3	2.60	0.41
86:v:218:ILE:HD12	86:v:250:ARG:HH12	1.85	0.41
1:AA:719:G:H22	1:AA:799:A:H1'	1.84	0.41
1:AA:1012:A:H2'	1:AA:1013:A:O4'	2.19	0.41
1:AA:1160:A:H2'	1:AA:1161:A:C8	2.55	0.41
1:AA:1462:G:H2'	1:AA:1463:G:C8	2.55	0.41
3:AC:77:ASP:OD2	17:AH:140:TYR:OH	2.37	0.41
4:AE:113:LEU:HD12	14:AW:152:ARG:HB3	2.02	0.41
11:AP:123:THR:HG23	11:AP:124:TYR:CD2	2.55	0.41
20:AS:40:PRO:HB2	20:AS:41:LEU:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AD:243:VAL:HG11	29:AD:268:PHE:HE1	1.85	0.41
32:A:1770:G:H2'	32:A:1771:C:H6	1.85	0.41
32:A:1872:U:H2'	32:A:1873:A:O4'	2.20	0.41
32:A:2100:C:H1'	32:A:2135:A:C8	2.55	0.41
32:A:2261:C:C2	42:S:184:ARG:HD2	2.54	0.41
32:A:2314:C:H2'	32:A:2315:A:C4	2.55	0.41
32:A:2339:G:H4'	50:2:55:PRO:HB2	2.02	0.41
32:A:2745:A:H2'	32:A:2745:A:N3	2.34	0.41
32:A:2930:U:H2'	32:A:2931:A:H8	1.85	0.41
32:A:3165:C:H2'	32:A:3166:U:C6	2.56	0.41
36:H:85:ASP:OD1	36:H:86:THR:N	2.52	0.41
42:S:95:LEU:HD23	42:S:95:LEU:H	1.85	0.41
57:i:126:LYS:HG2	57:i:127:PHE:H	1.85	0.41
72:7:103:SER:HB3	72:7:115:MET:HE3	2.03	0.41
73:9:64:ASP:OD1	73:9:64:ASP:N	2.52	0.41
75:c:245:LEU:HB3	75:c:250:VAL:HB	2.01	0.41
76:d:147:GLU:HB2	76:d:159:ARG:HH22	1.85	0.41
1:AA:1022:A:H2'	1:AA:1023:C:C6	2.55	0.41
4:AE:6:LEU:HD13	4:AE:93:ILE:HG12	2.03	0.41
4:AE:107:GLY:HA3	11:AP:64:LYS:HA	2.03	0.41
6:AJ:66:PHE:HE1	6:AJ:68:ARG:HE	1.69	0.41
7:AK:54:ILE:HG23	7:AK:71:ALA:HB1	2.02	0.41
10:AO:236:PRO:HB2	10:AO:237:LYS:H	1.67	0.41
29:AD:286:GLU:HB2	29:AD:288:HIS:CE1	2.55	0.41
32:A:1701:U:H4'	50:2:61:LYS:HB3	2.03	0.41
32:A:1818:A:H4'	43:T:88:TRP:NE1	2.36	0.41
32:A:1910:C:H2'	32:A:1911:C:C6	2.55	0.41
32:A:1992:C:N3	34:D:274:ARG:HB2	2.35	0.41
32:A:2043:C:O2'	32:A:2866:A:N3	2.37	0.41
32:A:2077:C:O2'	44:W:59:HIS:NE2	2.39	0.41
32:A:2276:C:N4	32:A:2290:A:H61	2.19	0.41
40:O:45:PRO:HG2	40:O:48:ARG:HD2	2.02	0.41
40:O:91:GLN:OE1	48:O:153:THR:OG1	2.29	0.41
75:c:67:ASP:HB3	75:c:70:ALA:HB3	2.02	0.41
7:AK:80:ARG:HD3	7:AK:86:ARG:HH12	1.84	0.41
9:AN:89:GLY:HA3	18:AL:174:TYR:HB2	2.02	0.41
19:AR:106:MET:HE1	19:AR:114:ALA:HB2	2.03	0.41
22:AV:90:TYR:CE1	83:Q:55:GLN:HB3	2.55	0.41
25:A1:64:GLN:NE2	28:A4:81:ASP:OD1	2.53	0.41
32:A:2032:G:H2'	32:A:2033:A:C8	2.54	0.41
32:A:2174:G:C2	63:J:102:ARG:O	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2366:G:OP1	67:U:79:ARG:NE	2.52	0.41
32:A:2367:A:H2'	32:A:2368:C:C6	2.56	0.41
32:A:2656:U:H5''	69:E:229:ALA:HB3	2.03	0.41
32:A:2910:A:C2	88:A7:71:P5P:H8	2.55	0.41
32:A:2945:A:O2'	32:A:2947:U:O4	2.38	0.41
36:H:74:HIS:CE1	36:H:75:ARG:HG2	2.55	0.41
51:3:183:ARG:HE	71:6:354:GLN:NE2	2.18	0.41
60:o:28:SER:OG	60:o:29:LEU:N	2.53	0.41
70:5:300:ARG:HA	70:5:303:ARG:HE	1.85	0.41
72:7:148:MET:HE1	72:7:255:HIS:HB2	2.03	0.41
76:d:48:PRO:HB2	76:d:50:PHE:CD1	2.54	0.41
82:s:185:VAL:HG21	82:s:200:LEU:HD22	2.02	0.41
86:v:399:ALA:HA	86:v:409:VAL:HG22	2.02	0.41
86:v:641:ALA:C	86:v:643:LEU:H	2.26	0.41
1:AA:798:C:H2'	1:AA:799:A:C8	2.55	0.41
1:AA:1215:U:H2'	1:AA:1216:C:O4'	2.20	0.41
4:AE:47:LEU:HD13	4:AE:51:ILE:HD12	2.02	0.41
13:AT:63:GLN:NE2	13:AT:65:MET:SD	2.93	0.41
22:AV:131:ASN:HD21	22:AV:134:GLN:HB3	1.85	0.41
24:AZ:26:THR:OG1	24:AZ:27:ASN:N	2.54	0.41
32:A:1760:G:OP1	61:q:59:LYS:NZ	2.53	0.41
32:A:2253:U:H2'	32:A:2254:C:C6	2.56	0.41
32:A:2675:G:H5''	43:T:167:MET:HG3	2.03	0.41
32:A:2953:U:H1'	65:N:181:HIS:CE1	2.55	0.41
32:A:3002:G:H2'	32:A:3003:A:H8	1.85	0.41
38:L:100:PHE:HB3	83:Q:158:GLN:HE21	1.86	0.41
45:X:14:LEU:O	45:X:18:GLU:HG3	2.21	0.41
55:e:203:LYS:O	55:e:237:LEU:N	2.47	0.41
64:I:78:LEU:CD1	80:I:118:TRP:CZ3	3.02	0.41
64:I:144:LEU:N	64:I:145:PRO:HD2	2.35	0.41
72:7:284:HIS:HB3	72:7:323:MET:HE2	2.02	0.41
82:s:175:PRO:HA	82:s:178:ASP:OD2	2.20	0.41
83:Q:118:ARG:HE	83:Q:134:LEU:HD12	1.86	0.41
1:AA:774:G:H2'	1:AA:775:C:H6	1.86	0.41
1:AA:788:U:H2'	1:AA:789:U:C6	2.56	0.41
1:AA:1003:A:H2'	1:AA:1004:G:C8	2.56	0.41
1:AA:1279:C:H2'	1:AA:1280:C:C6	2.55	0.41
1:AA:1489:G:O2'	1:AA:1583:A:O2'	2.35	0.41
22:AV:85:ILE:HD13	22:AV:116:CYS:HA	2.03	0.41
26:A0:164:VAL:HG13	26:A0:193:VAL:HG21	2.02	0.41
32:A:1735:A:H8	36:H:69:ARG:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1823:A:O2'	74:a:126:HIS:ND1	2.54	0.41
32:A:1893:A:H4'	32:A:1894:G:H5'	2.03	0.41
32:A:2100:C:H2'	32:A:2101:C:C6	2.56	0.41
32:A:2469:A:H2'	32:A:2470:G:H8	1.84	0.41
32:A:2584:C:H2'	32:A:2585:G:C8	2.56	0.41
35:F:227:PRO:HG2	35:F:230:ILE:HG22	2.03	0.41
55:e:128:PHE:HB2	59:m:73:ARG:HB3	2.02	0.41
55:e:205:LEU:HB3	77:f:171:LEU:HD11	2.02	0.41
70:5:187:LEU:HD22	70:5:411:PHE:HZ	1.85	0.41
72:7:163:MET:HE1	72:7:165:ASN:HD21	1.85	0.41
79:k:8:LEU:HD21	79:k:95:ARG:HB2	2.02	0.41
86:v:174:ASN:ND2	92:v:802:GCP:N7	2.69	0.41
86:v:208:GLU:HG2	86:v:209:GLY:H	1.86	0.41
1:AA:780:C:H42	18:AL:196:ARG:HH22	1.68	0.41
1:AA:805:C:H6	1:AA:805:C:H2'	1.68	0.41
32:A:2288:A:H2'	32:A:2289:G:H8	1.86	0.41
32:A:3142:A:H4'	38:L:63:LYS:HB2	2.02	0.41
32:A:3145:A:H2'	32:A:3146:G:C8	2.56	0.41
32:A:3145:A:H2'	32:A:3146:G:H8	1.86	0.41
32:A:3177:A:H2'	32:A:3177:A:N3	2.36	0.41
34:D:184:LEU:HD13	34:D:226:ILE:HD11	2.03	0.41
39:M:200:ILE:O	39:M:272:GLY:N	2.52	0.41
49:1:55:LEU:HG	61:q:128:MET:HE1	2.02	0.41
55:e:151:ARG:NH1	55:e:254:TRP:O	2.52	0.41
67:U:143:ARG:HG2	76:d:282:ILE:HD11	2.03	0.41
71:6:224:HIS:HB2	71:6:231:GLU:HA	2.03	0.41
81:p:50:PRO:HA	81:p:53:GLN:HE21	1.86	0.41
81:p:153:LYS:HA	81:p:156:ASP:OD2	2.21	0.41
86:v:46:ILE:HG21	86:v:416:ASP:OD1	2.21	0.41
1:AA:1051:A:H2'	1:AA:1052:C:C6	2.55	0.41
1:AA:1363:C:H2'	1:AA:1364:U:C6	2.56	0.41
8:AM:111:ARG:HD2	10:AO:232:PRO:HB3	2.02	0.41
13:AT:71:THR:HG22	13:AT:73:SER:H	1.85	0.41
15:AX:265:ILE:HG13	15:AX:329:LEU:HD21	2.03	0.41
22:AV:90:TYR:CD1	83:Q:55:GLN:HB3	2.56	0.41
23:AY:284:LYS:HE3	23:AY:284:LYS:HB3	1.92	0.41
23:AY:289:VAL:HG12	28:A4:412:ASP:H	1.86	0.41
31:AG:157:SER:OG	31:AG:211:GLU:OE1	2.37	0.41
32:A:1882:A:OP2	56:g:97:TYR:OH	2.34	0.41
32:A:2015:G:N2	32:A:2037:U:O3'	2.53	0.41
32:A:2094:G:OP2	39:M:57:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2461:A:H2'	32:A:2462:A:H8	1.86	0.41
34:D:124:GLU:HB2	34:D:163:ILE:HG13	2.02	0.41
35:F:286:PHE:HB2	57:i:66:PHE:CG	2.56	0.41
39:M:230:PRO:HB2	81:p:62:PRO:HD3	2.03	0.41
46:Y:76:GLN:O	46:Y:78:LYS:N	2.54	0.41
63:J:170:GLU:C	63:J:174:PHE:CD2	2.99	0.41
64:I:116:LEU:HB3	64:I:121:ILE:HD11	2.02	0.41
64:I:124:LYS:NZ	64:I:125:VAL:O	2.50	0.41
66:P:72:PHE:HB2	66:P:73:PRO:HD2	2.02	0.41
67:U:35:GLN:CD	82:s:270:LYS:HD2	2.45	0.41
67:U:128:SER:O	67:U:131:GLU:HG3	2.20	0.41
70:5:355:LEU:HD13	70:5:376:VAL:HG22	2.02	0.41
77:f:162:LEU:HB3	77:f:167:ALA:HB2	2.03	0.41
1:AA:674:U:H4'	1:AA:826:A:H1'	2.02	0.41
1:AA:713:C:H2'	1:AA:714:A:O4'	2.21	0.41
1:AA:1046:A:H3'	1:AA:1049:A:H62	1.86	0.41
1:AA:1109:A:H2'	1:AA:1110:A:C8	2.56	0.41
1:AA:1189:U:O2'	1:AA:1190:C:H5''	2.21	0.41
4:AE:37:ARG:NH2	21:AU:163:GLU:OE2	2.54	0.41
4:AE:40:GLU:HB2	4:AE:65:LEU:HB2	2.03	0.41
6:AJ:78:ARG:HB3	6:AJ:94:PHE:HE1	1.86	0.41
10:AO:57:LYS:O	10:AO:61:SER:OG	2.26	0.41
15:AX:264:GLY:N	15:AX:309:ALA:O	2.54	0.41
18:AL:72:LEU:HB2	18:AL:73:LYS:H	1.73	0.41
29:AD:282:ILE:HG12	29:AD:353:LEU:HB3	2.03	0.41
32:A:2214:A:H5'	80:l:126:ILE:CD1	2.51	0.41
32:A:2587:G:H2'	32:A:2588:C:C6	2.56	0.41
32:A:3013:G:N2	32:A:3024:U:O2	2.39	0.41
32:A:3092:U:H4'	32:A:3093:C:OP1	2.21	0.41
32:A:3130:A:H4'	86:v:98:ARG:NH2	2.35	0.41
36:H:124:LEU:HB2	36:H:125:PRO:HD3	2.02	0.41
39:M:193:PHE:HE2	39:M:200:ILE:HG12	1.86	0.41
41:R:83:TYR:HB3	41:R:84:PRO:HD3	2.02	0.41
43:T:159:HIS:HB3	43:T:160:GLY:H	1.72	0.41
49:1:61:LYS:CG	88:A7:1:P5P:C5'	2.60	0.41
57:i:39:PRO:HG2	75:c:35:PHE:HD1	1.85	0.41
61:q:110:GLU:HA	61:q:113:LYS:HG2	2.03	0.41
66:P:151:TRP:CD1	66:P:152:GLU:HG3	2.56	0.41
68:V:124:ASP:HA	68:V:125:PRO:HD3	1.93	0.41
70:5:63:LYS:HD3	70:5:65:HIS:NE2	2.35	0.41
70:5:120:ALA:HB1	70:5:314:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:6:179:VAL:H	81:p:194:HIS:CD2	2.39	0.41
71:6:275:GLN:HA	71:6:311:MET:HA	2.03	0.41
72:7:195:THR:OG1	72:7:196:LYS:N	2.53	0.41
74:a:75:ILE:HG12	75:c:257:LEU:HB2	2.02	0.41
77:f:92:ASN:OD1	77:f:94:HIS:NE2	2.54	0.41
82:s:188:LEU:HD22	82:s:426:LEU:HD21	2.02	0.41
88:A7:24:Y5P:H4A	88:A7:25:Y5P:H4	2.02	0.41
1:AA:833:A:H2'	1:AA:834:G:C8	2.56	0.41
1:AA:1575:U:H2'	1:AA:1576:G:C8	2.56	0.41
3:AC:72:HIS:HB3	3:AC:112:ARG:HH11	1.85	0.41
15:AX:155:ILE:HB	15:AX:262:VAL:HA	2.03	0.41
18:AL:114:ILE:HD12	18:AL:183:GLY:HA3	2.03	0.41
20:AS:89:ASN:HB3	20:AS:92:PHE:HB2	2.01	0.41
26:A0:63:ARG:HB3	26:A0:137:HIS:CD2	2.55	0.41
29:AD:305:MET:N	29:AD:305:MET:SD	2.94	0.41
32:A:2532:U:H2'	32:A:2533:A:H8	1.86	0.41
32:A:3122:U:H5'	32:A:3124:U:C6	2.56	0.41
35:F:59:ARG:NH2	56:g:114:GLU:OE2	2.55	0.41
43:T:61:PRO:HA	76:d:229:GLY:HA2	2.03	0.41
45:X:54:PRO:C	45:X:56:ASN:H	2.29	0.41
45:X:111:GLU:HA	45:X:126:THR:HA	2.02	0.41
51:3:179:LYS:O	71:6:370:ARG:NH2	2.49	0.41
56:g:132:LEU:HD21	56:g:153:PHE:HZ	1.86	0.41
66:P:52:ASN:ND2	66:P:54:ARG:O	2.54	0.41
69:E:94:SER:HB3	69:E:182:THR:HG21	2.03	0.41
71:6:92:LEU:HB2	71:6:170:ARG:HG3	2.03	0.41
76:d:185:PHE:HZ	76:d:188:SER:HB2	1.86	0.41
83:Q:226:PRO:HB2	83:Q:227:LYS:H	1.64	0.41
83:Q:227:LYS:HE2	83:Q:227:LYS:HB3	1.88	0.41
86:v:67:LEU:CD1	86:v:72:ARG:HD3	2.51	0.41
86:v:559:LEU:HD21	86:v:608:ARG:HB3	2.01	0.41
2:AB:117:ASP:HB3	2:AB:120:GLN:NE2	2.36	0.40
10:AO:72:PRO:HD2	10:AO:75:ALA:HB2	2.03	0.40
14:AW:122:CYS:SG	14:AW:123:VAL:N	2.94	0.40
17:AH:74:LYS:HB3	17:AH:175:THR:HG23	2.03	0.40
23:AY:353:LEU:HD23	24:AZ:22:VAL:HG21	2.03	0.40
32:A:1791:G:O2'	32:A:2006:C:O2'	2.37	0.40
32:A:2187:C:H42	63:J:103:GLN:HA	1.84	0.40
32:A:2241:A:H2'	62:r:192:TRP:HE3	1.85	0.40
32:A:2523:C:O2	34:D:87:HIS:ND1	2.54	0.40
32:A:2734:A:H2'	32:A:2735:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D:223:THR:HG22	34:D:296:VAL:HG21	2.03	0.40
45:X:156:LYS:NZ	70:5:70:LEU:CG	2.80	0.40
45:X:173:ASP:O	45:X:188:TYR:OH	2.38	0.40
48:0:136:GLU:OE2	48:0:139:ARG:NH1	2.54	0.40
61:q:107:GLN:O	61:q:110:GLU:HG3	2.20	0.40
63:J:123:ILE:O	63:J:126:GLN:NE2	2.54	0.40
65:N:36:VAL:HG12	80:l:128:ARG:CD	2.48	0.40
86:v:284:ARG:HG2	86:v:316:TYR:HA	2.03	0.40
1:AA:654:U:O2'	1:AA:1167:A:OP1	2.29	0.40
15:AX:384:SER:OG	15:AX:387:ASN:O	2.39	0.40
25:A1:286:THR:HG22	25:A1:288:GLU:H	1.85	0.40
30:AF:57:GLU:OE1	30:AF:58:LEU:N	2.54	0.40
32:A:1781:A:N6	32:A:1795:A:OP2	2.55	0.40
32:A:1836:A:N3	74:a:130:HIS:HB3	2.36	0.40
32:A:2753:A:H2'	32:A:2754:A:C8	2.50	0.40
58:j:112:LYS:NZ	71:6:308:GLN:O	2.55	0.40
61:q:148:ALA:HA	61:q:151:GLU:HG2	2.03	0.40
62:r:193:LYS:HE2	62:r:196:HIS:HB3	2.04	0.40
70:5:339:PRO:HB2	70:5:358:GLN:HE21	1.86	0.40
72:7:114:ASP:HB3	72:7:267:PRO:HB2	2.03	0.40
82:s:189:SER:HB3	82:s:190:PRO:HD3	2.02	0.40
1:AA:712:C:H42	21:AU:27:ARG:HB2	1.85	0.40
1:AA:889:G:H21	1:AA:901:G:H4'	1.85	0.40
1:AA:1471:A:H2'	1:AA:1472:G:H8	1.85	0.40
15:AX:56:PRO:HA	15:AX:59:HIS:CD2	2.57	0.40
15:AX:84:PRO:HA	15:AX:85:PRO:HD3	1.95	0.40
16:A2:86:MET:O	16:A2:90:GLN:HG2	2.21	0.40
28:A4:108:LEU:HD11	29:AD:154:VAL:HB	2.04	0.40
32:A:2093:U:O2	32:A:2266:U:O2'	2.37	0.40
32:A:2650:C:H2'	32:A:2651:A:H8	1.85	0.40
32:A:2934:G:H22	32:A:2937:A:H3'	1.86	0.40
45:X:163:ARG:HH21	70:5:55:LEU:HD11	1.85	0.40
48:0:173:ARG:HE	48:0:175:ILE:HD11	1.86	0.40
55:e:257:LYS:NZ	55:e:273:ARG:HB2	2.36	0.40
63:J:132:LEU:HA	64:I:117:ARG:HE	1.84	0.40
63:J:133:GLN:H	64:I:117:ARG:CZ	2.33	0.40
65:N:33:LEU:CA	80:l:125:ASN:HD21	2.33	0.40
65:N:33:LEU:CD2	80:l:125:ASN:HD22	2.31	0.40
77:f:119:ILE:HD12	77:f:159:ILE:HG21	2.03	0.40
78:h:57:SER:OG	78:h:136:ASP:OD2	2.33	0.40
86:v:527:GLU:HA	86:v:645:ILE:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:A7:57:Y5P:H4A	88:A7:58:Y5P:H4	2.04	0.40
1:AA:782:A:OP2	6:AJ:38:ARG:HD2	2.21	0.40
1:AA:873:G:H2'	1:AA:874:G:H8	1.86	0.40
1:AA:1085:C:H2'	1:AA:1086:C:H6	1.87	0.40
3:AC:142:LEU:HD23	3:AC:142:LEU:HA	1.91	0.40
3:AC:150:PRO:HD3	23:AY:309:LYS:HB3	2.04	0.40
22:AV:107:TRP:CD1	22:AV:107:TRP:H	2.39	0.40
30:AF:200:LEU:HD13	30:AF:200:LEU:HA	1.95	0.40
32:A:1897:A:H2'	32:A:1898:A:H8	1.86	0.40
32:A:2144:A:N6	32:A:2257:C:H42	2.20	0.40
32:A:2198:A:N1	63:J:150:SER:HB2	2.37	0.40
32:A:2343:G:N3	32:A:2343:G:H3'	2.37	0.40
32:A:2926:A:O2'	32:A:3087:C:OP1	2.29	0.40
35:F:79:LEU:HD22	78:h:94:SER:HB3	2.02	0.40
35:F:167:MET:HA	35:F:170:ARG:HE	1.87	0.40
38:L:59:HIS:HB3	38:L:74:LEU:HD12	2.02	0.40
39:M:238:ARG:O	81:p:155:ARG:NH2	2.55	0.40
44:W:126:LEU:HD23	44:W:128:LYS:NZ	2.37	0.40
55:e:152:LYS:HB2	55:e:157:LEU:HD21	2.03	0.40
76:d:122:ILE:HA	76:d:125:ILE:HG12	2.02	0.40
86:v:175:LYS:CB	92:v:802:GCP:C6	2.99	0.40
1:AA:977:A:H1'	5:AI:182:PRO:HB3	2.04	0.40
5:AI:147:ILE:HD13	5:AI:170:LEU:HD13	2.04	0.40
12:AQ:30:LEU:HD22	12:AQ:35:LEU:HD13	2.03	0.40
15:AX:159:HIS:HB3	15:AX:314:GLY:HA3	2.04	0.40
18:AL:66:PRO:HA	18:AL:67:PRO:HD3	1.95	0.40
22:AV:168:MET:HE3	22:AV:168:MET:HB3	1.93	0.40
25:A1:110:ASN:HD22	25:A1:110:ASN:H	1.68	0.40
32:A:1671:G:O2'	32:A:1672:C:H5''	2.22	0.40
32:A:1863:A:H2'	32:A:1864:A:C8	2.57	0.40
32:A:2174:G:O2'	63:J:101:ALA:C	2.62	0.40
32:A:2610:U:H2'	32:A:2611:C:C6	2.56	0.40
32:A:2853:A:N1	32:A:2878:G:O2'	2.50	0.40
36:H:53:THR:HG21	45:X:130:ARG:HD2	2.04	0.40
40:O:142:LEU:HB2	72:7:135:PRO:HD2	2.03	0.40
55:e:211:GLY:H	55:e:233:PHE:HB2	1.85	0.40
62:r:63:PRO:HA	62:r:64:PRO:HD3	1.98	0.40
64:I:188:ARG:CZ	79:k:55:VAL:H	2.35	0.40
67:U:11:ARG:NH1	70:5:80:ARG:HH11	2.20	0.40
82:s:376:THR:HB	82:s:389:ARG:HB2	2.04	0.40
86:v:47:ARG:O	86:v:116:ILE:HA	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	
2	AB	218/296 (74%)	187 (86%)	27 (12%)	4 (2%)	6	28
3	AC	130/167 (78%)	107 (82%)	22 (17%)	1 (1%)	16	47
4	AE	120/125 (96%)	98 (82%)	18 (15%)	4 (3%)	3	15
5	AI	134/194 (69%)	113 (84%)	18 (13%)	3 (2%)	5	24
6	AJ	106/138 (77%)	92 (87%)	12 (11%)	2 (2%)	6	27
7	AK	99/128 (77%)	88 (89%)	8 (8%)	3 (3%)	3	17
8	AM	114/137 (83%)	103 (90%)	10 (9%)	1 (1%)	14	45
9	AN	105/130 (81%)	85 (81%)	18 (17%)	2 (2%)	6	27
10	AO	188/258 (73%)	166 (88%)	18 (10%)	4 (2%)	5	25
11	AP	94/142 (66%)	82 (87%)	10 (11%)	2 (2%)	5	25
12	AQ	84/87 (97%)	71 (84%)	13 (16%)	0	100	100
13	AT	166/173 (96%)	149 (90%)	16 (10%)	1 (1%)	21	53
14	AW	95/187 (51%)	77 (81%)	15 (16%)	3 (3%)	3	16
15	AX	351/398 (88%)	319 (91%)	28 (8%)	4 (1%)	11	40
16	A2	114/118 (97%)	96 (84%)	17 (15%)	1 (1%)	14	45
17	AH	120/201 (60%)	101 (84%)	16 (13%)	3 (2%)	4	21
18	AL	172/257 (67%)	154 (90%)	15 (9%)	3 (2%)	7	30
19	AR	290/360 (81%)	263 (91%)	26 (9%)	1 (0%)	36	67
20	AS	133/190 (70%)	119 (90%)	10 (8%)	4 (3%)	3	17
21	AU	175/205 (85%)	163 (93%)	12 (7%)	0	100	100
22	AV	363/414 (88%)	319 (88%)	36 (10%)	8 (2%)	5	24
23	AY	118/395 (30%)	107 (91%)	10 (8%)	1 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AZ	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
25	A1	273/323 (84%)	242 (89%)	25 (9%)	6 (2%)	5	24
26	A0	212/218 (97%)	185 (87%)	22 (10%)	5 (2%)	4	22
27	A3	70/199 (35%)	64 (91%)	6 (9%)	0	100	100
28	A4	541/689 (78%)	465 (86%)	66 (12%)	10 (2%)	6	28
29	AD	341/430 (79%)	306 (90%)	31 (9%)	4 (1%)	10	38
30	AF	206/242 (85%)	180 (87%)	23 (11%)	3 (2%)	8	33
31	AG	311/396 (78%)	272 (88%)	37 (12%)	2 (1%)	21	53
34	D	237/305 (78%)	208 (88%)	27 (11%)	2 (1%)	16	47
35	F	248/311 (80%)	217 (88%)	27 (11%)	4 (2%)	7	31
36	H	96/267 (36%)	84 (88%)	10 (10%)	2 (2%)	5	25
37	K	175/178 (98%)	153 (87%)	16 (9%)	6 (3%)	3	15
38	L	113/145 (78%)	102 (90%)	10 (9%)	1 (1%)	14	45
39	M	285/296 (96%)	252 (88%)	26 (9%)	7 (2%)	4	21
40	O	150/175 (86%)	128 (85%)	19 (13%)	3 (2%)	6	26
41	R	138/149 (93%)	123 (89%)	10 (7%)	5 (4%)	2	14
42	S	154/205 (75%)	135 (88%)	15 (10%)	4 (3%)	4	20
43	T	164/212 (77%)	148 (90%)	13 (8%)	3 (2%)	6	28
44	W	109/148 (74%)	97 (89%)	11 (10%)	1 (1%)	14	45
45	X	241/256 (94%)	212 (88%)	24 (10%)	5 (2%)	5	25
46	Y	174/250 (70%)	161 (92%)	7 (4%)	6 (3%)	3	15
47	Z	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
48	0	106/188 (56%)	93 (88%)	10 (9%)	3 (3%)	4	19
49	1	50/65 (77%)	42 (84%)	7 (14%)	1 (2%)	6	26
50	2	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	5	23
51	3	93/188 (50%)	84 (90%)	8 (9%)	1 (1%)	11	40
52	4	36/103 (35%)	34 (94%)	2 (6%)	0	100	100
53	8	97/206 (47%)	85 (88%)	12 (12%)	0	100	100
54	b	146/155 (94%)	129 (88%)	14 (10%)	3 (2%)	5	25
55	e	211/279 (76%)	188 (89%)	22 (10%)	1 (0%)	24	58
56	g	130/166 (78%)	109 (84%)	17 (13%)	4 (3%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	i	95/128 (74%)	75 (79%)	20 (21%)	0	100	100
58	j	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	11	40
59	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	5	23
60	o	92/102 (90%)	79 (86%)	10 (11%)	3 (3%)	3	15
61	q	166/222 (75%)	154 (93%)	10 (6%)	2 (1%)	10	38
62	r	160/196 (82%)	139 (87%)	16 (10%)	5 (3%)	3	16
63	J	173/192 (90%)	152 (88%)	15 (9%)	6 (4%)	3	14
64	I	177/261 (68%)	164 (93%)	12 (7%)	1 (1%)	21	53
65	N	220/251 (88%)	203 (92%)	16 (7%)	1 (0%)	24	58
66	P	141/179 (79%)	123 (87%)	14 (10%)	4 (3%)	4	19
67	U	150/153 (98%)	122 (81%)	26 (17%)	2 (1%)	9	36
68	V	204/216 (94%)	179 (88%)	25 (12%)	0	100	100
69	E	304/348 (87%)	268 (88%)	32 (10%)	4 (1%)	9	36
70	5	392/423 (93%)	347 (88%)	41 (10%)	4 (1%)	12	42
71	6	352/380 (93%)	302 (86%)	47 (13%)	3 (1%)	14	45
72	7	295/338 (87%)	260 (88%)	28 (10%)	7 (2%)	4	22
73	9	122/137 (89%)	106 (87%)	15 (12%)	1 (1%)	16	47
74	a	106/142 (75%)	95 (90%)	8 (8%)	3 (3%)	4	19
75	c	287/332 (86%)	265 (92%)	18 (6%)	4 (1%)	9	34
76	d	255/306 (83%)	216 (85%)	33 (13%)	6 (2%)	4	22
77	f	144/194 (74%)	121 (84%)	22 (15%)	1 (1%)	18	50
78	h	108/158 (68%)	93 (86%)	13 (12%)	2 (2%)	6	27
79	k	94/112 (84%)	85 (90%)	9 (10%)	0	100	100
80	l	70/138 (51%)	62 (89%)	7 (10%)	1 (1%)	9	34
81	p	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	34
82	s	391/439 (89%)	342 (88%)	41 (10%)	8 (2%)	6	26
83	Q	238/292 (82%)	211 (89%)	20 (8%)	7 (3%)	3	18
84	TA	43/198 (22%)	32 (74%)	11 (26%)	0	100	100
84	TB	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
84	TC	69/198 (35%)	57 (83%)	11 (16%)	1 (1%)	9	34
86	v	710/751 (94%)	566 (80%)	117 (16%)	27 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	14720/19244 (76%)	12876 (88%)	1589 (11%)	255 (2%)	9	30

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AI	68	GLY
22	AV	35	VAL
28	A4	203	PRO
40	O	111	PRO
41	R	137	GLU
42	S	147	PRO
42	S	165	GLU
45	X	18	GLU
48	0	113	CYS
56	g	78	PRO
63	J	34	PRO
63	J	35	LEU
63	J	157	LYS
63	J	160	SER
66	P	73	PRO
72	7	60	PRO
75	c	251	SER
76	d	67	ILE
82	s	132	GLU
83	Q	226	PRO
84	TC	169	PRO
86	v	208	GLU
86	v	319	ASN
86	v	320	PRO
86	v	336	LYS
86	v	436	ASN
2	AB	185	PRO
4	AE	71	PRO
10	AO	97	ARG
10	AO	98	ASN
10	AO	236	PRO
15	AX	156	PRO
15	AX	371	ALA
17	AH	124	VAL
20	AS	40	PRO
26	A0	214	LYS
28	A4	407	PRO

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Mol	Chain	Res	Type
28	A4	541	PRO
29	AD	291	PHE
30	AF	71	THR
36	H	103	GLU
37	K	101	VAL
39	M	47	ARG
39	M	280	LYS
40	O	14	VAL
41	R	135	GLY
41	R	143	SER
62	r	136	PRO
62	r	167	PRO
66	P	68	TRP
67	U	111	PHE
69	E	317	PRO
70	5	70	LEU
72	7	230	PHE
72	7	270	PRO
76	d	176	ILE
76	d	236	GLU
78	h	83	PRO
82	s	131	PRO
83	Q	58	PRO
83	Q	60	PRO
86	v	148	VAL
86	v	271	GLU
86	v	272	LYS
86	v	566	LYS
86	v	744	VAL
86	v	745	LYS
2	AB	172	ARG
5	AI	143	GLY
6	AJ	70	PRO
9	AN	11	ARG
19	AR	183	LYS
20	AS	110	GLY
22	AV	121	ALA
22	AV	132	LYS
22	AV	155	GLU
22	AV	156	ASN
25	A1	61	ALA
28	A4	382	PRO

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Mol	Chain	Res	Type
28	A4	470	GLN
29	AD	423	SER
30	AF	80	GLY
30	AF	201	MET
31	AG	391	PHE
35	F	91	PRO
38	L	94	PRO
39	M	242	TYR
45	X	92	ALA
45	X	220	GLU
45	X	221	LYS
46	Y	77	GLU
55	e	265	LYS
56	g	53	PRO
56	g	55	THR
58	j	40	TYR
60	o	15	ARG
62	r	143	SER
65	N	55	ARG
72	7	167	VAL
72	7	281	SER
74	a	44	ASN
74	a	79	ASP
75	c	183	GLU
77	f	122	GLU
82	s	133	PRO
86	v	77	HIS
86	v	175	LYS
86	v	318	PRO
86	v	334	ASP
86	v	346	SER
86	v	435	ALA
86	v	743	PRO
4	AE	14	GLN
4	AE	54	HIS
6	AJ	49	LEU
7	AK	62	ILE
14	AW	110	ASN
16	A2	101	PRO
18	AL	71	LEU
22	AV	321	GLU
25	A1	73	ALA

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Mol	Chain	Res	Type
25	A1	76	PHE
25	A1	98	ALA
25	A1	131	THR
28	A4	136	HIS
28	A4	385	PRO
29	AD	416	GLY
36	H	61	LYS
37	K	5	SER
37	K	24	LYS
37	K	143	GLU
37	K	151	ILE
37	K	153	LYS
39	M	260	LYS
39	M	266	PHE
40	O	128	ASN
42	S	196	ASN
43	T	69	ARG
44	W	72	HIS
45	X	176	LEU
46	Y	94	SER
46	Y	162	ARG
46	Y	202	LEU
49	1	60	LYS
50	2	50	GLY
54	b	116	ARG
59	m	70	GLU
61	q	128	MET
61	q	161	GLN
64	I	38	ARG
69	E	82	ASP
70	5	73	PRO
70	5	114	LEU
71	6	289	PRO
72	7	123	CYS
75	c	120	LYS
75	c	186	VAL
78	h	80	SER
80	l	104	PRO
82	s	163	VAL
82	s	272	PRO
82	s	350	ASP
82	s	404	THR

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Mol	Chain	Res	Type
2	AB	103	GLU
4	AE	15	ARG
5	AI	60	PHE
7	AK	82	SER
10	AO	51	TYR
11	AP	57	PRO
14	AW	109	GLU
17	AH	179	GLN
17	AH	184	ILE
18	AL	146	ARG
20	AS	109	LEU
22	AV	135	TYR
25	A1	55	PRO
26	A0	182	GLY
39	M	267	PHE
39	M	279	ASP
41	R	136	LYS
42	S	138	ALA
43	T	158	TYR
46	Y	204	TYR
48	0	163	GLU
54	b	113	ILE
60	o	52	PRO
66	P	118	SER
66	P	173	ARG
67	U	146	GLY
69	E	125	GLN
69	E	344	SER
71	6	76	GLU
72	7	287	GLN
73	9	27	PRO
74	a	104	GLU
76	d	82	ALA
76	d	289	PRO
76	d	290	GLU
81	p	72	ILE
83	Q	67	ARG
83	Q	229	TRP
86	v	104	SER
86	v	151	VAL
86	v	217	LEU
86	v	262	GLU

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Mol	Chain	Res	Type
86	v	549	TYR
86	v	559	LEU
86	v	567	LEU
7	AK	63	LEU
13	AT	105	ILE
14	AW	144	LEU
15	AX	339	PRO
26	A0	54	ALA
26	A0	181	ASN
28	A4	488	PRO
35	F	128	TRP
35	F	283	LEU
43	T	94	ILE
46	Y	183	GLN
48	0	116	LEU
51	3	95	THR
54	b	117	LYS
86	v	42	PRO
20	AS	129	GLY
28	A4	365	ILE
31	AG	210	VAL
35	F	124	GLY
60	o	61	GLY
83	Q	228	PRO
11	AP	56	ASN
15	AX	338	ASP
18	AL	114	ILE
22	AV	176	PRO
56	g	36	PRO
70	5	286	PRO
28	A4	606	PRO
29	AD	195	GLY
34	D	98	GLY
34	D	207	ILE
41	R	138	PRO
63	J	36	GLY
83	Q	215	VAL
86	v	46	ILE
2	AB	202	ILE
3	AC	114	GLY
8	AM	62	GLY
23	AY	314	PRO

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Mol	Chain	Res	Type
26	A0	75	GLY
62	r	140	VAL
62	r	156	PRO
71	6	79	GLY
81	p	173	VAL
82	s	130	GLU
9	AN	85	VAL
63	J	32	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	193/249 (78%)	191 (99%)	2 (1%)	68	83
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AE	104/107 (97%)	103 (99%)	1 (1%)	68	83
5	AI	104/147 (71%)	102 (98%)	2 (2%)	50	75
6	AJ	93/118 (79%)	93 (100%)	0	100	100
7	AK	91/113 (80%)	91 (100%)	0	100	100
8	AM	95/113 (84%)	94 (99%)	1 (1%)	65	82
9	AN	93/115 (81%)	92 (99%)	1 (1%)	65	82
10	AO	171/230 (74%)	170 (99%)	1 (1%)	78	88
11	AP	87/123 (71%)	86 (99%)	1 (1%)	65	82
12	AQ	78/79 (99%)	78 (100%)	0	100	100
13	AT	153/157 (98%)	152 (99%)	1 (1%)	76	87
14	AW	84/158 (53%)	84 (100%)	0	100	100
15	AX	312/351 (89%)	311 (100%)	1 (0%)	86	91
16	A2	99/101 (98%)	97 (98%)	2 (2%)	48	75
17	AH	112/180 (62%)	111 (99%)	1 (1%)	70	85
18	AL	157/226 (70%)	156 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AR	262/318 (82%)	260 (99%)	2 (1%)	73	86
20	AS	116/164 (71%)	114 (98%)	2 (2%)	53	77
21	AU	153/174 (88%)	153 (100%)	0	100	100
22	AV	328/364 (90%)	324 (99%)	4 (1%)	63	82
23	AY	111/357 (31%)	110 (99%)	1 (1%)	70	85
24	AZ	89/95 (94%)	89 (100%)	0	100	100
25	A1	253/291 (87%)	253 (100%)	0	100	100
26	A0	186/190 (98%)	186 (100%)	0	100	100
27	A3	66/166 (40%)	64 (97%)	2 (3%)	36	67
28	A4	83/609 (14%)	83 (100%)	0	100	100
29	AD	286/357 (80%)	286 (100%)	0	100	100
30	AF	185/209 (88%)	181 (98%)	4 (2%)	45	73
31	AG	273/342 (80%)	272 (100%)	1 (0%)	84	90
34	D	193/245 (79%)	193 (100%)	0	100	100
35	F	217/262 (83%)	215 (99%)	2 (1%)	70	85
36	H	88/228 (39%)	88 (100%)	0	100	100
37	K	155/156 (99%)	155 (100%)	0	100	100
38	L	98/124 (79%)	97 (99%)	1 (1%)	68	83
39	M	245/249 (98%)	245 (100%)	0	100	100
40	O	133/150 (89%)	132 (99%)	1 (1%)	73	86
41	R	118/126 (94%)	117 (99%)	1 (1%)	73	86
42	S	141/180 (78%)	141 (100%)	0	100	100
43	T	146/182 (80%)	145 (99%)	1 (1%)	76	87
44	W	91/119 (76%)	91 (100%)	0	100	100
45	X	217/227 (96%)	212 (98%)	5 (2%)	44	72
46	Y	159/223 (71%)	157 (99%)	2 (1%)	61	81
47	Z	111/147 (76%)	111 (100%)	0	100	100
48	0	97/164 (59%)	97 (100%)	0	100	100
49	1	49/60 (82%)	48 (98%)	1 (2%)	48	75
50	2	40/72 (56%)	39 (98%)	1 (2%)	42	71
51	3	88/166 (53%)	86 (98%)	2 (2%)	44	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	4	37/89 (42%)	37 (100%)	0	100	100
53	8	91/190 (48%)	91 (100%)	0	100	100
54	b	130/135 (96%)	130 (100%)	0	100	100
55	e	188/236 (80%)	186 (99%)	2 (1%)	65	82
56	g	122/148 (82%)	119 (98%)	3 (2%)	42	71
57	i	86/110 (78%)	84 (98%)	2 (2%)	44	72
58	j	74/97 (76%)	74 (100%)	0	100	100
59	m	40/113 (35%)	40 (100%)	0	100	100
60	o	80/87 (92%)	79 (99%)	1 (1%)	61	81
61	q	114/178 (64%)	113 (99%)	1 (1%)	70	85
62	r	147/169 (87%)	146 (99%)	1 (1%)	76	87
63	J	138/150 (92%)	135 (98%)	3 (2%)	45	73
64	I	164/232 (71%)	160 (98%)	4 (2%)	43	72
65	N	189/211 (90%)	188 (100%)	1 (0%)	81	89
66	P	125/154 (81%)	124 (99%)	1 (1%)	73	86
67	U	126/135 (93%)	125 (99%)	1 (1%)	73	86
68	V	184/191 (96%)	182 (99%)	2 (1%)	65	82
69	E	260/290 (90%)	259 (100%)	1 (0%)	84	90
70	5	353/368 (96%)	350 (99%)	3 (1%)	73	86
71	6	313/332 (94%)	308 (98%)	5 (2%)	55	78
72	7	272/303 (90%)	272 (100%)	0	100	100
73	9	104/112 (93%)	103 (99%)	1 (1%)	68	83
74	a	101/133 (76%)	101 (100%)	0	100	100
75	c	253/288 (88%)	253 (100%)	0	100	100
76	d	224/274 (82%)	220 (98%)	4 (2%)	51	76
77	f	122/173 (70%)	122 (100%)	0	100	100
78	h	104/148 (70%)	103 (99%)	1 (1%)	68	83
79	k	81/90 (90%)	79 (98%)	2 (2%)	42	71
80	l	67/116 (58%)	67 (100%)	0	100	100
81	p	134/181 (74%)	131 (98%)	3 (2%)	45	73
82	s	336/381 (88%)	335 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	Q	221/256 (86%)	220 (100%)	1 (0%)	81	89
84	TA	39/158 (25%)	39 (100%)	0	100	100
84	TB	26/158 (16%)	26 (100%)	0	100	100
86	v	598/630 (95%)	576 (96%)	22 (4%)	30	62
All	All	12561/16442 (76%)	12447 (99%)	114 (1%)	68	85

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	186	THR
2	AB	236	VAL
4	AE	88	VAL
5	AI	81	GLU
5	AI	181	ILE
8	AM	69	ASN
9	AN	77	VAL
10	AO	115	VAL
11	AP	123	THR
13	AT	153	VAL
15	AX	217	GLU
16	A2	71	GLN
16	A2	104	LEU
17	AH	175	THR
18	AL	72	LEU
19	AR	136	VAL
19	AR	337	GLN
20	AS	67	GLU
20	AS	120	GLU
22	AV	52	ASP
22	AV	135	TYR
22	AV	161	LEU
22	AV	338	HIS
23	AY	310	LEU
27	A3	190	GLN
27	A3	191	THR
30	AF	39	PRO
30	AF	64	TYR
30	AF	71	THR
30	AF	72	GLN
31	AG	210	VAL
35	F	77	VAL

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Mol	Chain	Res	Type
35	F	262	THR
38	L	36	THR
40	O	14	VAL
41	R	95	VAL
43	T	211	THR
45	X	55	LYS
45	X	124	THR
45	X	126	THR
45	X	179	GLU
45	X	243	LEU
46	Y	77	GLU
46	Y	205	VAL
49	1	58	GLU
50	2	70	LEU
51	3	173	VAL
51	3	188	VAL
55	e	260	LEU
55	e	265	LYS
56	g	36	PRO
56	g	66	TYR
56	g	77	ASP
57	i	44	VAL
57	i	98	VAL
60	o	93	ASP
61	q	82	LEU
62	r	146	GLN
63	J	126	GLN
63	J	135	VAL
63	J	191	LYS
64	I	34	THR
64	I	98	VAL
64	I	104	LEU
64	I	158	GLU
65	N	59	VAL
66	P	72	PHE
67	U	6	VAL
68	V	45	VAL
68	V	193	THR
69	E	118	VAL
70	5	46	LEU
70	5	69	TRP
70	5	70	LEU

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Mol	Chain	Res	Type
71	6	168	VAL
71	6	171	VAL
71	6	187	VAL
71	6	204	VAL
71	6	288	SER
73	9	57	VAL
76	d	186	VAL
76	d	205	GLN
76	d	238	VAL
76	d	266	VAL
78	h	117	LEU
79	k	11	ARG
79	k	75	ILE
81	p	61	VAL
81	p	95	VAL
81	p	194	HIS
82	s	206	VAL
83	Q	55	GLN
86	v	72	ARG
86	v	85	VAL
86	v	88	VAL
86	v	102	ILE
86	v	124	HIS
86	v	125	VAL
86	v	129	ILE
86	v	145	LEU
86	v	170	LEU
86	v	200	PHE
86	v	208	GLU
86	v	264	LEU
86	v	328	ILE
86	v	338	LYS
86	v	393	VAL
86	v	446	VAL
86	v	489	LYS
86	v	491	THR
86	v	492	VAL
86	v	533	VAL
86	v	619	VAL
86	v	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (262) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	69	HIS
2	AB	134	HIS
2	AB	157	ASN
2	AB	201	ASN
2	AB	266	GLN
3	AC	75	ASN
3	AC	156	GLN
4	AE	14	GLN
4	AE	92	ASN
5	AI	87	HIS
6	AJ	105	HIS
8	AM	75	HIS
9	AN	56	GLN
10	AO	65	GLN
10	AO	103	ASN
10	AO	155	GLN
11	AP	115	GLN
12	AQ	53	GLN
12	AQ	65	ASN
13	AT	14	GLN
13	AT	33	ASN
13	AT	51	ASN
13	AT	59	ASN
14	AW	91	GLN
14	AW	106	HIS
14	AW	135	GLN
15	AX	59	HIS
15	AX	81	HIS
15	AX	90	GLN
15	AX	164	ASN
15	AX	180	GLN
15	AX	299	ASN
15	AX	326	GLN
15	AX	387	ASN
16	A2	15	ASN
16	A2	71	GLN
16	A2	90	GLN
16	A2	105	ASN
17	AH	179	GLN
19	AR	86	ASN
19	AR	288	GLN
19	AR	305	HIS
19	AR	315	GLN

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Mol	Chain	Res	Type
19	AR	337	GLN
19	AR	356	HIS
21	AU	147	GLN
21	AU	151	GLN
21	AU	159	GLN
21	AU	161	GLN
21	AU	201	GLN
22	AV	78	ASN
22	AV	87	HIS
22	AV	100	ASN
22	AV	134	GLN
22	AV	156	ASN
22	AV	261	GLN
22	AV	316	GLN
22	AV	342	GLN
22	AV	381	GLN
22	AV	388	GLN
24	AZ	63	GLN
24	AZ	76	GLN
25	A1	64	GLN
25	A1	261	ASN
25	A1	268	GLN
25	A1	301	ASN
26	A0	192	ASN
27	A3	129	ASN
27	A3	190	GLN
28	A4	72	GLN
28	A4	79	ASN
28	A4	122	ASN
28	A4	136	HIS
29	AD	145	ASN
29	AD	227	ASN
29	AD	278	HIS
29	AD	292	HIS
29	AD	356	GLN
29	AD	360	GLN
29	AD	361	GLN
30	AF	72	GLN
30	AF	103	ASN
30	AF	113	GLN
30	AF	197	GLN
30	AF	216	GLN

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Mol	Chain	Res	Type
31	AG	87	HIS
31	AG	101	GLN
31	AG	139	GLN
31	AG	265	GLN
31	AG	301	GLN
31	AG	308	GLN
31	AG	318	HIS
34	D	128	GLN
34	D	165	ASN
34	D	195	ASN
34	D	205	GLN
34	D	235	GLN
35	F	58	HIS
35	F	74	GLN
35	F	103	GLN
35	F	208	HIS
35	F	223	HIS
36	H	77	HIS
36	H	126	GLN
36	H	148	GLN
37	K	26	GLN
37	K	48	HIS
37	K	94	GLN
38	L	72	GLN
38	L	80	GLN
38	L	104	ASN
38	L	142	GLN
39	M	264	GLN
39	M	276	ASN
40	O	141	HIS
40	O	146	ASN
41	R	125	HIS
42	S	84	ASN
42	S	140	ASN
43	T	79	GLN
43	T	151	GLN
43	T	201	GLN
43	T	210	HIS
44	W	80	HIS
45	X	215	GLN
45	X	236	GLN
45	X	240	GLN

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Mol	Chain	Res	Type
46	Y	88	GLN
46	Y	89	GLN
46	Y	92	ASN
46	Y	117	GLN
46	Y	157	GLN
46	Y	183	GLN
47	Z	47	GLN
47	Z	98	GLN
47	Z	102	ASN
48	0	106	ASN
48	0	170	GLN
49	1	31	ASN
51	3	154	GLN
53	8	144	GLN
54	b	24	GLN
54	b	90	HIS
54	b	102	GLN
55	e	54	GLN
55	e	126	GLN
55	e	175	GLN
55	e	179	GLN
55	e	212	HIS
55	e	245	GLN
56	g	73	GLN
57	i	65	ASN
57	i	89	GLN
57	i	120	HIS
57	i	124	HIS
58	j	30	GLN
58	j	63	GLN
60	o	85	HIS
60	o	91	GLN
60	o	94	HIS
60	o	96	ASN
61	q	81	GLN
61	q	112	GLN
61	q	139	GLN
61	q	142	ASN
61	q	157	GLN
62	r	65	ASN
62	r	69	GLN
62	r	146	GLN

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Mol	Chain	Res	Type
62	r	184	ASN
63	J	103	GLN
63	J	116	HIS
63	J	126	GLN
63	J	133	GLN
64	I	91	GLN
64	I	115	GLN
64	I	150	HIS
64	I	193	ASN
65	N	110	ASN
65	N	181	HIS
67	U	98	GLN
68	V	92	ASN
69	E	52	HIS
69	E	125	GLN
69	E	137	ASN
69	E	227	GLN
69	E	294	ASN
70	5	165	GLN
70	5	186	GLN
70	5	191	GLN
70	5	221	GLN
70	5	269	ASN
70	5	302	HIS
70	5	343	GLN
70	5	360	ASN
70	5	385	HIS
70	5	420	HIS
71	6	101	GLN
71	6	111	GLN
71	6	320	GLN
71	6	332	HIS
71	6	354	GLN
72	7	45	ASN
72	7	69	HIS
72	7	139	ASN
72	7	165	ASN
72	7	198	ASN
72	7	231	GLN
72	7	284	HIS
72	7	285	ASN
73	9	113	ASN

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Mol	Chain	Res	Type
74	a	44	ASN
74	a	62	HIS
75	c	48	GLN
75	c	77	HIS
75	c	94	ASN
75	c	155	ASN
75	c	193	GLN
75	c	204	GLN
75	c	315	ASN
76	d	77	HIS
76	d	119	GLN
76	d	161	HIS
76	d	205	GLN
76	d	286	GLN
77	f	136	GLN
77	f	158	GLN
79	k	35	GLN
79	k	93	HIS
80	l	124	GLN
80	l	125	ASN
80	l	129	HIS
81	p	53	GLN
81	p	123	HIS
81	p	146	ASN
81	p	194	HIS
82	s	152	GLN
82	s	154	HIS
82	s	207	HIS
82	s	238	ASN
82	s	239	ASN
82	s	240	GLN
82	s	300	HIS
82	s	391	ASN
82	s	397	GLN
82	s	423	HIS
83	Q	55	GLN
83	Q	158	GLN
83	Q	172	GLN
83	Q	213	GLN
83	Q	262	GLN
86	v	43	ASN
86	v	54	HIS

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Mol	Chain	Res	Type
86	v	124	HIS
86	v	188	GLN
86	v	324	GLN
86	v	349	ASN
86	v	367	GLN
86	v	548	GLN
86	v	616	HIS
86	v	622	ASN
86	v	636	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	940/954 (98%)	191 (20%)	7 (0%)
32	A	1523/1559 (97%)	347 (22%)	18 (1%)
33	B	51/73 (69%)	6 (11%)	1 (1%)
All	All	2514/2586 (97%)	544 (21%)	26 (1%)

All (544) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	650	U
1	AA	651	A
1	AA	674	U
1	AA	676	G
1	AA	680	U
1	AA	688	A
1	AA	690	U
1	AA	691	A
1	AA	704	U
1	AA	711	U
1	AA	718	A
1	AA	721	U
1	AA	732	A
1	AA	745	A
1	AA	753	A
1	AA	761	A
1	AA	764	A
1	AA	766	G
1	AA	781	A
1	AA	782	A

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Mol	Chain	Res	Type
1	AA	791	G
1	AA	795	A
1	AA	796	G
1	AA	807	A
1	AA	814	A
1	AA	827	A
1	AA	828	C
1	AA	830	U
1	AA	831	U
1	AA	832	U
1	AA	835	C
1	AA	837	A
1	AA	846	A
1	AA	847	G
1	AA	856	A
1	AA	860	A
1	AA	868	C
1	AA	870	C
1	AA	872	G
1	AA	883	U
1	AA	890	C
1	AA	891	C
1	AA	899	G
1	AA	903	U
1	AA	907	A
1	AA	919	A
1	AA	921	U
1	AA	930	G
1	AA	931	C
1	AA	933	G
1	AA	938	A
1	AA	939	A
1	AA	942	A
1	AA	948	U
1	AA	950	A
1	AA	954	C
1	AA	956	C
1	AA	965	C
1	AA	966	A
1	AA	967	A
1	AA	992	U
1	AA	993	A

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Mol	Chain	Res	Type
1	AA	1001	C
1	AA	1011	C
1	AA	1014	A
1	AA	1015	A
1	AA	1022	A
1	AA	1042	U
1	AA	1046	A
1	AA	1065	C
1	AA	1069	A
1	AA	1081	U
1	AA	1082	A
1	AA	1105	C
1	AA	1109	A
1	AA	1117	A
1	AA	1118	A
1	AA	1119	U
1	AA	1120	C
1	AA	1121	A
1	AA	1126	A
1	AA	1138	G
1	AA	1143	C
1	AA	1151	C
1	AA	1152	A
1	AA	1154	A
1	AA	1167	A
1	AA	1187	U
1	AA	1188	A
1	AA	1189	U
1	AA	1190	C
1	AA	1193	U
1	AA	1199	G
1	AA	1215	U
1	AA	1220	A
1	AA	1223	C
1	AA	1225	C
1	AA	1234	C
1	AA	1235	U
1	AA	1246	U
1	AA	1247	G
1	AA	1248	C
1	AA	1249	U
1	AA	1250	C

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Mol	Chain	Res	Type
1	AA	1255	U
1	AA	1259	U
1	AA	1270	U
1	AA	1271	C
1	AA	1272	A
1	AA	1273	G
1	AA	1283	A
1	AA	1284	U
1	AA	1285	G
1	AA	1290	C
1	AA	1292	A
1	AA	1295	A
1	AA	1296	A
1	AA	1300	A
1	AA	1301	G
1	AA	1311	C
1	AA	1312	C
1	AA	1326	A
1	AA	1327	G
1	AA	1328	G
1	AA	1331	A
1	AA	1332	A
1	AA	1333	G
1	AA	1342	C
1	AA	1343	A
1	AA	1353	A
1	AA	1354	A
1	AA	1355	G
1	AA	1356	A
1	AA	1357	A
1	AA	1365	A
1	AA	1367	A
1	AA	1369	U
1	AA	1374	A
1	AA	1376	C
1	AA	1377	C
1	AA	1378	C
1	AA	1379	A
1	AA	1383	A
1	AA	1389	G
1	AA	1392	A
1	AA	1405	C

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Mol	Chain	Res	Type
1	AA	1406	U
1	AA	1407	U
1	AA	1408	A
1	AA	1418	G
1	AA	1419	G
1	AA	1420	U
1	AA	1421	G
1	AA	1422	G
1	AA	1425	U
1	AA	1430	A
1	AA	1446	A
1	AA	1447	G
1	AA	1449	G
1	AA	1478	A
1	AA	1481	C
1	AA	1482	A
1	AA	1502	A
1	AA	1505	A
1	AA	1512	A
1	AA	1513	A
1	AA	1514	A
1	AA	1518	C
1	AA	1519	A
1	AA	1522	U
1	AA	1523	A
1	AA	1525	C
1	AA	1526	U
1	AA	1527	A
1	AA	1533	C
1	AA	1534	C
1	AA	1535	U
1	AA	1536	A
1	AA	1537	C
1	AA	1539	C
1	AA	1540	A
1	AA	1548	A
1	AA	1558	A
1	AA	1562	G
1	AA	1564	A
1	AA	1568	U
1	AA	1582	G
1	AA	1594	G

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Mol	Chain	Res	Type
1	AA	1595	G
1	AA	1599	A
1	AA	1600	A
32	A	1678	C
32	A	1679	U
32	A	1680	A
32	A	1681	G
32	A	1689	C
32	A	1690	C
32	A	1700	U
32	A	1702	A
32	A	1704	U
32	A	1708	A
32	A	1709	G
32	A	1711	C
32	A	1713	A
32	A	1714	C
32	A	1715	C
32	A	1716	U
32	A	1717	U
32	A	1724	A
32	A	1727	A
32	A	1728	U
32	A	1734	C
32	A	1735	A
32	A	1736	A
32	A	1748	G
32	A	1750	G
32	A	1751	A
32	A	1762	A
32	A	1763	A
32	A	1766	U
32	A	1767	G
32	A	1770	G
32	A	1777	A
32	A	1781	A
32	A	1782	G
32	A	1794	A
32	A	1800	G
32	A	1806	U
32	A	1807	U
32	A	1808	A

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Mol	Chain	Res	Type
32	A	1809	U
32	A	1810	A
32	A	1817	C
32	A	1823	A
32	A	1824	U
32	A	1827	C
32	A	1828	A
32	A	1832	A
32	A	1833	C
32	A	1836	A
32	A	1839	C
32	A	1840	C
32	A	1844	A
32	A	1849	C
32	A	1853	A
32	A	1854	U
32	A	1855	A
32	A	1856	A
32	A	1867	A
32	A	1869	A
32	A	1872	U
32	A	1882	A
32	A	1883	G
32	A	1893	A
32	A	1901	C
32	A	1903	C
32	A	1917	A
32	A	1918	G
32	A	1935	A
32	A	1936	A
32	A	1937	A
32	A	1938	A
32	A	1940	A
32	A	1944	C
32	A	1958	G
32	A	1965	A
32	A	1968	G
32	A	1985	G
32	A	1987	G
32	A	1992	C
32	A	1994	A
32	A	1995	A

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Mol	Chain	Res	Type
32	A	2000	C
32	A	2001	C
32	A	2002	G
32	A	2011	G
32	A	2015	G
32	A	2016	C
32	A	2021	U
32	A	2022	G
32	A	2031	A
32	A	2036	C
32	A	2037	U
32	A	2039	A
32	A	2040	G
32	A	2060	A
32	A	2065	A
32	A	2066	C
32	A	2067	C
32	A	2069	U
32	A	2079	C
32	A	2083	U
32	A	2092	C
32	A	2093	U
32	A	2097	A
32	A	2098	G
32	A	2111	C
32	A	2113	G
32	A	2125	C
32	A	2126	U
32	A	2132	A
32	A	2136	C
32	A	2142	A
32	A	2154	A
32	A	2158	U
32	A	2166	C
32	A	2168	U
32	A	2171	U
32	A	2172	A
32	A	2173	G
32	A	2180	A
32	A	2181	A
32	A	2183	C
32	A	2184	A

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Mol	Chain	Res	Type
32	A	2187	C
32	A	2190	C
32	A	2193	U
32	A	2194	U
32	A	2198	A
32	A	2199	A
32	A	2201	G
32	A	2203	G
32	A	2205	U
32	A	2210	C
32	A	2215	C
32	A	2217	C
32	A	2218	C
32	A	2219	C
32	A	2220	A
32	A	2222	U
32	A	2224	C
32	A	2228	A
32	A	2229	A
32	A	2230	A
32	A	2235	C
32	A	2237	A
32	A	2241	A
32	A	2245	A
32	A	2246	A
32	A	2250	A
32	A	2252	C
32	A	2256	U
32	A	2262	C
32	A	2263	C
32	A	2264	A
32	A	2283	C
32	A	2284	C
32	A	2297	A
32	A	2300	G
32	A	2315	A
32	A	2322	C
32	A	2331	C
32	A	2332	C
32	A	2343	G
32	A	2345	G
32	A	2350	A

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Mol	Chain	Res	Type
32	A	2351	U
32	A	2356	A
32	A	2357	C
32	A	2360	U
32	A	2361	G
32	A	2362	A
32	A	2364	C
32	A	2365	U
32	A	2371	U
32	A	2374	A
32	A	2379	C
32	A	2381	A
32	A	2390	A
32	A	2393	C
32	A	2396	C
32	A	2404	U
32	A	2407	U
32	A	2414	C
32	A	2415	C
32	A	2434	A
32	A	2443	C
32	A	2444	A
32	A	2447	A
32	A	2449	G
32	A	2458	A
32	A	2471	G
32	A	2478	G
32	A	2482	A
32	A	2484	C
32	A	2493	C
32	A	2507	A
32	A	2508	C
32	A	2511	C
32	A	2520	C
32	A	2521	A
32	A	2522	U
32	A	2524	A
32	A	2527	A
32	A	2530	A
32	A	2531	U
32	A	2532	U
32	A	2540	C

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Mol	Chain	Res	Type
32	A	2546	G
32	A	2549	C
32	A	2557	C
32	A	2558	A
32	A	2559	U
32	A	2560	G
32	A	2570	C
32	A	2575	U
32	A	2578	C
32	A	2581	A
32	A	2592	G
32	A	2593	G
32	A	2594	U
32	A	2601	A
32	A	2607	U
32	A	2618	U
32	A	2619	A
32	A	2625	C
32	A	2626	U
32	A	2627	G
32	A	2629	A
32	A	2630	U
32	A	2632	A
32	A	2633	A
32	A	2634	U
32	A	2635	G
32	A	2638	U
32	A	2645	G
32	A	2654	U
32	A	2655	G
32	A	2656	U
32	A	2660	U
32	A	2683	C
32	A	2686	G
32	A	2694	A
32	A	2696	A
32	A	2706	A
32	A	2712	G
32	A	2714	A
32	A	2715	A
32	A	2718	C
32	A	2719	G

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Mol	Chain	Res	Type
32	A	2723	A
32	A	2724	G
32	A	2725	A
32	A	2732	G
32	A	2739	U
32	A	2740	A
32	A	2749	A
32	A	2750	U
32	A	2755	A
32	A	2756	C
32	A	2757	A
32	A	2758	G
32	A	2760	A
32	A	2803	A
32	A	2804	A
32	A	2805	A
32	A	2810	G
32	A	2814	G
32	A	2831	G
32	A	2832	A
32	A	2833	A
32	A	2843	C
32	A	2844	G
32	A	2847	C
32	A	2849	G
32	A	2854	U
32	A	2864	U
32	A	2865	C
32	A	2879	A
32	A	2881	C
32	A	2893	A
32	A	2906	C
32	A	2910	A
32	A	2912	C
32	A	2913	A
32	A	2917	G
32	A	2918	A
32	A	2926	A
32	A	2928	C
32	A	2935	A
32	A	2946	A
32	A	2963	A

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Mol	Chain	Res	Type
32	A	2965	A
32	A	2977	G
32	A	2978	U
32	A	2984	A
32	A	2985	C
32	A	2989	G
32	A	2990	A
32	A	2992	G
32	A	2994	U
32	A	3000	A
32	A	3005	A
32	A	3007	C
32	A	3016	G
32	A	3022	G
32	A	3042	U
32	A	3043	C
32	A	3053	A
32	A	3054	G
32	A	3060	C
32	A	3068	G
32	A	3069	A
32	A	3070	G
32	A	3072	U
32	A	3093	C
32	A	3096	U
32	A	3098	U
32	A	3100	U
32	A	3109	U
32	A	3113	A
32	A	3123	G
32	A	3129	A
32	A	3135	A
32	A	3150	U
32	A	3152	C
32	A	3155	C
32	A	3158	A
32	A	3168	C
32	A	3169	C
32	A	3172	C
32	A	3180	A
32	A	3182	A
32	A	3184	C

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Mol	Chain	Res	Type
32	A	3189	C
32	A	3190	A
32	A	3197	U
32	A	3200	U
32	A	3201	A
32	A	3204	C
32	A	3207	A
32	A	3208	C
32	A	3210	C
32	A	3211	C
32	A	3212	C
32	A	3217	A
32	A	3218	A
32	A	3228	U
33	B	1608	G
33	B	1611	G
33	B	1614	U
33	B	1615	A
33	B	1644	G
33	B	1645	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	717	G
1	AA	947	U
1	AA	953	U
1	AA	1021	U
1	AA	1246	U
1	AA	1406	U
1	AA	1429	C
32	A	1703	C
32	A	1805	A
32	A	1806	U
32	A	1807	U
32	A	1823	A
32	A	1871	A
32	A	1994	A
32	A	2165	C
32	A	2182	G
32	A	2245	A
32	A	2457	A

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Mol	Chain	Res	Type
32	A	2507	A
32	A	2559	U
32	A	2905	A
32	A	2989	G
32	A	3041	U
32	A	3092	U
32	A	3196	G
33	B	1607	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	P5P	A7	18	88	20,23,24	1.00	3 (15%)	27,33,36	2.04	4 (14%)
88	P5P	A7	20	88	20,23,24	0.98	3 (15%)	27,33,36	2.01	5 (18%)
87	P5P	A5	6	87	20,23,24	1.05	3 (15%)	27,33,36	2.03	5 (18%)
88	P5P	A7	14	88	20,23,24	1.01	2 (10%)	27,33,36	1.99	3 (11%)
87	Y5P	A5	4	87	14,19,20	4.80	2 (14%)	18,26,29	1.83	3 (16%)
88	P5P	A7	15	88	20,23,24	1.06	3 (15%)	27,33,36	1.99	5 (18%)
88	Y5P	A7	25	88	14,19,20	4.33	2 (14%)	18,26,29	1.39	3 (16%)
88	P5P	A7	27	88	20,23,24	0.99	2 (10%)	27,33,36	2.08	4 (14%)
88	P5P	A7	52	88	20,23,24	1.13	3 (15%)	27,33,36	1.97	5 (18%)
88	Y5P	A7	53	88	14,19,20	4.65	2 (14%)	18,26,29	1.55	3 (16%)
88	Y5P	A7	55	88	14,19,20	4.46	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	66	88	14,19,20	4.60	2 (14%)	18,26,29	1.48	2 (11%)
88	Y5P	A7	9	88	14,19,20	4.65	2 (14%)	18,26,29	1.78	3 (16%)
88	Y5P	A7	61	88	14,19,20	4.46	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A7	21	88	14,19,20	4.38	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	70	88	14,19,20	4.48	2 (14%)	18,26,29	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	P5P	A7	6	88	20,23,24	1.02	3 (15%)	27,33,36	2.10	5 (18%)
88	Y5P	A7	59	88	14,19,20	4.76	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A7	58	88	14,19,20	4.57	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	24	88	14,19,20	4.17	2 (14%)	18,26,29	1.36	2 (11%)
87	Y5P	A5	8	87	14,19,20	4.66	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A7	42	88	20,23,24	0.97	3 (15%)	27,33,36	2.03	4 (14%)
88	Y5P	A7	44	88	14,19,20	4.69	2 (14%)	18,26,29	1.45	2 (11%)
88	Y5P	A7	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.41	3 (16%)
88	P5P	A7	10	88	20,23,24	0.99	2 (10%)	27,33,36	1.98	4 (14%)
87	P5P	A5	5	87	20,23,24	1.07	3 (15%)	27,33,36	1.97	4 (14%)
87	Y5P	A5	7	87	14,19,20	4.60	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	40	88	20,23,24	1.00	3 (15%)	27,33,36	2.05	5 (18%)
88	P5P	A7	1	88	20,20,24	0.97	1 (5%)	28,29,36	1.95	4 (14%)
88	Y5P	A7	56	88	14,19,20	4.55	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	46	88	14,19,20	4.53	2 (14%)	18,26,29	1.49	3 (16%)
87	P5P	A5	2	87	20,23,24	1.10	2 (10%)	27,33,36	1.98	4 (14%)
88	P5P	A7	26	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	P5P	A7	16	88	20,23,24	1.08	3 (15%)	27,33,36	2.14	6 (22%)
88	P5P	A7	45	88	20,23,24	1.05	2 (10%)	27,33,36	2.15	4 (14%)
88	Y5P	A7	47	88	14,19,20	4.57	2 (14%)	18,26,29	1.52	3 (16%)
87	P5P	A5	9	87	20,23,24	1.01	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	22	88	14,19,20	4.28	2 (14%)	18,26,29	1.42	3 (16%)
88	P5P	A7	41	88	20,23,24	1.04	3 (15%)	27,33,36	1.94	5 (18%)
88	P5P	A7	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.08	5 (18%)
88	Y5P	A7	50	88	14,19,20	4.53	2 (14%)	18,26,29	1.39	2 (11%)
88	P5P	A7	54	88	20,23,24	1.08	3 (15%)	27,33,36	1.93	3 (11%)
88	Y5P	A7	68	88	14,19,20	4.73	2 (14%)	18,26,29	1.69	4 (22%)
88	P5P	A7	43	88	20,23,24	1.11	2 (10%)	27,33,36	2.08	4 (14%)
88	Y5P	A7	63	88	14,19,20	4.55	2 (14%)	18,26,29	1.49	3 (16%)
88	P5P	A7	11	88	20,23,24	0.98	3 (15%)	27,33,36	2.09	5 (18%)
88	Y5P	A7	51	88	14,19,20	4.35	2 (14%)	18,26,29	1.44	3 (16%)
88	P5P	A7	5	88	20,23,24	1.00	2 (10%)	27,33,36	2.02	4 (14%)
88	P5P	A7	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	Y5P	A7	12	88	14,19,20	4.28	2 (14%)	18,26,29	1.39	3 (16%)
87	Y5P	A5	3	87	14,19,20	4.47	2 (14%)	18,26,29	1.63	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	P5P	A7	4	88	20,23,24	1.07	3 (15%)	27,33,36	2.13	5 (18%)
88	P5P	A7	23	88	20,23,24	1.03	3 (15%)	27,33,36	1.92	4 (14%)
88	P5P	A7	71	32,88	20,23,24	0.96	3 (15%)	27,33,36	1.91	3 (11%)
87	Y5P	A5	10	87	14,19,20	4.50	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A7	2	88	20,23,24	1.02	2 (10%)	27,33,36	2.12	4 (14%)
88	Y5P	A7	17	88	14,19,20	4.60	2 (14%)	18,26,29	1.42	2 (11%)
87	Y5P	A5	1	87	14,19,20	4.81	2 (14%)	18,26,29	1.85	3 (16%)
88	Y5P	A7	3	88	14,19,20	4.38	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	65	88	14,19,20	4.62	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A7	67	88	14,19,20	4.64	2 (14%)	18,26,29	1.61	3 (16%)
88	P5P	A7	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.05	5 (18%)
88	Y5P	A7	60	88	14,19,20	4.45	2 (14%)	18,26,29	1.57	2 (11%)
88	Y5P	A7	13	88	14,19,20	4.19	2 (14%)	18,26,29	1.28	2 (11%)
88	Y5P	A7	38	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A7	64	88	14,19,20	4.52	2 (14%)	18,26,29	1.35	2 (11%)
88	Y5P	A7	69	88	14,19,20	4.64	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A7	19	88	20,23,24	1.04	3 (15%)	27,33,36	2.15	5 (18%)
88	Y5P	A7	57	88	14,19,20	4.47	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	62	88	14,19,20	4.41	2 (14%)	18,26,29	1.49	3 (16%)
88	P5P	A7	7	88	20,23,24	0.97	2 (10%)	27,33,36	2.07	4 (14%)
88	Y5P	A7	8	88	14,19,20	4.65	2 (14%)	18,26,29	1.41	3 (16%)
87	P5P	A5	11	87	20,23,24	1.01	3 (15%)	27,33,36	1.97	5 (18%)

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
88	P5P	A7	18	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	20	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	6	87	-	0/7/25/26	0/3/3/3
88	P5P	A7	14	88	-	2/7/25/26	0/3/3/3
87	Y5P	A5	4	87	-	7/7/33/34	0/2/2/2
88	P5P	A7	15	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	25	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	27	88	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	P5P	A7	52	88	-	6/7/25/26	0/3/3/3
88	Y5P	A7	53	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	55	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	9	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	61	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	21	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	6	88	-	4/7/25/26	0/3/3/3
88	Y5P	A7	59	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	58	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	24	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	8	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	42	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	44	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	37	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	10	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	5	87	-	2/7/25/26	0/3/3/3
87	Y5P	A5	7	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	40	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	1	88	-	0/6/22/26	0/3/3/3
88	Y5P	A7	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	46	88	-	3/7/33/34	0/2/2/2
87	P5P	A5	2	87	-	2/7/25/26	0/3/3/3
88	P5P	A7	26	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	16	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	45	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	47	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	9	87	-	0/7/25/26	0/3/3/3
88	Y5P	A7	22	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	41	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	48	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	50	88	-	4/7/33/34	0/2/2/2
88	P5P	A7	54	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	68	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	43	88	-	5/7/25/26	0/3/3/3
88	Y5P	A7	63	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	11	88	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	51	88	-	2/7/33/34	0/2/2/2
88	P5P	A7	5	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	39	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	12	88	-	3/7/33/34	0/2/2/2
87	Y5P	A5	3	87	-	4/7/33/34	0/2/2/2
88	P5P	A7	4	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	71	32,88	-	1/7/25/26	0/3/3/3
87	Y5P	A5	10	87	-	1/7/33/34	0/2/2/2
88	P5P	A7	2	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	17	88	-	2/7/33/34	0/2/2/2
87	Y5P	A5	1	87	-	7/7/33/34	0/2/2/2
88	Y5P	A7	3	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	65	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	49	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	60	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	13	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	38	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	64	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	69	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	19	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	57	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	62	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A7	8	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	11	87	-	0/7/25/26	0/3/3/3

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	53	Y5P	C4-N3	-13.51	1.33	1.46
88	A7	67	Y5P	C4-N3	-13.44	1.33	1.46
88	A7	44	Y5P	C4-N3	-13.31	1.33	1.46
87	A5	1	Y5P	C4-N3	-13.23	1.33	1.46
88	A7	66	Y5P	C4-N3	-13.23	1.33	1.46
88	A7	70	Y5P	C4-N3	-13.23	1.33	1.46
87	A5	4	Y5P	C4-N3	-13.21	1.33	1.46
88	A7	64	Y5P	C4-N3	-13.07	1.34	1.46
88	A7	8	Y5P	C4-N3	-12.94	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	9	Y5P	C4-N3	-12.88	1.34	1.46
88	A7	65	Y5P	C4-N3	-12.87	1.34	1.46
88	A7	59	Y5P	C4-N3	-12.84	1.34	1.46
88	A7	60	Y5P	C4-N3	-12.84	1.34	1.46
88	A7	58	Y5P	C4-N3	-12.82	1.34	1.46
88	A7	47	Y5P	C4-N3	-12.80	1.34	1.46
88	A7	3	Y5P	C4-N3	-12.79	1.34	1.46
88	A7	68	Y5P	C4-N3	-12.79	1.34	1.46
88	A7	46	Y5P	C4-N3	-12.76	1.34	1.46
87	A5	7	Y5P	C4-N3	-12.67	1.34	1.46
88	A7	17	Y5P	C4-N3	-12.57	1.34	1.46
88	A7	51	Y5P	C4-N3	-12.50	1.34	1.46
88	A7	57	Y5P	C4-N3	-12.49	1.34	1.46
88	A7	62	Y5P	C4-N3	-12.47	1.34	1.46
88	A7	38	Y5P	C4-N3	-12.42	1.34	1.46
88	A7	21	Y5P	C4-N3	-12.41	1.34	1.46
87	A5	8	Y5P	C4-N3	-12.41	1.34	1.46
88	A7	63	Y5P	C4-N3	-12.41	1.34	1.46
88	A7	69	Y5P	C4-N3	-12.40	1.34	1.46
88	A7	50	Y5P	C4-N3	-12.36	1.34	1.46
88	A7	22	Y5P	C4-N3	-12.33	1.34	1.46
87	A5	10	Y5P	C4-N3	-12.28	1.34	1.46
88	A7	37	Y5P	C4-N3	-12.27	1.34	1.46
87	A5	3	Y5P	C4-N3	-12.24	1.34	1.46
88	A7	55	Y5P	C4-N3	-12.22	1.34	1.46
88	A7	61	Y5P	C4-N3	-12.17	1.34	1.46
88	A7	59	Y5P	C2-N3	12.11	1.36	1.27
88	A7	68	Y5P	C2-N3	12.11	1.36	1.27
88	A7	56	Y5P	C4-N3	-12.11	1.34	1.46
88	A7	25	Y5P	C4-N3	-12.10	1.34	1.46
88	A7	24	Y5P	C4-N3	-11.97	1.35	1.46
87	A5	8	Y5P	C2-N3	11.93	1.36	1.27
88	A7	69	Y5P	C2-N3	11.90	1.36	1.27
87	A5	4	Y5P	C2-N3	11.86	1.36	1.27
88	A7	13	Y5P	C4-N3	-11.86	1.35	1.46
87	A5	1	Y5P	C2-N3	11.86	1.36	1.27
88	A7	56	Y5P	C2-N3	11.73	1.36	1.27
88	A7	12	Y5P	C4-N3	-11.66	1.35	1.46
88	A7	17	Y5P	C2-N3	11.57	1.36	1.27
88	A7	63	Y5P	C2-N3	11.41	1.36	1.27
88	A7	50	Y5P	C2-N3	11.40	1.36	1.27
88	A7	9	Y5P	C2-N3	11.39	1.36	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	8	Y5P	C2-N3	11.38	1.36	1.27
87	A5	7	Y5P	C2-N3	11.37	1.36	1.27
87	A5	10	Y5P	C2-N3	11.36	1.36	1.27
88	A7	44	Y5P	C2-N3	11.29	1.36	1.27
88	A7	65	Y5P	C2-N3	11.28	1.36	1.27
88	A7	47	Y5P	C2-N3	11.18	1.36	1.27
88	A7	55	Y5P	C2-N3	11.13	1.36	1.27
88	A7	61	Y5P	C2-N3	11.10	1.36	1.27
88	A7	58	Y5P	C2-N3	11.05	1.36	1.27
87	A5	3	Y5P	C2-N3	11.04	1.36	1.27
88	A7	57	Y5P	C2-N3	10.90	1.35	1.27
88	A7	46	Y5P	C2-N3	10.88	1.35	1.27
88	A7	67	Y5P	C2-N3	10.85	1.35	1.27
88	A7	66	Y5P	C2-N3	10.80	1.35	1.27
88	A7	53	Y5P	C2-N3	10.75	1.35	1.27
88	A7	12	Y5P	C2-N3	10.66	1.35	1.27
88	A7	62	Y5P	C2-N3	10.63	1.35	1.27
88	A7	37	Y5P	C2-N3	10.58	1.35	1.27
88	A7	25	Y5P	C2-N3	10.55	1.35	1.27
88	A7	64	Y5P	C2-N3	10.46	1.35	1.27
88	A7	60	Y5P	C2-N3	10.43	1.35	1.27
88	A7	38	Y5P	C2-N3	10.39	1.35	1.27
88	A7	21	Y5P	C2-N3	10.39	1.35	1.27
88	A7	51	Y5P	C2-N3	10.31	1.35	1.27
88	A7	70	Y5P	C2-N3	10.21	1.35	1.27
88	A7	13	Y5P	C2-N3	10.06	1.35	1.27
88	A7	3	Y5P	C2-N3	10.05	1.35	1.27
88	A7	22	Y5P	C2-N3	9.86	1.35	1.27
88	A7	24	Y5P	C2-N3	9.79	1.35	1.27
88	A7	1	P5P	C6-N1	2.73	1.40	1.34
88	A7	2	P5P	C6-N1	2.71	1.40	1.34
88	A7	54	P5P	C6-N1	2.71	1.40	1.34
88	A7	15	P5P	C6-N1	2.65	1.39	1.34
88	A7	52	P5P	C6-N1	2.64	1.39	1.34
88	A7	39	P5P	C6-N1	2.62	1.39	1.34
88	A7	18	P5P	C6-N1	2.60	1.39	1.34
88	A7	43	P5P	C6-N1	2.59	1.39	1.34
88	A7	48	P5P	C6-N1	2.58	1.39	1.34
88	A7	26	P5P	C6-N1	2.55	1.39	1.34
88	A7	4	P5P	C6-N1	2.55	1.39	1.34
87	A5	11	P5P	C6-N1	2.55	1.39	1.34
88	A7	23	P5P	C6-N1	2.55	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	19	P5P	C6-N1	2.54	1.39	1.34
87	A5	6	P5P	C6-N1	2.54	1.39	1.34
88	A7	4	P5P	C6-C5	2.54	1.43	1.39
87	A5	2	P5P	C6-N1	2.52	1.39	1.34
88	A7	49	P5P	C6-N1	2.52	1.39	1.34
88	A7	6	P5P	C6-N1	2.50	1.39	1.34
88	A7	41	P5P	C6-N1	2.48	1.39	1.34
88	A7	71	P5P	C6-N1	2.48	1.39	1.34
88	A7	7	P5P	C6-N1	2.47	1.39	1.34
87	A5	9	P5P	C6-N1	2.46	1.39	1.34
87	A5	5	P5P	C6-N1	2.45	1.39	1.34
88	A7	16	P5P	C6-N1	2.45	1.39	1.34
88	A7	14	P5P	C6-N1	2.40	1.39	1.34
88	A7	6	P5P	C6-C5	2.40	1.42	1.39
88	A7	48	P5P	C6-C5	2.38	1.42	1.39
88	A7	10	P5P	C6-N1	2.38	1.39	1.34
88	A7	11	P5P	C6-N1	2.37	1.39	1.34
88	A7	27	P5P	C6-N1	2.36	1.39	1.34
88	A7	40	P5P	C6-N1	2.36	1.39	1.34
88	A7	5	P5P	C6-N1	2.34	1.39	1.34
88	A7	15	P5P	C2-N1	2.32	1.38	1.33
88	A7	54	P5P	C2-N1	2.30	1.38	1.33
88	A7	2	P5P	C2-N1	2.30	1.38	1.33
88	A7	18	P5P	C2-N1	2.29	1.38	1.33
88	A7	54	P5P	C6-C5	2.29	1.42	1.39
88	A7	26	P5P	C6-C5	2.28	1.42	1.39
88	A7	45	P5P	C6-N1	2.28	1.39	1.34
88	A7	42	P5P	C6-N1	2.27	1.39	1.34
87	A5	9	P5P	C2-N1	2.27	1.37	1.33
88	A7	14	P5P	C2-N1	2.27	1.37	1.33
88	A7	39	P5P	C6-C5	2.26	1.42	1.39
87	A5	5	P5P	C2-N1	2.26	1.37	1.33
88	A7	23	P5P	C6-C5	2.26	1.42	1.39
88	A7	20	P5P	C6-N1	2.25	1.39	1.34
88	A7	52	P5P	C2-N1	2.25	1.37	1.33
87	A5	6	P5P	C2-N1	2.25	1.37	1.33
88	A7	43	P5P	C2-N1	2.25	1.37	1.33
87	A5	11	P5P	C2-N1	2.23	1.37	1.33
88	A7	40	P5P	C6-C5	2.22	1.42	1.39
87	A5	2	P5P	C2-N1	2.22	1.37	1.33
88	A7	41	P5P	C2-N1	2.22	1.37	1.33
88	A7	5	P5P	C6-C5	2.21	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	19	P5P	C2-N1	2.21	1.37	1.33
88	A7	52	P5P	C6-C5	2.20	1.42	1.39
88	A7	48	P5P	C2-N1	2.18	1.37	1.33
87	A5	11	P5P	C6-C5	2.16	1.42	1.39
88	A7	16	P5P	C6-C5	2.15	1.42	1.39
88	A7	71	P5P	C2-N1	2.14	1.37	1.33
88	A7	45	P5P	C2-N1	2.14	1.37	1.33
88	A7	20	P5P	C6-C5	2.14	1.42	1.39
88	A7	26	P5P	C2-N1	2.13	1.37	1.33
88	A7	42	P5P	C2-N1	2.13	1.37	1.33
88	A7	16	P5P	C2-N1	2.13	1.37	1.33
88	A7	27	P5P	C6-C5	2.13	1.42	1.39
87	A5	5	P5P	C6-C5	2.13	1.42	1.39
88	A7	23	P5P	C2-N1	2.12	1.37	1.33
88	A7	11	P5P	C6-C5	2.12	1.42	1.39
88	A7	49	P5P	C6-C5	2.12	1.42	1.39
88	A7	18	P5P	C6-C5	2.12	1.42	1.39
88	A7	15	P5P	C6-C5	2.11	1.42	1.39
88	A7	39	P5P	C2-N1	2.09	1.37	1.33
88	A7	10	P5P	C2-N1	2.09	1.37	1.33
88	A7	49	P5P	C2-N1	2.09	1.37	1.33
88	A7	41	P5P	C6-C5	2.08	1.42	1.39
88	A7	40	P5P	C2-N1	2.07	1.37	1.33
88	A7	19	P5P	C6-C5	2.07	1.42	1.39
88	A7	11	P5P	C2-N1	2.06	1.37	1.33
87	A5	9	P5P	C6-C5	2.06	1.42	1.39
88	A7	4	P5P	C2-N1	2.06	1.37	1.33
87	A5	6	P5P	C6-C5	2.05	1.42	1.39
88	A7	20	P5P	C2-N1	2.03	1.37	1.33
88	A7	7	P5P	C2-N1	2.03	1.37	1.33
88	A7	71	P5P	C6-C5	2.03	1.42	1.39
88	A7	42	P5P	C6-C5	2.01	1.42	1.39
88	A7	6	P5P	C2-N1	2.01	1.37	1.33

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	45	P5P	C6-N1-C2	8.80	126.18	115.80
88	A7	27	P5P	C6-N1-C2	8.66	126.02	115.80
88	A7	2	P5P	C6-N1-C2	8.60	125.95	115.80
88	A7	11	P5P	C6-N1-C2	8.58	125.93	115.80
88	A7	7	P5P	C6-N1-C2	8.52	125.85	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	26	P5P	C6-N1-C2	8.52	125.85	115.80
88	A7	4	P5P	C6-N1-C2	8.50	125.84	115.80
88	A7	39	P5P	C6-N1-C2	8.49	125.82	115.80
88	A7	19	P5P	C6-N1-C2	8.43	125.75	115.80
88	A7	40	P5P	C6-N1-C2	8.39	125.70	115.80
88	A7	5	P5P	C6-N1-C2	8.38	125.69	115.80
88	A7	18	P5P	C6-N1-C2	8.37	125.68	115.80
88	A7	49	P5P	C6-N1-C2	8.37	125.68	115.80
88	A7	6	P5P	C6-N1-C2	8.34	125.65	115.80
88	A7	1	P5P	C6-N1-C2	8.26	125.55	115.80
88	A7	48	P5P	C6-N1-C2	8.21	125.49	115.80
88	A7	20	P5P	C6-N1-C2	8.21	125.48	115.80
88	A7	10	P5P	C6-N1-C2	8.20	125.48	115.80
88	A7	42	P5P	C6-N1-C2	8.18	125.45	115.80
88	A7	16	P5P	C6-N1-C2	8.12	125.38	115.80
87	A5	5	P5P	C6-N1-C2	8.10	125.37	115.80
87	A5	11	P5P	C6-N1-C2	8.09	125.35	115.80
87	A5	6	P5P	C6-N1-C2	8.06	125.31	115.80
87	A5	9	P5P	C6-N1-C2	8.05	125.31	115.80
88	A7	43	P5P	C6-N1-C2	8.05	125.30	115.80
88	A7	14	P5P	C6-N1-C2	8.00	125.24	115.80
87	A5	2	P5P	C6-N1-C2	7.92	125.14	115.80
88	A7	71	P5P	C6-N1-C2	7.91	125.14	115.80
88	A7	23	P5P	C6-N1-C2	7.90	125.13	115.80
88	A7	15	P5P	C6-N1-C2	7.90	125.13	115.80
88	A7	52	P5P	C6-N1-C2	7.81	125.02	115.80
88	A7	41	P5P	C6-N1-C2	7.79	124.99	115.80
88	A7	54	P5P	C6-N1-C2	7.78	124.99	115.80
88	A7	44	Y5P	C5-C4-N3	4.82	121.92	114.15
88	A7	67	Y5P	C5-C4-N3	4.80	121.89	114.15
88	A7	70	Y5P	C5-C4-N3	4.79	121.87	114.15
88	A7	68	Y5P	C5-C4-N3	4.79	121.87	114.15
88	A7	9	Y5P	C1'-N1-C6	-4.72	110.78	120.77
87	A5	4	Y5P	C5-C4-N3	4.71	121.74	114.15
88	A7	17	Y5P	C5-C4-N3	4.71	121.74	114.15
87	A5	8	Y5P	C5-C4-N3	4.70	121.73	114.15
88	A7	69	Y5P	C5-C4-N3	4.68	121.69	114.15
88	A7	66	Y5P	C5-C4-N3	4.67	121.68	114.15
87	A5	1	Y5P	C5-C4-N3	4.66	121.66	114.15
88	A7	58	Y5P	C5-C4-N3	4.64	121.63	114.15
87	A5	10	Y5P	C5-C4-N3	4.63	121.61	114.15
87	A5	7	Y5P	C5-C4-N3	4.59	121.55	114.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	60	Y5P	C5-C4-N3	4.58	121.54	114.15
87	A5	3	Y5P	C5-C4-N3	4.57	121.51	114.15
88	A7	46	Y5P	C5-C4-N3	4.56	121.51	114.15
88	A7	3	Y5P	C5-C4-N3	4.56	121.50	114.15
88	A7	56	Y5P	C5-C4-N3	4.54	121.46	114.15
88	A7	55	Y5P	C5-C4-N3	4.53	121.45	114.15
87	A5	1	Y5P	C1'-N1-C6	-4.52	111.20	120.77
88	A7	59	Y5P	C5-C4-N3	4.51	121.42	114.15
88	A7	47	Y5P	C5-C4-N3	4.51	121.42	114.15
88	A7	45	P5P	C5-C6-N1	-4.50	110.69	121.90
88	A7	53	Y5P	C5-C4-N3	4.49	121.39	114.15
88	A7	65	Y5P	C5-C4-N3	4.49	121.38	114.15
88	A7	22	Y5P	C5-C4-N3	4.47	121.35	114.15
88	A7	8	Y5P	C5-C4-N3	4.46	121.35	114.15
88	A7	50	Y5P	C5-C4-N3	4.45	121.33	114.15
88	A7	38	Y5P	C5-C4-N3	4.44	121.31	114.15
88	A7	4	P5P	C5-C6-N1	-4.43	110.87	121.90
88	A7	62	Y5P	C5-C4-N3	4.41	121.26	114.15
88	A7	19	P5P	C5-C6-N1	-4.40	110.95	121.90
88	A7	57	Y5P	C5-C4-N3	4.39	121.23	114.15
88	A7	63	Y5P	C5-C4-N3	4.37	121.20	114.15
88	A7	14	P5P	C5-C6-N1	-4.35	111.05	121.90
87	A5	4	Y5P	C1'-N1-C6	-4.35	111.58	120.77
88	A7	25	Y5P	C5-C4-N3	4.34	121.16	114.15
88	A7	51	Y5P	C5-C4-N3	4.34	121.15	114.15
88	A7	11	P5P	C5-C6-N1	-4.34	111.10	121.90
88	A7	27	P5P	C5-C6-N1	-4.33	111.12	121.90
88	A7	61	Y5P	C5-C4-N3	4.30	121.09	114.15
88	A7	1	P5P	C5-C6-N1	-4.29	111.21	121.90
88	A7	37	Y5P	C5-C4-N3	4.29	121.07	114.15
88	A7	2	P5P	C5-C6-N1	-4.29	111.23	121.90
88	A7	12	Y5P	C5-C4-N3	4.28	121.05	114.15
88	A7	18	P5P	C5-C6-N1	-4.28	111.25	121.90
88	A7	40	P5P	C5-C6-N1	-4.27	111.26	121.90
88	A7	39	P5P	C5-C6-N1	-4.25	111.31	121.90
88	A7	26	P5P	C5-C6-N1	-4.24	111.33	121.90
88	A7	6	P5P	C5-C6-N1	-4.23	111.36	121.90
88	A7	21	Y5P	C5-C4-N3	4.23	120.97	114.15
88	A7	9	Y5P	C5-C4-N3	4.22	120.96	114.15
88	A7	5	P5P	C5-C6-N1	-4.22	111.38	121.90
87	A5	5	P5P	C5-C6-N1	-4.22	111.39	121.90
88	A7	42	P5P	C5-C6-N1	-4.22	111.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	A5	11	P5P	C5-C6-N1	-4.21	111.41	121.90
88	A7	7	P5P	C5-C6-N1	-4.21	111.41	121.90
88	A7	41	P5P	C5-C6-N1	-4.21	111.42	121.90
88	A7	71	P5P	C5-C6-N1	-4.21	111.42	121.90
87	A5	6	P5P	C5-C6-N1	-4.21	111.42	121.90
87	A5	9	P5P	C5-C6-N1	-4.20	111.43	121.90
88	A7	64	Y5P	C5-C4-N3	4.20	120.92	114.15
88	A7	24	Y5P	C5-C4-N3	4.20	120.92	114.15
87	A5	2	P5P	C5-C6-N1	-4.20	111.45	121.90
88	A7	48	P5P	C5-C6-N1	-4.19	111.45	121.90
88	A7	49	P5P	C5-C6-N1	-4.19	111.46	121.90
88	A7	16	P5P	C5-C6-N1	-4.19	111.47	121.90
88	A7	15	P5P	C5-C6-N1	-4.16	111.53	121.90
88	A7	54	P5P	C5-C6-N1	-4.15	111.56	121.90
88	A7	43	P5P	C5-C6-N1	-4.14	111.59	121.90
88	A7	10	P5P	C5-C6-N1	-4.14	111.59	121.90
88	A7	23	P5P	C5-C6-N1	-4.13	111.61	121.90
88	A7	20	P5P	C5-C6-N1	-4.10	111.69	121.90
88	A7	52	P5P	C5-C6-N1	-4.07	111.75	121.90
88	A7	13	Y5P	C5-C4-N3	4.06	120.70	114.15
88	A7	14	P5P	C6-C5-C4	3.18	119.72	116.24
88	A7	45	P5P	C6-C5-C4	3.05	119.57	116.24
88	A7	60	Y5P	O4'-C1'-N1	3.02	113.85	108.08
88	A7	47	Y5P	O4'-C1'-N1	3.00	113.80	108.08
88	A7	59	Y5P	O4'-C1'-N1	2.98	113.78	108.08
88	A7	55	Y5P	O4'-C1'-N1	2.94	113.70	108.08
88	A7	66	Y5P	O4'-C1'-N1	2.94	113.69	108.08
88	A7	6	P5P	O4'-C1'-N9	2.94	113.73	108.09
88	A7	16	P5P	C1'-N9-C8	-2.89	120.67	127.09
88	A7	53	Y5P	C1'-N1-C6	-2.84	114.77	120.77
87	A5	3	Y5P	O4'-C1'-N1	2.83	113.49	108.08
88	A7	68	Y5P	C1'-N1-C6	-2.82	114.80	120.77
88	A7	3	Y5P	O4'-C1'-N1	2.80	113.43	108.08
88	A7	56	Y5P	O4'-C1'-N1	2.80	113.42	108.08
88	A7	57	Y5P	O4'-C1'-N1	2.79	113.41	108.08
88	A7	48	P5P	O4'-C1'-N9	2.76	113.39	108.09
88	A7	19	P5P	O4'-C1'-N9	2.75	113.38	108.09
88	A7	8	Y5P	O4'-C1'-N1	2.74	113.31	108.08
88	A7	42	P5P	C6-C5-C4	2.71	119.20	116.24
88	A7	62	Y5P	O4'-C1'-N1	2.70	113.24	108.08
88	A7	52	P5P	N1-C2-N3	-2.69	122.75	127.33
88	A7	41	P5P	C6-C5-C4	2.69	119.18	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	2	P5P	N1-C2-N3	-2.69	122.76	127.33
88	A7	61	Y5P	O4'-C1'-N1	2.69	113.21	108.08
88	A7	65	Y5P	O4'-C1'-N1	2.67	113.18	108.08
88	A7	52	P5P	O4'-C1'-N9	2.67	113.21	108.09
88	A7	12	Y5P	O4'-C1'-N1	2.66	113.16	108.08
88	A7	27	P5P	C6-C5-C4	2.66	119.15	116.24
88	A7	24	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A7	67	Y5P	O4'-C1'-N1	2.65	113.13	108.08
88	A7	16	P5P	C4-N9-C1'	2.64	132.81	126.63
88	A7	63	Y5P	O4'-C1'-N1	2.64	113.12	108.08
88	A7	43	P5P	N1-C2-N3	-2.63	122.85	127.33
88	A7	19	P5P	C6-C5-C4	2.63	119.11	116.24
88	A7	18	P5P	N1-C2-N3	-2.62	122.88	127.33
88	A7	40	P5P	C6-C5-C4	2.62	119.10	116.24
88	A7	6	P5P	N1-C2-N3	-2.62	122.89	127.33
87	A5	6	P5P	O3'-C3'-C2'	2.61	120.20	111.82
88	A7	37	Y5P	O4'-C1'-N1	2.59	113.02	108.08
88	A7	26	P5P	N1-C2-N3	-2.58	122.94	127.33
88	A7	21	Y5P	O4'-C1'-N1	2.58	113.00	108.08
88	A7	7	P5P	N1-C2-N3	-2.57	122.97	127.33
88	A7	25	Y5P	O4'-C1'-N1	2.56	112.97	108.08
87	A5	9	P5P	C6-C5-C4	2.56	119.04	116.24
88	A7	11	P5P	C6-C5-C4	2.56	119.04	116.24
87	A5	11	P5P	C6-C5-C4	2.56	119.03	116.24
87	A5	6	P5P	C6-C5-C4	2.55	119.03	116.24
88	A7	46	Y5P	O4'-C1'-N1	2.55	112.94	108.08
88	A7	27	P5P	N1-C2-N3	-2.54	123.01	127.33
87	A5	2	P5P	C6-C5-C4	2.54	119.02	116.24
88	A7	39	P5P	N1-C2-N3	-2.54	123.01	127.33
88	A7	49	P5P	N1-C2-N3	-2.54	123.02	127.33
87	A5	10	Y5P	O4'-C1'-N1	2.54	112.92	108.08
88	A7	15	P5P	C6-C5-C4	2.54	119.01	116.24
88	A7	2	P5P	C6-C5-C4	2.53	119.01	116.24
87	A5	5	P5P	C6-C5-C4	2.53	119.01	116.24
88	A7	5	P5P	N1-C2-N3	-2.52	123.05	127.33
88	A7	5	P5P	C6-C5-C4	2.52	118.99	116.24
88	A7	45	P5P	N1-C2-N3	-2.49	123.09	127.33
88	A7	49	P5P	C6-C5-C4	2.49	118.96	116.24
88	A7	20	P5P	N1-C2-N3	-2.49	123.10	127.33
88	A7	16	P5P	C6-C5-C4	2.48	118.96	116.24
88	A7	10	P5P	N1-C2-N3	-2.47	123.13	127.33
88	A7	71	P5P	C6-C5-C4	2.47	118.94	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	18	P5P	C6-C5-C4	2.44	118.91	116.24
88	A7	11	P5P	N1-C2-N3	-2.44	123.19	127.33
88	A7	70	Y5P	N1-C2-N3	-2.42	118.67	125.39
88	A7	9	Y5P	N1-C2-N3	-2.42	118.68	125.39
88	A7	40	P5P	N1-C2-N3	-2.42	123.22	127.33
88	A7	7	P5P	C6-C5-C4	2.41	118.88	116.24
88	A7	51	Y5P	N1-C2-N3	-2.40	118.72	125.39
88	A7	40	P5P	O4'-C1'-N9	2.40	112.70	108.09
88	A7	38	Y5P	O4'-C1'-N1	2.40	112.66	108.08
88	A7	58	Y5P	O4'-C1'-N1	2.40	112.65	108.08
88	A7	69	Y5P	O4'-C1'-N1	2.39	112.65	108.08
88	A7	49	P5P	O4'-C1'-N9	2.39	112.68	108.09
88	A7	10	P5P	C6-C5-C4	2.38	118.84	116.24
88	A7	22	Y5P	O4'-C1'-N1	2.37	112.61	108.08
88	A7	20	P5P	C6-C5-C4	2.36	118.83	116.24
88	A7	6	P5P	C6-C5-C4	2.36	118.83	116.24
87	A5	4	Y5P	N1-C2-N3	-2.36	118.84	125.39
88	A7	48	P5P	N1-C2-N3	-2.36	123.32	127.33
87	A5	1	Y5P	N1-C2-N3	-2.36	118.85	125.39
88	A7	19	P5P	N1-C2-N3	-2.35	123.34	127.33
88	A7	4	P5P	O4'-C1'-N9	2.34	112.59	108.09
88	A7	26	P5P	C6-C5-C4	2.33	118.79	116.24
88	A7	51	Y5P	O4'-C1'-N1	2.33	112.53	108.08
87	A5	2	P5P	N1-C2-N3	-2.33	123.37	127.33
88	A7	1	P5P	C6-C5-C4	2.32	118.78	116.24
88	A7	43	P5P	C6-C5-C4	2.31	118.77	116.24
88	A7	53	Y5P	N1-C2-N3	-2.30	119.02	125.39
87	A5	3	Y5P	N1-C2-N3	-2.30	119.02	125.39
88	A7	1	P5P	N1-C2-N3	-2.29	123.43	127.33
88	A7	23	P5P	C6-C5-C4	2.28	118.73	116.24
88	A7	41	P5P	O4'-C1'-N9	2.27	112.45	108.09
88	A7	23	P5P	N1-C2-N3	-2.27	123.47	127.33
88	A7	13	Y5P	O4'-C1'-N1	2.26	112.40	108.08
88	A7	68	Y5P	O4'-C1'-N1	2.25	112.38	108.08
88	A7	39	P5P	C6-C5-C4	2.25	118.70	116.24
88	A7	4	P5P	N1-C2-N3	-2.25	123.51	127.33
87	A5	6	P5P	N1-C2-N3	-2.24	123.52	127.33
88	A7	68	Y5P	N1-C2-N3	-2.24	119.18	125.39
88	A7	64	Y5P	O4'-C1'-N1	2.24	112.35	108.08
88	A7	50	Y5P	N1-C2-N3	-2.23	119.19	125.39
87	A5	7	Y5P	N1-C2-N3	-2.23	119.20	125.39
88	A7	44	Y5P	N1-C2-N3	-2.22	119.22	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	15	P5P	N1-C2-N3	-2.21	123.57	127.33
88	A7	15	P5P	O4'-C1'-N9	2.21	112.33	108.09
88	A7	16	P5P	N1-C2-N3	-2.20	123.58	127.33
87	A5	7	Y5P	O4'-C1'-N1	2.20	112.27	108.08
88	A7	54	P5P	N1-C2-N3	-2.19	123.60	127.33
88	A7	46	Y5P	N1-C2-N3	-2.19	119.33	125.39
88	A7	20	P5P	O4'-C1'-N9	2.19	112.29	108.09
87	A5	11	P5P	N1-C2-N3	-2.18	123.62	127.33
88	A7	8	Y5P	N1-C2-N3	-2.18	119.34	125.39
87	A5	9	P5P	N1-C2-N3	-2.18	123.62	127.33
87	A5	8	Y5P	N1-C2-N3	-2.18	119.34	125.39
88	A7	52	P5P	C6-C5-C4	2.18	118.62	116.24
88	A7	69	Y5P	N1-C2-N3	-2.17	119.37	125.39
88	A7	63	Y5P	N1-C2-N3	-2.16	119.39	125.39
87	A5	8	Y5P	O4'-C1'-N1	2.16	112.20	108.08
88	A7	17	Y5P	N1-C2-N3	-2.16	119.41	125.39
88	A7	37	Y5P	N1-C2-N3	-2.14	119.45	125.39
88	A7	39	P5P	O4'-C1'-N9	2.14	112.19	108.09
87	A5	5	P5P	N1-C2-N3	-2.13	123.71	127.33
88	A7	55	Y5P	N1-C2-N3	-2.13	119.49	125.39
87	A5	10	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A7	62	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A7	21	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A7	47	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A7	3	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A7	56	Y5P	N1-C2-N3	-2.12	119.52	125.39
88	A7	59	Y5P	N1-C2-N3	-2.11	119.52	125.39
88	A7	42	P5P	N1-C2-N3	-2.11	123.75	127.33
88	A7	48	P5P	C6-C5-C4	2.08	118.52	116.24
88	A7	67	Y5P	N1-C2-N3	-2.07	119.64	125.39
87	A5	11	P5P	O4'-C1'-N9	2.07	112.07	108.09
88	A7	65	Y5P	N1-C2-N3	-2.07	119.64	125.39
88	A7	61	Y5P	N1-C2-N3	-2.07	119.64	125.39
88	A7	25	Y5P	N1-C2-N3	-2.05	119.69	125.39
88	A7	26	P5P	O4'-C1'-N9	2.05	112.03	108.09
88	A7	57	Y5P	N1-C2-N3	-2.05	119.71	125.39
88	A7	11	P5P	O4'-C1'-N9	2.03	111.99	108.09
88	A7	12	Y5P	N1-C2-N3	-2.02	119.78	125.39
88	A7	22	Y5P	N1-C2-N3	-2.02	119.80	125.39
88	A7	41	P5P	N1-C2-N3	-2.01	123.91	127.33
88	A7	38	Y5P	N1-C2-N3	-2.01	119.82	125.39
88	A7	58	Y5P	N1-C2-N3	-2.01	119.83	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	4	P5P	C6-C5-C4	2.00	118.43	116.24

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	A5	1	Y5P	O4'-C4'-C5'-O5'
87	A5	1	Y5P	C3'-C4'-C5'-O5'
87	A5	2	P5P	O4'-C4'-C5'-O5'
87	A5	4	Y5P	O4'-C4'-C5'-O5'
87	A5	4	Y5P	C3'-C4'-C5'-O5'
87	A5	5	P5P	O4'-C4'-C5'-O5'
87	A5	7	Y5P	O4'-C4'-C5'-O5'
87	A5	7	Y5P	O4'-C1'-N1-C2
87	A5	8	Y5P	O4'-C4'-C5'-O5'
87	A5	8	Y5P	O4'-C1'-N1-C2
88	A7	3	Y5P	O4'-C1'-N1-C2
88	A7	9	Y5P	C2'-C1'-N1-C2
88	A7	14	P5P	O4'-C4'-C5'-O5'
88	A7	21	Y5P	O4'-C4'-C5'-O5'
88	A7	21	Y5P	C3'-C4'-C5'-O5'
88	A7	22	Y5P	O4'-C4'-C5'-O5'
88	A7	24	Y5P	O4'-C1'-N1-C2
88	A7	25	Y5P	O4'-C1'-N1-C2
88	A7	37	Y5P	O4'-C1'-N1-C2
88	A7	43	P5P	O4'-C4'-C5'-O5'
88	A7	43	P5P	C4'-C5'-O5'-P
88	A7	46	Y5P	O4'-C4'-C5'-O5'
88	A7	46	Y5P	O4'-C1'-N1-C2
88	A7	51	Y5P	O4'-C1'-N1-C2
88	A7	52	P5P	O4'-C4'-C5'-O5'
88	A7	57	Y5P	O4'-C1'-N1-C2
88	A7	61	Y5P	O4'-C1'-N1-C2
88	A7	62	Y5P	O4'-C1'-N1-C2
88	A7	63	Y5P	O4'-C1'-N1-C2
88	A7	71	P5P	C4'-C5'-O5'-P
87	A5	10	Y5P	O4'-C1'-N1-C2
88	A7	8	Y5P	O4'-C1'-N1-C2
88	A7	12	Y5P	O4'-C1'-N1-C2
88	A7	13	Y5P	O4'-C1'-N1-C2
88	A7	21	Y5P	O4'-C1'-N1-C2
88	A7	22	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
88	A7	38	Y5P	O4'-C1'-N1-C2
88	A7	47	Y5P	O4'-C1'-N1-C2
88	A7	50	Y5P	O4'-C1'-N1-C2
88	A7	55	Y5P	O4'-C1'-N1-C2
88	A7	56	Y5P	O4'-C1'-N1-C2
88	A7	58	Y5P	O4'-C1'-N1-C2
88	A7	59	Y5P	O4'-C1'-N1-C2
88	A7	60	Y5P	O4'-C1'-N1-C2
88	A7	64	Y5P	O4'-C1'-N1-C2
88	A7	65	Y5P	O4'-C1'-N1-C2
88	A7	66	Y5P	O4'-C1'-N1-C2
88	A7	69	Y5P	O4'-C1'-N1-C2
87	A5	3	Y5P	O4'-C4'-C5'-O5'
87	A5	5	P5P	C3'-C4'-C5'-O5'
87	A5	7	Y5P	C3'-C4'-C5'-O5'
87	A5	8	Y5P	C3'-C4'-C5'-O5'
88	A7	6	P5P	C3'-C4'-C5'-O5'
88	A7	14	P5P	C3'-C4'-C5'-O5'
88	A7	16	P5P	C3'-C4'-C5'-O5'
88	A7	22	Y5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	C3'-C4'-C5'-O5'
88	A7	45	P5P	C3'-C4'-C5'-O5'
88	A7	46	Y5P	C3'-C4'-C5'-O5'
88	A7	52	P5P	C3'-C4'-C5'-O5'
88	A7	52	P5P	O4'-C1'-N9-C8
88	A7	9	Y5P	C2'-C1'-N1-C6
87	A5	2	P5P	C3'-C4'-C5'-O5'
88	A7	45	P5P	O4'-C4'-C5'-O5'
88	A7	58	Y5P	O4'-C4'-C5'-O5'
88	A7	58	Y5P	C3'-C4'-C5'-O5'
88	A7	52	P5P	O4'-C1'-N9-C4
88	A7	67	Y5P	O4'-C1'-N1-C2
88	A7	70	Y5P	O4'-C1'-N1-C2
87	A5	1	Y5P	C4'-C5'-O5'-P
87	A5	4	Y5P	C4'-C5'-O5'-P
87	A5	1	Y5P	C2'-C1'-N1-C6
87	A5	4	Y5P	C2'-C1'-N1-C6
87	A5	3	Y5P	C3'-C4'-C5'-O5'
88	A7	6	P5P	O4'-C4'-C5'-O5'
88	A7	7	P5P	O4'-C4'-C5'-O5'
88	A7	50	Y5P	C4'-C5'-O5'-P
88	A7	16	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
88	A7	70	Y5P	O4'-C4'-C5'-O5'
88	A7	12	Y5P	C3'-C4'-C5'-O5'
88	A7	50	Y5P	C3'-C4'-C5'-O5'
88	A7	18	P5P	C4'-C5'-O5'-P
88	A7	70	Y5P	C3'-C4'-C5'-O5'
87	A5	1	Y5P	C2'-C1'-N1-C2
88	A7	7	P5P	C3'-C4'-C5'-O5'
87	A5	1	Y5P	O4'-C1'-N1-C2
87	A5	4	Y5P	O4'-C1'-N1-C2
88	A7	5	P5P	C3'-C4'-C5'-O5'
88	A7	64	Y5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	C2'-C1'-N9-C8
88	A7	12	Y5P	O4'-C4'-C5'-O5'
88	A7	54	P5P	C4'-C5'-O5'-P
88	A7	56	Y5P	C4'-C5'-O5'-P
88	A7	56	Y5P	O4'-C4'-C5'-O5'
87	A5	4	Y5P	C2'-C1'-N1-C2
87	A5	4	Y5P	O4'-C1'-N1-C6
88	A7	53	Y5P	O4'-C1'-N1-C6
88	A7	6	P5P	C4'-C5'-O5'-P
88	A7	7	P5P	C4'-C5'-O5'-P
88	A7	17	Y5P	C4'-C5'-O5'-P
88	A7	51	Y5P	C4'-C5'-O5'-P
88	A7	38	Y5P	C3'-C4'-C5'-O5'
88	A7	68	Y5P	O4'-C1'-N1-C6
88	A7	9	Y5P	O4'-C1'-N1-C2
88	A7	17	Y5P	O4'-C1'-N1-C2
88	A7	44	Y5P	O4'-C1'-N1-C2
88	A7	65	Y5P	C4'-C5'-O5'-P
87	A5	1	Y5P	O4'-C1'-N1-C6
88	A7	50	Y5P	O4'-C4'-C5'-O5'
88	A7	53	Y5P	C2'-C1'-N1-C6
87	A5	3	Y5P	O4'-C1'-N1-C2
88	A7	44	Y5P	C2'-C1'-N1-C2
88	A7	52	P5P	C4'-C5'-O5'-P
88	A7	5	P5P	O4'-C4'-C5'-O5'
88	A7	6	P5P	C2'-C1'-N9-C8
87	A5	3	Y5P	C2'-C1'-N1-C2
88	A7	53	Y5P	O4'-C1'-N1-C2
88	A7	56	Y5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	O4'-C1'-N9-C8
88	A7	52	P5P	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
88	A7	27	P5P	C3'-C4'-C5'-O5'
88	A7	64	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

25 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A7	20	P5P	1	0
87	A5	4	Y5P	3	0
88	A7	25	Y5P	1	0
88	A7	61	Y5P	1	0
88	A7	21	Y5P	2	0
88	A7	70	Y5P	4	0
88	A7	59	Y5P	1	0
88	A7	58	Y5P	1	0
88	A7	24	Y5P	1	0
88	A7	1	P5P	9	0
88	A7	47	Y5P	1	0
88	A7	22	Y5P	1	0
88	A7	48	P5P	1	0
88	A7	63	Y5P	1	0
88	A7	12	Y5P	1	0
88	A7	71	P5P	6	0
87	A5	10	Y5P	4	0
87	A5	1	Y5P	7	0
88	A7	65	Y5P	2	0
88	A7	60	Y5P	4	0
88	A7	13	Y5P	1	0
88	A7	64	Y5P	3	0
88	A7	69	Y5P	2	0
88	A7	57	Y5P	1	0
88	A7	62	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 137 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
92	GCP	v	802	89	32,34,34	1.67	6 (18%)	49,54,54	1.87	10 (20%)
91	GDP	AX	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)

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
92	GCP	v	802	89	-	5/19/38/38	0/3/3/3
91	GDP	AX	500	-	-	1/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	v	802	GCP	PG-O1G	5.53	1.61	1.50
91	AX	500	GDP	C5-C4	3.22	1.47	1.38
92	v	802	GCP	PG-O3G	3.06	1.61	1.55
92	v	802	GCP	C5-C4	3.03	1.47	1.38
92	v	802	GCP	PG-O2G	-2.61	1.49	1.55
91	AX	500	GDP	C6-N1	-2.40	1.34	1.38
92	v	802	GCP	PB-O2B	2.25	1.61	1.56
92	v	802	GCP	C4-N9	-2.22	1.32	1.38
91	AX	500	GDP	C5-N7	-2.05	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AX	500	GDP	C5-C4-N3	-6.34	118.30	128.39
92	v	802	GCP	PB-O3A-PA	-5.90	113.13	132.37
91	AX	500	GDP	C2-N3-C4	5.15	121.17	112.30
92	v	802	GCP	C2-N3-C4	4.82	120.60	112.30
91	AX	500	GDP	N9-C4-N3	4.71	135.37	125.95
92	v	802	GCP	C5-C4-N3	-4.63	121.02	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	v	802	GCP	C6-C5-N7	4.11	137.77	130.29
92	v	802	GCP	N9-C4-N3	3.24	132.44	125.95
91	AX	500	GDP	C6-C5-N7	3.12	135.96	130.29
91	AX	500	GDP	C4-C5-N7	-2.55	106.63	110.67
92	v	802	GCP	O4'-C1'-N9	2.54	114.12	108.36
92	v	802	GCP	C6-C5-C4	-2.41	115.20	118.83
92	v	802	GCP	C4-C5-N7	-2.30	107.02	110.67
92	v	802	GCP	C1'-N9-C4	-2.25	119.83	126.49
91	AX	500	GDP	C3'-C2'-C1'	2.15	105.53	101.46
92	v	802	GCP	O6-C6-C5	-2.11	120.96	126.53
91	AX	500	GDP	O6-C6-C5	-2.09	121.01	126.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

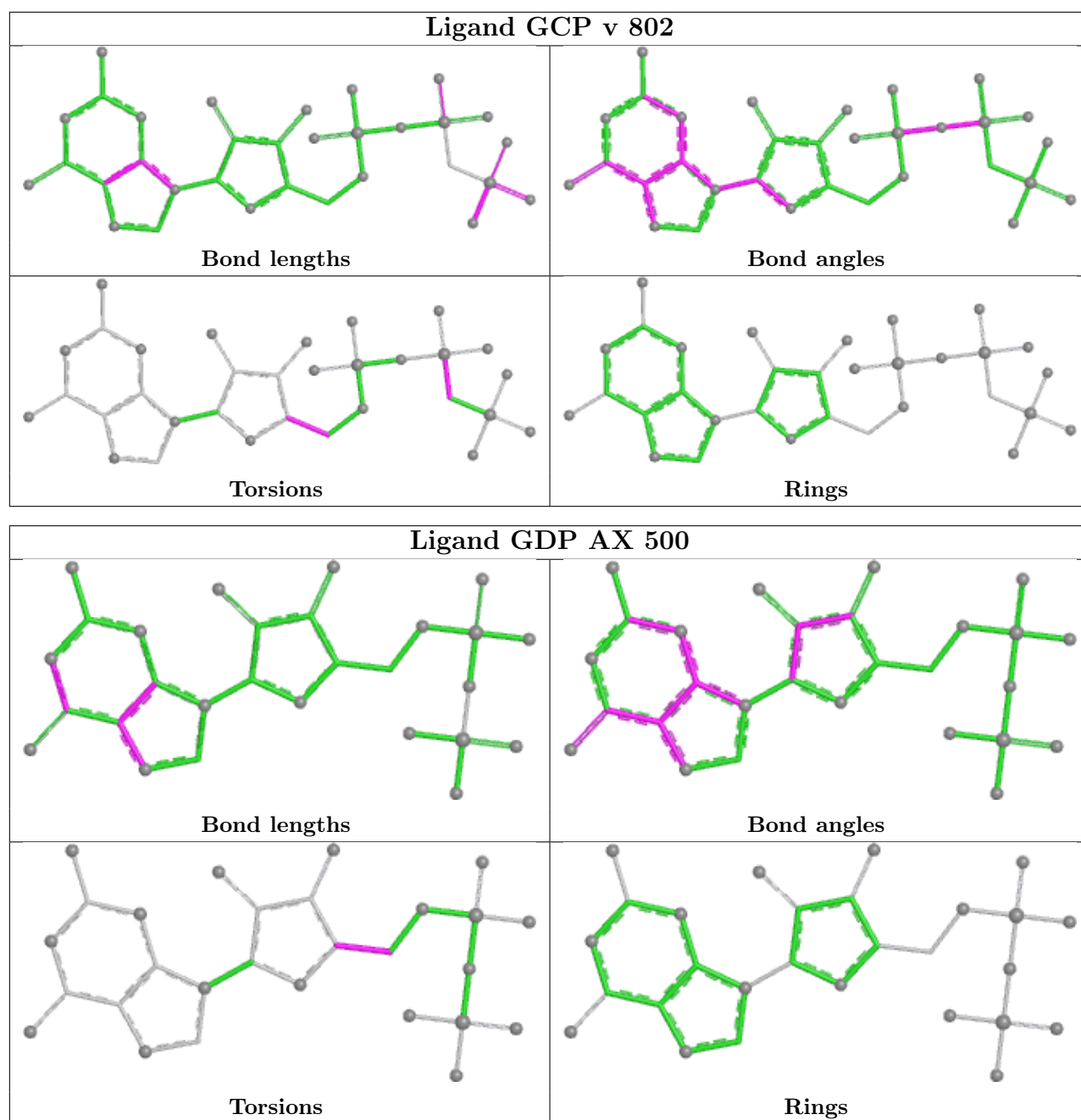
Mol	Chain	Res	Type	Atoms
92	v	802	GCP	PG-C3B-PB-O1B
92	v	802	GCP	PG-C3B-PB-O3A
92	v	802	GCP	O4'-C4'-C5'-O5'
92	v	802	GCP	C3'-C4'-C5'-O5'
92	v	802	GCP	PG-C3B-PB-O2B
91	AX	500	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	v	802	GCP	33	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks
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Mol	Chain	Number of breaks
85	u	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	414:UNK	C	601:UNK	N	48.04
1	u	106:UNK	C	301:UNK	N	30.89
1	u	315:UNK	C	399:UNK	N	19.09
1	u	615:UNK	C	700:UNK	N	18.25

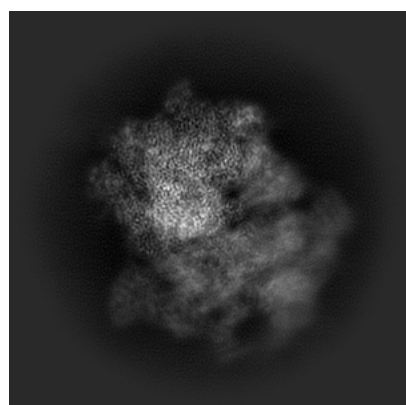
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21233. These allow visual inspection of the internal detail of the map and identification of artifacts.

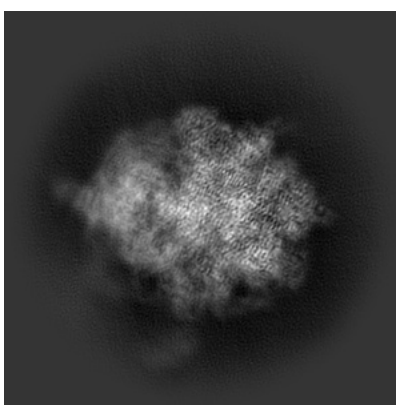
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

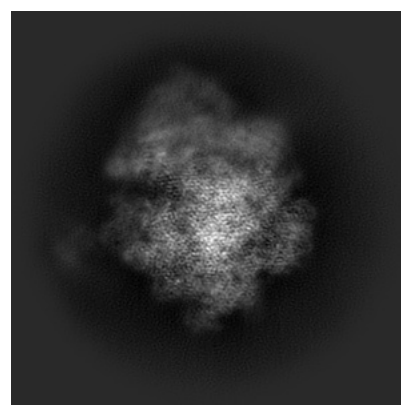
6.1.1 Primary map



X



Y

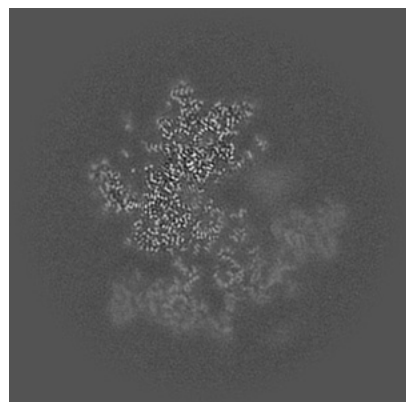


Z

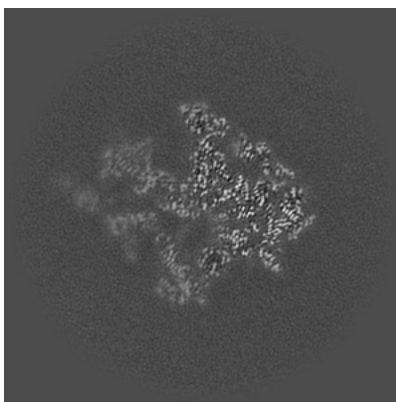
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

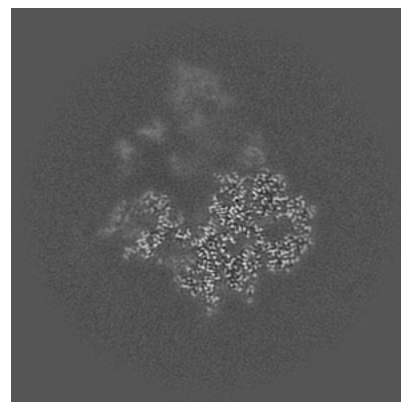
6.2.1 Primary map



X Index: 200



Y Index: 200

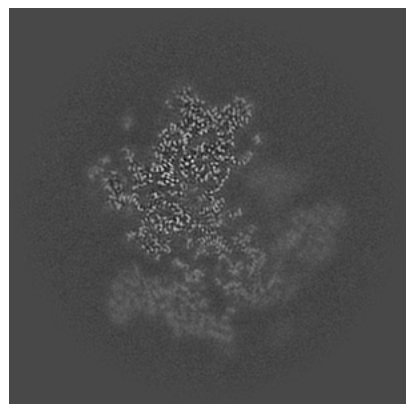


Z Index: 200

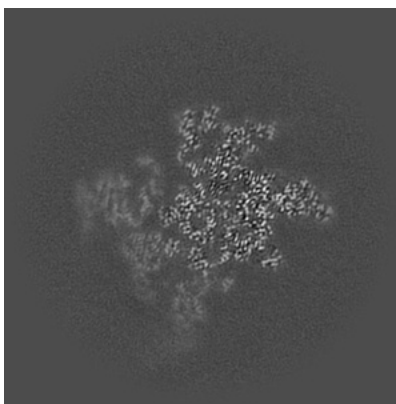
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

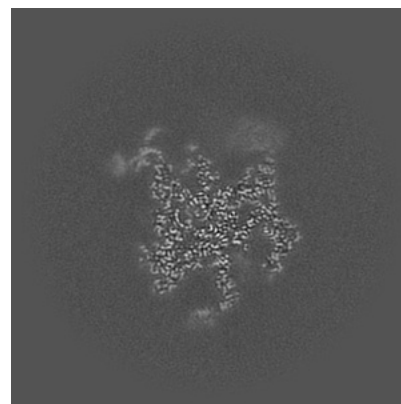
6.3.1 Primary map



X Index: 205



Y Index: 172

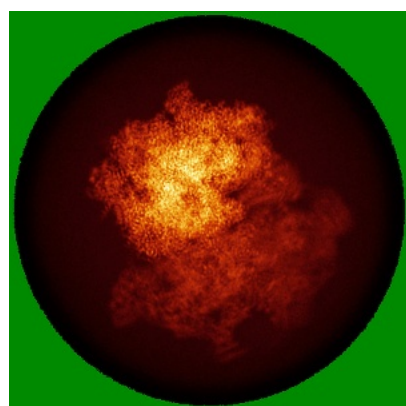


Z Index: 243

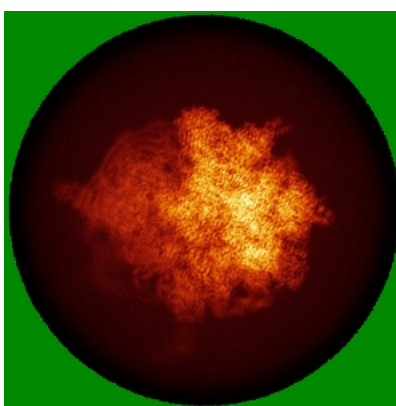
The images above show the largest variance slices of the map in three orthogonal directions.

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

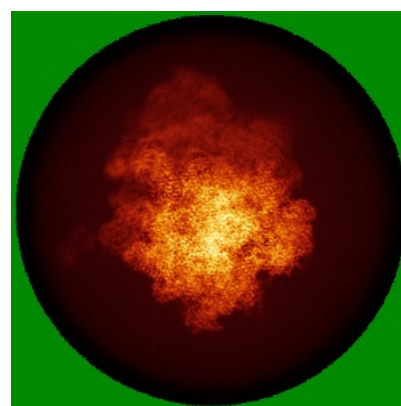
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

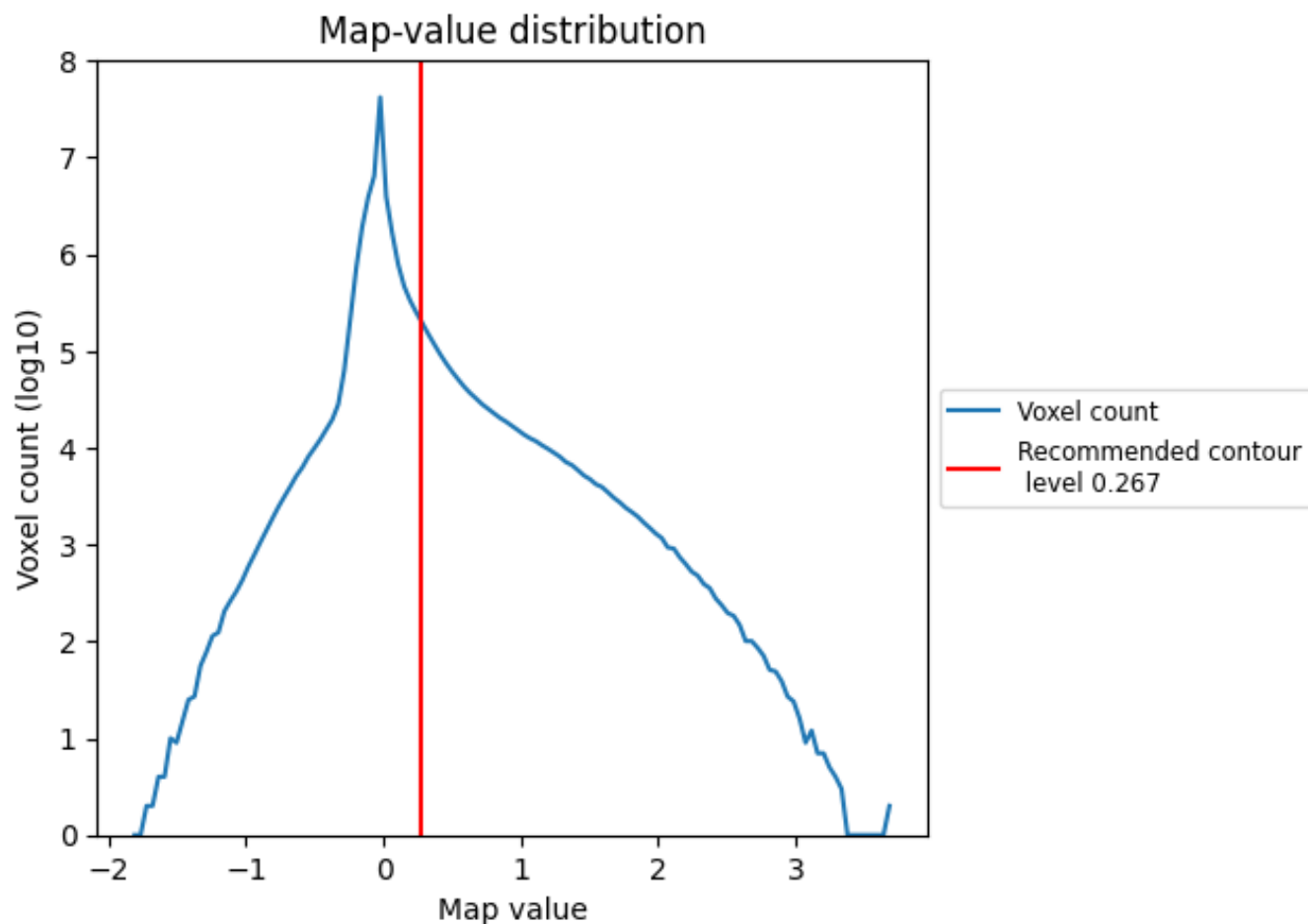
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

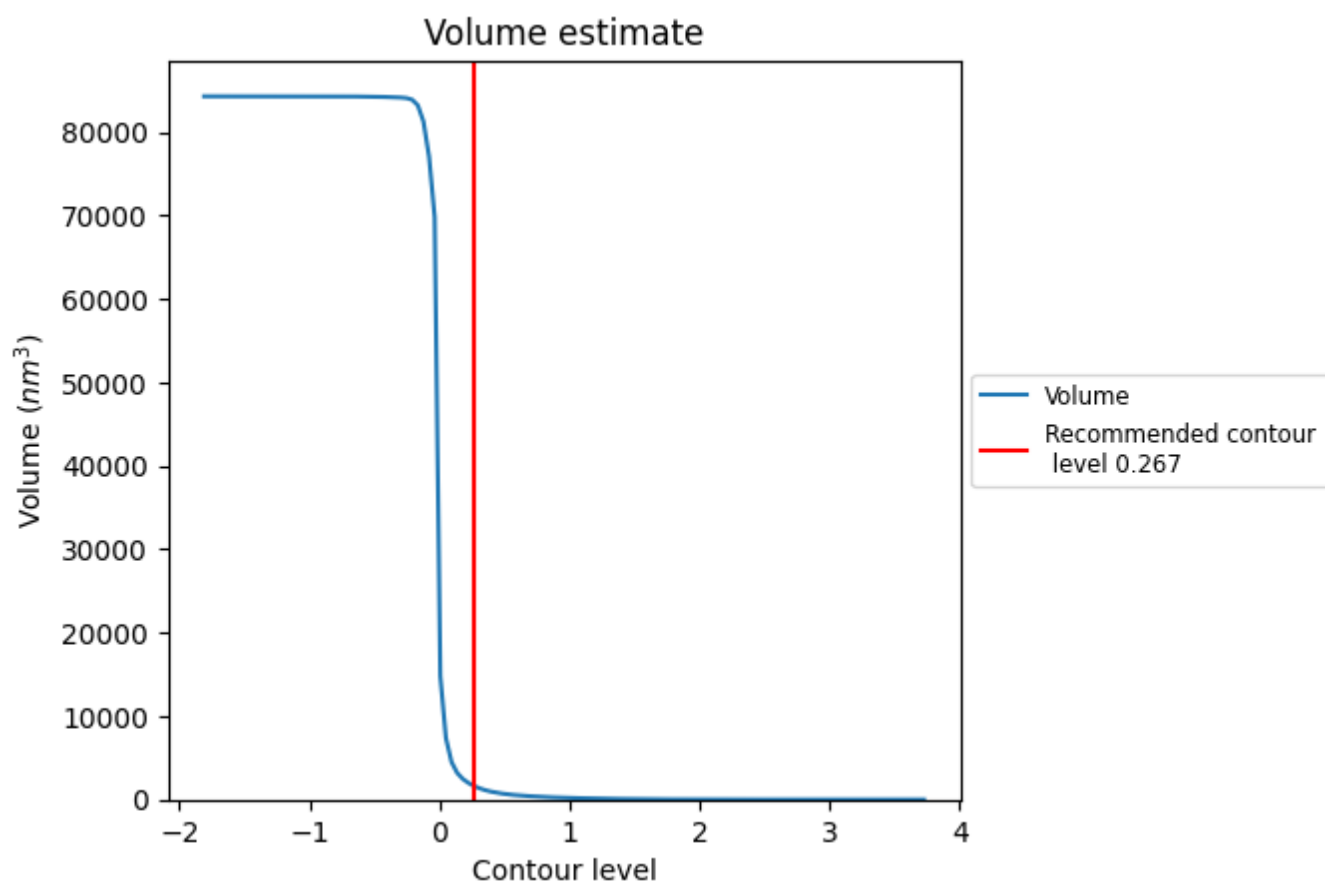
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

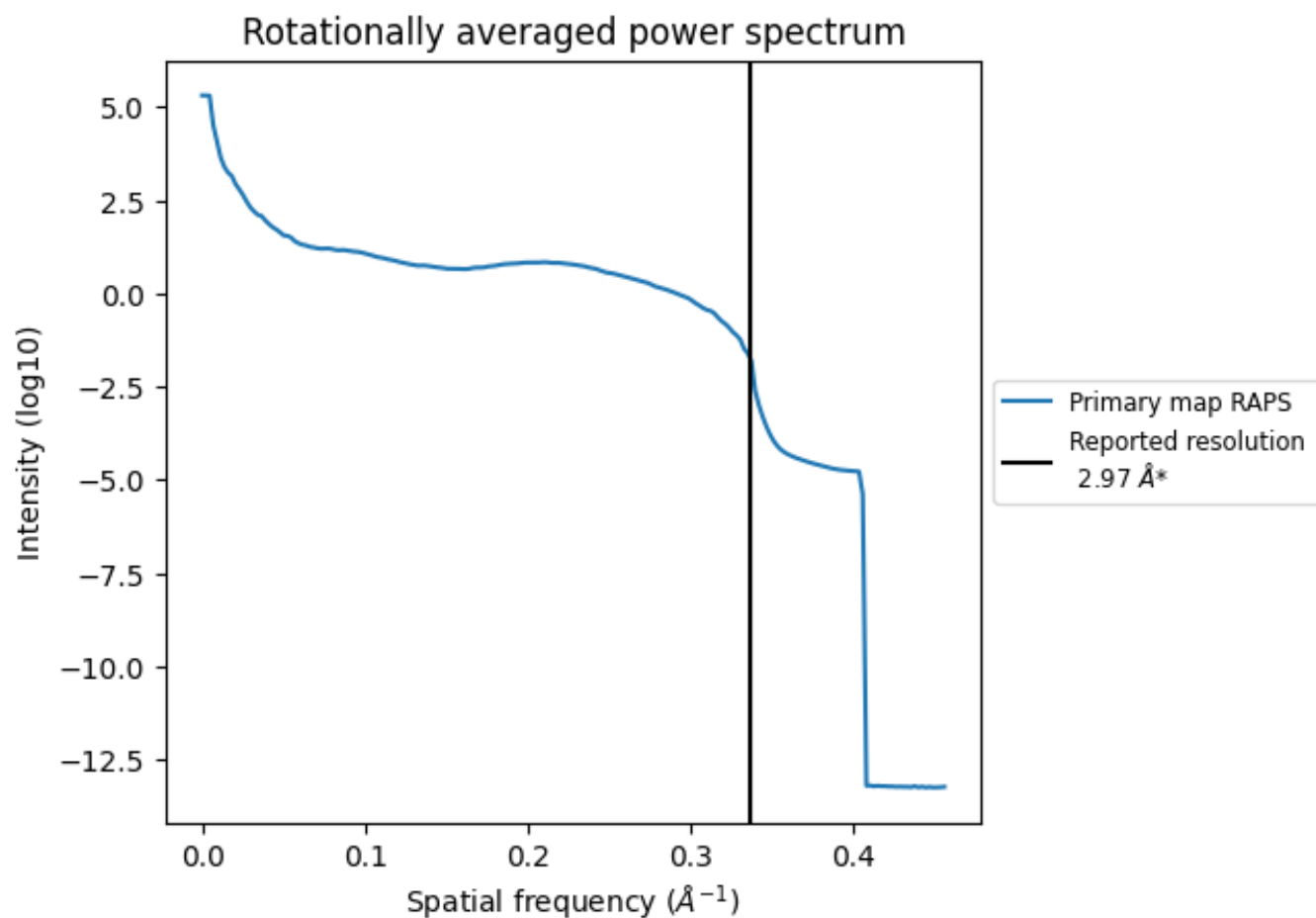
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1618 nm^3 ; this corresponds to an approximate mass of 1461 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 0.337 Å⁻¹

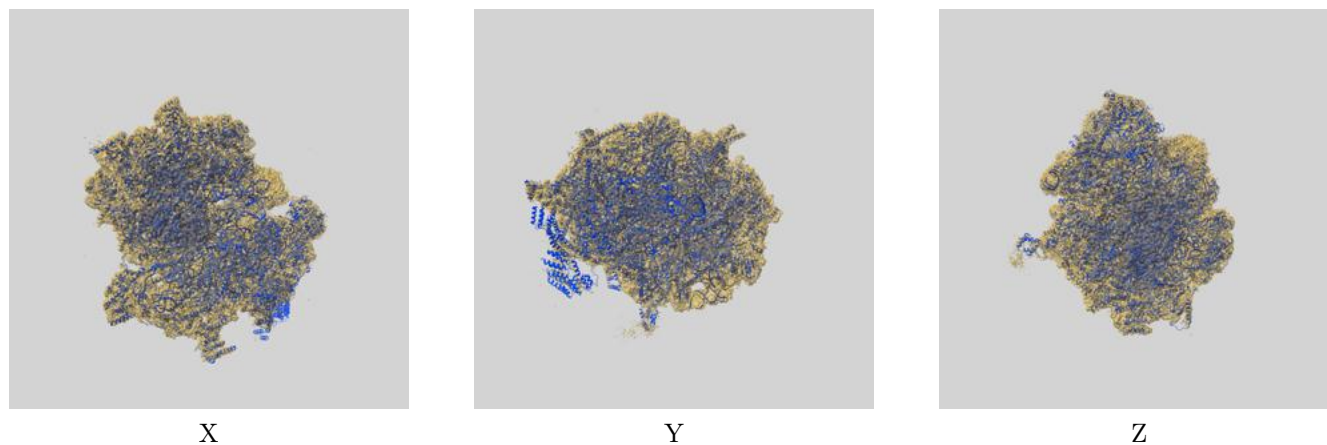
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

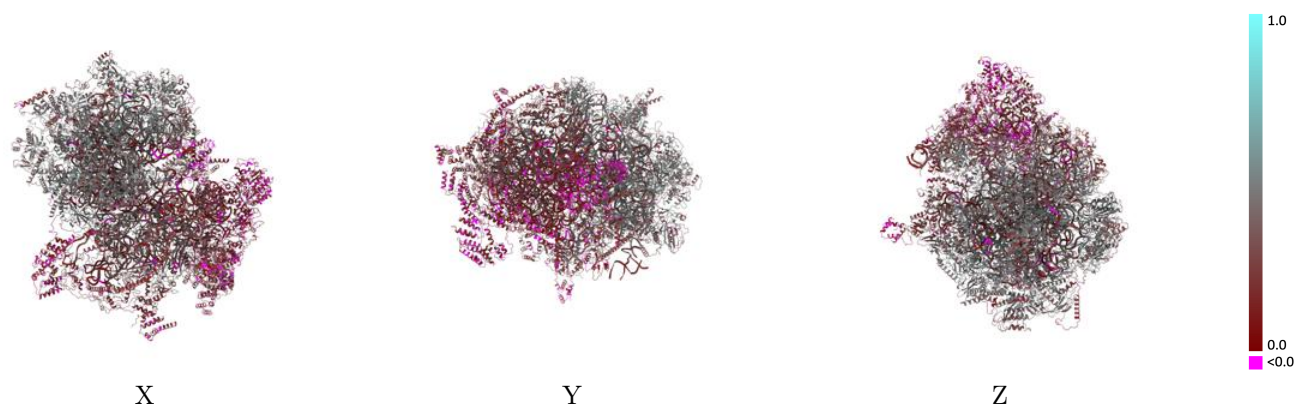
This section contains information regarding the fit between EMDB map EMD-21233 and PDB model 6VLZ. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



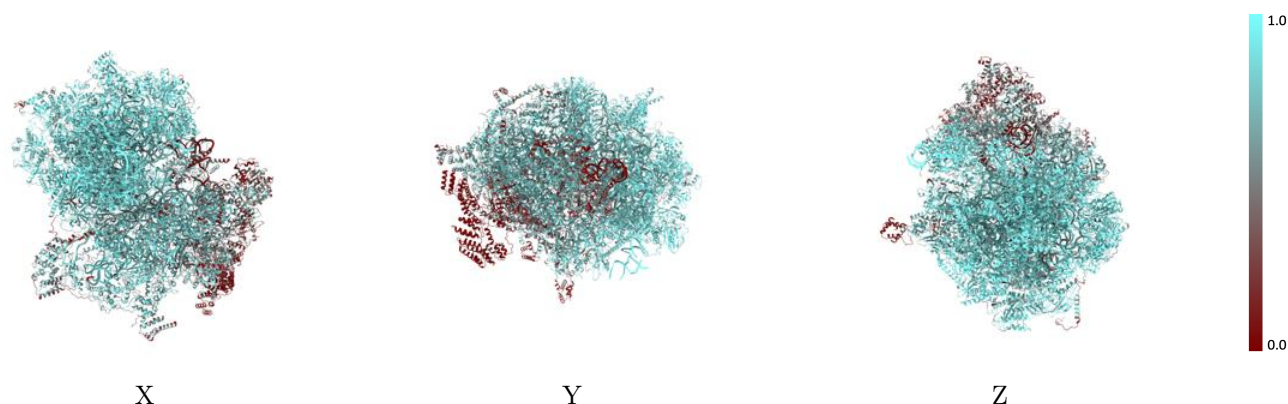
The images above show the 3D surface view of the map at the recommended contour level 0.267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



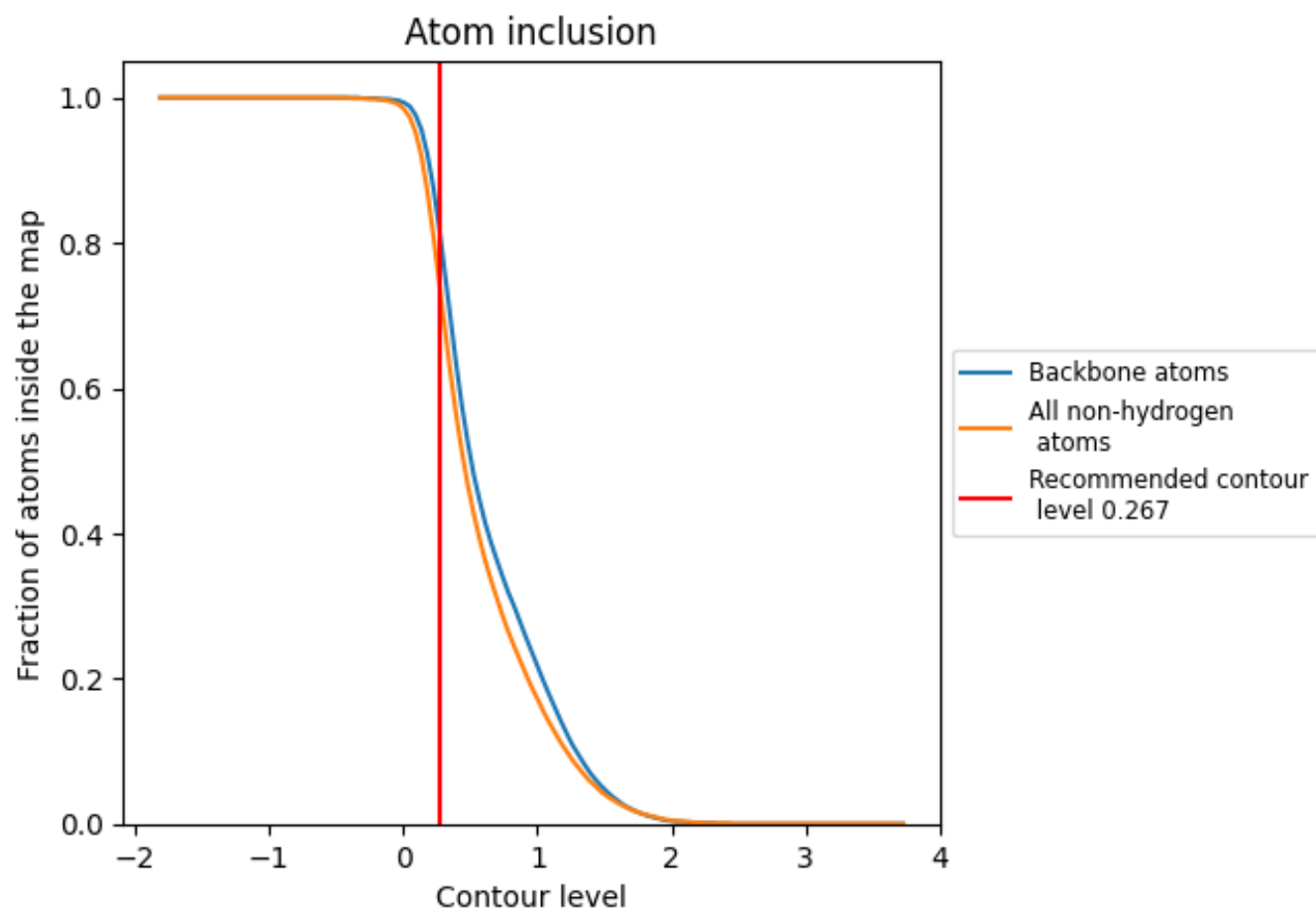
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.267).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.3170
0	 0.8580	 0.4350
1	 0.8410	 0.4250
2	 0.9110	 0.4820
3	 0.8970	 0.4990
4	 0.8590	 0.4400
5	 0.8880	 0.4360
6	 0.8750	 0.4050
7	 0.8610	 0.4030
8	 0.7270	 0.2300
9	 0.8720	 0.4070
A	 0.8440	 0.3320
A0	 0.6790	 0.2400
A1	 0.3650	 0.1370
A2	 0.4450	 0.2500
A3	 0.7270	 0.3760
A4	 0.1020	 0.1390
A5	 0.0240	 0.0310
A7	 0.1290	 0.0240
AA	 0.8170	 0.2590
AB	 0.6750	 0.2520
AC	 0.4550	 0.1700
AD	 0.5850	 0.2880
AE	 0.5540	 0.2510
AF	 0.4060	 0.2070
AG	 0.5010	 0.1720
AH	 0.4080	 0.1910
AI	 0.6400	 0.2880
AJ	 0.6970	 0.3530
AK	 0.6190	 0.1700
AL	 0.6750	 0.3090
AM	 0.7240	 0.2890
AN	 0.7960	 0.3620
AO	 0.6780	 0.2530
AP	 0.6310	 0.2770



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Chain	Atom inclusion	Q-score
AQ	 0.7190	 0.3230
AR	 0.6150	 0.2080
AS	 0.5480	 0.2090
AT	 0.7510	 0.3280
AU	 0.6650	 0.2020
AV	 0.5190	 0.1380
AW	 0.6120	 0.2510
AX	 0.3530	 0.0800
AY	 0.3590	 0.1320
AZ	 0.4080	 0.1530
B	 0.9480	 0.2870
D	 0.8650	 0.4350
E	 0.8820	 0.4590
F	 0.8880	 0.4590
H	 0.8360	 0.3920
I	 0.6890	 0.2600
J	 0.7400	 0.2690
K	 0.9050	 0.4740
L	 0.8510	 0.4540
M	 0.8910	 0.4500
N	 0.8540	 0.4300
O	 0.8740	 0.4370
P	 0.8810	 0.4120
Q	 0.8070	 0.4040
R	 0.8890	 0.4660
S	 0.9020	 0.4580
T	 0.8910	 0.4670
TA	 0.1310	 0.0810
TB	 0.1550	 0.0700
TC	 0.0340	 0.1480
U	 0.8680	 0.4330
V	 0.8590	 0.4160
W	 0.8830	 0.4550
X	 0.8800	 0.4430
Y	 0.8900	 0.4430
Z	 0.8800	 0.4520
a	 0.7980	 0.3920
b	 0.9000	 0.4710
c	 0.8610	 0.4180
d	 0.7530	 0.3680
e	 0.6990	 0.1610
f	 0.7010	 0.2860

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Chain	Atom inclusion	Q-score
g	 0.8720	 0.4180
h	 0.8210	 0.3580
i	 0.9010	 0.4680
j	 0.8450	 0.4100
k	 0.7430	 0.2880
l	 0.7680	 0.2830
m	 0.7420	 0.2190
o	 0.8580	 0.4220
p	 0.7950	 0.3700
q	 0.7480	 0.3460
r	 0.8750	 0.4280
s	 0.8800	 0.4360
u	 0.4740	 0.1660
v	 0.6950	 0.2920