



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:35 AM UTC

PDB ID : 6VMI / pdb_00006vmi
EMDB ID : EMD-21242
Title : Structure of the human mitochondrial ribosome-EF-G1 complex (ClassIII)
Authors : Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on : 2020-01-28
Resolution : 2.96 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:

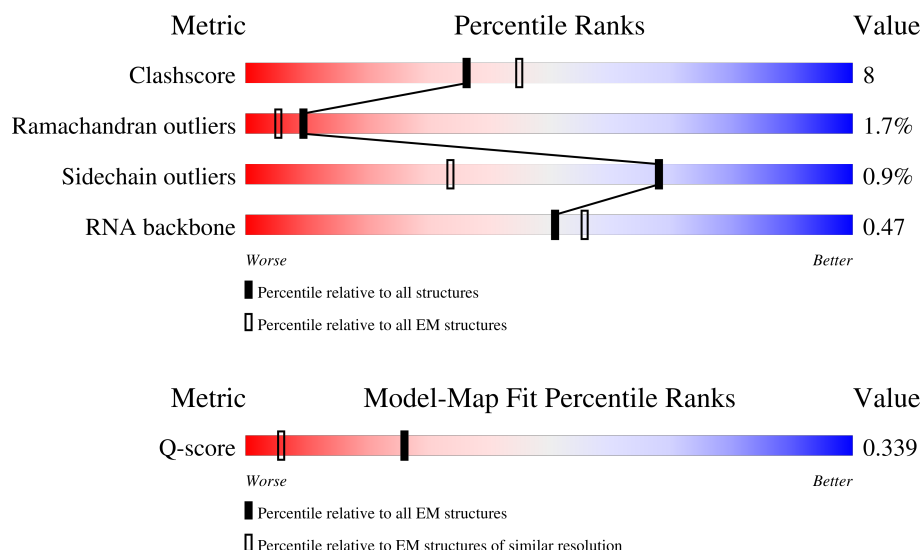
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.96 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.



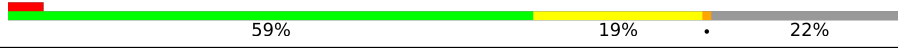
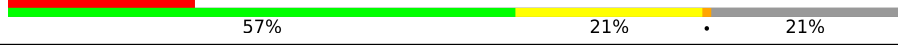
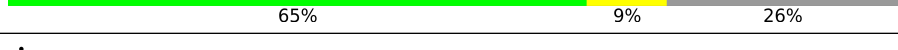
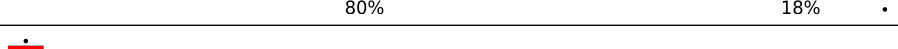
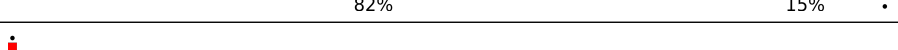
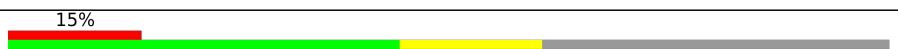
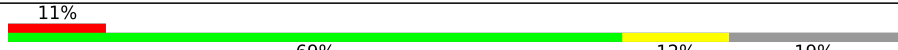
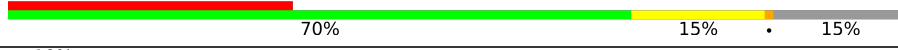
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	

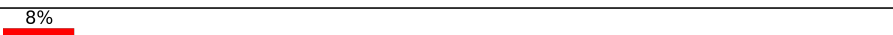
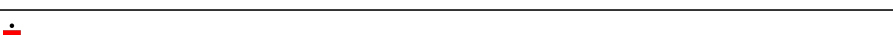
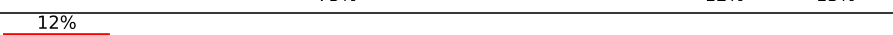
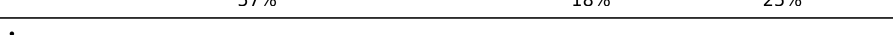
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Mol	Chain	Length	Quality of chain
29	AD	430	
30	AF	242	
31	AG	396	
32	A	1559	
33	B	73	
34	D	305	
35	F	311	
36	H	267	
37	K	178	
38	L	145	
39	M	296	
40	O	175	
41	R	149	
42	S	205	
43	T	212	
44	W	148	
45	X	256	
46	Y	250	
47	Z	161	
48	0	188	
49	1	65	
50	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	A6	71	
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	P5P	A5	2	-	-	X	-
88	Y5P	A6	35	-	-	X	-
88	Y5P	A6	36	-	-	X	-
88	Y5P	A6	69	-	-	X	-
88	Y5P	A6	70	-	-	X	-
88	P5P	A7	71	-	-	X	-
92	GCP	v	802	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 176217 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	variant	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		

- 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	variant	UNP Q13084
X	149	SER	PRO	variant	UNP Q13084
X	150	GLY	LYS	variant	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 P-site and E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	A6	71	Total	C	N	O	P	0	0
			1368	670	204	424	70		

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

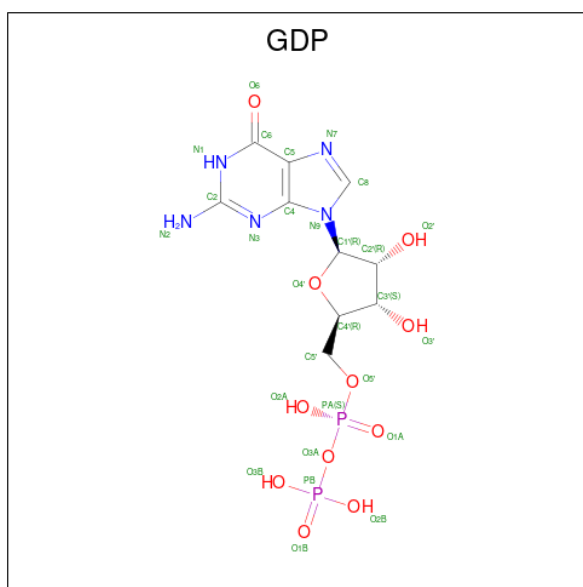
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	27	Total	Mg	0
			27	27	
89	AC	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).

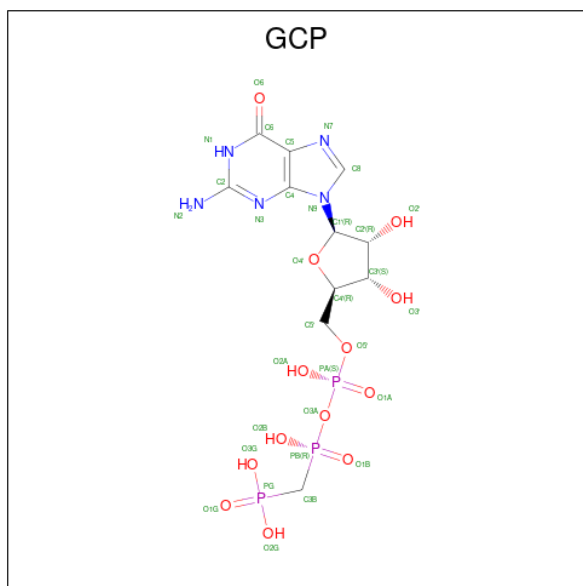
Mol	Chain	Residues	Atoms		AltConf
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

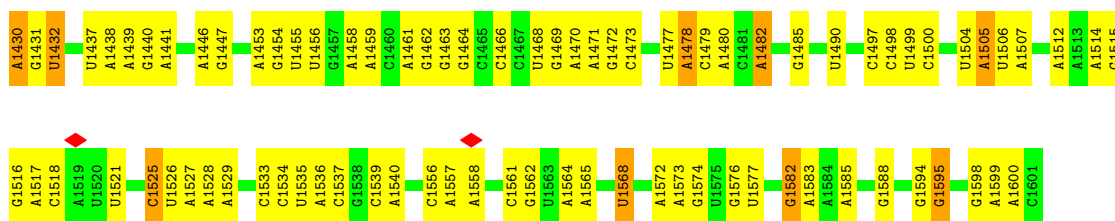


Mol	Chain	Residues	Atoms					AltConf
91	AX	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 92 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).

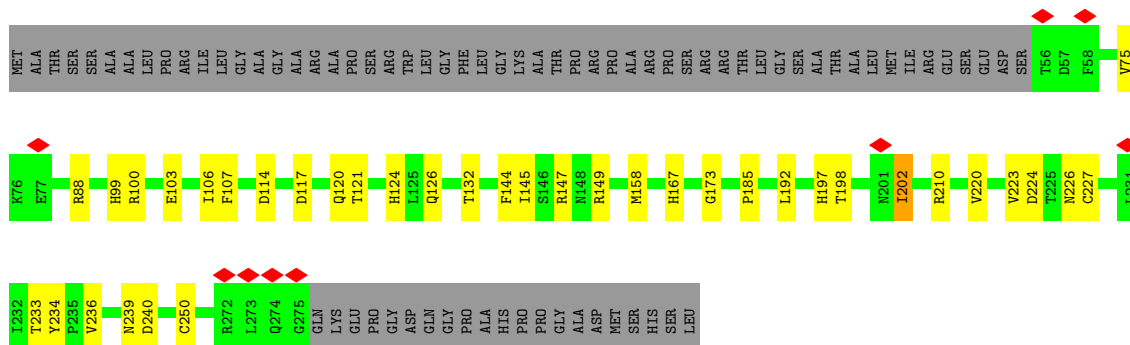


Mol	Chain	Residues	Atoms					AltConf
92	v	1	Total 32	C 11	N 5	O 13	P 3	0



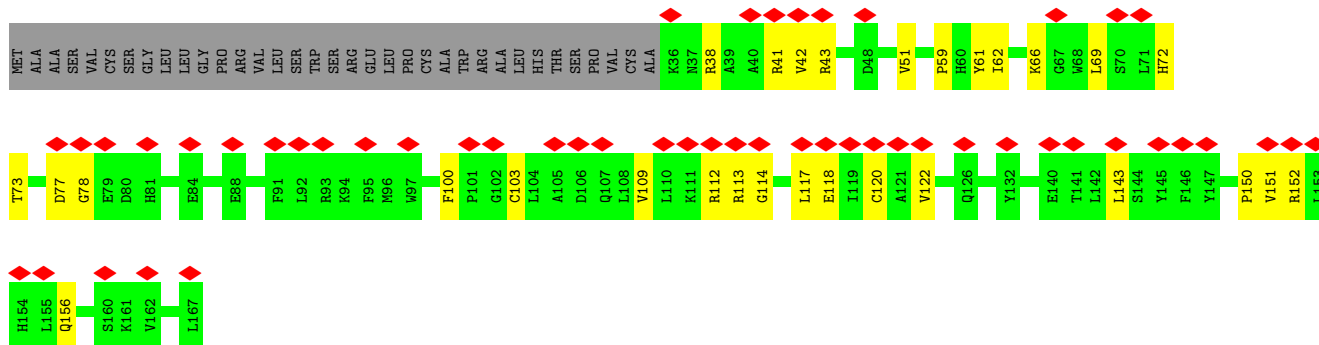
- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain AB: 61% 12% 26%



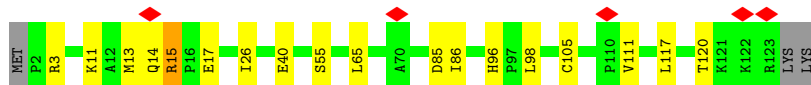
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC: 31% 62% 17% 21%



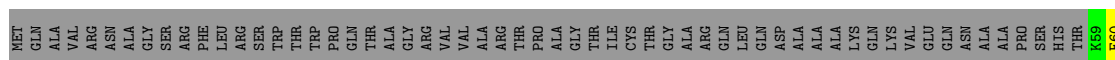
- Molecule 4: 28S ribosomal protein S6, mitochondrial

Chain AE: 83% 14% ..



- Molecule 5: 28S ribosomal protein S11, mitochondrial

Chain AI: 58% 12% 30%

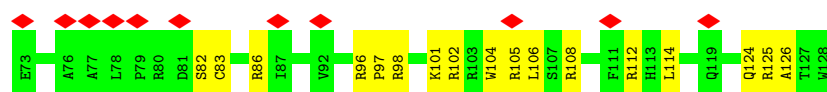
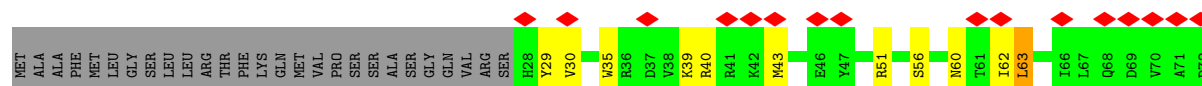




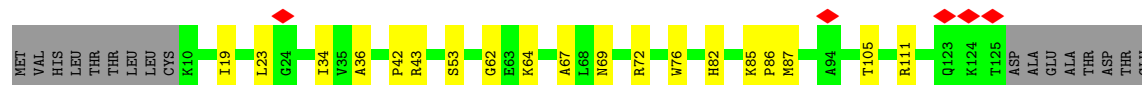
- Molecule 6: 28S ribosomal protein S12, mitochondrial



- Molecule 7: 28S ribosomal protein S14, mitochondrial



- Molecule 8: 28S ribosomal protein S16, mitochondrial

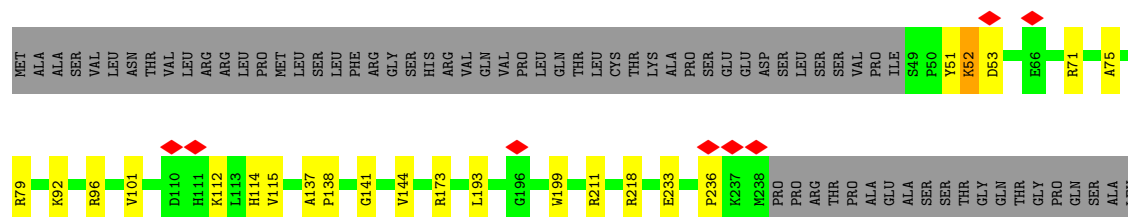


- Molecule 9: 28S ribosomal protein S17, mitochondrial

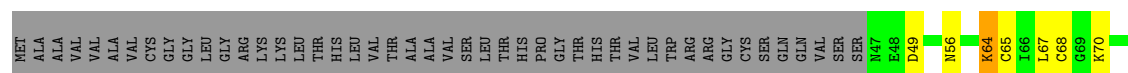


- Molecule 10: 28S ribosomal protein S18b, mitochondrial

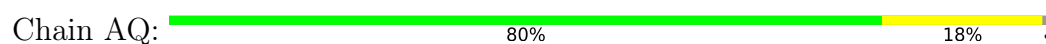




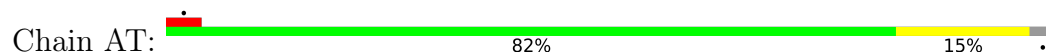
- Molecule 11: 28S ribosomal protein S18c, mitochondrial



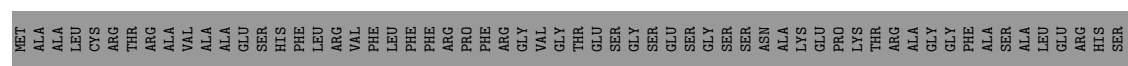
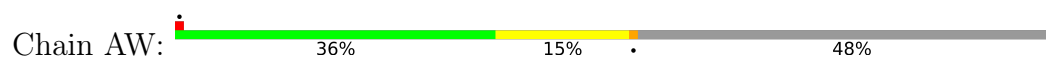
- Molecule 12: 28S ribosomal protein S21, mitochondrial



- Molecule 13: 28S ribosomal protein S25, mitochondrial

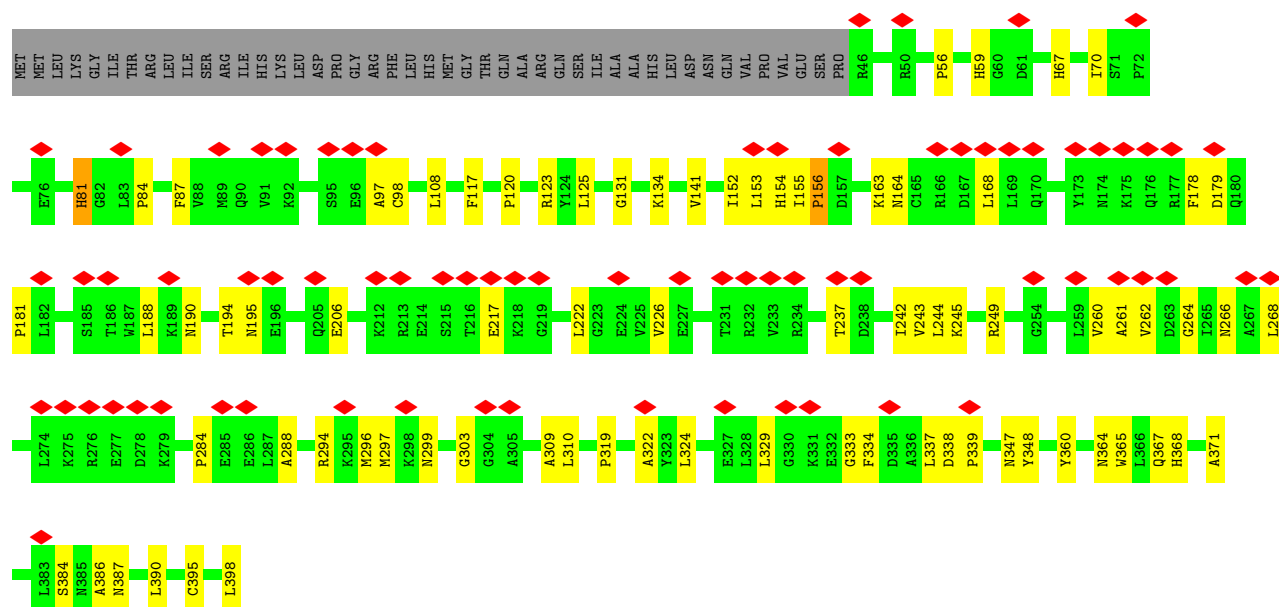


- Molecule 14: 28S ribosomal protein S28, mitochondrial

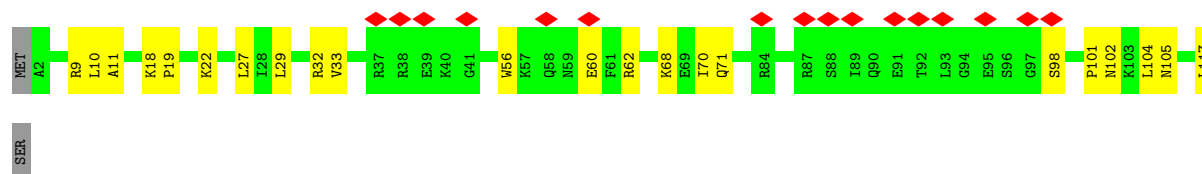
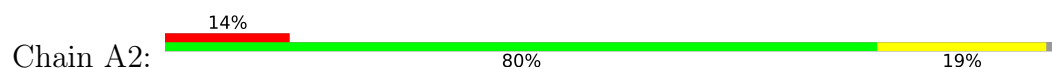


- Molecule 15: 28S ribosomal protein S29, mitochondrial

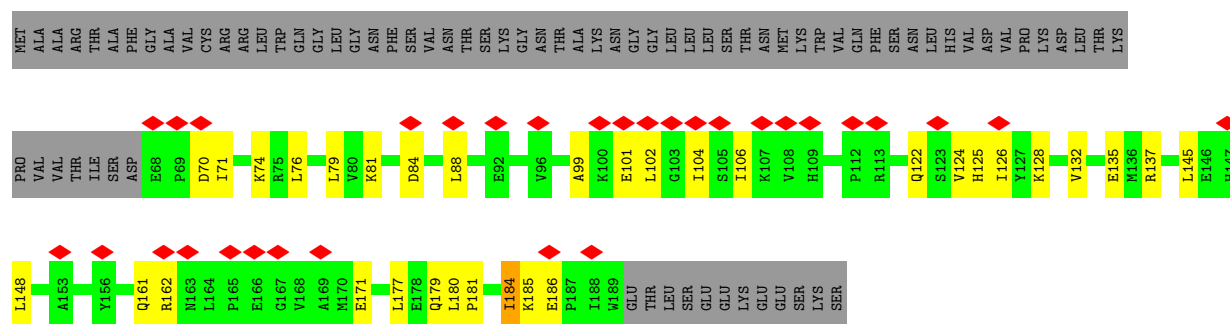




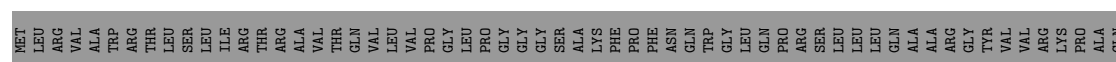
- Molecule 16: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



- Molecule 17: 28S ribosomal protein S10, mitochondrial

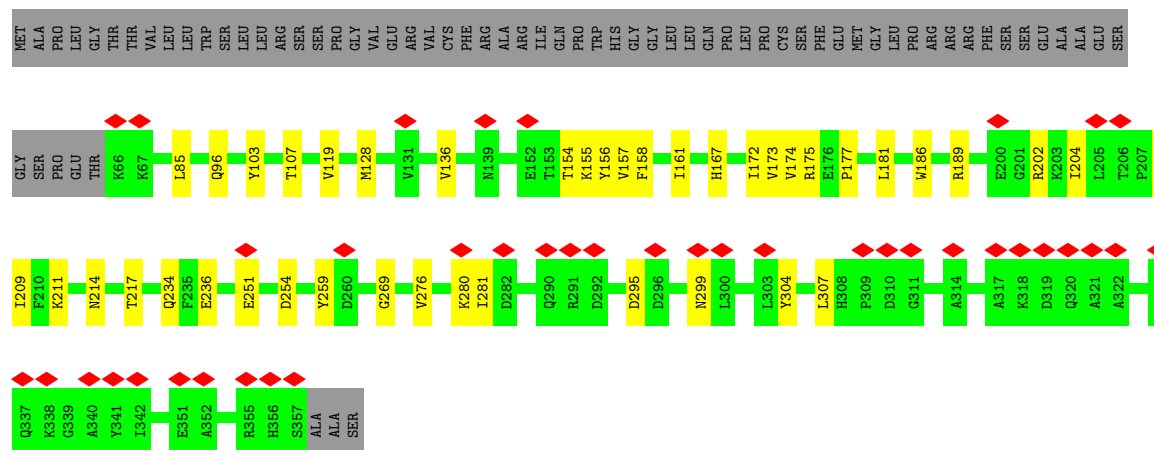
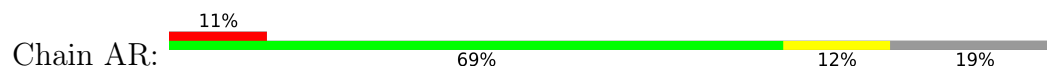


- Molecule 18: 28S ribosomal protein S15, mitochondrial

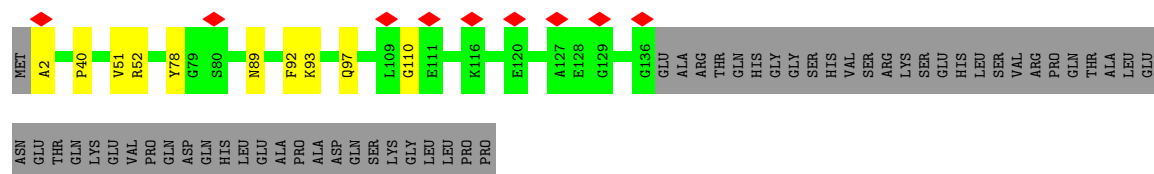




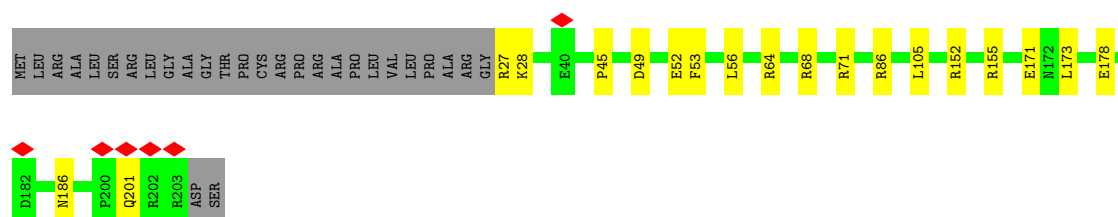
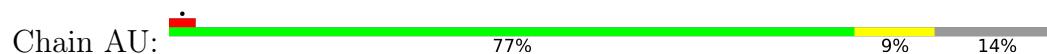
- Molecule 19: 28S ribosomal protein S22, mitochondrial



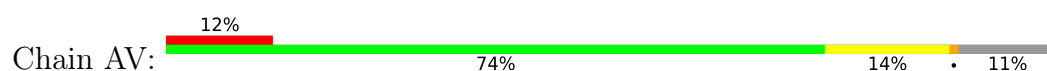
- Molecule 20: 28S ribosomal protein S23, mitochondrial

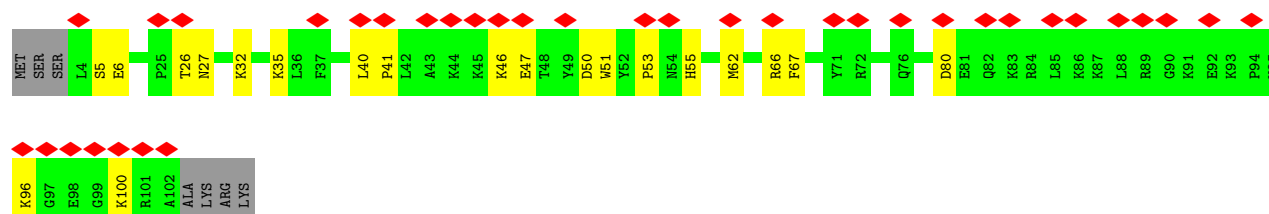
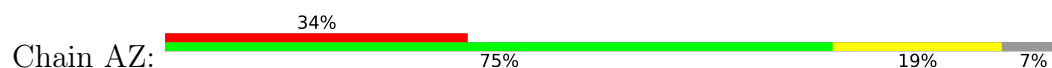
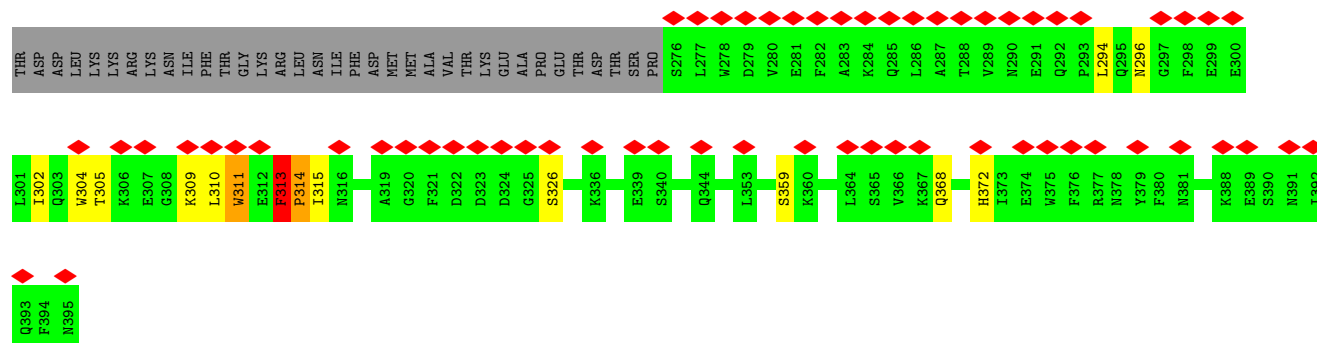


- Molecule 21: 28S ribosomal protein S26, mitochondrial

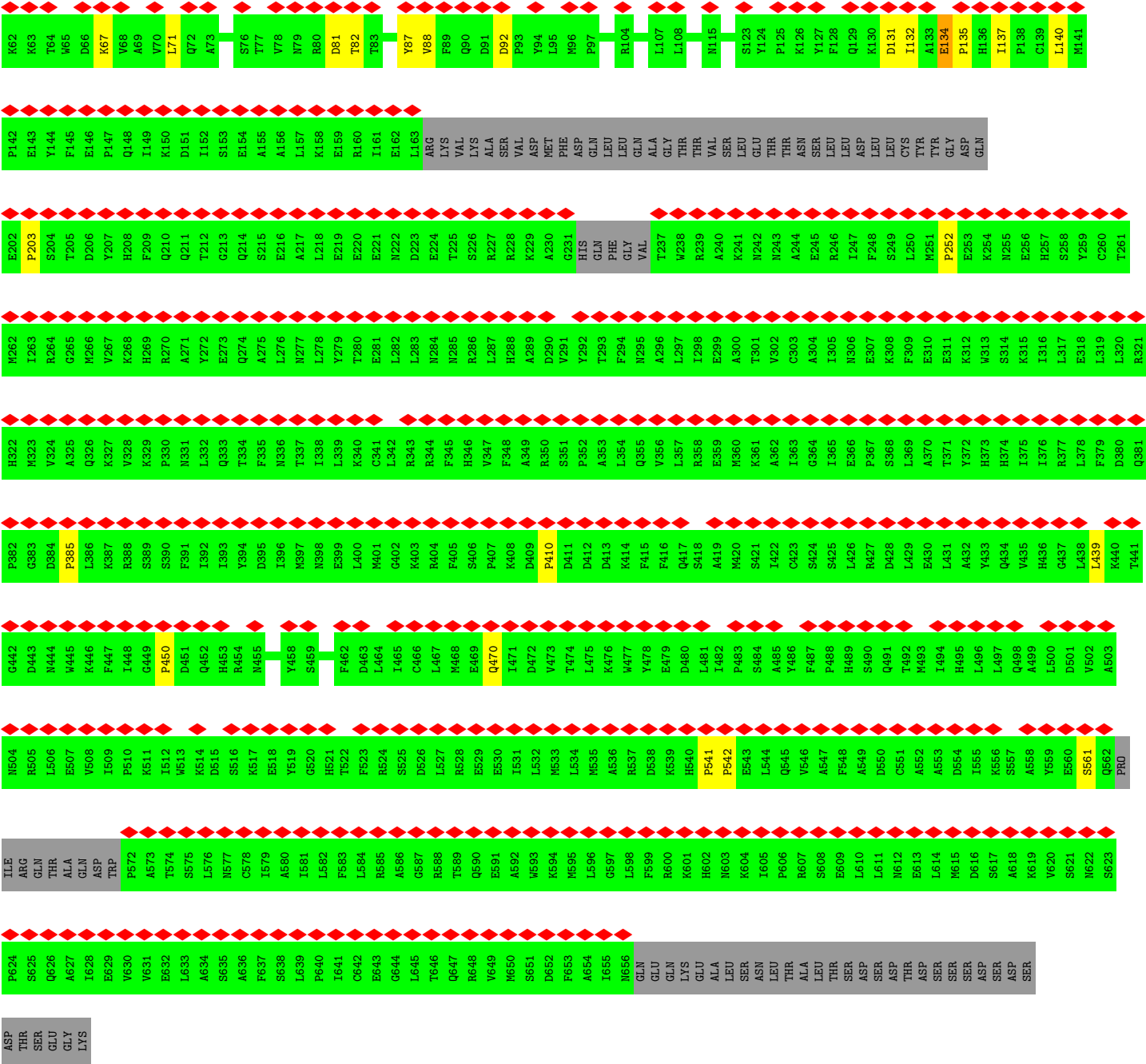


- Molecule 22: 28S ribosomal protein S27, mitochondrial

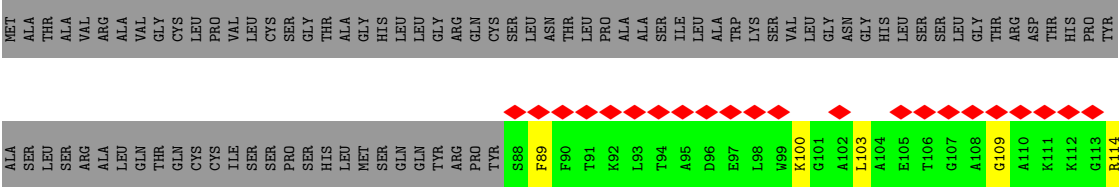


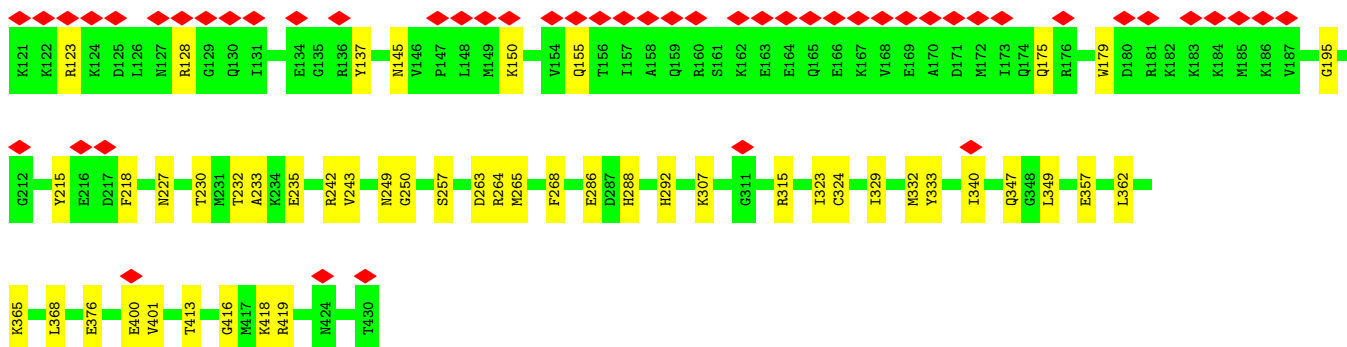


- Chain A4: 
- | Residue | Category |
|---------|----------|
| MET | Red |
| ALA | Red |
| VAL | Red |
| VAL | Red |
| SER | Red |
| ALA | Red |
| VAL | Red |
| ARG | Red |
| TRP | Red |
| LEU | Red |
| GLY | Red |
| ARG | Red |
| SER | Red |
| ARG | Red |
| LEU | Red |
| GLY | Red |
| GLN | Red |
| PRO | Red |
| LEU | Red |
| THR | Red |
| GLY | Red |
| ARG | Red |
| ALA | Red |
| GLY | Red |
| LEU | Red |
| CYS | Red |
| GLU | Red |
| GLN | Red |
| ALA | Red |
| ARG | Red |
| SER | Red |
| CYS | Red |
| ARG | Red |
| PHE | Red |
| TYR | Red |
| SER | Red |
| GLY | Red |
| SER | Red |
| THR | Red |
| LEU | Red |
| SER | Red |
| LYS | Red |
| VAL | Red |
| GLU | Red |
| GLY | Red |
| THR | Red |
| ASP | Red |
| VAL | Red |
| THR | Red |
| GLY | Red |
| ILE | Red |
| GLU | Red |
| E56 | Green |
| V57 | Green |
| V58 | Green |
| T59 | Green |

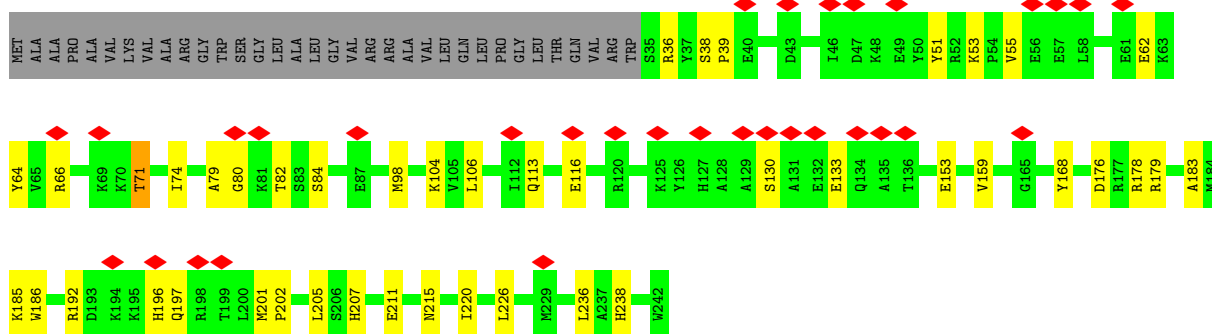


• Molecule 29: 28S ribosomal protein S5, mitochondrial

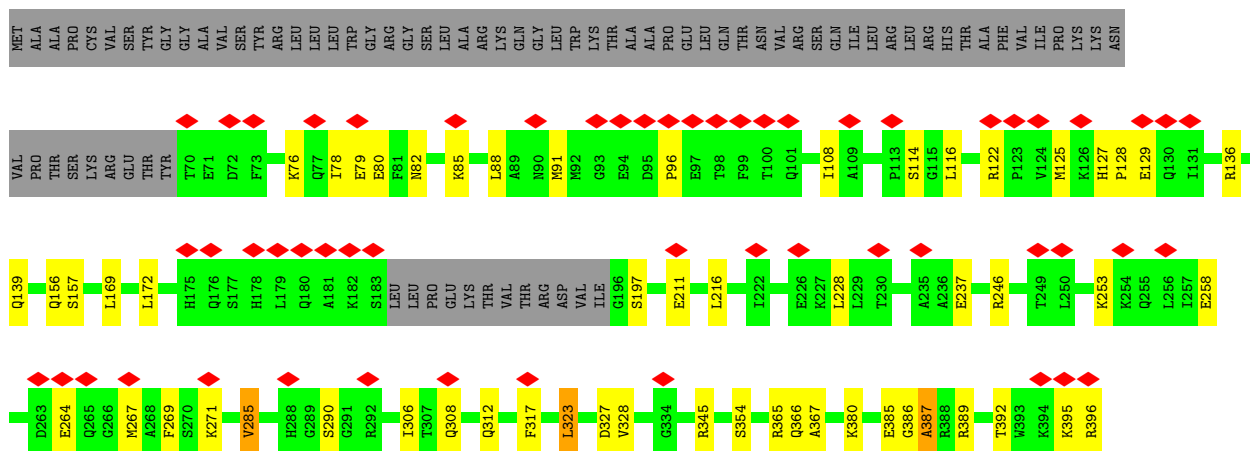




• Molecule 30: 28S ribosomal protein S7, mitochondrial



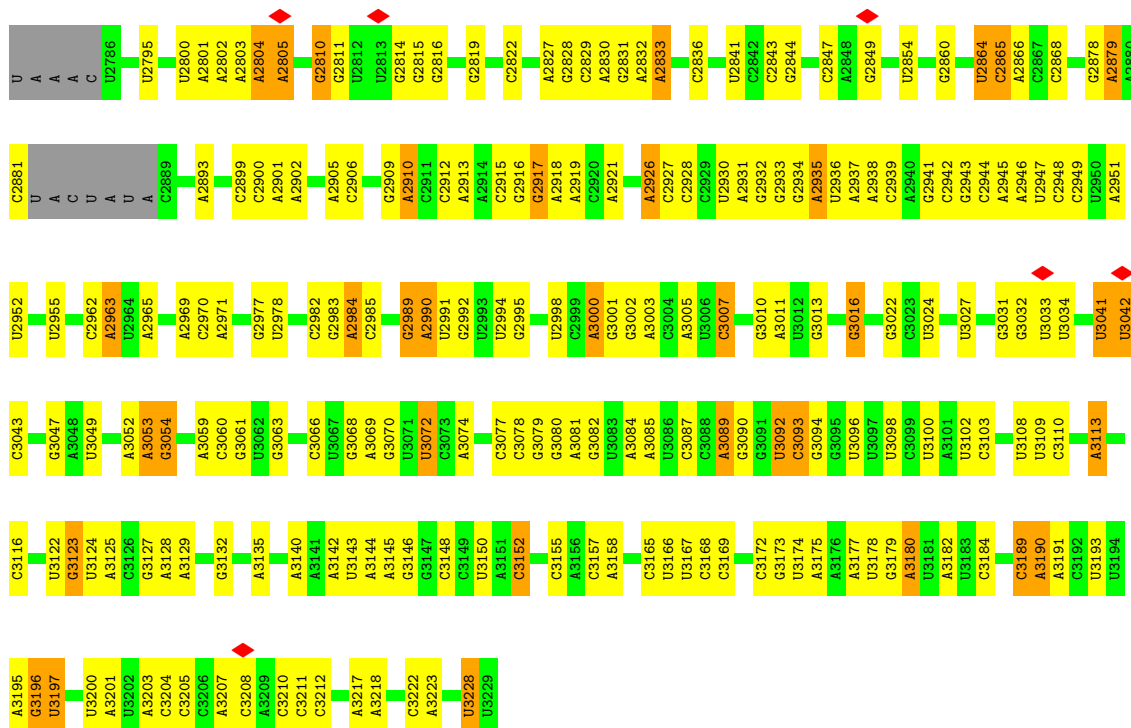
• Molecule 31: 28S ribosomal protein S9, mitochondrial



• Molecule 32: 16S rRNA



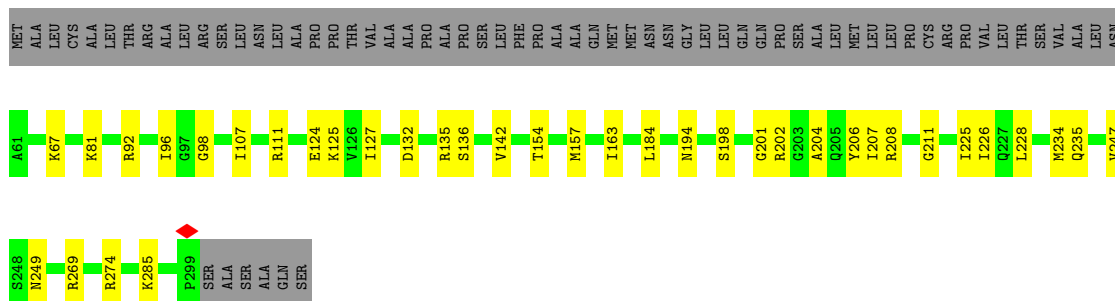
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G2719	A2644	G2571	G2471	C2380	U2301	A2181	A2084	C1903	A1823	A1752
A2723	G2645	A2576	A2472	A2381	A2302	G2182	A2085	A1907	U1824	A1753
G2724	G2646	A2577	A2473	A2382	A2303	A2185	A2086	A1908	C1827	G1754
A2725	G2647	A2578	A2474	U2383	G2304	A2186	U2087	A1909	A1828	A1755
A2726	C2650	A2579	G2478	A2384	U2307	A2187	U2088	C1910	A1829	A1756
C2727	G2651	C2577	A2482	A2388	A2308	U2171	C2092	C1911	G1830	G1760
G2728	A2652	A2578	U2483	C2389	U2311	A2172	G2093	A1912	A1831	A1761
U2729	C2653	C2579	C2484	A2390	A2312	G2173	G2094	G1915	C1832	A1762
G2730	G2654	U2580	C2489	A2393	A2313	G2174	A2097	G1916	C1833	A1763
C2731	G2655	A2581	C2490	C2394	C2314	C2175	G2098	A1917	A1834	A1764
A2732	U2656	C2582	A2491	A2395	A2315	A2180	U2099	G1918	A1835	G1765
G2733	C2657	G2583	A2492	C2396	U2316	A2181	G2099	U1924	C1836	C1766
U2734	U2658	C2584	C2493	A2397	A2317	G2182	C2100	U1925	A1837	U1766
C2735	G2659	G2585	A2494	C2398	A2318	A2183	C2101	A1926	C1838	G1767
A2736	U2660	U2586	A2503	C2399	A2319	C2184	A2102	C1927	C1839	G1768
U2737	U2661	C2587	A2504	U2404	A2320	A2185	A2103	A1928	C1840	C1769
G2738	U2662	C2588	A2505	U2407	A2321	G2186	A2104	C1930	A1844	G1770
A2739	A2663	A2589	A2506	A2408	C2322	C2187	G2105	A1935	U1848	C1771
C2740	U2664	A2590	U2507	C2414	U2325	A2188	G2108	C1936	U1849	A1772
U2741	U2665	C2591	C2508	C2415	U2326	C2189	A2109	A1937	C1849	A1777
A2742	U2666	G2592	A2509	U2420	U2330	A2191	A2110	A1938	C1852	A1781
U2743	U2667	G2593	A2510	G2421	C2331	C2192	G2111	G1939	A1853	G1782
C2744	A2668	U2594	C2511	U2422	C2332	A2193	G2112	A1940	U1854	U1783
A2745	U2669	C2595	G2512	A2423	G2333	U2194	G2113	C1941	A1855	
U2746	C2670	A2596	G2513	A2424	C2334	A2195	U2117	C1942	A1856	
U2747	G2671	A2601	A2514	C2425	U2335	A2196	C2123	C1943	C1857	G1787
A2748	U2672	C2603	A2515	C2426	A2264	G2197	A2124	C1944	A1859	A1789
U2749	U2673	U2606	A2516	C2427	A2265	A2198	U2125	C1951	A1860	A1790
C2750	U2674	U2607	A2517	A2428	U2266	A2199	U2126	U1952	U1861	G1791
A2751	C2675	C2608	A2518	A2429	U2267	A2200	C2136	U1953	U1862	G1792
U2752	A2676	A2609	A2519	A2430	G2268	G2201	U2137	U1954	A1863	G1793
C2753	U2677	U2610	A2520	A2431	C2272	C2202	A2132	A1794	A1864	A1795
A2754	A2678	C2611	A2521	G2440	A2273	G2203	A2133	G1958	A1867	
U2755	C2679	U2612	A2522	C2441	U2274	U2204	A2134	A1959	G1868	A1798
C2756	U2680	G2613	A2523	U2442	C2275	C2205	A2135	A1960	A1869	U1799
A2757	G2681	A2614	A2524	C2443	U2276	C2206	C2136	U1979	U1870	G1800
U2758	U2682	U2615	A2525	A2444	U2277	A2207	U2138	A1965	A1871	A1803
C2759	G2683	A2616	A2526	A2445	A2278	A2208	U2139	G1966	U1872	A1804
A2760	U2684	U2617	A2527	A2446	A2279	G2209	A2142	G1967	A1873	A1805
C	G2685	U2618	A2528	A2447	C2280	C2210	G2143	G1968	U1877	U1806
C	C2686	A2619	A2529	G2448	A2281	U2211	A2144	U1979	A1881	A1807
C	C2687	U2620	A2530	G2449	C2282	C2212	G2145	A1980	A1882	A1808
C	U2688	G2621	A2531	A2453	C2283	A2213	A2146	G1981	A1883	A1809
C	G2689	U2622	A2532	A2454	C2284	C2214	G2147	G1982	A1884	A1810
C	U2690	C2623	A2533	A2455	C2285	A2215	A2151	G1985	C1812	C1813
C	G2691	U2624	A2534	A2456	C2286	C2216	A2152	A1986	C1814	A1814
C	U2692	C2625	A2535	A2457	C2287	C2217	A2153	G1987	A1815	A1816
C	A2693	U2626	A2536	A2458	C2288	C2218	A2154	C1992	G1899	C1817
C	C2694	G2627	A2537	A2459	C2289	C2219	A2155	A1994	A1900	A1818
C	U2695	U2628	A2538	A2460	C2290	U2222	A2156			
C	A2696	A2629	A2539	A2461	C2291	A2223	U2157			
C	G2697	U2630	A2540	A2462	C2292	C2224	U2158			
C	U2698	A2631	A2541	A2463	C2293	C2225	U2159			
C	C2700	U2632	A2542	A2464	C2294	U2226				
C	A2701	A2633	A2543	A2465	C2295	C2227				
C	C2702	G2634	A2544	A2466	C2296	C2228				
C	U2703	U2635	A2545	A2467	A2297	C2229				
C	A2704	C2636	A2546	A2468	A2298	U2229				
C	C2705	U2637	A2547			U2230				
C	U2706	A2638	A2548			U2231				
C	G2707		A2549			U2232				
C	A2708		A2550			U2233				
C	U2709		A2551			U2234				
C	C2710		A2552			U2235				
C	A2711		A2553			U2236				
C	G2712		A2554			U2237				
C	U2713		A2555			U2238				
C	C2714		A2556			U2239				
C	A2715		A2557			U2240				
C			A2558			U2241				
C			U2559			U2242				
C			A2560			U2243				
C						U2244				
C						U2245				
C						U2246				
C						U2247				
C						U2248				
C						U2249				
C						U2250				
C						U2251				
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C						U2339				
C										



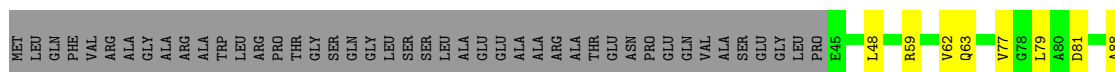
• Molecule 33: tRNA^{Val}

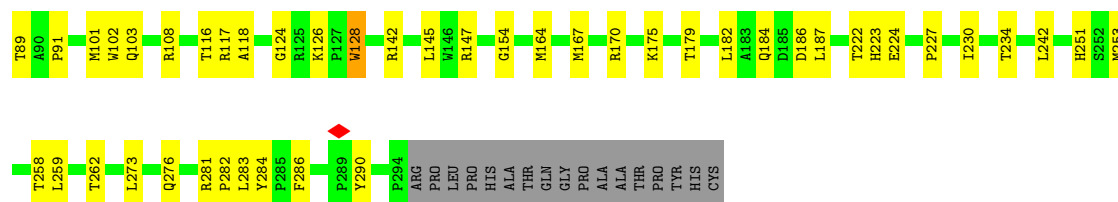


• Molecule 34: 39S ribosomal protein L2, mitochondrial

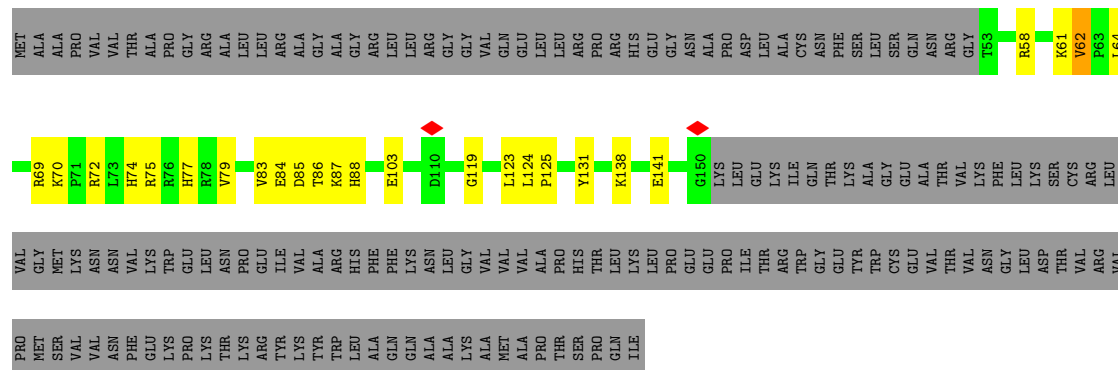


• Molecule 35: 39S ribosomal protein L4, mitochondrial

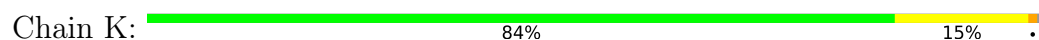




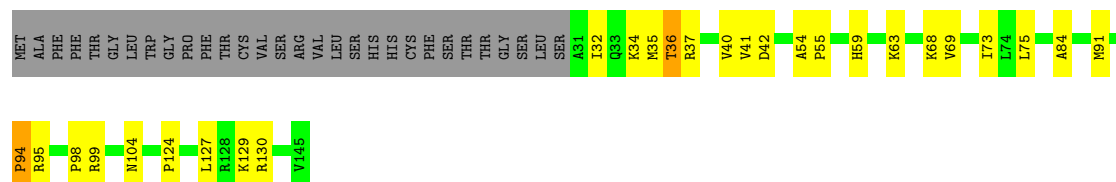
- Molecule 36: 39S ribosomal protein L9, mitochondrial



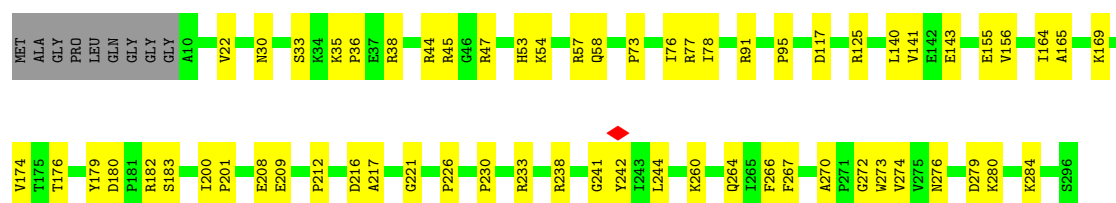
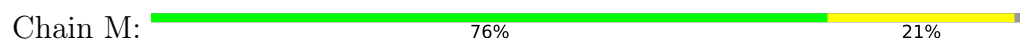
- Molecule 37: 39S ribosomal protein L13, mitochondrial



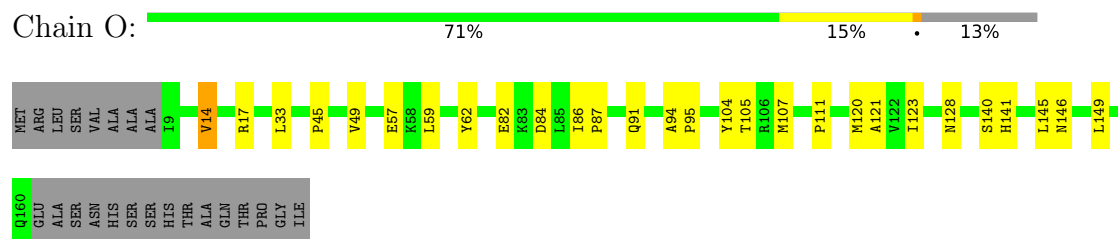
- Molecule 38: 39S ribosomal protein L14, mitochondrial



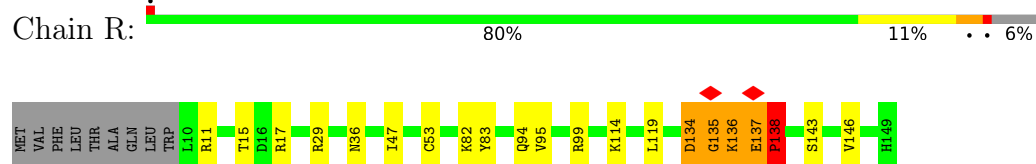
- Molecule 39: 39S ribosomal protein L15, mitochondrial



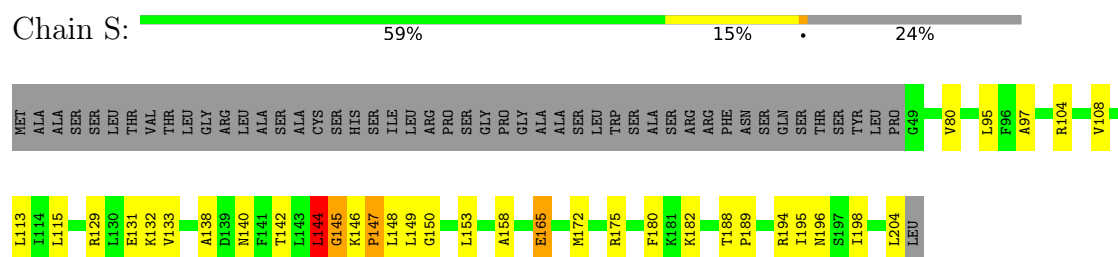
- Molecule 40: 39S ribosomal protein L17, mitochondrial



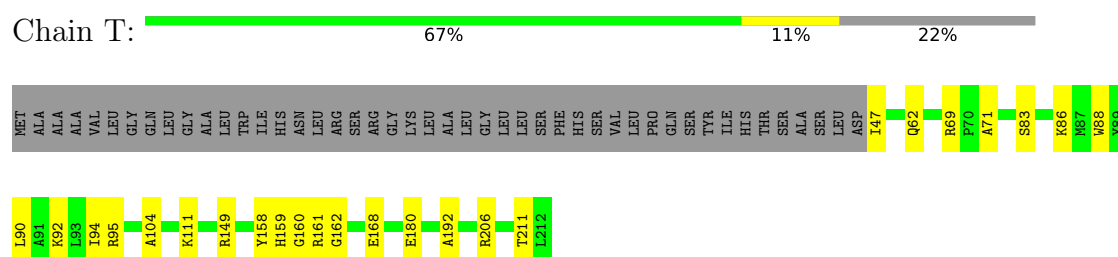
- Molecule 41: 39S ribosomal protein L20, mitochondrial



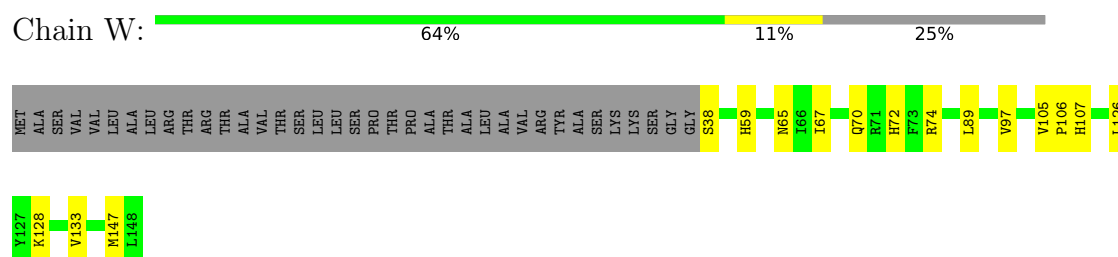
- Molecule 42: 39S ribosomal protein L21, mitochondrial



- Molecule 43: 39S ribosomal protein L22, mitochondrial



- Molecule 44: 39S ribosomal protein L27, mitochondrial



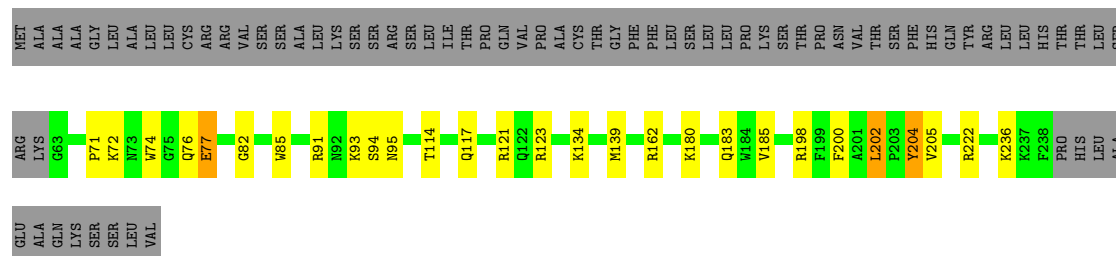
- Molecule 45: 39S ribosomal protein L28, mitochondrial

Chain X:  80% 14% 5%



- Molecule 46: 39S ribosomal protein L47, mitochondrial

Chain Y:  59% 10% 30%



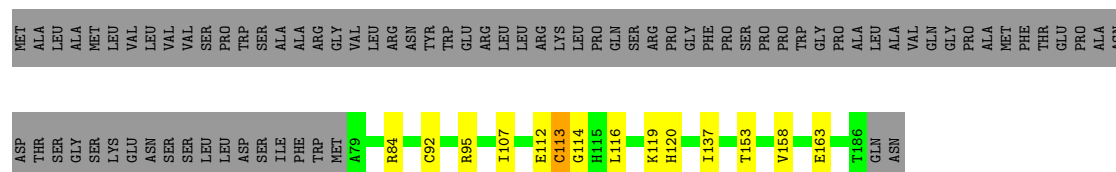
- Molecule 47: 39S ribosomal protein L30, mitochondrial

Chain Z:  63% 12% 25%



- Molecule 48: 39S ribosomal protein L32, mitochondrial

Chain 0:  50% 7% 43%

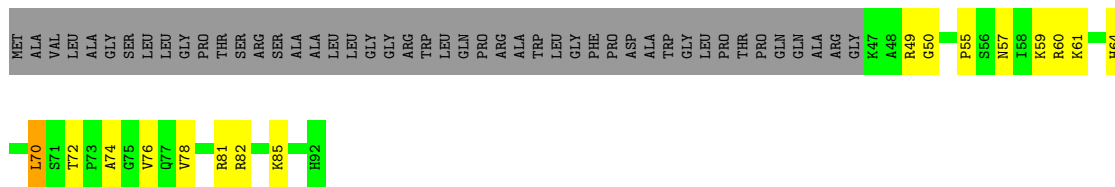


- Molecule 49: 39S ribosomal protein L33, mitochondrial

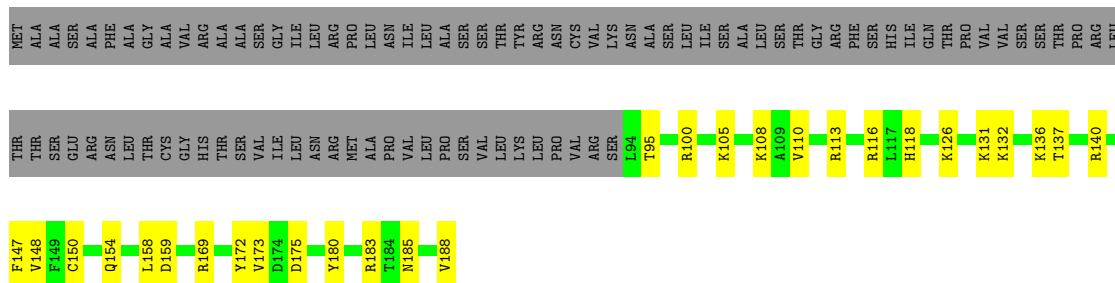
Chain 1:  63% 17% 20%



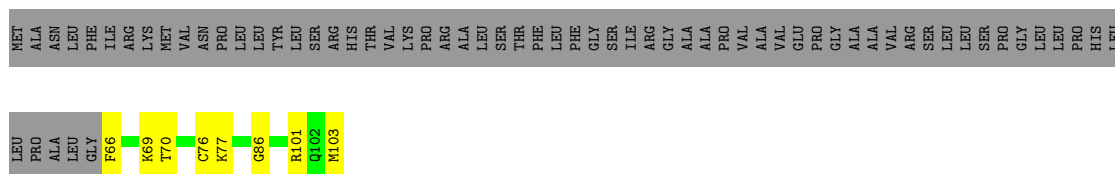
- Molecule 50: 39S ribosomal protein L34, mitochondrial



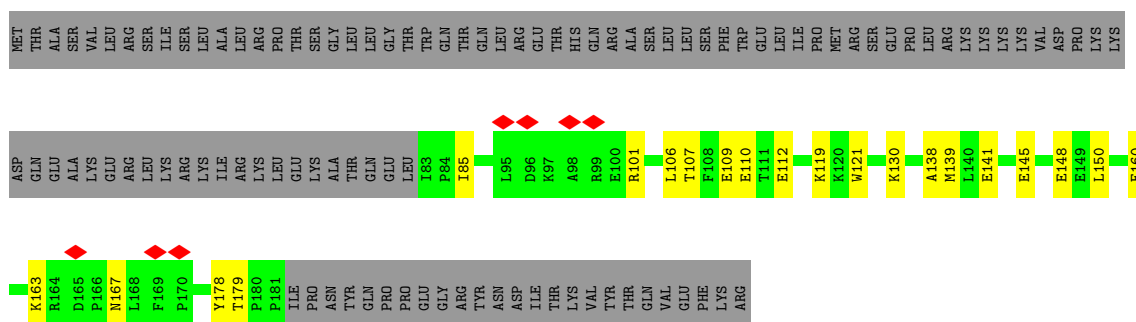
- Molecule 51: 39S ribosomal protein L35, mitochondrial



- Molecule 52: 39S ribosomal protein L36, mitochondrial



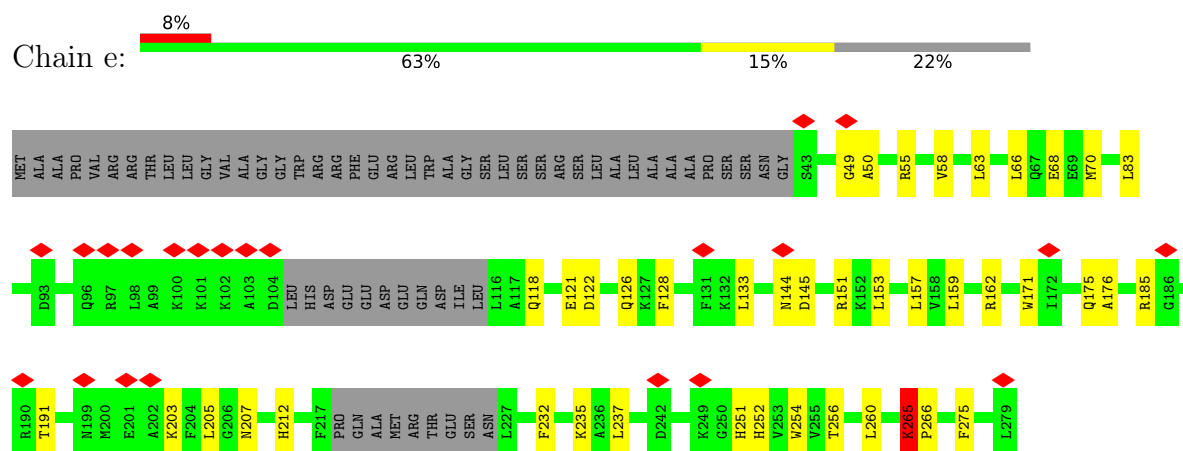
- Molecule 53: 39S ribosomal protein L40, mitochondrial



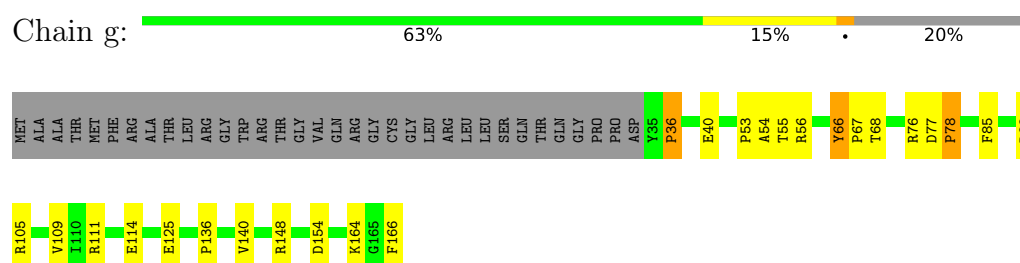
- Molecule 54: 39S ribosomal protein L43, mitochondrial



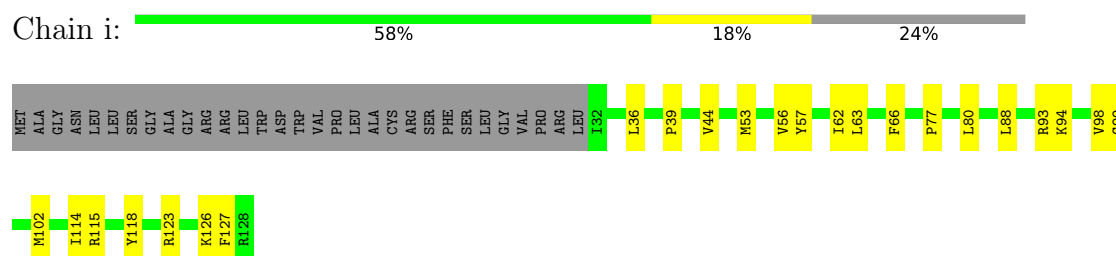
- Molecule 55: 39S ribosomal protein L46, mitochondrial



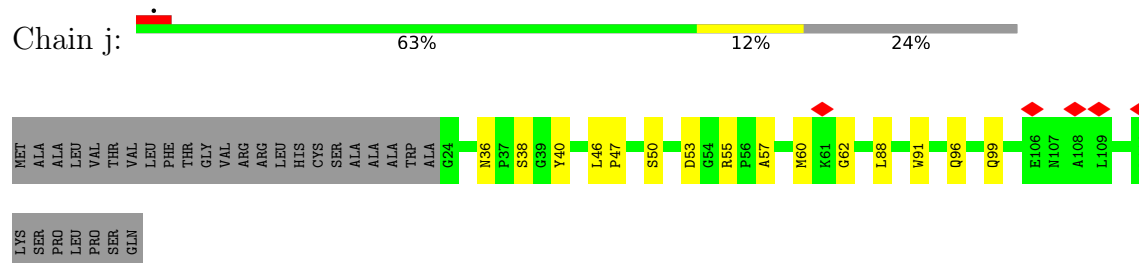
- Molecule 56: 39S ribosomal protein L49, mitochondrial



- Molecule 57: 39S ribosomal protein L51, mitochondrial

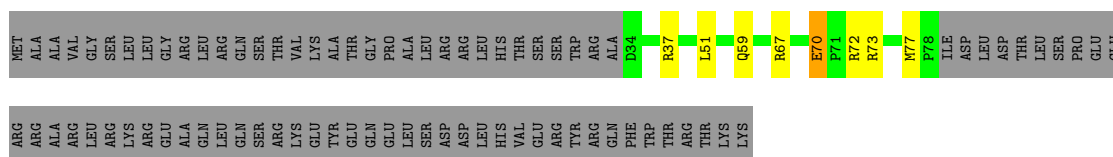


- Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



- Molecule 59: 39S ribosomal protein L55, mitochondrial

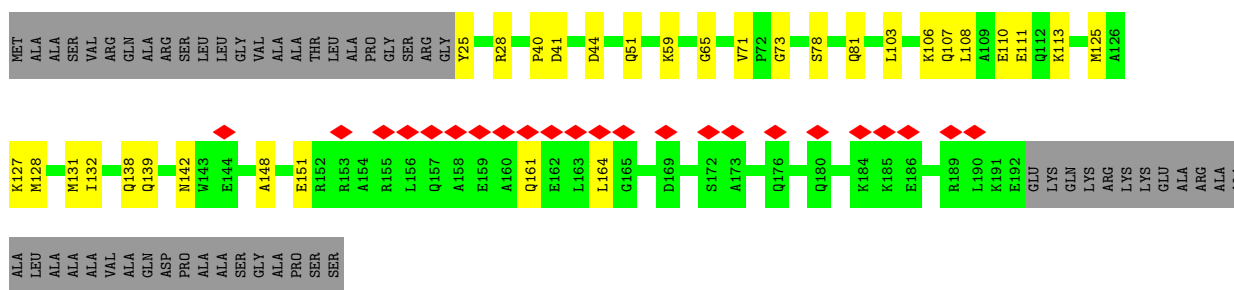




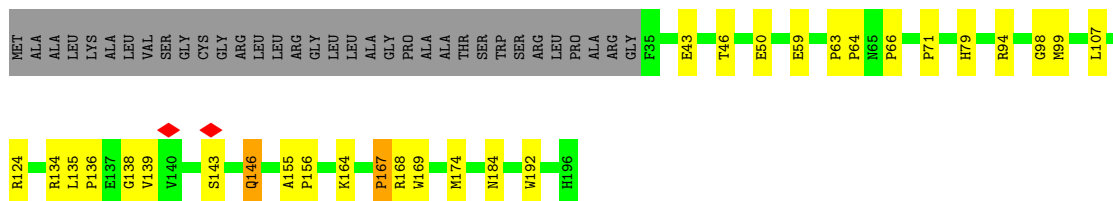
- Molecule 60: Ribosomal protein 63, mitochondrial



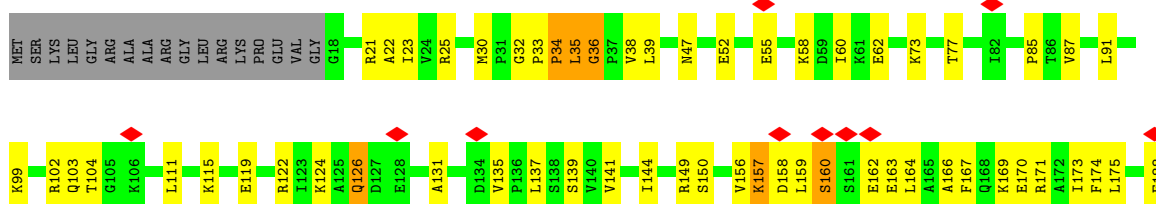
- Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 62: 39S ribosomal protein S18a, mitochondrial

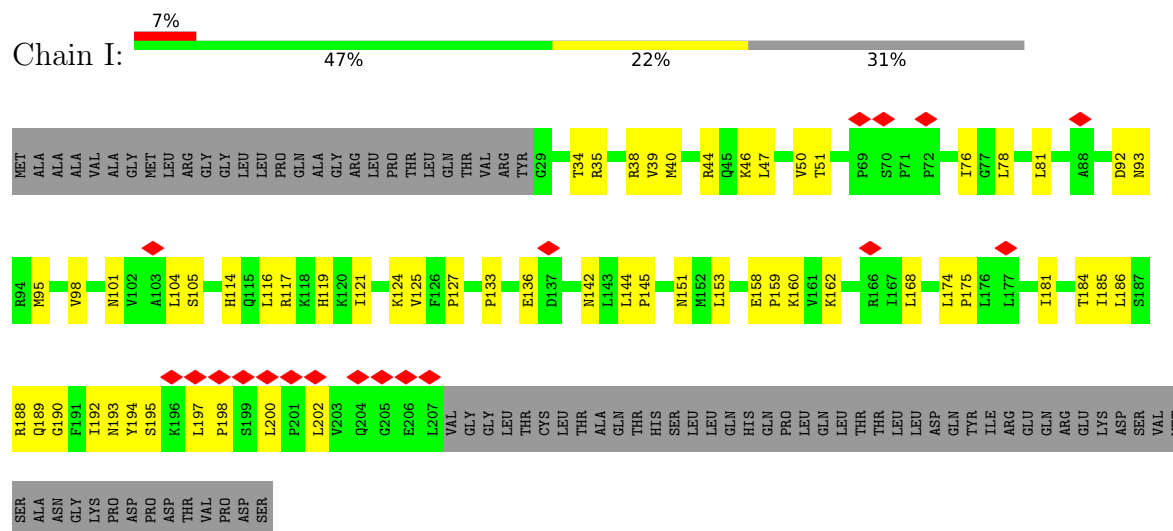


- Molecule 63: 39S ribosomal protein L11, mitochondrial

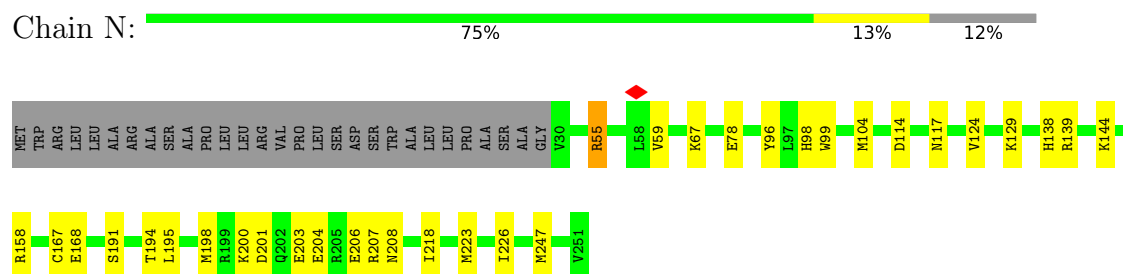




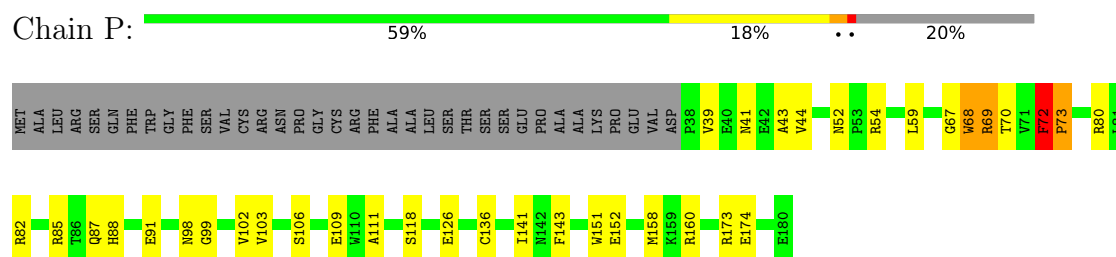
- Molecule 64: 39S ribosomal protein L10, mitochondrial



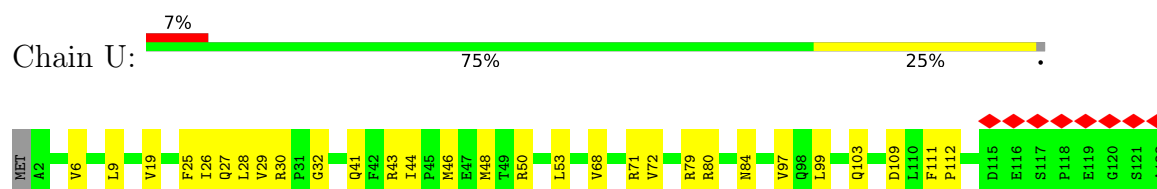
- Molecule 65: 39S ribosomal protein L16, mitochondrial



- Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA_b



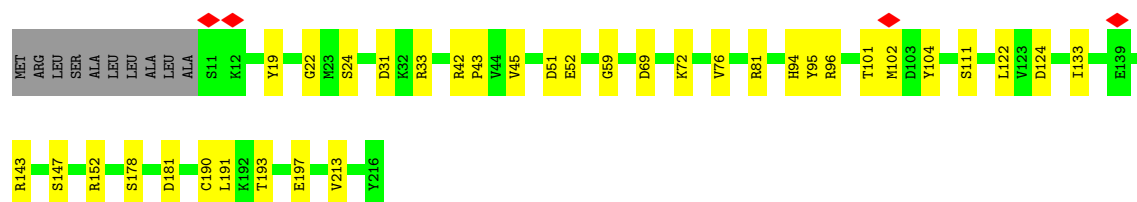
- Molecule 67: 39S ribosomal protein L23, mitochondrial





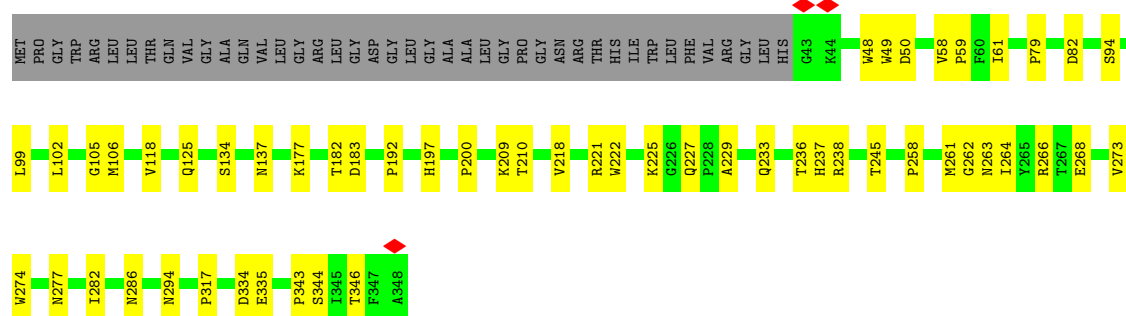
- Molecule 68: 39S ribosomal protein L24, mitochondrial

Chain V: 79% 16% 5%



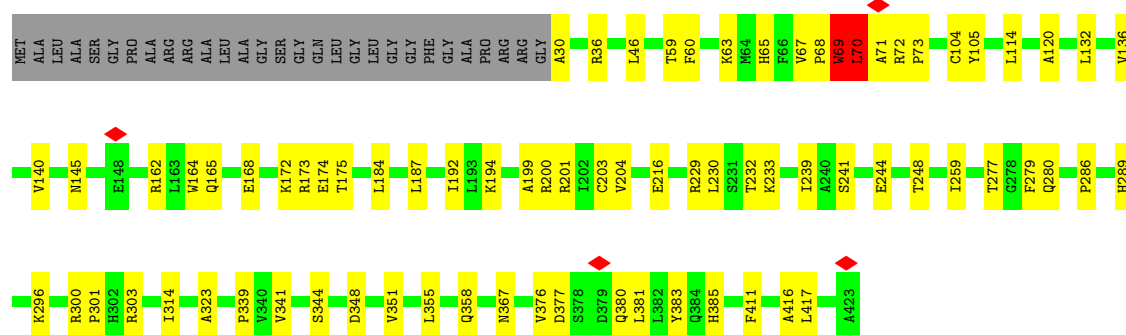
- Molecule 69: 39S ribosomal protein L3, mitochondrial

Chain E: 72% 16% 12%



- Molecule 70: 39S ribosomal protein L37, mitochondrial

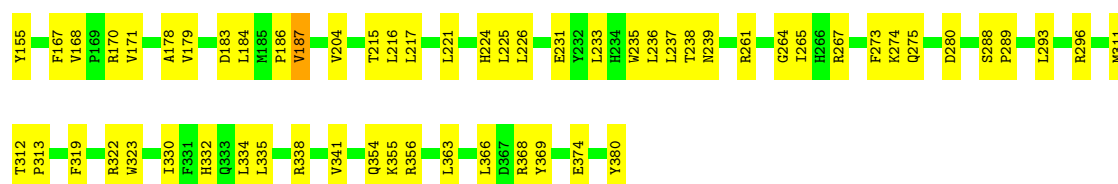
Chain 5: 75% 18% 7%



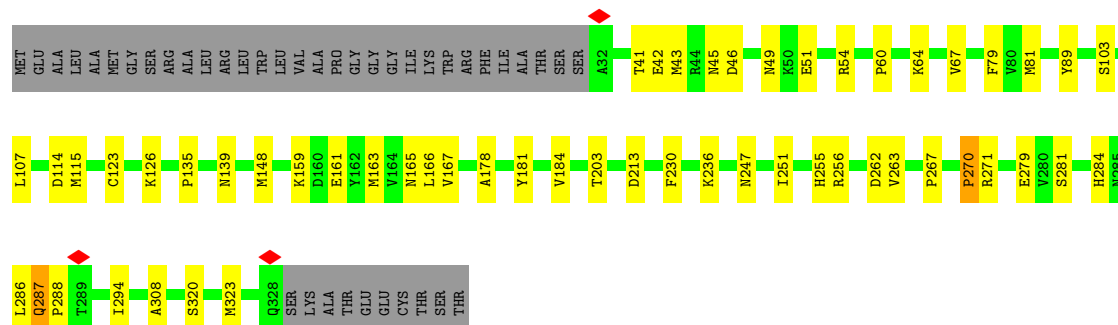
- Molecule 71: 39S ribosomal protein L38, mitochondrial

Chain 6: 74% 19% 7%

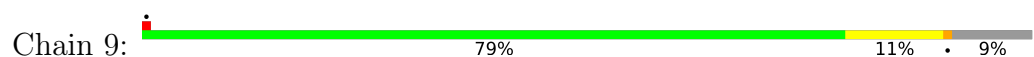




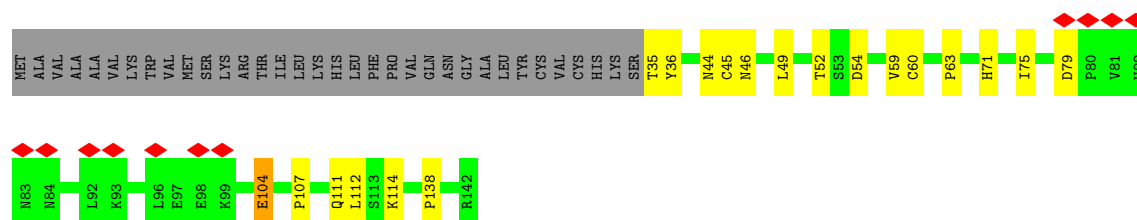
- Molecule 72: 39S ribosomal protein L39, mitochondrial



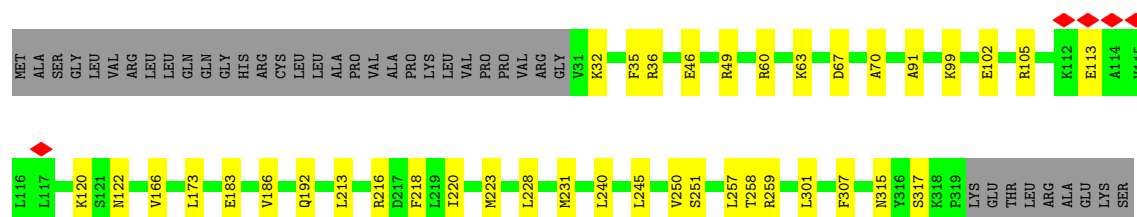
- Molecule 73: 39S ribosomal protein L41, mitochondrial



- Molecule 74: 39S ribosomal protein L42, mitochondrial



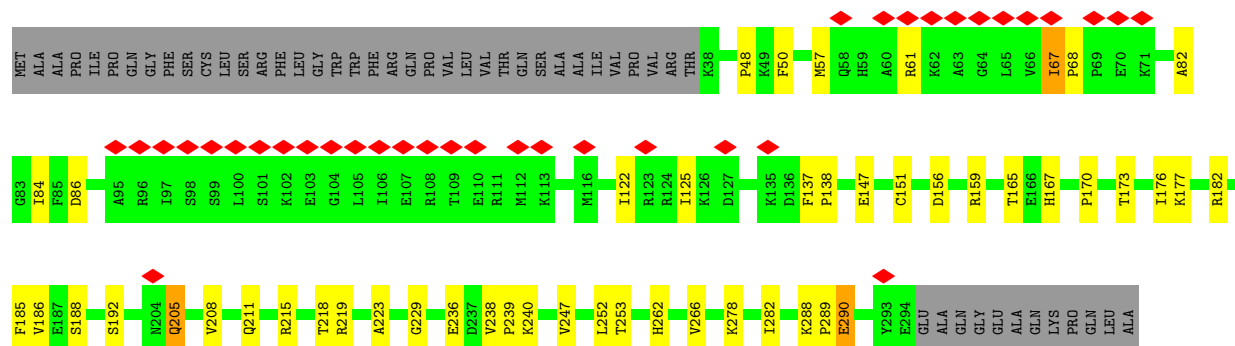
- Molecule 75: 39S ribosomal protein L44, mitochondrial



ILE
THR
ALA
SER

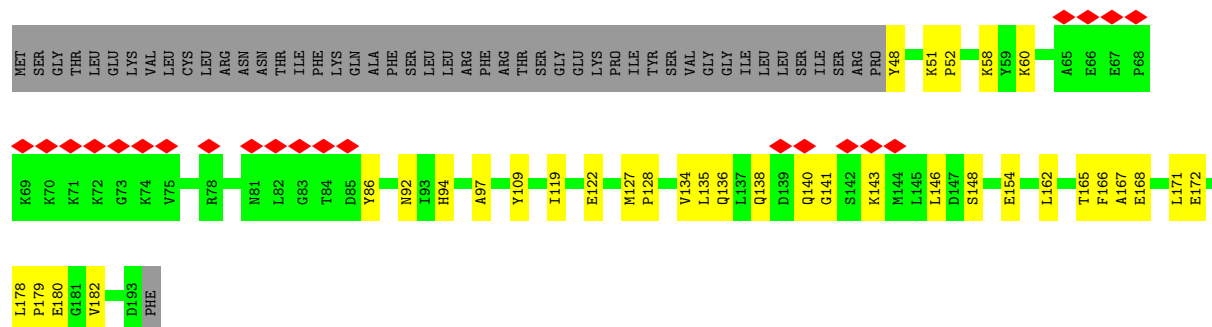
- Molecule 76: 39S ribosomal protein L45, mitochondrial

Chain d: 



- Molecule 77: 39S ribosomal protein L48, mitochondrial

Chain f: 



- Molecule 78: 39S ribosomal protein L50, mitochondrial

Chain h: 

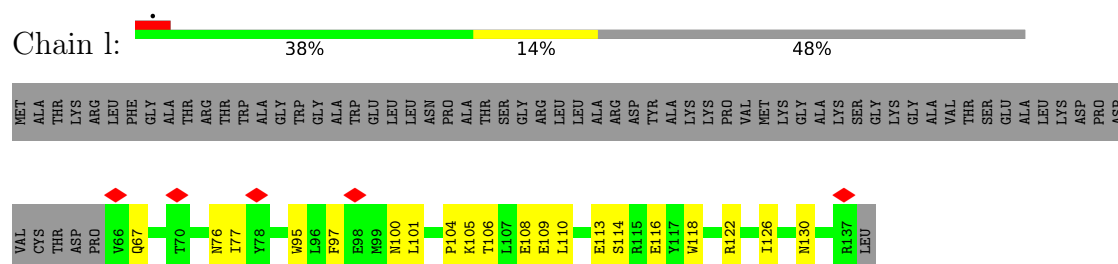


- Molecule 79: 39S ribosomal protein L53, mitochondrial

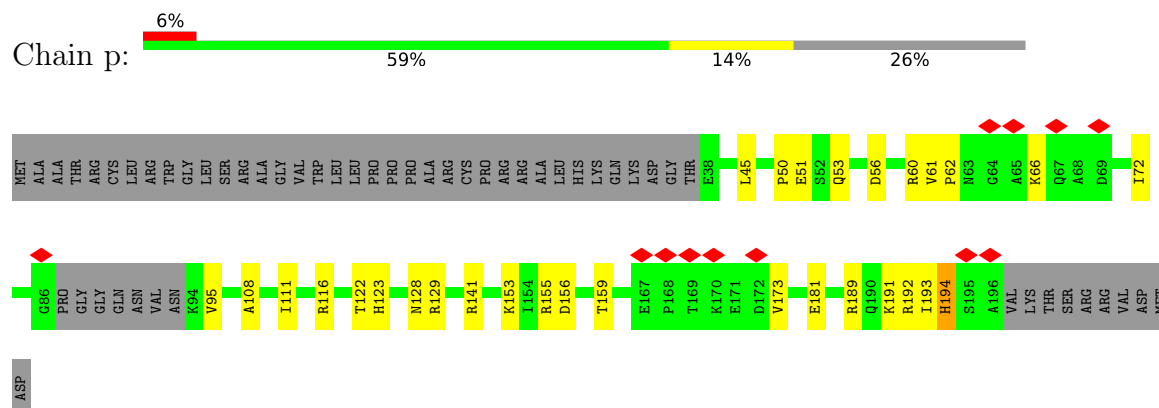
Chain k: 



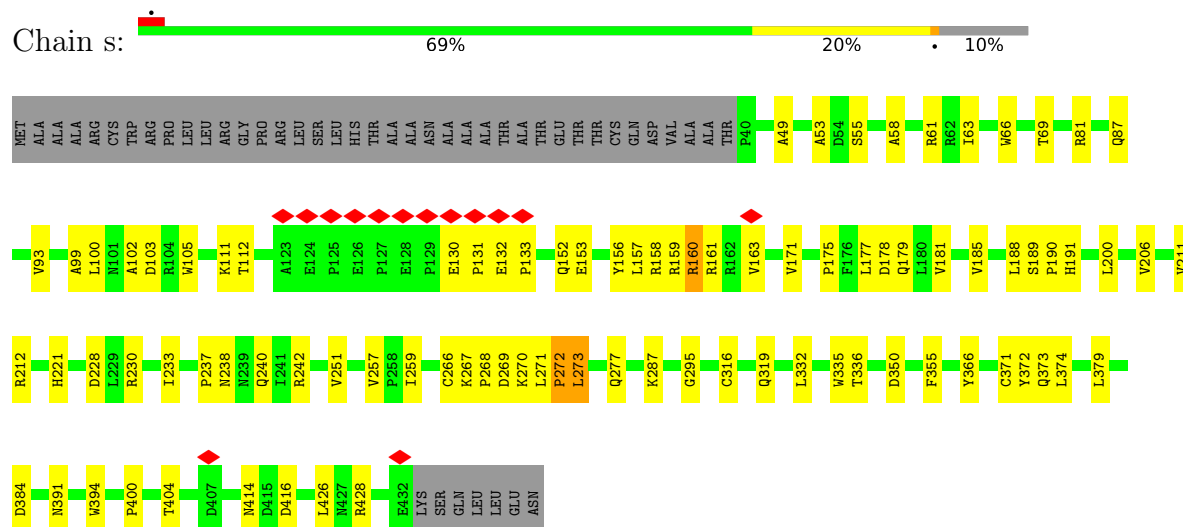
- Molecule 80: 39S ribosomal protein L54, mitochondrial



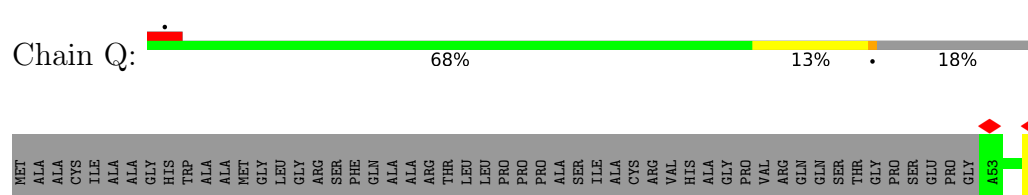
- Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial

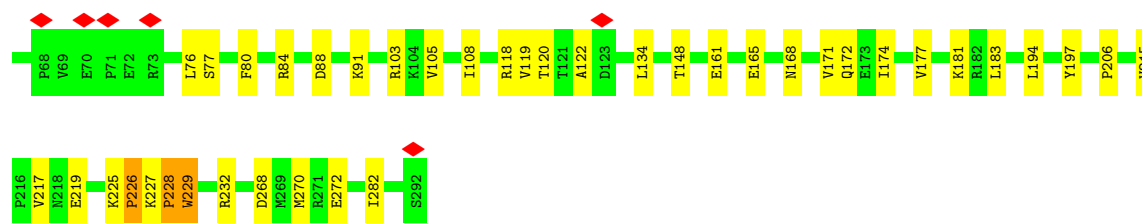


- Molecule 82: 39S ribosomal protein S30, mitochondrial

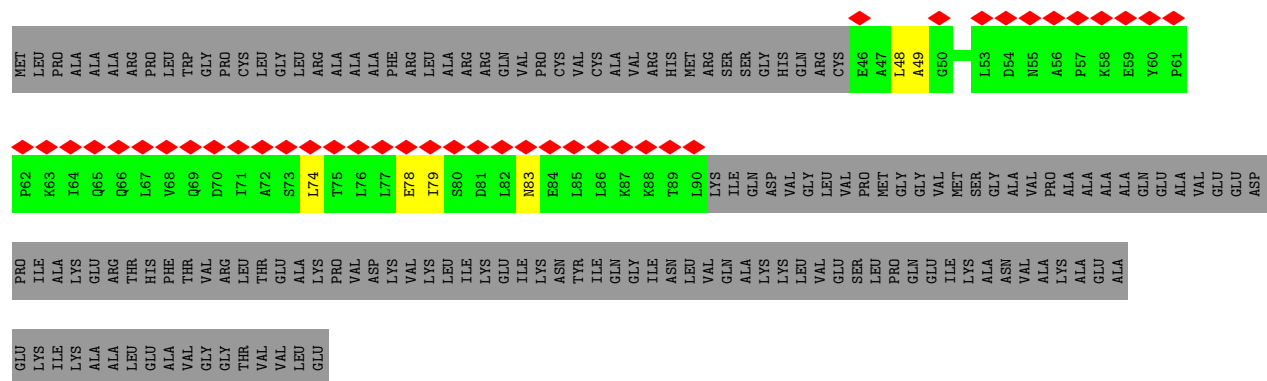


- Molecule 83: 39S ribosomal protein L19, mitochondrial

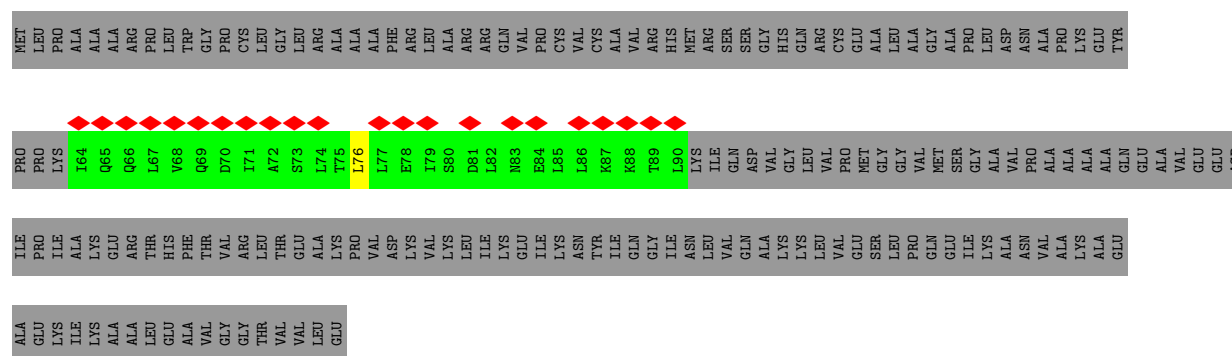




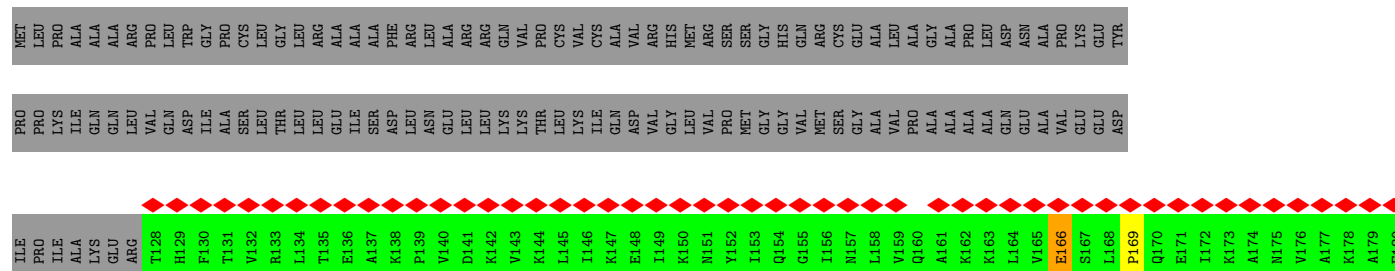
- Molecule 84: 39S ribosomal protein L12, mitochondrial

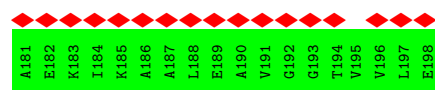


- Molecule 84: 39S ribosomal protein L12, mitochondrial

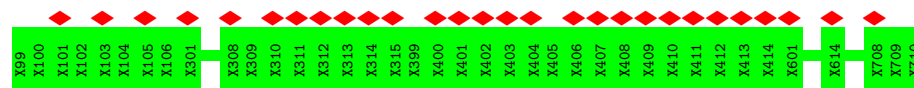
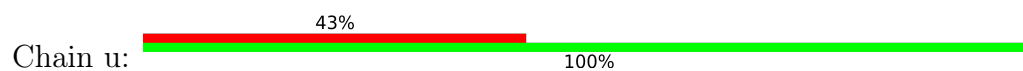


- Molecule 84: 39S ribosomal protein L12, mitochondrial

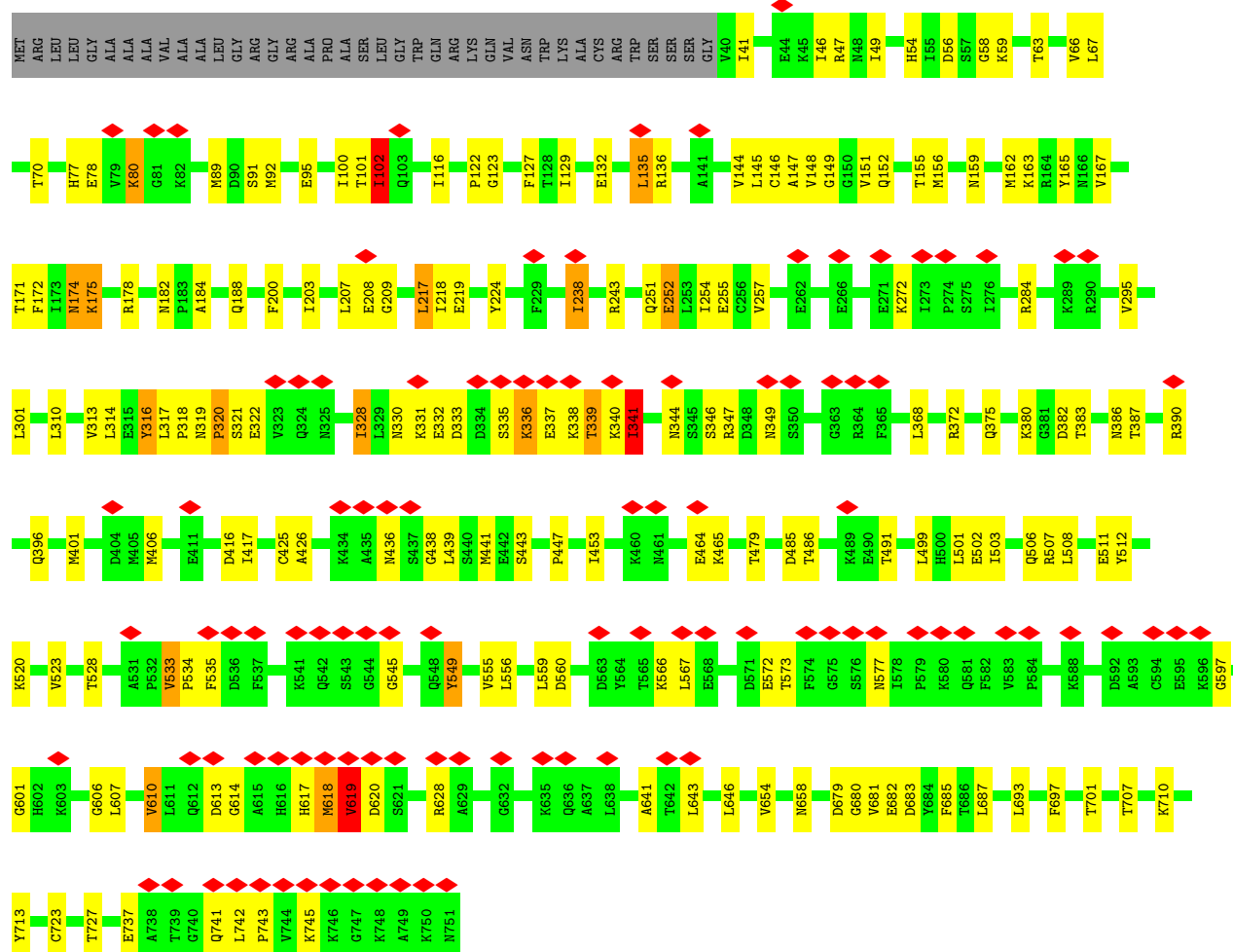




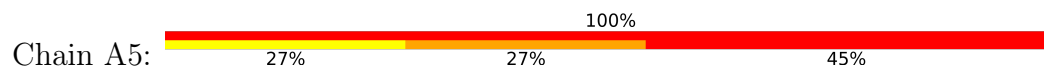
• Molecule 85: P-site finger

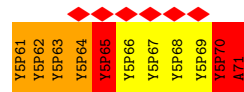


• Molecule 86: Elongation factor G, mitochondrial



• Molecule 87: mRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150347	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	4.076	Depositor
Minimum map value	-1.966	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.267	Depositor
Map size (Å)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: P5P, GDP, Y5P, MG, GCP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.07	0/22406	0.17	0/34881
2	AB	0.07	0/1830	0.22	0/2477
3	AC	0.08	0/1112	0.28	0/1505
4	AE	0.09	0/989	0.33	0/1335
5	AI	0.07	0/1031	0.25	0/1390
6	AJ	0.09	0/854	0.27	0/1148
7	AK	0.09	0/879	0.30	0/1182
8	AM	0.10	0/941	0.34	0/1265
9	AN	0.07	0/864	0.22	0/1169
10	AO	0.07	0/1624	0.23	0/2209
11	AP	0.07	0/791	0.21	0/1062
12	AQ	0.09	0/752	0.26	0/1001
13	AT	0.07	0/1402	0.20	0/1883
14	AW	0.08	0/778	0.27	0/1048
15	AX	0.08	0/2932	0.23	0/3968
16	A2	0.08	0/939	0.26	0/1256
17	AH	0.08	0/1037	0.22	0/1403
18	AL	0.09	0/1475	0.25	0/1970
19	AR	0.07	0/2435	0.20	0/3288
20	AS	0.08	0/1138	0.22	0/1533
21	AU	0.10	0/1521	0.26	0/2039
22	AV	0.08	0/3071	0.21	0/4147
23	AY	0.14	0/1046	0.41	4/1410 (0.3%)
24	AZ	0.07	0/851	0.20	0/1133
25	A1	0.07	0/2277	0.21	0/3079
26	A0	0.08	0/1827	0.26	0/2473
27	A3	0.10	0/650	0.29	0/855
28	A4	0.06	0/3028	0.18	0/4197
29	AD	0.07	0/2783	0.22	0/3724
30	AF	0.09	0/1765	0.25	0/2369
31	AG	0.08	0/2642	0.23	0/3538
32	A	0.10	2/36246 (0.0%)	0.21	2/56422 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B	0.06	0/1328	0.15	0/2056
34	D	0.07	0/1904	0.24	0/2561
35	F	0.08	0/2071	0.26	0/2817
36	H	0.10	0/820	0.28	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	0.28	0/3185
40	O	0.10	0/1269	0.28	0/1708
41	R	0.12	0/1174	0.54	7/1572 (0.4%)
42	S	0.11	0/1276	0.47	3/1729 (0.2%)
43	T	0.08	0/1402	0.24	0/1886
44	W	0.07	0/893	0.22	0/1204
45	X	0.08	0/2081	0.24	0/2812
46	Y	0.08	0/1552	0.25	0/2079
47	Z	0.07	0/1003	0.24	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	0.26	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	0.25	0/1152
54	b	0.08	0/1202	0.27	0/1626
55	e	0.08	0/1797	0.25	0/2422
56	g	0.12	0/1132	0.31	0/1543
57	i	0.10	0/849	0.28	0/1135
58	j	0.09	0/755	0.25	0/1016
59	m	0.09	0/379	0.28	0/510
60	o	0.10	0/818	0.34	0/1097
61	q	0.11	0/1325	0.41	2/1799 (0.1%)
62	r	0.08	0/1362	0.25	0/1846
63	J	0.27	1/1348 (0.1%)	0.37	0/1813
64	I	0.09	0/1467	0.28	0/1984
65	N	0.08	0/1833	0.25	0/2468
66	P	0.22	0/1191	0.41	1/1611 (0.1%)
67	U	0.11	0/1254	0.27	0/1700
68	V	0.08	0/1727	0.24	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	0.07	0/923	0.23	0/1254
75	c	0.08	0/2371	0.24	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	0.23	0/1249
79	k	0.10	0/754	0.26	0/1017
80	l	0.08	0/636	0.23	0/860
81	p	0.09	0/1246	0.25	0/1675
82	s	0.11	0/3262	0.42	5/4435 (0.1%)
83	Q	0.12	0/2044	0.29	0/2757
84	TA	0.12	0/349	0.38	0/475
84	TB	0.05	0/212	0.16	0/286
84	TC	0.10	0/351	0.59	2/488 (0.4%)
86	v	0.26	3/5647 (0.1%)	0.51	15/7623 (0.2%)
All	All	0.10	7/181965 (0.0%)	0.26	41/258102 (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
23	AY	0	1
41	R	0	1
42	S	0	1
66	P	0	1
82	s	0	1
84	TC	0	1
86	v	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	v	174	ASN	C-N	12.20	1.50	1.33
63	J	188	GLU	C-N	8.20	1.45	1.34
86	v	175	LYS	N-CA	8.11	1.56	1.46
32	A	3089	A	C3'-O3'	-6.20	1.32	1.42
86	v	175	LYS	CA-C	5.54	1.60	1.52
70	5	69	TRP	NE1-CE2	-5.40	1.31	1.37
32	A	3089	A	C2'-C1'	-5.33	1.45	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	s	160	ARG	CA-C-N	-11.64	105.31	121.84
82	s	160	ARG	C-N-CA	-11.64	105.31	121.84
86	v	339	THR	N-CA-C	10.60	125.52	109.41
32	A	3089	A	C4'-C3'-O3'	10.54	128.80	113.00
42	S	144	LEU	CA-C-N	-9.37	103.04	121.41
42	S	144	LEU	C-N-CA	-9.37	103.04	121.41
86	v	175	LYS	CA-CB-CG	8.78	131.66	114.10
86	v	339	THR	CA-C-N	8.39	136.91	122.81
86	v	339	THR	C-N-CA	8.39	136.91	122.81
42	S	145	GLY	N-CA-C	8.04	132.24	113.18
41	R	138	PRO	CA-C-N	7.72	136.28	121.54
41	R	138	PRO	C-N-CA	7.72	136.28	121.54
86	v	174	ASN	CA-C-N	7.38	135.64	121.54
86	v	174	ASN	C-N-CA	7.38	135.64	121.54
86	v	316	TYR	N-CA-C	6.49	124.63	110.80
23	AY	313	PHE	CA-CB-CG	-6.41	107.39	113.80
41	R	134	ASP	CA-C-N	6.28	133.72	121.41
41	R	134	ASP	C-N-CA	6.28	133.72	121.41
86	v	320	PRO	CA-C-N	-6.22	109.66	121.54
86	v	320	PRO	C-N-CA	-6.22	109.66	121.54
86	v	175	LYS	N-CA-CB	-6.18	100.04	110.49
41	R	136	LYS	CA-C-N	6.17	136.85	121.80
41	R	136	LYS	C-N-CA	6.17	136.85	121.80
23	AY	313	PHE	CB-CA-C	6.06	122.79	110.31
66	P	72	PHE	N-CA-CB	5.98	121.02	110.37
84	TC	166	GLU	CA-C-N	5.90	129.49	120.82
84	TC	166	GLU	C-N-CA	5.90	129.49	120.82
82	s	161	ARG	CB-CA-C	-5.89	107.94	116.54
32	A	3089	A	N9-C1'-C2'	-5.55	103.67	112.00
41	R	135	GLY	N-CA-C	5.51	126.23	113.18
86	v	618	MET	N-CA-C	-5.33	99.06	108.23
86	v	619	VAL	CA-C-N	5.19	131.46	121.54
86	v	619	VAL	C-N-CA	5.19	131.46	121.54
23	AY	311	TRP	CA-C-N	-5.19	112.79	120.94
23	AY	311	TRP	C-N-CA	-5.19	112.79	120.94
86	v	341	ILE	N-CA-CB	5.15	119.73	111.23
82	s	273	LEU	CA-C-N	5.15	130.55	122.21
82	s	273	LEU	C-N-CA	5.15	130.55	122.21
61	q	164	LEU	CA-C-N	-5.13	111.36	121.41
61	q	164	LEU	C-N-CA	-5.13	111.36	121.41
86	v	175	LYS	N-CA-C	-5.01	100.13	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	AY	313	PHE	Peptide
66	P	72	PHE	Peptide
41	R	134	ASP	Peptide
42	S	144	LEU	Peptide
84	TC	166	GLU	Peptide
82	s	160	ARG	Peptide
86	v	321	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20030	0	10172	283	0
2	AB	1787	0	1779	24	0
3	AC	1082	0	1088	20	0
4	AE	972	0	1001	11	0
5	AI	1011	0	1052	14	0
6	AJ	838	0	887	18	0
7	AK	861	0	885	22	0
8	AM	920	0	951	12	0
9	AN	846	0	908	12	0
10	AO	1570	0	1533	14	0
11	AP	774	0	803	15	0
12	AQ	740	0	754	14	0
13	AT	1371	0	1395	14	0
14	AW	766	0	785	19	0
15	AX	2860	0	2856	45	0
16	A2	925	0	962	16	0
17	AH	1014	0	1036	23	0
18	AL	1451	0	1543	13	0
19	AR	2388	0	2410	28	0
20	AS	1111	0	1115	5	0
21	AU	1499	0	1512	20	0
22	AV	3009	0	3006	32	0
23	AY	1016	0	962	15	0
24	AZ	833	0	853	13	0
25	A1	2231	0	2261	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A0	1781	0	1791	34	0
27	A3	639	0	715	10	0
28	A4	3010	0	1760	10	0
29	AD	2731	0	2804	52	0
30	AF	1724	0	1765	25	0
31	AG	2587	0	2570	36	0
32	A	32395	0	16450	608	0
33	B	1191	0	607	12	0
34	D	1866	0	1927	26	0
35	F	2013	0	2044	34	0
36	H	806	0	849	16	0
37	K	1451	0	1448	15	0
38	L	889	0	941	17	0
39	M	2305	0	2378	44	0
40	O	1245	0	1283	16	0
41	R	1153	0	1214	14	0
42	S	1251	0	1322	28	0
43	T	1368	0	1410	16	0
44	W	871	0	897	13	0
45	X	2027	0	2040	24	0
46	Y	1517	0	1561	25	0
47	Z	978	0	1030	13	0
48	0	880	0	904	9	0
49	1	433	0	475	6	0
50	2	376	0	406	13	0
51	3	831	0	883	20	0
52	4	342	0	362	7	0
53	8	836	0	844	18	0
54	b	1178	0	1180	10	0
55	e	1762	0	1767	28	0
56	g	1096	0	1081	18	0
57	i	827	0	857	18	0
58	j	740	0	741	9	0
59	m	372	0	387	5	0
60	o	797	0	804	15	0
61	q	1294	0	1178	20	0
62	r	1322	0	1350	21	0
63	J	1330	0	1407	103	0
64	I	1435	0	1521	41	0
65	N	1786	0	1817	21	0
66	P	1165	0	1162	35	0
67	U	1224	0	1191	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	V	1682	0	1692	23	0
69	E	2410	0	2418	37	0
70	5	3210	0	3206	94	0
71	6	2948	0	2841	53	0
72	7	2410	0	2415	31	0
73	9	997	0	987	11	0
74	a	896	0	847	15	0
75	c	2322	0	2338	22	0
76	d	2075	0	2037	30	0
77	f	1126	0	1106	24	0
78	h	894	0	881	8	0
79	k	743	0	758	11	0
80	l	619	0	611	24	0
81	p	1227	0	1239	22	0
82	s	3178	0	3124	53	0
83	Q	1995	0	2036	29	0
84	TA	345	0	364	5	0
84	TB	213	0	234	1	0
84	TC	352	0	169	0	0
85	u	325	0	76	0	0
86	v	5546	0	5501	170	0
87	A5	213	0	122	29	0
88	A6	1368	0	790	73	0
88	A7	1197	0	690	39	0
89	A	97	0	0	0	0
89	AA	27	0	0	0	0
89	AC	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	10	3	0
92	v	32	0	14	44	0
All	All	176217	0	148138	2448	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 (2448) 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)
63:J:171:ARG:HA	63:J:174:PHE:CE2	1.29	1.66
70:5:60:PHE:CD1	70:5:71:ALA:HB1	1.25	1.63
70:5:68:PRO:HG2	70:5:69:TRP:CE3	1.24	1.62
86:v:175:LYS:HE2	92:v:802:GCP:C4	1.38	1.51
45:X:156:LYS:NZ	70:5:70:LEU:HD23	1.24	1.44
32:A:2909:G:N2	88:A7:71:P5P:H2	1.34	1.41
70:5:68:PRO:HG2	70:5:69:TRP:CZ3	1.54	1.40
86:v:59:LYS:HD2	92:v:802:GCP:O2G	1.19	1.35
63:J:174:PHE:CE1	63:J:175:LEU:CD2	2.11	1.34
70:5:68:PRO:CG	70:5:69:TRP:CZ3	2.13	1.31
32:A:2919:A:H4'	88:A7:71:P5P:O3'	1.13	1.30
32:A:3110:C:H42	32:A:3203:A:N6	1.31	1.27
63:J:174:PHE:CE1	63:J:175:LEU:HD22	1.69	1.27
63:J:111:LEU:HD13	63:J:170:GLU:OE2	1.23	1.27
70:5:60:PHE:CD1	70:5:71:ALA:CB	2.19	1.26
32:A:2909:G:N2	88:A7:71:P5P:C2	1.97	1.25
70:5:60:PHE:HE1	70:5:71:ALA:C	1.42	1.25
70:5:68:PRO:CG	70:5:69:TRP:CE3	2.20	1.24
32:A:2909:G:C2	88:A7:71:P5P:N1	2.08	1.22
63:J:171:ARG:CA	63:J:174:PHE:CE2	2.25	1.20
29:AD:264:ARG:NH2	87:A5:3:Y5P:H2'	1.55	1.18
86:v:175:LYS:HB3	92:v:802:GCP:C5	1.47	1.17
32:A:2919:A:C4'	88:A7:71:P5P:O3'	1.94	1.15
29:AD:128:ARG:NH2	87:A5:7:Y5P:O3'	1.79	1.14
70:5:67:VAL:HG23	70:5:71:ALA:HB3	1.16	1.14
63:J:159:LEU:HB3	63:J:162:GLU:HB3	1.28	1.12
86:v:175:LYS:CE	92:v:802:GCP:C4	2.27	1.12
29:AD:265:MET:HE3	87:A5:4:Y5P:H5	1.20	1.12
32:A:3110:C:N4	32:A:3203:A:H61	1.47	1.12
86:v:175:LYS:HE2	92:v:802:GCP:C5	1.79	1.12
70:5:60:PHE:HD1	70:5:71:ALA:CB	1.58	1.10
86:v:175:LYS:NZ	92:v:802:GCP:O4'	1.84	1.10
45:X:156:LYS:NZ	70:5:70:LEU:CD2	2.13	1.10
29:AD:265:MET:CG	87:A5:4:Y5P:H4A	1.82	1.10
32:A:2962:C:H42	32:A:3016:G:N2	1.49	1.10
70:5:60:PHE:CE1	70:5:71:ALA:C	2.29	1.10
29:AD:265:MET:HG2	87:A5:4:Y5P:C4	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:v:175:LYS:HE2	92:v:802:GCP:N9	1.70	1.07
86:v:175:LYS:CE	92:v:802:GCP:N9	2.18	1.06
32:A:3125:A:N6	32:A:3132:G:H21	1.52	1.06
86:v:175:LYS:NZ	92:v:802:GCP:C1'	2.19	1.05
70:5:68:PRO:HG3	70:5:69:TRP:HZ3	1.18	1.04
32:A:2939:C:N4	32:A:2991:U:H3	1.55	1.04
32:A:3125:A:H62	32:A:3132:G:N2	1.57	1.03
70:5:67:VAL:CG2	70:5:71:ALA:HB3	1.89	1.03
86:v:175:LYS:HZ1	92:v:802:GCP:C1'	1.72	1.03
86:v:175:LYS:CB	92:v:802:GCP:C5	2.34	1.02
70:5:60:PHE:HE1	70:5:71:ALA:O	1.39	1.02
32:A:2962:C:N4	32:A:3016:G:H22	1.58	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	1.02
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	1.01
32:A:3089:A:H3'	32:A:3089:A:N3	1.74	1.01
63:J:159:LEU:HD13	63:J:162:GLU:HG2	1.40	1.00
1:AA:1078:A:H8	88:A6:35:Y5P:O2'	1.43	1.00
70:5:67:VAL:CG2	70:5:71:ALA:CB	2.39	1.00
86:v:59:LYS:CD	92:v:802:GCP:O2G	2.10	0.99
45:X:156:LYS:HZ3	70:5:70:LEU:CD2	1.71	0.98
70:5:68:PRO:CG	70:5:69:TRP:HZ3	1.63	0.98
32:A:2588:C:H42	32:A:2592:G:H22	0.98	0.98
32:A:3125:A:H62	32:A:3132:G:H21	1.07	0.98
63:J:174:PHE:CE1	63:J:175:LEU:HD23	1.99	0.98
86:v:58:GLY:CA	92:v:802:GCP:O2A	2.12	0.98
1:AA:1197:G:H1	1:AA:1425:U:H3	1.12	0.97
29:AD:265:MET:HG2	87:A5:4:Y5P:H4A	0.99	0.97
32:A:2909:G:C2	88:A7:71:P5P:C2	2.46	0.97
29:AD:264:ARG:NH2	87:A5:3:Y5P:C2'	2.28	0.96
32:A:1721:C:H42	32:A:1730:U:H3	0.96	0.95
32:A:2468:A:H61	32:A:2659:C:N4	1.64	0.95
63:J:174:PHE:HE1	63:J:175:LEU:CD2	1.65	0.95
45:X:156:LYS:HZ3	70:5:70:LEU:HD23	1.17	0.93
31:AG:395:LYS:HZ3	88:A6:31:Y5P:HA1	1.32	0.92
29:AD:265:MET:HE3	87:A5:4:Y5P:C5	1.99	0.92
63:J:189:ALA:O	63:J:192:LYS:HD3	1.70	0.92
32:A:2962:C:H42	32:A:3016:G:H22	0.96	0.92
32:A:3010:G:H1	32:A:3027:U:H3	1.10	0.91
25:A1:49:ARG:NH2	87:A5:11:P5P:N9	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2549:C:H42	32:A:2565:A:H62	1.17	0.91
1:AA:1078:A:H5'	88:A6:36:Y5P:HA1	1.53	0.90
86:v:56:ASP:HA	92:v:802:GCP:H5'2	1.53	0.90
63:J:171:ARG:HA	63:J:174:PHE:HE2	1.10	0.90
32:A:2909:G:H22	88:A7:71:P5P:H2	1.12	0.90
32:A:3013:G:H1	32:A:3024:U:H3	1.19	0.90
63:J:111:LEU:CD1	63:J:170:GLU:OE2	2.18	0.90
29:AD:120:LYS:NZ	87:A5:2:P5P:H2	1.87	0.89
86:v:58:GLY:HA2	92:v:802:GCP:O2A	1.71	0.89
63:J:167:PHE:O	63:J:171:ARG:CD	2.21	0.89
25:A1:49:ARG:HH22	87:A5:11:P5P:C4	1.86	0.88
86:v:59:LYS:HD2	92:v:802:GCP:PG	2.14	0.88
33:B:1607:U:H3	33:B:1664:G:H1	1.20	0.88
45:X:156:LYS:HZ2	70:5:70:LEU:CD2	1.83	0.88
32:A:3089:A:N6	88:A6:69:Y5P:O5'	2.08	0.87
86:v:175:LYS:CE	92:v:802:GCP:C8	2.52	0.87
63:J:171:ARG:NH2	80:l:76:ASN:O	2.07	0.87
25:A1:49:ARG:NH2	87:A5:11:P5P:C1'	2.38	0.86
32:A:2374:A:H62	82:s:272:PRO:HB2	1.39	0.86
70:5:69:TRP:H	70:5:69:TRP:HE3	1.18	0.86
32:A:1721:C:N4	32:A:1730:U:H3	1.74	0.86
63:J:174:PHE:HE1	63:J:175:LEU:HD22	1.23	0.86
32:A:2549:C:N4	32:A:2565:A:H62	1.72	0.85
32:A:3110:C:N4	32:A:3203:A:N6	2.13	0.85
32:A:3049:U:H3	32:A:3053:A:H62	1.21	0.85
63:J:170:GLU:O	63:J:174:PHE:CD2	2.30	0.84
32:A:2588:C:H42	32:A:2592:G:N2	1.74	0.84
32:A:3072:U:OP1	88:A6:71:P5P:H5'2	1.76	0.84
63:J:156:VAL:O	63:J:157:LYS:O	1.95	0.84
86:v:508:LEU:O	86:v:512:TYR:HB3	1.77	0.84
1:AA:1078:A:H5'	88:A6:36:Y5P:P	2.17	0.84
32:A:2588:C:N4	32:A:2592:G:H22	1.75	0.84
1:AA:1078:A:H5'	88:A6:36:Y5P:C5'	2.06	0.83
32:A:3110:C:H42	32:A:3203:A:H61	0.84	0.83
70:5:60:PHE:CE1	70:5:71:ALA:HB1	2.10	0.83
32:A:3033:U:H5''	32:A:3034:U:H5'	1.60	0.83
32:A:1724:A:H61	32:A:2040:G:N2	1.76	0.83
1:AA:1078:A:P	88:A6:36:Y5P:HA1	2.18	0.83
1:AA:1078:A:OP1	88:A6:36:Y5P:HA1	1.79	0.82
32:A:1711:C:OP2	70:5:72:ARG:NH2	2.12	0.82
32:A:2613:U:H3	32:A:2619:A:H61	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2939:C:H42	32:A:2991:U:H3	0.82	0.81
31:AG:395:LYS:NZ	88:A6:31:Y5P:HA1	1.94	0.81
32:A:2203:G:N2	32:A:2208:A:H62	1.77	0.81
86:v:330:ASN:O	86:v:339:THR:OG1	1.99	0.81
70:5:69:TRP:HE3	70:5:69:TRP:N	1.79	0.81
29:AD:264:ARG:HH21	87:A5:3:Y5P:H2'	1.46	0.80
32:A:3179:G:H21	32:A:3190:A:N6	1.80	0.80
70:5:68:PRO:HG2	70:5:69:TRP:HE3	0.97	0.80
29:AD:264:ARG:HH21	87:A5:3:Y5P:C2'	1.92	0.80
32:A:2174:G:N2	63:J:102:ARG:O	2.14	0.79
70:5:68:PRO:HG3	70:5:69:TRP:CZ3	1.97	0.79
32:A:2549:C:H42	32:A:2565:A:N6	1.80	0.79
32:A:2203:G:H21	32:A:2208:A:N6	1.80	0.79
63:J:159:LEU:HD13	63:J:162:GLU:CG	2.14	0.78
29:AD:120:LYS:HZ3	87:A5:2:P5P:H2	1.45	0.78
86:v:175:LYS:HE3	92:v:802:GCP:C8	2.14	0.78
63:J:174:PHE:CD1	63:J:175:LEU:HD22	2.19	0.77
39:M:140:LEU:HB2	39:M:156:VAL:HG11	1.66	0.77
32:A:2816:G:N2	88:A6:69:Y5P:H4	1.99	0.77
46:Y:200:PHE:CB	70:5:68:PRO:HG3	2.15	0.77
32:A:2909:G:N3	88:A7:71:P5P:N1	2.33	0.76
32:A:2919:A:H4'	88:A7:71:P5P:C3'	2.15	0.76
86:v:175:LYS:HB3	92:v:802:GCP:N7	1.99	0.76
63:J:159:LEU:O	63:J:163:GLU:CG	2.33	0.76
32:A:1724:A:N6	32:A:2040:G:N2	2.32	0.76
86:v:47:ARG:NH2	86:v:314:LEU:O	2.16	0.76
32:A:2468:A:H61	32:A:2659:C:H42	1.34	0.76
82:s:99:ALA:HB1	82:s:271:LEU:HD23	1.66	0.75
86:v:340:LYS:O	86:v:341:ILE:HG12	1.86	0.75
86:v:175:LYS:HE2	92:v:802:GCP:C8	2.16	0.75
32:A:3089:A:C8	88:A6:70:Y5P:OP1	2.40	0.75
63:J:164:LEU:HD22	80:l:77:ILE:HB	1.66	0.75
88:A7:59:Y5P:H4A	88:A7:60:Y5P:H4	1.68	0.75
20:AS:2:ALA:N	29:AD:215:TYR:HH	1.84	0.74
32:A:2468:A:N6	32:A:2659:C:H42	1.83	0.74
61:q:78:SER:H	61:q:81:GLN:HE21	1.34	0.74
32:A:2214:A:O2'	80:l:122:ARG:NH1	2.21	0.74
32:A:3179:G:N2	32:A:3190:A:H62	1.86	0.74
63:J:190:ALA:O	63:J:192:LYS:HG2	1.88	0.74
63:J:25:ARG:NH1	80:l:67:GLN:OE1	2.21	0.74
32:A:3110:C:N3	32:A:3203:A:N1	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:O:113:CYS:SG	48:O:114:GLY:N	2.61	0.74
32:A:3089:A:N6	88:A6:68:Y5P:HB2	2.02	0.73
1:AA:1078:A:C5'	88:A6:36:Y5P:HA1	2.17	0.73
25:A1:49:ARG:NH2	87:A5:11:P5P:H1'	2.04	0.73
86:v:301:LEU:HD22	92:v:802:GCP:C2	2.18	0.73
63:J:164:LEU:CD2	80:l:77:ILE:O	2.36	0.73
1:AA:1078:A:O4'	88:A6:35:Y5P:O3'	2.06	0.73
32:A:2910:A:C2	88:A7:71:P5P:C8	2.72	0.73
88:A7:61:Y5P:H4A	88:A7:62:Y5P:H4	1.69	0.72
86:v:332:GLU:HG2	86:v:339:THR:OG1	1.88	0.72
29:AD:264:ARG:HH22	87:A5:3:Y5P:H2'	1.49	0.72
86:v:175:LYS:NZ	92:v:802:GCP:N9	2.36	0.72
32:A:2203:G:H21	32:A:2208:A:H62	1.34	0.72
88:A6:69:Y5P:H2'	88:A6:70:Y5P:HA1	1.72	0.72
86:v:320:PRO:O	86:v:322:GLU:N	2.23	0.72
63:J:158:ASP:OD2	80:l:97:PHE:CE1	2.42	0.72
66:P:72:PHE:CD2	66:P:73:PRO:HD2	2.25	0.72
32:A:2910:A:C4	88:A7:71:P5P:N7	2.58	0.72
34:D:111:ARG:HH22	34:D:163:ILE:HD12	1.54	0.72
56:g:77:ASP:HB2	56:g:78:PRO:HD2	1.72	0.71
61:q:127:LYS:O	61:q:131:MET:HG3	1.90	0.71
15:AX:387:ASN:HD22	15:AX:390:LEU:H	1.38	0.71
31:AG:136:ARG:HH21	31:AG:156:GLN:HE21	1.38	0.71
1:AA:1110:A:H61	1:AA:1131:C:H42	1.36	0.71
64:I:81:LEU:HD11	80:l:113:GLU:HA	1.70	0.71
86:v:175:LYS:HZ3	92:v:802:GCP:C1'	2.03	0.71
63:J:158:ASP:OD2	80:l:97:PHE:HE1	1.73	0.71
1:AA:1078:A:C8	88:A6:35:Y5P:HA	2.26	0.71
46:Y:200:PHE:HB2	70:5:68:PRO:HG3	1.72	0.71
45:X:156:LYS:HZ2	70:5:70:LEU:HD23	0.88	0.71
63:J:170:GLU:O	63:J:174:PHE:HD2	1.73	0.71
54:b:49:ARG:HG3	54:b:50:GLU:HG3	1.71	0.70
70:5:60:PHE:CE1	70:5:71:ALA:CB	2.73	0.70
70:5:69:TRP:CE3	70:5:69:TRP:N	2.58	0.70
32:A:2919:A:O2'	88:A7:71:P5P:H5'2	1.90	0.70
32:A:1724:A:N6	32:A:2040:G:H21	1.89	0.70
32:A:2919:A:C3'	88:A7:71:P5P:O3'	2.39	0.70
1:AA:780:C:N3	18:AL:196:ARG:NH2	2.39	0.70
32:A:2472:A:N3	32:A:2474:C:N4	2.39	0.70
32:A:3089:A:N9	88:A6:70:Y5P:OP1	2.23	0.70
70:5:69:TRP:O	70:5:70:LEU:C	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:990:U:H3	1:AA:997:A:H61	1.39	0.70
86:v:313:VAL:O	86:v:317:LEU:HB2	1.90	0.70
32:A:1783:U:H3	32:A:1794:A:H62	1.39	0.69
32:A:2085:A:H2'	32:A:2086:A:H8	1.57	0.69
86:v:332:GLU:H	86:v:339:THR:HB	1.57	0.69
39:M:276:ASN:HD21	61:q:65:GLY:HA2	1.57	0.69
32:A:3089:A:N7	88:A6:69:Y5P:P	2.65	0.69
43:T:71:ALA:H	43:T:180:GLU:HG2	1.58	0.69
63:J:189:ALA:O	63:J:192:LYS:CD	2.39	0.69
86:v:313:VAL:HB	86:v:317:LEU:HD12	1.73	0.69
1:AA:1078:A:OP1	88:A6:35:Y5P:H2'	1.92	0.69
76:d:165:THR:HG23	76:d:167:HIS:H	1.57	0.69
1:AA:713:C:H5''	8:AM:42:PRO:HG3	1.75	0.69
25:A1:86:ARG:HG2	25:A1:98:ALA:HA	1.75	0.69
32:A:3122:U:H4'	32:A:3123:G:H4'	1.75	0.68
3:AC:113:ARG:NH2	17:AH:161:GLN:O	2.26	0.68
63:J:164:LEU:HD21	80:l:77:ILE:O	1.93	0.68
32:A:2339:G:H21	32:A:2427:C:H5'	1.57	0.68
32:A:3089:A:N3	32:A:3089:A:O5'	2.27	0.68
32:A:3089:A:H61	88:A6:68:Y5P:HB2	1.57	0.68
82:s:332:LEU:HD13	82:s:372:TYR:HB2	1.75	0.68
86:v:59:LYS:NZ	92:v:802:GCP:H3B1	2.08	0.68
51:3:172:TYR:HB2	51:3:175:ASP:HB2	1.76	0.68
83:Q:225:LYS:HB3	83:Q:226:PRO:HD2	1.75	0.68
32:A:3082:G:N2	32:A:3085:A:OP2	2.26	0.68
36:H:62:VAL:HG22	36:H:64:LEU:H	1.58	0.68
86:v:101:THR:HG23	86:v:122:PRO:HA	1.75	0.68
32:A:2586:U:HO2'	88:A6:12:Y5P:HD	1.34	0.68
13:AT:78:PHE:HB2	13:AT:86:VAL:HB	1.77	0.67
32:A:2472:A:OP2	32:A:2653:C:N4	2.27	0.67
66:P:72:PHE:HZ	71:6:54:PHE:HE2	1.42	0.67
1:AA:947:U:O2	1:AA:1046:A:N7	2.28	0.67
32:A:2222:U:H5'	32:A:2223:A:H5'	1.76	0.67
51:3:147:PHE:HB2	71:6:363:LEU:HB2	1.75	0.67
1:AA:1230:C:N4	1:AA:1446:A:O2'	2.28	0.67
25:A1:49:ARG:NH2	87:A5:11:P5P:C4	2.54	0.67
1:AA:846:A:H61	26:A0:53:ARG:HH22	1.42	0.67
25:A1:313:LYS:HE3	25:A1:317:LYS:HE3	1.77	0.67
32:A:1838:C:H4'	37:K:116:LEU:HD12	1.75	0.67
84:TA:74:LEU:HD11	84:TA:79:ILE:HG13	1.77	0.67
31:AG:396:ARG:NH2	88:A6:31:Y5P:OP2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1834:U:H3	43:T:206:ARG:HA	1.59	0.67
63:J:170:GLU:HA	63:J:173:ILE:HG12	1.76	0.67
46:Y:114:THR:HG22	67:U:28:LEU:H	1.60	0.67
86:v:318:PRO:HA	86:v:319:ASN:HB3	1.75	0.67
75:c:216:ARG:HG3	75:c:220:ILE:HD12	1.76	0.66
78:h:127:LEU:O	78:h:131:ASN:ND2	2.28	0.66
92:v:802:GCP:O2B	92:v:802:GCP:O3G	2.13	0.66
47:Z:78:ARG:O	47:Z:83:LYS:NZ	2.28	0.66
32:A:2232:A:H1'	32:A:3002:G:H21	1.59	0.66
86:v:58:GLY:N	92:v:802:GCP:O2A	2.28	0.66
86:v:78:GLU:OE2	92:v:802:GCP:O1A	2.13	0.66
32:A:2753:A:H2'	32:A:2754:A:H8	1.60	0.66
32:A:2625:C:O2'	32:A:2627:G:OP1	2.14	0.66
32:A:2554:A:N3	34:D:285:LYS:NZ	2.44	0.65
32:A:2998:U:H5''	69:E:225:LYS:HB2	1.78	0.65
86:v:41:ILE:HG23	86:v:46:ILE:HD11	1.78	0.65
1:AA:1265:C:H2'	1:AA:1266:A:H8	1.61	0.65
23:AY:296:ASN:HB3	25:A1:71:PRO:HG3	1.76	0.65
32:A:3179:G:H21	32:A:3190:A:H62	1.42	0.65
86:v:330:ASN:HD22	86:v:441:MET:HE2	1.61	0.65
1:AA:1169:G:H2'	1:AA:1170:G:H8	1.61	0.65
1:AA:1504:U:O4	1:AA:1505:A:N6	2.30	0.65
32:A:2909:G:C2	88:A7:71:P5P:H2	2.15	0.65
32:A:3049:U:H3	32:A:3053:A:N6	1.95	0.65
71:6:184:LEU:HG	71:6:186:PRO:HD3	1.79	0.65
1:AA:1490:U:H1'	1:AA:1582:G:H21	1.62	0.65
70:5:68:PRO:CG	70:5:69:TRP:HE3	1.81	0.65
42:S:146:LYS:O	42:S:148:LEU:N	2.30	0.65
26:A0:130:GLU:HG2	26:A0:207:GLN:HB2	1.79	0.65
32:A:2503:A:H1'	32:A:3094:G:H21	1.62	0.64
77:f:134:VAL:HB	77:f:148:SER:HB2	1.79	0.64
32:A:1744:A:H62	32:A:1754:G:H21	1.45	0.64
57:i:94:LYS:NZ	57:i:102:MET:SD	2.70	0.64
31:AG:253:LYS:O	31:AG:365:ARG:NH1	2.30	0.64
63:J:33:PRO:O	63:J:35:LEU:N	2.30	0.64
32:A:2173:G:N3	63:J:150:SER:HB2	2.13	0.64
51:3:126:LYS:HE3	51:3:148:VAL:HG21	1.78	0.64
65:N:124:VAL:HG12	65:N:158:ARG:HE	1.62	0.64
32:A:1907:A:N3	32:A:2930:U:O2'	2.29	0.64
82:s:63:ILE:HA	82:s:66:TRP:HD1	1.61	0.64
22:AV:49:CYS:SG	22:AV:50:LEU:N	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:K:37:ILE:HG23	37:K:42:LEU:HB2	1.79	0.64
63:J:22:ALA:HB1	63:J:35:LEU:HD21	1.79	0.64
31:AG:258:GLU:HB2	31:AG:354:SER:HB2	1.80	0.64
1:AA:705:C:H41	26:A0:137:HIS:HB2	1.62	0.64
1:AA:886:C:N4	1:AA:887:G:O6	2.31	0.64
1:AA:1197:G:N2	1:AA:1425:U:O2	2.31	0.64
25:A1:49:ARG:HH21	87:A5:11:P5P:C1'	2.09	0.64
32:A:2910:A:N3	88:A7:71:P5P:C8	2.61	0.64
64:I:47:LEU:HD22	65:N:226:ILE:HG12	1.78	0.64
86:v:91:SER:HA	86:v:95:GLU:HB2	1.80	0.63
86:v:436:ASN:OD1	86:v:439:LEU:HD21	1.97	0.63
1:AA:730:A:N6	1:AA:745:A:N7	2.46	0.63
32:A:1867:A:H62	32:A:2295:C:H5	1.47	0.63
35:F:89:THR:HG22	35:F:179:THR:HG21	1.81	0.63
1:AA:674:U:H4'	1:AA:826:A:H1'	1.81	0.63
32:A:1682:C:OP1	46:Y:222:ARG:NH1	2.31	0.63
32:A:2186:C:O2'	63:J:103:GLN:NE2	2.30	0.63
86:v:330:ASN:HB3	86:v:341:ILE:HG13	1.81	0.63
22:AV:117:LEU:HA	22:AV:121:ALA:HB2	1.80	0.63
32:A:1881:A:OP2	56:g:111:ARG:NH2	2.30	0.63
32:A:2819:G:H21	44:W:38:SER:HB3	1.62	0.63
1:AA:1148:A:N6	1:AA:1149:G:O6	2.32	0.63
3:AC:109:VAL:HB	3:AC:120:CYS:HB2	1.80	0.63
32:A:1674:A:N7	43:T:47:ILE:N	2.46	0.63
32:A:2350:A:H61	32:A:2360:U:H2'	1.63	0.63
32:A:3049:U:O4	32:A:3053:A:N7	2.32	0.63
1:AA:1320:G:OP1	3:AC:41:ARG:NH1	2.32	0.63
25:A1:64:GLN:NE2	28:A4:81:ASP:OD1	2.31	0.63
82:s:242:ARG:HA	82:s:295:GLY:HA2	1.80	0.63
25:A1:169:ARG:HD2	25:A1:213:PRO:HA	1.81	0.63
32:A:2155:A:N6	62:r:169:TRP:O	2.31	0.63
71:6:261:ARG:HD3	71:6:341:VAL:HG12	1.81	0.63
29:AD:150:LYS:HB2	29:AD:155:GLN:HE21	1.63	0.62
69:E:227:GLN:NE2	69:E:236:THR:O	2.32	0.62
5:AI:178:ASN:HA	12:AQ:10:ARG:HH11	1.64	0.62
32:A:2307:U:H1'	48:0:84:ARG:HG3	1.80	0.62
32:A:3089:A:C1'	88:A6:70:Y5P:OP1	2.47	0.62
32:A:3179:G:N2	32:A:3190:A:N6	2.47	0.62
63:J:35:LEU:HD12	63:J:39:LEU:HD11	1.81	0.62
41:R:83:TYR:OH	41:R:99:ARG:NH1	2.32	0.62
42:S:140:ASN:HD22	74:a:63:PRO:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:i:99:GLY:HA2	57:i:102:MET:HE2	1.81	0.62
82:s:177:LEU:HD23	82:s:238:ASN:HD22	1.64	0.62
32:A:3089:A:H62	88:A6:69:Y5P:P	2.22	0.62
31:AG:127:HIS:HD2	31:AG:129:GLU:HG2	1.64	0.62
32:A:1924:U:H5''	34:D:81:LYS:HB2	1.80	0.62
32:A:2948:C:H2'	32:A:2949:C:C6	2.34	0.62
29:AD:227:ASN:OD1	87:A5:1:Y5P:H4A	2.00	0.62
32:A:1795:A:H5'	35:F:147:ARG:HH12	1.64	0.62
46:Y:121:ARG:NH1	67:U:30:ARG:O	2.32	0.62
81:p:111:ILE:O	81:p:116:ARG:NH2	2.32	0.62
1:AA:1528:A:H2'	1:AA:1529:A:H8	1.65	0.62
12:AQ:69:ALA:O	12:AQ:73:ASN:ND2	2.32	0.62
32:A:3125:A:N6	32:A:3132:G:N2	2.25	0.62
63:J:174:PHE:CZ	63:J:175:LEU:HD23	2.35	0.62
28:A4:134:GLU:H	28:A4:135:PRO:HD2	1.65	0.62
32:A:2363:A:OP2	32:A:2432:A:N6	2.32	0.62
65:N:218:ILE:HG23	65:N:223:MET:HB2	1.80	0.62
71:6:330:ILE:O	71:6:334:LEU:HB2	2.00	0.61
32:A:2472:A:H1'	32:A:2474:C:H41	1.66	0.61
32:A:2917:G:O6	39:M:77:ARG:NH2	2.33	0.61
84:TA:74:LEU:HD13	84:TA:78:GLU:HB3	1.82	0.61
1:AA:1154:A:OP2	27:A3:155:ARG:NH2	2.33	0.61
8:AM:23:LEU:HB2	8:AM:43:ARG:HH22	1.66	0.61
40:O:140:SER:O	40:O:146:ASN:ND2	2.32	0.61
63:J:171:ARG:CA	63:J:174:PHE:CD2	2.73	0.61
32:A:2373:A:OP1	67:U:50:ARG:NH2	2.34	0.61
60:o:22:ARG:HH21	64:I:39:VAL:HG13	1.65	0.61
86:v:59:LYS:HZ3	92:v:802:GCP:H3B1	1.64	0.61
32:A:1811:A:H61	75:c:49:ARG:HH21	1.48	0.61
55:e:58:VAL:HB	55:e:153:LEU:HB2	1.81	0.61
59:m:59:GLN:NE2	59:m:77:MET:O	2.33	0.61
81:p:192:ARG:HG3	81:p:193:ILE:HG22	1.82	0.61
86:v:320:PRO:C	86:v:322:GLU:H	2.08	0.61
1:AA:1340:C:H4'	24:AZ:100:LYS:HE3	1.82	0.61
70:5:201:ARG:HG2	70:5:232:THR:HG22	1.82	0.61
24:AZ:66:ARG:NH2	24:AZ:80:ASP:OD2	2.33	0.61
25:A1:163:VAL:H	28:A4:134:GLU:HG3	1.66	0.61
21:AU:45:PRO:HB3	26:A0:53:ARG:HH21	1.66	0.61
40:O:141:HIS:HD2	40:O:146:ASN:HB3	1.66	0.61
48:0:119:LYS:O	48:0:120:HIS:ND1	2.34	0.61
63:J:167:PHE:HB3	63:J:171:ARG:CZ	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:996:A:H3'	1:AA:997:A:H8	1.66	0.61
2:AB:223:VAL:HG23	2:AB:227:CYS:HB2	1.83	0.61
1:AA:1430:A:N6	1:AA:1459:A:OP2	2.32	0.60
7:AK:43:MET:HE2	7:AK:82:SER:HB3	1.82	0.60
32:A:1955:G:N2	32:A:1960:A:H61	1.99	0.60
32:A:2173:G:N2	63:J:150:SER:O	2.31	0.60
32:A:3089:A:H3'	32:A:3089:A:C4	2.35	0.60
32:A:3063:G:O2'	32:A:3066:C:OP2	2.19	0.60
32:A:2143:G:H2'	32:A:2144:A:H8	1.65	0.60
32:A:2388:A:H61	34:D:127:ILE:HG21	1.66	0.60
63:J:174:PHE:CD1	63:J:175:LEU:N	2.69	0.60
1:AA:1479:C:H5'	1:AA:1485:G:H21	1.66	0.60
32:A:2028:G:H4'	32:A:2047:U:H4'	1.82	0.60
32:A:2468:A:N6	32:A:2659:C:N4	2.38	0.60
61:q:41:ASP:HB3	61:q:44:ASP:HB2	1.82	0.60
22:AV:250:ILE:HG22	22:AV:252:LYS:H	1.65	0.60
32:A:2376:A:O2'	73:9:28:ARG:NH2	2.34	0.60
63:J:55:GLU:HA	63:J:58:LYS:HE2	1.84	0.60
82:s:237:PRO:HG2	82:s:240:GLN:HE21	1.66	0.60
86:v:175:LYS:CE	92:v:802:GCP:C5	2.69	0.60
31:AG:395:LYS:NZ	88:A6:31:Y5P:C5'	2.63	0.60
1:AA:1021:U:OP2	16:A2:9:ARG:NH2	2.34	0.60
1:AA:1260:A:N6	1:AA:1330:C:O2	2.35	0.60
26:A0:133:HIS:O	26:A0:139:TRP:NE1	2.35	0.60
32:A:3010:G:N2	32:A:3027:U:O2	2.32	0.60
1:AA:850:U:O2	21:AU:27:ARG:NH2	2.34	0.60
1:AA:1441:A:O2'	7:AK:101:LYS:NZ	2.32	0.60
15:AX:348:TYR:OH	91:AX:500:GDP:N2	2.35	0.60
32:A:3000:A:H2'	32:A:3001:G:H8	1.66	0.60
34:D:96:ILE:O	34:D:269:ARG:NH1	2.35	0.60
40:O:33:LEU:HD21	40:O:59:LEU:HD22	1.83	0.60
69:E:343:PRO:HA	83:Q:105:VAL:HG21	1.83	0.60
72:7:107:LEU:HB3	72:7:126:LYS:HB3	1.84	0.60
30:AF:176:ASP:OD1	30:AF:179:ARG:NH2	2.35	0.60
64:I:189:GLN:O	64:I:193:ASN:ND2	2.35	0.60
75:c:60:ARG:HD2	75:c:63:LYS:HD2	1.82	0.60
1:AA:712:C:H42	21:AU:27:ARG:HB2	1.66	0.60
1:AA:1078:A:H5'	88:A6:36:Y5P:OP1	2.02	0.60
32:A:2112:A:H1'	32:A:2943:G:H21	1.66	0.60
39:M:91:ARG:NH2	39:M:209:GLU:OE2	2.33	0.60
32:A:2520:C:O2	32:A:2528:G:N2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:v:503:ILE:HG13	86:v:506:GLN:HE21	1.66	0.59
47:Z:147:VAL:HG13	47:Z:148:GLN:HG3	1.84	0.59
32:A:2508:C:H2'	32:A:2509:A:C8	2.37	0.59
1:AA:773:U:H2'	1:AA:774:G:H8	1.68	0.59
86:v:346:SER:OG	86:v:349:ASN:ND2	2.35	0.59
1:AA:867:C:O2'	1:AA:869:C:N4	2.36	0.59
1:AA:1234:C:O2'	7:AK:40:ARG:NH1	2.35	0.59
32:A:2598:A:N6	32:A:2625:C:O5'	2.36	0.59
30:AF:74:ILE:HG13	31:AG:366:GLN:HA	1.84	0.59
32:A:1911:C:H2'	32:A:1912:A:H8	1.67	0.59
64:I:142:ASN:ND2	84:TA:49:ALA:O	2.35	0.59
1:AA:1078:A:C8	88:A6:35:Y5P:O2'	2.32	0.59
2:AB:149:ARG:NH2	12:AQ:84:TRP:O	2.36	0.59
65:N:167:CYS:SG	65:N:168:GLU:N	2.76	0.59
76:d:67:ILE:H	76:d:68:PRO:CD	2.15	0.59
86:v:344:ASN:OD1	86:v:375:GLN:NE2	2.35	0.59
15:AX:81:HIS:HB3	15:AX:156:PRO:HG3	1.84	0.59
26:A0:88:GLN:NE2	26:A0:202:ASP:OD2	2.36	0.59
32:A:1882:A:OP1	56:g:93:ASN:ND2	2.35	0.59
32:A:2453:G:O6	32:A:2672:A:N6	2.36	0.59
38:L:99:ARG:HB3	83:Q:161:GLU:HB2	1.84	0.59
40:O:104:TYR:HD1	40:O:105:THR:HG23	1.67	0.59
48:O:112:GLU:O	48:O:114:GLY:N	2.36	0.59
63:J:174:PHE:CD1	63:J:174:PHE:C	2.79	0.59
4:AE:40:GLU:HB2	4:AE:65:LEU:HB2	1.85	0.59
39:M:182:ARG:HE	39:M:201:PRO:HG3	1.68	0.59
70:5:174:GLU:HG3	70:5:296:LYS:HB3	1.84	0.59
57:i:77:PRO:HD2	57:i:80:LEU:HD11	1.85	0.59
76:d:182:ARG:HB2	76:d:223:ALA:HB3	1.85	0.59
49:1:20:MET:HB3	49:1:56:PHE:HB3	1.85	0.58
55:e:49:GLY:HA2	55:e:232:PHE:H	1.66	0.58
61:q:71:VAL:HG22	61:q:73:GLY:H	1.67	0.58
70:5:201:ARG:HB3	70:5:230:LEU:HD11	1.85	0.58
88:A7:63:Y5P:H4A	88:A7:64:Y5P:H4	1.85	0.58
32:A:1852:C:O2'	32:A:1854:U:OP2	2.19	0.58
32:A:2366:G:H2'	32:A:2367:A:H8	1.68	0.58
32:A:2822:C:O2'	32:A:2915:C:OP2	2.21	0.58
32:A:3113:A:OP1	32:A:3167:U:O2'	2.20	0.58
46:Y:72:LYS:O	46:Y:76:GLN:NE2	2.36	0.58
79:k:10:LEU:O	79:k:46:ASN:ND2	2.36	0.58
81:p:108:ALA:O	81:p:116:ARG:NH2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:62:ILE:HA	3:AC:66:LYS:HB3	1.84	0.58
4:AE:15:ARG:NH1	21:AU:178:GLU:OE1	2.35	0.58
1:AA:1216:C:H2'	1:AA:1217:G:H8	1.68	0.58
1:AA:1526:U:H3	26:A0:76:LEU:HD21	1.68	0.58
32:A:2827:A:N6	32:A:2828:G:O6	2.36	0.58
82:s:49:ALA:O	82:s:61:ARG:NH1	2.37	0.58
82:s:159:ARG:NH2	82:s:171:VAL:O	2.36	0.58
1:AA:1078:A:OP1	88:A6:36:Y5P:C5'	2.51	0.58
19:AR:175:ARG:HE	19:AR:181:LEU:HD13	1.68	0.58
32:A:2039:A:H62	32:A:2729:U:H1'	1.68	0.58
1:AA:815:C:O2	1:AA:818:C:N4	2.36	0.58
1:AA:1012:A:H4'	1:AA:1093:C:H4'	1.86	0.58
15:AX:134:LYS:NZ	91:AX:500:GDP:O1B	2.36	0.58
32:A:1952:U:H2'	32:A:1953:A:C8	2.39	0.58
32:A:2816:G:N2	88:A6:69:Y5P:C4	2.66	0.58
32:A:2909:G:H21	88:A7:70:Y5P:C2	2.17	0.58
8:AM:34:ILE:HG22	8:AM:87:MET:HE1	1.86	0.58
32:A:2196:A:O2'	32:A:2213:A:N1	2.34	0.58
33:B:1628:C:H2'	33:B:1629:A:H8	1.69	0.58
72:7:115:MET:HB3	72:7:270:PRO:HB3	1.85	0.58
86:v:619:VAL:HG23	86:v:620:ASP:H	1.68	0.58
32:A:2658:U:OP1	69:E:225:LYS:NZ	2.37	0.58
46:Y:198:ARG:NH2	50:2:70:LEU:O	2.36	0.58
69:E:346:THR:HG22	83:Q:172:GLN:HE22	1.69	0.58
86:v:556:LEU:HD23	86:v:607:LEU:HD11	1.84	0.58
15:AX:153:LEU:HD23	15:AX:260:VAL:HG22	1.85	0.58
29:AD:120:LYS:NZ	87:A5:2:P5P:C2	2.64	0.58
32:A:2048:U:O4	32:A:2092:C:N3	2.36	0.58
32:A:2466:A:H2'	32:A:2467:A:C8	2.38	0.58
34:D:211:GLY:H	34:D:247:VAL:HB	1.69	0.58
69:E:294:ASN:HD21	83:Q:88:ASP:HB2	1.68	0.58
82:s:271:LEU:O	82:s:273:LEU:N	2.36	0.58
1:AA:1101:U:HO2'	1:AA:1576:G:HO2'	1.50	0.58
3:AC:78:GLY:O	25:A1:167:ARG:NH1	2.36	0.58
9:AN:100:CYS:SG	9:AN:101:ALA:N	2.77	0.58
13:AT:63:GLN:NE2	13:AT:65:MET:SD	2.73	0.58
26:A0:200:PRO:HG2	26:A0:203:TYR:HB2	1.85	0.58
32:A:2274:A:OP1	75:c:36:ARG:NH1	2.36	0.58
58:j:53:ASP:OD2	58:j:55:ARG:NH2	2.37	0.58
70:5:216:GLU:OE2	70:5:367:ASN:ND2	2.36	0.58
32:A:1821:A:OP2	48:0:95:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AR:202:ARG:NH1	19:AR:234:GLN:O	2.37	0.57
32:A:1951:C:H2'	32:A:1952:U:C6	2.39	0.57
32:A:2795:U:O2	36:H:87:LYS:NZ	2.35	0.57
32:A:3108:U:O2	69:E:266:ARG:NH2	2.36	0.57
32:A:3174:U:N3	32:A:3196:G:O6	2.37	0.57
53:8:160:GLU:O	55:e:207:ASN:ND2	2.36	0.57
61:q:128:MET:O	61:q:132:ILE:HG12	2.04	0.57
86:v:175:LYS:HZ3	92:v:802:GCP:H1'	1.67	0.57
32:A:3127:G:H2'	32:A:3128:A:H2'	1.84	0.57
58:j:60:MET:N	58:j:60:MET:SD	2.77	0.57
63:J:102:ARG:HG3	63:J:103:GLN:HG2	1.87	0.57
63:J:156:VAL:HG21	63:J:159:LEU:HD12	1.86	0.57
79:k:65:ASP:HA	79:k:75:ILE:HA	1.86	0.57
1:AA:1439:A:H2'	1:AA:1440:G:H8	1.69	0.57
7:AK:51:ARG:NH1	7:AK:83:CYS:SG	2.78	0.57
14:AW:80:PHE:HA	14:AW:83:MET:HE2	1.86	0.57
32:A:1864:A:OP2	41:R:17:ARG:NH1	2.38	0.57
32:A:1999:A:H4'	50:2:49:ARG:HE	1.70	0.57
32:A:2016:C:O2	32:A:2931:A:O2'	2.20	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
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
86:v:618:MET:O	88:A6:34:P5P:OP1	2.22	0.57
86:v:658:ASN:ND2	86:v:683:ASP:O	2.37	0.57
1:AA:735:A:N6	1:AA:740:G:C6	2.73	0.57
14:AW:124:CYS:SG	14:AW:125:ARG:N	2.77	0.57
25:A1:56:ARG:HD3	25:A1:60:MET:HE3	1.86	0.57
25:A1:114:LEU:HB2	25:A1:119:ILE:HD11	1.87	0.57
86:v:63:THR:HA	86:v:66:VAL:HG22	1.86	0.57
1:AA:1329:U:O2'	1:AA:1332:A:OP2	2.23	0.57
3:AC:100:PHE:HB3	3:AC:103:CYS:HB2	1.85	0.57
29:AD:128:ARG:HH21	87:A5:8:Y5P:P	2.26	0.57
32:A:1813:C:H41	57:i:36:LEU:HD21	1.70	0.57
32:A:3157:C:O2'	83:Q:84:ARG:O	2.23	0.57
39:M:284:LYS:HB2	56:g:40:GLU:HB3	1.87	0.57
66:P:102:VAL:HG23	66:P:103:VAL:HG12	1.87	0.57
5:AI:109:PHE:O	5:AI:138:ARG:NH1	2.38	0.57
22:AV:44:GLU:OE2	22:AV:78:ASN:ND2	2.37	0.57
23:AY:368:GLN:O	23:AY:372:HIS:ND1	2.35	0.57
25:A1:211:ARG:NH1	25:A1:221:TYR:OH	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A0:36:VAL:HB	26:A0:43:ARG:HE	1.69	0.57
63:J:85:PRO:O	63:J:124:LYS:NZ	2.38	0.57
1:AA:1052:C:H4'	18:AL:149:LYS:HB3	1.87	0.57
1:AA:1246:U:OP2	1:AA:1247:G:N2	2.38	0.57
32:A:2290:A:H1'	35:F:108:ARG:HH12	1.69	0.57
32:A:3196:G:H4'	32:A:3197:U:O5'	2.05	0.57
66:P:43:ALA:HB1	71:6:226:LEU:HD13	1.87	0.57
1:AA:1239:C:H2'	1:AA:1240:A:H8	1.70	0.57
5:AI:71:SER:O	5:AI:74:ARG:NH1	2.28	0.57
11:AP:49:ASP:OD1	14:AW:85:ARG:NH1	2.36	0.57
32:A:2325:U:OP2	82:s:55:SER:OG	2.22	0.57
1:AA:939:A:OP1	27:A3:132:LYS:NZ	2.37	0.57
32:A:1749:C:OP2	32:A:2899:C:O2'	2.22	0.57
32:A:2868:C:O2'	39:M:77:ARG:NH1	2.38	0.57
32:A:3116:C:H42	32:A:3140:A:H61	1.53	0.57
40:O:49:VAL:HG21	40:O:121:ALA:HB3	1.87	0.57
86:v:617:HIS:ND1	86:v:619:VAL:HG13	2.20	0.57
5:AI:159:LEU:O	5:AI:163:HIS:ND1	2.36	0.56
32:A:1731:A:H61	57:i:115:ARG:HG2	1.70	0.56
32:A:3031:G:H2'	32:A:3032:G:C8	2.40	0.56
63:J:171:ARG:HG3	63:J:174:PHE:HE2	1.70	0.56
64:I:76:ILE:HD12	64:I:78:LEU:HD13	1.86	0.56
2:AB:198:THR:OG1	2:AB:227:CYS:SG	2.62	0.56
22:AV:66:PRO:HB3	22:AV:99:PRO:HD2	1.86	0.56
32:A:2209:G:H3'	32:A:2210:C:H5''	1.87	0.56
68:V:124:ASP:OD2	68:V:152:ARG:NH1	2.38	0.56
68:V:190:CYS:SG	68:V:191:LEU:N	2.78	0.56
82:s:371:CYS:HB2	82:s:394:TRP:HB2	1.85	0.56
1:AA:949:U:OP2	18:AL:167:LYS:NZ	2.36	0.56
1:AA:1016:U:O4	11:AP:112:LYS:NZ	2.35	0.56
1:AA:1078:A:C5'	88:A6:36:Y5P:OP1	2.54	0.56
1:AA:1556:C:OP1	6:AJ:71:LYS:NZ	2.38	0.56
86:v:549:TYR:HB3	86:v:619:VAL:HG21	1.87	0.56
1:AA:675:A:N6	1:AA:676:G:O6	2.38	0.56
1:AA:919:A:OP2	10:AO:96:ARG:NH1	2.39	0.56
1:AA:1319:A:OP1	7:AK:125:ARG:NH1	2.38	0.56
10:AO:173:ARG:NH2	19:AR:236:GLU:OE2	2.38	0.56
32:A:2461:A:OP1	69:E:238:ARG:N	2.39	0.56
42:S:142:THR:OG1	74:a:60:CYS:SG	2.64	0.56
43:T:90:LEU:HD21	43:T:111:LYS:HD2	1.87	0.56
44:W:105:VAL:HG12	66:P:72:PHE:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Z:68:ILE:HD11	47:Z:122:LEU:HD13	1.88	0.56
15:AX:364:ASN:O	15:AX:367:GLN:NE2	2.38	0.56
17:AH:162:ARG:CZ	23:AY:313:PHE:CE1	2.89	0.56
29:AD:120:LYS:HZ2	87:A5:2:P5P:H2	1.67	0.56
32:A:2110:A:OP2	65:N:67:LYS:NZ	2.39	0.56
32:A:2257:C:OP1	58:j:62:GLY:N	2.38	0.56
46:Y:93:LYS:NZ	68:V:181:ASP:O	2.38	0.56
68:V:52:GLU:HB3	68:V:143:ARG:HH22	1.70	0.56
69:E:209:LYS:NZ	69:E:263:ASN:OD1	2.34	0.56
69:E:218:VAL:HB	69:E:258:PRO:HG3	1.86	0.56
1:AA:976:A:OP1	12:AQ:2:ALA:N	2.38	0.56
1:AA:1568:U:O4'	1:AA:1595:G:N2	2.38	0.56
30:AF:53:LYS:NZ	30:AF:55:VAL:O	2.38	0.56
32:A:2938:A:OP1	32:A:2984:A:N6	2.39	0.56
44:W:105:VAL:HG12	66:P:72:PHE:HE1	1.71	0.56
45:X:128:THR:OG1	45:X:129:MET:N	2.35	0.56
45:X:181:PRO:HB3	45:X:184:ARG:HH11	1.71	0.56
68:V:178:SER:OG	68:V:181:ASP:OD2	2.24	0.56
86:v:339:THR:OG1	86:v:340:LYS:N	2.36	0.56
1:AA:829:C:H1'	1:AA:857:G:H22	1.70	0.56
1:AA:1116:A:N6	2:AB:100:ARG:O	2.32	0.56
9:AN:17:VAL:HG22	9:AN:28:VAL:HG22	1.87	0.56
32:A:1725:C:O2	32:A:2921:A:N6	2.39	0.56
32:A:1911:C:H2'	32:A:1912:A:C8	2.40	0.56
32:A:1979:U:H2'	32:A:1980:A:H8	1.71	0.56
32:A:2489:C:N4	32:A:2647:G:O6	2.39	0.56
32:A:2661:U:H2'	32:A:2662:A:H8	1.70	0.56
86:v:146:CYS:SG	86:v:147:ALA:N	2.75	0.56
16:A2:101:PRO:O	16:A2:105:ASN:ND2	2.39	0.56
27:A3:189:TRP:NE1	27:A3:191:THR:OG1	2.38	0.56
55:e:235:LYS:NZ	77:f:172:GLU:OE1	2.37	0.56
69:E:105:GLY:HA3	83:Q:91:LYS:HD2	1.88	0.56
75:c:173:LEU:HD21	75:c:218:PHE:HE1	1.70	0.56
79:k:63:CYS:HA	79:k:77:ARG:HA	1.87	0.56
1:AA:715:G:N3	1:AA:816:A:O2'	2.39	0.56
1:AA:1226:C:OP1	17:AH:128:LYS:NZ	2.38	0.56
32:A:1916:G:N2	32:A:1998:U:OP2	2.35	0.56
32:A:2083:U:O4	32:A:2084:A:N6	2.38	0.56
32:A:2103:A:N3	47:Z:35:LYS:N	2.53	0.56
32:A:2277:U:H2'	32:A:2278:A:H8	1.71	0.56
57:i:53:MET:HE3	57:i:56:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:J:111:LEU:HD13	63:J:170:GLU:CD	2.23	0.56
1:AA:845:A:OP1	21:AU:64:ARG:NH2	2.39	0.56
24:AZ:62:MET:HG3	29:AD:89:PHE:HZ	1.69	0.56
41:R:47:ILE:HG12	42:S:172:MET:HE1	1.87	0.56
63:J:159:LEU:O	63:J:163:GLU:CB	2.54	0.56
71:6:184:LEU:HD13	81:p:191:LYS:HD3	1.88	0.56
4:AE:105:CYS:O	11:AP:64:LYS:NZ	2.39	0.55
32:A:2805:A:H2	45:X:99:LYS:HE3	1.70	0.55
56:g:105:ARG:HH12	60:o:83:PRO:HD3	1.70	0.55
72:7:135:PRO:O	72:7:139:ASN:ND2	2.39	0.55
86:v:184:ALA:O	86:v:188:GLN:NE2	2.38	0.55
86:v:425:CYS:SG	86:v:426:ALA:N	2.80	0.55
12:AQ:83:PRO:HB3	14:AW:108:VAL:HG21	1.88	0.55
13:AT:143:VAL:HG21	13:AT:146:GLN:HE21	1.71	0.55
14:AW:92:MET:O	14:AW:98:LYS:NZ	2.36	0.55
32:A:2020:U:O4	39:M:58:GLN:NE2	2.39	0.55
32:A:2173:G:H21	63:J:150:SER:CA	2.19	0.55
32:A:2383:U:O4	32:A:2384:A:N6	2.39	0.55
45:X:36:ARG:NH2	45:X:149:SER:OG	2.38	0.55
70:5:69:TRP:O	70:5:71:ALA:N	2.38	0.55
1:AA:1194:C:OP1	30:AF:185:LYS:NZ	2.38	0.55
29:AD:362:LEU:HA	29:AD:365:LYS:HG2	1.87	0.55
32:A:1849:C:OP2	39:M:53:HIS:NE2	2.40	0.55
32:A:2713:C:H2'	32:A:2714:A:C4	2.40	0.55
32:A:3089:A:H61	88:A6:68:Y5P:C5'	2.18	0.55
35:F:230:ILE:HG13	35:F:242:LEU:HD11	1.87	0.55
71:6:184:LEU:HD22	81:p:191:LYS:HB2	1.87	0.55
72:7:41:THR:O	72:7:45:ASN:ND2	2.39	0.55
88:A6:69:Y5P:H5	88:A6:70:Y5P:N3	2.20	0.55
1:AA:845:A:H1'	21:AU:53:PHE:HE1	1.70	0.55
15:AX:268:LEU:O	15:AX:294:ARG:NH2	2.40	0.55
42:S:144:LEU:HB3	42:S:145:GLY:HA2	1.89	0.55
42:S:150:GLY:H	42:S:153:LEU:HD12	1.72	0.55
73:9:27:PRO:O	73:9:31:ARG:NE	2.37	0.55
1:AA:1141:C:OP1	27:A3:139:ASN:ND2	2.39	0.55
32:A:3089:A:N6	88:A6:69:Y5P:P	2.79	0.55
84:TA:79:ILE:O	84:TA:83:ASN:ND2	2.35	0.55
1:AA:890:C:H4'	1:AA:891:C:H5	1.71	0.55
8:AM:105:THR:HG21	21:AU:56:LEU:HD12	1.88	0.55
32:A:1834:U:OP2	54:b:116:ARG:NH1	2.38	0.55
32:A:2536:G:H2'	32:A:2537:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3174:U:H2'	32:A:3175:A:C8	2.41	0.55
83:Q:225:LYS:O	83:Q:226:PRO:O	2.24	0.55
86:v:132:GLU:O	86:v:136:ARG:HG2	2.07	0.55
86:v:224:TYR:HB2	86:v:238:ILE:HD11	1.89	0.55
1:AA:832:U:H2'	1:AA:833:A:H8	1.71	0.55
1:AA:1078:A:H5'	88:A6:35:Y5P:O3'	2.06	0.55
1:AA:1275:A:O2'	1:AA:1300:A:N6	2.40	0.55
15:AX:244:LEU:HB3	15:AX:296:MET:HE3	1.87	0.55
32:A:1756:A:O2'	45:X:61:ARG:NH2	2.39	0.55
32:A:2466:A:H2'	32:A:2467:A:H8	1.71	0.55
32:A:2971:A:OP1	65:N:98:HIS:NE2	2.36	0.55
32:A:3089:A:C5	88:A6:69:Y5P:P	3.00	0.55
50:2:78:VAL:HG22	50:2:81:ARG:HH21	1.72	0.55
64:I:95:MET:HE3	64:I:159:PRO:HB3	1.88	0.55
86:v:441:MET:HG3	86:v:443:SER:H	1.71	0.55
1:AA:1078:A:C4'	88:A6:36:Y5P:OP1	2.55	0.55
1:AA:1402:A:OP1	7:AK:51:ARG:NH1	2.40	0.55
1:AA:802:C:O3'	1:AA:816:A:N6	2.40	0.55
32:A:2017:U:OP1	39:M:54:LYS:NZ	2.40	0.55
34:D:204:ALA:O	34:D:208:ARG:NH1	2.39	0.55
27:A3:132:LYS:HG2	27:A3:135:ARG:HH21	1.72	0.55
32:A:1783:U:O4	32:A:1794:A:N7	2.40	0.55
32:A:2172:A:C8	63:J:23:ILE:HB	2.42	0.55
32:A:2737:U:O2'	32:A:3084:A:N3	2.34	0.55
72:7:165:ASN:HB2	72:7:184:VAL:HB	1.89	0.55
82:s:191:HIS:O	82:s:428:ARG:NH2	2.40	0.55
86:v:47:ARG:O	86:v:116:ILE:HA	2.07	0.55
86:v:330:ASN:CB	86:v:341:ILE:HG13	2.37	0.55
4:AE:11:LYS:HB2	4:AE:13:MET:HE1	1.89	0.54
32:A:2691:U:H2'	32:A:2692:G:C8	2.42	0.54
35:F:222:THR:O	35:F:224:GLU:N	2.35	0.54
51:3:183:ARG:NH1	71:6:355:LYS:O	2.40	0.54
53:8:121:TRP:HB2	55:e:70:MET:HE3	1.88	0.54
66:P:109:GLU:HG2	66:P:111:ALA:H	1.70	0.54
86:v:503:ILE:HA	86:v:506:GLN:HG2	1.89	0.54
86:v:681:VAL:HG13	86:v:683:ASP:H	1.71	0.54
6:AJ:127:ARG:NH1	6:AJ:133:GLY:O	2.41	0.54
10:AO:211:ARG:NH2	26:A0:90:ASP:OD2	2.40	0.54
13:AT:77:ARG:NH2	13:AT:85:GLN:OE1	2.36	0.54
23:AY:326:SER:O	25:A1:217:GLN:NE2	2.40	0.54
29:AD:324:CYS:HB2	29:AD:329:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2442:U:OP1	82:s:81:ARG:NH2	2.39	0.54
55:e:55:ARG:HD3	55:e:157:LEU:HD13	1.88	0.54
77:f:127:MET:SD	77:f:127:MET:N	2.81	0.54
82:s:212:ARG:HD3	82:s:379:LEU:HB3	1.88	0.54
1:AA:1562:G:H1'	1:AA:1583:A:H2	1.72	0.54
15:AX:154:HIS:HA	15:AX:261:ALA:HB3	1.89	0.54
32:A:2661:U:H2'	32:A:2662:A:C8	2.42	0.54
32:A:2661:U:OP2	69:E:238:ARG:NH2	2.40	0.54
32:A:2694:A:O2'	32:A:2941:G:N2	2.39	0.54
32:A:2816:G:N2	88:A6:69:Y5P:C5	2.71	0.54
34:D:136:SER:O	34:D:249:ASN:ND2	2.39	0.54
64:I:125:VAL:HG12	64:I:153:LEU:H	1.72	0.54
66:P:72:PHE:HB2	66:P:73:PRO:CD	2.38	0.54
73:9:53:ILE:HG22	73:9:55:GLU:H	1.72	0.54
1:AA:752:C:O2'	1:AA:793:C:N4	2.41	0.54
5:AI:149:VAL:HG11	5:AI:162:MET:HE3	1.89	0.54
13:AT:80:LEU:HD12	13:AT:84:GLU:HB2	1.89	0.54
32:A:1782:G:N2	32:A:1794:A:OP2	2.41	0.54
42:S:132:LYS:HA	42:S:148:LEU:HD13	1.89	0.54
46:Y:121:ARG:HH22	67:U:32:GLY:HA2	1.73	0.54
50:2:70:LEU:HD22	50:2:76:VAL:HG22	1.90	0.54
53:8:85:ILE:HB	77:f:128:PRO:HG3	1.89	0.54
60:o:31:ALA:HB1	64:I:46:LYS:HE3	1.90	0.54
61:q:139:GLN:HA	61:q:142:ASN:HD21	1.72	0.54
76:d:170:PRO:HA	76:d:173:THR:HG22	1.90	0.54
3:AC:117:LEU:HB2	3:AC:151:VAL:HG22	1.88	0.54
13:AT:132:ARG:NH1	13:AT:136:LEU:O	2.41	0.54
31:AG:78:ILE:O	31:AG:82:ASN:ND2	2.34	0.54
46:Y:95:ASN:ND2	68:V:197:GLU:OE1	2.41	0.54
49:1:17:LEU:HB3	49:1:63:ARG:HB3	1.90	0.54
62:r:135:LEU:HD11	62:r:139:VAL:HG13	1.90	0.54
66:P:91:GLU:HG3	66:P:106:SER:HB3	1.89	0.54
67:U:68:VAL:HG22	67:U:97:VAL:HG12	1.89	0.54
77:f:178:LEU:HD12	77:f:179:PRO:HD2	1.90	0.54
86:v:318:PRO:HA	86:v:319:ASN:CB	2.35	0.54
1:AA:929:A:H3'	29:AD:419:ARG:HH22	1.73	0.54
32:A:2043:C:O2'	32:A:2866:A:N3	2.32	0.54
32:A:2367:A:N3	46:Y:123:ARG:NH1	2.49	0.54
63:J:190:ALA:C	63:J:192:LYS:HG2	2.33	0.54
32:A:1798:A:N3	68:V:42:ARG:NH2	2.55	0.54
32:A:1965:A:H2'	32:A:1966:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2816:G:H22	88:A6:69:Y5P:C5	2.21	0.54
32:A:2933:G:N2	32:A:2936:U:O2	2.36	0.54
32:A:3089:A:C4	32:A:3089:A:C3'	2.91	0.54
61:q:103:LEU:HA	61:q:106:LYS:HZ3	1.73	0.54
1:AA:889:G:H21	1:AA:901:G:H4'	1.73	0.54
32:A:1936:A:OP1	32:A:1938:A:N6	2.41	0.54
32:A:3007:C:N4	32:A:3054:G:N7	2.55	0.54
32:A:3189:C:HO2'	62:r:155:ALA:H	1.53	0.54
32:A:3190:A:H4'	62:r:124:ARG:HH21	1.73	0.54
47:Z:75:THR:HB	47:Z:83:LYS:HG2	1.89	0.54
64:I:133:PRO:HA	64:I:136:GLU:HG2	1.90	0.54
3:AC:143:LEU:HD23	3:AC:151:VAL:HG11	1.89	0.54
33:B:1611:G:O6	33:B:1644:G:N2	2.34	0.54
52:4:76:CYS:SG	52:4:77:LYS:N	2.80	0.54
63:J:30:MET:N	63:J:30:MET:SD	2.81	0.54
29:AD:292:HIS:HE1	29:AD:357:GLU:H	1.56	0.54
32:A:2108:G:O2'	32:A:2111:C:N4	2.36	0.54
66:P:72:PHE:CZ	71:6:54:PHE:HE2	2.25	0.54
32:A:1966:G:H2'	32:A:1967:U:C6	2.43	0.53
32:A:2160:A:N6	52:4:70:THR:O	2.41	0.53
41:R:29:ARG:NH2	41:R:36:ASN:O	2.41	0.53
1:AA:944:U:H2'	1:AA:945:G:H8	1.73	0.53
2:AB:117:ASP:HB3	2:AB:120:GLN:HE22	1.72	0.53
32:A:1745:U:O4	51:3:108:LYS:NZ	2.40	0.53
32:A:1903:C:H41	39:M:58:GLN:HG2	1.73	0.53
32:A:3011:A:O2'	32:A:3173:G:N2	2.32	0.53
44:W:147:MET:HE3	71:6:338:ARG:HB2	1.89	0.53
55:e:265:LYS:H	55:e:266:PRO:HD2	1.73	0.53
56:g:54:ALA:O	56:g:56:ARG:N	2.41	0.53
9:AN:64:VAL:HG22	9:AN:84:ILE:HA	1.90	0.53
32:A:1679:U:H4'	68:V:43:PRO:HD2	1.91	0.53
32:A:2370:A:OP1	67:U:41:GLN:NE2	2.42	0.53
32:A:2571:G:H1	32:A:2586:U:H3	1.54	0.53
56:g:154:ASP:OD1	56:g:154:ASP:N	2.37	0.53
63:J:174:PHE:HE1	63:J:175:LEU:HD21	1.68	0.53
64:I:189:GLN:HA	64:I:192:ILE:HG12	1.90	0.53
9:AN:18:ILE:HD11	9:AN:29:ARG:HB3	1.89	0.53
22:AV:47:HIS:HA	22:AV:78:ASN:HD21	1.73	0.53
72:7:159:LYS:HG2	72:7:161:GLU:H	1.73	0.53
86:v:144:VAL:HG22	86:v:172:PHE:HB3	1.90	0.53
1:AA:1252:G:H5''	7:AK:30:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1416:A:H3'	1:AA:1417:A:H8	1.73	0.53
2:AB:132:THR:HG22	2:AB:192:LEU:HD21	1.91	0.53
15:AX:360:TYR:HB3	15:AX:365:TRP:HB3	1.90	0.53
32:A:1953:A:N6	32:A:1965:A:H61	2.06	0.53
32:A:2200:A:H5'	80:l:130:ASN:HB3	1.90	0.53
32:A:2206:C:N3	63:J:34:PRO:HD3	2.24	0.53
32:A:2289:G:H2'	32:A:2290:A:C8	2.44	0.53
32:A:2955:U:OP2	32:A:2963:A:N6	2.41	0.53
63:J:167:PHE:O	63:J:171:ARG:HD2	2.06	0.53
1:AA:1103:A:O2'	1:AA:1574:G:N2	2.42	0.53
1:AA:1294:A:OP2	2:AB:147:ARG:NH2	2.42	0.53
15:AX:384:SER:OG	15:AX:387:ASN:O	2.26	0.53
26:A0:78:ARG:HB2	26:A0:97:LEU:HD12	1.89	0.53
32:A:2469:A:H2'	32:A:2470:G:C8	2.43	0.53
32:A:2632:A:H2'	32:A:2635:G:H21	1.74	0.53
37:K:26:GLN:HE22	37:K:149:ARG:H	1.56	0.53
43:T:149:ARG:NH1	43:T:168:GLU:OE2	2.40	0.53
55:e:157:LEU:HG	55:e:256:THR:HG22	1.91	0.53
1:AA:704:U:N3	26:A0:57:ASP:OD2	2.41	0.53
1:AA:734:C:H4'	21:AU:71:ARG:HH11	1.73	0.53
2:AB:103:GLU:OE2	20:AS:52:ARG:NH2	2.42	0.53
32:A:1824:U:OP2	32:A:2706:A:O2'	2.26	0.53
32:A:1884:G:H1'	32:A:1895:C:H1'	1.91	0.53
32:A:3205:C:OP1	69:E:177:LYS:NZ	2.37	0.53
62:r:71:PRO:HD2	62:r:107:LEU:HD23	1.91	0.53
1:AA:1428:G:O2'	1:AA:1432:U:O2'	2.23	0.53
32:A:2134:A:H4'	32:A:2135:A:H5'	1.91	0.53
32:A:2995:G:O2'	32:A:3042:U:OP1	2.27	0.53
35:F:103:GLN:HE22	35:F:251:HIS:H	1.56	0.53
1:AA:773:U:H2'	1:AA:774:G:C8	2.44	0.53
1:AA:1369:U:H4'	30:AF:106:LEU:HD21	1.91	0.53
82:s:266:CYS:SG	82:s:267:LYS:N	2.81	0.53
1:AA:881:A:N3	1:AA:915:C:O2'	2.36	0.53
1:AA:1221:A:H3'	1:AA:1222:A:H8	1.74	0.53
1:AA:1426:U:H2'	1:AA:1427:A:C8	2.43	0.53
22:AV:274:LYS:NZ	22:AV:278:GLU:OE2	2.40	0.53
32:A:2111:C:OP1	64:I:35:ARG:NH1	2.42	0.53
32:A:3089:A:C8	88:A6:70:Y5P:P	3.02	0.53
34:D:201:GLY:O	70:5:30:ALA:N	2.41	0.53
35:F:62:VAL:HG13	78:h:118:HIS:HB2	1.90	0.53
67:U:132:GLU:OE2	67:U:136:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:5:104:CYS:SG	70:5:105:TYR:N	2.81	0.53
80:l:106:THR:OG1	80:l:108:GLU:OE1	2.27	0.53
1:AA:1206:G:O6	1:AA:1359:U:O2	2.27	0.52
51:3:183:ARG:NH2	71:6:356:ARG:O	2.39	0.52
2:AB:145:ILE:HG12	2:AB:167:HIS:HB3	1.90	0.52
4:AE:117:LEU:HD13	16:A2:10:LEU:HD12	1.91	0.52
14:AW:141:ARG:HB2	14:AW:171:GLY:H	1.73	0.52
18:AL:131:LEU:HD12	18:AL:165:MET:HE2	1.90	0.52
32:A:1744:A:H62	32:A:1754:G:N2	2.07	0.52
32:A:2144:A:H1'	42:S:188:THR:HG21	1.91	0.52
32:A:2507:A:O2'	32:A:2508:C:OP1	2.25	0.52
32:A:2601:A:N7	32:A:3077:C:O2'	2.37	0.52
32:A:2942:C:H2'	32:A:2943:G:C8	2.44	0.52
33:B:1637:C:OP1	71:6:52:ARG:NH1	2.41	0.52
63:J:156:VAL:O	63:J:157:LYS:C	2.51	0.52
63:J:191:LYS:HA	63:J:191:LYS:HE3	1.92	0.52
64:I:186:LEU:HG	64:I:190:GLY:HA3	1.91	0.52
70:5:377:ASP:OD1	70:5:380:GLN:NE2	2.42	0.52
82:s:87:GLN:O	82:s:277:GLN:NE2	2.42	0.52
82:s:105:TRP:HZ3	82:s:268:PRO:HA	1.73	0.52
1:AA:991:G:H21	1:AA:996:A:H2	1.58	0.52
1:AA:1271:C:H5	1:AA:1320:G:H21	1.55	0.52
2:AB:75:VAL:HG23	2:AB:126:GLN:HE22	1.74	0.52
14:AW:104:ILE:HG13	14:AW:114:ILE:HG12	1.91	0.52
32:A:2673:G:H2'	32:A:2674:U:H6	1.74	0.52
32:A:3089:A:H5''	32:A:3090:G:H5''	1.91	0.52
39:M:73:PRO:HD2	39:M:76:ILE:HD12	1.91	0.52
64:I:181:ILE:O	64:I:184:THR:OG1	2.22	0.52
75:c:213:LEU:HD22	75:c:216:ARG:HH21	1.74	0.52
19:AR:295:ASP:O	19:AR:299:ASN:ND2	2.31	0.52
32:A:1673:U:C4	32:A:1674:A:H1'	2.45	0.52
32:A:2365:U:H2'	32:A:2366:G:C8	2.45	0.52
32:A:3148:C:O2'	69:E:106:MET:SD	2.67	0.52
34:D:198:SER:HB3	34:D:206:TYR:HE2	1.74	0.52
37:K:20:LEU:HD22	37:K:141:LEU:HD13	1.91	0.52
38:L:69:VAL:HG12	38:L:127:LEU:HD21	1.90	0.52
86:v:129:ILE:HD13	86:v:479:THR:HB	1.91	0.52
32:A:1834:U:H4'	74:a:138:PRO:HB2	1.91	0.52
32:A:2075:U:O2'	32:A:2833:A:N7	2.42	0.52
32:A:2508:C:H2'	32:A:2509:A:H8	1.74	0.52
44:W:106:PRO:O	66:P:72:PHE:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:78:LEU:HD11	80:l:118:TRP:CE3	2.45	0.52
70:5:132:LEU:HD21	70:5:377:ASP:HB2	1.91	0.52
86:v:335:SER:O	86:v:337:GLU:N	2.42	0.52
1:AA:807:A:H1'	1:AA:808:C:H5	1.75	0.52
1:AA:1190:C:O2'	1:AA:1191:C:O4'	2.24	0.52
14:AW:146:ASP:OD1	14:AW:147:LEU:N	2.41	0.52
17:AH:101:GLU:OE1	25:A1:120:LYS:NZ	2.35	0.52
32:A:2175:C:H5''	63:J:99:LYS:HE2	1.90	0.52
39:M:78:ILE:O	51:3:113:ARG:NH1	2.38	0.52
61:q:138:GLN:O	61:q:142:ASN:ND2	2.43	0.52
63:J:171:ARG:CA	63:J:174:PHE:HE2	1.96	0.52
64:I:119:HIS:O	64:I:160:LYS:NZ	2.40	0.52
69:E:334:ASP:OD1	69:E:335:GLU:N	2.43	0.52
86:v:47:ARG:HB2	86:v:116:ILE:HG13	1.90	0.52
88:A6:69:Y5P:H4A	88:A6:70:Y5P:C2	2.39	0.52
11:AP:65:CYS:HB2	11:AP:68:CYS:HB2	1.91	0.52
19:AR:103:TYR:OH	29:AD:307:LYS:NZ	2.43	0.52
32:A:2048:U:O2'	32:A:2267:U:O2'	2.26	0.52
32:A:2603:C:H4'	32:A:3090:G:H1'	1.92	0.52
32:A:2654:U:H2'	32:A:2655:G:H5''	1.91	0.52
35:F:276:GLN:HE21	57:i:62:ILE:HG23	1.74	0.52
66:P:68:TRP:O	66:P:70:THR:N	2.42	0.52
71:6:332:HIS:HD2	81:p:129:ARG:HD2	1.74	0.52
1:AA:717:G:H4'	1:AA:718:A:O5'	2.09	0.52
7:AK:104:TRP:HB2	7:AK:106:LEU:HD22	1.92	0.52
10:AO:79:ARG:HD2	10:AO:141:GLY:HA2	1.91	0.52
22:AV:110:HIS:NE2	22:AV:375:TYR:OH	2.34	0.52
32:A:3189:C:C6	52:4:86:GLY:HA2	2.45	0.52
37:K:20:LEU:HB2	37:K:141:LEU:HD22	1.91	0.52
38:L:98:PRO:HG3	38:L:124:PRO:HB3	1.92	0.52
39:M:30:ASN:OD1	60:o:86:ARG:NH2	2.42	0.52
63:J:159:LEU:CB	63:J:162:GLU:HB3	2.20	0.52
3:AC:77:ASP:N	3:AC:77:ASP:OD1	2.43	0.52
6:AJ:99:GLY:O	6:AJ:127:ARG:NH2	2.43	0.52
16:A2:11:ALA:HB2	16:A2:19:PRO:HB3	1.91	0.52
17:AH:125:HIS:CD2	17:AH:126:ILE:HG13	2.44	0.52
22:AV:195:ASP:OD1	22:AV:196:PHE:N	2.41	0.52
27:A3:174:ARG:HA	27:A3:177:TRP:CE2	2.44	0.52
31:AG:290:SER:H	31:AG:327:ASP:HB2	1.74	0.52
32:A:1868:G:OP2	32:A:1868:G:N2	2.39	0.52
32:A:2027:A:O2'	32:A:2048:U:OP1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2145:G:N1	32:A:2256:U:O4	2.42	0.52
54:b:78:GLU:HG2	54:b:84:VAL:HG22	1.91	0.52
55:e:122:ASP:O	55:e:126:GLN:NE2	2.43	0.52
63:J:159:LEU:O	63:J:163:GLU:HG3	2.09	0.52
88:A6:62:Y5P:H4A	88:A6:63:Y5P:H4	1.92	0.52
15:AX:365:TRP:NE1	15:AX:395:CYS:O	2.41	0.52
32:A:2642:C:H2'	32:A:2643:G:C8	2.44	0.52
32:A:2899:C:H5'	51:3:113:ARG:HH22	1.75	0.52
32:A:2982:C:N4	32:A:2983:G:O6	2.43	0.52
58:j:36:ASN:ND2	58:j:38:SER:OG	2.35	0.52
60:o:15:ARG:HG2	60:o:18:ILE:HG12	1.92	0.52
71:6:217:LEU:HD13	71:6:236:LEU:HD13	1.91	0.52
72:7:79:PHE:HB3	72:7:81:MET:HE2	1.92	0.52
79:k:49:CYS:SG	79:k:50:SER:N	2.84	0.52
1:AA:683:G:OP1	13:AT:160:ARG:NH1	2.43	0.51
22:AV:43:ARG:NH2	22:AV:375:TYR:OH	2.40	0.51
32:A:2860:G:O2'	44:W:65:ASN:OD1	2.24	0.51
32:A:3089:A:N6	88:A6:69:Y5P:HA	2.25	0.51
62:r:63:PRO:HG2	62:r:66:PRO:HG3	1.91	0.51
1:AA:1078:A:OP1	88:A6:35:Y5P:C2'	2.57	0.51
1:AA:1239:C:H2'	1:AA:1240:A:C8	2.45	0.51
24:AZ:40:LEU:HD12	24:AZ:41:PRO:HD2	1.92	0.51
32:A:1737:A:N6	32:A:1760:G:H21	2.07	0.51
32:A:2373:A:H1'	32:A:2374:A:H8	1.75	0.51
39:M:169:LYS:NZ	39:M:241:GLY:O	2.32	0.51
1:AA:1078:A:H4'	88:A6:36:Y5P:OP1	2.09	0.51
13:AT:105:ILE:HA	21:AU:105:LEU:HD13	1.91	0.51
19:AR:156:TYR:HB2	19:AR:175:ARG:HB3	1.92	0.51
57:i:57:TYR:OH	61:q:28:ARG:O	2.26	0.51
77:f:136:GLN:HB2	77:f:146:LEU:HB2	1.91	0.51
83:Q:148:THR:HG22	83:Q:165:GLU:HG2	1.92	0.51
83:Q:225:LYS:O	83:Q:229:TRP:NE1	2.28	0.51
86:v:171:THR:HB	86:v:295:VAL:HG12	1.91	0.51
1:AA:1440:G:H2'	1:AA:1441:A:H8	1.76	0.51
7:AK:102:ARG:HA	24:AZ:51:TRP:HH2	1.74	0.51
11:AP:124:TYR:HB3	12:AQ:9:ALA:HB2	1.90	0.51
29:AD:264:ARG:NH2	87:A5:3:Y5P:C3'	2.73	0.51
30:AF:207:HIS:NE2	30:AF:211:GLU:OE2	2.43	0.51
32:A:2173:G:H21	63:J:150:SER:C	2.17	0.51
32:A:2257:C:H2'	32:A:2258:A:C4	2.46	0.51
32:A:2277:U:H2'	32:A:2278:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2292:G:H5'	35:F:154:GLY:HA2	1.92	0.51
38:L:68:LYS:NZ	38:L:91:MET:SD	2.83	0.51
1:AA:719:G:H1	1:AA:799:A:H1'	1.76	0.51
16:A2:102:ASN:HA	16:A2:105:ASN:HD21	1.76	0.51
31:AG:312:GLN:OE1	31:AG:345:ARG:NH1	2.43	0.51
32:A:2155:A:O2'	32:A:2156:A:O4'	2.24	0.51
32:A:2192:A:H4'	63:J:139:SER:HB3	1.92	0.51
32:A:2724:G:O2'	32:A:2726:C:N4	2.38	0.51
39:M:155:GLU:OE2	39:M:179:TYR:OH	2.29	0.51
70:5:280:GLN:HE21	82:s:158:ARG:HH22	1.56	0.51
86:v:182:ASN:OD1	86:v:182:ASN:N	2.43	0.51
86:v:485:ASP:OD1	86:v:486:THR:N	2.42	0.51
17:AH:186:GLU:OE2	25:A1:181:ASN:ND2	2.44	0.51
32:A:2065:A:OP1	77:f:48:TYR:N	2.43	0.51
32:A:2085:A:H2'	32:A:2086:A:C8	2.43	0.51
32:A:3123:G:N2	32:A:3132:G:OP2	2.41	0.51
39:M:95:PRO:HB2	71:6:380:TYR:HB3	1.92	0.51
51:3:137:THR:HG23	51:3:140:ARG:H	1.75	0.51
64:I:40:MET:HB3	64:I:44:ARG:HD3	1.92	0.51
1:AA:944:U:H2'	1:AA:945:G:C8	2.46	0.51
1:AA:1264:C:O2'	17:AH:122:GLN:O	2.28	0.51
15:AX:188:LEU:HD22	15:AX:226:VAL:HG13	1.93	0.51
32:A:2620:G:H2'	32:A:2621:G:H8	1.76	0.51
41:R:114:LYS:NZ	74:a:45:CYS:O	2.37	0.51
45:X:69:ILE:HG22	45:X:86:ILE:HG12	1.91	0.51
82:s:105:TRP:CE2	82:s:271:LEU:HD13	2.46	0.51
1:AA:664:G:O2'	1:AA:1166:A:N1	2.33	0.51
3:AC:38:ARG:HD2	3:AC:43:ARG:HH21	1.75	0.51
3:AC:122:VAL:HG12	3:AC:156:GLN:HB3	1.92	0.51
11:AP:78:GLN:NE2	11:AP:132:ASP:OD2	2.42	0.51
31:AG:267:MET:N	31:AG:267:MET:SD	2.84	0.51
32:A:1883:G:N7	35:F:281:ARG:NH1	2.59	0.51
32:A:2951:A:O2'	52:4:103:MET:SD	2.68	0.51
32:A:2952:U:HO2'	52:4:70:THR:HG1	1.55	0.51
42:S:165:GLU:HA	42:S:189:PRO:HA	1.91	0.51
55:e:159:LEU:HD11	55:e:252:HIS:HB2	1.92	0.51
65:N:114:ASP:OD2	65:N:117:ASN:ND2	2.44	0.51
80:l:100:ASN:OD1	80:l:101:LEU:N	2.43	0.51
86:v:58:GLY:C	92:v:802:GCP:O2A	2.53	0.51
86:v:572:GLU:HG2	86:v:610:VAL:HG12	1.93	0.51
1:AA:1068:A:H4'	1:AA:1588:G:H4'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:150:PRO:HB3	23:AY:309:LYS:HD3	1.92	0.51
9:AN:11:ARG:HA	9:AN:68:ALA:HB2	1.93	0.51
32:A:1767:G:H2'	32:A:1768:G:C8	2.46	0.51
32:A:2244:U:OP2	41:R:82:LYS:NZ	2.39	0.51
69:E:218:VAL:HG23	69:E:222:TRP:HD1	1.75	0.51
7:AK:62:ILE:HG13	7:AK:63:LEU:H	1.76	0.51
17:AH:79:LEU:HB3	17:AH:171:GLU:HB2	1.93	0.51
32:A:2173:G:H21	63:J:150:SER:HA	1.76	0.51
32:A:3179:G:H2'	32:A:3180:A:C8	2.46	0.51
35:F:234:THR:O	61:q:25:TYR:N	2.43	0.51
53:8:107:THR:HG23	53:8:110:GLU:H	1.76	0.51
66:P:72:PHE:CG	66:P:73:PRO:HD2	2.45	0.51
1:AA:826:A:H62	6:AJ:55:ARG:HG3	1.76	0.50
1:AA:1380:G:H1'	15:AX:163:LYS:HE2	1.93	0.50
1:AA:1470:A:H2'	1:AA:1471:A:H8	1.76	0.50
15:AX:56:PRO:HA	15:AX:59:HIS:HD2	1.75	0.50
24:AZ:53:PRO:O	24:AZ:55:HIS:ND1	2.44	0.50
25:A1:237:GLU:O	25:A1:241:LYS:NZ	2.40	0.50
32:A:1743:U:H2'	32:A:1744:A:C8	2.46	0.50
32:A:2214:A:O3'	80:l:122:ARG:NH1	2.44	0.50
32:A:3063:G:OP1	32:A:3063:G:N2	2.44	0.50
42:S:129:ARG:NH1	42:S:131:GLU:OE2	2.44	0.50
63:J:131:ALA:O	64:I:117:ARG:NH1	2.44	0.50
67:U:153:LEU:HD21	76:d:240:LYS:HD3	1.93	0.50
83:Q:268:ASP:O	83:Q:270:MET:N	2.44	0.50
86:v:152:GLN:N	86:v:155:THR:OG1	2.44	0.50
29:AD:227:ASN:OD1	87:A5:1:Y5P:C5	2.60	0.50
32:A:2077:C:O2'	44:W:59:HIS:NE2	2.40	0.50
32:A:2815:G:C8	32:A:2937:A:H4'	2.46	0.50
32:A:2864:U:H5'	32:A:2865:C:H4'	1.94	0.50
51:3:132:LYS:O	51:3:136:LYS:NZ	2.35	0.50
66:P:143:PHE:HB3	66:P:174:GLU:HG2	1.93	0.50
68:V:22:GLY:O	68:V:24:SER:N	2.42	0.50
70:5:173:ARG:NH1	70:5:348:ASP:O	2.41	0.50
86:v:175:LYS:HE2	92:v:802:GCP:N7	2.24	0.50
1:AA:1002:C:H2'	1:AA:1003:A:H8	1.74	0.50
1:AA:1292:A:H2'	31:AG:216:LEU:HD13	1.94	0.50
1:AA:1437:U:H2'	1:AA:1438:A:H8	1.76	0.50
1:AA:1600:A:N1	16:A2:98:SER:OG	2.42	0.50
43:T:62:GLN:HG3	76:d:229:GLY:HA3	1.94	0.50
60:o:35:MET:HG2	60:o:38:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:864:U:H2'	1:AA:865:A:C8	2.47	0.50
1:AA:1369:U:O4	30:AF:192:ARG:NE	2.41	0.50
15:AX:329:LEU:HB3	15:AX:333:GLY:HA3	1.91	0.50
19:AR:128:MET:HE1	19:AR:269:GLY:HA3	1.93	0.50
23:AY:305:THR:O	28:A4:67:LYS:NZ	2.37	0.50
29:AD:265:MET:CE	87:A5:4:Y5P:C5	2.84	0.50
32:A:1737:A:H62	32:A:1760:G:H21	1.60	0.50
32:A:3152:C:O4'	38:L:95:ARG:NH1	2.45	0.50
35:F:282:PRO:O	35:F:284:TYR:N	2.44	0.50
44:W:67:ILE:N	44:W:89:LEU:O	2.43	0.50
51:3:116:ARG:NH2	51:3:159:ASP:OD1	2.45	0.50
69:E:48:TRP:HD1	69:E:50:ASP:H	1.60	0.50
72:7:89:TYR:HB2	72:7:115:MET:HG3	1.93	0.50
83:Q:227:LYS:N	83:Q:228:PRO:HD3	2.27	0.50
86:v:465:LYS:HB2	86:v:512:TYR:HE1	1.76	0.50
1:AA:947:U:O2'	1:AA:948:U:OP1	2.26	0.50
32:A:1742:G:O2'	32:A:1754:G:O6	2.29	0.50
38:L:34:LYS:HE2	38:L:59:HIS:HA	1.93	0.50
63:J:159:LEU:O	63:J:163:GLU:HG2	2.11	0.50
72:7:287:GLN:H	72:7:288:PRO:HD2	1.76	0.50
82:s:178:ASP:HA	82:s:181:VAL:HG12	1.94	0.50
1:AA:1067:A:H5''	5:AI:189:ARG:HG2	1.94	0.50
16:A2:19:PRO:HG2	16:A2:22:LYS:HE2	1.93	0.50
32:A:2214:A:O2'	80:l:122:ARG:HD3	2.12	0.50
32:A:2673:G:H2'	32:A:2674:U:C6	2.46	0.50
32:A:3066:C:O2'	69:E:233:GLN:OE1	2.24	0.50
64:I:119:HIS:CE1	64:I:160:LYS:HD2	2.46	0.50
74:a:104:GLU:HG2	74:a:107:PRO:HD2	1.93	0.50
8:AM:69:ASN:ND2	19:AR:161:ILE:O	2.44	0.50
32:A:2909:G:N7	51:3:131:LYS:NZ	2.58	0.50
44:W:97:VAL:HG22	44:W:133:VAL:HG22	1.92	0.50
53:8:179:THR:HG21	55:e:133:LEU:HB2	1.94	0.50
65:N:203:GLU:HA	65:N:206:GLU:HG2	1.92	0.50
72:7:213:ASP:OD2	72:7:271:ARG:NH1	2.45	0.50
88:A6:21:Y5P:H4A	88:A6:22:Y5P:H4	1.94	0.50
1:AA:1207:U:H4'	1:AA:1218:A:H61	1.77	0.50
32:A:1673:U:O2	32:A:1816:G:C6	2.65	0.50
32:A:2138:U:O2'	32:A:2151:A:N3	2.37	0.50
32:A:2910:A:N3	88:A7:71:P5P:N7	2.60	0.50
49:1:55:LEU:HD12	61:q:131:MET:HE2	1.94	0.50
64:I:92:ASP:OD1	64:I:93:ASN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:E:182:THR:OG1	69:E:183:ASP:N	2.45	0.50
70:5:230:LEU:HD23	70:5:289:HIS:HD2	1.77	0.50
76:d:48:PRO:HB2	76:d:50:PHE:HD1	1.77	0.50
86:v:320:PRO:C	86:v:322:GLU:N	2.67	0.50
1:AA:1285:G:O3'	29:AD:242:ARG:NH1	2.45	0.50
32:A:1794:A:OP1	35:F:142:ARG:NH2	2.43	0.50
32:A:2025:C:OP2	42:S:182:LYS:NZ	2.35	0.50
32:A:3143:U:H2'	32:A:3144:A:C8	2.46	0.50
32:A:3143:U:H2'	32:A:3144:A:H8	1.76	0.50
37:K:168:ARG:HB3	62:r:59:GLU:HA	1.93	0.50
53:8:167:ASN:HD22	55:e:185:ARG:HH22	1.59	0.50
63:J:156:VAL:HG21	63:J:159:LEU:CD1	2.40	0.50
81:p:156:ASP:HA	81:p:159:THR:HG22	1.94	0.50
86:v:78:GLU:HG3	92:v:802:GCP:H3'	1.93	0.50
29:AD:120:LYS:HZ3	87:A5:2:P5P:C2	2.21	0.49
32:A:1930:C:O2'	32:A:1944:C:N4	2.45	0.49
32:A:2232:A:O2'	32:A:3002:G:N3	2.44	0.49
32:A:2255:C:H2'	32:A:2256:U:H5	1.77	0.49
72:7:166:LEU:HD22	72:7:181:TYR:HE2	1.76	0.49
78:h:137:ARG:NH2	78:h:141:ASP:O	2.45	0.49
1:AA:1106:C:O2'	1:AA:1108:C:OP2	2.25	0.49
4:AE:85:ASP:OD1	4:AE:86:ILE:N	2.45	0.49
13:AT:150:PRO:HB3	13:AT:155:LEU:HG	1.94	0.49
23:AY:359:SER:HB3	25:A1:211:ARG:HH21	1.77	0.49
26:A0:99:ARG:HB2	26:A0:115:TRP:HB2	1.93	0.49
32:A:1741:A:H4'	32:A:1742:G:H4'	1.94	0.49
32:A:1814:A:N3	32:A:1862:U:O2'	2.44	0.49
42:S:204:LEU:HD11	74:a:59:VAL:HG21	1.94	0.49
63:J:34:PRO:O	63:J:36:GLY:N	2.41	0.49
68:V:147:SER:HB3	68:V:152:ARG:H	1.76	0.49
72:7:49:ASN:OD1	72:7:256:ARG:NH1	2.44	0.49
83:Q:76:LEU:HD21	83:Q:282:ILE:HD11	1.93	0.49
1:AA:735:A:O2'	21:AU:68:ARG:NH2	2.45	0.49
1:AA:1214:A:N6	1:AA:1351:G:O2'	2.44	0.49
1:AA:1426:U:H2'	1:AA:1427:A:H8	1.77	0.49
32:A:2586:U:H2'	32:A:2587:G:C8	2.46	0.49
55:e:63:LEU:HD21	55:e:68:GLU:HB2	1.94	0.49
70:5:351:VAL:HG12	70:5:381:LEU:HG	1.93	0.49
72:7:64:LYS:NZ	76:d:278:LYS:O	2.45	0.49
76:d:57:MET:SD	76:d:57:MET:N	2.85	0.49
79:k:10:LEU:HD22	79:k:42:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Q:119:VAL:HG22	83:Q:174:ILE:HG23	1.95	0.49
83:Q:181:LYS:HB2	83:Q:217:VAL:HG22	1.94	0.49
19:AR:167:HIS:O	19:AR:189:ARG:NH2	2.38	0.49
22:AV:179:GLN:NE2	22:AV:367:CYS:SG	2.86	0.49
29:AD:175:GLN:OE1	29:AD:179:TRP:NE1	2.46	0.49
32:A:1860:A:H2'	32:A:1861:U:C6	2.48	0.49
32:A:2747:U:N3	32:A:2802:A:N1	2.60	0.49
32:A:2860:G:OP2	71:6:368:ARG:NH1	2.46	0.49
39:M:273:TRP:HE1	39:M:284:LYS:HG2	1.76	0.49
63:J:60:ILE:HG22	63:J:62:GLU:H	1.78	0.49
86:v:174:ASN:OD1	86:v:175:LYS:N	2.38	0.49
32:A:1954:U:H5'	32:A:2462:A:H4'	1.95	0.49
32:A:2588:C:O2	32:A:2592:G:O6	2.31	0.49
34:D:107:ILE:HG13	34:D:135:ARG:HH12	1.76	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
56:g:125:GLU:HG3	56:g:136:PRO:HD2	1.93	0.49
68:V:33:ARG:NH2	76:d:61:ARG:O	2.44	0.49
77:f:165:THR:O	77:f:168:GLU:HG3	2.12	0.49
86:v:46:ILE:HG21	86:v:416:ASP:OD1	2.12	0.49
88:A6:69:Y5P:C5	88:A6:70:Y5P:C2	2.91	0.49
1:AA:1098:C:OP1	1:AA:1151:C:N4	2.46	0.49
1:AA:1453:A:H2'	1:AA:1454:G:H8	1.78	0.49
1:AA:1478:A:N6	1:AA:1565:A:O2'	2.45	0.49
15:AX:163:LYS:HG3	15:AX:164:ASN:HD22	1.78	0.49
26:A0:88:GLN:OE1	26:A0:201:TRP:NE1	2.39	0.49
30:AF:168:TYR:HB3	30:AF:236:LEU:HD13	1.94	0.49
32:A:2370:A:OP2	67:U:71:ARG:NH2	2.45	0.49
32:A:2538:C:H2'	32:A:2539:A:O4'	2.12	0.49
32:A:3195:A:OP2	32:A:3196:G:O2'	2.27	0.49
60:o:12:ILE:HG21	60:o:16:GLN:HB3	1.94	0.49
68:V:51:ASP:OD1	68:V:81:ARG:NH2	2.42	0.49
71:6:322:ARG:NH1	81:p:181:GLU:OE1	2.46	0.49
72:7:286:LEU:HD23	72:7:286:LEU:H	1.78	0.49
74:a:45:CYS:SG	74:a:46:ASN:N	2.85	0.49
86:v:207:LEU:O	86:v:209:GLY:N	2.45	0.49
1:AA:658:G:H21	1:AA:1286:A:H1'	1.77	0.49
1:AA:1216:C:H2'	1:AA:1217:G:C8	2.46	0.49
15:AX:155:ILE:HD12	15:AX:262:VAL:HB	1.95	0.49
24:AZ:32:LYS:HA	24:AZ:35:LYS:HG2	1.95	0.49
32:A:1800:G:H22	32:A:1803:A:H5'	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2930:U:H2'	32:A:2931:A:C8	2.47	0.49
65:N:78:GLU:HG2	65:N:158:ARG:HH12	1.77	0.49
75:c:223:MET:HE3	75:c:231:MET:HE1	1.93	0.49
15:AX:334:PHE:HA	15:AX:337:LEU:HG	1.95	0.49
17:AH:74:LYS:HB2	17:AH:177:LEU:HD21	1.94	0.49
32:A:2302:U:H2'	32:A:2303:A:C8	2.48	0.49
32:A:2317:G:H2'	32:A:2318:A:H8	1.76	0.49
32:A:2919:A:C3'	88:A7:71:P5P:HO3'	2.26	0.49
46:Y:117:GLN:HG2	67:U:29:VAL:HG22	1.94	0.49
55:e:162:ARG:HB3	55:e:251:HIS:HB2	1.94	0.49
72:7:42:GLU:HA	72:7:45:ASN:HD21	1.76	0.49
82:s:112:THR:HG22	82:s:391:ASN:HB2	1.93	0.49
83:Q:77:SER:HB3	83:Q:80:PHE:HD2	1.78	0.49
83:Q:168:ASN:HB3	83:Q:171:VAL:HG23	1.94	0.49
86:v:122:PRO:O	92:v:802:GCP:O2G	2.31	0.49
32:A:2715:A:O2'	69:E:245:THR:O	2.26	0.49
77:f:138:GLN:OE1	77:f:141:GLY:N	2.42	0.49
82:s:228:ASP:O	82:s:230:ARG:NH1	2.46	0.49
82:s:316:CYS:HB3	82:s:319:GLN:HB2	1.94	0.49
1:AA:1078:A:OP1	88:A6:36:Y5P:C4'	2.61	0.49
1:AA:1358:A:O2'	88:A6:27:P5P:O5'	2.29	0.49
18:AL:69:SER:HA	18:AL:93:SER:HB2	1.94	0.49
32:A:2190:C:O2'	63:J:149:ARG:NH2	2.45	0.49
32:A:2710:C:H2'	32:A:2711:A:H8	1.78	0.49
64:I:168:LEU:HB2	64:I:174:LEU:HD23	1.93	0.49
65:N:247:MET:N	65:N:247:MET:SD	2.85	0.49
66:P:44:VAL:HA	71:6:225:LEU:HB3	1.95	0.49
1:AA:1490:U:OP1	27:A3:142:LYS:NZ	2.40	0.48
4:AE:120:THR:HG21	20:AS:51:VAL:HG21	1.94	0.48
15:AX:284:PRO:HB2	15:AX:294:ARG:HH21	1.78	0.48
19:AR:276:VAL:HA	19:AR:281:ILE:HD11	1.95	0.48
32:A:2174:G:H21	63:J:102:ARG:C	2.20	0.48
36:H:58:ARG:HH11	36:H:77:HIS:HB3	1.78	0.48
50:2:57:ASN:OD1	50:2:60:ARG:NH2	2.39	0.48
62:r:50:GLU:OE2	79:k:77:ARG:NH1	2.46	0.48
86:v:742:LEU:HD23	86:v:742:LEU:H	1.77	0.48
1:AA:1028:G:N7	16:A2:18:LYS:NZ	2.60	0.48
15:AX:123:ARG:NH2	15:AX:297:MET:O	2.40	0.48
31:AG:116:LEU:O	31:AG:122:ARG:NH2	2.47	0.48
32:A:2576:A:N3	86:v:628:ARG:NH2	2.61	0.48
35:F:63:GLN:HA	35:F:81:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:194:TYR:HA	64:I:197:LEU:HD23	1.95	0.48
86:v:380:LYS:NZ	86:v:396:GLN:O	2.45	0.48
10:AO:193:LEU:HD23	10:AO:193:LEU:H	1.76	0.48
22:AV:219:VAL:HG22	22:AV:352:LEU:HD11	1.95	0.48
26:A0:62:SER:OG	26:A0:63:ARG:N	2.46	0.48
31:AG:380:LYS:HG3	31:AG:387:ALA:H	1.78	0.48
32:A:2740:A:H2'	32:A:2741:A:H8	1.78	0.48
33:B:1622:A:H2'	33:B:1623:G:C8	2.48	0.48
65:N:204:GLU:OE2	65:N:208:ASN:ND2	2.46	0.48
70:5:241:SER:N	70:5:244:GLU:OE2	2.40	0.48
75:c:102:GLU:HA	75:c:105:ARG:HG2	1.94	0.48
82:s:266:CYS:SG	82:s:270:LYS:HG3	2.54	0.48
86:v:681:VAL:HG22	86:v:682:GLU:H	1.77	0.48
1:AA:1365:A:O2'	1:AA:1418:G:N2	2.46	0.48
1:AA:1416:A:H3'	1:AA:1417:A:C8	2.48	0.48
3:AC:69:LEU:HD23	25:A1:107:LYS:HE2	1.96	0.48
6:AJ:105:HIS:HE2	86:v:491:THR:HG21	1.78	0.48
15:AX:324:LEU:HD13	25:A1:304:GLU:HB3	1.94	0.48
17:AH:180:LEU:HD22	17:AH:184:ILE:HD13	1.96	0.48
24:AZ:67:PHE:HB3	29:AD:137:TYR:HE1	1.77	0.48
32:A:1800:G:H2'	32:A:1805:A:H61	1.79	0.48
32:A:1980:A:OP2	50:2:59:LYS:NZ	2.44	0.48
32:A:2930:U:H2'	32:A:2931:A:H8	1.79	0.48
53:8:150:LEU:HB2	55:e:212:HIS:HE1	1.78	0.48
58:j:88:LEU:HD11	60:o:53:TYR:HE2	1.78	0.48
65:N:96:TYR:OH	65:N:129:LYS:NZ	2.46	0.48
68:V:52:GLU:OE1	68:V:52:GLU:N	2.46	0.48
82:s:93:VAL:HB	82:s:233:ILE:HG12	1.95	0.48
83:Q:177:VAL:HA	83:Q:206:PRO:HB3	1.96	0.48
86:v:203:ILE:HG12	86:v:217:LEU:HD23	1.94	0.48
86:v:372:ARG:HD3	86:v:417:ILE:HG13	1.95	0.48
1:AA:1431:G:OP2	30:AF:36:ARG:HB2	2.12	0.48
1:AA:1462:G:H2'	1:AA:1463:G:C8	2.48	0.48
11:AP:78:GLN:HE21	11:AP:82:GLN:HG3	1.79	0.48
25:A1:244:THR:HG22	25:A1:246:ALA:H	1.79	0.48
32:A:3089:A:C6	88:A6:69:Y5P:HA	2.48	0.48
58:j:50:SER:HA	58:j:57:ALA:HB2	1.96	0.48
63:J:33:PRO:HB2	63:J:34:PRO:HD2	1.95	0.48
66:P:39:VAL:HG12	66:P:41:ASN:H	1.78	0.48
69:E:134:SER:OG	69:E:137:ASN:ND2	2.46	0.48
1:AA:1014:A:H4'	5:AI:184:ASN:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1056:A:O2'	1:AA:1577:U:O2	2.30	0.48
1:AA:1337:U:H2'	1:AA:1338:A:H8	1.77	0.48
9:AN:18:ILE:HD12	9:AN:27:LYS:HG2	1.96	0.48
31:AG:108:ILE:HD11	31:AG:125:MET:HE2	1.95	0.48
32:A:2521:A:N6	34:D:202:ARG:O	2.43	0.48
32:A:2536:G:H2'	32:A:2537:G:C8	2.48	0.48
35:F:102:TRP:HE1	35:F:164:MET:HA	1.78	0.48
62:r:79:HIS:HB3	62:r:184:ASN:HA	1.96	0.48
70:5:204:VAL:HG11	70:5:279:PHE:HZ	1.78	0.48
83:Q:120:THR:HG23	83:Q:172:GLN:HB2	1.95	0.48
10:AO:71:ARG:NH2	10:AO:75:ALA:O	2.47	0.48
26:A0:78:ARG:HH12	26:A0:144:LYS:HB2	1.79	0.48
32:A:1829:A:H2'	32:A:1830:G:C8	2.49	0.48
32:A:3080:G:H2'	32:A:3081:A:H8	1.78	0.48
64:I:198:PRO:HB2	64:I:202:LEU:HD11	1.95	0.48
88:A6:69:Y5P:H5	88:A6:70:Y5P:C4	2.44	0.48
26:A0:62:SER:OG	26:A0:66:GLN:OE1	2.27	0.48
26:A0:83:LYS:HE3	26:A0:138:ASP:HA	1.96	0.48
30:AF:186:TRP:HH2	30:AF:226:LEU:HD22	1.77	0.48
32:A:1955:G:N2	32:A:1960:A:N6	2.61	0.48
32:A:2829:C:OP2	32:A:2830:A:O2'	2.31	0.48
32:A:2901:A:H2'	32:A:2902:A:H8	1.79	0.48
38:L:32:ILE:HG23	38:L:36:THR:HG21	1.96	0.48
69:E:79:PRO:HG3	69:E:192:PRO:HD2	1.95	0.48
70:5:60:PHE:CD1	70:5:71:ALA:CA	2.95	0.48
77:f:135:LEU:HD23	77:f:135:LEU:H	1.78	0.48
86:v:54:HIS:O	86:v:59:LYS:NZ	2.46	0.48
86:v:162:MET:HG2	86:v:167:VAL:HB	1.96	0.48
86:v:520:LYS:HE2	86:v:697:PHE:HB3	1.96	0.48
19:AR:254:ASP:OD1	19:AR:259:TYR:OH	2.32	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:2466:A:H5''	83:Q:232:ARG:HE	1.77	0.48
32:A:3000:A:H2'	32:A:3001:G:C8	2.48	0.48
32:A:3032:G:N2	32:A:3052:A:N3	2.45	0.48
32:A:3089:A:C6	88:A6:69:Y5P:O5'	2.66	0.48
35:F:253:MET:HE3	35:F:259:LEU:HD22	1.95	0.48
37:K:171:THR:HG22	62:r:59:GLU:H	1.79	0.48
39:M:44:ARG:HG3	39:M:45:ARG:HG3	1.96	0.48
39:M:216:ASP:OD1	39:M:217:ALA:N	2.46	0.48
39:M:264:GLN:HE22	39:M:270:ALA:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:8:106:LEU:HD22	53:8:110:GLU:HG2	1.95	0.48
59:m:37:ARG:HH21	77:f:109:TYR:HE1	1.62	0.48
63:J:171:ARG:HD2	63:J:171:ARG:N	2.28	0.48
70:5:145:ASN:HA	70:5:194:LYS:HE2	1.96	0.48
82:s:66:TRP:HA	82:s:69:THR:HG22	1.95	0.48
1:AA:1287:A:H2'	1:AA:1288:G:H8	1.79	0.48
1:AA:1439:A:H2'	1:AA:1440:G:C8	2.49	0.48
1:AA:1514:A:H2'	1:AA:1515:G:C8	2.49	0.48
6:AJ:67:THR:HG22	6:AJ:79:LYS:HA	1.95	0.48
10:AO:92:LYS:HA	10:AO:144:VAL:HB	1.96	0.48
12:AQ:70:ARG:HH12	14:AW:151:SER:HB2	1.78	0.48
19:AR:136:VAL:O	19:AR:186:TRP:NE1	2.40	0.48
29:AD:329:ILE:HG21	29:AD:332:MET:HE3	1.95	0.48
31:AG:169:LEU:HB2	31:AG:228:LEU:HD21	1.95	0.48
40:O:62:TYR:OH	83:Q:272:GLU:OE1	2.30	0.48
53:8:139:MET:HG2	55:e:275:PHE:HA	1.95	0.48
67:U:80:ARG:NH1	67:U:84:ASN:OD1	2.47	0.48
76:d:192:SER:OG	76:d:215:ARG:O	2.29	0.48
1:AA:1247:G:H22	24:AZ:96:LYS:HG3	1.79	0.47
30:AF:215:ASN:HA	30:AF:220:ILE:HG13	1.95	0.47
32:A:2126:U:O4	47:Z:76:ARG:NH1	2.37	0.47
32:A:2314:C:H2'	32:A:2315:A:C5	2.49	0.47
34:D:194:ASN:HD22	34:D:247:VAL:HG22	1.79	0.47
39:M:176:THR:HB	39:M:221:GLY:HA2	1.95	0.47
49:1:17:LEU:HD11	49:1:31:ASN:HB3	1.96	0.47
71:6:274:LYS:N	71:6:312:THR:O	2.47	0.47
72:7:51:GLU:OE2	72:7:54:ARG:NH2	2.44	0.47
80:l:114:SER:OG	80:l:116:GLU:OE1	2.32	0.47
82:s:111:LYS:NZ	82:s:384:ASP:OD1	2.45	0.47
1:AA:944:U:O2'	1:AA:1025:A:N3	2.36	0.47
11:AP:140:TYR:O	11:AP:142:GLU:N	2.45	0.47
15:AX:242:ILE:HA	15:AX:245:LYS:HE2	1.95	0.47
17:AH:76:LEU:HG	17:AH:145:LEU:HB2	1.95	0.47
32:A:1728:U:H3	32:A:1750:G:H1	1.61	0.47
32:A:2081:U:H2'	32:A:2082:G:C8	2.49	0.47
32:A:2105:G:HO2'	32:A:2829:C:HO2'	1.60	0.47
32:A:2620:G:H2'	32:A:2621:G:C8	2.49	0.47
70:5:244:GLU:O	70:5:248:THR:OG1	2.30	0.47
81:p:56:ASP:OD2	81:p:60:ARG:NH2	2.46	0.47
82:s:251:VAL:O	82:s:373:GLN:NE2	2.42	0.47
82:s:366:TYR:HA	82:s:400:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AM:111:ARG:NH1	10:AO:233:GLU:O	2.46	0.47
22:AV:76:ILE:HD13	22:AV:112:TRP:HB2	1.96	0.47
32:A:1863:A:H2'	32:A:1864:A:H8	1.80	0.47
32:A:1951:C:H2'	32:A:1952:U:H6	1.79	0.47
32:A:2804:A:H2'	32:A:2805:A:C8	2.49	0.47
59:m:70:GLU:O	59:m:72:ARG:N	2.45	0.47
63:J:171:ARG:HG3	63:J:174:PHE:CE2	2.48	0.47
66:P:72:PHE:HZ	71:6:54:PHE:CE2	2.27	0.47
68:V:96:ARG:NE	68:V:111:SER:OG	2.47	0.47
71:6:147:HIS:HA	71:6:150:ARG:HG2	1.97	0.47
72:7:262:ASP:OD1	72:7:263:VAL:N	2.46	0.47
86:v:284:ARG:CG	86:v:316:TYR:HD1	2.27	0.47
88:A6:20:P5P:C6	88:A6:21:Y5P:H4	2.44	0.47
1:AA:806:C:OP2	1:AA:807:A:N6	2.46	0.47
1:AA:1146:C:OP1	27:A3:161:ARG:NH2	2.47	0.47
1:AA:1314:C:O2	30:AF:36:ARG:HA	2.14	0.47
1:AA:1438:A:H2'	1:AA:1439:A:C8	2.50	0.47
1:AA:1479:C:O2	1:AA:1482:A:O2'	2.32	0.47
1:AA:1506:U:H2'	1:AA:1507:A:C8	2.49	0.47
19:AR:154:THR:OG1	19:AR:155:LYS:N	2.46	0.47
30:AF:130:SER:OG	30:AF:133:GLU:OE1	2.33	0.47
35:F:186:ASP:HB3	35:F:258:THR:HA	1.96	0.47
36:H:70:LYS:HB2	36:H:72:ARG:HH12	1.78	0.47
68:V:19:TYR:OH	68:V:31:ASP:OD2	2.33	0.47
1:AA:1287:A:OP1	29:AD:230:THR:OG1	2.28	0.47
22:AV:175:VAL:O	22:AV:177:SER:N	2.47	0.47
31:AG:114:SER:O	31:AG:122:ARG:NH1	2.45	0.47
32:A:1737:A:O2'	57:i:93:ARG:NH2	2.38	0.47
32:A:2559:U:H4'	32:A:2560:G:O5'	2.13	0.47
32:A:2584:C:H2'	32:A:2585:G:C8	2.50	0.47
32:A:2800:U:H2'	32:A:2801:A:N7	2.30	0.47
32:A:2919:A:HO2'	88:A7:71:P5P:H5'2	1.76	0.47
32:A:2943:G:H2'	32:A:2944:C:C6	2.50	0.47
56:g:85:PHE:N	56:g:114:GLU:O	2.47	0.47
62:r:174:MET:N	62:r:174:MET:SD	2.88	0.47
1:AA:887:G:H2'	1:AA:888:U:H6	1.80	0.47
1:AA:1473:C:O3'	16:A2:32:ARG:NH1	2.45	0.47
1:AA:1506:U:H2'	1:AA:1507:A:H8	1.80	0.47
19:AR:208:ILE:HA	19:AR:211:LYS:HZ2	1.80	0.47
25:A1:84:PRO:HG3	31:AG:80:GLU:HB3	1.97	0.47
26:A0:88:GLN:O	26:A0:89:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:F:182:LEU:HD13	35:F:187:LEU:HD23	1.94	0.47
42:S:133:VAL:HG23	42:S:149:LEU:HB2	1.96	0.47
76:d:67:ILE:H	76:d:68:PRO:HD2	1.79	0.47
88:A6:61:Y5P:H4A	88:A6:62:Y5P:H4	1.96	0.47
1:AA:747:A:H2'	1:AA:748:G:H8	1.79	0.47
1:AA:891:C:H5''	6:AJ:76:ALA:HA	1.96	0.47
1:AA:1139:A:H2'	1:AA:1140:A:C8	2.50	0.47
14:AW:157:THR:HG21	16:A2:117:LEU:HB2	1.95	0.47
19:AR:107:THR:HG22	29:AD:368:LEU:HD22	1.96	0.47
32:A:1676:A:C4	57:i:36:LEU:HD23	2.50	0.47
32:A:1833:C:O5'	54:b:116:ARG:NH1	2.48	0.47
32:A:2117:U:O2'	32:A:2836:C:O2	2.27	0.47
32:A:2233:U:N3	32:A:2688:C:OP1	2.36	0.47
32:A:2989:G:O2'	32:A:2990:A:OP2	2.30	0.47
35:F:48:LEU:HD11	78:h:95:ARG:HB2	1.97	0.47
63:J:160:SER:O	63:J:163:GLU:HG3	2.15	0.47
68:V:69:ASP:HB2	68:V:72:LYS:HD2	1.96	0.47
70:5:60:PHE:CD1	70:5:67:VAL:HG22	2.50	0.47
70:5:63:LYS:HD2	70:5:67:VAL:HG11	1.96	0.47
76:d:67:ILE:HG22	76:d:68:PRO:HD3	1.97	0.47
1:AA:1284:U:O2'	29:AD:347:GLN:OE1	2.22	0.47
2:AB:99:HIS:HB2	2:AB:226:ASN:HA	1.96	0.47
30:AF:153:GLU:HA	30:AF:183:ALA:HB2	1.97	0.47
32:A:2668:A:H2'	32:A:2669:A:H8	1.80	0.47
39:M:226:PRO:HD3	81:p:45:LEU:HD11	1.97	0.47
42:S:194:ARG:HD3	54:b:18:GLY:HA3	1.96	0.47
64:I:81:LEU:HD11	80:l:113:GLU:CA	2.40	0.47
76:d:84:ILE:HA	76:d:211:GLN:HE22	1.80	0.47
86:v:654:VAL:HG12	86:v:713:TYR:HB3	1.96	0.47
86:v:680:GLY:HA2	86:v:685:PHE:HA	1.96	0.47
1:AA:985:U:H2'	1:AA:986:G:C8	2.50	0.47
5:AI:84:PRO:HB3	5:AI:101:SER:HA	1.97	0.47
7:AK:108:ARG:HH12	17:AH:124:VAL:HA	1.80	0.47
17:AH:70:ASP:OD1	17:AH:71:ILE:N	2.48	0.47
32:A:1770:G:O3'	41:R:11:ARG:NH1	2.48	0.47
32:A:1808:A:OP2	76:d:177:LYS:NZ	2.47	0.47
32:A:2944:C:H2'	32:A:2945:A:O4'	2.14	0.47
36:H:119:GLY:HA2	36:H:123:LEU:HD12	1.96	0.47
58:j:46:LEU:HD12	58:j:47:PRO:HD2	1.96	0.47
1:AA:1078:A:C5'	88:A6:36:Y5P:C5'	2.84	0.47
5:AI:98:GLN:HB2	5:AI:109:PHE:HD1	1.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AH:104:ILE:HG12	17:AH:148:LEU:HD21	1.95	0.47
22:AV:29:LEU:HB2	22:AV:364:LEU:HD21	1.97	0.47
32:A:1868:G:H21	32:A:1868:G:P	2.38	0.47
32:A:1881:A:H62	56:g:111:ARG:HD3	1.80	0.47
32:A:2214:A:HO2'	80:l:122:ARG:NH1	2.13	0.47
32:A:2298:A:H61	35:F:145:LEU:HD22	1.78	0.47
36:H:119:GLY:HA2	36:H:123:LEU:HB2	1.97	0.47
58:j:96:GLN:O	58:j:99:GLN:HG3	2.15	0.47
83:Q:165:GLU:HB2	83:Q:168:ASN:HB2	1.95	0.47
86:v:175:LYS:HB2	92:v:802:GCP:N1	2.13	0.47
1:AA:710:U:H4'	1:AA:712:C:C5	2.51	0.46
3:AC:118:GLU:OE2	3:AC:152:ARG:NH2	2.48	0.46
10:AO:199:TRP:NE1	26:A0:166:TYR:O	2.35	0.46
26:A0:41:LEU:HD21	26:A0:59:ARG:HH21	1.80	0.46
29:AD:400:GLU:HG2	29:AD:401:VAL:HG23	1.96	0.46
32:A:1788:C:O2	50:2:64:HIS:NE2	2.32	0.46
32:A:1925:A:H2'	32:A:1926:A:C8	2.50	0.46
32:A:2527:A:O4'	34:D:67:LYS:NZ	2.42	0.46
34:D:225:ILE:HA	34:D:235:GLN:HA	1.97	0.46
49:1:65:LEU:HD23	49:1:65:LEU:H	1.80	0.46
81:p:128:ASN:OD1	81:p:129:ARG:N	2.43	0.46
1:AA:774:G:H2'	1:AA:775:C:C6	2.50	0.46
5:AI:149:VAL:HG21	5:AI:162:MET:HG2	1.97	0.46
7:AK:105:ARG:NH1	24:AZ:50:ASP:O	2.48	0.46
16:A2:10:LEU:HD11	16:A2:27:LEU:HD12	1.97	0.46
17:AH:102:LEU:HD21	25:A1:123:CYS:HB3	1.97	0.46
29:AD:323:ILE:HD11	29:AD:349:LEU:HD23	1.98	0.46
31:AG:78:ILE:HG12	31:AG:128:PRO:HG2	1.97	0.46
32:A:1678:C:HO2'	32:A:1679:U:H6	1.63	0.46
32:A:1822:U:O2	32:A:2707:A:O2'	2.29	0.46
32:A:1828:A:H4'	32:A:1829:A:H8	1.79	0.46
32:A:2927:C:H4'	32:A:3074:A:H4'	1.97	0.46
46:Y:183:GLN:HE21	68:V:213:VAL:HG21	1.81	0.46
63:J:159:LEU:O	63:J:163:GLU:HB3	2.14	0.46
77:f:48:TYR:HB3	77:f:51:LYS:HG2	1.98	0.46
86:v:102:ILE:HA	86:v:122:PRO:HB3	1.96	0.46
86:v:147:ALA:O	86:v:149:GLY:N	2.49	0.46
1:AA:1262:C:H5''	29:AD:100:LYS:HE2	1.96	0.46
32:A:1790:A:OP1	50:2:82:ARG:NH2	2.48	0.46
32:A:1830:G:H2'	32:A:1831:G:H8	1.79	0.46
32:A:2170:G:O3'	63:J:124:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2366:G:H2'	32:A:2367:A:C8	2.48	0.46
36:H:84:GLU:OE1	45:X:44:ARG:NH2	2.48	0.46
70:5:172:LYS:O	70:5:175:THR:HG22	2.16	0.46
71:6:293:LEU:HD11	71:6:335:LEU:HD13	1.97	0.46
72:7:67:VAL:HG13	72:7:79:PHE:HB2	1.96	0.46
86:v:619:VAL:HB	86:v:620:ASP:OD1	2.15	0.46
1:AA:941:G:H4'	1:AA:942:A:H5''	1.96	0.46
5:AI:176:THR:HG21	12:AQ:7:PHE:HD2	1.80	0.46
23:AY:294:LEU:HD13	28:A4:88:VAL:HG22	1.96	0.46
32:A:2190:C:H4'	63:J:149:ARG:NH2	2.31	0.46
32:A:2317:G:H2'	32:A:2318:A:C8	2.50	0.46
39:M:179:TYR:HB3	39:M:183:SER:HB2	1.97	0.46
46:Y:185:VAL:HG22	67:U:9:LEU:HD21	1.97	0.46
70:5:67:VAL:CG2	70:5:71:ALA:HB2	2.41	0.46
71:6:155:TYR:O	71:6:267:ARG:NH1	2.36	0.46
82:s:99:ALA:HB3	82:s:102:ALA:HB2	1.97	0.46
86:v:331:LYS:NZ	86:v:333:ASP:OD1	2.49	0.46
86:v:401:MET:HE2	86:v:401:MET:HA	1.97	0.46
6:AJ:66:PHE:HE1	6:AJ:68:ARG:HE	1.64	0.46
32:A:2003:A:OP2	32:A:2734:A:O2'	2.33	0.46
32:A:2919:A:O2'	88:A7:71:P5P:C5'	2.62	0.46
32:A:3089:A:C5	88:A6:69:Y5P:OP1	2.68	0.46
32:A:3144:A:H2'	32:A:3145:A:H8	1.80	0.46
35:F:63:GLN:HG2	35:F:81:ASP:HB3	1.97	0.46
37:K:153:LYS:HE2	37:K:158:TYR:HA	1.96	0.46
64:I:188:ARG:NH1	79:k:53:ALA:O	2.46	0.46
71:6:216:LEU:HB3	71:6:237:LEU:HD23	1.96	0.46
76:d:208:VAL:HG22	76:d:253:THR:HG23	1.98	0.46
82:s:153:GLU:HA	82:s:157:LEU:HD12	1.97	0.46
82:s:336:THR:HB	82:s:374:LEU:HD22	1.96	0.46
83:Q:103:ARG:HE	83:Q:108:ILE:HD12	1.79	0.46
1:AA:1062:G:H2'	1:AA:1063:A:C8	2.51	0.46
19:AR:85:LEU:HD13	19:AR:119:VAL:HG13	1.98	0.46
19:AR:172:ILE:HG13	19:AR:189:ARG:HG3	1.97	0.46
23:AY:304:TRP:HB3	23:AY:310:LEU:HD13	1.97	0.46
28:A4:92:ASP:N	28:A4:92:ASP:OD1	2.47	0.46
30:AF:82:THR:HG22	30:AF:84:SER:H	1.79	0.46
32:A:1703:C:O2'	32:A:1704:U:OP2	2.26	0.46
32:A:1724:A:N6	32:A:2040:G:C2	2.79	0.46
32:A:1848:U:H5''	39:M:53:HIS:CE1	2.51	0.46
32:A:2032:G:H2'	32:A:2033:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2212:C:H2'	32:A:2213:A:C8	2.51	0.46
32:A:2439:U:H2'	32:A:2440:G:H8	1.80	0.46
35:F:175:LYS:HG2	35:F:273:LEU:HD13	1.97	0.46
35:F:184:GLN:HE22	39:M:22:VAL:HG23	1.81	0.46
36:H:131:TYR:HB3	45:X:139:TYR:HD1	1.81	0.46
66:P:59:LEU:HD11	71:6:264:GLY:HA2	1.98	0.46
70:5:140:VAL:HB	70:5:416:ALA:HB2	1.96	0.46
71:6:239:ASN:ND2	71:6:280:ASP:OD1	2.40	0.46
71:6:265:ILE:HD12	71:6:322:ARG:HG2	1.97	0.46
77:f:138:GLN:HE22	77:f:140:GLN:HG3	1.81	0.46
82:s:267:LYS:HG2	82:s:269:ASP:H	1.79	0.46
86:v:330:ASN:HB3	86:v:341:ILE:CG1	2.45	0.46
86:v:528:THR:HG22	86:v:646:LEU:HD11	1.98	0.46
1:AA:992:U:O2'	1:AA:994:A:OP2	2.23	0.46
15:AX:120:PRO:HB2	15:AX:299:ASN:HB2	1.98	0.46
32:A:1754:G:H5''	51:3:100:ARG:CZ	2.46	0.46
32:A:2080:U:OP1	60:o:67:ARG:NH1	2.49	0.46
34:D:142:VAL:HG11	34:D:163:ILE:HD11	1.98	0.46
39:M:141:VAL:HG12	39:M:143:GLU:H	1.81	0.46
55:e:176:ALA:HA	55:e:191:THR:HG21	1.98	0.46
63:J:174:PHE:CZ	63:J:175:LEU:CD2	2.87	0.46
65:N:55:ARG:HG2	65:N:99:TRP:CG	2.50	0.46
66:P:85:ARG:HD2	66:P:158:MET:HE3	1.98	0.46
68:V:59:GLY:H	68:V:76:VAL:HG13	1.81	0.46
70:5:184:LEU:HD22	70:5:411:PHE:HE1	1.81	0.46
70:5:203:CYS:O	82:s:179:GLN:NE2	2.39	0.46
82:s:257:VAL:HG22	82:s:259:ILE:H	1.81	0.46
82:s:414:ASN:ND2	82:s:416:ASP:OD1	2.49	0.46
88:A7:64:Y5P:H4A	88:A7:65:Y5P:C2	2.46	0.46
1:AA:812:A:O2'	1:AA:813:A:O4'	2.28	0.46
1:AA:924:A:O2'	6:AJ:56:PRO:HB3	2.16	0.46
1:AA:1572:A:H2'	1:AA:1573:A:H8	1.80	0.46
9:AN:24:LYS:H	9:AN:56:GLN:HE21	1.64	0.46
18:AL:138:TYR:HB2	18:AL:155:LEU:HD13	1.98	0.46
26:A0:71:LEU:HD13	26:A0:78:ARG:HG3	1.98	0.46
32:A:1742:G:H2'	51:3:105:LYS:HA	1.97	0.46
32:A:1769:C:O2'	32:A:2276:C:O2	2.30	0.46
32:A:1783:U:H3	32:A:1794:A:N6	2.09	0.46
32:A:1787:G:N2	32:A:1790:A:OP2	2.49	0.46
32:A:2606:U:H4'	32:A:2607:U:H3'	1.97	0.46
35:F:126:LYS:NZ	35:F:128:TRP:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:K:52:ASP:O	43:T:206:ARG:NH1	2.47	0.46
41:R:15:THR:HG22	75:c:32:LYS:HB3	1.98	0.46
2:AB:158:MET:HG3	2:AB:250:CYS:HB3	1.98	0.46
8:AM:72:ARG:HG3	8:AM:76:TRP:CD1	2.51	0.46
15:AX:181:PRO:HA	15:AX:237:THR:HB	1.98	0.46
21:AU:152:ARG:HA	21:AU:155:ARG:HE	1.81	0.46
29:AD:103:LEU:HD11	29:AD:123:ARG:HB2	1.96	0.46
31:AG:380:LYS:HE2	31:AG:386:GLY:HA2	1.98	0.46
32:A:1747:G:O2'	32:A:1750:G:O6	2.24	0.46
32:A:1852:C:O2'	32:A:1856:A:N6	2.49	0.46
32:A:2236:C:OP1	60:o:9:ARG:N	2.49	0.46
35:F:116:THR:HG23	35:F:118:ALA:H	1.80	0.46
46:Y:200:PHE:HB3	70:5:68:PRO:HG3	1.96	0.46
55:e:162:ARG:HH11	55:e:171:TRP:HB2	1.80	0.46
66:P:41:ASN:HB3	71:6:293:LEU:HD13	1.96	0.46
69:E:99:LEU:HD11	69:E:197:HIS:HB3	1.96	0.46
70:5:67:VAL:HB	70:5:68:PRO:HD2	1.97	0.46
71:6:31:PRO:HA	77:f:52:PRO:HB3	1.97	0.46
1:AA:936:G:H4'	1:AA:1107:U:H2'	1.96	0.46
17:AH:106:ILE:HG21	17:AH:145:LEU:HD23	1.97	0.46
30:AF:51:TYR:HE2	31:AG:367:ALA:HB2	1.80	0.46
32:A:1792:G:OP2	50:2:85:LYS:NZ	2.44	0.46
32:A:1861:U:H3	32:A:2304:G:H1	1.63	0.46
32:A:1955:G:H21	32:A:1960:A:N6	2.14	0.46
32:A:2068:C:OP2	77:f:58:LYS:NZ	2.39	0.46
32:A:2173:G:H2'	32:A:2174:G:H8	1.81	0.46
32:A:2235:C:O2'	62:r:164:LYS:O	2.28	0.46
32:A:2395:A:H1'	70:5:385:HIS:HB2	1.97	0.46
32:A:2519:G:C5	34:D:228:LEU:HD13	2.51	0.46
32:A:3079:G:N1	32:A:3090:G:O6	2.49	0.46
36:H:87:LYS:HG3	36:H:88:HIS:CD2	2.51	0.46
38:L:55:PRO:HB2	38:L:75:LEU:HD11	1.97	0.46
39:M:165:ALA:O	39:M:169:LYS:HG2	2.16	0.46
46:Y:91:ARG:NH1	73:9:83:GLU:OE1	2.48	0.46
47:Z:41:ILE:HD13	47:Z:114:LYS:HZ3	1.80	0.46
74:a:111:GLN:HA	74:a:114:LYS:HG2	1.98	0.46
1:AA:851:A:H5'	1:AA:853:C:N4	2.31	0.45
28:A4:131:ASP:OD1	28:A4:132:ILE:N	2.49	0.45
32:A:1721:C:O2'	57:i:123:ARG:NH2	2.50	0.45
32:A:2318:A:H2'	32:A:2319:A:C8	2.51	0.45
32:A:2740:A:N3	32:A:2921:A:O2'	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2952:U:H5'	52:4:69:LYS:HD3	1.99	0.45
32:A:3108:U:H3	69:E:264:ILE:HG21	1.81	0.45
63:J:73:LYS:HD2	63:J:77:THR:HB	1.97	0.45
65:N:198:MET:HA	65:N:201:ASP:OD2	2.17	0.45
81:p:51:GLU:OE1	81:p:51:GLU:N	2.48	0.45
1:AA:768:A:H4'	9:AN:24:LYS:HB2	1.98	0.45
11:AP:84:VAL:HG23	11:AP:91:ILE:HD13	1.98	0.45
37:K:134:PRO:HD2	37:K:137:ILE:HD12	1.98	0.45
51:3:110:VAL:HG13	51:3:158:LEU:HD22	1.97	0.45
57:i:63:LEU:HD23	57:i:63:LEU:H	1.81	0.45
63:J:191:LYS:HE3	63:J:192:LYS:N	2.31	0.45
76:d:147:GLU:OE1	76:d:159:ARG:NH2	2.49	0.45
86:v:49:ILE:HG21	86:v:317:LEU:HD13	1.98	0.45
88:A6:24:Y5P:H4A	88:A6:25:Y5P:H4	1.97	0.45
25:A1:91:VAL:HG22	25:A1:92:LYS:H	1.81	0.45
32:A:1753:A:OP1	57:i:118:TYR:OH	2.32	0.45
39:M:233:ARG:HH12	39:M:244:LEU:HD21	1.81	0.45
40:O:94:ALA:HB3	40:O:95:PRO:HD3	1.98	0.45
66:P:44:VAL:HG13	71:6:225:LEU:HD13	1.99	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	1.80	0.45
72:7:43:MET:HA	72:7:46:ASP:OD2	2.16	0.45
72:7:203:THR:HG21	72:7:279:GLU:HG2	1.98	0.45
75:c:258:THR:HG22	75:c:259:ARG:HG3	1.98	0.45
86:v:301:LEU:CD2	92:v:802:GCP:C2	2.90	0.45
17:AH:181:PRO:HG2	17:AH:184:ILE:HB	1.98	0.45
23:AY:294:LEU:HB3	28:A4:87:TYR:HB3	1.98	0.45
32:A:1816:G:H2'	32:A:1817:C:C6	2.52	0.45
32:A:1827:C:O4'	32:A:2698:G:N2	2.49	0.45
55:e:66:LEU:HD23	55:e:66:LEU:H	1.82	0.45
70:5:204:VAL:HG13	82:s:152:GLN:HE21	1.82	0.45
74:a:52:THR:HG22	74:a:54:ASP:H	1.81	0.45
86:v:465:LYS:HB2	86:v:512:TYR:CE1	2.51	0.45
1:AA:1468:U:H2'	1:AA:1469:G:H8	1.81	0.45
4:AE:3:ARG:HD2	4:AE:96:HIS:CG	2.52	0.45
8:AM:53:SER:H	8:AM:67:ALA:HB3	1.82	0.45
11:AP:67:LEU:HD21	11:AP:79:LEU:HD21	1.97	0.45
12:AQ:76:MET:HE1	12:AQ:79:ASN:HD22	1.81	0.45
13:AT:144:GLU:HB3	19:AR:204:ILE:HD12	1.97	0.45
26:A0:132:GLU:HG2	26:A0:207:GLN:HG2	1.98	0.45
29:AD:109:GLY:HA2	29:AD:114:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1830:G:H2'	32:A:1831:G:C8	2.51	0.45
32:A:1942:C:H2'	32:A:1943:A:O4'	2.16	0.45
32:A:1979:U:H2'	32:A:1980:A:C8	2.51	0.45
32:A:2018:G:H2'	32:A:2019:G:C8	2.51	0.45
32:A:2395:A:H2'	32:A:2396:C:H5''	1.97	0.45
32:A:2420:U:O2'	73:9:23:SER:OG	2.28	0.45
32:A:2507:A:HO2'	32:A:2508:C:P	2.38	0.45
32:A:2747:U:H2'	32:A:2748:A:C8	2.52	0.45
32:A:2934:G:H22	32:A:2937:A:H3'	1.81	0.45
40:O:45:PRO:HA	40:O:120:MET:HA	1.97	0.45
40:O:82:GLU:O	40:O:84:ASP:N	2.41	0.45
62:r:43:GLU:O	62:r:46:THR:OG1	2.31	0.45
67:U:99:LEU:HD13	67:U:103:GLN:HB2	1.99	0.45
70:5:60:PHE:CE1	70:5:71:ALA:CA	2.98	0.45
70:5:344:SER:HB3	70:5:355:LEU:HD23	1.98	0.45
77:f:97:ALA:HB2	77:f:182:VAL:HA	1.98	0.45
82:s:63:ILE:HA	82:s:66:TRP:CD1	2.47	0.45
86:v:382:ASP:OD1	86:v:383:THR:N	2.50	0.45
86:v:618:MET:C	88:A6:34:P5P:OP1	2.59	0.45
1:AA:710:U:O2'	21:AU:28:LYS:O	2.35	0.45
1:AA:1006:U:H2'	1:AA:1007:G:C8	2.51	0.45
12:AQ:67:GLU:HG3	14:AW:154:LEU:HD12	1.98	0.45
32:A:2018:G:H2'	32:A:2019:G:H8	1.80	0.45
32:A:2841:U:H5'	65:N:144:LYS:HD3	1.97	0.45
32:A:3123:G:O6	86:v:80:LYS:NZ	2.49	0.45
32:A:3193:U:H4'	62:r:138:GLY:HA3	1.97	0.45
43:T:192:ALA:HB1	74:a:112:LEU:HD21	1.98	0.45
66:P:136:CYS:HB2	66:P:141:ILE:HG23	1.97	0.45
75:c:105:ARG:NH1	75:c:113:GLU:OE2	2.49	0.45
75:c:315:ASN:HD21	75:c:317:SER:HB2	1.82	0.45
86:v:679:ASP:OD1	86:v:679:ASP:N	2.48	0.45
88:A7:12:Y5P:H4A	88:A7:13:Y5P:H4	1.99	0.45
1:AA:681:U:O4	1:AA:682:A:N6	2.49	0.45
1:AA:985:U:H2'	1:AA:986:G:H8	1.82	0.45
1:AA:1361:G:H2'	1:AA:1362:G:C8	2.52	0.45
6:AJ:78:ARG:HB3	6:AJ:94:PHE:HE1	1.82	0.45
10:AO:218:ARG:NH1	22:AV:315:GLU:O	2.49	0.45
14:AW:108:VAL:O	14:AW:110:ASN:N	2.50	0.45
19:AR:158:PHE:HB2	19:AR:173:VAL:HG13	1.98	0.45
19:AR:276:VAL:HG11	19:AR:307:LEU:HD12	1.98	0.45
22:AV:79:ILE:HG23	22:AV:84:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A1:87:MET:HE3	25:A1:104:GLU:HB3	1.98	0.45
30:AF:98:MET:O	30:AF:192:ARG:NH2	2.50	0.45
32:A:1744:A:N6	32:A:1754:G:H21	2.13	0.45
32:A:1770:G:H2'	32:A:1771:C:C6	2.52	0.45
32:A:2212:C:H2'	32:A:2213:A:H8	1.82	0.45
32:A:2610:U:H2'	32:A:2611:C:C6	2.52	0.45
32:A:2665:U:OP2	40:O:17:ARG:NH1	2.49	0.45
36:H:58:ARG:HD3	36:H:77:HIS:HB3	1.99	0.45
71:6:90:ILE:HG13	71:6:167:PHE:HB3	1.99	0.45
76:d:151:CYS:HB2	76:d:156:ASP:HB3	1.98	0.45
77:f:119:ILE:HD13	77:f:166:PHE:HE2	1.80	0.45
10:AO:51:TYR:HE2	10:AO:112:LYS:HD3	1.81	0.45
16:A2:68:LYS:O	16:A2:71:GLN:HG3	2.17	0.45
29:AD:249:ASN:OD1	29:AD:250:GLY:N	2.50	0.45
32:A:2024:C:OP1	42:S:182:LYS:HA	2.17	0.45
37:K:58:VAL:HG22	37:K:126:HIS:HB2	1.99	0.45
38:L:129:LYS:HE3	38:L:130:ARG:HH12	1.81	0.45
41:R:137:GLU:HB3	41:R:138:PRO:HD3	1.98	0.45
64:I:78:LEU:HD11	80:I:118:TRP:CZ3	2.52	0.45
64:I:105:SER:N	79:k:40:GLU:OE2	2.48	0.45
68:V:101:THR:OG1	68:V:104:TYR:O	2.29	0.45
76:d:288:LYS:O	76:d:290:GLU:N	2.50	0.45
86:v:301:LEU:HD22	92:v:802:GCP:N3	2.32	0.45
86:v:641:ALA:O	86:v:643:LEU:N	2.39	0.45
1:AA:747:A:H2'	1:AA:748:G:C8	2.51	0.45
1:AA:1233:C:O2	1:AA:1402:A:N6	2.49	0.45
1:AA:1438:A:H2'	1:AA:1439:A:H8	1.82	0.45
17:AH:81:LYS:NZ	17:AH:171:GLU:OE2	2.49	0.45
22:AV:335:LYS:O	22:AV:338:HIS:ND1	2.49	0.45
32:A:2123:C:OP1	47:Z:76:ARG:NH2	2.50	0.45
32:A:2524:A:N1	34:D:92:ARG:HD3	2.31	0.45
32:A:2667:U:C2	32:A:2668:A:C8	3.05	0.45
32:A:3092:U:H2'	32:A:3093:C:C6	2.51	0.45
70:5:168:GLU:OE1	70:5:168:GLU:N	2.49	0.45
77:f:94:HIS:ND1	77:f:154:GLU:OE2	2.45	0.45
86:v:453:ILE:HG12	86:v:501:LEU:HD13	1.99	0.45
86:v:620:ASP:OD1	86:v:620:ASP:N	2.49	0.45
1:AA:674:U:H2'	1:AA:675:A:C8	2.52	0.45
1:AA:888:U:O4	1:AA:905:A:N7	2.50	0.45
1:AA:1265:C:H2'	1:AA:1266:A:C8	2.48	0.45
10:AO:51:TYR:O	10:AO:53:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:210:LEU:HB3	22:AV:211:PRO:HD3	1.99	0.45
31:AG:197:SER:OG	31:AG:246:ARG:O	2.32	0.45
32:A:1828:A:H4'	32:A:1829:A:C8	2.52	0.45
38:L:37:ARG:HD2	38:L:54:ALA:HB3	1.99	0.45
39:M:36:PRO:HB2	39:M:38:ARG:HH22	1.82	0.45
45:X:117:GLU:O	45:X:175:GLN:NE2	2.46	0.45
53:8:150:LEU:HB2	55:e:212:HIS:CE1	2.51	0.45
53:8:163:LYS:HA	77:f:86:TYR:HB2	1.98	0.45
62:r:94:ARG:HD2	62:r:98:GLY:HA3	1.99	0.45
67:U:19:VAL:HB	73:9:136:LEU:HD23	1.98	0.45
71:6:66:GLN:HG2	71:6:75:ARG:HH22	1.82	0.45
72:7:166:LEU:HB2	72:7:236:LYS:HE2	1.99	0.45
86:v:58:GLY:H	92:v:802:GCP:PA	2.40	0.45
86:v:100:ILE:HG22	92:v:802:GCP:O1G	2.17	0.45
86:v:251:GLN:HA	86:v:254:ILE:HG12	1.99	0.45
86:v:545:GLY:O	88:A6:34:P5P:O2'	2.34	0.45
32:A:1981:G:H2'	32:A:1982:G:H8	1.82	0.44
32:A:2245:A:H4'	32:A:2246:A:OP1	2.17	0.44
32:A:2745:A:H2'	32:A:2745:A:N3	2.32	0.44
32:A:3089:A:N7	88:A6:69:Y5P:O5'	2.50	0.44
38:L:73:ILE:O	38:L:84:ALA:N	2.51	0.44
86:v:507:ARG:O	86:v:511:GLU:HG2	2.16	0.44
1:AA:1304:C:H5''	1:AA:1319:A:H2	1.82	0.44
1:AA:1529:A:H1'	22:AV:66:PRO:HD3	1.99	0.44
32:A:1899:G:H21	39:M:35:LYS:HD3	1.80	0.44
33:B:1642:G:H4'	53:8:119:LYS:HE3	1.99	0.44
40:O:149:LEU:HD22	69:E:61:ILE:HD11	1.99	0.44
44:W:107:HIS:CD2	66:P:72:PHE:HB3	2.52	0.44
70:5:136:VAL:HG11	70:5:417:LEU:HD23	1.99	0.44
70:5:200:ARG:HD3	70:5:233:LYS:HB2	1.99	0.44
71:6:45:LEU:O	71:6:50:LYS:NZ	2.40	0.44
71:6:273:PHE:HA	71:6:313:PRO:HA	1.99	0.44
86:v:685:PHE:HE2	86:v:687:LEU:HB2	1.81	0.44
1:AA:1109:A:H2'	1:AA:1110:A:C8	2.53	0.44
1:AA:1361:G:H2'	1:AA:1362:G:H8	1.82	0.44
14:AW:154:LEU:HB3	14:AW:155:GLY:H	1.68	0.44
32:A:2004:G:H2'	32:A:2005:C:C6	2.52	0.44
32:A:2263:C:H4'	42:S:175:ARG:HH12	1.82	0.44
32:A:2900:C:H2'	32:A:2901:A:H8	1.82	0.44
39:M:238:ARG:HB3	81:p:155:ARG:HH22	1.82	0.44
40:O:86:ILE:HB	40:O:87:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Z:71:ARG:HA	47:Z:117:ILE:HG22	1.99	0.44
56:g:88:ARG:NH2	56:g:166:PHE:O	2.50	0.44
69:E:58:VAL:HB	69:E:59:PRO:HD3	1.99	0.44
86:v:341:ILE:HD13	86:v:341:ILE:HA	1.91	0.44
86:v:560:ASP:OD1	86:v:560:ASP:N	2.44	0.44
3:AC:42:VAL:HG11	3:AC:51:VAL:HG11	2.00	0.44
6:AJ:70:PRO:HB2	6:AJ:71:LYS:H	1.66	0.44
15:AX:206:GLU:HB2	15:AX:249:ARG:HH12	1.83	0.44
19:AR:157:VAL:HG13	19:AR:174:VAL:HG22	1.99	0.44
32:A:1862:U:H2'	32:A:1863:A:H8	1.82	0.44
32:A:1877:U:H1'	39:M:33:SER:HB2	1.99	0.44
32:A:2362:A:N6	32:A:2432:A:O4'	2.50	0.44
43:T:92:LYS:HA	43:T:95:ARG:HG2	1.98	0.44
45:X:234:LEU:HD23	45:X:238:LEU:HD23	1.99	0.44
54:b:54:PHE:HD2	54:b:63:ILE:HD11	1.82	0.44
61:q:108:LEU:O	61:q:111:GLU:HG3	2.18	0.44
63:J:47:ASN:HB3	86:v:682:GLU:HG3	1.99	0.44
67:U:27:GLN:HB2	67:U:43:ARG:HB3	1.99	0.44
83:Q:183:LEU:HD21	83:Q:219:GLU:HG2	1.98	0.44
86:v:559:LEU:HD12	86:v:606:GLY:HA2	1.99	0.44
1:AA:810:G:H2'	1:AA:811:G:C8	2.52	0.44
1:AA:1204:C:O2'	1:AA:1225:C:N4	2.51	0.44
25:A1:67:PRO:HG3	25:A1:118:ALA:HB2	2.00	0.44
32:A:2213:A:N3	80:l:126:ILE:HD12	2.32	0.44
32:A:2307:U:H2'	32:A:2308:A:O4'	2.18	0.44
32:A:2371:U:O2	32:A:2422:U:H5''	2.17	0.44
46:Y:202:LEU:HB3	46:Y:204:TYR:CE2	2.52	0.44
55:e:151:ARG:NH1	55:e:254:TRP:O	2.50	0.44
66:P:72:PHE:HB2	66:P:73:PRO:HD2	1.99	0.44
86:v:135:LEU:HD22	86:v:136:ARG:HH21	1.83	0.44
86:v:723:CYS:SG	86:v:727:THR:OG1	2.54	0.44
88:A6:69:Y5P:C2'	88:A6:70:Y5P:HA1	2.45	0.44
88:A7:21:Y5P:H4A	88:A7:22:Y5P:H4	2.00	0.44
1:AA:932:C:OP2	9:AN:38:TYR:OH	2.36	0.44
6:AJ:102:LEU:HD21	6:AJ:132:CYS:HB3	1.98	0.44
11:AP:67:LEU:HA	11:AP:70:LYS:HD3	2.00	0.44
23:AY:326:SER:O	25:A1:216:ARG:NH2	2.51	0.44
32:A:2256:U:H2'	32:A:2257:C:C6	2.52	0.44
32:A:3089:A:C2	32:A:3090:G:OP1	2.70	0.44
32:A:3089:A:O4'	88:A6:70:Y5P:OP1	2.35	0.44
47:Z:140:LYS:HG2	47:Z:141:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:J:141:VAL:HA	63:J:144:ILE:HG22	2.00	0.44
64:I:175:PRO:HB3	79:k:53:ALA:HB1	2.00	0.44
67:U:109:ASP:CG	67:U:112:PRO:HD3	2.42	0.44
15:AX:179:ASP:HB3	15:AX:288:ALA:HB3	1.99	0.44
15:AX:319:PRO:HG2	15:AX:322:ALA:HB2	2.00	0.44
91:AX:500:GDP:H8	91:AX:500:GDP:H2'	1.72	0.44
29:AD:315:ARG:HB2	29:AD:333:TYR:HD1	1.81	0.44
31:AG:269:PHE:HZ	31:AG:271:LYS:HE3	1.83	0.44
32:A:1994:A:O2'	32:A:1995:A:OP2	2.23	0.44
32:A:2708:C:H4'	48:0:92:CYS:HB3	2.00	0.44
33:B:1625:A:N7	66:P:87:GLN:NE2	2.58	0.44
42:S:115:LEU:HB3	54:b:118:PRO:HB2	2.00	0.44
59:m:51:LEU:HB3	59:m:67:ARG:HB3	2.00	0.44
66:P:80:ARG:HH12	66:P:82:ARG:HD3	1.82	0.44
67:U:48:MET:HE2	67:U:53:LEU:HA	1.99	0.44
86:v:549:TYR:OH	88:A6:25:Y5P:HB2	2.18	0.44
1:AA:713:C:H2'	1:AA:714:A:O4'	2.18	0.44
2:AB:88:ARG:HH11	14:AW:118:GLY:H	1.64	0.44
6:AJ:95:ILE:HG13	6:AJ:125:VAL:HG21	2.00	0.44
22:AV:61:PHE:HZ	22:AV:95:PHE:HD1	1.64	0.44
29:AD:218:PHE:HA	29:AD:249:ASN:HA	2.00	0.44
32:A:2597:C:H2'	32:A:2598:A:C8	2.53	0.44
32:A:2656:U:H5''	69:E:229:ALA:HB3	2.00	0.44
32:A:3122:U:H5'	32:A:3124:U:H6	1.83	0.44
32:A:3146:G:N2	69:E:268:GLU:OE2	2.51	0.44
42:S:158:ALA:HA	42:S:195:ILE:HA	2.00	0.44
54:b:141:ARG:H	74:a:71:HIS:HA	1.83	0.44
76:d:219:ARG:NH1	76:d:239:PRO:O	2.47	0.44
79:k:13:VAL:HA	79:k:68:PHE:HA	2.00	0.44
82:s:53:ALA:HB3	82:s:58:ALA:HB2	1.99	0.44
86:v:175:LYS:NZ	92:v:802:GCP:C4	2.76	0.44
1:AA:733:U:O3'	8:AM:82:HIS:NE2	2.41	0.44
1:AA:760:A:O2'	1:AA:781:A:N6	2.51	0.44
1:AA:809:G:H2'	1:AA:810:G:H8	1.82	0.44
1:AA:1343:A:O2'	1:AA:1345:G:N7	2.41	0.44
1:AA:1358:A:O2'	88:A6:27:P5P:P	2.76	0.44
1:AA:1371:U:H2'	1:AA:1372:C:H6	1.83	0.44
2:AB:233:THR:HG23	2:AB:234:TYR:HD1	1.82	0.44
22:AV:173:PHE:CZ	22:AV:211:PRO:HG3	2.53	0.44
24:AZ:5:SER:OG	24:AZ:6:GLU:N	2.50	0.44
29:AD:120:LYS:HZ2	87:A5:2:P5P:C2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AF:178:ARG:HA	30:AF:178:ARG:HD2	1.85	0.44
32:A:1689:C:H2'	32:A:1690:C:C5	2.53	0.44
32:A:2743:U:H2'	32:A:2744:U:C6	2.53	0.44
32:A:2744:U:O2	32:A:2745:A:N6	2.50	0.44
32:A:2910:A:N3	88:A7:71:P5P:H8	2.32	0.44
33:B:1625:A:OP2	71:6:56:ARG:NH2	2.50	0.44
45:X:180:ASP:N	45:X:180:ASP:OD1	2.51	0.44
63:J:52:GLU:O	63:J:55:GLU:HG3	2.18	0.44
65:N:195:LEU:HA	65:N:198:MET:HG2	2.00	0.44
68:V:102:MET:SD	68:V:102:MET:N	2.81	0.44
71:6:178:ALA:HA	81:p:194:HIS:CD2	2.53	0.44
72:7:247:ASN:HD21	72:7:251:ILE:H	1.64	0.44
77:f:162:LEU:HB3	77:f:167:ALA:HB2	2.00	0.44
82:s:188:LEU:HD22	82:s:426:LEU:HD21	2.00	0.44
86:v:162:MET:HE3	86:v:162:MET:HB3	1.87	0.44
86:v:737:GLU:OE1	86:v:741:GLN:NE2	2.48	0.44
88:A7:47:Y5P:H4A	88:A7:48:P5P:N7	2.32	0.44
88:A7:64:Y5P:H4A	88:A7:65:Y5P:N3	2.33	0.44
1:AA:1388:C:H2'	1:AA:1389:G:C4	2.53	0.43
2:AB:106:ILE:HD13	2:AB:114:ASP:HB3	1.99	0.43
3:AC:72:HIS:HB3	3:AC:112:ARG:HB2	2.00	0.43
32:A:2065:A:C8	44:W:74:ARG:HG3	2.53	0.43
32:A:2216:A:H5''	64:I:127:PRO:HB3	2.00	0.43
34:D:225:ILE:HG13	34:D:235:GLN:HB3	1.99	0.43
43:T:161:ARG:HG2	43:T:162:GLY:H	1.83	0.43
70:5:60:PHE:CG	70:5:67:VAL:HG22	2.52	0.43
86:v:159:ASN:HA	86:v:162:MET:HE3	2.00	0.43
86:v:284:ARG:HG2	86:v:316:TYR:HD1	1.83	0.43
1:AA:688:A:OP2	1:AA:829:C:N4	2.42	0.43
1:AA:1380:G:N2	15:AX:164:ASN:OD1	2.51	0.43
11:AP:96:ILE:HG22	11:AP:136:CYS:HB2	2.00	0.43
19:AR:96:GLN:HE21	29:AD:376:GLU:HA	1.84	0.43
31:AG:172:LEU:HD11	31:AG:237:GLU:HG2	1.99	0.43
32:A:2935:A:H3'	32:A:2936:U:H2'	1.99	0.43
48:0:137:ILE:HD13	48:0:158:VAL:HG11	2.00	0.43
70:5:279:PHE:HA	82:s:156:TYR:HE2	1.83	0.43
71:6:183:ASP:HB3	81:p:189:ARG:HB3	1.99	0.43
88:A7:20:P5P:C6	88:A7:21:Y5P:H4	2.48	0.43
1:AA:839:A:H2'	1:AA:840:A:C8	2.53	0.43
1:AA:945:G:H1'	18:AL:153:ARG:HH21	1.83	0.43
1:AA:1138:G:H2'	1:AA:1139:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1477:U:H2'	1:AA:1479:C:H41	1.84	0.43
7:AK:35:TRP:NE1	7:AK:39:LYS:HE3	2.34	0.43
19:AR:276:VAL:HG13	19:AR:304:TYR:HD1	1.83	0.43
26:A0:37:ASP:HB3	26:A0:40:THR:HB	1.99	0.43
31:AG:306:ILE:HG22	31:AG:308:GLN:H	1.82	0.43
32:A:1830:G:H4'	41:R:53:CYS:HB2	1.99	0.43
33:B:1663:C:H2'	33:B:1664:G:H8	1.83	0.43
49:1:35:ASN:OD1	49:1:36:ARG:N	2.51	0.43
83:Q:194:LEU:HD12	83:Q:197:TYR:HE2	1.83	0.43
2:AB:197:HIS:NE2	2:AB:240:ASP:O	2.51	0.43
14:AW:122:CYS:HB3	14:AW:165:ALA:HB3	2.01	0.43
23:AY:313:PHE:HB3	23:AY:314:PRO:HD2	2.00	0.43
32:A:1862:U:H2'	32:A:1863:A:C8	2.54	0.43
32:A:3078:C:N4	32:A:3079:G:O6	2.52	0.43
32:A:3144:A:H2'	32:A:3145:A:C8	2.53	0.43
43:T:83:SER:HB3	43:T:86:LYS:HD2	2.00	0.43
56:g:140:VAL:H	60:o:85:HIS:CD2	2.36	0.43
66:P:98:ASN:OD1	66:P:99:GLY:N	2.51	0.43
71:6:233:LEU:O	71:6:296:ARG:NH1	2.46	0.43
75:c:240:LEU:HD23	75:c:301:LEU:HD21	2.00	0.43
1:AA:1281:U:OP1	2:AB:210:ARG:NH1	2.51	0.43
1:AA:1455:U:H2'	1:AA:1456:U:H6	1.84	0.43
21:AU:186:ASN:HB2	21:AU:201:GLN:HE21	1.84	0.43
31:AG:88:LEU:HA	31:AG:91:MET:HG2	2.00	0.43
32:A:1907:A:H2'	32:A:1908:A:C8	2.53	0.43
32:A:2533:A:H2'	32:A:2534:G:C8	2.54	0.43
34:D:125:LYS:HD3	70:5:259:ILE:HD11	1.99	0.43
65:N:104:MET:HE3	65:N:104:MET:HB3	1.94	0.43
70:5:239:ILE:HG12	70:5:341:VAL:HG21	2.00	0.43
75:c:91:ALA:O	75:c:122:ASN:ND2	2.52	0.43
83:Q:122:ALA:HB2	83:Q:172:GLN:HE21	1.84	0.43
86:v:335:SER:O	86:v:336:LYS:C	2.59	0.43
1:AA:818:C:H2'	1:AA:819:A:H8	1.83	0.43
13:AT:71:THR:HG22	13:AT:73:SER:H	1.84	0.43
15:AX:222:LEU:HD11	15:AX:243:VAL:HG13	2.01	0.43
26:A0:95:TRP:HE1	26:A0:204:PRO:HG3	1.83	0.43
26:A0:120:PHE:CD1	26:A0:121:LYS:HG2	2.54	0.43
32:A:1805:A:O2'	32:A:1806:U:OP1	2.31	0.43
32:A:3089:A:N6	88:A6:68:Y5P:C5'	2.77	0.43
34:D:154:THR:HG22	34:D:157:MET:HE3	2.01	0.43
38:L:41:VAL:HG11	38:L:104:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:b:45:GLU:O	54:b:49:ARG:HG2	2.18	0.43
69:E:94:SER:HB3	69:E:182:THR:HG21	2.00	0.43
76:d:137:PHE:N	76:d:138:PRO:HD2	2.34	0.43
86:v:549:TYR:CB	86:v:619:VAL:HG21	2.48	0.43
86:v:613:ASP:OD1	86:v:614:GLY:N	2.52	0.43
1:AA:702:C:N3	1:AA:842:C:O2'	2.44	0.43
1:AA:855:A:H2'	1:AA:856:A:C8	2.53	0.43
1:AA:945:G:H2'	1:AA:946:U:C6	2.54	0.43
1:AA:1078:A:C8	88:A6:35:Y5P:C4'	3.00	0.43
1:AA:1164:U:H2'	1:AA:1165:C:C6	2.54	0.43
1:AA:1479:C:H2'	1:AA:1480:A:C8	2.53	0.43
19:AR:251:GLU:OE2	19:AR:280:LYS:NZ	2.51	0.43
28:A4:137:ILE:HB	28:A4:140:LEU:HD23	2.00	0.43
29:AD:286:GLU:HB2	29:AD:288:HIS:CE1	2.53	0.43
30:AF:196:HIS:CG	30:AF:197:GLN:H	2.37	0.43
31:AG:395:LYS:HZ2	88:A6:31:Y5P:C5'	2.31	0.43
32:A:2919:A:O2'	88:A7:71:P5P:O3'	2.36	0.43
32:A:2945:A:O2'	32:A:2947:U:O4	2.36	0.43
32:A:3041:U:H4'	32:A:3042:U:OP1	2.18	0.43
32:A:3228:U:OP2	69:E:49:TRP:NE1	2.50	0.43
34:D:132:ASP:OD2	34:D:135:ARG:NH1	2.51	0.43
37:K:22:ASP:OD1	37:K:23:GLY:N	2.51	0.43
37:K:51:SER:O	43:T:206:ARG:NH1	2.52	0.43
39:M:164:ILE:HG12	39:M:174:VAL:HG11	2.00	0.43
51:3:180:TYR:HD1	71:6:366:LEU:HD12	1.83	0.43
53:8:145:GLU:O	53:8:148:GLU:HG3	2.19	0.43
64:I:124:LYS:NZ	64:I:125:VAL:O	2.48	0.43
79:k:39:SER:OG	79:k:40:GLU:N	2.51	0.43
81:p:122:THR:HG23	81:p:123:HIS:CD2	2.54	0.43
86:v:67:LEU:O	86:v:70:THR:OG1	2.36	0.43
19:AR:155:LYS:HB3	19:AR:177:PRO:HD3	1.99	0.43
22:AV:168:MET:HE3	22:AV:168:MET:HB3	1.92	0.43
29:AD:117:ARG:HD2	87:A5:2:P5P:N7	2.34	0.43
32:A:1881:A:N7	56:g:111:ARG:NE	2.67	0.43
32:A:2139:U:O4	47:Z:77:ARG:NH1	2.52	0.43
32:A:2374:A:H62	82:s:272:PRO:CB	2.21	0.43
32:A:2425:A:C6	82:s:221:HIS:HA	2.54	0.43
41:R:119:LEU:HD23	74:a:49:LEU:HD13	2.00	0.43
44:W:70:GLN:NE2	44:W:74:ARG:HB3	2.33	0.43
70:5:63:LYS:HB2	70:5:65:HIS:CE1	2.54	0.43
76:d:218:THR:OG1	76:d:219:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:832:U:H2'	1:AA:833:A:C8	2.54	0.43
1:AA:1066:C:H2'	1:AA:1067:A:C8	2.54	0.43
1:AA:1261:C:H2'	1:AA:1262:C:H6	1.84	0.43
17:AH:99:ALA:HB1	17:AH:104:ILE:HB	2.00	0.43
32:A:2584:C:H2'	32:A:2585:G:H8	1.83	0.43
32:A:3089:A:C5	88:A6:69:Y5P:O5'	2.72	0.43
40:O:145:LEU:HD11	72:7:308:ALA:HB2	2.01	0.43
42:S:146:LYS:O	42:S:147:PRO:C	2.62	0.43
46:Y:236:LYS:HE3	46:Y:236:LYS:HB3	1.92	0.43
55:e:118:GLN:O	55:e:121:GLU:HG3	2.19	0.43
57:i:88:LEU:HD11	57:i:114:ILE:HG23	2.01	0.43
63:J:166:ALA:HA	63:J:169:LYS:HE3	2.01	0.43
70:5:162:ARG:NH1	70:5:383:TYR:OH	2.52	0.43
82:s:295:GLY:HA3	82:s:335:TRP:HZ2	1.83	0.43
86:v:368:LEU:HD21	86:v:406:MET:HE2	2.01	0.43
1:AA:1287:A:H2'	1:AA:1288:G:C8	2.54	0.43
3:AC:156:GLN:NE2	25:A1:78:PRO:HD2	2.34	0.43
7:AK:35:TRP:HE1	7:AK:39:LYS:HE3	1.84	0.43
15:AX:108:LEU:HD23	15:AX:141:VAL:HG21	2.00	0.43
15:AX:168:LEU:HD21	15:AX:178:PHE:HB3	2.01	0.43
31:AG:76:LYS:O	31:AG:79:GLU:HG3	2.19	0.43
32:A:2280:C:H2'	32:A:2281:A:H8	1.84	0.43
32:A:2587:G:H2'	32:A:2588:C:C6	2.54	0.43
32:A:3178:U:O2'	62:r:134:ARG:NH1	2.51	0.43
39:M:273:TRP:NE1	39:M:284:LYS:HG2	2.33	0.43
51:3:118:HIS:CD2	51:3:169:ARG:HB2	2.53	0.43
76:d:86:ASP:OD1	76:d:86:ASP:N	2.51	0.43
1:AA:774:G:H2'	1:AA:775:C:H6	1.83	0.42
1:AA:1528:A:H4'	26:A0:101:ARG:HD2	2.01	0.42
7:AK:112:ARG:HE	17:AH:132:VAL:HG11	1.84	0.42
10:AO:137:ALA:HB3	10:AO:138:PRO:HD3	2.00	0.42
12:AQ:38:ASP:OD1	12:AQ:42:ARG:NH2	2.52	0.42
18:AL:115:VAL:HG12	18:AL:179:LYS:HZ1	1.82	0.42
21:AU:49:ASP:HB3	21:AU:52:GLU:HB3	2.01	0.42
25:A1:176:LYS:HE2	25:A1:178:SER:HB2	2.00	0.42
32:A:2171:U:O2'	32:A:2173:G:OP2	2.35	0.42
32:A:2206:C:O2	63:J:34:PRO:HG3	2.19	0.42
32:A:3002:G:H2'	32:A:3003:A:C8	2.54	0.42
32:A:3222:C:H2'	32:A:3223:A:O4'	2.19	0.42
38:L:40:VAL:HG12	38:L:42:ASP:H	1.83	0.42
39:M:117:ASP:OD1	39:M:117:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:M:212:PRO:HD3	61:q:103:LEU:HD13	2.01	0.42
43:T:95:ARG:HD3	43:T:95:ARG:HA	1.90	0.42
69:E:233:GLN:HB2	69:E:237:HIS:HE1	1.84	0.42
70:5:192:ILE:HD11	70:5:199:ALA:HB2	2.00	0.42
78:h:70:LEU:HA	78:h:73:TYR:CD2	2.54	0.42
86:v:301:LEU:HB2	92:v:802:GCP:C5	2.49	0.42
12:AQ:70:ARG:NH2	14:AW:152:ARG:O	2.47	0.42
32:A:2100:C:H1'	32:A:2135:A:C8	2.54	0.42
32:A:2588:C:N3	32:A:2592:G:N1	2.50	0.42
35:F:59:ARG:NH1	35:F:88:ALA:O	2.50	0.42
42:S:175:ARG:HB2	42:S:180:PHE:HB3	2.01	0.42
46:Y:200:PHE:HB3	70:5:68:PRO:HD3	2.00	0.42
55:e:205:LEU:HB3	77:f:171:LEU:HD11	2.01	0.42
56:g:76:ARG:NH2	56:g:164:LYS:O	2.53	0.42
66:P:72:PHE:H	66:P:72:PHE:HD1	1.68	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
82:s:211:VAL:HG22	82:s:230:ARG:HG3	2.00	0.42
15:AX:226:VAL:HG22	15:AX:243:VAL:HG11	2.01	0.42
15:AX:266:ASN:HA	15:AX:329:LEU:HG	2.01	0.42
22:AV:182:SER:HA	22:AV:185:VAL:HG22	2.01	0.42
22:AV:321:GLU:HB3	22:AV:326:LYS:HE3	2.01	0.42
25:A1:212:CYS:SG	25:A1:217:GLN:HB2	2.59	0.42
31:AG:85:LYS:NZ	31:AG:96:PRO:O	2.53	0.42
32:A:1688:A:H2'	32:A:1689:C:H4'	2.01	0.42
32:A:1827:C:H5''	32:A:2698:G:H21	1.83	0.42
33:B:1609:U:O2	33:B:1616:A:N6	2.52	0.42
33:B:1642:G:H2'	33:B:1643:A:C8	2.55	0.42
34:D:228:LEU:HD21	34:D:234:MET:HE2	2.01	0.42
43:T:159:HIS:HB3	43:T:160:GLY:H	1.71	0.42
64:I:185:ILE:HD11	84:TA:48:LEU:HD13	2.02	0.42
68:V:51:ASP:HA	68:V:81:ARG:HH22	1.85	0.42
75:c:99:LYS:O	75:c:102:GLU:HG3	2.18	0.42
86:v:92:MET:N	86:v:95:GLU:OE1	2.42	0.42
86:v:742:LEU:N	86:v:743:PRO:HD2	2.34	0.42
1:AA:837:A:N1	1:AA:853:C:O2'	2.52	0.42
1:AA:902:G:N2	1:AA:902:G:OP2	2.52	0.42
6:AJ:127:ARG:HG3	6:AJ:134:HIS:HA	2.00	0.42
7:AK:56:SER:O	7:AK:60:ASN:ND2	2.52	0.42
13:AT:66:MET:N	13:AT:66:MET:SD	2.93	0.42
18:AL:94:LEU:HD13	18:AL:102:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:393:GLU:OE2	22:AV:397:ARG:NH2	2.51	0.42
23:AY:302:ILE:HG23	28:A4:71:LEU:HD11	2.01	0.42
26:A0:129:ARG:NH2	26:A0:204:PRO:O	2.53	0.42
32:A:2067:C:H4'	77:f:60:LYS:HD2	2.00	0.42
32:A:2087:U:H2'	32:A:2088:U:C6	2.55	0.42
32:A:2094:G:O2'	32:A:2265:A:N3	2.49	0.42
32:A:2369:A:O2'	32:A:2370:A:O4'	2.26	0.42
32:A:2919:A:O2'	88:A7:71:P5P:C4'	2.68	0.42
32:A:3032:G:H2'	32:A:3033:U:O4'	2.19	0.42
32:A:3102:U:H2'	32:A:3103:C:H6	1.84	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
46:Y:71:PRO:HA	46:Y:74:TRP:CE2	2.55	0.42
53:8:138:ALA:O	53:8:141:GLU:HG3	2.19	0.42
62:r:167:PRO:HB2	62:r:168:ARG:H	1.63	0.42
63:J:119:GLU:HA	63:J:122:ARG:HG2	2.01	0.42
64:I:81:LEU:HD11	80:l:113:GLU:C	2.45	0.42
65:N:200:LYS:O	65:N:203:GLU:HG3	2.20	0.42
69:E:102:LEU:HD21	69:E:294:ASN:HA	2.00	0.42
69:E:221:ARG:HG3	69:E:261:MET:HG3	2.01	0.42
70:5:60:PHE:HD1	70:5:71:ALA:HB1	0.69	0.42
75:c:166:VAL:HG21	75:c:192:GLN:HG3	2.01	0.42
86:v:619:VAL:HA	88:A6:34:P5P:OP1	2.19	0.42
1:AA:712:C:N3	21:AU:27:ARG:HD2	2.34	0.42
1:AA:741:A:OP1	21:AU:86:ARG:NH2	2.53	0.42
1:AA:1515:G:O3'	18:AL:223:ARG:NH1	2.53	0.42
1:AA:1561:C:H2'	1:AA:1562:G:C8	2.54	0.42
1:AA:1572:A:H2'	1:AA:1573:A:C8	2.53	0.42
2:AB:239:ASN:OD1	14:AW:119:LYS:NZ	2.43	0.42
7:AK:96:ARG:HH22	7:AK:108:ARG:HH11	1.67	0.42
11:AP:115:GLN:HB3	11:AP:122:VAL:HG22	2.01	0.42
32:A:2034:A:H4'	32:A:2916:G:N7	2.34	0.42
32:A:2537:G:H2'	32:A:2538:C:C6	2.54	0.42
32:A:2579:C:C4	32:A:2580:U:C4	3.07	0.42
32:A:2734:A:H2'	32:A:2735:G:H8	1.84	0.42
37:K:27:PRO:HD3	37:K:149:ARG:HD2	2.01	0.42
39:M:208:GLU:OE2	61:q:106:LYS:NZ	2.43	0.42
40:O:57:GLU:HA	40:O:104:TYR:HE1	1.84	0.42
46:Y:202:LEU:HB3	46:Y:204:TYR:HE2	1.85	0.42
55:e:144:ASN:OD1	55:e:145:ASP:N	2.53	0.42
64:I:50:VAL:HG13	64:I:51:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:116:LEU:HB3	64:I:121:ILE:HD11	2.01	0.42
65:N:191:SER:H	65:N:194:THR:HG1	1.61	0.42
67:U:26:ILE:HG22	67:U:44:ILE:HG22	2.01	0.42
70:5:204:VAL:HB	70:5:229:ARG:HG3	2.01	0.42
71:6:187:VAL:HG23	71:6:319:PHE:HB3	2.01	0.42
86:v:254:ILE:HA	86:v:257:VAL:HG22	2.01	0.42
1:AA:1180:U:H2'	1:AA:1181:G:H8	1.84	0.42
2:AB:144:PHE:O	2:AB:167:HIS:N	2.48	0.42
5:AI:78:LYS:HB3	5:AI:82:GLU:HG3	2.01	0.42
15:AX:67:HIS:HB3	15:AX:98:CYS:HB3	2.01	0.42
22:AV:79:ILE:HD13	22:AV:85:ILE:HD13	2.01	0.42
31:AG:317:PHE:HB3	31:AG:323:LEU:HD23	2.02	0.42
32:A:2017:U:H2'	32:A:2018:G:H8	1.84	0.42
32:A:2079:C:H42	60:o:60:ARG:NH2	2.17	0.42
32:A:2094:G:OP2	39:M:57:ARG:NH2	2.53	0.42
32:A:2145:G:N3	42:S:104:ARG:NH1	2.67	0.42
32:A:2207:A:H2	63:J:38:VAL:HB	1.84	0.42
32:A:2919:A:C4'	88:A7:71:P5P:O2'	2.67	0.42
36:H:138:LYS:O	36:H:141:GLU:HG3	2.19	0.42
54:b:65:VAL:HB	78:h:154:ILE:HG22	2.01	0.42
75:c:46:GLU:HG2	75:c:49:ARG:HH12	1.83	0.42
83:Q:118:ARG:HE	83:Q:134:LEU:HD12	1.85	0.42
83:Q:227:LYS:HB3	83:Q:227:LYS:HE2	1.84	0.42
86:v:386:ASN:OD1	86:v:387:THR:N	2.52	0.42
1:AA:678:U:OP1	86:v:390:ARG:NH1	2.50	0.42
2:AB:202:ILE:HD12	2:AB:202:ILE:HA	1.96	0.42
32:A:2267:U:H2'	32:A:2268:G:H8	1.84	0.42
32:A:2366:G:OP1	67:U:79:ARG:NE	2.52	0.42
32:A:2550:A:N6	32:A:2590:A:N1	2.67	0.42
53:8:109:GLU:O	53:8:112:GLU:HG3	2.20	0.42
56:g:66:TYR:O	56:g:68:THR:HG23	2.19	0.42
62:r:94:ARG:NE	62:r:99:MET:O	2.53	0.42
62:r:146:GLN:HE21	62:r:146:GLN:HB2	1.67	0.42
64:I:190:GLY:HA2	64:I:193:ASN:HD21	1.84	0.42
70:5:59:THR:OG1	70:5:60:PHE:N	2.52	0.42
71:6:235:TRP:CE2	71:6:237:LEU:HD21	2.55	0.42
72:7:178:ALA:HB2	72:7:320:SER:HB2	2.00	0.42
72:7:184:VAL:HG22	72:7:294:ILE:HG22	2.02	0.42
86:v:156:MET:SD	86:v:710:LYS:NZ	2.93	0.42
1:AA:665:C:H2'	1:AA:666:C:C6	2.55	0.42
1:AA:1249:U:H5	7:AK:29:TYR:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1378:C:H42	15:AX:131:GLY:HA3	1.85	0.42
2:AB:120:GLN:O	2:AB:124:HIS:ND1	2.40	0.42
20:AS:93:LYS:HD2	20:AS:97:GLN:HG2	2.00	0.42
32:A:2366:G:H5''	67:U:79:ARG:HH21	1.85	0.42
32:A:3165:C:H2'	32:A:3166:U:C6	2.55	0.42
35:F:167:MET:HA	35:F:170:ARG:HE	1.85	0.42
42:S:95:LEU:HD23	42:S:95:LEU:H	1.84	0.42
73:9:131:TYR:HB3	73:9:132:PRO:HD3	2.01	0.42
1:AA:925:U:H2'	1:AA:926:A:H8	1.83	0.42
1:AA:997:A:H4'	1:AA:1074:G:H4'	2.02	0.42
4:AE:96:HIS:HD2	4:AE:98:LEU:HB2	1.84	0.42
16:A2:60:GLU:HG3	16:A2:62:ARG:HD3	2.02	0.42
29:AD:232:THR:OG1	29:AD:233:ALA:N	2.37	0.42
32:A:2015:G:N2	32:A:2037:U:O3'	2.52	0.42
32:A:2469:A:H2'	32:A:2470:G:H8	1.84	0.42
32:A:2579:C:C5	32:A:2580:U:C4	3.08	0.42
32:A:2969:A:H2'	32:A:2970:C:C6	2.55	0.42
32:A:2989:G:H5''	32:A:2990:A:H5'	2.02	0.42
42:S:97:ALA:N	42:S:108:VAL:O	2.47	0.42
45:X:79:LEU:HB2	45:X:125:VAL:HG11	2.02	0.42
63:J:115:LYS:HG3	63:J:158:ASP:OD1	2.20	0.42
63:J:191:LYS:HE3	63:J:191:LYS:CA	2.49	0.42
69:E:210:THR:OG1	69:E:262:GLY:O	2.34	0.42
73:9:64:ASP:OD1	73:9:64:ASP:N	2.52	0.42
76:d:48:PRO:HB2	76:d:50:PHE:CD1	2.55	0.42
76:d:205:GLN:HE21	76:d:205:GLN:HB2	1.68	0.42
1:AA:776:A:O3'	1:AA:777:G:H8	2.03	0.42
1:AA:1109:A:H2'	1:AA:1110:A:H8	1.84	0.42
7:AK:126:ALA:HA	17:AH:135:GLU:HG3	2.01	0.42
8:AM:19:ILE:HA	8:AM:36:ALA:HA	2.02	0.42
16:A2:56:TRP:HZ2	16:A2:70:ILE:HD12	1.84	0.42
22:AV:226:TYR:CE2	22:AV:280:LEU:HD22	2.55	0.42
24:AZ:26:THR:OG1	24:AZ:27:ASN:N	2.53	0.42
26:A0:63:ARG:HB3	26:A0:137:HIS:CD2	2.54	0.42
32:A:1696:C:OP2	46:Y:180:LYS:NZ	2.38	0.42
32:A:2169:A:OP2	63:J:21:ARG:NH2	2.53	0.42
32:A:2188:A:C2	63:J:104:THR:HG21	2.55	0.42
32:A:2276:C:N4	32:A:2290:A:H61	2.18	0.42
32:A:2311:U:H2'	32:A:2312:A:H8	1.83	0.42
32:A:2439:U:H2'	32:A:2440:G:C8	2.55	0.42
32:A:2470:G:O2'	38:L:35:MET:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:74:HIS:CE1	36:H:75:ARG:HG2	2.55	0.42
36:H:85:ASP:OD1	36:H:86:THR:N	2.52	0.42
52:4:66:PHE:HB3	52:4:101:ARG:HB2	2.01	0.42
53:8:101:ARG:HH21	55:e:83:LEU:HA	1.85	0.42
57:i:126:LYS:HG2	57:i:127:PHE:H	1.85	0.42
63:J:137:LEU:HB2	80:l:95:TRP:HH2	1.85	0.42
63:J:190:ALA:HA	63:J:192:LYS:HE2	2.01	0.42
70:5:201:ARG:HD3	70:5:230:LEU:HD21	2.01	0.42
72:7:103:SER:HB3	72:7:115:MET:HE3	2.02	0.42
72:7:163:MET:HE1	72:7:165:ASN:HD21	1.84	0.42
73:9:45:THR:OG1	73:9:46:SER:N	2.52	0.42
80:l:105:LYS:HB3	80:l:110:LEU:HD21	2.01	0.42
82:s:103:ASP:N	82:s:103:ASP:OD1	2.53	0.42
1:AA:1284:U:H5	29:AD:257:SER:HA	1.85	0.41
15:AX:125:LEU:HD11	15:AX:310:LEU:HB2	2.02	0.41
16:A2:33:VAL:HG21	16:A2:104:LEU:HB3	2.00	0.41
22:AV:250:ILE:HD11	26:A0:146:GLU:HG3	2.01	0.41
26:A0:99:ARG:O	26:A0:115:TRP:N	2.38	0.41
32:A:1827:C:O2'	32:A:1844:A:OP1	2.31	0.41
32:A:1872:U:H2'	32:A:1873:A:O4'	2.20	0.41
32:A:2069:U:O2'	32:A:2070:C:O4'	2.31	0.41
32:A:2080:U:H5	47:Z:105:SER:HB3	1.85	0.41
32:A:2093:U:O2	32:A:2266:U:O2'	2.36	0.41
32:A:2172:A:H8	63:J:23:ILE:HB	1.82	0.41
36:H:79:VAL:HG11	45:X:91:TYR:CZ	2.55	0.41
37:K:21:LEU:HB3	37:K:59:ILE:HG12	2.01	0.41
39:M:180:ASP:OD1	39:M:180:ASP:N	2.53	0.41
46:Y:82:GLY:HA2	46:Y:134:LYS:HZ3	1.84	0.41
50:2:72:THR:HG22	50:2:74:ALA:H	1.85	0.41
64:I:101:ASN:H	64:I:151:ASN:HA	1.85	0.41
75:c:245:LEU:HB3	75:c:250:VAL:HB	2.01	0.41
76:d:247:VAL:HG13	76:d:262:HIS:HB3	2.02	0.41
1:AA:894:C:N4	6:AJ:117:ASP:OD2	2.49	0.41
1:AA:1598:G:OP1	12:AQ:57:TYR:OH	2.32	0.41
32:A:2295:C:OP2	41:R:17:ARG:NH2	2.52	0.41
32:A:3013:G:N2	32:A:3024:U:O2	2.39	0.41
46:Y:85:TRP:HH2	73:9:70:LEU:HD11	1.84	0.41
69:E:200:PRO:HA	69:E:273:VAL:HG13	2.02	0.41
75:c:67:ASP:HB3	75:c:70:ALA:HB3	2.02	0.41
76:d:185:PHE:HZ	76:d:188:SER:HB2	1.85	0.41
86:v:252:GLU:O	86:v:255:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:v:464:GLU:CD	86:v:464:GLU:H	2.28	0.41
23:AY:296:ASN:ND2	25:A1:68:SER:O	2.41	0.41
26:A0:81:THR:HG22	26:A0:94:TYR:HB3	2.02	0.41
32:A:1701:U:H4'	50:2:61:LYS:HB3	2.02	0.41
32:A:2288:A:H2'	32:A:2289:G:H8	1.85	0.41
32:A:2390:A:H4'	70:5:301:PRO:HD3	2.02	0.41
32:A:2900:C:H2'	32:A:2901:A:C8	2.55	0.41
62:r:63:PRO:HA	62:r:64:PRO:HD3	1.96	0.41
64:I:144:LEU:N	64:I:145:PRO:HD2	2.35	0.41
66:P:72:PHE:CB	66:P:73:PRO:HD2	2.51	0.41
70:5:63:LYS:HD3	70:5:65:HIS:NE2	2.35	0.41
76:d:208:VAL:HG23	76:d:252:LEU:HB2	2.02	0.41
86:v:218:ILE:HG23	86:v:219:GLU:HG2	2.00	0.41
1:AA:845:A:H4'	21:AU:56:LEU:HD21	2.02	0.41
1:AA:1525:C:OP1	22:AV:392:ARG:NH1	2.54	0.41
2:AB:117:ASP:O	2:AB:121:THR:OG1	2.36	0.41
5:AI:176:THR:HG22	12:AQ:11:THR:HG22	2.02	0.41
13:AT:2:PRO:HB2	13:AT:8:PRO:HB3	2.01	0.41
13:AT:111:GLU:HG2	13:AT:114:ARG:HH12	1.85	0.41
15:AX:117:PHE:HB3	15:AX:303:GLY:HA2	2.01	0.41
18:AL:175:ASP:O	18:AL:178:GLU:HG3	2.21	0.41
19:AR:214:ASN:HA	19:AR:217:THR:HG22	2.02	0.41
29:AD:413:THR:HA	29:AD:418:LYS:HB2	2.02	0.41
32:A:1770:G:H2'	32:A:1771:C:H6	1.85	0.41
32:A:2032:G:H2'	32:A:2033:A:C8	2.54	0.41
35:F:227:PRO:HG2	35:F:230:ILE:HG22	2.02	0.41
55:e:50:ALA:HA	55:e:175:GLN:HA	2.03	0.41
60:o:55:THR:O	60:o:57:GLU:N	2.43	0.41
66:P:87:GLN:HG3	66:P:88:HIS:CD2	2.54	0.41
71:6:224:HIS:HB2	71:6:231:GLU:HA	2.03	0.41
78:h:73:TYR:HE1	78:h:100:LEU:HG	1.85	0.41
82:s:185:VAL:HG21	82:s:200:LEU:HD22	2.02	0.41
86:v:533:VAL:HB	86:v:535:PHE:HE2	1.84	0.41
1:AA:1437:U:H2'	1:AA:1438:A:C8	2.54	0.41
15:AX:84:PRO:HG2	15:AX:87:PHE:HB3	2.02	0.41
32:A:2314:C:H2'	32:A:2315:A:C4	2.56	0.41
32:A:2461:A:H2'	32:A:2462:A:H8	1.86	0.41
32:A:2575:U:H2'	32:A:2581:A:N6	2.35	0.41
32:A:2810:G:H2'	32:A:2811:G:H8	1.85	0.41
32:A:2909:G:N2	88:A7:71:P5P:N1	2.33	0.41
32:A:2919:A:O2'	88:A7:71:P5P:H4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:3190:A:H2'	32:A:3191:A:C8	2.55	0.41
45:X:14:LEU:O	45:X:18:GLU:HG3	2.21	0.41
46:Y:139:MET:HE1	67:U:25:PHE:HE1	1.86	0.41
71:6:275:GLN:HA	71:6:311:MET:HA	2.03	0.41
82:s:355:PHE:HB2	82:s:374:LEU:HB3	2.02	0.41
86:v:436:ASN:CG	86:v:439:LEU:HD21	2.44	0.41
86:v:573:THR:OG1	86:v:577:ASN:ND2	2.54	0.41
86:v:597:GLY:HA3	86:v:601:GLY:HA2	2.03	0.41
1:AA:810:G:H2'	1:AA:811:G:H8	1.86	0.41
1:AA:1174:U:H2'	1:AA:1175:G:H8	1.85	0.41
1:AA:1230:C:H5''	7:AK:98:ARG:HD2	2.01	0.41
1:AA:1233:C:O2'	7:AK:86:ARG:NH1	2.54	0.41
1:AA:1265:C:H5'	17:AH:122:GLN:HE21	1.85	0.41
1:AA:1370:U:H2'	1:AA:1371:U:C6	2.55	0.41
1:AA:1440:G:H2'	1:AA:1441:A:C8	2.56	0.41
2:AB:220:VAL:HG22	2:AB:234:TYR:HB2	2.02	0.41
18:AL:169:LEU:HA	18:AL:172:THR:HG22	2.03	0.41
31:AG:385:GLU:HB3	31:AG:389:ARG:HG3	2.02	0.41
32:A:1760:G:OP1	61:q:59:LYS:NZ	2.54	0.41
32:A:2100:C:H2'	32:A:2101:C:C6	2.56	0.41
32:A:2311:U:H2'	32:A:2312:A:C8	2.55	0.41
32:A:2665:U:H2'	32:A:2666:U:H6	1.84	0.41
32:A:2688:C:H2'	32:A:2689:C:C6	2.55	0.41
32:A:2693:A:H4'	32:A:2694:A:H8	1.84	0.41
32:A:3145:A:H2'	32:A:3146:G:C8	2.56	0.41
40:O:91:GLN:OE1	48:0:153:THR:OG1	2.29	0.41
42:S:113:LEU:HD21	42:S:194:ARG:HH11	1.85	0.41
45:X:209:GLU:OE2	70:5:69:TRP:NE1	2.51	0.41
64:I:114:HIS:HA	64:I:117:ARG:HG2	2.02	0.41
66:P:67:GLY:O	66:P:69:ARG:N	2.54	0.41
70:5:187:LEU:HD22	70:5:411:PHE:HZ	1.85	0.41
70:5:300:ARG:HA	70:5:303:ARG:HE	1.85	0.41
70:5:355:LEU:HD13	70:5:376:VAL:HG22	2.02	0.41
72:7:148:MET:HE1	72:7:255:HIS:HB2	2.03	0.41
74:a:35:THR:OG1	74:a:36:TYR:N	2.53	0.41
86:v:310:LEU:HA	86:v:313:VAL:HG22	2.02	0.41
86:v:499:LEU:O	86:v:502:GLU:HG3	2.20	0.41
88:A6:69:Y5P:H5	88:A6:70:Y5P:C2	2.51	0.41
1:AA:848:U:H2'	1:AA:849:U:C6	2.56	0.41
2:AB:107:PHE:HB2	2:AB:117:ASP:HB2	2.02	0.41
14:AW:143:ARG:HE	14:AW:168:VAL:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:311:TRP:HE3	23:AY:315:ILE:HD13	1.85	0.41
26:A0:167:PRO:HG2	26:A0:170:LEU:HB2	2.03	0.41
30:AF:62:GLU:HG2	30:AF:66:ARG:HE	1.86	0.41
32:A:1771:C:H2'	32:A:1772:A:C8	2.55	0.41
32:A:2339:G:H4'	50:2:55:PRO:HB2	2.03	0.41
32:A:2615:A:H2	32:A:3047:G:H1'	1.85	0.41
32:A:3089:A:C6	88:A6:69:Y5P:P	3.14	0.41
34:D:124:GLU:HB2	34:D:163:ILE:HG13	2.03	0.41
38:L:73:ILE:HG13	38:L:84:ALA:HB3	2.01	0.41
39:M:200:ILE:O	39:M:272:GLY:N	2.52	0.41
41:R:146:VAL:CG2	42:S:146:LYS:HD3	2.51	0.41
57:i:39:PRO:HG2	75:c:35:PHE:HD1	1.85	0.41
63:J:170:GLU:C	63:J:174:PHE:CD2	2.99	0.41
66:P:72:PHE:CZ	71:6:54:PHE:CE2	3.06	0.41
66:P:151:TRP:CD1	66:P:152:GLU:HG3	2.56	0.41
67:U:46:MET:HE1	67:U:72:VAL:HG13	2.02	0.41
70:5:120:ALA:HB1	70:5:314:ILE:HG21	2.02	0.41
71:6:215:THR:HG22	71:6:238:THR:HA	2.02	0.41
82:s:175:PRO:HA	82:s:178:ASP:OD2	2.20	0.41
1:AA:815:C:O2'	1:AA:817:G:OP1	2.31	0.41
1:AA:1055:U:H2'	1:AA:1056:A:C8	2.55	0.41
1:AA:1471:A:H2'	1:AA:1472:G:H8	1.85	0.41
6:AJ:52:THR:O	6:AJ:53:GLU:HG3	2.20	0.41
8:AM:64:LYS:NZ	19:AR:155:LYS:O	2.53	0.41
32:A:1858:G:O2'	32:A:2298:A:OP1	2.39	0.41
32:A:2321:A:OP2	32:A:2322:C:N4	2.53	0.41
32:A:3092:U:H4'	32:A:3093:C:OP1	2.21	0.41
35:F:286:PHE:HB2	57:i:66:PHE:CG	2.56	0.41
43:T:104:ALA:HB1	48:0:107:ILE:HG21	2.03	0.41
51:3:185:ASN:ND2	71:6:369:TYR:O	2.47	0.41
72:7:114:ASP:HB3	72:7:267:PRO:HB2	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:56:ASP:HA	92:v:802:GCP:C5'	2.38	0.41
86:v:59:LYS:HE2	86:v:123:GLY:HA3	2.02	0.41
1:AA:675:A:H61	1:AA:922:C:H42	1.68	0.41
1:AA:735:A:N6	1:AA:740:G:N1	2.69	0.41
1:AA:782:A:N6	1:AA:950:A:H4'	2.36	0.41
1:AA:798:C:H2'	1:AA:799:A:C8	2.55	0.41
1:AA:1458:A:OP1	30:AF:104:LYS:NZ	2.35	0.41
1:AA:1499:U:H2'	1:AA:1500:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:41:ARG:HH21	3:AC:59:PRO:HD2	1.86	0.41
4:AE:13:MET:HG3	4:AE:17:GLU:HB2	2.02	0.41
10:AO:52:LYS:HG2	10:AO:114:HIS:HE1	1.86	0.41
11:AP:99:LEU:HD23	11:AP:103:LYS:HB3	2.03	0.41
15:AX:190:ASN:O	15:AX:194:THR:OG1	2.37	0.41
15:AX:368:HIS:HB2	15:AX:398:LEU:HD11	2.03	0.41
19:AR:209:ILE:HA	19:AR:214:ASN:HD22	1.86	0.41
20:AS:89:ASN:HB3	20:AS:92:PHE:HB2	2.03	0.41
26:A0:135:MET:SD	26:A0:135:MET:N	2.71	0.41
27:A3:151:ARG:NH2	32:A:2543:C:O2'	2.54	0.41
30:AF:79:ALA:HB1	31:AG:308:GLN:HE21	1.86	0.41
30:AF:113:GLN:O	30:AF:116:GLU:HG3	2.20	0.41
32:A:1735:A:H8	36:H:69:ARG:HB3	1.84	0.41
32:A:1737:A:H62	32:A:1760:G:N2	2.19	0.41
32:A:2241:A:H2'	62:r:192:TRP:HE3	1.85	0.41
32:A:2650:C:H2'	32:A:2651:A:H8	1.84	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:H8	1.86	0.41
35:F:281:ARG:HG3	39:M:125:ARG:HD3	2.03	0.41
39:M:230:PRO:HB2	81:p:62:PRO:HD3	2.03	0.41
42:S:108:VAL:HG12	42:S:198:ILE:HD11	2.02	0.41
51:3:150:CYS:HB2	51:3:154:GLN:HE21	1.84	0.41
53:8:130:LYS:HE3	53:8:130:LYS:HB3	1.91	0.41
55:e:128:PHE:HB2	59:m:73:ARG:HB3	2.03	0.41
64:I:162:LYS:HG3	64:I:195:SER:HB2	2.03	0.41
64:I:200:LEU:HD13	84:TB:76:LEU:HD12	2.02	0.41
66:P:126:GLU:OE1	66:P:160:ARG:NH2	2.54	0.41
70:5:164:TRP:HD1	82:s:287:LYS:HD2	1.86	0.41
71:6:179:VAL:H	81:p:194:HIS:CD2	2.38	0.41
71:6:221:LEU:HB2	71:6:267:ARG:HG3	2.02	0.41
75:c:228:LEU:HD22	75:c:307:PHE:HB3	2.03	0.41
77:f:92:ASN:OD1	77:f:94:HIS:NE2	2.54	0.41
1:AA:1307:G:H21	3:AC:61:TYR:HE1	1.68	0.41
1:AA:1498:C:H2'	1:AA:1499:U:H6	1.86	0.41
4:AE:26:ILE:HG21	21:AU:173:LEU:HD22	2.03	0.41
8:AM:85:LYS:HB2	8:AM:86:PRO:HD3	2.02	0.41
15:AX:348:TYR:HB2	15:AX:386:ALA:HB1	2.03	0.41
32:A:1818:A:H4'	43:T:88:TRP:NE1	2.36	0.41
32:A:2080:U:O2'	60:o:59:GLU:O	2.29	0.41
32:A:2919:A:O3'	88:A7:71:P5P:O3'	2.39	0.41
55:e:203:LYS:O	55:e:237:LEU:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:j:91:TRP:CE2	60:o:58:GLN:HG2	2.56	0.41
61:q:107:GLN:O	61:q:110:GLU:HG3	2.20	0.41
67:U:128:SER:O	67:U:131:GLU:HG3	2.20	0.41
72:7:148:MET:HE3	72:7:262:ASP:HB3	2.03	0.41
86:v:328:ILE:O	86:v:341:ILE:HG21	2.21	0.41
86:v:332:GLU:HB2	86:v:338:LYS:O	2.21	0.41
1:AA:799:A:H2'	1:AA:800:C:C6	2.56	0.40
1:AA:1078:A:C5'	88:A6:35:Y5P:O3'	2.69	0.40
1:AA:1165:C:H2'	1:AA:1166:A:C8	2.56	0.40
1:AA:1573:A:H2'	1:AA:1574:G:C8	2.56	0.40
5:AI:125:GLY:H	30:AF:238:HIS:CE1	2.39	0.40
14:AW:107:ILE:HG12	14:AW:112:LEU:HG	2.04	0.40
15:AX:70:ILE:HB	15:AX:97:ALA:HB3	2.03	0.40
29:AD:243:VAL:HG21	29:AD:268:PHE:HE1	1.86	0.40
32:A:1863:A:H2'	32:A:1864:A:C8	2.56	0.40
32:A:2878:G:O6	32:A:2879:A:N6	2.54	0.40
32:A:2926:A:O2'	32:A:3087:C:OP1	2.29	0.40
32:A:3059:A:OP1	32:A:3061:G:O2'	2.33	0.40
32:A:3080:G:H2'	32:A:3081:A:C8	2.56	0.40
35:F:116:THR:OG1	35:F:117:ARG:N	2.54	0.40
61:q:110:GLU:HA	61:q:113:LYS:HG2	2.03	0.40
66:P:52:ASN:ND2	66:P:54:ARG:O	2.55	0.40
67:U:143:ARG:HG2	76:d:282:ILE:HD11	2.03	0.40
74:a:75:ILE:HG12	75:c:257:LEU:HB2	2.02	0.40
86:v:47:ARG:HE	86:v:314:LEU:HA	1.86	0.40
1:AA:712:C:N4	21:AU:28:LYS:O	2.54	0.40
1:AA:750:A:H4'	9:AN:47:LYS:HE2	2.04	0.40
1:AA:839:A:H2'	1:AA:840:A:H8	1.86	0.40
6:AJ:84:ARG:HB3	6:AJ:90:GLU:HG2	2.03	0.40
31:AG:285:VAL:HA	31:AG:328:VAL:HG12	2.02	0.40
32:A:1671:G:O2'	32:A:1672:C:H5''	2.22	0.40
32:A:2522:U:H5''	70:5:36:ARG:HH12	1.86	0.40
32:A:2943:G:H2'	32:A:2944:C:H6	1.86	0.40
32:A:3128:A:H61	86:v:701:THR:HA	1.86	0.40
32:A:3177:A:H2'	32:A:3177:A:N3	2.36	0.40
38:L:94:PRO:HB2	38:L:95:ARG:H	1.71	0.40
39:M:238:ARG:NH2	81:p:66:LYS:O	2.54	0.40
40:O:107:MET:HA	40:O:123:ILE:HG22	2.02	0.40
41:R:94:GLN:OE1	42:S:146:LYS:HE2	2.21	0.40
42:S:80:VAL:HG12	74:a:59:VAL:HB	2.02	0.40
61:q:148:ALA:HA	61:q:151:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:I:162:LYS:HE2	64:I:162:LYS:HB2	1.92	0.40
70:5:165:GLN:HE21	70:5:165:GLN:HB3	1.68	0.40
70:5:339:PRO:HB2	70:5:358:GLN:HE21	1.86	0.40
72:7:284:HIS:HB3	72:7:323:MET:HE2	2.03	0.40
88:A7:24:Y5P:H4A	88:A7:25:Y5P:H4	2.02	0.40
1:AA:826:A:H61	6:AJ:56:PRO:HD2	1.86	0.40
1:AA:1032:C:H1'	11:AP:116:ILE:HG21	2.04	0.40
15:AX:152:ILE:H	15:AX:195:ASN:HD22	1.68	0.40
16:A2:29:LEU:H	16:A2:29:LEU:HD23	1.87	0.40
32:A:1676:A:C2	57:i:36:LEU:HB2	2.56	0.40
32:A:1893:A:H4'	32:A:1894:G:H5'	2.03	0.40
32:A:2017:U:H5'	32:A:2932:G:H4'	2.03	0.40
32:A:2253:U:H2'	32:A:2254:C:C6	2.57	0.40
32:A:2459:A:N6	32:A:2668:A:H4'	2.36	0.40
34:D:184:LEU:HD13	34:D:226:ILE:HD11	2.04	0.40
36:H:124:LEU:HB2	36:H:125:PRO:HD3	2.02	0.40
45:X:54:PRO:C	45:X:56:ASN:H	2.29	0.40
63:J:126:GLN:HE21	63:J:126:GLN:HB2	1.72	0.40
65:N:138:HIS:ND1	65:N:139:ARG:O	2.55	0.40
65:N:204:GLU:OE1	65:N:207:ARG:NH2	2.52	0.40
68:V:94:HIS:HB2	68:V:95:TYR:H	1.76	0.40
69:E:274:TRP:HE1	69:E:286:ASN:HB2	1.85	0.40
82:s:189:SER:HB3	82:s:190:PRO:HD3	2.02	0.40
86:v:56:ASP:CA	92:v:802:GCP:H5'2	2.38	0.40
86:v:534:PRO:HB3	86:v:555:VAL:HG13	2.03	0.40
88:A7:57:Y5P:H4A	88:A7:58:Y5P:H4	2.04	0.40
1:AA:950:A:H2'	1:AA:951:G:H8	1.87	0.40
1:AA:1002:C:H2'	1:AA:1003:A:C8	2.54	0.40
1:AA:1238:C:H2'	1:AA:1239:C:C6	2.57	0.40
1:AA:1497:C:H2'	1:AA:1498:C:C6	2.56	0.40
3:AC:120:CYS:HB3	25:A1:106:LEU:HD11	2.02	0.40
15:AX:264:GLY:N	15:AX:309:ALA:O	2.55	0.40
22:AV:151:PHE:O	22:AV:156:ASN:ND2	2.44	0.40
22:AV:317:LEU:H	22:AV:320:GLU:HB2	1.85	0.40
24:AZ:46:LYS:HG3	24:AZ:47:GLU:HG3	2.02	0.40
25:A1:149:ILE:HG23	25:A1:175:VAL:HG22	2.02	0.40
30:AF:201:MET:HB3	30:AF:202:PRO:HD3	2.04	0.40
31:AG:157:SER:OG	31:AG:211:GLU:OE1	2.27	0.40
32:A:1910:C:H2'	32:A:1911:C:C6	2.55	0.40
32:A:2272:C:N3	32:A:2273:A:N6	2.70	0.40
32:A:2288:A:O2'	35:F:101:MET:SD	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:2755:A:O2'	45:X:112:ARG:NH2	2.54	0.40
32:A:2910:A:C2	88:A7:71:P5P:H8	2.54	0.40
32:A:3002:G:H2'	32:A:3003:A:H8	1.86	0.40
33:B:1666:U:H2'	33:B:1667:C:C6	2.57	0.40
35:F:79:LEU:HD22	78:h:94:SER:HB3	2.02	0.40
44:W:126:LEU:HD23	44:W:128:LYS:NZ	2.37	0.40
47:Z:73:LYS:HB3	47:Z:116:LEU:HA	2.03	0.40
51:3:183:ARG:HE	71:6:354:GLN:NE2	2.18	0.40
61:q:40:PRO:HG3	61:q:51:GLN:HB3	2.03	0.40
67:U:141:ASP:HB3	67:U:144:ARG:HG2	2.02	0.40
76:d:122:ILE:HA	76:d:125:ILE:HG12	2.03	0.40
82:s:270:LYS:HD3	82:s:270:LYS:HA	1.65	0.40
83:Q:226:PRO:HB2	83:Q:227:LYS:H	1.70	0.40
86:v:175:LYS:CE	92:v:802:GCP:N7	2.84	0.40
86:v:313:VAL:CB	86:v:317:LEU:HD12	2.46	0.40
7:AK:124:GLN:HE22	17:AH:137:ARG:HE	1.68	0.40
9:AN:31:THR:HG22	9:AN:46:ARG:HB3	2.04	0.40
9:AN:69:LEU:HD21	9:AN:80:GLU:HB2	2.03	0.40
18:AL:208:LEU:HD23	27:A3:173:LEU:HD22	2.04	0.40
21:AU:171:GLU:OE1	21:AU:171:GLU:N	2.44	0.40
25:A1:254:GLU:HG3	25:A1:255:ASN:HD22	1.85	0.40
32:A:1992:C:N3	34:D:274:ARG:HB2	2.36	0.40
32:A:2332:C:H2'	32:A:2333:G:C8	2.57	0.40
32:A:2677:A:H2'	32:A:2678:A:C8	2.56	0.40
32:A:2694:A:HO2'	32:A:2941:G:H21	1.62	0.40
56:g:66:TYR:O	56:g:68:THR:N	2.52	0.40
63:J:87:VAL:HG12	63:J:91:LEU:HD13	2.03	0.40
63:J:171:ARG:CG	63:J:174:PHE:HE2	2.32	0.40
63:J:191:LYS:C	63:J:191:LYS:HD3	2.47	0.40
71:6:92:LEU:HB2	71:6:170:ARG:HG3	2.04	0.40
80:l:108:GLU:OE1	80:l:109:GLU:HG3	2.22	0.40
86:v:127:PHE:HZ	86:v:503:ILE:HG21	1.85	0.40
86:v:523:VAL:HG23	86:v:693:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	193 (88%)	21 (10%)	4 (2%)	6	19
3	AC	130/167 (78%)	110 (85%)	19 (15%)	1 (1%)	16	37
4	AE	120/125 (96%)	102 (85%)	15 (12%)	3 (2%)	4	13
5	AI	134/194 (69%)	117 (87%)	12 (9%)	5 (4%)	2	6
6	AJ	106/138 (77%)	88 (83%)	15 (14%)	3 (3%)	4	11
7	AK	99/128 (77%)	87 (88%)	10 (10%)	2 (2%)	6	16
8	AM	114/137 (83%)	101 (89%)	12 (10%)	1 (1%)	14	34
9	AN	105/130 (81%)	83 (79%)	21 (20%)	1 (1%)	12	32
10	AO	188/258 (73%)	170 (90%)	15 (8%)	3 (2%)	7	21
11	AP	94/142 (66%)	79 (84%)	12 (13%)	3 (3%)	3	8
12	AQ	84/87 (97%)	75 (89%)	9 (11%)	0	100	100
13	AT	166/173 (96%)	149 (90%)	17 (10%)	0	100	100
14	AW	95/187 (51%)	78 (82%)	15 (16%)	2 (2%)	5	16
15	AX	351/398 (88%)	318 (91%)	27 (8%)	6 (2%)	7	20
16	A2	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
17	AH	120/201 (60%)	96 (80%)	20 (17%)	4 (3%)	3	7
18	AL	172/257 (67%)	151 (88%)	17 (10%)	4 (2%)	5	14
19	AR	290/360 (81%)	253 (87%)	36 (12%)	1 (0%)	36	59
20	AS	133/190 (70%)	122 (92%)	8 (6%)	3 (2%)	5	14
21	AU	175/205 (85%)	164 (94%)	11 (6%)	0	100	100
22	AV	363/414 (88%)	312 (86%)	42 (12%)	9 (2%)	4	13
23	AY	118/395 (30%)	105 (89%)	12 (10%)	1 (1%)	16	37
24	AZ	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
25	A1	273/323 (84%)	247 (90%)	23 (8%)	3 (1%)	11	29
26	A0	212/218 (97%)	183 (86%)	27 (13%)	2 (1%)	14	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	A3	70/199 (35%)	65 (93%)	4 (6%)	1 (1%)	9	24
28	A4	541/689 (78%)	468 (86%)	61 (11%)	12 (2%)	5	15
29	AD	341/430 (79%)	298 (87%)	38 (11%)	5 (2%)	8	23
30	AF	206/242 (85%)	184 (89%)	19 (9%)	3 (2%)	8	23
31	AG	311/396 (78%)	274 (88%)	35 (11%)	2 (1%)	21	45
34	D	237/305 (78%)	207 (87%)	28 (12%)	2 (1%)	16	37
35	F	248/311 (80%)	217 (88%)	26 (10%)	5 (2%)	6	16
36	H	96/267 (36%)	83 (86%)	11 (12%)	2 (2%)	5	16
37	K	175/178 (98%)	153 (87%)	16 (9%)	6 (3%)	3	7
38	L	113/145 (78%)	101 (89%)	11 (10%)	1 (1%)	14	34
39	M	285/296 (96%)	252 (88%)	26 (9%)	7 (2%)	4	13
40	O	150/175 (86%)	128 (85%)	19 (13%)	3 (2%)	6	16
41	R	138/149 (93%)	124 (90%)	9 (6%)	5 (4%)	2	6
42	S	154/205 (75%)	135 (88%)	15 (10%)	4 (3%)	4	12
43	T	164/212 (77%)	148 (90%)	13 (8%)	3 (2%)	6	19
44	W	109/148 (74%)	96 (88%)	12 (11%)	1 (1%)	14	34
45	X	241/256 (94%)	213 (88%)	22 (9%)	6 (2%)	4	13
46	Y	174/250 (70%)	161 (92%)	8 (5%)	5 (3%)	3	10
47	Z	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
48	0	106/188 (56%)	93 (88%)	10 (9%)	3 (3%)	4	11
49	1	50/65 (77%)	42 (84%)	7 (14%)	1 (2%)	6	16
50	2	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	5	14
51	3	93/188 (50%)	84 (90%)	8 (9%)	1 (1%)	11	29
52	4	36/103 (35%)	33 (92%)	3 (8%)	0	100	100
53	8	97/206 (47%)	84 (87%)	13 (13%)	0	100	100
54	b	146/155 (94%)	129 (88%)	14 (10%)	3 (2%)	5	16
55	e	211/279 (76%)	188 (89%)	22 (10%)	1 (0%)	24	49
56	g	130/166 (78%)	111 (85%)	14 (11%)	5 (4%)	2	6
57	i	95/128 (74%)	75 (79%)	20 (21%)	0	100	100
58	j	91/123 (74%)	83 (91%)	7 (8%)	1 (1%)	11	29
59	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	5	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	o	92/102 (90%)	78 (85%)	11 (12%)	3 (3%)	3	7
61	q	166/222 (75%)	154 (93%)	10 (6%)	2 (1%)	10	28
62	r	160/196 (82%)	139 (87%)	17 (11%)	4 (2%)	4	13
63	J	173/192 (90%)	152 (88%)	15 (9%)	6 (4%)	3	7
64	I	177/261 (68%)	164 (93%)	12 (7%)	1 (1%)	21	45
65	N	220/251 (88%)	203 (92%)	16 (7%)	1 (0%)	24	49
66	P	141/179 (79%)	123 (87%)	13 (9%)	5 (4%)	3	7
67	U	150/153 (98%)	121 (81%)	27 (18%)	2 (1%)	9	26
68	V	204/216 (94%)	179 (88%)	25 (12%)	0	100	100
69	E	304/348 (87%)	268 (88%)	32 (10%)	4 (1%)	9	26
70	5	392/423 (93%)	347 (88%)	41 (10%)	4 (1%)	12	32
71	6	352/380 (93%)	302 (86%)	47 (13%)	3 (1%)	14	34
72	7	295/338 (87%)	260 (88%)	28 (10%)	7 (2%)	4	13
73	9	122/137 (89%)	106 (87%)	15 (12%)	1 (1%)	16	37
74	a	106/142 (75%)	95 (90%)	8 (8%)	3 (3%)	4	11
75	c	287/332 (86%)	266 (93%)	17 (6%)	4 (1%)	9	24
76	d	255/306 (83%)	215 (84%)	34 (13%)	6 (2%)	4	13
77	f	144/194 (74%)	122 (85%)	21 (15%)	1 (1%)	18	40
78	h	108/158 (68%)	93 (86%)	13 (12%)	2 (2%)	6	17
79	k	94/112 (84%)	86 (92%)	8 (8%)	0	100	100
80	l	70/138 (51%)	62 (89%)	7 (10%)	1 (1%)	9	24
81	p	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	24
82	s	391/439 (89%)	342 (88%)	40 (10%)	9 (2%)	5	14
83	Q	238/292 (82%)	216 (91%)	16 (7%)	6 (2%)	4	13
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	24
86	v	710/751 (94%)	565 (80%)	128 (18%)	17 (2%)	4	13
All	All	14720/19244 (76%)	12885 (88%)	1589 (11%)	246 (2%)	9	20

All (246) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	AL	71	LEU
23	AY	314	PRO
28	A4	252	PRO
28	A4	450	PRO
28	A4	542	PRO
30	AF	38	SER
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	341	ILE
5	AI	145	ILE
6	AJ	70	PRO
10	AO	236	PRO
14	AW	109	GLU
15	AX	156	PRO
15	AX	371	ALA
17	AH	185	LYS
18	AL	199	HIS
20	AS	40	PRO
26	A0	60	ARG
27	A3	130	VAL
28	A4	439	LEU
28	A4	541	PRO
29	AD	235	GLU
30	AF	71	THR
31	AG	387	ALA
36	H	103	GLU
37	K	101	VAL

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Mol	Chain	Res	Type
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
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
77	f	122	GLU
78	h	83	PRO
82	s	131	PRO
86	v	272	LYS
86	v	336	LYS
86	v	745	LYS
2	AB	202	ILE
3	AC	114	GLY
4	AE	15	ARG
5	AI	79	LYS
6	AJ	49	LEU
6	AJ	104	GLU
8	AM	62	GLY
9	AN	97	GLY
10	AO	52	LYS
14	AW	154	LEU
17	AH	179	GLN
18	AL	85	ASP
19	AR	334	THR
20	AS	110	GLY
22	AV	155	GLU
22	AV	156	ASN
22	AV	347	ILE
25	A1	71	PRO
28	A4	203	PRO
28	A4	410	PRO
35	F	91	PRO
38	L	94	PRO

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Mol	Chain	Res	Type
39	M	242	TYR
45	X	92	ALA
45	X	220	GLU
45	X	221	LYS
46	Y	77	GLU
56	g	53	PRO
56	g	55	THR
58	j	40	TYR
60	o	15	ARG
61	q	161	GLN
62	r	143	SER
65	N	55	ARG
66	P	68	TRP
72	7	167	VAL
72	7	281	SER
74	a	44	ASN
74	a	79	ASP
75	c	183	GLU
78	h	80	SER
82	s	133	PRO
83	Q	228	PRO
86	v	148	VAL
86	v	208	GLU
86	v	217	LEU
2	AB	173	GLY
4	AE	14	GLN
5	AI	69	GLU
5	AI	116	GLY
15	AX	81	HIS
15	AX	347	ASN
17	AH	184	ILE
20	AS	78	TYR
22	AV	197	SER
22	AV	291	THR
22	AV	321	GLU
28	A4	82	THR
29	AD	145	ASN
29	AD	416	GLY
30	AF	80	GLY
31	AG	323	LEU
36	H	61	LYS
37	K	5	SER

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Mol	Chain	Res	Type
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
46	Y	204	TYR
49	1	60	LYS
50	2	50	GLY
54	b	116	ARG
55	e	265	LYS
59	m	70	GLU
64	I	38	ARG
69	E	82	ASP
70	5	73	PRO
70	5	114	LEU
71	6	289	PRO
75	c	120	LYS
75	c	186	VAL
80	l	104	PRO
82	s	272	PRO
82	s	350	ASP
82	s	404	THR
83	Q	60	PRO
86	v	77	HIS
86	v	347	ARG
86	v	549	TYR
86	v	566	LYS
2	AB	224	ASP
11	AP	64	LYS
11	AP	141	ARG
15	AX	339	PRO
17	AH	84	ASP
18	AL	114	ILE

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Mol	Chain	Res	Type
25	A1	183	ASP
28	A4	134	GLU
28	A4	385	PRO
28	A4	470	GLN
28	A4	561	SER
29	AD	263	ASP
39	M	267	PHE
39	M	279	ASP
42	S	138	ALA
43	T	158	TYR
48	0	163	GLU
54	b	113	ILE
60	o	52	PRO
61	q	125	MET
66	P	69	ARG
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	123	CYS
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
82	s	163	VAL
86	v	567	LEU
2	AB	185	PRO
4	AE	55	SER
5	AI	60	PHE
25	A1	76	PHE
35	F	124	GLY
35	F	128	TRP
35	F	223	HIS
35	F	283	LEU
41	R	136	LYS
48	0	116	LEU
51	3	95	THR

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Mol	Chain	Res	Type
54	b	117	LYS
82	s	100	LEU
83	Q	229	TRP
86	v	151	VAL
86	v	438	GLY
86	v	447	PRO
7	AK	63	LEU
7	AK	97	PRO
15	AX	338	ASP
22	AV	35	VAL
26	A0	182	GLY
43	T	94	ILE
60	o	61	GLY
29	AD	195	GLY
56	g	36	PRO
62	r	156	PRO
70	5	286	PRO
11	AP	56	ASN
22	AV	136	GLY
22	AV	212	GLY
34	D	98	GLY
41	R	138	PRO
45	X	19	GLY
56	g	67	PRO
63	J	36	GLY
81	p	173	VAL
83	Q	58	PRO
83	Q	215	VAL
86	v	238	ILE
10	AO	101	VAL
34	D	207	ILE
71	6	79	GLY
82	s	130	GLU
86	v	102	ILE
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%)	192 (100%)	1 (0%)	81	90
3	AC	115/143 (80%)	114 (99%)	1 (1%)	70	83
4	AE	104/107 (97%)	103 (99%)	1 (1%)	68	82
5	AI	104/147 (71%)	103 (99%)	1 (1%)	68	82
6	AJ	93/118 (79%)	93 (100%)	0	100	100
7	AK	91/113 (80%)	90 (99%)	1 (1%)	65	80
8	AM	95/113 (84%)	95 (100%)	0	100	100
9	AN	93/115 (81%)	92 (99%)	1 (1%)	65	80
10	AO	171/230 (74%)	170 (99%)	1 (1%)	78	89
11	AP	87/123 (71%)	87 (100%)	0	100	100
12	AQ	78/79 (99%)	78 (100%)	0	100	100
13	AT	153/157 (98%)	151 (99%)	2 (1%)	61	78
14	AW	84/158 (53%)	84 (100%)	0	100	100
15	AX	312/351 (89%)	311 (100%)	1 (0%)	86	92
16	A2	99/101 (98%)	99 (100%)	0	100	100
17	AH	112/180 (62%)	111 (99%)	1 (1%)	70	83
18	AL	157/226 (70%)	156 (99%)	1 (1%)	78	89
19	AR	262/318 (82%)	262 (100%)	0	100	100
20	AS	116/164 (71%)	116 (100%)	0	100	100
21	AU	153/174 (88%)	153 (100%)	0	100	100
22	AV	328/364 (90%)	325 (99%)	3 (1%)	70	83
23	AY	111/357 (31%)	111 (100%)	0	100	100
24	AZ	89/95 (94%)	89 (100%)	0	100	100
25	A1	253/291 (87%)	250 (99%)	3 (1%)	63	79
26	A0	186/190 (98%)	186 (100%)	0	100	100
27	A3	66/166 (40%)	64 (97%)	2 (3%)	36	60
28	A4	83/609 (14%)	83 (100%)	0	100	100
29	AD	286/357 (80%)	285 (100%)	1 (0%)	86	92
30	AF	185/209 (88%)	180 (97%)	5 (3%)	39	64
31	AG	273/342 (80%)	269 (98%)	4 (2%)	57	76
34	D	193/245 (79%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	F	217/262 (83%)	215 (99%)	2 (1%)	70	83
36	H	88/228 (39%)	86 (98%)	2 (2%)	44	67
37	K	155/156 (99%)	155 (100%)	0	100	100
38	L	98/124 (79%)	97 (99%)	1 (1%)	68	82
39	M	245/249 (98%)	244 (100%)	1 (0%)	84	92
40	O	133/150 (89%)	132 (99%)	1 (1%)	73	85
41	R	118/126 (94%)	117 (99%)	1 (1%)	73	85
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	67
46	Y	159/223 (71%)	157 (99%)	2 (1%)	61	78
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	71
50	2	40/72 (56%)	39 (98%)	1 (2%)	42	66
51	3	88/166 (53%)	86 (98%)	2 (2%)	44	67
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	80
56	g	122/148 (82%)	120 (98%)	2 (2%)	55	75
57	i	86/110 (78%)	84 (98%)	2 (2%)	44	67
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	78
61	q	114/178 (64%)	114 (100%)	0	100	100
62	r	147/169 (87%)	146 (99%)	1 (1%)	76	87
63	J	138/150 (92%)	135 (98%)	3 (2%)	45	69
64	I	164/232 (71%)	160 (98%)	4 (2%)	43	67
65	N	189/211 (90%)	188 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	P	125/154 (81%)	124 (99%)	1 (1%)	73	85
67	U	126/135 (93%)	125 (99%)	1 (1%)	73	85
68	V	184/191 (96%)	182 (99%)	2 (1%)	65	80
69	E	260/290 (90%)	259 (100%)	1 (0%)	84	92
70	5	353/368 (96%)	350 (99%)	3 (1%)	73	85
71	6	313/332 (94%)	308 (98%)	5 (2%)	55	75
72	7	272/303 (90%)	272 (100%)	0	100	100
73	9	104/112 (93%)	103 (99%)	1 (1%)	68	82
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	72
77	f	122/173 (70%)	121 (99%)	1 (1%)	73	85
78	h	104/148 (70%)	103 (99%)	1 (1%)	68	82
79	k	81/90 (90%)	79 (98%)	2 (2%)	42	66
80	l	67/116 (58%)	67 (100%)	0	100	100
81	p	134/181 (74%)	131 (98%)	3 (2%)	45	69
82	s	336/381 (88%)	335 (100%)	1 (0%)	86	92
83	Q	221/256 (86%)	221 (100%)	0	100	100
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%)	582 (97%)	16 (3%)	39	64
All	All	12561/16442 (76%)	12453 (99%)	108 (1%)	68	83

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	236	VAL
3	AC	73	THR
4	AE	111	VAL
5	AI	181	ILE
7	AK	114	LEU
9	AN	77	VAL
10	AO	115	VAL
13	AT	88	VAL
13	AT	153	VAL

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Mol	Chain	Res	Type
15	AX	217	GLU
17	AH	88	LEU
18	AL	71	LEU
22	AV	129	LEU
22	AV	146	LEU
22	AV	338	HIS
25	A1	114	LEU
25	A1	171	VAL
25	A1	281	GLU
27	A3	159	GLU
27	A3	190	GLN
29	AD	340	ILE
30	AF	39	PRO
30	AF	64	TYR
30	AF	71	THR
30	AF	159	VAL
30	AF	205	LEU
31	AG	139	GLN
31	AG	264	GLU
31	AG	285	VAL
31	AG	392	THR
35	F	77	VAL
35	F	262	THR
36	H	62	VAL
36	H	83	VAL
38	L	36	THR
39	M	274	VAL
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

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Mol	Chain	Res	Type
55	e	265	LYS
56	g	36	PRO
56	g	66	TYR
57	i	44	VAL
57	i	98	VAL
60	o	93	ASP
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
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
77	f	143	LYS
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
86	v	80	LYS

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Mol	Chain	Res	Type
86	v	89	MET
86	v	102	ILE
86	v	135	LEU
86	v	145	LEU
86	v	163	LYS
86	v	165	TYR
86	v	178	ARG
86	v	200	PHE
86	v	243	ARG
86	v	252	GLU
86	v	328	ILE
86	v	533	VAL
86	v	610	VAL
86	v	619	VAL
86	v	707	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (266) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	126	GLN
2	AB	150	GLN
2	AB	157	ASN
3	AC	107	GLN
3	AC	156	GLN
4	AE	14	GLN
4	AE	57	GLN
4	AE	59	ASN
4	AE	96	HIS
5	AI	96	GLN
5	AI	98	GLN
5	AI	104	ASN
6	AJ	134	HIS
7	AK	124	GLN
8	AM	39	ASN
9	AN	56	GLN
10	AO	65	GLN
10	AO	80	ASN
10	AO	146	GLN
10	AO	155	GLN
10	AO	166	HIS
10	AO	204	ASN
11	AP	78	GLN

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Mol	Chain	Res	Type
11	AP	82	GLN
11	AP	115	GLN
12	AQ	79	ASN
12	AQ	85	GLN
13	AT	56	GLN
13	AT	59	ASN
13	AT	101	HIS
14	AW	91	GLN
14	AW	106	HIS
14	AW	135	GLN
15	AX	59	HIS
15	AX	302	HIS
15	AX	387	ASN
16	A2	58	GLN
16	A2	105	ASN
17	AH	133	GLN
18	AL	107	GLN
18	AL	199	HIS
19	AR	88	GLN
19	AR	96	GLN
19	AR	167	HIS
19	AR	214	ASN
19	AR	224	HIS
19	AR	229	ASN
19	AR	277	ASN
19	AR	312	GLN
19	AR	315	GLN
19	AR	337	GLN
21	AU	65	GLN
21	AU	110	GLN
21	AU	131	GLN
21	AU	139	GLN
21	AU	159	GLN
21	AU	161	GLN
21	AU	201	GLN
22	AV	78	ASN
22	AV	100	ASN
22	AV	122	GLN
22	AV	131	ASN
22	AV	179	GLN
22	AV	245	HIS
22	AV	261	GLN

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Mol	Chain	Res	Type
22	AV	381	GLN
22	AV	388	GLN
22	AV	407	GLN
23	AY	349	HIS
25	A1	110	ASN
25	A1	217	GLN
25	A1	255	ASN
25	A1	268	GLN
25	A1	301	ASN
26	A0	111	HIS
26	A0	192	ASN
26	A0	207	GLN
27	A3	190	GLN
28	A4	136	HIS
29	AD	145	ASN
29	AD	155	GLN
29	AD	278	HIS
29	AD	292	HIS
29	AD	356	GLN
29	AD	360	GLN
30	AF	103	ASN
30	AF	113	GLN
30	AF	233	ASN
30	AF	238	HIS
31	AG	127	HIS
31	AG	139	GLN
31	AG	156	GLN
31	AG	220	GLN
31	AG	296	ASN
31	AG	308	GLN
31	AG	384	GLN
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

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Mol	Chain	Res	Type
36	H	126	GLN
36	H	148	GLN
37	K	26	GLN
37	K	48	HIS
38	L	72	GLN
38	L	80	GLN
38	L	104	ASN
38	L	142	GLN
39	M	71	GLN
39	M	198	GLN
39	M	264	GLN
39	M	276	ASN
40	O	100	GLN
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	108	GLN
45	X	215	GLN
45	X	236	GLN
45	X	240	GLN
46	Y	88	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

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Mol	Chain	Res	Type
54	b	102	GLN
55	e	54	GLN
55	e	126	GLN
55	e	179	GLN
55	e	245	GLN
56	g	73	GLN
56	g	102	HIS
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
62	r	184	ASN
63	J	103	GLN
63	J	126	GLN
64	I	91	GLN
64	I	114	HIS
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

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Mol	Chain	Res	Type
70	5	65	HIS
70	5	165	GLN
70	5	191	GLN
70	5	221	GLN
70	5	269	ASN
70	5	280	GLN
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	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
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

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Mol	Chain	Res	Type
80	l	129	HIS
81	p	53	GLN
81	p	123	HIS
81	p	146	ASN
81	p	194	HIS
82	s	154	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	237	ASN
83	Q	262	GLN
86	v	48	ASN
86	v	115	ASN
86	v	154	GLN
86	v	188	GLN
86	v	189	GLN
86	v	231	GLN
86	v	259	ASN
86	v	303	ASN
86	v	349	ASN
86	v	375	GLN
86	v	488	ASN
86	v	506	GLN
86	v	577	ASN
86	v	741	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	940/954 (98%)	190 (20%)	10 (1%)
32	A	1523/1559 (97%)	345 (22%)	18 (1%)
33	B	51/73 (69%)	6 (11%)	1 (1%)
All	All	2514/2586 (97%)	541 (21%)	29 (1%)

All (541) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	650	U
1	AA	651	A
1	AA	663	A
1	AA	676	G
1	AA	680	U
1	AA	689	U
1	AA	690	U
1	AA	691	A
1	AA	694	C
1	AA	701	G
1	AA	704	U
1	AA	711	U
1	AA	718	A
1	AA	721	U
1	AA	736	C
1	AA	737	C
1	AA	745	A
1	AA	753	A
1	AA	761	A
1	AA	764	A
1	AA	766	G
1	AA	770	C
1	AA	771	A
1	AA	783	A
1	AA	791	G
1	AA	794	U
1	AA	795	A
1	AA	796	G
1	AA	807	A
1	AA	808	C
1	AA	812	A
1	AA	817	G
1	AA	826	A
1	AA	827	A
1	AA	828	C
1	AA	829	C
1	AA	830	U
1	AA	835	C
1	AA	837	A
1	AA	842	C
1	AA	843	G
1	AA	846	A

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Mol	Chain	Res	Type
1	AA	847	G
1	AA	860	A
1	AA	868	C
1	AA	870	C
1	AA	877	G
1	AA	883	U
1	AA	890	C
1	AA	891	C
1	AA	899	G
1	AA	904	C
1	AA	907	A
1	AA	919	A
1	AA	921	U
1	AA	922	C
1	AA	931	C
1	AA	933	G
1	AA	938	A
1	AA	942	A
1	AA	948	U
1	AA	954	C
1	AA	957	C
1	AA	965	C
1	AA	966	A
1	AA	967	A
1	AA	992	U
1	AA	993	A
1	AA	1001	C
1	AA	1011	C
1	AA	1015	A
1	AA	1017	A
1	AA	1018	G
1	AA	1022	A
1	AA	1042	U
1	AA	1046	A
1	AA	1049	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	1116	A

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Mol	Chain	Res	Type
1	AA	1118	A
1	AA	1119	U
1	AA	1120	C
1	AA	1121	A
1	AA	1126	A
1	AA	1129	U
1	AA	1138	G
1	AA	1143	C
1	AA	1151	C
1	AA	1154	A
1	AA	1167	A
1	AA	1179	G
1	AA	1180	U
1	AA	1187	U
1	AA	1188	A
1	AA	1189	U
1	AA	1193	U
1	AA	1214	A
1	AA	1215	U
1	AA	1220	A
1	AA	1223	C
1	AA	1225	C
1	AA	1231	A
1	AA	1235	U
1	AA	1236	C
1	AA	1237	A
1	AA	1238	C
1	AA	1245	U
1	AA	1246	U
1	AA	1247	G
1	AA	1248	C
1	AA	1249	U
1	AA	1250	C
1	AA	1251	A
1	AA	1254	C
1	AA	1261	C
1	AA	1270	U
1	AA	1271	C
1	AA	1272	A
1	AA	1283	A
1	AA	1284	U
1	AA	1292	A

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Mol	Chain	Res	Type
1	AA	1295	A
1	AA	1296	A
1	AA	1300	A
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	1345	G
1	AA	1348	G
1	AA	1353	A
1	AA	1354	A
1	AA	1355	G
1	AA	1356	A
1	AA	1367	A
1	AA	1369	U
1	AA	1374	A
1	AA	1377	C
1	AA	1378	C
1	AA	1383	A
1	AA	1390	A
1	AA	1404	A
1	AA	1405	C
1	AA	1406	U
1	AA	1407	U
1	AA	1408	A
1	AA	1417	A
1	AA	1420	U
1	AA	1430	A
1	AA	1432	U
1	AA	1447	G
1	AA	1461	A
1	AA	1464	G
1	AA	1466	C
1	AA	1478	A
1	AA	1482	A
1	AA	1505	A
1	AA	1512	A

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Mol	Chain	Res	Type
1	AA	1516	G
1	AA	1517	A
1	AA	1518	C
1	AA	1521	U
1	AA	1525	C
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	1557	A
1	AA	1558	A
1	AA	1564	A
1	AA	1568	U
1	AA	1582	G
1	AA	1585	A
1	AA	1594	G
1	AA	1595	G
1	AA	1599	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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	2147	G
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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	2601	A
32	A	2607	U
32	A	2618	U
32	A	2619	A
32	A	2625	C
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

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Mol	Chain	Res	Type
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
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	2746	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	717	G

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Mol	Chain	Res	Type
1	AA	828	C
1	AA	947	U
1	AA	953	U
1	AA	1021	U
1	AA	1166	A
1	AA	1246	U
1	AA	1406	U
1	AA	1429	C
1	AA	1535	U
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
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 [i](#)

144 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	Y5P	A6	70	88	14,19,20	4.52	2 (14%)	18,26,29	1.46	2 (11%)
88	P5P	A7	42	88	20,23,24	0.98	3 (15%)	27,33,36	2.04	4 (14%)
88	Y5P	A6	61	88	14,19,20	4.57	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A6	25	88	14,19,20	4.34	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A7	24	88	14,19,20	4.16	2 (14%)	18,26,29	1.36	2 (11%)
88	P5P	A6	43	88	20,23,24	1.09	3 (15%)	27,33,36	2.01	4 (14%)
88	Y5P	A6	65	88	14,19,20	4.42	2 (14%)	18,26,29	1.42	3 (16%)
88	P5P	A6	32	88	20,23,24	0.96	3 (15%)	27,33,36	1.93	4 (14%)
88	Y5P	A7	21	88	14,19,20	4.36	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	1	88	20,20,24	0.97	2 (10%)	28,29,36	1.97	4 (14%)
88	Y5P	A6	24	88	14,19,20	4.16	2 (14%)	18,26,29	1.36	2 (11%)
88	P5P	A6	23	88	20,23,24	1.01	3 (15%)	27,33,36	1.94	4 (14%)
88	P5P	A6	71	32,88	20,23,24	1.00	3 (15%)	27,33,36	1.96	4 (14%)
88	P5P	A7	5	88	20,23,24	1.00	2 (10%)	27,33,36	2.02	4 (14%)
88	P5P	A7	41	88	20,23,24	1.04	3 (15%)	27,33,36	1.94	5 (18%)
88	P5P	A6	15	88	20,23,24	1.08	3 (15%)	27,33,36	2.02	5 (18%)
88	P5P	A6	18	88	20,23,24	1.03	3 (15%)	27,33,36	1.97	4 (14%)
88	P5P	A6	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.04	5 (18%)
87	Y5P	A5	1	87	14,19,20	4.80	2 (14%)	18,26,29	1.85	3 (16%)
88	Y5P	A6	66	88	14,19,20	4.54	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	51	88	14,19,20	4.36	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	43	88	20,23,24	1.11	2 (10%)	27,33,36	2.08	4 (14%)
88	P5P	A6	14	88	20,23,24	1.00	2 (10%)	27,33,36	1.99	3 (11%)
88	Y5P	A7	44	88	14,19,20	4.69	2 (14%)	18,26,29	1.45	2 (11%)
88	Y5P	A7	9	88	14,19,20	4.67	2 (14%)	18,26,29	1.78	3 (16%)
88	P5P	A6	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.09	5 (18%)
88	Y5P	A7	69	88	14,19,20	4.66	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A6	26	88	20,23,24	1.00	3 (15%)	27,33,36	2.07	5 (18%)
88	Y5P	A7	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	55	88	14,19,20	4.52	2 (14%)	18,26,29	1.52	3 (16%)
88	Y5P	A7	17	88	14,19,20	4.61	2 (14%)	18,26,29	1.42	2 (11%)
88	Y5P	A6	36	88	14,19,20	4.42	2 (14%)	18,26,29	1.36	3 (16%)
87	P5P	A5	6	87	20,23,24	1.05	3 (15%)	27,33,36	2.04	5 (18%)
88	Y5P	A6	69	88	14,19,20	4.64	2 (14%)	18,26,29	1.96	6 (33%)
88	P5P	A7	10	88	20,23,24	0.99	2 (10%)	27,33,36	1.97	4 (14%)

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	4 (14%)
88	Y5P	A6	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	46	88	14,19,20	4.49	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A6	20	88	20,23,24	1.00	3 (15%)	27,33,36	1.96	5 (18%)
88	P5P	A6	41	88	20,23,24	1.02	2 (10%)	27,33,36	1.95	4 (14%)
88	Y5P	A6	3	88	14,19,20	4.43	2 (14%)	18,26,29	1.50	3 (16%)
88	P5P	A7	11	88	20,23,24	0.99	3 (15%)	27,33,36	2.10	5 (18%)
88	P5P	A6	4	88	20,23,24	1.00	3 (15%)	27,33,36	1.95	5 (18%)
88	Y5P	A7	64	88	14,19,20	4.53	2 (14%)	18,26,29	1.34	2 (11%)
88	Y5P	A6	30	88	14,19,20	4.48	2 (14%)	18,26,29	1.47	3 (16%)
88	Y5P	A7	63	88	14,19,20	4.53	2 (14%)	18,26,29	1.49	3 (16%)
88	Y5P	A6	53	88	14,19,20	4.69	2 (14%)	18,26,29	1.50	4 (22%)
88	Y5P	A7	67	88	14,19,20	4.66	2 (14%)	18,26,29	1.61	3 (16%)
88	P5P	A6	52	88	20,23,24	1.14	3 (15%)	27,33,36	1.98	5 (18%)
88	Y5P	A6	63	88	14,19,20	4.62	2 (14%)	18,26,29	1.52	3 (16%)
88	P5P	A7	19	88	20,23,24	1.03	3 (15%)	27,33,36	2.14	5 (18%)
88	Y5P	A6	22	88	14,19,20	4.29	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A7	52	88	20,23,24	1.13	3 (15%)	27,33,36	1.98	5 (18%)
88	P5P	A7	14	88	20,23,24	1.01	2 (10%)	27,33,36	1.99	3 (11%)
88	Y5P	A6	67	88	14,19,20	4.68	2 (14%)	18,26,29	1.52	3 (16%)
88	P5P	A7	7	88	20,23,24	0.98	2 (10%)	27,33,36	2.07	4 (14%)
88	Y5P	A6	8	88	14,19,20	4.63	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	12	88	14,19,20	4.33	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A6	42	88	20,23,24	0.98	2 (10%)	27,33,36	2.00	4 (14%)
88	P5P	A7	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
87	P5P	A5	2	87	20,23,24	1.10	2 (10%)	27,33,36	1.98	4 (14%)
88	Y5P	A6	21	88	14,19,20	4.38	2 (14%)	18,26,29	1.38	3 (16%)
88	Y5P	A7	8	88	14,19,20	4.65	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	58	88	14,19,20	4.55	2 (14%)	18,26,29	1.41	3 (16%)
88	P5P	A7	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.08	5 (18%)
88	Y5P	A7	25	88	14,19,20	4.31	2 (14%)	18,26,29	1.39	3 (16%)
88	Y5P	A7	50	88	14,19,20	4.54	2 (14%)	18,26,29	1.39	2 (11%)
88	Y5P	A6	64	88	14,19,20	4.52	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	68	88	14,19,20	4.78	2 (14%)	18,26,29	1.71	4 (22%)
88	Y5P	A7	13	88	14,19,20	4.20	2 (14%)	18,26,29	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A7	62	88	14,19,20	4.40	2 (14%)	18,26,29	1.49	3 (16%)
88	Y5P	A6	59	88	14,19,20	4.79	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	5	88	20,23,24	1.02	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	65	88	14,19,20	4.61	2 (14%)	18,26,29	1.46	3 (16%)
87	P5P	A5	9	87	20,23,24	1.00	3 (15%)	27,33,36	1.95	4 (14%)
88	Y5P	A7	53	88	14,19,20	4.66	2 (14%)	18,26,29	1.55	3 (16%)
87	Y5P	A5	10	87	14,19,20	4.49	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A7	6	88	20,23,24	1.02	3 (15%)	27,33,36	2.11	5 (18%)
88	P5P	A6	40	88	20,23,24	1.02	3 (15%)	27,33,36	2.05	5 (18%)
87	Y5P	A5	3	87	14,19,20	4.49	2 (14%)	18,26,29	1.62	3 (16%)
88	Y5P	A7	57	88	14,19,20	4.46	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	7	88	20,23,24	1.03	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A6	47	88	14,19,20	4.58	2 (14%)	18,26,29	1.51	3 (16%)
88	P5P	A7	71	88	20,23,24	0.99	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	61	88	14,19,20	4.46	2 (14%)	18,26,29	1.42	3 (16%)
87	Y5P	A5	8	87	14,19,20	4.64	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A6	9	88	14,19,20	4.66	2 (14%)	18,26,29	1.78	4 (22%)
88	P5P	A6	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	P5P	A7	18	88	20,23,24	1.00	3 (15%)	27,33,36	2.04	4 (14%)
88	Y5P	A7	70	88	14,19,20	4.51	2 (14%)	18,26,29	1.45	2 (11%)
88	P5P	A7	54	88	20,23,24	1.08	3 (15%)	27,33,36	1.94	3 (11%)
88	Y5P	A7	56	88	14,19,20	4.54	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	12	88	14,19,20	4.27	2 (14%)	18,26,29	1.39	3 (16%)
88	Y5P	A6	17	88	14,19,20	4.65	2 (14%)	18,26,29	1.42	2 (11%)
88	P5P	A7	1	88	20,20,24	0.99	2 (10%)	28,29,36	1.96	4 (14%)
88	P5P	A7	23	88	20,23,24	1.02	3 (15%)	27,33,36	1.92	4 (14%)
88	P5P	A7	2	88	20,23,24	1.03	2 (10%)	27,33,36	2.11	4 (14%)
88	P5P	A6	10	88	20,23,24	1.03	3 (15%)	27,33,36	1.98	4 (14%)
88	Y5P	A6	31	88	14,19,20	4.59	2 (14%)	18,26,29	1.45	3 (16%)
87	Y5P	A5	7	87	14,19,20	4.58	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	15	88	20,23,24	1.06	3 (15%)	27,33,36	2.00	5 (18%)
88	P5P	A7	40	88	20,23,24	1.00	3 (15%)	27,33,36	2.05	5 (18%)
88	P5P	A6	34	88	20,23,24	0.98	3 (15%)	27,33,36	1.91	4 (14%)
88	Y5P	A7	55	88	14,19,20	4.47	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	66	88	14,19,20	4.58	2 (14%)	18,26,29	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A6	29	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A6	45	88	20,23,24	1.08	3 (15%)	27,33,36	2.03	4 (14%)
88	Y5P	A7	59	88	14,19,20	4.76	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A6	57	88	14,19,20	4.48	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A6	50	88	14,19,20	4.60	2 (14%)	18,26,29	1.38	2 (11%)
88	P5P	A7	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.06	5 (18%)
88	P5P	A7	26	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
87	Y5P	A5	4	87	14,19,20	4.79	2 (14%)	18,26,29	1.82	3 (16%)
87	P5P	A5	5	87	20,23,24	1.07	3 (15%)	27,33,36	1.97	4 (14%)
88	Y5P	A6	33	88	14,19,20	4.41	2 (14%)	18,26,29	1.44	3 (16%)
88	P5P	A7	27	88	20,23,24	0.99	3 (15%)	27,33,36	2.07	4 (14%)
88	P5P	A7	45	88	20,23,24	1.05	3 (15%)	27,33,36	2.16	4 (14%)
88	P5P	A6	11	88	20,23,24	0.97	2 (10%)	27,33,36	2.09	4 (14%)
88	Y5P	A7	58	88	14,19,20	4.59	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A6	56	88	14,19,20	4.56	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	60	88	14,19,20	4.45	2 (14%)	18,26,29	1.56	2 (11%)
88	P5P	A6	6	88	20,23,24	1.04	3 (15%)	27,33,36	1.98	4 (14%)
88	Y5P	A7	68	88	14,19,20	4.72	2 (14%)	18,26,29	1.69	4 (22%)
88	P5P	A6	2	88	20,23,24	0.95	2 (10%)	27,33,36	1.96	4 (14%)
88	P5P	A6	27	88	20,23,24	0.99	2 (10%)	27,33,36	2.08	4 (14%)
88	Y5P	A7	46	88	14,19,20	4.51	2 (14%)	18,26,29	1.48	3 (16%)
87	P5P	A5	11	87	20,23,24	1.00	3 (15%)	27,33,36	1.97	5 (18%)
88	P5P	A6	16	88	20,23,24	1.11	3 (15%)	27,33,36	2.14	6 (22%)
88	Y5P	A6	60	88	14,19,20	4.51	2 (14%)	18,26,29	1.54	3 (16%)
88	Y5P	A7	3	88	14,19,20	4.38	2 (14%)	18,26,29	1.50	3 (16%)
88	P5P	A6	28	88	20,23,24	1.01	3 (15%)	27,33,36	2.09	4 (14%)
88	P5P	A6	54	88	20,23,24	1.07	3 (15%)	27,33,36	1.95	4 (14%)
88	P5P	A7	20	88	20,23,24	0.98	3 (15%)	27,33,36	2.01	5 (18%)
88	P5P	A6	19	88	20,23,24	0.99	2 (10%)	27,33,36	2.11	5 (18%)
88	P5P	A7	16	88	20,23,24	1.07	3 (15%)	27,33,36	2.14	6 (22%)
88	Y5P	A6	51	88	14,19,20	4.42	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	38	88	14,19,20	4.33	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	13	88	14,19,20	4.26	2 (14%)	18,26,29	1.28	2 (11%)
88	Y5P	A6	35	88	14,19,20	4.40	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	62	88	14,19,20	4.57	2 (14%)	18,26,29	1.50	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A7	47	88	14,19,20	4.59	2 (14%)	18,26,29	1.53	3 (16%)
88	Y5P	A7	22	88	14,19,20	4.29	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A7	38	88	14,19,20	4.36	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	44	88	14,19,20	4.68	2 (14%)	18,26,29	1.46	2 (11%)

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	Y5P	A6	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	42	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	61	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	25	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	24	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	43	88	-	4/7/25/26	0/3/3/3
88	Y5P	A6	65	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	32	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	21	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	1	88	-	0/6/22/26	0/3/3/3
88	Y5P	A6	24	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	71	32,88	-	1/7/25/26	0/3/3/3
88	P5P	A7	5	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	41	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	15	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	18	88	-	1/7/25/26	0/3/3/3
88	P5P	A6	48	88	-	0/7/25/26	0/3/3/3
87	Y5P	A5	1	87	-	7/7/33/34	0/2/2/2
88	Y5P	A6	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	51	88	-	2/7/33/34	0/2/2/2
88	P5P	A7	43	88	-	5/7/25/26	0/3/3/3
88	P5P	A6	14	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	44	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	9	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	49	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	69	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	26	88	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	37	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	55	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	17	88	-	2/7/33/34	0/2/2/2
88	Y5P	A6	36	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	6	87	-	0/7/25/26	0/3/3/3
88	Y5P	A6	69	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	10	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	4	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	37	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	46	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	20	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	41	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	3	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	11	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	4	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	64	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	30	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	63	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	53	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	52	88	-	6/7/25/26	0/3/3/3
88	Y5P	A6	63	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	19	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	22	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	52	88	-	6/7/25/26	0/3/3/3
88	P5P	A7	14	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A6	8	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	12	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	42	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	39	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	2	87	-	2/7/25/26	0/3/3/3
88	Y5P	A6	21	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	8	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	58	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	48	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	25	88	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	50	88	-	4/7/33/34	0/2/2/2
88	Y5P	A6	64	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	68	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	62	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	59	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	5	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	65	88	-	2/7/33/34	0/2/2/2
87	P5P	A5	9	87	-	0/7/25/26	0/3/3/3
88	Y5P	A7	53	88	-	4/7/33/34	0/2/2/2
87	Y5P	A5	10	87	-	1/7/33/34	0/2/2/2
88	P5P	A7	6	88	-	4/7/25/26	0/3/3/3
88	P5P	A6	40	88	-	0/7/25/26	0/3/3/3
87	Y5P	A5	3	87	-	4/7/33/34	0/2/2/2
88	Y5P	A7	57	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A6	47	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	71	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	61	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	8	87	-	3/7/33/34	0/2/2/2
88	Y5P	A6	9	88	-	5/7/33/34	0/2/2/2
88	P5P	A6	39	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	18	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	54	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	12	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	17	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	1	88	-	0/6/22/26	0/3/3/3
88	P5P	A7	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	2	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	10	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	31	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	7	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	15	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	40	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	34	88	-	0/7/25/26	0/3/3/3
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A6	29	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	45	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	59	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	57	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	50	88	-	4/7/33/34	0/2/2/2
88	P5P	A7	49	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	26	88	-	0/7/25/26	0/3/3/3
87	Y5P	A5	4	87	-	7/7/33/34	0/2/2/2
87	P5P	A5	5	87	-	2/7/25/26	0/3/3/3
88	Y5P	A6	33	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	27	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	45	88	-	2/7/25/26	0/3/3/3
88	P5P	A6	11	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	58	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	60	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	6	88	-	3/7/25/26	0/3/3/3
88	Y5P	A7	68	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	2	88	-	1/7/25/26	0/3/3/3
88	P5P	A6	27	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	46	88	-	3/7/33/34	0/2/2/2
87	P5P	A5	11	87	-	0/7/25/26	0/3/3/3
88	P5P	A6	16	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	60	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	3	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	28	88	-	2/7/25/26	0/3/3/3
88	P5P	A6	54	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	20	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	19	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	16	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	51	88	-	2/7/33/34	0/2/2/2
88	Y5P	A6	38	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	13	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	35	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	62	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	47	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	22	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	38	88	-	2/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A6	44	88	-	2/7/33/34	0/2/2/2

All (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A6	69	Y5P	C4-N3	-14.56	1.32	1.46
88	A6	53	Y5P	C4-N3	-13.91	1.33	1.46
88	A6	8	Y5P	C4-N3	-13.70	1.33	1.46
88	A7	53	Y5P	C4-N3	-13.56	1.33	1.46
88	A7	67	Y5P	C4-N3	-13.50	1.33	1.46
88	A7	44	Y5P	C4-N3	-13.32	1.33	1.46
88	A6	44	Y5P	C4-N3	-13.29	1.33	1.46
87	A5	4	Y5P	C4-N3	-13.24	1.33	1.46
88	A6	68	Y5P	C4-N3	-13.23	1.33	1.46
87	A5	1	Y5P	C4-N3	-13.21	1.33	1.46
88	A7	66	Y5P	C4-N3	-13.18	1.33	1.46
88	A7	64	Y5P	C4-N3	-13.03	1.34	1.46
88	A7	9	Y5P	C4-N3	-12.95	1.34	1.46
88	A7	8	Y5P	C4-N3	-12.92	1.34	1.46
88	A7	58	Y5P	C4-N3	-12.88	1.34	1.46
88	A7	47	Y5P	C4-N3	-12.88	1.34	1.46
88	A7	65	Y5P	C4-N3	-12.85	1.34	1.46
88	A7	59	Y5P	C4-N3	-12.84	1.34	1.46
88	A7	60	Y5P	C4-N3	-12.81	1.34	1.46
88	A7	68	Y5P	C4-N3	-12.80	1.34	1.46
88	A7	3	Y5P	C4-N3	-12.78	1.34	1.46
88	A6	30	Y5P	C4-N3	-12.76	1.34	1.46
88	A6	9	Y5P	C4-N3	-12.74	1.34	1.46
88	A7	46	Y5P	C4-N3	-12.73	1.34	1.46
88	A6	58	Y5P	C4-N3	-12.73	1.34	1.46
88	A6	63	Y5P	C4-N3	-12.72	1.34	1.46
88	A6	62	Y5P	C4-N3	-12.70	1.34	1.46
87	A5	7	Y5P	C4-N3	-12.68	1.34	1.46
88	A6	67	Y5P	C4-N3	-12.68	1.34	1.46
88	A6	59	Y5P	C4-N3	-12.66	1.34	1.46
88	A6	17	Y5P	C4-N3	-12.61	1.34	1.46
88	A7	17	Y5P	C4-N3	-12.60	1.34	1.46
88	A6	47	Y5P	C4-N3	-12.56	1.34	1.46
88	A7	51	Y5P	C4-N3	-12.55	1.34	1.46
88	A6	22	Y5P	C4-N3	-12.51	1.34	1.46
88	A6	46	Y5P	C4-N3	-12.48	1.34	1.46
88	A6	64	Y5P	C4-N3	-12.44	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	62	Y5P	C4-N3	-12.43	1.34	1.46
88	A7	69	Y5P	C4-N3	-12.43	1.34	1.46
88	A6	59	Y5P	C2-N3	12.41	1.37	1.27
88	A6	51	Y5P	C4-N3	-12.41	1.34	1.46
88	A7	57	Y5P	C4-N3	-12.41	1.34	1.46
88	A6	65	Y5P	C4-N3	-12.39	1.34	1.46
88	A6	61	Y5P	C4-N3	-12.39	1.34	1.46
88	A6	60	Y5P	C4-N3	-12.38	1.34	1.46
88	A7	50	Y5P	C4-N3	-12.37	1.34	1.46
88	A7	21	Y5P	C4-N3	-12.37	1.34	1.46
88	A7	22	Y5P	C4-N3	-12.36	1.34	1.46
88	A7	38	Y5P	C4-N3	-12.36	1.34	1.46
88	A7	63	Y5P	C4-N3	-12.35	1.34	1.46
88	A6	50	Y5P	C4-N3	-12.35	1.34	1.46
87	A5	8	Y5P	C4-N3	-12.34	1.34	1.46
87	A5	3	Y5P	C4-N3	-12.28	1.34	1.46
88	A7	37	Y5P	C4-N3	-12.27	1.34	1.46
88	A6	21	Y5P	C4-N3	-12.26	1.34	1.46
87	A5	10	Y5P	C4-N3	-12.26	1.34	1.46
88	A6	57	Y5P	C4-N3	-12.25	1.34	1.46
88	A6	55	Y5P	C4-N3	-12.24	1.34	1.46
88	A6	38	Y5P	C4-N3	-12.23	1.34	1.46
88	A7	61	Y5P	C4-N3	-12.22	1.34	1.46
88	A6	3	Y5P	C4-N3	-12.19	1.34	1.46
88	A7	55	Y5P	C4-N3	-12.19	1.34	1.46
88	A6	37	Y5P	C4-N3	-12.16	1.34	1.46
88	A6	56	Y5P	C4-N3	-12.15	1.34	1.46
88	A7	59	Y5P	C2-N3	12.14	1.36	1.27
88	A6	66	Y5P	C4-N3	-12.09	1.34	1.46
88	A7	25	Y5P	C4-N3	-12.07	1.34	1.46
88	A7	56	Y5P	C4-N3	-12.06	1.34	1.46
88	A7	68	Y5P	C2-N3	12.04	1.36	1.27
88	A6	25	Y5P	C4-N3	-12.03	1.34	1.46
88	A6	31	Y5P	C2-N3	12.01	1.36	1.27
88	A6	31	Y5P	C4-N3	-12.00	1.35	1.46
88	A6	29	Y5P	C4-N3	-11.99	1.35	1.46
88	A6	36	Y5P	C4-N3	-11.99	1.35	1.46
88	A7	69	Y5P	C2-N3	11.98	1.36	1.27
88	A7	24	Y5P	C4-N3	-11.95	1.35	1.46
88	A7	70	Y5P	C4-N3	-11.94	1.35	1.46
87	A5	8	Y5P	C2-N3	11.93	1.36	1.27
88	A6	70	Y5P	C4-N3	-11.93	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A6	13	Y5P	C4-N3	-11.91	1.35	1.46
88	A6	68	Y5P	C2-N3	11.89	1.36	1.27
87	A5	1	Y5P	C2-N3	11.86	1.36	1.27
88	A7	13	Y5P	C4-N3	-11.86	1.35	1.46
88	A6	67	Y5P	C2-N3	11.82	1.36	1.27
88	A6	50	Y5P	C2-N3	11.78	1.36	1.27
88	A7	70	Y5P	C2-N3	11.77	1.36	1.27
88	A6	17	Y5P	C2-N3	11.76	1.36	1.27
88	A6	24	Y5P	C4-N3	-11.76	1.35	1.46
88	A6	70	Y5P	C2-N3	11.75	1.36	1.27
87	A5	4	Y5P	C2-N3	11.75	1.36	1.27
88	A6	35	Y5P	C4-N3	-11.75	1.35	1.46
88	A6	12	Y5P	C4-N3	-11.73	1.35	1.46
88	A6	56	Y5P	C2-N3	11.72	1.36	1.27
88	A7	56	Y5P	C2-N3	11.70	1.36	1.27
88	A6	66	Y5P	C2-N3	11.70	1.36	1.27
88	A6	33	Y5P	C4-N3	-11.65	1.35	1.46
88	A7	12	Y5P	C4-N3	-11.64	1.35	1.46
88	A7	17	Y5P	C2-N3	11.62	1.36	1.27
88	A6	9	Y5P	C2-N3	11.58	1.36	1.27
88	A6	61	Y5P	C2-N3	11.53	1.36	1.27
88	A6	63	Y5P	C2-N3	11.52	1.36	1.27
88	A6	47	Y5P	C2-N3	11.46	1.36	1.27
88	A7	50	Y5P	C2-N3	11.46	1.36	1.27
88	A7	9	Y5P	C2-N3	11.46	1.36	1.27
88	A6	33	Y5P	C2-N3	11.42	1.36	1.27
88	A6	55	Y5P	C2-N3	11.40	1.36	1.27
88	A7	8	Y5P	C2-N3	11.40	1.36	1.27
88	A7	63	Y5P	C2-N3	11.38	1.36	1.27
87	A5	10	Y5P	C2-N3	11.31	1.36	1.27
88	A6	62	Y5P	C2-N3	11.29	1.36	1.27
88	A6	60	Y5P	C2-N3	11.29	1.36	1.27
88	A6	44	Y5P	C2-N3	11.28	1.36	1.27
88	A7	65	Y5P	C2-N3	11.27	1.36	1.27
87	A5	7	Y5P	C2-N3	11.26	1.36	1.27
88	A6	64	Y5P	C2-N3	11.25	1.36	1.27
88	A7	44	Y5P	C2-N3	11.23	1.36	1.27
88	A6	35	Y5P	C2-N3	11.23	1.36	1.27
88	A6	57	Y5P	C2-N3	11.22	1.36	1.27
88	A7	55	Y5P	C2-N3	11.20	1.36	1.27
88	A7	47	Y5P	C2-N3	11.19	1.36	1.27
88	A6	36	Y5P	C2-N3	11.13	1.36	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A5	3	Y5P	C2-N3	11.11	1.36	1.27
88	A7	58	Y5P	C2-N3	11.08	1.36	1.27
88	A6	3	Y5P	C2-N3	11.08	1.36	1.27
88	A7	61	Y5P	C2-N3	11.07	1.36	1.27
88	A6	58	Y5P	C2-N3	11.05	1.36	1.27
88	A6	46	Y5P	C2-N3	10.99	1.36	1.27
88	A7	57	Y5P	C2-N3	10.98	1.35	1.27
88	A6	29	Y5P	C2-N3	10.91	1.35	1.27
88	A6	12	Y5P	C2-N3	10.87	1.35	1.27
88	A7	67	Y5P	C2-N3	10.86	1.35	1.27
88	A6	51	Y5P	C2-N3	10.79	1.35	1.27
88	A7	66	Y5P	C2-N3	10.79	1.35	1.27
88	A7	46	Y5P	C2-N3	10.78	1.35	1.27
88	A6	30	Y5P	C2-N3	10.74	1.35	1.27
88	A6	25	Y5P	C2-N3	10.73	1.35	1.27
88	A6	37	Y5P	C2-N3	10.71	1.35	1.27
88	A7	53	Y5P	C2-N3	10.71	1.35	1.27
88	A7	12	Y5P	C2-N3	10.65	1.35	1.27
88	A6	65	Y5P	C2-N3	10.64	1.35	1.27
88	A7	62	Y5P	C2-N3	10.61	1.35	1.27
88	A7	37	Y5P	C2-N3	10.59	1.35	1.27
88	A6	21	Y5P	C2-N3	10.52	1.35	1.27
88	A7	64	Y5P	C2-N3	10.52	1.35	1.27
88	A7	25	Y5P	C2-N3	10.49	1.35	1.27
88	A7	60	Y5P	C2-N3	10.45	1.35	1.27
88	A6	53	Y5P	C2-N3	10.41	1.35	1.27
88	A7	38	Y5P	C2-N3	10.39	1.35	1.27
88	A6	13	Y5P	C2-N3	10.39	1.35	1.27
88	A6	38	Y5P	C2-N3	10.36	1.35	1.27
88	A7	21	Y5P	C2-N3	10.36	1.35	1.27
88	A6	8	Y5P	C2-N3	10.34	1.35	1.27
88	A7	51	Y5P	C2-N3	10.32	1.35	1.27
88	A7	13	Y5P	C2-N3	10.08	1.35	1.27
88	A7	3	Y5P	C2-N3	10.08	1.35	1.27
88	A6	24	Y5P	C2-N3	9.99	1.35	1.27
88	A7	22	Y5P	C2-N3	9.90	1.35	1.27
88	A6	22	Y5P	C2-N3	9.78	1.35	1.27
88	A7	24	Y5P	C2-N3	9.76	1.35	1.27
88	A6	69	Y5P	C2-N3	9.18	1.34	1.27
88	A7	1	P5P	C6-N1	2.74	1.40	1.34
88	A7	2	P5P	C6-N1	2.74	1.40	1.34
88	A6	1	P5P	C6-N1	2.73	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A6	18	P5P	C6-N1	2.71	1.40	1.34
88	A7	54	P5P	C6-N1	2.69	1.40	1.34
88	A7	15	P5P	C6-N1	2.67	1.39	1.34
88	A7	52	P5P	C6-N1	2.62	1.39	1.34
88	A6	54	P5P	C6-N1	2.62	1.39	1.34
88	A6	52	P5P	C6-N1	2.62	1.39	1.34
88	A6	6	P5P	C6-N1	2.61	1.39	1.34
88	A7	39	P5P	C6-N1	2.61	1.39	1.34
88	A7	18	P5P	C6-N1	2.60	1.39	1.34
88	A6	26	P5P	C6-N1	2.60	1.39	1.34
88	A7	43	P5P	C6-N1	2.60	1.39	1.34
88	A7	48	P5P	C6-N1	2.60	1.39	1.34
88	A6	15	P5P	C6-N1	2.59	1.39	1.34
88	A6	39	P5P	C6-N1	2.58	1.39	1.34
88	A7	26	P5P	C6-N1	2.57	1.39	1.34
88	A6	48	P5P	C6-N1	2.56	1.39	1.34
88	A7	4	P5P	C6-N1	2.56	1.39	1.34
88	A7	4	P5P	C6-C5	2.55	1.43	1.39
88	A7	71	P5P	C6-N1	2.55	1.39	1.34
88	A6	7	P5P	C6-N1	2.54	1.39	1.34
88	A7	19	P5P	C6-N1	2.54	1.39	1.34
88	A6	71	P5P	C6-N1	2.53	1.39	1.34
88	A7	23	P5P	C6-N1	2.53	1.39	1.34
88	A6	49	P5P	C6-N1	2.52	1.39	1.34
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	A6	34	P5P	C6-N1	2.51	1.39	1.34
87	A5	11	P5P	C6-N1	2.50	1.39	1.34
88	A6	10	P5P	C6-N1	2.50	1.39	1.34
88	A6	43	P5P	C6-N1	2.50	1.39	1.34
87	A5	6	P5P	C6-N1	2.50	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	A6	2	P5P	C6-N1	2.48	1.39	1.34
87	A5	9	P5P	C6-N1	2.47	1.39	1.34
88	A7	7	P5P	C6-N1	2.47	1.39	1.34
88	A6	4	P5P	C6-N1	2.46	1.39	1.34
88	A6	19	P5P	C6-N1	2.45	1.39	1.34
88	A6	23	P5P	C6-N1	2.44	1.39	1.34
87	A5	5	P5P	C6-N1	2.43	1.39	1.34
88	A6	28	P5P	C6-N1	2.43	1.39	1.34
88	A6	14	P5P	C6-N1	2.42	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	6	P5P	C6-C5	2.42	1.42	1.39
88	A7	10	P5P	C6-N1	2.41	1.39	1.34
88	A7	16	P5P	C6-N1	2.40	1.39	1.34
88	A7	14	P5P	C6-N1	2.39	1.39	1.34
88	A6	48	P5P	C6-C5	2.39	1.42	1.39
88	A7	11	P5P	C6-N1	2.38	1.39	1.34
88	A6	16	P5P	C6-N1	2.37	1.39	1.34
88	A7	48	P5P	C6-C5	2.37	1.42	1.39
88	A7	5	P5P	C6-N1	2.37	1.39	1.34
88	A7	40	P5P	C6-N1	2.37	1.39	1.34
88	A6	28	P5P	C6-C5	2.36	1.42	1.39
88	A6	45	P5P	C6-N1	2.35	1.39	1.34
88	A6	5	P5P	C6-N1	2.35	1.39	1.34
88	A6	14	P5P	C2-N1	2.35	1.38	1.33
88	A7	27	P5P	C6-N1	2.33	1.39	1.34
88	A6	18	P5P	C2-N1	2.33	1.38	1.33
88	A6	11	P5P	C6-N1	2.33	1.39	1.34
88	A7	54	P5P	C2-N1	2.32	1.38	1.33
88	A6	42	P5P	C6-N1	2.32	1.39	1.34
88	A6	27	P5P	C6-N1	2.32	1.39	1.34
88	A6	41	P5P	C6-N1	2.32	1.39	1.34
88	A6	32	P5P	C6-N1	2.30	1.39	1.34
88	A7	26	P5P	C6-C5	2.30	1.42	1.39
88	A7	15	P5P	C2-N1	2.30	1.38	1.33
88	A6	40	P5P	C6-N1	2.30	1.39	1.34
88	A7	2	P5P	C2-N1	2.30	1.38	1.33
88	A6	40	P5P	C6-C5	2.29	1.42	1.39
88	A7	42	P5P	C6-N1	2.29	1.39	1.34
88	A6	39	P5P	C6-C5	2.28	1.42	1.39
88	A7	54	P5P	C6-C5	2.28	1.42	1.39
88	A7	18	P5P	C2-N1	2.28	1.37	1.33
88	A6	6	P5P	C6-C5	2.27	1.42	1.39
88	A6	20	P5P	C6-N1	2.27	1.39	1.34
88	A6	52	P5P	C6-C5	2.27	1.42	1.39
88	A6	54	P5P	C6-C5	2.27	1.42	1.39
88	A7	52	P5P	C6-C5	2.27	1.42	1.39
88	A7	39	P5P	C6-C5	2.27	1.42	1.39
88	A6	52	P5P	C2-N1	2.27	1.37	1.33
88	A6	71	P5P	C2-N1	2.26	1.37	1.33
88	A7	20	P5P	C6-N1	2.26	1.39	1.34
88	A7	71	P5P	C2-N1	2.26	1.37	1.33
87	A5	6	P5P	C2-N1	2.26	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	45	P5P	C6-N1	2.26	1.39	1.34
88	A7	43	P5P	C2-N1	2.26	1.37	1.33
87	A5	11	P5P	C2-N1	2.26	1.37	1.33
88	A7	14	P5P	C2-N1	2.25	1.37	1.33
88	A6	7	P5P	C2-N1	2.25	1.37	1.33
88	A7	52	P5P	C2-N1	2.24	1.37	1.33
87	A5	5	P5P	C2-N1	2.24	1.37	1.33
87	A5	9	P5P	C2-N1	2.24	1.37	1.33
88	A6	15	P5P	C2-N1	2.24	1.37	1.33
88	A6	54	P5P	C2-N1	2.23	1.37	1.33
88	A6	45	P5P	C6-C5	2.23	1.42	1.39
88	A6	18	P5P	C6-C5	2.23	1.42	1.39
88	A7	23	P5P	C6-C5	2.22	1.42	1.39
88	A7	41	P5P	C2-N1	2.22	1.37	1.33
87	A5	2	P5P	C2-N1	2.21	1.37	1.33
88	A6	16	P5P	C6-C5	2.20	1.42	1.39
88	A7	48	P5P	C2-N1	2.20	1.37	1.33
88	A7	71	P5P	C6-C5	2.20	1.42	1.39
88	A6	34	P5P	C2-N1	2.20	1.37	1.33
88	A6	71	P5P	C6-C5	2.19	1.42	1.39
88	A7	19	P5P	C2-N1	2.19	1.37	1.33
88	A6	41	P5P	C2-N1	2.19	1.37	1.33
88	A6	49	P5P	C6-C5	2.19	1.42	1.39
88	A7	5	P5P	C6-C5	2.19	1.42	1.39
88	A7	40	P5P	C6-C5	2.18	1.42	1.39
88	A6	48	P5P	C2-N1	2.18	1.37	1.33
88	A7	11	P5P	C6-C5	2.18	1.42	1.39
88	A6	20	P5P	C6-C5	2.17	1.42	1.39
88	A6	42	P5P	C2-N1	2.17	1.37	1.33
88	A6	10	P5P	C2-N1	2.16	1.37	1.33
88	A6	26	P5P	C6-C5	2.16	1.42	1.39
88	A6	4	P5P	C2-N1	2.16	1.37	1.33
88	A7	16	P5P	C6-C5	2.15	1.42	1.39
88	A7	16	P5P	C2-N1	2.15	1.37	1.33
88	A6	23	P5P	C6-C5	2.14	1.42	1.39
88	A6	45	P5P	C2-N1	2.14	1.37	1.33
88	A6	27	P5P	C6-C5	2.14	1.42	1.39
88	A6	6	P5P	C2-N1	2.14	1.37	1.33
88	A7	18	P5P	C6-C5	2.13	1.42	1.39
88	A6	19	P5P	C2-N1	2.13	1.37	1.33
88	A7	15	P5P	C6-C5	2.13	1.42	1.39
87	A5	11	P5P	C6-C5	2.13	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A5	5	P5P	C6-C5	2.13	1.42	1.39
88	A6	32	P5P	C2-N1	2.13	1.37	1.33
88	A7	42	P5P	C2-N1	2.12	1.37	1.33
88	A6	5	P5P	C6-C5	2.12	1.42	1.39
88	A6	39	P5P	C2-N1	2.12	1.37	1.33
88	A6	16	P5P	C2-N1	2.12	1.37	1.33
88	A6	11	P5P	C6-C5	2.12	1.42	1.39
88	A7	26	P5P	C2-N1	2.12	1.37	1.33
88	A7	45	P5P	C2-N1	2.12	1.37	1.33
88	A6	23	P5P	C2-N1	2.12	1.37	1.33
88	A7	20	P5P	C6-C5	2.12	1.42	1.39
88	A7	49	P5P	C6-C5	2.11	1.42	1.39
88	A7	23	P5P	C2-N1	2.11	1.37	1.33
88	A7	49	P5P	C2-N1	2.11	1.37	1.33
88	A7	39	P5P	C2-N1	2.11	1.37	1.33
88	A7	27	P5P	C6-C5	2.10	1.42	1.39
88	A6	26	P5P	C2-N1	2.10	1.37	1.33
88	A7	40	P5P	C2-N1	2.10	1.37	1.33
88	A6	5	P5P	C2-N1	2.09	1.37	1.33
88	A6	49	P5P	C2-N1	2.09	1.37	1.33
88	A6	4	P5P	C6-C5	2.09	1.42	1.39
88	A7	10	P5P	C2-N1	2.09	1.37	1.33
88	A6	20	P5P	C2-N1	2.08	1.37	1.33
88	A6	43	P5P	C6-C5	2.08	1.42	1.39
88	A7	41	P5P	C6-C5	2.08	1.42	1.39
87	A5	6	P5P	C6-C5	2.08	1.42	1.39
88	A6	15	P5P	C6-C5	2.08	1.42	1.39
88	A6	43	P5P	C2-N1	2.07	1.37	1.33
88	A7	19	P5P	C6-C5	2.07	1.42	1.39
88	A6	7	P5P	C6-C5	2.06	1.42	1.39
88	A6	32	P5P	C6-C5	2.05	1.42	1.39
88	A7	11	P5P	C2-N1	2.05	1.37	1.33
88	A7	4	P5P	C2-N1	2.04	1.37	1.33
88	A6	40	P5P	C2-N1	2.04	1.37	1.33
88	A6	1	P5P	C2-N1	2.04	1.37	1.33
88	A7	7	P5P	C2-N1	2.04	1.37	1.33
88	A7	42	P5P	C6-C5	2.03	1.42	1.39
88	A7	20	P5P	C2-N1	2.02	1.37	1.33
88	A7	27	P5P	C2-N1	2.02	1.37	1.33
88	A7	6	P5P	C2-N1	2.02	1.37	1.33
88	A7	1	P5P	C2-N1	2.02	1.37	1.33
88	A6	34	P5P	C6-C5	2.02	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	A5	9	P5P	C6-C5	2.01	1.42	1.39
88	A6	2	P5P	C2-N1	2.01	1.37	1.33
88	A6	28	P5P	C2-N1	2.01	1.37	1.33
88	A6	10	P5P	C6-C5	2.00	1.42	1.39
88	A7	45	P5P	C6-C5	2.00	1.42	1.39

All (513) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	45	P5P	C6-N1-C2	8.85	126.25	115.80
88	A6	27	P5P	C6-N1-C2	8.68	126.05	115.80
88	A6	28	P5P	C6-N1-C2	8.65	126.01	115.80
88	A7	27	P5P	C6-N1-C2	8.63	125.98	115.80
88	A7	11	P5P	C6-N1-C2	8.61	125.97	115.80
88	A6	11	P5P	C6-N1-C2	8.61	125.96	115.80
88	A7	2	P5P	C6-N1-C2	8.57	125.91	115.80
88	A7	7	P5P	C6-N1-C2	8.53	125.87	115.80
88	A7	4	P5P	C6-N1-C2	8.52	125.85	115.80
88	A7	39	P5P	C6-N1-C2	8.51	125.84	115.80
88	A7	26	P5P	C6-N1-C2	8.50	125.84	115.80
88	A6	39	P5P	C6-N1-C2	8.50	125.84	115.80
88	A6	26	P5P	C6-N1-C2	8.48	125.81	115.80
88	A6	49	P5P	C6-N1-C2	8.47	125.80	115.80
88	A7	19	P5P	C6-N1-C2	8.41	125.73	115.80
88	A6	40	P5P	C6-N1-C2	8.40	125.72	115.80
88	A7	49	P5P	C6-N1-C2	8.40	125.71	115.80
88	A7	40	P5P	C6-N1-C2	8.39	125.70	115.80
88	A7	6	P5P	C6-N1-C2	8.38	125.69	115.80
88	A7	5	P5P	C6-N1-C2	8.36	125.67	115.80
88	A7	18	P5P	C6-N1-C2	8.36	125.66	115.80
88	A6	19	P5P	C6-N1-C2	8.31	125.61	115.80
88	A7	1	P5P	C6-N1-C2	8.25	125.54	115.80
88	A7	42	P5P	C6-N1-C2	8.22	125.51	115.80
88	A7	20	P5P	C6-N1-C2	8.22	125.51	115.80
88	A6	45	P5P	C6-N1-C2	8.21	125.49	115.80
88	A6	10	P5P	C6-N1-C2	8.21	125.49	115.80
88	A7	48	P5P	C6-N1-C2	8.21	125.49	115.80
88	A6	1	P5P	C6-N1-C2	8.20	125.48	115.80
88	A7	10	P5P	C6-N1-C2	8.18	125.46	115.80
88	A6	48	P5P	C6-N1-C2	8.17	125.44	115.80
88	A6	16	P5P	C6-N1-C2	8.16	125.43	115.80
88	A6	5	P5P	C6-N1-C2	8.15	125.41	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	16	P5P	C6-N1-C2	8.13	125.40	115.80
87	A5	5	P5P	C6-N1-C2	8.12	125.39	115.80
88	A6	42	P5P	C6-N1-C2	8.11	125.38	115.80
88	A6	71	P5P	C6-N1-C2	8.10	125.36	115.80
87	A5	11	P5P	C6-N1-C2	8.09	125.35	115.80
87	A5	6	P5P	C6-N1-C2	8.08	125.34	115.80
88	A6	15	P5P	C6-N1-C2	8.05	125.30	115.80
87	A5	9	P5P	C6-N1-C2	8.05	125.30	115.80
88	A6	23	P5P	C6-N1-C2	8.04	125.29	115.80
88	A6	6	P5P	C6-N1-C2	8.04	125.29	115.80
88	A7	14	P5P	C6-N1-C2	8.03	125.28	115.80
88	A6	14	P5P	C6-N1-C2	8.03	125.27	115.80
88	A6	7	P5P	C6-N1-C2	8.02	125.27	115.80
88	A6	20	P5P	C6-N1-C2	8.02	125.27	115.80
88	A7	43	P5P	C6-N1-C2	8.02	125.27	115.80
88	A7	71	P5P	C6-N1-C2	8.00	125.25	115.80
88	A6	4	P5P	C6-N1-C2	8.00	125.24	115.80
88	A6	2	P5P	C6-N1-C2	7.99	125.23	115.80
88	A6	32	P5P	C6-N1-C2	7.97	125.20	115.80
88	A7	15	P5P	C6-N1-C2	7.94	125.17	115.80
87	A5	2	P5P	C6-N1-C2	7.94	125.17	115.80
88	A6	34	P5P	C6-N1-C2	7.92	125.15	115.80
88	A6	18	P5P	C6-N1-C2	7.91	125.14	115.80
88	A7	23	P5P	C6-N1-C2	7.90	125.12	115.80
88	A7	52	P5P	C6-N1-C2	7.86	125.08	115.80
88	A6	54	P5P	C6-N1-C2	7.85	125.07	115.80
88	A6	41	P5P	C6-N1-C2	7.85	125.07	115.80
88	A6	52	P5P	C6-N1-C2	7.83	125.04	115.80
88	A7	54	P5P	C6-N1-C2	7.83	125.04	115.80
88	A6	43	P5P	C6-N1-C2	7.81	125.02	115.80
88	A7	41	P5P	C6-N1-C2	7.80	125.01	115.80
88	A6	69	Y5P	C5-C4-N3	5.02	122.24	114.15
88	A6	67	Y5P	C5-C4-N3	4.88	122.02	114.15
88	A6	44	Y5P	C5-C4-N3	4.85	121.96	114.15
88	A7	44	Y5P	C5-C4-N3	4.82	121.93	114.15
88	A7	67	Y5P	C5-C4-N3	4.82	121.92	114.15
88	A7	68	Y5P	C5-C4-N3	4.78	121.85	114.15
88	A6	68	Y5P	C5-C4-N3	4.73	121.78	114.15
88	A7	9	Y5P	C1'-N1-C6	-4.72	110.79	120.77
88	A6	66	Y5P	C5-C4-N3	4.72	121.76	114.15
87	A5	8	Y5P	C5-C4-N3	4.71	121.75	114.15
88	A7	17	Y5P	C5-C4-N3	4.70	121.73	114.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	A5	4	Y5P	C5-C4-N3	4.70	121.73	114.15
88	A7	69	Y5P	C5-C4-N3	4.69	121.72	114.15
88	A6	31	Y5P	C5-C4-N3	4.68	121.69	114.15
88	A7	70	Y5P	C5-C4-N3	4.67	121.67	114.15
88	A6	63	Y5P	C5-C4-N3	4.66	121.67	114.15
87	A5	1	Y5P	C5-C4-N3	4.66	121.66	114.15
88	A6	70	Y5P	C5-C4-N3	4.65	121.65	114.15
88	A6	17	Y5P	C5-C4-N3	4.65	121.65	114.15
88	A7	66	Y5P	C5-C4-N3	4.65	121.64	114.15
88	A7	58	Y5P	C5-C4-N3	4.64	121.63	114.15
87	A5	10	Y5P	C5-C4-N3	4.63	121.62	114.15
88	A6	3	Y5P	C5-C4-N3	4.63	121.61	114.15
88	A6	62	Y5P	C5-C4-N3	4.62	121.59	114.15
88	A6	9	Y5P	C1'-N1-C6	-4.62	111.01	120.77
88	A6	61	Y5P	C5-C4-N3	4.61	121.59	114.15
88	A6	30	Y5P	C5-C4-N3	4.60	121.57	114.15
87	A5	7	Y5P	C5-C4-N3	4.59	121.55	114.15
88	A6	60	Y5P	C5-C4-N3	4.58	121.53	114.15
88	A6	58	Y5P	C5-C4-N3	4.57	121.51	114.15
88	A6	64	Y5P	C5-C4-N3	4.56	121.50	114.15
88	A7	60	Y5P	C5-C4-N3	4.55	121.49	114.15
88	A6	59	Y5P	C5-C4-N3	4.55	121.49	114.15
88	A7	46	Y5P	C5-C4-N3	4.55	121.49	114.15
87	A5	3	Y5P	C5-C4-N3	4.55	121.48	114.15
88	A7	56	Y5P	C5-C4-N3	4.54	121.48	114.15
88	A7	3	Y5P	C5-C4-N3	4.54	121.48	114.15
87	A5	1	Y5P	C1'-N1-C6	-4.53	111.18	120.77
88	A6	55	Y5P	C5-C4-N3	4.53	121.46	114.15
88	A7	47	Y5P	C5-C4-N3	4.53	121.45	114.15
88	A7	55	Y5P	C5-C4-N3	4.52	121.44	114.15
88	A6	47	Y5P	C5-C4-N3	4.52	121.43	114.15
88	A6	56	Y5P	C5-C4-N3	4.52	121.43	114.15
88	A6	22	Y5P	C5-C4-N3	4.51	121.43	114.15
88	A6	46	Y5P	C5-C4-N3	4.51	121.43	114.15
88	A7	45	P5P	C5-C6-N1	-4.51	110.67	121.90
88	A6	33	Y5P	C5-C4-N3	4.50	121.41	114.15
88	A7	59	Y5P	C5-C4-N3	4.50	121.41	114.15
88	A7	53	Y5P	C5-C4-N3	4.49	121.39	114.15
88	A6	38	Y5P	C5-C4-N3	4.49	121.39	114.15
88	A7	65	Y5P	C5-C4-N3	4.48	121.38	114.15
88	A7	50	Y5P	C5-C4-N3	4.48	121.37	114.15
88	A7	22	Y5P	C5-C4-N3	4.47	121.35	114.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	65	Y5P	C5-C4-N3	4.47	121.35	114.15
88	A7	8	Y5P	C5-C4-N3	4.45	121.33	114.15
88	A7	38	Y5P	C5-C4-N3	4.45	121.33	114.15
88	A6	50	Y5P	C5-C4-N3	4.45	121.32	114.15
88	A6	53	Y5P	C5-C4-N3	4.44	121.31	114.15
88	A6	8	Y5P	C5-C4-N3	4.43	121.30	114.15
88	A7	4	P5P	C5-C6-N1	-4.43	110.87	121.90
88	A7	57	Y5P	C5-C4-N3	4.42	121.28	114.15
88	A7	62	Y5P	C5-C4-N3	4.41	121.27	114.15
88	A6	57	Y5P	C5-C4-N3	4.41	121.26	114.15
88	A7	19	P5P	C5-C6-N1	-4.39	110.97	121.90
88	A6	12	Y5P	C5-C4-N3	4.39	121.22	114.15
88	A7	14	P5P	C5-C6-N1	-4.36	111.05	121.90
88	A7	63	Y5P	C5-C4-N3	4.35	121.17	114.15
88	A6	28	P5P	C5-C6-N1	-4.35	111.06	121.90
88	A7	11	P5P	C5-C6-N1	-4.35	111.06	121.90
88	A7	25	Y5P	C5-C4-N3	4.35	121.16	114.15
87	A5	4	Y5P	C1'-N1-C6	-4.35	111.58	120.77
88	A6	14	P5P	C5-C6-N1	-4.35	111.08	121.90
88	A6	11	P5P	C5-C6-N1	-4.34	111.10	121.90
88	A6	29	Y5P	C5-C4-N3	4.34	121.14	114.15
88	A6	25	Y5P	C5-C4-N3	4.33	121.14	114.15
88	A6	37	Y5P	C5-C4-N3	4.33	121.13	114.15
88	A7	51	Y5P	C5-C4-N3	4.33	121.13	114.15
88	A7	37	Y5P	C5-C4-N3	4.32	121.12	114.15
88	A7	61	Y5P	C5-C4-N3	4.31	121.10	114.15
88	A7	1	P5P	C5-C6-N1	-4.31	111.17	121.90
88	A6	27	P5P	C5-C6-N1	-4.31	111.17	121.90
88	A6	19	P5P	C5-C6-N1	-4.31	111.18	121.90
88	A7	27	P5P	C5-C6-N1	-4.30	111.18	121.90
88	A6	40	P5P	C5-C6-N1	-4.30	111.19	121.90
88	A7	2	P5P	C5-C6-N1	-4.29	111.21	121.90
88	A6	45	P5P	C5-C6-N1	-4.28	111.24	121.90
88	A7	40	P5P	C5-C6-N1	-4.27	111.26	121.90
88	A7	12	Y5P	C5-C4-N3	4.26	121.03	114.15
88	A7	18	P5P	C5-C6-N1	-4.26	111.28	121.90
88	A6	39	P5P	C5-C6-N1	-4.26	111.28	121.90
88	A7	39	P5P	C5-C6-N1	-4.26	111.29	121.90
88	A6	18	P5P	C5-C6-N1	-4.26	111.29	121.90
88	A6	6	P5P	C5-C6-N1	-4.26	111.30	121.90
88	A7	26	P5P	C5-C6-N1	-4.25	111.32	121.90
88	A6	51	Y5P	C5-C4-N3	4.24	120.99	114.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	9	Y5P	C5-C4-N3	4.24	120.99	114.15
88	A7	6	P5P	C5-C6-N1	-4.24	111.34	121.90
88	A7	42	P5P	C5-C6-N1	-4.23	111.35	121.90
88	A6	9	Y5P	C5-C4-N3	4.23	120.97	114.15
88	A6	21	Y5P	C5-C4-N3	4.23	120.97	114.15
88	A7	21	Y5P	C5-C4-N3	4.23	120.97	114.15
88	A6	26	P5P	C5-C6-N1	-4.23	111.37	121.90
88	A7	5	P5P	C5-C6-N1	-4.23	111.37	121.90
88	A6	5	P5P	C5-C6-N1	-4.23	111.37	121.90
88	A6	49	P5P	C5-C6-N1	-4.22	111.38	121.90
88	A6	24	Y5P	C5-C4-N3	4.22	120.96	114.15
88	A6	1	P5P	C5-C6-N1	-4.22	111.39	121.90
88	A6	41	P5P	C5-C6-N1	-4.22	111.39	121.90
88	A6	10	P5P	C5-C6-N1	-4.22	111.40	121.90
87	A5	5	P5P	C5-C6-N1	-4.21	111.41	121.90
88	A6	71	P5P	C5-C6-N1	-4.21	111.41	121.90
88	A7	49	P5P	C5-C6-N1	-4.21	111.41	121.90
88	A7	7	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	41	P5P	C5-C6-N1	-4.20	111.43	121.90
88	A7	48	P5P	C5-C6-N1	-4.20	111.43	121.90
87	A5	2	P5P	C5-C6-N1	-4.20	111.44	121.90
88	A7	24	Y5P	C5-C4-N3	4.20	120.92	114.15
88	A6	16	P5P	C5-C6-N1	-4.19	111.45	121.90
87	A5	11	P5P	C5-C6-N1	-4.19	111.46	121.90
88	A6	36	Y5P	C5-C4-N3	4.19	120.91	114.15
88	A7	71	P5P	C5-C6-N1	-4.19	111.46	121.90
88	A6	48	P5P	C5-C6-N1	-4.19	111.47	121.90
88	A7	64	Y5P	C5-C4-N3	4.19	120.90	114.15
88	A7	15	P5P	C5-C6-N1	-4.18	111.49	121.90
88	A6	15	P5P	C5-C6-N1	-4.17	111.50	121.90
88	A7	16	P5P	C5-C6-N1	-4.17	111.51	121.90
88	A6	34	P5P	C5-C6-N1	-4.17	111.51	121.90
88	A7	54	P5P	C5-C6-N1	-4.17	111.52	121.90
88	A6	4	P5P	C5-C6-N1	-4.17	111.52	121.90
88	A6	42	P5P	C5-C6-N1	-4.17	111.52	121.90
88	A6	13	Y5P	C5-C4-N3	4.16	120.85	114.15
88	A6	7	P5P	C5-C6-N1	-4.15	111.55	121.90
88	A6	23	P5P	C5-C6-N1	-4.15	111.55	121.90
88	A6	32	P5P	C5-C6-N1	-4.14	111.58	121.90
88	A6	54	P5P	C5-C6-N1	-4.13	111.60	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	10	P5P	C5-C6-N1	-4.13	111.61	121.90
88	A7	23	P5P	C5-C6-N1	-4.13	111.62	121.90
88	A7	43	P5P	C5-C6-N1	-4.12	111.63	121.90
88	A6	43	P5P	C5-C6-N1	-4.12	111.64	121.90
88	A7	20	P5P	C5-C6-N1	-4.10	111.69	121.90
88	A6	52	P5P	C5-C6-N1	-4.10	111.70	121.90
88	A6	35	Y5P	C5-C4-N3	4.09	120.75	114.15
88	A7	52	P5P	C5-C6-N1	-4.09	111.71	121.90
88	A7	13	Y5P	C5-C4-N3	4.06	120.69	114.15
88	A6	20	P5P	C5-C6-N1	-4.05	111.81	121.90
88	A6	2	P5P	C5-C6-N1	-3.92	112.14	121.90
88	A6	69	Y5P	O3'-C3'-C4'	3.27	120.46	111.08
88	A7	14	P5P	C6-C5-C4	3.15	119.68	116.24
88	A6	35	Y5P	O4'-C1'-N1	3.12	114.03	108.08
88	A6	14	P5P	C6-C5-C4	3.12	119.65	116.24
88	A6	68	Y5P	C1'-N1-C6	-3.07	114.27	120.77
88	A6	60	Y5P	O4'-C1'-N1	3.07	113.93	108.08
88	A7	45	P5P	C6-C5-C4	3.02	119.55	116.24
88	A6	69	Y5P	C2'-C1'-N1	-3.02	105.87	113.31
88	A7	60	Y5P	O4'-C1'-N1	3.02	113.84	108.08
88	A7	47	Y5P	O4'-C1'-N1	2.99	113.79	108.08
88	A7	59	Y5P	O4'-C1'-N1	2.97	113.75	108.08
88	A6	45	P5P	C6-C5-C4	2.93	119.45	116.24
88	A7	6	P5P	O4'-C1'-N9	2.93	113.71	108.09
88	A7	66	Y5P	O4'-C1'-N1	2.93	113.67	108.08
88	A6	55	Y5P	O4'-C1'-N1	2.93	113.67	108.08
88	A7	55	Y5P	O4'-C1'-N1	2.93	113.67	108.08
88	A6	68	Y5P	O4'-C1'-N1	2.92	113.65	108.08
88	A6	16	P5P	C1'-N9-C8	-2.90	120.65	127.09
88	A6	1	P5P	N1-C2-N3	-2.90	122.40	127.33
88	A7	16	P5P	C1'-N9-C8	-2.87	120.72	127.09
88	A6	41	P5P	C6-C5-C4	2.85	119.35	116.24
88	A7	53	Y5P	C1'-N1-C6	-2.83	114.78	120.77
87	A5	3	Y5P	O4'-C1'-N1	2.82	113.47	108.08
88	A7	3	Y5P	O4'-C1'-N1	2.82	113.46	108.08
88	A7	68	Y5P	C1'-N1-C6	-2.81	114.83	120.77
88	A7	56	Y5P	O4'-C1'-N1	2.81	113.44	108.08
88	A6	47	Y5P	O4'-C1'-N1	2.79	113.40	108.08
88	A7	57	Y5P	O4'-C1'-N1	2.79	113.40	108.08
88	A7	48	P5P	O4'-C1'-N9	2.77	113.42	108.09
88	A7	19	P5P	O4'-C1'-N9	2.77	113.41	108.09
88	A6	63	Y5P	O4'-C1'-N1	2.77	113.36	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	8	Y5P	O4'-C1'-N1	2.76	113.35	108.08
88	A6	59	Y5P	O4'-C1'-N1	2.74	113.31	108.08
88	A7	8	Y5P	O4'-C1'-N1	2.74	113.31	108.08
88	A6	29	Y5P	O4'-C1'-N1	2.73	113.29	108.08
88	A6	52	P5P	O4'-C1'-N9	2.73	113.33	108.09
88	A7	42	P5P	C6-C5-C4	2.72	119.22	116.24
88	A7	62	Y5P	O4'-C1'-N1	2.72	113.27	108.08
88	A6	40	P5P	C6-C5-C4	2.71	119.20	116.24
88	A6	61	Y5P	O4'-C1'-N1	2.70	113.24	108.08
88	A7	52	P5P	N1-C2-N3	-2.70	122.74	127.33
88	A6	56	Y5P	O4'-C1'-N1	2.70	113.23	108.08
88	A7	61	Y5P	O4'-C1'-N1	2.69	113.22	108.08
88	A6	52	P5P	N1-C2-N3	-2.68	122.78	127.33
88	A6	57	Y5P	O4'-C1'-N1	2.68	113.19	108.08
88	A7	12	Y5P	O4'-C1'-N1	2.67	113.18	108.08
88	A7	41	P5P	C6-C5-C4	2.67	119.16	116.24
88	A7	65	Y5P	O4'-C1'-N1	2.66	113.17	108.08
88	A7	2	P5P	N1-C2-N3	-2.66	122.81	127.33
88	A6	24	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A7	67	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A7	24	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A6	12	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A6	30	Y5P	O4'-C1'-N1	2.65	113.14	108.08
88	A7	43	P5P	N1-C2-N3	-2.65	122.83	127.33
88	A7	6	P5P	N1-C2-N3	-2.65	122.83	127.33
88	A7	52	P5P	O4'-C1'-N9	2.64	113.16	108.09
88	A7	40	P5P	C6-C5-C4	2.64	119.13	116.24
88	A6	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	A6	11	P5P	C6-C5-C4	2.64	119.12	116.24
88	A6	49	P5P	N1-C2-N3	-2.64	122.85	127.33
88	A6	25	Y5P	O4'-C1'-N1	2.63	113.10	108.08
88	A6	2	P5P	N1-C2-N3	-2.63	122.86	127.33
88	A6	28	P5P	N1-C2-N3	-2.63	122.87	127.33
88	A6	27	P5P	C6-C5-C4	2.62	119.11	116.24
88	A7	27	P5P	C6-C5-C4	2.62	119.11	116.24
88	A7	19	P5P	C6-C5-C4	2.62	119.11	116.24
88	A6	19	P5P	O4'-C1'-N9	2.62	113.11	108.09
88	A7	16	P5P	C4-N9-C1'	2.62	132.75	126.63
88	A7	18	P5P	N1-C2-N3	-2.61	122.89	127.33
87	A5	6	P5P	O3'-C3'-C2'	2.61	120.19	111.82
88	A6	5	P5P	C6-C5-C4	2.59	119.08	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	26	P5P	N1-C2-N3	-2.59	122.92	127.33
88	A6	66	Y5P	O4'-C1'-N1	2.59	113.03	108.08
88	A7	21	Y5P	O4'-C1'-N1	2.59	113.02	108.08
87	A5	9	P5P	C6-C5-C4	2.59	119.07	116.24
88	A6	49	P5P	O4'-C1'-N9	2.58	113.04	108.09
88	A7	7	P5P	N1-C2-N3	-2.58	122.95	127.33
88	A7	26	P5P	N1-C2-N3	-2.57	122.96	127.33
88	A7	2	P5P	C6-C5-C4	2.57	119.05	116.24
88	A7	25	Y5P	O4'-C1'-N1	2.57	112.98	108.08
88	A6	7	P5P	C6-C5-C4	2.57	119.05	116.24
88	A7	39	P5P	N1-C2-N3	-2.57	122.97	127.33
88	A7	37	Y5P	O4'-C1'-N1	2.56	112.98	108.08
88	A6	42	P5P	C6-C5-C4	2.56	119.05	116.24
88	A7	49	P5P	N1-C2-N3	-2.56	122.97	127.33
88	A6	36	Y5P	O4'-C1'-N1	2.56	112.97	108.08
88	A7	11	P5P	C6-C5-C4	2.56	119.04	116.24
87	A5	10	Y5P	O4'-C1'-N1	2.55	112.95	108.08
87	A5	6	P5P	C6-C5-C4	2.55	119.03	116.24
88	A7	5	P5P	C6-C5-C4	2.55	119.03	116.24
88	A6	39	P5P	N1-C2-N3	-2.55	123.00	127.33
88	A6	27	P5P	N1-C2-N3	-2.55	123.00	127.33
88	A7	27	P5P	N1-C2-N3	-2.54	123.00	127.33
88	A6	31	Y5P	O4'-C1'-N1	2.54	112.94	108.08
88	A7	15	P5P	C6-C5-C4	2.54	119.02	116.24
88	A6	19	P5P	C6-C5-C4	2.54	119.02	116.24
88	A6	15	P5P	C6-C5-C4	2.53	119.01	116.24
88	A7	46	Y5P	O4'-C1'-N1	2.53	112.91	108.08
88	A7	49	P5P	C6-C5-C4	2.53	119.01	116.24
87	A5	11	P5P	C6-C5-C4	2.52	119.00	116.24
87	A5	2	P5P	C6-C5-C4	2.52	118.99	116.24
87	A5	5	P5P	C6-C5-C4	2.52	118.99	116.24
88	A7	5	P5P	N1-C2-N3	-2.51	123.06	127.33
88	A6	62	Y5P	O4'-C1'-N1	2.51	112.87	108.08
88	A7	45	P5P	N1-C2-N3	-2.50	123.08	127.33
88	A6	49	P5P	C6-C5-C4	2.50	118.98	116.24
88	A6	48	P5P	O4'-C1'-N9	2.50	112.89	108.09
88	A6	43	P5P	N1-C2-N3	-2.50	123.08	127.33
88	A6	16	P5P	C6-C5-C4	2.49	118.96	116.24
88	A7	20	P5P	N1-C2-N3	-2.49	123.10	127.33
88	A6	20	P5P	N1-C2-N3	-2.49	123.10	127.33
88	A6	69	Y5P	O4'-C1'-N1	2.49	112.82	108.08
88	A6	28	P5P	C6-C5-C4	2.48	118.95	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	3	Y5P	O4'-C1'-N1	2.48	112.81	108.08
88	A6	15	P5P	O4'-C1'-N9	2.48	112.84	108.09
88	A6	46	Y5P	O4'-C1'-N1	2.47	112.80	108.08
88	A6	4	P5P	C6-C5-C4	2.47	118.94	116.24
88	A6	6	P5P	C6-C5-C4	2.47	118.94	116.24
88	A6	40	P5P	O4'-C1'-N9	2.46	112.82	108.09
88	A7	10	P5P	N1-C2-N3	-2.46	123.14	127.33
88	A6	6	P5P	N1-C2-N3	-2.46	123.14	127.33
88	A6	10	P5P	C6-C5-C4	2.46	118.93	116.24
88	A6	10	P5P	N1-C2-N3	-2.46	123.15	127.33
88	A6	37	Y5P	O4'-C1'-N1	2.45	112.77	108.08
88	A7	11	P5P	N1-C2-N3	-2.45	123.17	127.33
88	A7	16	P5P	C6-C5-C4	2.44	118.91	116.24
88	A7	18	P5P	C6-C5-C4	2.44	118.91	116.24
88	A7	40	P5P	N1-C2-N3	-2.43	123.20	127.33
88	A6	33	Y5P	O4'-C1'-N1	2.43	112.72	108.08
88	A6	51	Y5P	N1-C2-N3	-2.43	118.66	125.39
88	A6	11	P5P	N1-C2-N3	-2.42	123.22	127.33
88	A7	40	P5P	O4'-C1'-N9	2.42	112.73	108.09
88	A6	32	P5P	C6-C5-C4	2.41	118.88	116.24
88	A7	38	Y5P	O4'-C1'-N1	2.41	112.67	108.08
88	A6	26	P5P	C6-C5-C4	2.41	118.87	116.24
88	A7	9	Y5P	N1-C2-N3	-2.40	118.72	125.39
88	A6	44	Y5P	N1-C2-N3	-2.40	118.73	125.39
88	A6	7	P5P	N1-C2-N3	-2.40	123.25	127.33
88	A7	49	P5P	O4'-C1'-N9	2.40	112.70	108.09
88	A7	51	Y5P	N1-C2-N3	-2.40	118.73	125.39
88	A6	18	P5P	N1-C2-N3	-2.40	123.25	127.33
88	A7	58	Y5P	O4'-C1'-N1	2.40	112.65	108.08
88	A6	71	P5P	C6-C5-C4	2.39	118.86	116.24
88	A7	69	Y5P	O4'-C1'-N1	2.39	112.64	108.08
88	A7	10	P5P	C6-C5-C4	2.39	118.85	116.24
88	A6	34	P5P	C6-C5-C4	2.38	118.84	116.24
88	A6	23	P5P	C6-C5-C4	2.38	118.84	116.24
88	A7	1	P5P	C6-C5-C4	2.38	118.84	116.24
88	A6	38	Y5P	O4'-C1'-N1	2.38	112.62	108.08
88	A7	7	P5P	C6-C5-C4	2.38	118.84	116.24
88	A7	4	P5P	O4'-C1'-N9	2.37	112.65	108.09
88	A7	22	Y5P	O4'-C1'-N1	2.37	112.60	108.08
88	A7	48	P5P	N1-C2-N3	-2.36	123.31	127.33
87	A5	1	Y5P	N1-C2-N3	-2.36	118.84	125.39
88	A7	6	P5P	C6-C5-C4	2.36	118.82	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	64	Y5P	O4'-C1'-N1	2.36	112.58	108.08
88	A7	20	P5P	C6-C5-C4	2.35	118.81	116.24
88	A6	67	Y5P	O4'-C1'-N1	2.35	112.57	108.08
88	A6	65	Y5P	O4'-C1'-N1	2.35	112.57	108.08
87	A5	4	Y5P	N1-C2-N3	-2.34	118.89	125.39
87	A5	2	P5P	N1-C2-N3	-2.34	123.35	127.33
88	A7	26	P5P	C6-C5-C4	2.34	118.80	116.24
88	A6	40	P5P	N1-C2-N3	-2.33	123.37	127.33
88	A7	19	P5P	N1-C2-N3	-2.33	123.37	127.33
88	A7	51	Y5P	O4'-C1'-N1	2.33	112.52	108.08
88	A6	22	Y5P	O4'-C1'-N1	2.32	112.51	108.08
88	A6	68	Y5P	N1-C2-N3	-2.32	118.96	125.39
88	A6	48	P5P	N1-C2-N3	-2.32	123.39	127.33
88	A7	1	P5P	N1-C2-N3	-2.31	123.40	127.33
88	A6	23	P5P	N1-C2-N3	-2.31	123.40	127.33
88	A6	9	Y5P	N1-C2-N3	-2.31	118.98	125.39
88	A7	53	Y5P	N1-C2-N3	-2.30	119.01	125.39
87	A5	3	Y5P	N1-C2-N3	-2.30	119.02	125.39
88	A6	20	P5P	O4'-C1'-N9	2.29	112.49	108.09
88	A6	45	P5P	N1-C2-N3	-2.29	123.44	127.33
88	A7	43	P5P	C6-C5-C4	2.29	118.74	116.24
88	A7	71	P5P	C6-C5-C4	2.29	118.74	116.24
88	A6	19	P5P	N1-C2-N3	-2.29	123.44	127.33
88	A6	65	Y5P	N1-C2-N3	-2.28	119.06	125.39
88	A6	53	Y5P	N1-C2-N3	-2.28	119.06	125.39
88	A6	18	P5P	C6-C5-C4	2.28	118.73	116.24
88	A6	71	P5P	N1-C2-N3	-2.28	123.46	127.33
88	A7	41	P5P	O4'-C1'-N9	2.27	112.46	108.09
88	A6	21	Y5P	O4'-C1'-N1	2.27	112.42	108.08
88	A7	39	P5P	C6-C5-C4	2.27	118.73	116.24
88	A7	23	P5P	C6-C5-C4	2.27	118.72	116.24
88	A6	15	P5P	N1-C2-N3	-2.27	123.47	127.33
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	A6	52	P5P	C6-C5-C4	2.26	118.72	116.24
88	A7	4	P5P	N1-C2-N3	-2.26	123.49	127.33
88	A6	2	P5P	C6-C5-C4	2.26	118.71	116.24
87	A5	6	P5P	N1-C2-N3	-2.25	123.50	127.33
88	A6	39	P5P	C6-C5-C4	2.25	118.70	116.24
88	A6	50	Y5P	N1-C2-N3	-2.25	119.16	125.39
88	A7	71	P5P	N1-C2-N3	-2.24	123.52	127.33
88	A7	68	Y5P	O4'-C1'-N1	2.24	112.36	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	58	Y5P	O4'-C1'-N1	2.24	112.36	108.08
88	A7	68	Y5P	N1-C2-N3	-2.24	119.18	125.39
88	A6	30	Y5P	N1-C2-N3	-2.24	119.18	125.39
88	A6	43	P5P	C6-C5-C4	2.24	118.69	116.24
88	A7	16	P5P	N1-C2-N3	-2.24	123.53	127.33
88	A6	16	P5P	N1-C2-N3	-2.23	123.53	127.33
88	A7	54	P5P	N1-C2-N3	-2.23	123.53	127.33
88	A6	20	P5P	C6-C5-C4	2.23	118.68	116.24
87	A5	7	Y5P	O4'-C1'-N1	2.23	112.33	108.08
88	A7	44	Y5P	N1-C2-N3	-2.23	119.21	125.39
88	A7	15	P5P	N1-C2-N3	-2.23	123.55	127.33
88	A6	3	Y5P	N1-C2-N3	-2.23	119.22	125.39
87	A5	7	Y5P	N1-C2-N3	-2.22	119.22	125.39
88	A7	50	Y5P	N1-C2-N3	-2.22	119.22	125.39
88	A6	62	Y5P	N1-C2-N3	-2.22	119.23	125.39
88	A7	64	Y5P	O4'-C1'-N1	2.22	112.32	108.08
88	A6	51	Y5P	O4'-C1'-N1	2.22	112.31	108.08
88	A6	63	Y5P	N1-C2-N3	-2.21	119.26	125.39
88	A7	15	P5P	O4'-C1'-N9	2.20	112.31	108.09
88	A6	46	Y5P	N1-C2-N3	-2.20	119.29	125.39
88	A7	46	Y5P	N1-C2-N3	-2.20	119.30	125.39
88	A6	41	P5P	O4'-C1'-N9	2.20	112.31	108.09
88	A6	47	Y5P	N1-C2-N3	-2.19	119.32	125.39
88	A6	64	Y5P	N1-C2-N3	-2.19	119.32	125.39
88	A6	67	Y5P	N1-C2-N3	-2.18	119.33	125.39
88	A7	20	P5P	O4'-C1'-N9	2.18	112.28	108.09
87	A5	11	P5P	N1-C2-N3	-2.18	123.62	127.33
88	A6	60	Y5P	N1-C2-N3	-2.18	119.35	125.39
88	A7	69	Y5P	N1-C2-N3	-2.18	119.35	125.39
88	A7	52	P5P	C6-C5-C4	2.18	118.62	116.24
88	A6	66	Y5P	N1-C2-N3	-2.18	119.35	125.39
88	A6	54	P5P	N1-C2-N3	-2.18	123.63	127.33
87	A5	8	Y5P	O4'-C1'-N1	2.17	112.23	108.08
88	A7	70	Y5P	N1-C2-N3	-2.16	119.39	125.39
88	A7	8	Y5P	N1-C2-N3	-2.16	119.39	125.39
87	A5	8	Y5P	N1-C2-N3	-2.16	119.39	125.39
88	A6	17	Y5P	N1-C2-N3	-2.16	119.39	125.39
88	A7	17	Y5P	N1-C2-N3	-2.16	119.40	125.39
88	A7	63	Y5P	N1-C2-N3	-2.16	119.40	125.39
87	A5	9	P5P	N1-C2-N3	-2.16	123.66	127.33
88	A6	48	P5P	C6-C5-C4	2.16	118.60	116.24
88	A6	70	Y5P	N1-C2-N3	-2.15	119.42	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	A5	5	P5P	N1-C2-N3	-2.15	123.68	127.33
88	A7	39	P5P	O4'-C1'-N9	2.15	112.21	108.09
88	A6	29	Y5P	N1-C2-N3	-2.14	119.45	125.39
88	A6	69	Y5P	O3'-C3'-C2'	-2.14	104.96	111.82
88	A6	21	Y5P	N1-C2-N3	-2.14	119.47	125.39
88	A7	62	Y5P	N1-C2-N3	-2.14	119.47	125.39
88	A7	55	Y5P	N1-C2-N3	-2.13	119.47	125.39
88	A7	37	Y5P	N1-C2-N3	-2.13	119.47	125.39
88	A7	3	Y5P	N1-C2-N3	-2.13	119.47	125.39
88	A6	55	Y5P	N1-C2-N3	-2.13	119.47	125.39
88	A7	42	P5P	N1-C2-N3	-2.13	123.71	127.33
87	A5	10	Y5P	N1-C2-N3	-2.13	119.49	125.39
88	A6	61	Y5P	N1-C2-N3	-2.13	119.49	125.39
88	A6	13	Y5P	O4'-C1'-N1	2.13	112.14	108.08
88	A6	53	Y5P	C1'-N1-C6	-2.12	116.28	120.77
88	A7	47	Y5P	N1-C2-N3	-2.12	119.50	125.39
88	A6	35	Y5P	N1-C2-N3	-2.12	119.51	125.39
88	A6	37	Y5P	N1-C2-N3	-2.12	119.52	125.39
88	A6	56	Y5P	N1-C2-N3	-2.12	119.52	125.39
88	A6	39	P5P	O4'-C1'-N9	2.12	112.15	108.09
88	A7	48	P5P	C6-C5-C4	2.12	118.56	116.24
88	A7	21	Y5P	N1-C2-N3	-2.11	119.53	125.39
88	A6	31	Y5P	N1-C2-N3	-2.11	119.53	125.39
88	A7	59	Y5P	N1-C2-N3	-2.11	119.55	125.39
88	A6	53	Y5P	O4'-C1'-N1	2.10	112.09	108.08
88	A6	36	Y5P	N1-C2-N3	-2.10	119.56	125.39
88	A6	4	P5P	O4'-C1'-N9	2.10	112.12	108.09
88	A6	42	P5P	N1-C2-N3	-2.10	123.77	127.33
88	A6	69	Y5P	C6-N1-C2	2.10	123.06	118.65
88	A6	32	P5P	N1-C2-N3	-2.10	123.77	127.33
88	A7	56	Y5P	N1-C2-N3	-2.10	119.58	125.39
87	A5	11	P5P	O4'-C1'-N9	2.09	112.11	108.09
88	A6	59	Y5P	N1-C2-N3	-2.09	119.59	125.39
88	A6	9	Y5P	C2'-C1'-N1	2.09	118.43	113.31
88	A6	1	P5P	C6-C5-C4	2.08	118.52	116.24
88	A6	4	P5P	N1-C2-N3	-2.08	123.80	127.33
88	A6	26	P5P	O4'-C1'-N9	2.08	112.08	108.09
88	A7	26	P5P	O4'-C1'-N9	2.08	112.08	108.09
88	A7	65	Y5P	N1-C2-N3	-2.08	119.63	125.39
88	A7	61	Y5P	N1-C2-N3	-2.07	119.64	125.39
88	A7	67	Y5P	N1-C2-N3	-2.07	119.64	125.39
88	A6	5	P5P	N1-C2-N3	-2.07	123.81	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A6	33	Y5P	N1-C2-N3	-2.06	119.66	125.39
88	A6	58	Y5P	N1-C2-N3	-2.06	119.67	125.39
88	A7	25	Y5P	N1-C2-N3	-2.05	119.72	125.39
88	A6	54	P5P	C6-C5-C4	2.04	118.47	116.24
88	A6	34	P5P	N1-C2-N3	-2.04	123.87	127.33
88	A7	57	Y5P	N1-C2-N3	-2.04	119.74	125.39
88	A7	12	Y5P	N1-C2-N3	-2.04	119.74	125.39
88	A6	12	Y5P	N1-C2-N3	-2.03	119.77	125.39
88	A6	25	Y5P	N1-C2-N3	-2.03	119.77	125.39
88	A7	22	Y5P	N1-C2-N3	-2.03	119.77	125.39
88	A7	11	P5P	O4'-C1'-N9	2.02	111.98	108.09
88	A7	41	P5P	N1-C2-N3	-2.02	123.89	127.33
88	A6	8	Y5P	N1-C2-N3	-2.02	119.79	125.39
88	A7	58	Y5P	N1-C2-N3	-2.01	119.81	125.39
88	A6	22	Y5P	N1-C2-N3	-2.01	119.82	125.39
88	A6	57	Y5P	N1-C2-N3	-2.01	119.82	125.39
88	A6	38	Y5P	N1-C2-N3	-2.00	119.83	125.39
88	A7	38	Y5P	N1-C2-N3	-2.00	119.83	125.39

There are no chirality outliers.

All (230) 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	A6	9	Y5P	C2'-C1'-N1-C2
88	A7	9	Y5P	C2'-C1'-N1-C2
88	A6	14	P5P	O4'-C4'-C5'-O5'
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	A6	24	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
88	A7	24	Y5P	O4'-C1'-N1-C2
88	A6	25	Y5P	O4'-C1'-N1-C2
88	A7	25	Y5P	O4'-C1'-N1-C2
88	A6	29	Y5P	O4'-C1'-N1-C2
88	A6	30	Y5P	O4'-C1'-N1-C2
88	A6	33	Y5P	O4'-C1'-N1-C2
88	A6	35	Y5P	O4'-C1'-N1-C2
88	A6	37	Y5P	O4'-C1'-N1-C2
88	A7	37	Y5P	O4'-C1'-N1-C2
88	A6	43	P5P	O4'-C4'-C5'-O5'
88	A6	43	P5P	C4'-C5'-O5'-P
88	A7	43	P5P	O4'-C4'-C5'-O5'
88	A7	43	P5P	C4'-C5'-O5'-P
88	A6	46	Y5P	O4'-C4'-C5'-O5'
88	A6	46	Y5P	O4'-C1'-N1-C2
88	A7	46	Y5P	O4'-C4'-C5'-O5'
88	A7	46	Y5P	O4'-C1'-N1-C2
88	A6	51	Y5P	O4'-C1'-N1-C2
88	A7	51	Y5P	O4'-C1'-N1-C2
88	A6	52	P5P	O4'-C4'-C5'-O5'
88	A7	52	P5P	O4'-C4'-C5'-O5'
88	A6	57	Y5P	O4'-C1'-N1-C2
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	A6	67	Y5P	O4'-C1'-N1-C2
88	A6	69	Y5P	C3'-C4'-C5'-O5'
88	A6	71	P5P	C4'-C5'-O5'-P
88	A7	71	P5P	C4'-C5'-O5'-P
87	A5	10	Y5P	O4'-C1'-N1-C2
88	A6	3	Y5P	O4'-C1'-N1-C2
88	A6	8	Y5P	O4'-C1'-N1-C2
88	A7	8	Y5P	O4'-C1'-N1-C2
88	A6	12	Y5P	O4'-C1'-N1-C2
88	A7	12	Y5P	O4'-C1'-N1-C2
88	A6	13	Y5P	O4'-C1'-N1-C2
88	A7	13	Y5P	O4'-C1'-N1-C2
88	A6	21	Y5P	O4'-C1'-N1-C2
88	A7	21	Y5P	O4'-C1'-N1-C2
88	A6	22	Y5P	O4'-C1'-N1-C2
88	A7	22	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
88	A6	31	Y5P	O4'-C1'-N1-C2
88	A6	36	Y5P	O4'-C1'-N1-C2
88	A6	38	Y5P	O4'-C1'-N1-C2
88	A7	38	Y5P	O4'-C1'-N1-C2
88	A6	47	Y5P	O4'-C1'-N1-C2
88	A7	47	Y5P	O4'-C1'-N1-C2
88	A6	50	Y5P	O4'-C1'-N1-C2
88	A7	50	Y5P	O4'-C1'-N1-C2
88	A6	55	Y5P	O4'-C1'-N1-C2
88	A7	55	Y5P	O4'-C1'-N1-C2
88	A6	56	Y5P	O4'-C1'-N1-C2
88	A7	56	Y5P	O4'-C1'-N1-C2
88	A6	58	Y5P	O4'-C1'-N1-C2
88	A7	58	Y5P	O4'-C1'-N1-C2
88	A6	59	Y5P	O4'-C1'-N1-C2
88	A7	59	Y5P	O4'-C1'-N1-C2
88	A6	60	Y5P	O4'-C1'-N1-C2
88	A7	60	Y5P	O4'-C1'-N1-C2
88	A6	61	Y5P	O4'-C1'-N1-C2
88	A6	62	Y5P	O4'-C1'-N1-C2
88	A6	63	Y5P	O4'-C1'-N1-C2
88	A6	64	Y5P	O4'-C1'-N1-C2
88	A7	64	Y5P	O4'-C1'-N1-C2
88	A6	65	Y5P	O4'-C1'-N1-C2
88	A7	65	Y5P	O4'-C1'-N1-C2
88	A6	66	Y5P	O4'-C1'-N1-C2
88	A7	66	Y5P	O4'-C1'-N1-C2
88	A6	69	Y5P	O4'-C1'-N1-C2
88	A7	69	Y5P	O4'-C1'-N1-C2
88	A6	9	Y5P	C2'-C1'-N1-C6
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	A6	14	P5P	C3'-C4'-C5'-O5'
88	A7	14	P5P	C3'-C4'-C5'-O5'
88	A7	16	P5P	C3'-C4'-C5'-O5'
88	A6	21	Y5P	O4'-C4'-C5'-O5'
88	A6	21	Y5P	C3'-C4'-C5'-O5'
88	A6	22	Y5P	O4'-C4'-C5'-O5'
88	A6	22	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
88	A7	22	Y5P	C3'-C4'-C5'-O5'
88	A6	43	P5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	C3'-C4'-C5'-O5'
88	A7	45	P5P	C3'-C4'-C5'-O5'
88	A6	46	Y5P	C3'-C4'-C5'-O5'
88	A7	46	Y5P	C3'-C4'-C5'-O5'
88	A6	52	P5P	C3'-C4'-C5'-O5'
88	A7	52	P5P	C3'-C4'-C5'-O5'
88	A6	52	P5P	O4'-C1'-N9-C8
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	A6	6	P5P	C3'-C4'-C5'-O5'
88	A6	7	P5P	C3'-C4'-C5'-O5'
88	A6	7	P5P	O4'-C4'-C5'-O5'
88	A6	9	Y5P	O4'-C4'-C5'-O5'
88	A6	9	Y5P	C3'-C4'-C5'-O5'
88	A6	16	P5P	C3'-C4'-C5'-O5'
88	A6	28	P5P	O4'-C4'-C5'-O5'
88	A6	33	Y5P	O4'-C4'-C5'-O5'
88	A6	33	Y5P	C3'-C4'-C5'-O5'
88	A6	45	P5P	C3'-C4'-C5'-O5'
88	A6	45	P5P	O4'-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	A6	69	Y5P	O4'-C4'-C5'-O5'
88	A6	70	Y5P	O4'-C4'-C5'-O5'
88	A6	70	Y5P	C3'-C4'-C5'-O5'
88	A6	52	P5P	O4'-C1'-N9-C4
88	A7	52	P5P	O4'-C1'-N9-C4
88	A7	67	Y5P	O4'-C1'-N1-C2
88	A7	70	Y5P	O4'-C1'-N1-C2
88	A6	68	Y5P	O4'-C1'-N1-C6
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	A6	6	P5P	O4'-C4'-C5'-O5'
88	A7	6	P5P	O4'-C4'-C5'-O5'
88	A7	7	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
88	A6	13	Y5P	C3'-C4'-C5'-O5'
88	A6	50	Y5P	C3'-C4'-C5'-O5'
88	A6	50	Y5P	C4'-C5'-O5'-P
88	A7	50	Y5P	C4'-C5'-O5'-P
88	A6	16	P5P	O4'-C4'-C5'-O5'
88	A7	16	P5P	O4'-C4'-C5'-O5'
88	A6	56	Y5P	O4'-C4'-C5'-O5'
88	A7	70	Y5P	O4'-C4'-C5'-O5'
88	A6	18	P5P	C4'-C5'-O5'-P
88	A7	12	Y5P	C3'-C4'-C5'-O5'
88	A7	50	Y5P	C3'-C4'-C5'-O5'
88	A6	70	Y5P	O4'-C1'-N1-C2
88	A6	28	P5P	C3'-C4'-C5'-O5'
88	A7	70	Y5P	C3'-C4'-C5'-O5'
88	A7	18	P5P	C4'-C5'-O5'-P
88	A6	55	Y5P	O4'-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	A6	53	Y5P	C3'-C4'-C5'-O5'
88	A6	56	Y5P	C3'-C4'-C5'-O5'
88	A7	64	Y5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	C2'-C1'-N9-C8
88	A6	5	P5P	C3'-C4'-C5'-O5'
88	A6	58	Y5P	C3'-C4'-C5'-O5'
88	A7	12	Y5P	O4'-C4'-C5'-O5'
88	A6	53	Y5P	O4'-C1'-N1-C6
88	A6	17	Y5P	C4'-C5'-O5'-P
88	A6	51	Y5P	C4'-C5'-O5'-P
88	A7	54	P5P	C4'-C5'-O5'-P
88	A7	56	Y5P	C4'-C5'-O5'-P
88	A6	50	Y5P	O4'-C4'-C5'-O5'
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

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Mol	Chain	Res	Type	Atoms
88	A6	54	P5P	C4'-C5'-O5'-P
88	A6	13	Y5P	O4'-C4'-C5'-O5'
88	A7	38	Y5P	C3'-C4'-C5'-O5'
88	A6	9	Y5P	O4'-C1'-N1-C2
88	A7	68	Y5P	O4'-C1'-N1-C6
88	A6	56	Y5P	C4'-C5'-O5'-P
88	A6	12	Y5P	C3'-C4'-C5'-O5'
88	A7	9	Y5P	O4'-C1'-N1-C2
88	A7	17	Y5P	O4'-C1'-N1-C2
88	A6	17	Y5P	O4'-C1'-N1-C2
88	A7	44	Y5P	O4'-C1'-N1-C2
88	A7	65	Y5P	C4'-C5'-O5'-P
88	A6	6	P5P	C4'-C5'-O5'-P
88	A6	52	P5P	C4'-C5'-O5'-P
88	A6	60	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	A6	44	Y5P	O4'-C1'-N1-C2
88	A7	44	Y5P	C2'-C1'-N1-C2
88	A7	52	P5P	C4'-C5'-O5'-P
88	A6	7	P5P	C4'-C5'-O5'-P
88	A7	5	P5P	O4'-C4'-C5'-O5'
88	A6	53	Y5P	O4'-C4'-C5'-O5'
88	A6	5	P5P	O4'-C4'-C5'-O5'
88	A6	17	Y5P	C2'-C1'-N1-C2
88	A7	6	P5P	C2'-C1'-N9-C8
87	A5	3	Y5P	C2'-C1'-N1-C2
88	A6	44	Y5P	C2'-C1'-N1-C2
88	A6	55	Y5P	C3'-C4'-C5'-O5'
88	A6	43	P5P	C2'-C1'-N9-C8
88	A7	53	Y5P	O4'-C1'-N1-C2
88	A6	2	P5P	O4'-C4'-C5'-O5'
88	A7	56	Y5P	C3'-C4'-C5'-O5'
88	A7	43	P5P	O4'-C1'-N9-C8
88	A6	52	P5P	C2'-C1'-N9-C8
88	A7	52	P5P	C2'-C1'-N9-C8
88	A6	58	Y5P	O4'-C4'-C5'-O5'
88	A6	12	Y5P	O4'-C4'-C5'-O5'
88	A7	27	P5P	C3'-C4'-C5'-O5'
88	A7	53	Y5P	C3'-C4'-C5'-O5'

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

There are no ring outliers.

45 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A6	70	Y5P	12	0
88	A6	61	Y5P	1	0
88	A6	25	Y5P	2	0
88	A7	24	Y5P	1	0
88	A7	21	Y5P	2	0
88	A6	24	Y5P	1	0
88	A6	71	P5P	1	0
87	A5	1	Y5P	2	0
88	A6	36	Y5P	13	0
88	A6	69	Y5P	23	0
88	A6	20	P5P	1	0
88	A7	64	Y5P	3	0
88	A7	63	Y5P	1	0
88	A6	63	Y5P	1	0
88	A6	22	Y5P	1	0
88	A6	12	Y5P	1	0
87	A5	2	P5P	7	0
88	A6	21	Y5P	2	0
88	A7	48	P5P	1	0
88	A7	25	Y5P	1	0
88	A6	68	Y5P	4	0
88	A7	13	Y5P	1	0
88	A7	62	Y5P	1	0
88	A7	65	Y5P	2	0
87	A5	3	Y5P	6	0
88	A7	57	Y5P	1	0
88	A7	71	P5P	27	0
88	A7	61	Y5P	1	0
87	A5	8	Y5P	1	0
88	A7	70	Y5P	1	0
88	A7	12	Y5P	1	0
88	A6	31	Y5P	5	0
87	A5	7	Y5P	1	0
88	A6	34	P5P	4	0
88	A7	59	Y5P	1	0
87	A5	4	Y5P	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A7	58	Y5P	1	0
88	A7	60	Y5P	1	0
88	A6	27	P5P	2	0
87	A5	11	P5P	6	0
88	A7	20	P5P	1	0
88	A6	35	Y5P	9	0
88	A6	62	Y5P	2	0
88	A7	47	Y5P	1	0
88	A7	22	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	$\# Z > 2$
91	GDP	AX	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
92	GCP	v	802	89	32,34,34	1.67	6 (18%)	49,54,54	1.87	10 (20%)

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
91	GDP	AX	500	-	-	1/16/32/32	0/3/3/3
92	GCP	v	802	89	-	5/19/38/38	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	5.57	1.61	1.50
91	AX	500	GDP	C5-C4	3.18	1.47	1.38
92	v	802	GCP	C5-C4	3.05	1.47	1.38
92	v	802	GCP	PG-O3G	3.04	1.61	1.55
92	v	802	GCP	PG-O2G	-2.64	1.49	1.55
91	AX	500	GDP	C6-N1	-2.38	1.34	1.38
92	v	802	GCP	C4-N9	-2.23	1.32	1.38
92	v	802	GCP	PB-O2B	2.20	1.61	1.56
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	-6.32	118.32	128.39
92	v	802	GCP	PB-O3A-PA	-5.90	113.11	132.37
91	AX	500	GDP	C2-N3-C4	5.20	121.25	112.30
92	v	802	GCP	C2-N3-C4	4.83	120.62	112.30
92	v	802	GCP	C5-C4-N3	-4.69	120.92	128.39
91	AX	500	GDP	N9-C4-N3	4.66	135.26	125.95
92	v	802	GCP	C6-C5-N7	4.14	137.82	130.29
92	v	802	GCP	N9-C4-N3	3.22	132.39	125.95
91	AX	500	GDP	C6-C5-N7	3.15	136.03	130.29
92	v	802	GCP	O4'-C1'-N9	2.57	114.18	108.36
91	AX	500	GDP	C4-C5-N7	-2.57	106.60	110.67
92	v	802	GCP	C6-C5-C4	-2.37	115.26	118.83
92	v	802	GCP	C4-C5-N7	-2.37	106.91	110.67
91	AX	500	GDP	C3'-C2'-C1'	2.37	105.95	101.46
92	v	802	GCP	C1'-N9-C4	-2.22	119.94	126.49
92	v	802	GCP	O6-C6-C5	-2.11	120.97	126.53
91	AX	500	GDP	O6-C6-C5	-2.11	120.97	126.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

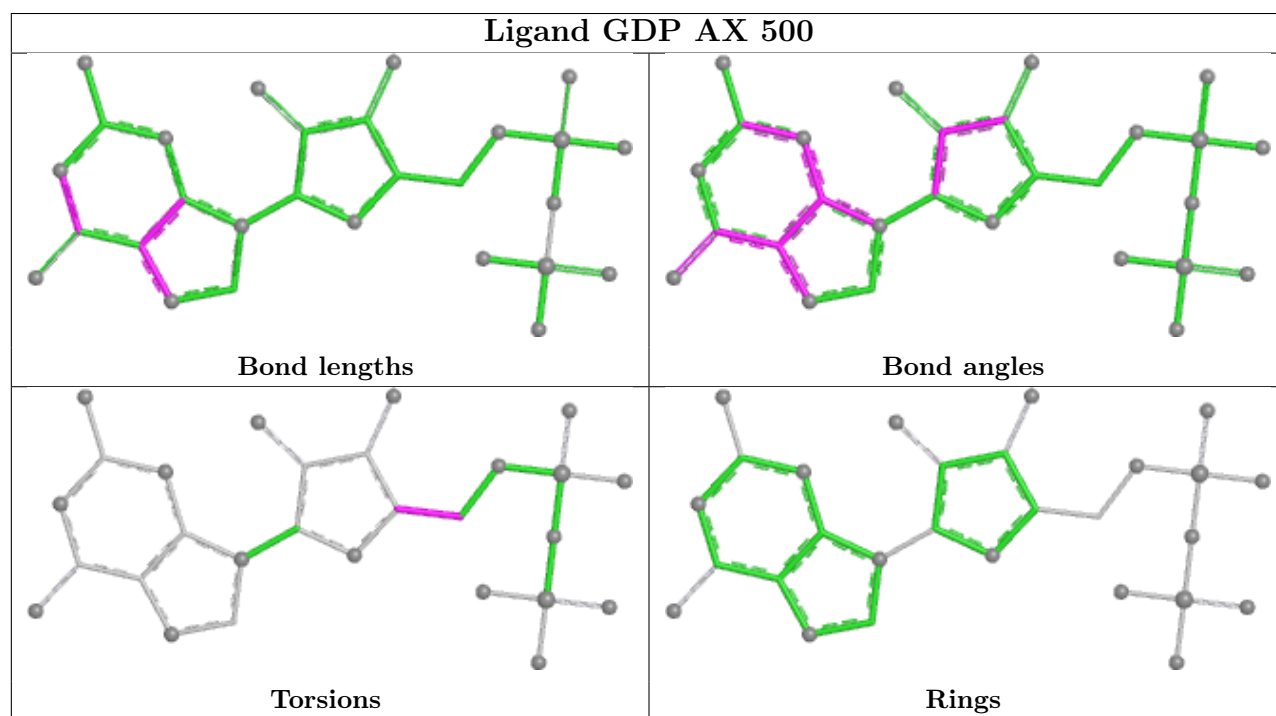
Mol	Chain	Res	Type	Atoms
92	v	802	GCP	PG-C3B-PB-O1B
92	v	802	GCP	PG-C3B-PB-O3A
92	v	802	GCP	O4'-C4'-C5'-O5'
92	v	802	GCP	C3'-C4'-C5'-O5'
92	v	802	GCP	PG-C3B-PB-O2B
91	AX	500	GDP	C3'-C4'-C5'-O5'

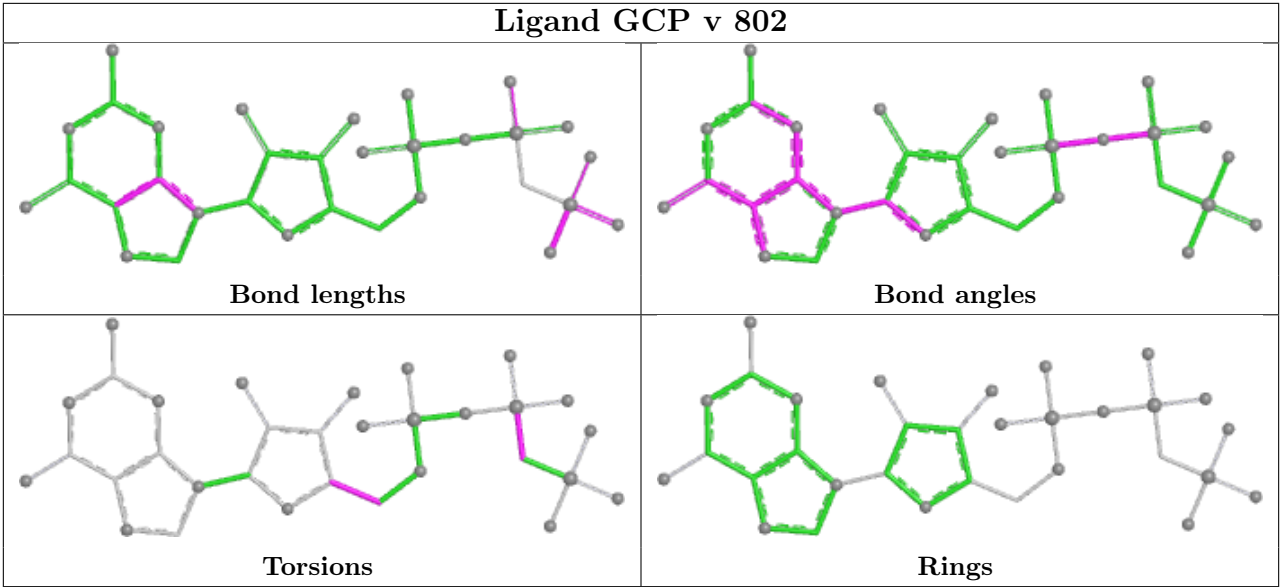
There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	AX	500	GDP	3	0
92	v	802	GCP	44	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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	30.88
1	u	315:UNK	C	399:UNK	N	19.09
1	u	615:UNK	C	700:UNK	N	18.25

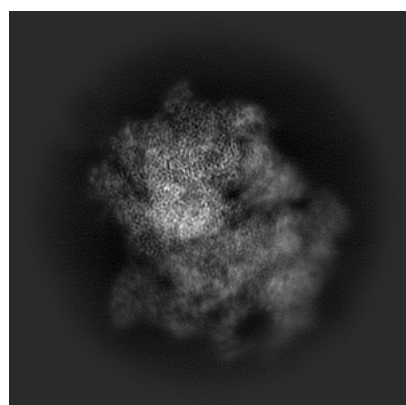
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21242. These allow visual inspection of the internal detail of the map and identification of artifacts.

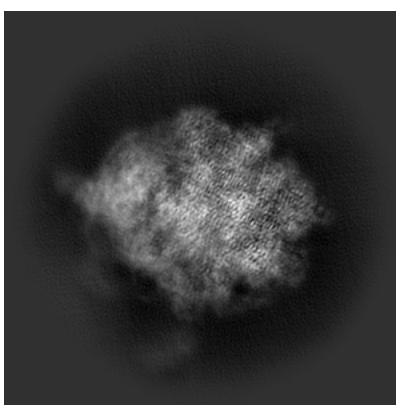
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

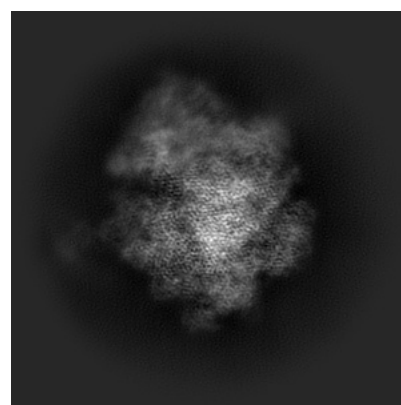
6.1.1 Primary map



X



Y

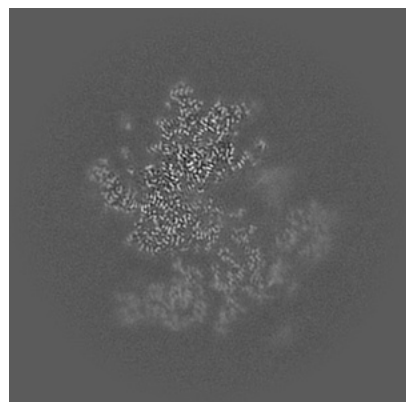


Z

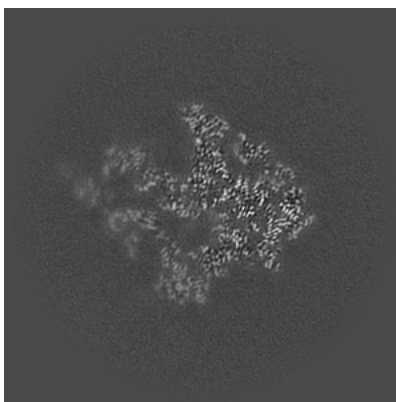
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

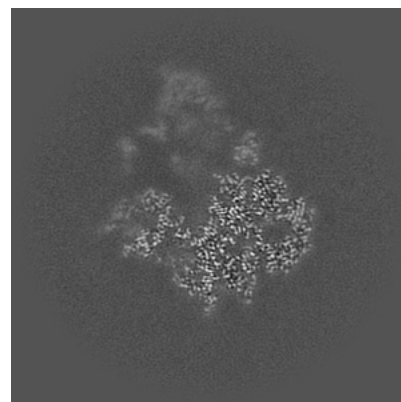
6.2.1 Primary map



X Index: 200



Y Index: 200

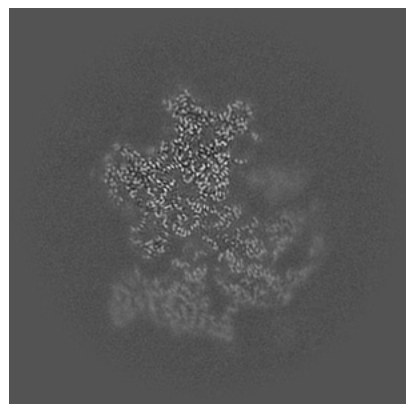


Z Index: 200

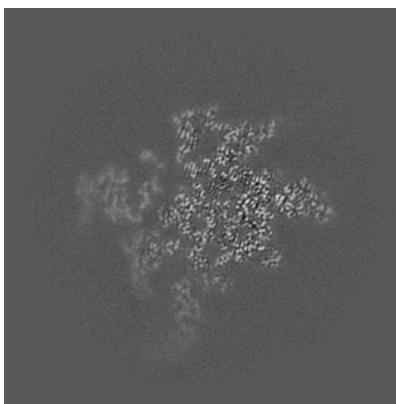
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

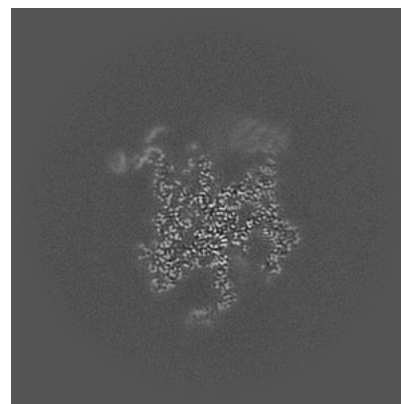
6.3.1 Primary map



X Index: 210



Y Index: 172

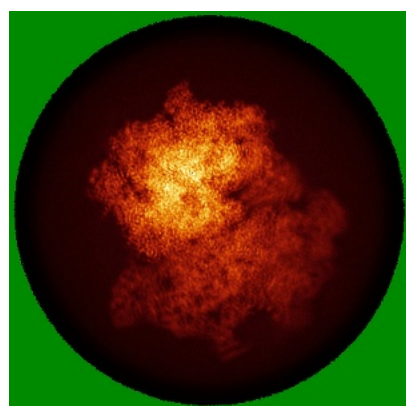


Z Index: 242

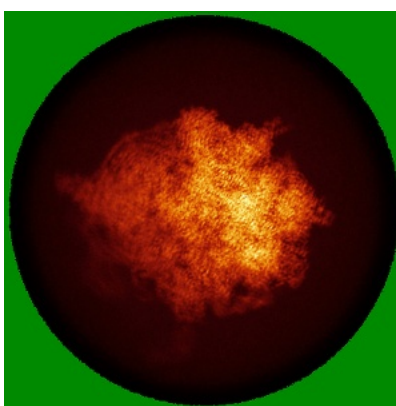
The images above show the largest variance slices of the map in three orthogonal directions.

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

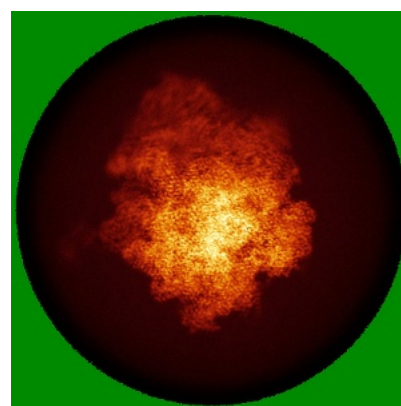
6.4.1 Primary map



X



Y

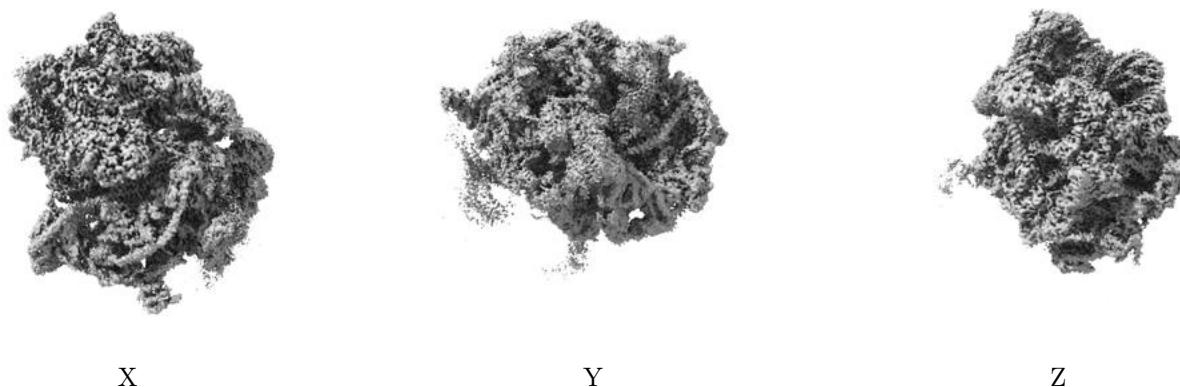


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

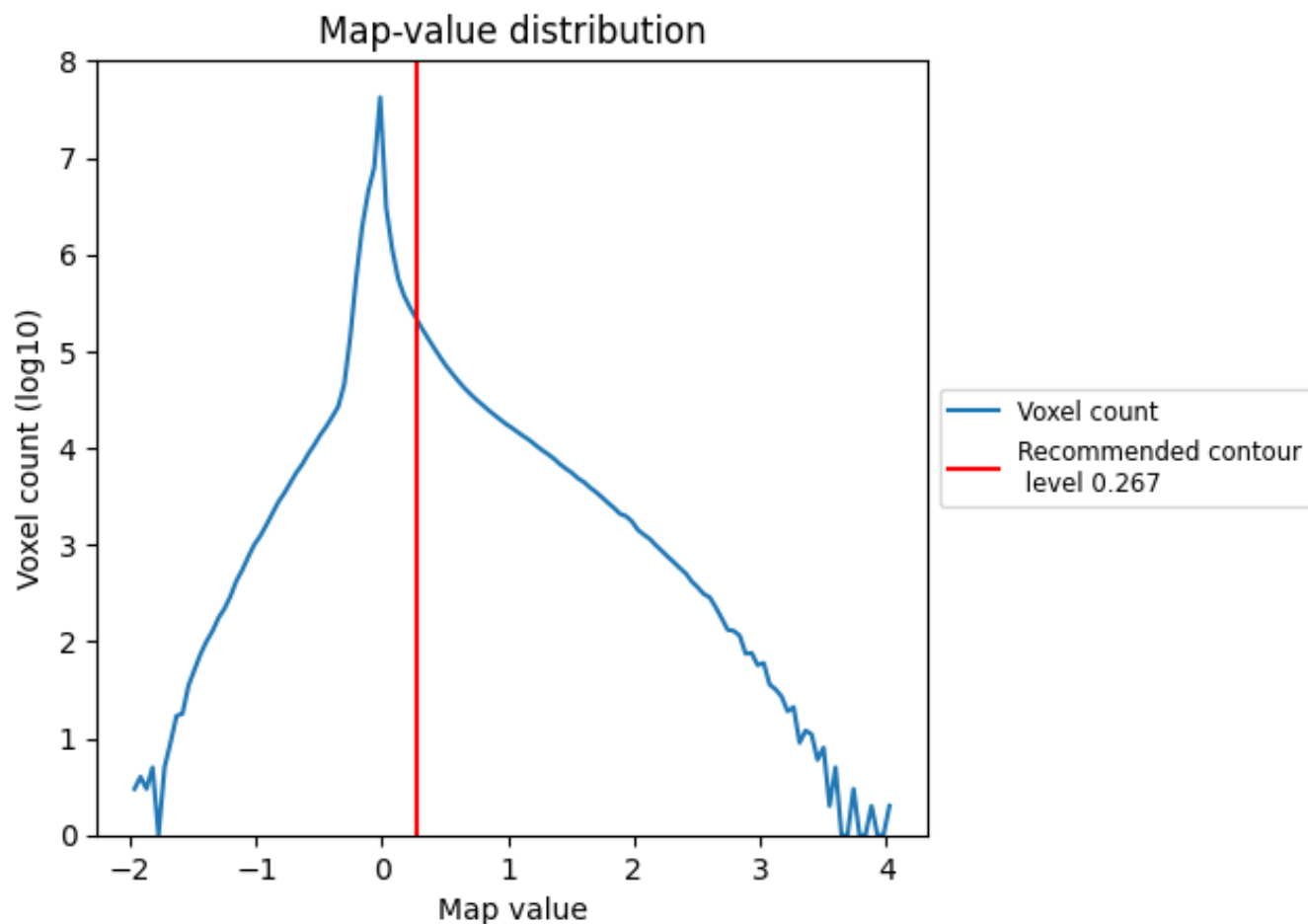
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

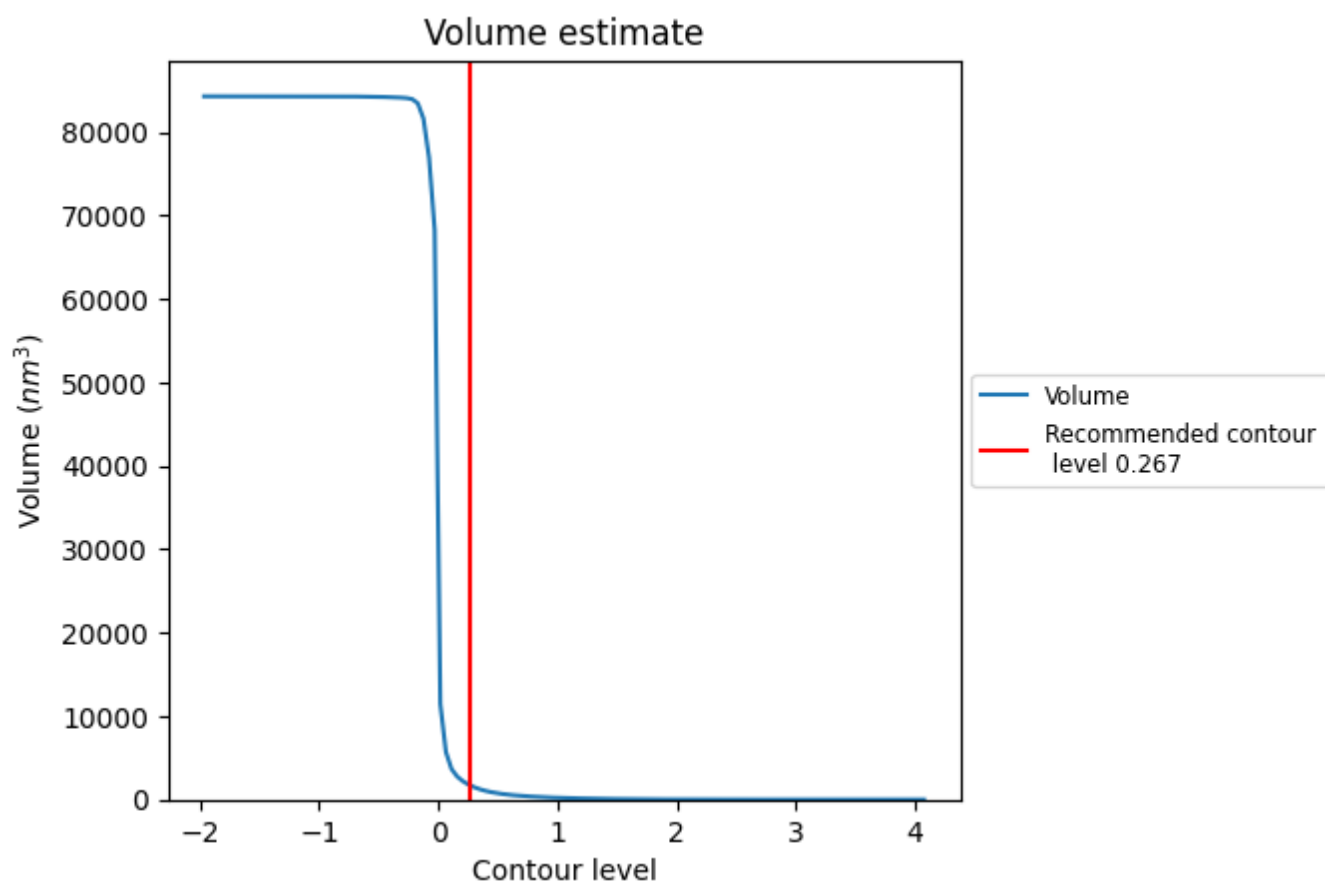
This section contains the results of statistical analysis of the map.

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.

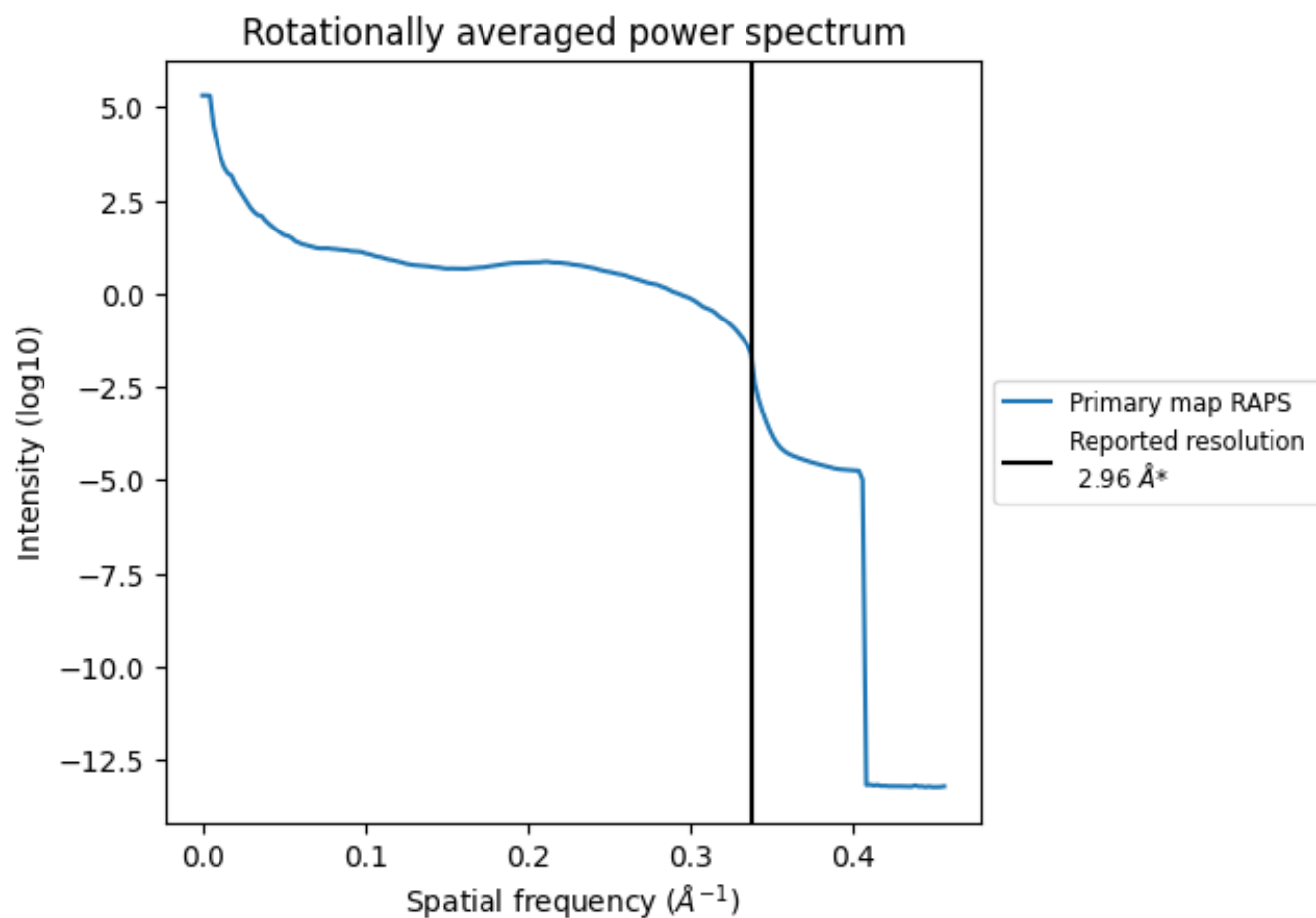
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1709 nm^3 ; this corresponds to an approximate mass of 1544 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 0.338 Å⁻¹

8 Fourier-Shell correlation

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

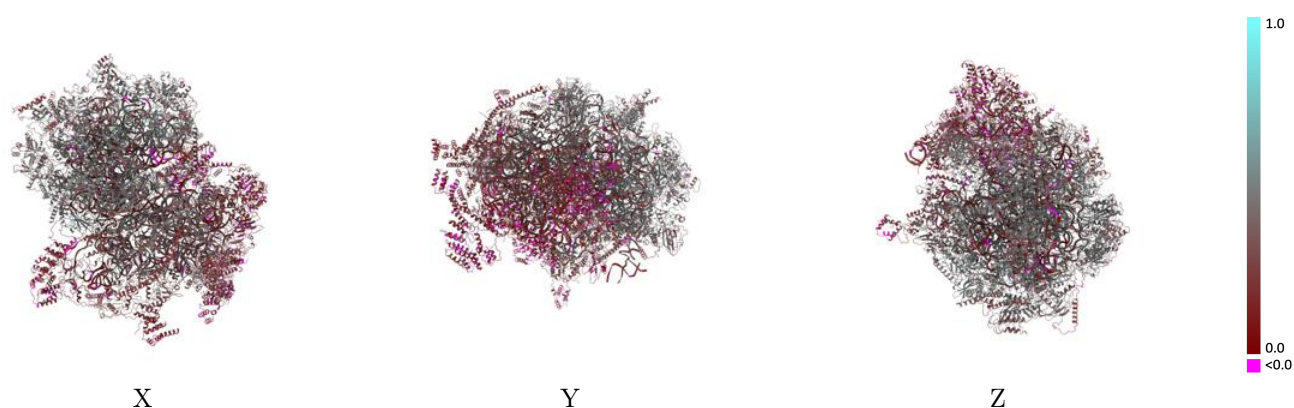
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21242 and PDB model 6VMI. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

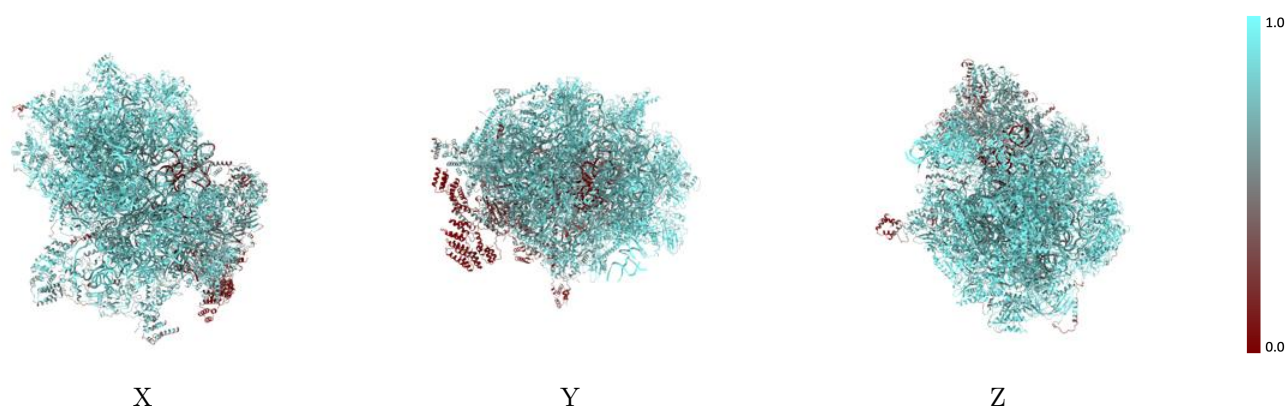
This section was not generated.

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



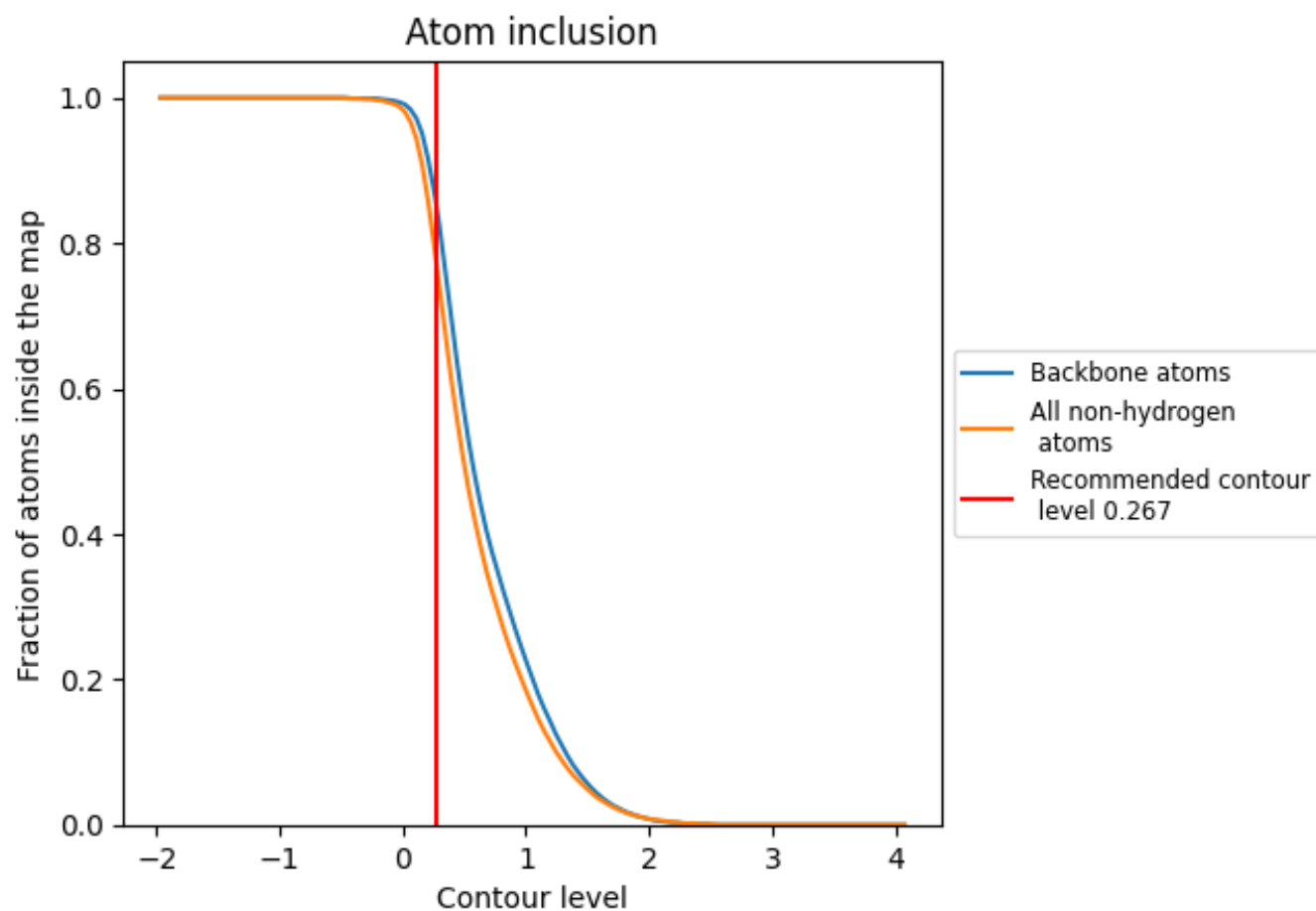
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 78% 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	 0.7820	 0.3390
0	 0.8790	 0.4430
1	 0.8550	 0.4410
2	 0.9060	 0.4680
3	 0.9010	 0.5010
4	 0.8990	 0.4740
5	 0.8980	 0.4400
6	 0.8850	 0.4090
7	 0.8660	 0.4100
8	 0.7540	 0.2460
9	 0.8800	 0.4210
A	 0.8460	 0.3360
A0	 0.7340	 0.2560
A1	 0.5090	 0.1810
A2	 0.6550	 0.3320
A3	 0.8090	 0.4300
A4	 0.1430	 0.1650
A5	 0.0470	 0.0780
A6	 0.0270	 0.0710
A7	 0.3890	 0.1280
AA	 0.8650	 0.2980
AB	 0.7760	 0.3190
AC	 0.5070	 0.1970
AD	 0.6200	 0.3110
AE	 0.7640	 0.3890
AF	 0.6420	 0.2680
AG	 0.6450	 0.2300
AH	 0.5830	 0.2180
AI	 0.8290	 0.4060
AJ	 0.7630	 0.3750
AK	 0.5980	 0.1710
AL	 0.7890	 0.3790
AM	 0.7740	 0.2970
AN	 0.8510	 0.4030
AO	 0.7700	 0.2930



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Chain	Atom inclusion	Q-score
AP	 0.7740	 0.3830
AQ	 0.8310	 0.4000
AR	 0.6720	 0.2350
AS	 0.7050	 0.2830
AT	 0.8030	 0.3480
AU	 0.7520	 0.2540
AV	 0.6780	 0.1770
AW	 0.7610	 0.3350
AX	 0.6230	 0.1760
AY	 0.4180	 0.1470
AZ	 0.4910	 0.1800
B	 0.9460	 0.2990
D	 0.8780	 0.4520
E	 0.8940	 0.4620
F	 0.8950	 0.4560
H	 0.8530	 0.4040
I	 0.7190	 0.3300
J	 0.7350	 0.2970
K	 0.9040	 0.4710
L	 0.8610	 0.4600
M	 0.8910	 0.4540
N	 0.8760	 0.4560
O	 0.8870	 0.4420
P	 0.9120	 0.4350
Q	 0.8490	 0.4350
R	 0.8930	 0.4580
S	 0.9030	 0.4520
T	 0.8850	 0.4580
TA	 0.1570	 0.1180
TB	 0.1830	 0.1980
TC	 0.0740	 0.1600
U	 0.8740	 0.4430
V	 0.8570	 0.4170
W	 0.8790	 0.4580
X	 0.8860	 0.4460
Y	 0.8940	 0.4480
Z	 0.8880	 0.4580
a	 0.7940	 0.3920
b	 0.8970	 0.4720
c	 0.8700	 0.4230
d	 0.7510	 0.3760
e	 0.7240	 0.2060

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Chain	Atom inclusion	Q-score
f	 0.7180	 0.3210
g	 0.8820	 0.4300
h	 0.8410	 0.3600
i	 0.9070	 0.4580
j	 0.8450	 0.4020
k	 0.8040	 0.3520
l	 0.7710	 0.3130
m	 0.8020	 0.2930
o	 0.8560	 0.4260
p	 0.8200	 0.3850
q	 0.7930	 0.3470
r	 0.8850	 0.4230
s	 0.8910	 0.4470
u	 0.5290	 0.1420
v	 0.6750	 0.3110