



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 09:04 PM EDT

PDB ID : 9Q2P / pdb_00009q2p
EMDB ID : EMD-72171
Title : Rabbit ribosomal 80S elongation complex with eEF1A, A*/T Ala-tRNA, P site Ala-tRNA, E site Ala-tRNA on NediV ORF
Authors : De, S.; Altomare, C.G.; Abaeva, I.S.; Dadhwal, P.; Garg, P.; Acosta-Reyes, F.; Brown, Z.P.; Pestova, T.V.; Hellen, C.U.T.; Frank, J.
Deposited on : 2025-08-15
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

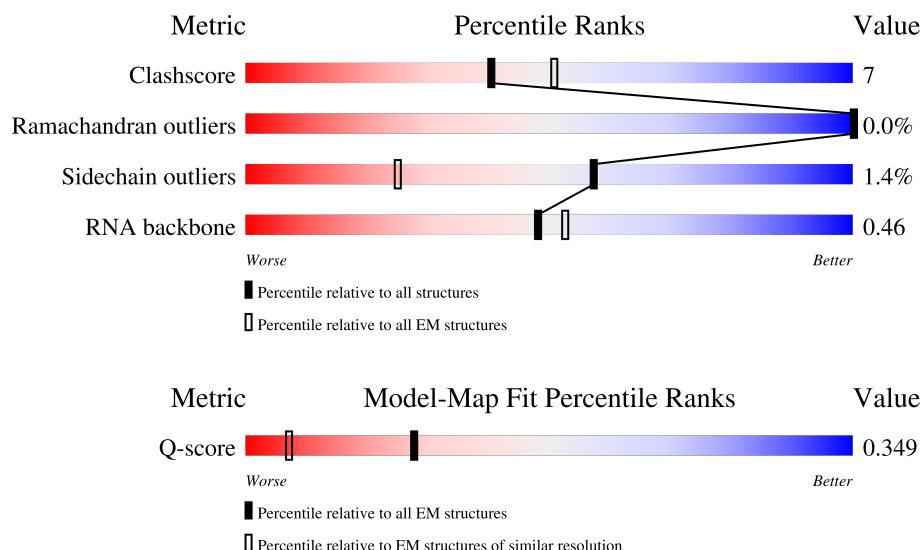
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)	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	14081 (2.50 - 3.50)

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	7	119	
2	A	248	
3	B	394	


























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Mol	Chain	Length	Quality of chain
4	C	362	 88% 12%
5	D	293	 89% 11%
6	E	216	 83% 16% .
7	F	225	 79% 20% .
8	G	240	 79% 18% .
9	H	190	 76% 24%
10	I	213	 83% 13% .
11	J	170	 82% 17% .
12	L	210	 90% 10%
13	M	138	 75% 25%
14	N	203	 80% 19%
15	O	199	 76% 23% .
16	P	153	 85% 14% .
17	Q	187	 84% 15% .
18	R	180	 81% 18% .
19	S	176	 74% 25% .
20	T	159	 81% 18% .
21	U	99	 87% 13%
22	V	139	 78% 22%
23	W	106	 92% 8% .
24	X	118	 82% 16% .
25	Y	134	 85% 15%
26	Z	135	 93% 7%
27	a	147	 84% 16% .
28	b	104	 83% 17%

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Mol	Chain	Length	Quality of chain
29	c	98	 74% 26%
30	d	107	 77% 23%
31	e	128	 89% 11%
32	f	109	 82% 18%
33	g	114	 82% 17% .
34	h	122	 84% 15% .
35	i	102	 86% 14%
36	j	86	 94% 6%
37	k	69	 83% 17%
38	l	50	 82% 18%
39	m	52	 71% 27% .
40	n	25	 80% 20%
41	o	104	 88% 12%
42	p	91	 76% 22% .
43	r	124	 86% 14%
44	s	196	 59% 39% .
45	t	153	 78% 11% 10% .
46	2	75	 60% 28% 12%
46	3	75	 72% 25% .
47	5	3543	 69% 26% 5%
48	8	156	 67% 24% 5% .
49	9	1697	 69% 26% 5%
50	AA	217	 77% 22%
51	BB	213	 81% 18% .
52	CC	221	 81% 19%






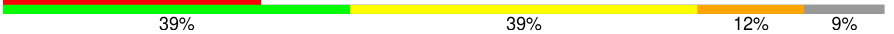
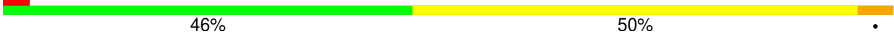

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Mol	Chain	Length	Quality of chain
53	DD	228	
54	EE	262	
55	FF	191	
56	GG	237	
57	HH	189	
58	II	206	
59	JJ	185	
60	KK	96	
61	LL	151	
62	MM	117	
63	NN	149	
64	OO	136	
65	PP	129	
66	QQ	142	
67	RR	132	
68	SS	144	
69	TT	141	
70	UU	100	
71	VV	83	
72	WW	129	
73	XX	141	
74	YY	124	
75	ZZ	75	
76	aa	101	
77	bb	83	

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Mol	Chain	Length	Quality of chain
78	cc	62	 71% 27% •
79	dd	55	 84% 16%
80	ee	57	 72% 28%
81	ff	68	 84% 16%
82	gg	313	 90% 10%
83	AT	76	 29% 39% 39% 12% 9%
84	EF	441	 46% 50% •
85	1	15	 13% 33% 53%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 385235 atoms, of which 164603 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	7	119	Total	C	H	N	O	P	0	0
			3824	1132	1286	454	834	118		

- Molecule 2 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	248	Total	C	H	N	O	S	0	0
			3891	1189	1993	389	314	6		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	394	Total	C	H	N	O	S	0	0
			6482	2020	3310	597	542	13		

- Molecule 4 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	362	Total	C	H	N	O	S	0	0
			5936	1812	3053	577	480	14		

- Molecule 5 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	293	Total	C	H	N	O	S	0	0
			4815	1512	2424	438	427	14		

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	216	Total	C	H	N	O	S	0	0
			3616	1115	1887	329	282	3		

- Molecule 7 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	225	Total	C	H	N	O	S	0	0
			3870	1205	1995	358	303	9		

- Molecule 8 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	233	Total	C	H	N	O	S	0	0
			3906	1199	2027	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 9 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 10 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	205	Total	C	H	N	O	S	0	0
			3376	1056	1712	321	274	13		

- Molecule 11 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	170	Total	C	H	N	O	S	0	0
			2761	861	1399	254	241	6		

- Molecule 12 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	210	Total	C	H	N	O	S	0	0
			3522	1065	1820	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 13 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	138	Total	C	H	N	O	S	0	0
			2348	727	1211	221	182	7		

- Molecule 14 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	199	Total	C	H	N	O	S	0	0
			3408	1051	1778	319	255	5		

- Molecule 16 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 17 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	187	Total	C	H	N	O	S	0	0
			3149	946	1634	315	250	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	4	ASP	ASN	conflict	UNP G1TFE0
Q	14	ARG	TRP	conflict	UNP G1TFE0
Q	53	MET	LEU	conflict	UNP G1TFE0
Q	58	ARG	TRP	conflict	UNP G1TFE0
Q	75	ARG	GLN	conflict	UNP G1TFE0
Q	80	ALA	PRO	conflict	UNP G1TFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	86	VAL	ILE	conflict	UNP G1TFE0
Q	104	ARG	HIS	conflict	UNP G1TFE0
Q	110	ARG	CYS	conflict	UNP G1TFE0
Q	137	VAL	GLY	conflict	UNP G1TFE0
Q	157	GLY	ARG	conflict	UNP G1TFE0
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 18 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	180	Total	C	H	N	O	S	0	0
			3160	930	1655	328	238	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 19 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	176	Total	C	H	N	O	S	0	0
			2961	928	1501	285	236	11		

- Molecule 20 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 21 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	99	Total	C	H	N	O	S	0	0
			1642	519	833	141	147	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	139	Total	C	H	N	O	S	0	0
			2131	648	1097	199	182	5		

- Molecule 23 is a protein called uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	106	Total	C	H	N	O	S	0	0
			1763	538	903	174	144	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	118	Total	C	H	N	O	S	0	0
			2007	618	1040	181	167	1		

- Molecule 25 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 27 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	147	Total	C	H	N	O	S	0	0
			2371	734	1209	239	185	4		

- Molecule 28 is a protein called eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	104	Total	C	H	N	O	S	0	0
			1768	527	920	189	129	3		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	98	Total	C	H	N	O	S	0	0
			1555	481	794	134	140	6		

- Molecule 30 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	e	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	3	ALA	SER	conflict	UNP G1TUN8
e	13	VAL	ILE	conflict	UNP G1TUN8
e	16	ARG	TRP	conflict	UNP G1TUN8
e	81	ASN	SER	conflict	UNP G1TUN8
e	98	GLU	LYS	conflict	UNP G1TUN8
e	108	ARG	CYS	conflict	UNP G1TUN8
e	115	ALA	VAL	conflict	UNP G1TUN8

- Molecule 32 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	g	114	Total	C	H	N	O	S	0	0
			1904	566	998	187	147	6		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	h	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

- Molecule 35 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	i	102	Total	C	H	N	O	S	0	0
			1746	520	916	176	129	5		

- Molecule 36 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	j	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 37 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	k	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	l	50	Total	C	H	N	O	S	0	0
			927	286	480	96	64	1		

- Molecule 39 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	m	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

- Molecule 40 is a protein called eL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	n	25	Total	C	H	N	O	S	0	0
			528	145	289	64	27	3		

- Molecule 41 is a protein called eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	o	104	Total	C	H	N	O	S	0	0
			1771	533	920	174	138	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	p	91	Total	C	H	N	O	S	0	0
			1464	445	756	136	120	7		

- Molecule 43 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	r	124	Total	C	H	N	O	S	0	0
			2045	616	1051	205	167	6		

- Molecule 44 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	s	196	Total	C	H	N	O	S	0	0
			3071	959	1564	263	276	9		

- Molecule 45 is a protein called uL11.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	t	137	Total	C	H	N	O	S	0	0
			2087	637	1066	187	194	3		

- Molecule 46 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	2	75	Total	C	H	N	O	P	0	0
			2408	712	813	285	524	74		
46	3	75	Total	C	H	N	O	P	0	0
			2408	712	813	285	524	74		

- Molecule 47 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	5	3543	Total	C	H	N	O	P	0	0
			114306	33826	38351	13895	24691	3543		

- Molecule 48 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	8	151	Total	C	H	N	O	P	0	0
			4836	1432	1628	564	1062	150		

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	9	1697	Total	C	H	N	O	P	0	0
			54517	16171	18288	6506	11856	1696		

- Molecule 50 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	AA	217	Total	C	H	N	O	S	0	0
			3418	1086	1708	300	316	8		

- Molecule 51 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	BB	213	Total	C	H	N	O	S	0	0
			3532	1098	1803	309	308	14		

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	CC	221	Total	C	H	N	O	S	0	0
			3522	1111	1806	295	301	9		

- Molecule 53 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	DD	228	Total	C	H	N	O	S	0	0
			3634	1126	1866	318	316	8		

- Molecule 54 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	EE	262	Total	C	H	N	O	S	0	0
			4253	1324	2177	386	358	8		

- Molecule 55 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	FF	185	Total	C	H	N	O	S	0	0
			2993	921	1522	277	266	7		

- Molecule 56 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	GG	237	Total	C	H	N	O	S	0	0
			4005	1199	2084	387	328	7		

- Molecule 57 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	HH	185	Total	C	H	N	O	S	0	0
			3070	952	1582	271	264	1		

- Molecule 58 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	II	206	Total	C	H	N	O	S	0	0
			3458	1058	1772	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 59 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	JJ	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 60 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	KK	96	Total	C	H	N	O	S	0	0
			1646	530	836	143	131	6		

- Molecule 61 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	LL	143	Total	C	H	N	O	S	0	0
			2424	749	1249	222	198	6		

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	MM	117	Total	C	H	N	O	S	0	0
			1847	570	939	161	169	8		

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	NN	149	Total	C	H	N	O	S	0	0
			2491	770	1289	228	203	1		

- Molecule 64 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	OO	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

- Molecule 65 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	PP	129	Total	C	H	N	O	S	0	0
			2162	670	1104	201	180	7		

- Molecule 66 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	QQ	142	Total	C	H	N	O	S	0	0
			2323	717	1195	213	195	3		

- Molecule 67 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	RR	132	Total	C	H	N	O	S	0	0
			2189	670	1121	199	195	4		

- Molecule 68 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	SS	144	Total	C	H	N	O	S	0	0
			2439	746	1249	241	202	1		

- Molecule 69 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	TT	141	Total	C	H	N	O	S	0	0
			2217	685	1123	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 70 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	UU	100	Total	C	H	N	O	S	0	0
			1657	498	862	152	141	4		

- Molecule 71 is a protein called eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	VV	83	Total	C	H	N	O	S	0	0
			1273	393	637	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 72 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	WW	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 73 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	XX	141	Total	C	H	N	O	S	0	0
			2265	693	1167	219	183	3		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	YY	124	Total	C	H	N	O	S	0	0
			2094	640	1083	198	168	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	ZZ	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 76 is a protein called eS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	aa	101	Total	C	H	N	O	S	0	0
			1677	507	863	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	28	ARG	CYS	conflict	UNP G1TFE8
aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 77 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	bb	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 78 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	cc	62	Total	C	H	N	O	S	0	0
			1002	297	514	97	92	2		

- Molecule 79 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	dd	55	Total	C	H	N	O	S	0	0
			907	286	448	94	74	5		

- Molecule 80 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	ee	57	Total	C	H	N	O	S	0	0
			959	282	502	101	73	1		

- Molecule 81 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	ff	68	Total	C	H	N	O	S	0	0
			1118	351	563	103	94	7		

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	gg	313	Total	C	H	N	O	S	0	0
			4829	1535	2393	424	465	12		

- Molecule 83 is a RNA chain called A*/T tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	AT	69	Total	C	H	N	O	P	0	0
			2220	656	749	265	482	68		

- Molecule 84 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms							AltConf	Trace
84	EF	441	Total	C	H	N	O	P	S	0	0
			6814	2148	3431	581	636	1	17		

- Molecule 85 is a RNA chain called NediV ORF.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	1	15	Total	C	H	N	O	P	0	0
			418	141	105	54	103	15		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	7	6	Total	Mg	0
			6	6	
86	A	1	Total	Mg	0
			1	1	
86	I	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	
86	a	1	Total	Mg	0
			1	1	
86	5	189	Total	Mg	0
			189	189	
86	8	5	Total	Mg	0
			5	5	
86	9	70	Total	Mg	0
			70	70	
86	EF	1	Total	Mg	0
			1	1	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

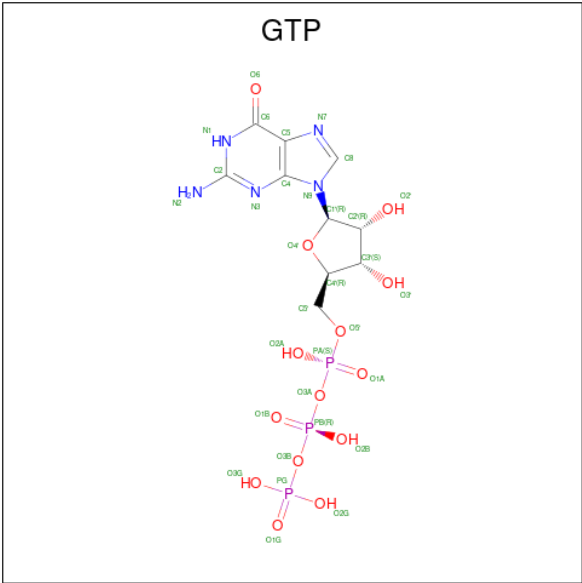
Mol	Chain	Residues	Atoms		AltConf
87	g	1	Total	Zn	0
			1	1	
87	j	1	Total	Zn	0
			1	1	
87	m	1	Total	Zn	0
			1	1	
87	o	1	Total	Zn	0
			1	1	
87	p	1	Total	Zn	0
			1	1	
87	aa	1	Total	Zn	0
			1	1	
87	dd	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	ff	1	Total	Zn	0
			1	1	

- Molecule 88 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).




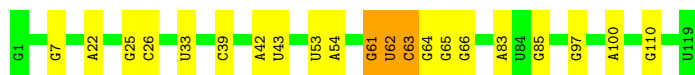
Mol	Chain	Residues	Atoms						AltConf
88	EF	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

3 Residue-property plots


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

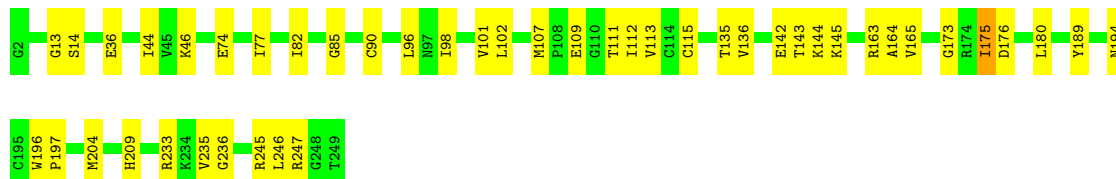
- Molecule 1: 5S ribosomal RNA

Chain 7: 




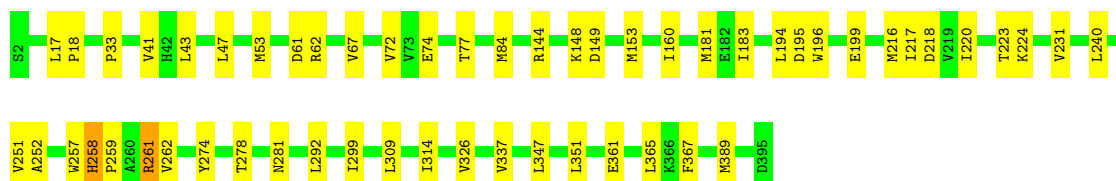
- Molecule 2: 60S ribosomal protein L8

Chain A: 




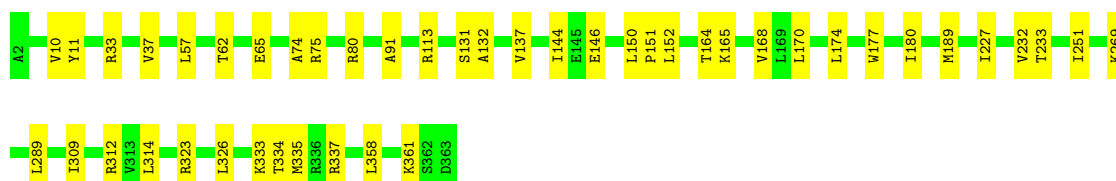
- Molecule 3: 60S ribosomal protein L3

Chain B: 

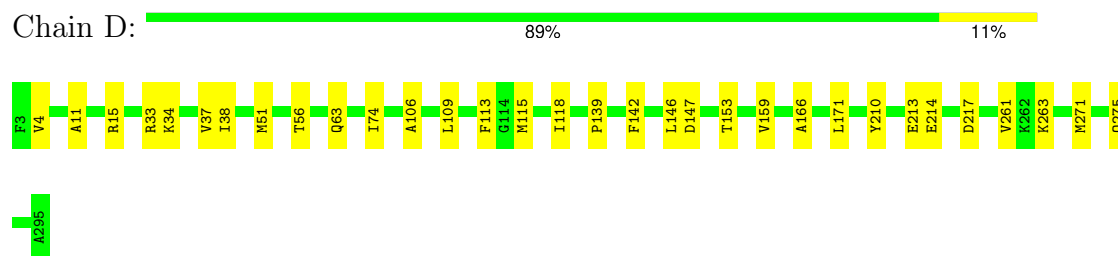


- Molecule 4: 60S ribosomal protein L4

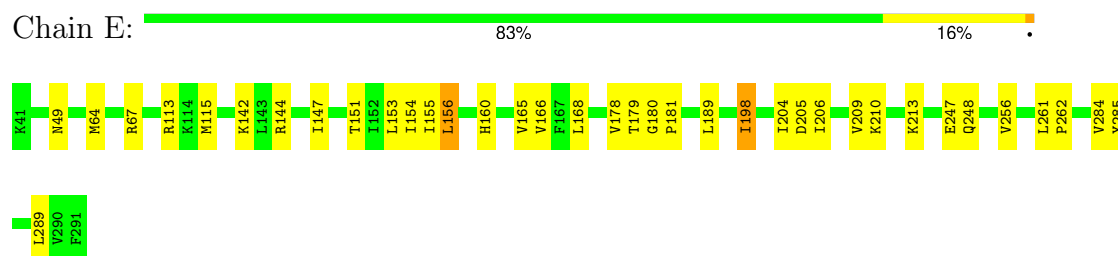
Chain C: 



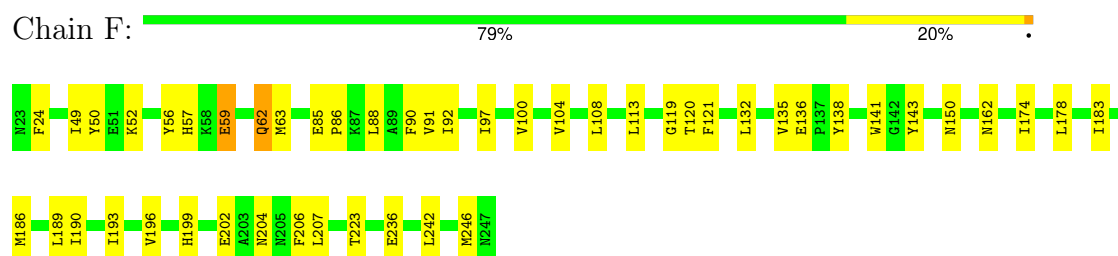
- Molecule 5: 60S ribosomal protein L5



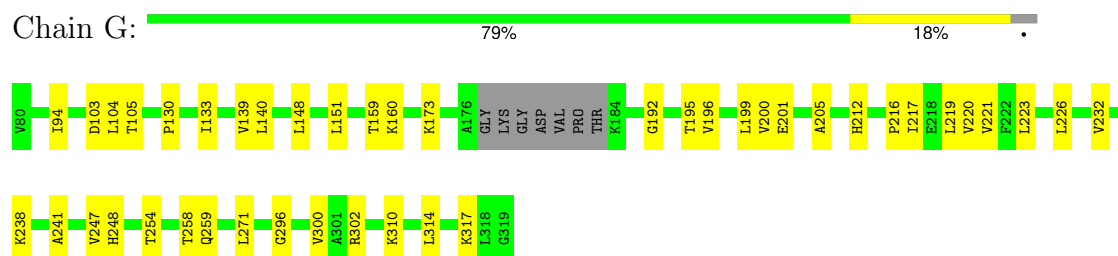
- Molecule 6: 60S ribosomal protein L6



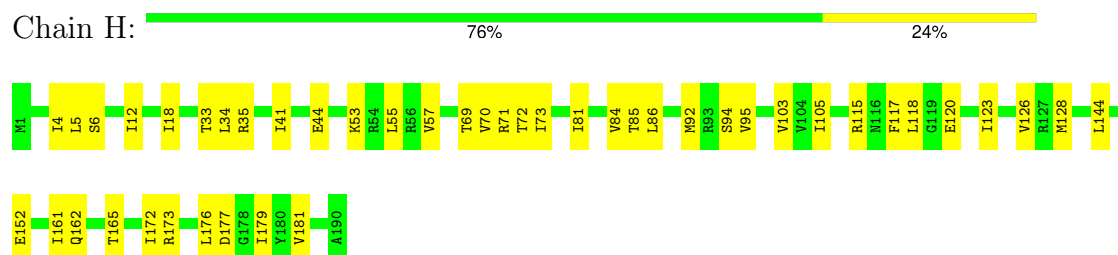
- Molecule 7: 60S ribosomal protein L7



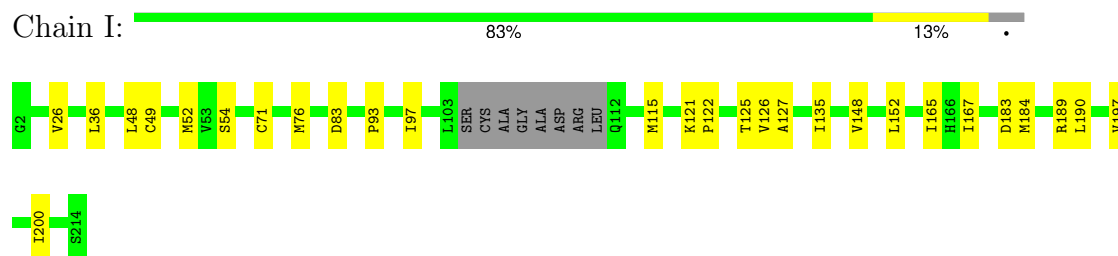
- Molecule 8: Large ribosomal subunit protein eL8



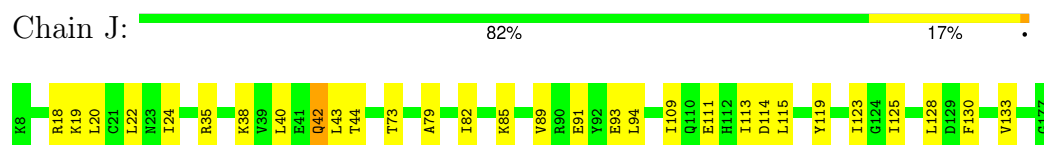
- Molecule 9: 60S ribosomal protein L9



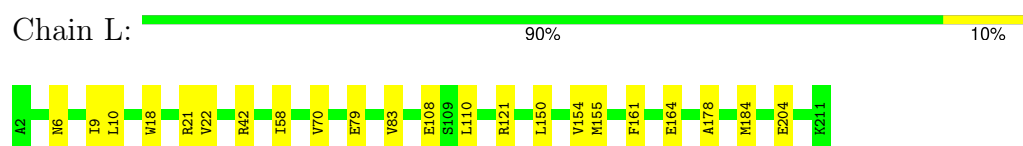
- Molecule 10: Ribosomal protein L10



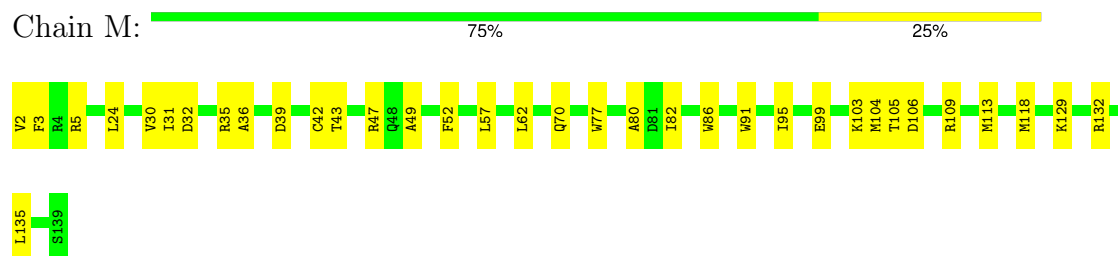
- Molecule 11: 60S ribosomal protein L11



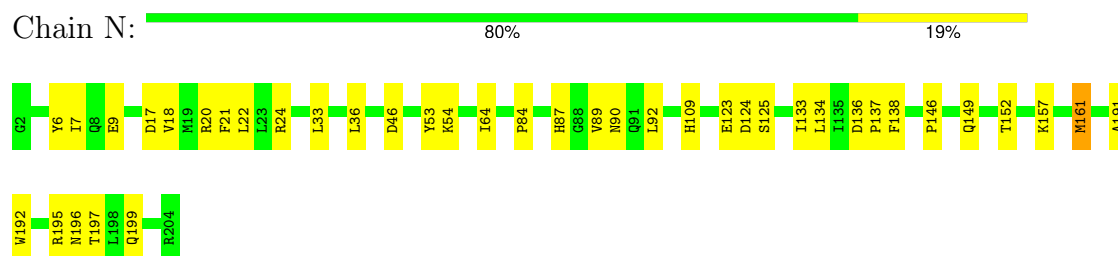
- Molecule 12: Large ribosomal subunit protein eL13



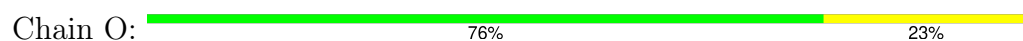
- Molecule 13: 60S ribosomal protein L14

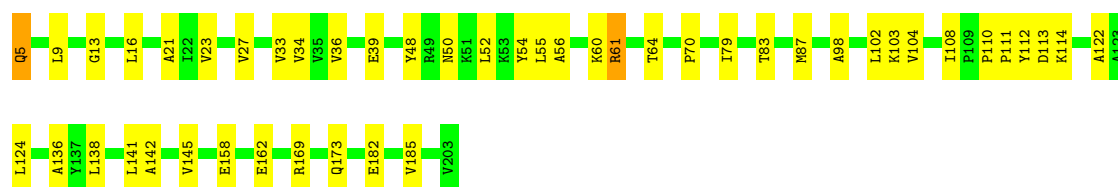


- Molecule 14: 60S ribosomal protein L15



- Molecule 15: Large ribosomal subunit protein uL13





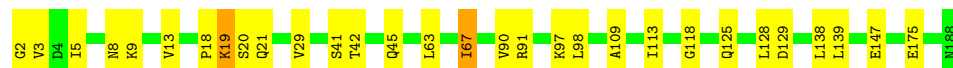
- Molecule 16: 60S ribosomal protein L17

Chain P: 85% 14%



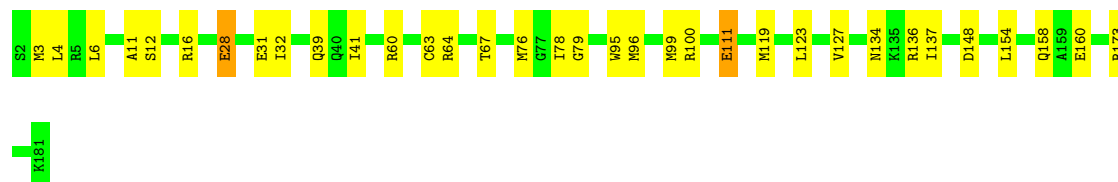
- Molecule 17: Large ribosomal subunit protein eL18

Chain Q: 84% 15%



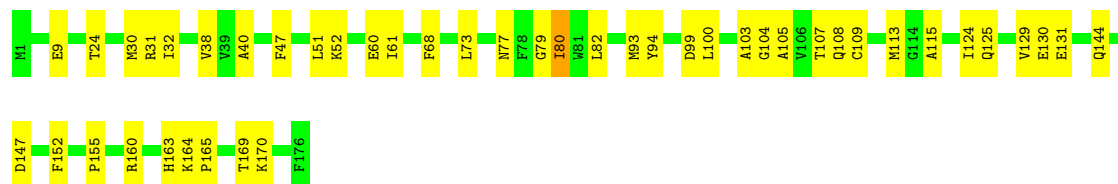
- Molecule 18: 60S ribosomal protein L19

Chain R: 81% 18%



- Molecule 19: 60S ribosomal protein L18a

Chain S: 74% 25%




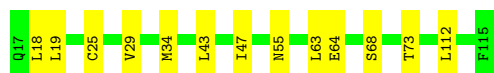
- Molecule 20: 60S ribosomal protein L21

Chain T: 81% 18%




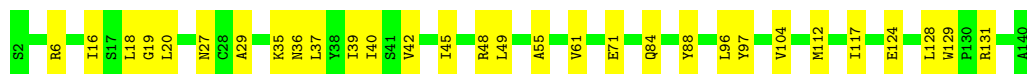
- Molecule 21: Large ribosomal subunit protein eL22

Chain U:  87% 13%



- Molecule 22: Large ribosomal subunit protein uL14

Chain V:  78% 22%




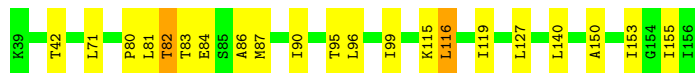
- Molecule 23: uL24

Chain W:  92% 8%




- Molecule 24: Large ribosomal subunit protein uL23

Chain X:  82% 16%



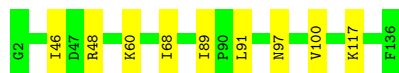
- Molecule 25: 60S ribosomal protein L26

Chain Y:  85% 15%




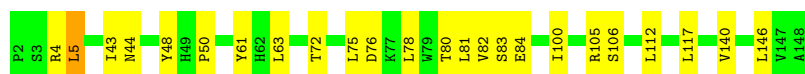
- Molecule 26: 60S ribosomal protein L27

Chain Z:  93% 7%




- Molecule 27: 60S ribosomal protein L27a

Chain a:  84% 16%



- Molecule 28: eL29

Chain b:  83% 17%



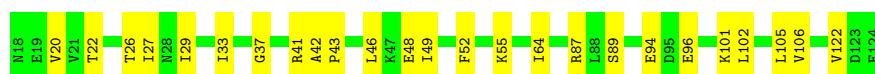
- Molecule 29: 60S ribosomal protein L30

Chain c: 74% 26%



- Molecule 30: 60S ribosomal protein L31

Chain d: 77% 23%



- Molecule 31: Large ribosomal subunit protein eL32

Chain e: 89% 11%



- Molecule 32: Large ribosomal subunit protein eL33

Chain f: 82% 18%



- Molecule 33: 60S ribosomal protein L34

Chain g: 82% 17% .



- Molecule 34: 60S ribosomal protein L35

Chain h: 84% 15% .



- Molecule 35: 60S ribosomal protein L36

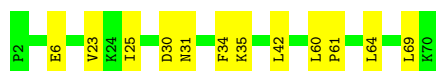
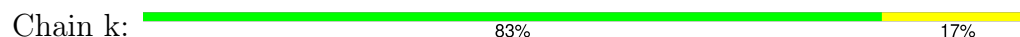
Chain i: 86% 14%



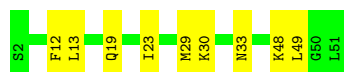
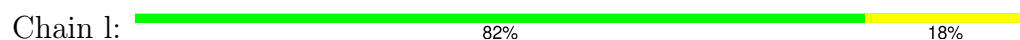
- Molecule 36: 60S ribosomal protein L37



- Molecule 37: Large ribosomal subunit protein eL38



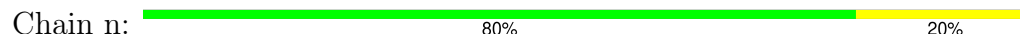
- Molecule 38: 60S ribosomal protein L39



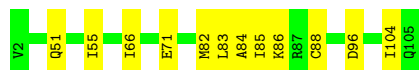
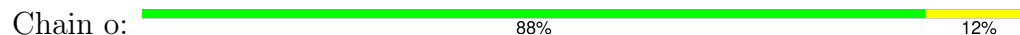
- Molecule 39: Large ribosomal subunit protein eL40



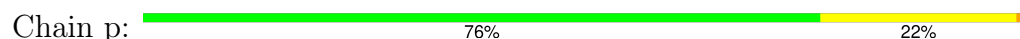
- Molecule 40: eL41



- Molecule 41: eL42



- Molecule 42: 60S ribosomal protein L37a





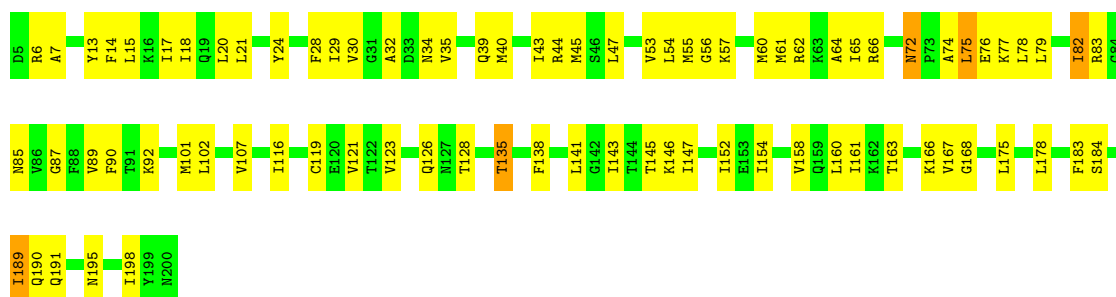
- Molecule 43: 60S ribosomal protein L28

Chain r: 86% 14%



- Molecule 44: 60S acidic ribosomal protein P0

Chain s: 59% 39% .



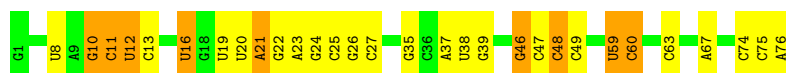
- Molecule 45: uL11

Chain t: 78% 11% 10%



- Molecule 46: tRNA

Chain 2: 60% 28% 12%



- Molecule 46: tRNA

Chain 3: 72% 25% .

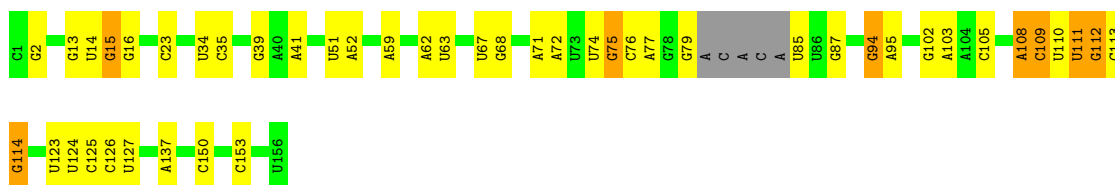


- Molecule 47: 28S ribosomal RNA

Chain 5: 69% 26% 5%

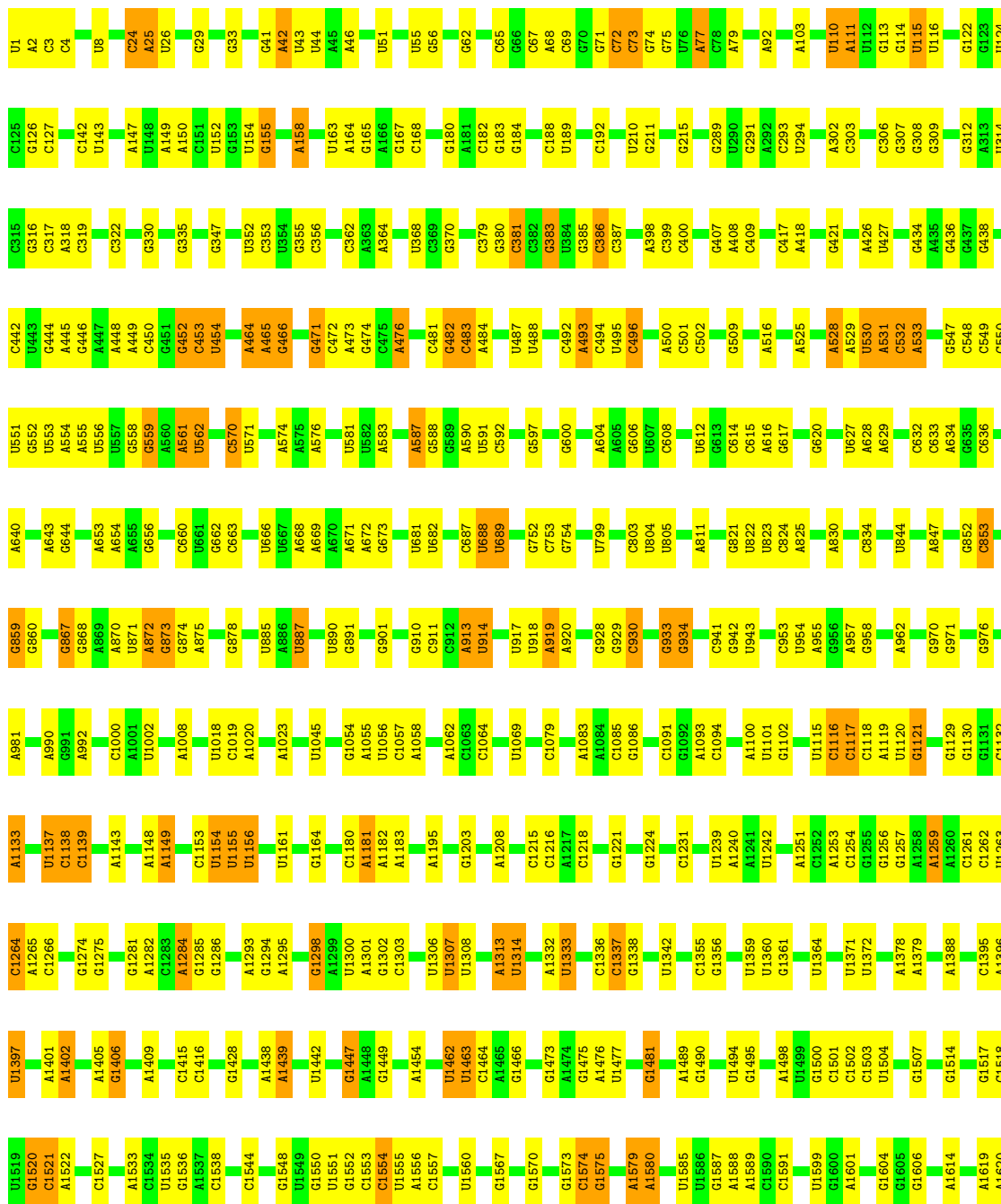


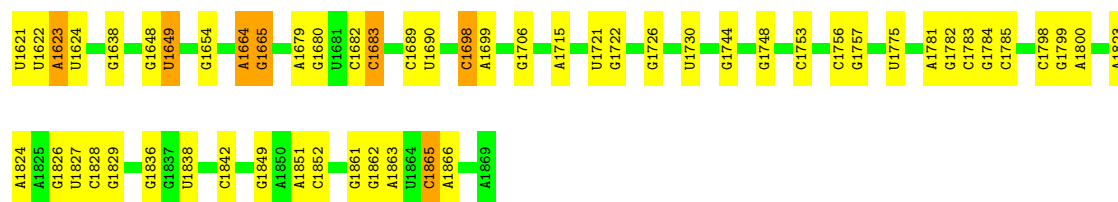




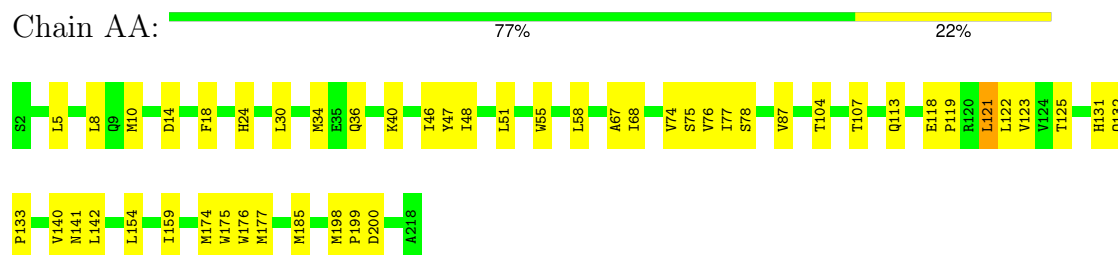
• Molecule 49: 18S ribosomal RNA

Chain 9: 69% 26% 5%

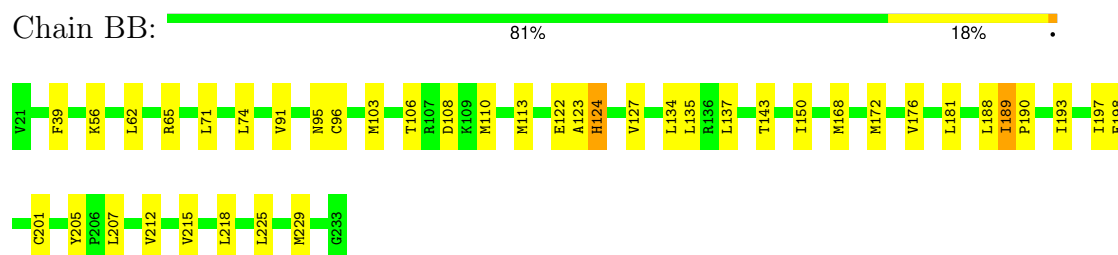




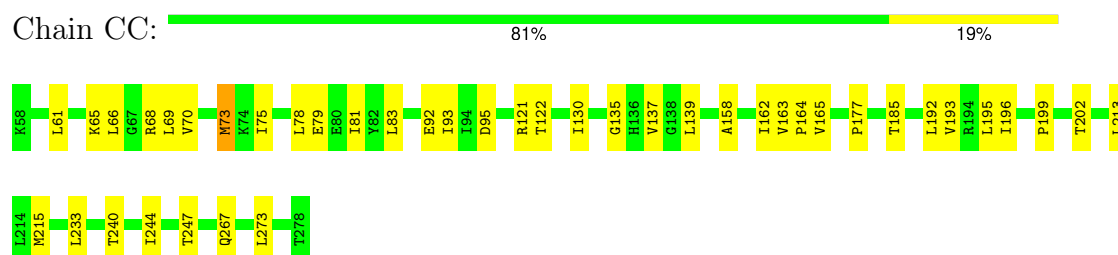
• Molecule 50: 40S_SA_C domain-containing protein



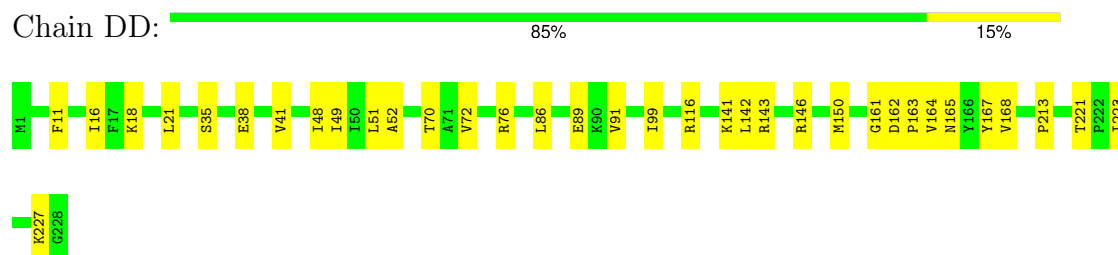
• Molecule 51: 40S ribosomal protein S3a



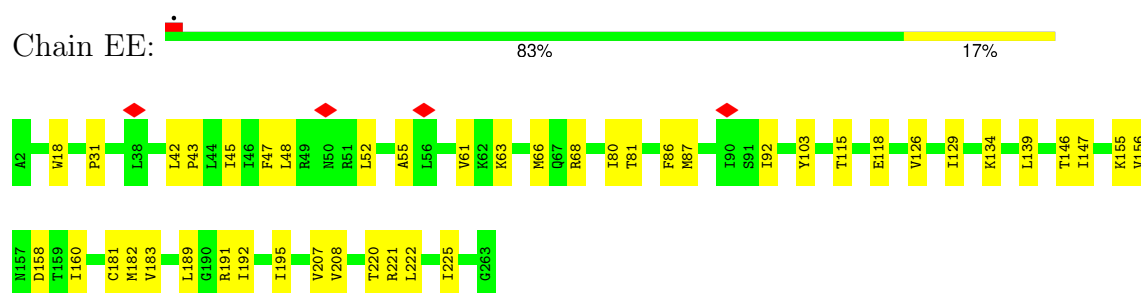
• Molecule 52: 40S ribosomal protein S2



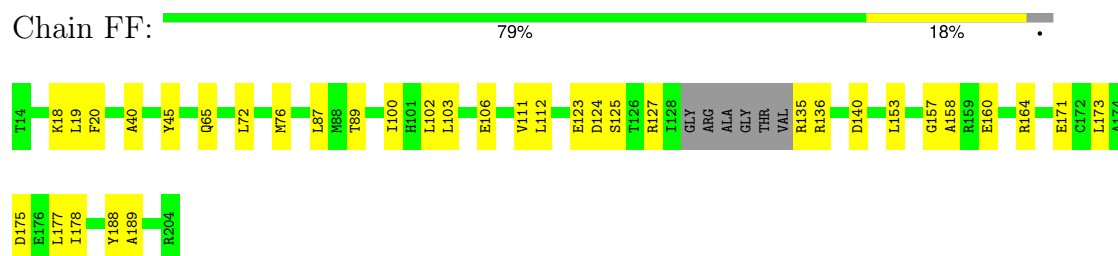
• Molecule 53: 40S ribosomal protein S3



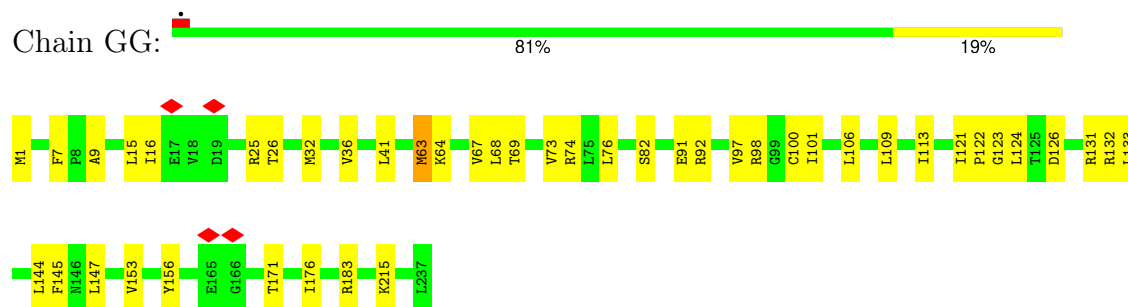
• Molecule 54: 40S ribosomal protein S4



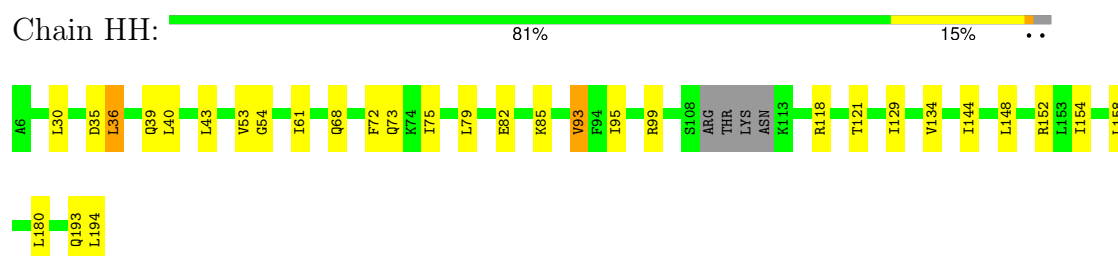
- Molecule 55: Small ribosomal subunit protein uS7



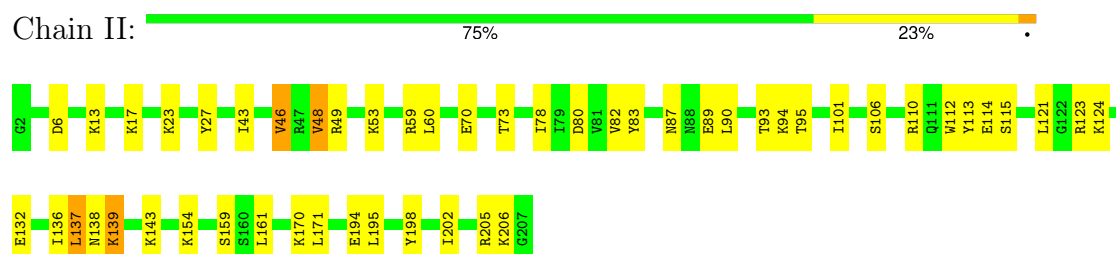
- Molecule 56: 40S ribosomal protein S6




- Molecule 57: Small ribosomal subunit protein eS7



- Molecule 58: 40S ribosomal protein S8




- Molecule 59: 40S ribosomal protein S9

Chain JJ:  88% 11%




- Molecule 60: 40S ribosomal protein S10

Chain KK:  85% 15%



- Molecule 61: Small ribosomal subunit protein uS17

Chain LL:  75% 19% 5%




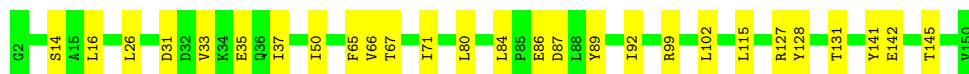
- Molecule 62: 40S ribosomal protein S12

Chain MM:  82% 17%




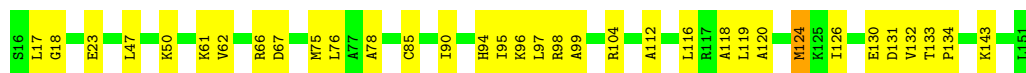
- Molecule 63: 40S ribosomal protein S13

Chain NN:  82% 18%



- Molecule 64: Small ribosomal subunit protein uS11

Chain OO:  75% 24%



- Molecule 65: Small ribosomal subunit protein uS19

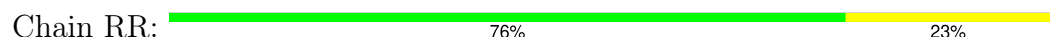
Chain PP:  86% 14%



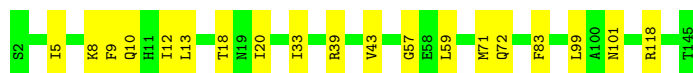
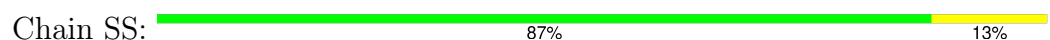
- Molecule 66: Small ribosomal subunit protein uS9



- Molecule 67: 40S ribosomal protein S17



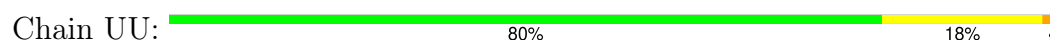
- Molecule 68: 40S ribosomal protein S18



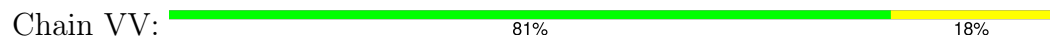
- Molecule 69: Small ribosomal subunit protein eS19



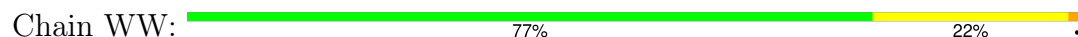
- Molecule 70: 40S ribosomal protein S20



- Molecule 71: eS21

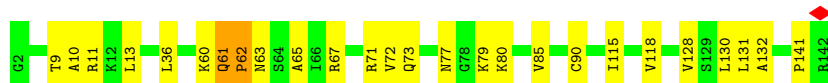
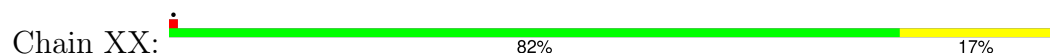


- Molecule 72: 40S ribosomal protein S15a

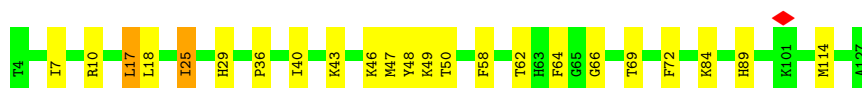
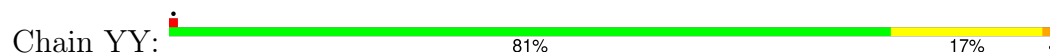




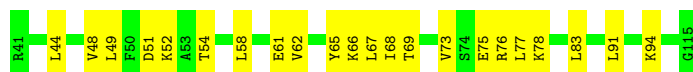
- Molecule 73: 40S ribosomal protein S23



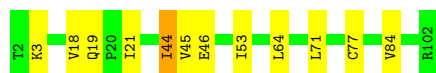
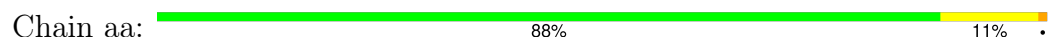
- Molecule 74: 40S ribosomal protein S24



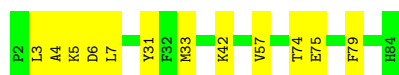
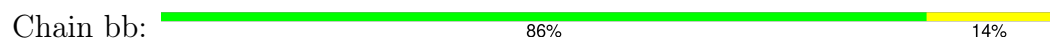
- Molecule 75: 40S ribosomal protein S25



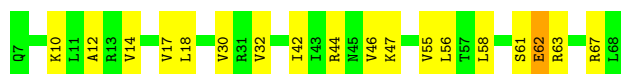
- Molecule 76: eS26



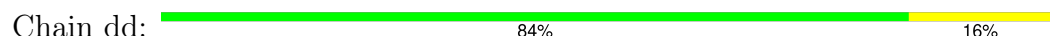
- Molecule 77: 40S ribosomal protein S27



- Molecule 78: 40S ribosomal protein S28



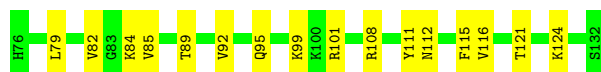
- Molecule 79: 40S ribosomal protein S29





- Molecule 80: Small ribosomal subunit protein eS30

Chain ee: 72% 28%



- Molecule 81: 40S ribosomal protein S27a

Chain ff: 84% 16%



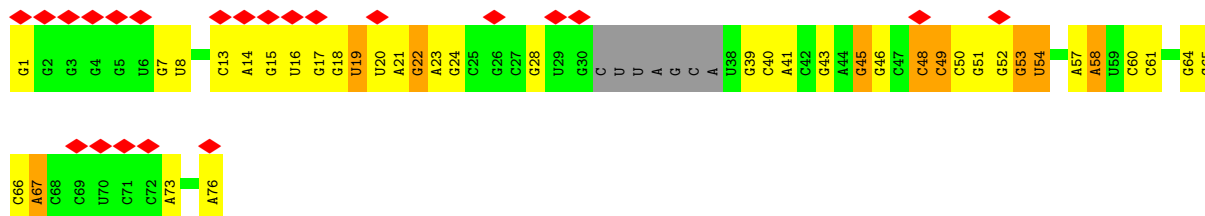
- Molecule 82: Receptor of activated protein C kinase 1

Chain gg: 90% 10%



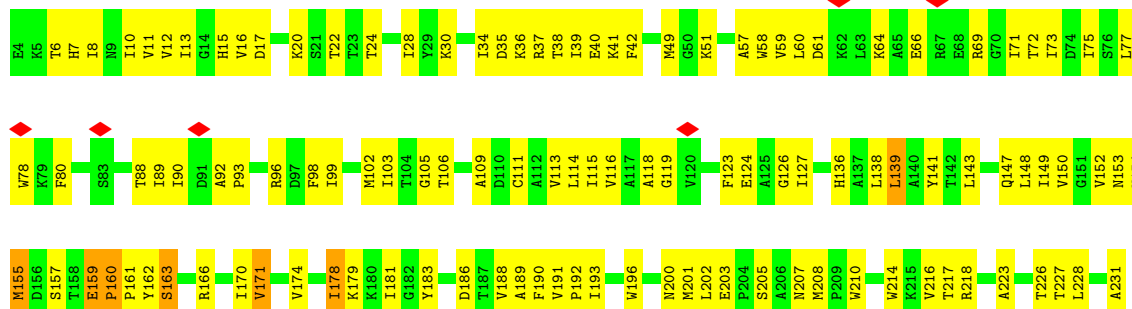
- Molecule 83: A*/T tRNA

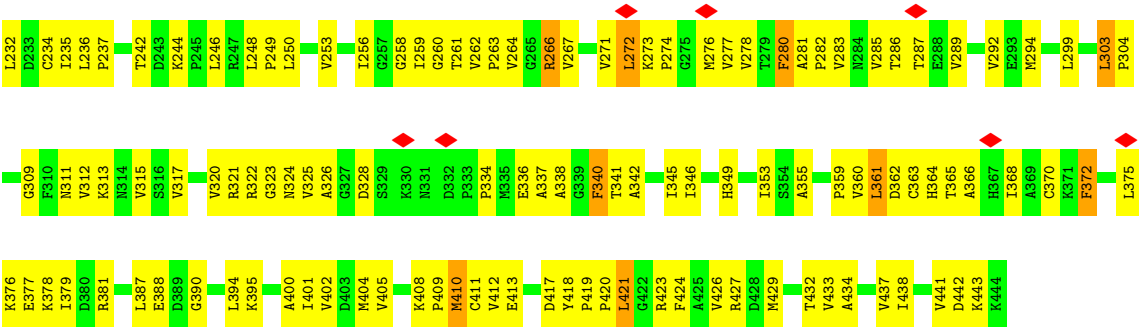
Chain AT: 29% 39% 39% 12% 9%



- Molecule 84: Elongation factor 1-alpha 1

Chain EF: 46% 50%





● Molecule 85: NediV ORF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	3.012	Depositor
Minimum map value	-1.422	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	849.92, 849.92, 849.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.66, 1.66, 1.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	7	0.09	0/2836	0.20	0/4421
2	A	0.14	0/1936	0.35	0/2596
3	B	0.14	0/3240	0.34	0/4339
4	C	0.13	0/2937	0.30	0/3946
5	D	0.11	0/2437	0.27	0/3264
6	E	0.13	0/1762	0.32	0/2362
7	F	0.13	0/1911	0.34	0/2549
8	G	0.12	0/1910	0.29	0/2569
9	H	0.15	0/1535	0.31	0/2063
10	I	0.15	0/1702	0.33	0/2272
11	J	0.11	0/1385	0.31	0/1852
12	L	0.11	0/1733	0.29	0/2316
13	M	0.14	0/1158	0.39	0/1547
14	N	0.14	0/1746	0.31	0/2338
15	O	0.15	0/1662	0.36	0/2222
16	P	0.18	0/1268	0.40	0/1700
17	Q	0.15	0/1539	0.36	0/2054
18	R	0.13	0/1521	0.34	0/2009
19	S	0.15	0/1499	0.39	0/2009
20	T	0.15	0/1326	0.40	0/1770
21	U	0.12	0/823	0.33	0/1104
22	V	0.26	1/1048 (0.1%)	0.39	0/1402
23	W	0.12	0/873	0.30	0/1158
24	X	0.12	0/984	0.31	0/1323
25	Y	0.14	0/1132	0.33	0/1504
26	Z	0.11	0/1130	0.27	0/1507
27	a	0.11	0/1191	0.26	0/1590
28	b	0.15	0/861	0.34	0/1138
29	c	0.15	0/771	0.39	0/1034
30	d	0.19	0/903	0.34	0/1216
31	e	0.11	0/1071	0.28	0/1429
32	f	0.20	0/895	0.39	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.15	0/916	0.36	0/1220
34	h	0.12	0/1021	0.31	0/1348
35	i	0.12	0/841	0.31	0/1112
36	j	0.09	0/720	0.25	0/952
37	k	0.14	0/575	0.32	0/761
38	l	0.16	0/459	0.49	0/608
39	m	0.38	1/435 (0.2%)	0.58	0/575
40	n	0.20	0/240	0.41	0/305
41	o	0.11	0/864	0.31	0/1140
42	p	0.16	0/718	0.38	0/953
43	r	0.11	0/1010	0.29	0/1354
44	s	0.20	0/1530	0.53	0/2064
45	t	0.08	0/1031	0.25	0/1392
46	2	0.12	0/1780	0.29	0/2771
46	3	0.08	0/1779	0.23	0/2767
47	5	0.10	0/84950	0.24	5/132471 (0.0%)
48	8	0.11	0/3581	0.24	0/5577
49	9	0.09	0/40503	0.23	0/63104
50	AA	0.13	0/1747	0.34	0/2374
51	BB	0.20	1/1756 (0.1%)	0.32	0/2350
52	CC	0.14	0/1753	0.37	1/2369 (0.0%)
53	DD	0.10	0/1796	0.27	0/2417
54	EE	0.11	0/2118	0.30	0/2849
55	FF	0.13	0/1492	0.31	0/2005
56	GG	0.10	0/1944	0.28	0/2587
57	HH	0.12	0/1510	0.31	0/2022
58	II	0.17	0/1715	0.50	0/2287
59	JJ	0.11	0/1550	0.28	0/2069
60	KK	0.12	0/834	0.31	0/1125
61	LL	0.13	0/1195	0.36	0/1597
62	MM	0.12	0/918	0.35	0/1233
63	NN	0.14	0/1226	0.33	0/1649
64	OO	0.13	0/1029	0.36	0/1380
65	PP	0.13	0/1079	0.36	0/1441
66	QQ	0.10	0/1146	0.28	0/1534
67	RR	0.12	0/1082	0.33	0/1452
68	SS	0.14	0/1208	0.35	0/1618
69	TT	0.11	0/1112	0.30	0/1489
70	UU	0.21	0/805	0.48	0/1081
71	VV	0.15	0/643	0.37	0/860
72	WW	0.17	0/1051	0.41	0/1406
73	XX	0.12	0/1116	0.32	0/1490
74	YY	0.13	0/1028	0.35	0/1366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	ZZ	0.16	0/604	0.38	0/810
76	aa	0.13	0/828	0.35	0/1109
77	bb	0.12	0/665	0.32	0/891
78	cc	0.12	0/490	0.37	0/656
79	dd	0.16	0/470	0.35	0/623
80	ee	0.11	0/462	0.31	0/607
81	ff	0.12	0/567	0.33	0/753
82	gg	0.09	0/2493	0.24	0/3394
83	AT	0.10	0/1642	0.27	0/2557
84	EF	0.20	0/3442	0.51	0/4656
85	1	0.68	4/348 (1.1%)	0.59	0/538
All	All	0.12	7/236542 (0.0%)	0.29	6/346919 (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
3	B	0	1
32	f	0	1
39	m	0	1
73	XX	0	1
84	EF	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	1	1493	G	C1'-N9	-7.04	1.37	1.48
51	BB	189	ILE	CA-CB	6.90	1.58	1.53
22	V	6	ARG	C-N	-6.55	1.30	1.33
85	1	1490	C	C1'-N1	5.52	1.56	1.48
85	1	1498	A	C1'-N9	-5.21	1.40	1.48
85	1	1492	C	C1'-N1	5.18	1.56	1.48
39	m	58	GLN	CG-CD	5.09	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	752	G	OP1-P-OP2	-13.33	79.61	119.60
47	5	751	G	OP2-P-O3'	-12.10	71.69	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	752	G	O5'-P-OP1	-10.12	77.65	108.00
47	5	751	G	OP1-P-O3'	9.48	136.45	108.00
47	5	752	G	O5'-P-OP2	7.45	130.36	108.00
52	CC	73	MET	CB-CG-SD	6.14	131.13	112.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	258	HIS	Peptide
84	EF	159	GLU	Peptide
73	XX	61	GLN	Peptide
32	f	106	TYR	Peptide
39	m	58	GLN	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	7	2538	1286	1286	8	0
2	A	1898	1993	1993	44	0
3	B	3172	3310	3310	61	0
4	C	2883	3053	3053	40	0
5	D	2391	2424	2424	34	0
6	E	1729	1887	1887	34	0
7	F	1875	1995	1995	38	0
8	G	1879	2027	2027	36	0
9	H	1516	1597	1597	51	0
10	I	1664	1712	1712	24	0
11	J	1362	1399	1399	27	0
12	L	1702	1820	1820	18	0
13	M	1137	1211	1211	28	0
14	N	1701	1749	1749	40	0
15	O	1630	1778	1778	37	0
16	P	1242	1274	1274	20	0
17	Q	1515	1634	1634	25	0
18	R	1505	1655	1655	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	1460	1501	1501	46	0
20	T	1298	1366	1366	36	0
21	U	809	833	833	13	0
22	V	1034	1097	1097	24	0
23	W	860	903	903	9	0
24	X	967	1040	1040	20	0
25	Y	1115	1205	1205	18	0
26	Z	1107	1182	1182	10	0
27	a	1162	1209	1209	20	0
28	b	848	920	920	17	0
29	c	761	794	794	24	0
30	d	888	930	930	23	0
31	e	1053	1147	1147	11	0
32	f	876	912	912	20	0
33	g	906	998	998	16	0
34	h	1013	1147	1147	15	0
35	i	830	916	916	15	0
36	j	705	737	737	6	0
37	k	569	637	637	9	0
38	l	447	480	480	7	0
39	m	429	465	465	14	0
40	n	239	289	289	8	0
41	o	851	920	920	14	0
42	p	708	756	756	24	0
43	r	994	1051	1051	10	0
44	s	1507	1564	1564	86	0
45	t	1021	1066	1065	10	0
46	2	1595	813	814	15	0
46	3	1595	813	815	8	0
47	5	75955	38351	38384	409	0
48	8	3208	1628	1629	20	0
49	9	36229	18288	18304	244	0
50	AA	1710	1708	1708	45	0
51	BB	1729	1803	1803	38	0
52	CC	1716	1806	1806	38	0
53	DD	1768	1866	1863	54	0
54	EE	2076	2177	2177	41	0
55	FF	1471	1522	1522	35	0
56	GG	1921	2084	2084	44	0
57	HH	1488	1582	1582	32	0
58	II	1686	1772	1772	43	0
59	JJ	1525	1640	1640	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	KK	810	836	836	14	0
61	LL	1175	1249	1249	28	0
62	MM	908	939	939	16	0
63	NN	1202	1289	1289	21	0
64	OO	1016	1039	1039	30	0
65	PP	1058	1104	1104	18	0
66	QQ	1128	1195	1195	12	0
67	RR	1068	1121	1121	27	0
68	SS	1190	1249	1249	24	0
69	TT	1094	1123	1123	20	0
70	UU	795	862	862	31	0
71	VV	636	637	637	24	0
72	WW	1034	1080	1080	42	0
73	XX	1098	1167	1167	23	0
74	YY	1011	1083	1083	21	0
75	ZZ	598	656	656	29	0
76	aa	814	863	863	13	0
77	bb	651	672	672	12	0
78	cc	488	514	514	17	0
79	dd	459	448	448	13	0
80	ee	457	502	502	31	0
81	ff	555	563	563	12	0
82	gg	2436	2393	2393	27	0
83	AT	1471	749	750	17	0
84	EF	3383	3431	3431	257	0
85	1	313	105	163	71	0
86	5	189	0	0	0	0
86	7	6	0	0	0	0
86	8	5	0	0	0	0
86	9	70	0	0	0	0
86	A	1	0	0	0	0
86	EF	1	0	0	0	0
86	I	1	0	0	0	0
86	P	1	0	0	0	0
86	V	1	0	0	0	0
86	a	1	0	0	0	0
87	aa	1	0	0	0	0
87	dd	1	0	0	0	0
87	ff	1	0	0	0	0
87	g	1	0	0	0	0
87	j	1	0	0	0	0
87	m	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	o	1	0	0	0	0
87	p	1	0	0	0	0
88	EF	32	12	12	3	0
All	All	220632	164603	164711	2683	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 7.

All (2683) 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)
53:DD:116:ARG:HH22	85:1:1504:U:C4'	1.31	1.40
53:DD:116:ARG:NH1	85:1:1504:U:OP1	1.56	1.37
53:DD:143:ARG:NH1	85:1:1503:A:C8	2.00	1.29
53:DD:116:ARG:NH2	85:1:1504:U:H4'	1.46	1.27
15:O:5:GLN:N	15:O:5:GLN:HE21	1.33	1.23
53:DD:116:ARG:HH22	85:1:1504:U:C5'	1.51	1.22
80:ee:124:LYS:NZ	85:1:1504:U:C6	2.07	1.22
53:DD:116:ARG:NH2	85:1:1504:U:H5'	1.60	1.15
53:DD:143:ARG:NE	85:1:1502:A:C4'	1.94	1.14
53:DD:143:ARG:CD	85:1:1502:A:H4'	1.77	1.13
84:EF:312:VAL:HG23	84:EF:315:VAL:HG21	1.14	1.11
49:9:1698:C:O2	85:1:1500:A:N1	1.85	1.08
49:9:1698:C:C2	85:1:1500:A:N6	2.20	1.07
80:ee:124:LYS:CE	85:1:1504:U:C6	2.42	1.03
53:DD:116:ARG:NH2	85:1:1504:U:C5'	2.16	1.02
85:1:1493:G:C6	85:1:1494:C:N4	2.29	1.01
49:9:1698:C:C2	85:1:1500:A:N1	2.30	1.00
53:DD:143:ARG:NE	85:1:1502:A:H4'	1.37	1.00
53:DD:143:ARG:NH1	85:1:1503:A:N7	2.04	1.00
53:DD:116:ARG:HH22	85:1:1504:U:H4'	0.85	0.99
80:ee:124:LYS:CE	85:1:1504:U:H6	1.76	0.99
53:DD:116:ARG:CZ	85:1:1504:U:H5'	1.98	0.93
80:ee:124:LYS:NZ	85:1:1504:U:C5	2.32	0.92
15:O:5:GLN:N	15:O:5:GLN:NE2	2.17	0.91
11:J:20:LEU:HD23	11:J:79:ALA:HB1	1.53	0.91
19:S:61:ILE:HD12	19:S:61:ILE:O	1.70	0.90
49:9:1698:C:C2	85:1:1500:A:C6	2.61	0.89
52:CC:73:MET:O	52:CC:73:MET:HE3	1.72	0.89
84:EF:277:VAL:HG22	84:EF:286:THR:HG22	1.56	0.88
49:9:1560:U:O2	49:9:1575:G:O6	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:ee:124:LYS:HE2	85:1:1504:U:H6	1.40	0.86
20:T:84:ILE:HD11	28:b:21:ILE:HG22	1.58	0.86
68:SS:71:MET:O	68:SS:71:MET:HE3	1.79	0.83
14:N:161:MET:HE1	47:5:55:G:O4'	1.78	0.82
71:VV:55:ILE:HD11	71:VV:69:ILE:HD11	1.61	0.82
80:ee:124:LYS:NZ	85:1:1504:U:O5'	2.11	0.82
71:VV:55:ILE:HG23	71:VV:59:ILE:HD11	1.61	0.81
51:BB:110:MET:HE2	51:BB:110:MET:HA	1.62	0.80
72:WW:52:ILE:HG22	72:WW:61:ILE:CD1	2.12	0.80
80:ee:124:LYS:HE3	85:1:1504:U:H2'	1.62	0.80
20:T:91:VAL:HG23	20:T:96:ILE:HD11	1.64	0.80
46:2:22:G:N7	46:2:46:G:O6	2.15	0.79
72:WW:52:ILE:HD12	72:WW:52:ILE:O	1.83	0.78
68:SS:10:GLN:HG3	68:SS:13:LEU:HD21	1.65	0.78
3:B:252:ALA:HB3	47:5:4457:U:O2	1.83	0.78
49:9:804:U:O2	49:9:859:G:O6	2.02	0.78
59:JJ:91:LYS:HE2	59:JJ:91:LYS:HA	1.65	0.78
10:I:200:ILE:O	10:I:200:ILE:HD12	1.83	0.78
3:B:216:MET:HA	3:B:216:MET:HE3	1.65	0.77
84:EF:114:LEU:HB3	84:EF:150:VAL:HG22	1.66	0.77
53:DD:70:THR:HG22	53:DD:86:LEU:HD13	1.65	0.77
80:ee:124:LYS:HE2	85:1:1504:U:C6	2.13	0.77
46:2:35:G:H1	85:1:1495:U:H3	1.32	0.77
9:H:4:ILE:HD11	19:S:152:PHE:HB3	1.67	0.76
44:s:62:ARG:HG3	44:s:82:ILE:HD12	1.68	0.76
53:DD:143:ARG:HE	85:1:1502:A:C4'	1.86	0.76
53:DD:143:ARG:HH12	85:1:1503:A:C8	1.43	0.76
14:N:161:MET:HE1	47:5:55:G:C1'	2.14	0.76
19:S:93:MET:HE3	19:S:94:TYR:H	1.51	0.76
56:GG:32:MET:HE3	56:GG:63:MET:HE3	1.68	0.75
49:9:1757:G:O6	49:9:1775:U:O2	2.04	0.75
84:EF:271:VAL:HG22	84:EF:303:LEU:HD22	1.70	0.74
84:EF:232:LEU:HA	84:EF:235:ILE:HD12	1.70	0.73
47:5:1918:U:O2	47:5:2064:G:O6	2.06	0.73
50:AA:174:MET:HE2	50:AA:174:MET:HA	1.68	0.73
18:R:3:MET:HE2	18:R:3:MET:HA	1.71	0.73
25:Y:55:VAL:HG13	25:Y:104:VAL:HG13	1.69	0.73
84:EF:250:LEU:HD13	84:EF:253:VAL:HG21	1.71	0.73
6:E:156:LEU:HD21	6:E:198:ILE:CD1	2.19	0.72
44:s:14:PHE:HD1	44:s:64:ALA:HB2	1.52	0.72
60:KK:49:MET:HA	60:KK:49:MET:HE3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:161:ILE:HD12	9:H:162:GLN:N	2.05	0.71
2:A:101:VAL:HG23	2:A:164:ALA:C	2.14	0.71
68:SS:71:MET:HE2	68:SS:99:LEU:HD21	1.73	0.71
70:UU:80:PHE:HB3	79:dd:52:PHE:CE2	2.25	0.71
84:EF:294:MET:CG	84:EF:299:LEU:HD11	2.20	0.71
53:DD:116:ARG:NH2	85:1:1504:U:C4'	2.15	0.71
58:II:115:SER:HA	58:II:137:LEU:HD21	1.72	0.71
49:9:1698:C:N1	85:1:1500:A:N6	2.39	0.70
57:HH:148:LEU:HD13	72:WW:42:MET:HE2	1.73	0.70
30:d:27:ILE:HD11	30:d:52:PHE:CZ	2.26	0.70
49:9:29:G:O2'	73:XX:131:LEU:HD11	1.91	0.70
4:C:152:LEU:HD11	4:C:174:LEU:HD12	1.72	0.70
54:EE:195:ILE:H	54:EE:195:ILE:HD12	1.57	0.69
84:EF:294:MET:HG2	84:EF:299:LEU:HD11	1.74	0.69
30:d:96:GLU:OE1	30:d:96:GLU:O	2.10	0.69
84:EF:368:ILE:HG23	84:EF:408:LYS:HB3	1.75	0.69
20:T:159:MET:HA	20:T:159:MET:HE3	1.73	0.69
22:V:45:ILE:HD12	22:V:45:ILE:O	1.91	0.69
84:EF:426:VAL:HG21	84:EF:434:ALA:HB3	1.75	0.69
9:H:41:ILE:HD11	9:H:69:THR:HB	1.74	0.69
30:d:64:ILE:HG22	30:d:106:VAL:HB	1.74	0.69
49:9:1698:C:N3	85:1:1500:A:N6	2.33	0.69
75:ZZ:77:LEU:O	75:ZZ:77:LEU:HD23	1.93	0.69
77:bb:42:LYS:NZ	77:bb:57:VAL:HG22	2.06	0.69
84:EF:361:LEU:HD13	84:EF:424:PHE:CD1	2.27	0.69
84:EF:246:LEU:HD21	84:EF:248:LEU:HG	1.75	0.69
3:B:224:LYS:HZ3	47:5:4625:C:P	2.17	0.68
3:B:314:ILE:HD11	3:B:326:VAL:HG11	1.76	0.68
22:V:40:ILE:HD11	47:5:3799:A:C4	2.28	0.68
84:EF:106:THR:OG1	84:EF:143:LEU:HD13	1.93	0.68
84:EF:114:LEU:HB2	84:EF:148:LEU:HD21	1.75	0.68
84:EF:261:THR:HB	84:EF:315:VAL:HG23	1.74	0.68
9:H:165:THR:HG21	9:H:179:ILE:HG22	1.76	0.68
13:M:118:MET:HE3	47:5:4929:C:O4'	1.94	0.68
44:s:135:THR:HG23	44:s:147:ILE:CG1	2.24	0.68
49:9:1698:C:C4	85:1:1500:A:N6	2.60	0.68
53:DD:21:LEU:HD21	53:DD:48:ILE:HD11	1.75	0.68
52:CC:135:GLY:O	52:CC:165:VAL:HG22	1.94	0.68
72:WW:52:ILE:HG22	72:WW:61:ILE:HD13	1.76	0.68
82:gg:5:MET:HE1	82:gg:312:VAL:HG22	1.75	0.68
7:F:174:ILE:CD1	7:F:178:LEU:HD12	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DD:143:ARG:HD3	85:1:1502:A:H4'	1.76	0.68
3:B:252:ALA:HB1	47:5:4524:G:C2	2.28	0.68
61:LL:136:LYS:HG3	61:LL:137:THR:HG23	1.76	0.67
84:EF:148:LEU:HD23	84:EF:188:VAL:HG13	1.76	0.67
19:S:169:THR:HG22	47:5:4875:G:H2'	1.76	0.67
7:F:90:PHE:CE2	7:F:92:ILE:HD11	2.29	0.67
32:f:101:ILE:HD12	32:f:101:ILE:O	1.95	0.67
72:WW:52:ILE:HG22	72:WW:61:ILE:HD12	1.76	0.67
85:1:1502:A:H1'	85:1:1503:A:N6	2.09	0.67
18:R:78:ILE:HD12	18:R:79:GLY:N	2.10	0.67
9:H:92:MET:HE1	9:H:161:ILE:HD11	1.74	0.67
20:T:154:ILE:HD12	20:T:154:ILE:O	1.94	0.67
77:bb:31:TYR:CD2	77:bb:33:MET:HE2	2.30	0.67
71:VV:41:LYS:HE2	71:VV:41:LYS:HA	1.77	0.67
84:EF:340:PHE:HB2	84:EF:412:VAL:HG21	1.77	0.66
3:B:148:LYS:N	3:B:148:LYS:HE2	2.11	0.66
78:cc:42:ILE:C	78:cc:42:ILE:HD12	2.21	0.66
44:s:135:THR:HG23	44:s:147:ILE:HG12	1.77	0.66
12:L:154:VAL:HG22	12:L:155:MET:HG3	1.78	0.66
40:n:20:MET:N	40:n:20:MET:HE2	2.11	0.66
62:MM:33:ARG:NH2	62:MM:91:LEU:HD11	2.11	0.66
49:9:442:C:H42	49:9:449:A:H62	1.44	0.66
15:O:48:TYR:CE1	15:O:52:LEU:HD21	2.31	0.66
16:P:48:LEU:HD11	16:P:91:LEU:HD11	1.76	0.66
9:H:12:ILE:O	9:H:12:ILE:HD12	1.96	0.65
12:L:108:GLU:OE2	35:i:17:VAL:HG13	1.94	0.65
53:DD:143:ARG:NH1	85:1:1503:A:C5	2.54	0.65
84:EF:426:VAL:CG2	84:EF:434:ALA:HB3	2.26	0.65
85:1:1501:U:H2'	85:1:1502:A:C2	2.31	0.65
3:B:47:LEU:HD12	3:B:84:MET:SD	2.37	0.65
26:Z:89:ILE:HG23	26:Z:91:LEU:CD2	2.26	0.65
6:E:115:MET:HE1	47:5:2261:G:H4'	1.77	0.65
33:g:25:THR:HG22	33:g:29:ARG:O	1.97	0.65
56:GG:106:LEU:HD13	56:GG:109:LEU:HD11	1.78	0.65
42:p:29:ILE:HD11	42:p:69:TRP:CD2	2.32	0.65
44:s:40:MET:HE2	47:5:1996:C:O2'	1.96	0.65
81:ff:130:VAL:HG11	81:ff:143:LYS:HZ2	1.61	0.65
84:EF:155:MET:HE3	84:EF:208:MET:HE3	1.78	0.65
13:M:57:LEU:HD12	13:M:57:LEU:O	1.96	0.65
30:d:46:LEU:HD13	30:d:49:ILE:HD11	1.79	0.65
51:BB:229:MET:HA	51:BB:229:MET:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:132:LEU:HD23	7:F:141:TRP:CD2	2.32	0.65
32:f:104:MET:HA	32:f:104:MET:HE3	1.77	0.65
35:i:57:ALA:HB2	35:i:73:ILE:HD11	1.79	0.65
53:DD:18:LYS:HE2	53:DD:18:LYS:HA	1.79	0.65
58:II:83:TYR:HB2	58:II:202:ILE:HG22	1.79	0.65
3:B:252:ALA:HB1	47:5:4524:G:N3	2.11	0.64
33:g:65:MET:HE2	33:g:65:MET:N	2.13	0.64
47:5:2638:G:H22	47:5:2697:A:H61	1.42	0.64
71:VV:11:LEU:HD23	71:VV:11:LEU:H	1.62	0.64
44:s:43:ILE:HG21	44:s:53:VAL:HG23	1.78	0.64
84:EF:340:PHE:CB	84:EF:412:VAL:HG21	2.27	0.64
16:P:140:MET:HE3	16:P:140:MET:H	1.62	0.64
20:T:48:VAL:HG21	20:T:94:GLU:HG2	1.78	0.64
44:s:138:PHE:HB2	44:s:145:THR:HG21	1.78	0.64
10:I:97:ILE:HD12	10:I:97:ILE:O	1.97	0.64
35:i:36:HIS:O	35:i:40:VAL:HG23	1.97	0.64
9:H:81:ILE:O	9:H:85:THR:HG22	1.97	0.64
14:N:6:TYR:HE1	35:i:40:VAL:HG22	1.63	0.64
71:VV:64:GLU:HG3	77:bb:3:LEU:HD21	1.78	0.64
41:o:82:MET:HE2	41:o:82:MET:H	1.63	0.64
80:ee:124:LYS:HZ1	85:1:1504:U:P	2.20	0.64
84:EF:150:VAL:HG23	84:EF:188:VAL:CG1	2.28	0.64
6:E:165:VAL:HG11	6:E:178:VAL:HG22	1.78	0.64
14:N:6:TYR:CD1	35:i:40:VAL:HG13	2.33	0.64
63:NN:66:VAL:HG13	63:NN:67:THR:HG23	1.79	0.64
53:DD:116:ARG:NH1	85:1:1504:U:H5'	2.13	0.64
84:EF:159:GLU:HG3	84:EF:160:PRO:HD3	1.80	0.64
84:EF:189:ALA:HB2	84:EF:216:VAL:HG12	1.80	0.64
11:J:119:TYR:CE1	68:SS:12:ILE:HD12	2.33	0.64
13:M:91:TRP:O	13:M:95:ILE:HG23	1.97	0.64
20:T:95:HIS:C	20:T:96:ILE:HD12	2.23	0.64
19:S:80:ILE:HD12	19:S:129:VAL:HG22	1.79	0.63
30:d:27:ILE:HD11	30:d:52:PHE:CE2	2.33	0.63
14:N:6:TYR:CE1	35:i:40:VAL:HG22	2.33	0.63
55:FF:100:ILE:HG21	55:FF:111:VAL:HG11	1.79	0.63
72:WW:69:LEU:HD11	72:WW:71:LYS:C	2.23	0.63
85:1:1493:G:N1	85:1:1494:C:C4	2.66	0.63
44:s:47:LEU:HD12	44:s:101:MET:HE1	1.80	0.63
44:s:161:ILE:HG12	44:s:167:VAL:HG22	1.78	0.63
84:EF:338:ALA:O	84:EF:405:VAL:HG13	1.99	0.63
6:E:156:LEU:HD21	6:E:198:ILE:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:WW:7:LEU:HD22	72:WW:34:ILE:HD12	1.79	0.63
84:EF:34:ILE:HG21	84:EF:39:ILE:HD12	1.80	0.63
29:c:45:LEU:HD12	29:c:47:ILE:HD11	1.81	0.63
84:EF:28:ILE:HD11	84:EF:89:ILE:HD13	1.80	0.63
11:J:91:GLU:OE1	11:J:91:GLU:O	2.16	0.63
84:EF:147:GLN:OE1	84:EF:235:ILE:HG23	1.98	0.63
14:N:64:ILE:C	14:N:64:ILE:HD12	2.23	0.63
14:N:161:MET:HE1	47:5:55:G:H1'	1.81	0.63
47:5:4993:G:O6	47:5:5058:A:N1	2.32	0.63
84:EF:75:ILE:CG2	84:EF:90:ILE:HG23	2.28	0.63
8:G:226:LEU:HD12	14:N:6:TYR:HE2	1.64	0.63
81:f:130:VAL:HG11	81:f:143:LYS:NZ	2.13	0.63
84:EF:313:LYS:O	84:EF:315:VAL:HG13	1.98	0.63
16:P:119:VAL:HG22	16:P:146:ILE:HD12	1.80	0.62
34:h:33:VAL:O	34:h:37:THR:HG23	1.99	0.62
13:M:24:LEU:HD11	13:M:86:TRP:CG	2.34	0.62
18:R:99:MET:HE1	18:R:127:VAL:O	1.99	0.62
51:BB:71:LEU:O	51:BB:71:LEU:HD23	1.99	0.62
52:CC:65:LYS:HE2	52:CC:273:LEU:HD13	1.81	0.62
9:H:4:ILE:HD11	19:S:152:PHE:CB	2.29	0.62
34:h:80:PRO:HD2	34:h:83:LEU:HD12	1.81	0.62
58:II:170:LYS:C	58:II:171:LEU:HD23	2.24	0.62
42:p:8:VAL:HG12	47:5:2876:G:OP1	2.00	0.62
54:EE:134:LYS:HE2	54:EE:134:LYS:HA	1.81	0.62
5:D:146:LEU:HD23	5:D:147:ASP:N	2.15	0.62
56:GG:63:MET:HE2	56:GG:64:LYS:N	2.15	0.62
77:bb:5:LYS:HD2	77:bb:7:LEU:HD23	1.80	0.62
55:FF:103:LEU:HD12	75:ZZ:66:LYS:NZ	2.15	0.62
75:ZZ:66:LYS:HD3	75:ZZ:66:LYS:C	2.25	0.62
18:R:95:TRP:CZ2	18:R:99:MET:HE3	2.34	0.61
84:EF:11:VAL:HG22	84:EF:13:ILE:HG23	1.82	0.61
84:EF:147:GLN:CD	84:EF:235:ILE:HG23	2.25	0.61
44:s:65:ILE:HG21	44:s:79:LEU:HG	1.83	0.61
7:F:186:MET:O	7:F:190:ILE:HG23	2.01	0.61
19:S:93:MET:HE3	19:S:93:MET:HA	1.82	0.61
68:SS:18:THR:HG21	68:SS:33:ILE:HA	1.83	0.61
53:DD:141:LYS:C	53:DD:142:LEU:HD12	2.26	0.61
44:s:14:PHE:CD1	44:s:64:ALA:HB2	2.35	0.61
49:9:1154:U:C5	52:CC:192:LEU:HD13	2.36	0.61
49:9:1698:C:C6	85:1:1500:A:N6	2.68	0.61
53:DD:51:LEU:CD1	53:DD:91:VAL:HG22	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:1091:C:HO2'	72:WW:2:VAL:N	1.98	0.61
64:OO:99:ALA:H	64:OO:133:THR:HG22	1.66	0.61
64:OO:131:ASP:OD1	64:OO:133:THR:HG23	2.00	0.61
6:E:64:MET:HE2	6:E:64:MET:HA	1.83	0.60
58:II:170:LYS:O	58:II:171:LEU:HD23	2.01	0.60
4:C:309:ILE:HD12	4:C:309:ILE:O	2.01	0.60
9:H:165:THR:HG21	9:H:179:ILE:CG2	2.31	0.60
13:M:104:MET:HA	13:M:104:MET:HE3	1.83	0.60
53:DD:161:GLY:O	53:DD:164:VAL:HG12	2.01	0.60
67:RR:58:MET:HE3	67:RR:58:MET:HA	1.83	0.60
9:H:103:VAL:HG21	9:H:144:LEU:HD11	1.83	0.60
15:O:5:GLN:HE21	15:O:5:GLN:CA	2.12	0.60
54:EE:181:CYS:HB2	54:EE:195:ILE:HD11	1.83	0.60
39:m:55:SER:O	39:m:58:GLN:HB2	2.01	0.60
50:AA:34:MET:HE1	50:AA:154:LEU:HD11	1.83	0.60
84:EF:20:LYS:HD2	84:EF:92:ALA:HB3	1.83	0.60
84:EF:248:LEU:CD2	84:EF:267:VAL:HG22	2.31	0.60
85:1:1493:G:C6	85:1:1494:C:C4	2.89	0.60
24:X:82:THR:HG22	24:X:155:ILE:HD13	1.84	0.60
84:EF:116:VAL:HG13	84:EF:123:PHE:CD2	2.35	0.60
84:EF:277:VAL:CG2	84:EF:286:THR:HG22	2.30	0.60
7:F:24:PHE:CG	7:F:24:PHE:O	2.55	0.60
56:GG:132:ARG:C	56:GG:133:LEU:HD12	2.26	0.60
25:Y:42:TYR:CG	25:Y:119:LEU:HD21	2.36	0.60
44:s:143:ILE:HG22	44:s:154:ILE:HG23	1.84	0.60
59:JJ:114:VAL:HG13	59:JJ:119:LEU:HD11	1.84	0.60
9:H:44:GLU:OE1	9:H:44:GLU:N	2.34	0.60
22:V:20:LEU:HD21	22:V:84:GLN:HB2	1.84	0.60
41:o:82:MET:HE2	41:o:82:MET:N	2.17	0.60
74:YY:25:ILE:HD12	74:YY:25:ILE:O	2.02	0.60
11:J:109:ILE:CD1	11:J:115:LEU:HD21	2.32	0.60
34:h:4:ILE:HD12	34:h:4:ILE:O	2.01	0.60
84:EF:250:LEU:HD13	84:EF:253:VAL:CG2	2.32	0.60
15:O:16:LEU:HD11	15:O:83:THR:HG21	1.83	0.60
57:HH:35:ASP:OD1	57:HH:36:LEU:HD22	2.02	0.59
19:S:24:THR:HG23	19:S:24:THR:O	2.00	0.59
29:c:96:ILE:HD12	29:c:96:ILE:O	2.01	0.59
32:f:9:ALA:HB3	32:f:101:ILE:CD1	2.32	0.59
84:EF:246:LEU:HD22	84:EF:328:ASP:H	1.66	0.59
7:F:135:VAL:O	7:F:135:VAL:HG12	2.00	0.59
13:M:31:ILE:HG22	13:M:32:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:144:ARG:HD3	3:B:148:LYS:HE3	1.84	0.59
9:H:34:LEU:HD13	9:H:84:VAL:HG22	1.84	0.59
44:s:121:VAL:HG21	44:s:161:ILE:HD13	1.84	0.59
57:HH:61:ILE:HD11	57:HH:95:ILE:HG13	1.85	0.59
27:a:81:LEU:HD21	27:a:106:SER:HB3	1.85	0.59
62:MM:46:GLN:OE1	62:MM:46:GLN:O	2.21	0.59
85:1:1493:G:O6	85:1:1494:C:N4	2.34	0.59
3:B:47:LEU:HD11	3:B:181:MET:HE3	1.84	0.59
21:U:29:VAL:HG22	21:U:34:MET:HE1	1.84	0.59
47:5:2657:G:H2'	47:5:2658:G:C4	2.38	0.59
49:9:616:A:C4'	80:ee:84:LYS:HZ3	2.15	0.59
5:D:106:ALA:HB1	5:D:171:LEU:HD23	1.84	0.59
19:S:51:LEU:HD22	19:S:52:LYS:HG2	1.84	0.59
50:AA:185:MET:HA	50:AA:185:MET:HE3	1.85	0.59
82:gg:265:ILE:HD12	82:gg:265:ILE:O	2.03	0.59
44:s:43:ILE:HG21	44:s:53:VAL:CG2	2.32	0.59
55:FF:76:MET:HE2	55:FF:76:MET:HA	1.83	0.59
2:A:245:ARG:NE	2:A:245:ARG:HA	2.17	0.58
80:ee:124:LYS:CE	85:1:1504:U:H2'	2.32	0.58
21:U:63:LEU:HD23	21:U:63:LEU:H	1.68	0.58
64:OO:119:LEU:HD12	64:OO:120:ALA:N	2.18	0.58
84:EF:11:VAL:HG12	84:EF:111:CYS:O	2.02	0.58
2:A:46:LYS:HE3	47:5:4121:G:H21	1.68	0.58
29:c:56:ARG:O	29:c:60:ILE:HG22	2.02	0.58
82:gg:4:GLN:C	82:gg:5:MET:HE2	2.28	0.58
84:EF:139:LEU:O	84:EF:143:LEU:HD12	2.03	0.58
45:t:116:MET:SD	45:t:132:ILE:HD11	2.43	0.58
24:X:90:ILE:HG22	24:X:95:THR:O	2.02	0.58
84:EF:216:VAL:HG11	84:EF:234:CYS:SG	2.44	0.58
10:I:48:LEU:HD21	10:I:167:ILE:HD11	1.85	0.58
39:m:51:ILE:HG23	39:m:52:ILE:HG22	1.84	0.58
47:5:132:G:N2	47:5:137:G:C6	2.71	0.58
69:TT:28:LEU:HD23	69:TT:110:LEU:HD21	1.84	0.58
7:F:85:GLU:N	7:F:85:GLU:OE1	2.36	0.58
29:c:48:LEU:HD21	29:c:60:ILE:HG21	1.85	0.58
49:9:957:A:H3'	49:9:958:G:H21	1.69	0.58
85:1:1493:G:N1	85:1:1494:C:N4	2.52	0.58
8:G:159:THR:HG22	8:G:160:LYS:H	1.67	0.58
53:DD:221:THR:O	53:DD:223:ILE:HD12	2.04	0.58
82:gg:44:LYS:HE2	82:gg:44:LYS:HA	1.84	0.58
3:B:389:MET:HE3	3:B:389:MET:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:95:VAL:HB	39:m:56:LEU:HD12	1.85	0.57
50:AA:34:MET:HE2	50:AA:34:MET:HA	1.86	0.57
58:II:106:SER:HB2	58:II:171:LEU:HD21	1.85	0.57
78:cc:42:ILE:HD13	78:cc:44:ARG:HG3	1.85	0.57
84:EF:149:ILE:CD1	84:EF:231:ALA:HB1	2.35	0.57
84:EF:341:THR:HG21	84:EF:376:LYS:HE3	1.84	0.57
34:h:17:LEU:HD13	34:h:61:ILE:HD11	1.86	0.57
50:AA:24:HIS:HB3	50:AA:51:LEU:HD21	1.85	0.57
64:OO:75:MET:SD	64:OO:75:MET:C	2.87	0.57
3:B:224:LYS:N	3:B:224:LYS:HD2	2.20	0.57
15:O:34:VAL:HG11	15:O:112:TYR:CE2	2.40	0.57
69:TT:110:LEU:HD12	69:TT:110:LEU:O	2.04	0.57
72:WW:7:LEU:HD12	72:WW:74:VAL:HG23	1.86	0.57
11:J:128:LEU:HD11	11:J:130:PHE:CE1	2.39	0.57
30:d:64:ILE:HG22	30:d:106:VAL:CB	2.35	0.57
44:s:123:VAL:O	44:s:123:VAL:HG12	2.05	0.57
49:9:1698:C:H1'	85:1:1500:A:N1	2.19	0.57
53:DD:51:LEU:HD11	53:DD:91:VAL:HG22	1.85	0.57
56:GG:64:LYS:HB2	56:GG:97:VAL:HG21	1.86	0.57
61:LL:96:ILE:HD13	73:XX:10:ALA:HB1	1.86	0.57
9:H:18:ILE:C	9:H:18:ILE:HD12	2.29	0.57
34:h:17:LEU:HB3	34:h:61:ILE:HD11	1.87	0.57
57:HH:40:LEU:HD23	57:HH:43:LEU:HD21	1.87	0.57
84:EF:181:ILE:O	84:EF:181:ILE:HG22	2.03	0.57
84:EF:193:ILE:HG21	84:EF:228:LEU:HB3	1.87	0.57
56:GG:1:MET:CE	56:GG:109:LEU:HD21	2.35	0.57
24:X:119:ILE:HG21	24:X:140:LEU:HD23	1.87	0.57
50:AA:77:ILE:HD13	50:AA:122:LEU:HD12	1.85	0.57
84:EF:191:VAL:HG22	84:EF:214:TRP:CE2	2.39	0.57
84:EF:191:VAL:HG22	84:EF:214:TRP:NE1	2.20	0.57
4:C:132:ALA:O	4:C:150:LEU:HD22	2.05	0.56
15:O:54:TYR:CD1	15:O:145:VAL:HG21	2.39	0.56
29:c:26:LYS:HE2	29:c:26:LYS:N	2.19	0.56
49:9:1154:U:H4'	49:9:1155:U:H3'	1.87	0.56
58:II:113:TYR:CE1	58:II:121:LEU:HD13	2.40	0.56
84:EF:148:LEU:O	84:EF:188:VAL:HG22	2.05	0.56
84:EF:312:VAL:CG2	84:EF:315:VAL:HG21	2.10	0.56
3:B:326:VAL:O	3:B:326:VAL:HG13	2.05	0.56
20:T:40:VAL:HG13	20:T:96:ILE:HG23	1.85	0.56
34:h:65:GLN:OE1	34:h:65:GLN:HA	2.05	0.56
41:o:66:ILE:C	41:o:66:ILE:HD12	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:GG:26:THR:HG22	56:GG:36:VAL:CG1	2.35	0.56
67:RR:50:ILE:O	67:RR:54:VAL:HG23	2.04	0.56
3:B:149:ASP:O	3:B:153:MET:HG3	2.05	0.56
6:E:49:ASN:HB3	6:E:64:MET:HE3	1.87	0.56
9:H:176:LEU:HD12	39:m:60:ALA:HB1	1.87	0.56
10:I:48:LEU:CD2	10:I:167:ILE:HD11	2.34	0.56
15:O:102:LEU:HD11	15:O:104:VAL:HG23	1.85	0.56
26:Z:46:ILE:HD13	26:Z:68:ILE:CG2	2.34	0.56
30:d:29:ILE:O	30:d:33:ILE:HG22	2.04	0.56
54:EE:45:ILE:HG13	54:EE:61:VAL:HG11	1.88	0.56
58:II:73:THR:HG23	58:II:73:THR:O	2.04	0.56
68:SS:20:ILE:HD11	68:SS:33:ILE:HD11	1.86	0.56
70:UU:80:PHE:CD1	79:dd:54:LYS:HB3	2.41	0.56
61:LL:72:ILE:C	61:LL:73:LEU:HD23	2.30	0.56
72:WW:34:ILE:O	72:WW:38:LEU:HD22	2.04	0.56
84:EF:200:ASN:HA	84:EF:227:THR:HG22	1.88	0.56
11:J:93:GLU:C	11:J:94:LEU:HD22	2.31	0.56
17:Q:18:PRO:HG3	17:Q:29:VAL:HG21	1.88	0.56
39:m:52:ILE:HG23	39:m:57:ARG:HH11	1.69	0.56
50:AA:58:LEU:HD12	50:AA:174:MET:SD	2.46	0.56
84:EF:148:LEU:HD23	84:EF:188:VAL:CG1	2.36	0.56
8:G:192:GLY:O	8:G:196:VAL:HG23	2.04	0.56
9:H:33:THR:C	9:H:34:LEU:HD12	2.31	0.56
10:I:49:CYS:O	10:I:167:ILE:HD12	2.06	0.56
84:EF:294:MET:HG3	84:EF:299:LEU:HD11	1.86	0.56
7:F:92:ILE:HD13	7:F:119:GLY:HA2	1.86	0.56
61:LL:103:GLU:OE1	73:XX:11:ARG:HB3	2.06	0.56
84:EF:256:ILE:HG12	84:EF:262:VAL:HG21	1.87	0.56
84:EF:263:PRO:CD	84:EF:312:VAL:HG22	2.35	0.56
58:II:138:ASN:C	58:II:139:LYS:HD2	2.31	0.56
84:EF:312:VAL:HG23	84:EF:315:VAL:CG2	2.10	0.56
2:A:235:VAL:HG12	2:A:236:GLY:H	1.70	0.56
19:S:130:GLU:OE2	19:S:131:GLU:N	2.39	0.56
34:h:17:LEU:HD13	34:h:61:ILE:CD1	2.35	0.56
53:DD:52:ALA:C	53:DD:91:VAL:HG23	2.30	0.56
44:s:116:ILE:C	44:s:116:ILE:HD12	2.31	0.56
49:9:885:U:O2	49:9:901:G:O6	2.24	0.56
58:II:23:LYS:H	58:II:23:LYS:HD3	1.71	0.56
62:MM:45:ARG:CZ	62:MM:45:ARG:HA	2.35	0.56
66:QQ:70:VAL:HG11	66:QQ:84:ILE:CD1	2.35	0.56
8:G:317:LYS:HD2	51:BB:225:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:HH:134:VAL:HG23	57:HH:134:VAL:O	2.07	0.55
70:UU:48:LEU:CD1	70:UU:91:LEU:HD22	2.36	0.55
84:EF:11:VAL:O	84:EF:11:VAL:HG13	2.06	0.55
12:L:79:GLU:O	12:L:83:VAL:HG23	2.07	0.55
30:d:48:GLU:HA	30:d:48:GLU:OE2	2.06	0.55
32:f:9:ALA:HB3	32:f:101:ILE:HD11	1.88	0.55
43:r:56:ASP:C	43:r:56:ASP:OD1	2.49	0.55
58:II:87:ASN:OD1	58:II:90:LEU:HD22	2.06	0.55
65:PP:83:MET:HE2	65:PP:83:MET:HA	1.88	0.55
77:bb:42:LYS:HZ2	77:bb:57:VAL:HG22	1.70	0.55
3:B:43:LEU:HB3	3:B:183:ILE:HG21	1.87	0.55
22:V:45:ILE:HD12	22:V:45:ILE:C	2.30	0.55
32:f:69:VAL:HG21	47:5:4944:C:O2	2.05	0.55
61:LL:18:GLN:O	61:LL:18:GLN:CD	2.49	0.55
61:LL:80:MET:N	61:LL:80:MET:HE3	2.21	0.55
84:EF:150:VAL:HG23	84:EF:188:VAL:HG12	1.88	0.55
84:EF:412:VAL:HG23	84:EF:441:VAL:HG13	1.87	0.55
20:T:72:VAL:HG13	20:T:74:ILE:HD11	1.88	0.55
59:JJ:45:ARG:HD3	59:JJ:46:VAL:HG13	1.88	0.55
84:EF:93:PRO:HD2	84:EF:102:MET:HB2	1.88	0.55
84:EF:294:MET:HG3	84:EF:299:LEU:HD21	1.89	0.55
2:A:98:ILE:HD13	42:p:80:LYS:HE3	1.88	0.55
21:U:25:CYS:HB3	21:U:112:LEU:HD23	1.89	0.55
24:X:95:THR:O	24:X:96:LEU:HD23	2.05	0.55
25:Y:1:MET:HE2	47:5:1368:A:HI'	1.89	0.55
50:AA:75:SER:HB3	50:AA:122:LEU:HD13	1.89	0.55
53:DD:72:VAL:CG2	60:KK:20:VAL:HG21	2.37	0.55
56:GG:25:ARG:HD2	56:GG:25:ARG:C	2.32	0.55
56:GG:113:ILE:H	56:GG:113:ILE:HD12	1.72	0.55
51:BB:205:TYR:O	51:BB:207:LEU:HD12	2.06	0.55
57:HH:144:ILE:HG22	72:WW:52:ILE:HG13	1.87	0.55
84:EF:423:ARG:HA	84:EF:437:VAL:HG12	1.89	0.55
2:A:36:GLU:OE1	2:A:36:GLU:HA	2.07	0.55
4:C:137:VAL:HG11	4:C:144:ILE:HD13	1.88	0.55
39:m:72:LYS:HD2	39:m:92:THR:HG21	1.88	0.55
45:t:56:LEU:HD11	45:t:82:ILE:HG21	1.89	0.55
84:EF:138:LEU:HD12	84:EF:181:ILE:HD11	1.89	0.55
1:7:61:G:H4'	5:D:271:MET:HE2	1.88	0.55
14:N:20:ARG:NH1	14:N:20:ARG:HB2	2.22	0.55
16:P:99:GLU:C	16:P:99:GLU:OE1	2.50	0.55
58:II:114:GLU:O	58:II:137:LEU:HD11	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:bb:42:LYS:HZ1	77:bb:57:VAL:HG22	1.72	0.55
16:P:147:GLU:N	16:P:147:GLU:OE2	2.39	0.55
22:V:19:GLY:C	22:V:20:LEU:HD22	2.32	0.55
28:b:103:LYS:HA	28:b:103:LYS:HE3	1.88	0.55
56:GG:32:MET:SD	56:GG:100:CYS:HB2	2.46	0.55
57:HH:95:ILE:O	57:HH:95:ILE:HD12	2.07	0.55
59:JJ:29:LEU:HD22	80:ee:115:PHE:CE1	2.42	0.55
7:F:183:ILE:HG21	7:F:189:LEU:HD12	1.89	0.55
19:S:93:MET:HE1	47:5:1952:G:H4'	1.89	0.55
42:p:57:CYS:O	42:p:61:MET:HA	2.07	0.55
50:AA:118:GLU:O	50:AA:118:GLU:CD	2.50	0.55
54:EE:195:ILE:HD12	54:EE:195:ILE:N	2.22	0.55
84:EF:214:TRP:CZ3	84:EF:216:VAL:HG13	2.42	0.55
29:c:106:ARG:H	29:c:106:ARG:HD2	1.72	0.54
40:n:15:ARG:NH1	49:9:1182:A:H5''	2.22	0.54
47:5:2845:A:H61	47:5:3843:C:H42	1.56	0.54
49:9:823:U:O4'	74:YY:64:PHE:CZ	2.61	0.54
49:9:1464:C:P	67:RR:63:ARG:NH2	2.80	0.54
50:AA:34:MET:CE	50:AA:154:LEU:HD11	2.37	0.54
21:U:43:LEU:O	21:U:47:ILE:HD13	2.07	0.54
57:HH:148:LEU:CD1	72:WW:42:MET:HE2	2.38	0.54
18:R:173:ARG:HE	18:R:173:ARG:HA	1.72	0.54
50:AA:185:MET:HE1	71:VV:39:VAL:HG23	1.89	0.54
84:EF:39:ILE:HA	84:EF:42:PHE:HB3	1.90	0.54
44:s:20:LEU:HD22	44:s:90:PHE:CB	2.38	0.54
49:9:616:A:P	73:XX:65:ALA:HB1	2.47	0.54
63:NN:89:TYR:HA	63:NN:92:ILE:HD12	1.89	0.54
69:TT:123:LEU:HD21	69:TT:131:LEU:HD11	1.89	0.54
84:EF:75:ILE:HG21	84:EF:90:ILE:HG23	1.90	0.54
8:G:139:VAL:HG11	8:G:238:LYS:HG3	1.88	0.54
27:a:78:LEU:HD13	27:a:78:LEU:O	2.08	0.54
47:5:1817:U:N3	47:5:1823:G:C6	2.75	0.54
56:GG:100:CYS:SG	56:GG:101:ILE:HD13	2.48	0.54
80:ee:108:ARG:HA	80:ee:108:ARG:NE	2.22	0.54
29:c:79:ILE:O	29:c:83:THR:HG23	2.07	0.54
33:g:85:LYS:O	33:g:88:ARG:HG2	2.07	0.54
40:n:15:ARG:HH12	49:9:1183:A:P	2.31	0.54
47:5:1971:C:C5	47:5:2000:G:H2'	2.43	0.54
52:CC:79:GLU:N	52:CC:79:GLU:OE1	2.40	0.54
11:J:19:LYS:C	11:J:20:LEU:HD22	2.33	0.54
28:b:32:LEU:N	28:b:32:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:UU:35:VAL:HA	70:UU:38:ASP:OD2	2.08	0.54
84:EF:155:MET:HB3	84:EF:162:TYR:CD2	2.42	0.54
84:EF:248:LEU:HD13	84:EF:272:LEU:HD12	1.89	0.54
8:G:217:ILE:HG22	8:G:221:VAL:CG1	2.37	0.54
49:9:962:A:H4'	55:FF:135:ARG:HH22	1.72	0.54
61:LL:125:ILE:HD12	61:LL:125:ILE:N	2.23	0.54
17:Q:138:LEU:HD21	47:5:1427:A:C6	2.43	0.54
62:MM:69:CYS:SG	62:MM:76:LEU:HD21	2.48	0.54
75:ZZ:54:THR:HB	75:ZZ:77:LEU:HD21	1.90	0.54
1:7:26:C:OP1	5:D:56:THR:HG21	2.08	0.54
16:P:112:LEU:HB3	16:P:150:LEU:HD12	1.90	0.54
29:c:37:MET:SD	29:c:97:ILE:HD11	2.47	0.54
44:s:28:PHE:CE1	44:s:189:ILE:HD12	2.43	0.54
47:5:4584:A:H62	47:5:4718:G:H21	1.54	0.54
62:MM:79:VAL:HG11	62:MM:85:LEU:HD12	1.90	0.54
82:gg:21:ILE:HG22	82:gg:31:ILE:HD11	1.89	0.54
84:EF:15:HIS:CD2	84:EF:16:VAL:HG12	2.43	0.54
84:EF:102:MET:SD	84:EF:136:HIS:CD2	3.01	0.54
84:EF:103:ILE:HG23	84:EF:143:LEU:HD11	1.89	0.54
2:A:98:ILE:H	2:A:98:ILE:HD12	1.73	0.53
10:I:83:ASP:OD1	10:I:83:ASP:O	2.26	0.53
39:m:52:ILE:HG23	39:m:57:ARG:NH1	2.22	0.53
49:9:494:C:H41	49:9:509:G:H21	1.54	0.53
53:DD:41:VAL:HG13	53:DD:41:VAL:O	2.08	0.53
63:NN:127:ARG:O	63:NN:131:THR:HG23	2.08	0.53
85:1:1498:A:H2'	85:1:1499:C:C5'	2.38	0.53
29:c:42:LYS:N	29:c:42:LYS:HD2	2.23	0.53
49:9:1139:C:H41	49:9:1149:A:H62	1.56	0.53
51:BB:103:MET:HE3	51:BB:103:MET:C	2.33	0.53
53:DD:143:ARG:NH1	85:1:1503:A:N9	2.53	0.53
57:HH:154:ILE:H	57:HH:154:ILE:HD12	1.72	0.53
85:1:1498:A:C2'	85:1:1499:C:H5'	2.38	0.53
5:D:115:MET:HE2	5:D:139:PRO:HG2	1.90	0.53
47:5:2634:C:C2	47:5:2635:U:C5	2.96	0.53
52:CC:215:MET:HA	52:CC:215:MET:HE3	1.89	0.53
14:N:124:ASP:OD1	14:N:125:SER:N	2.42	0.53
20:T:154:ILE:HD12	20:T:154:ILE:C	2.33	0.53
22:V:18:LEU:HD23	22:V:18:LEU:H	1.74	0.53
42:p:29:ILE:HD11	42:p:69:TRP:CE3	2.43	0.53
66:QQ:31:LEU:HD23	66:QQ:31:LEU:H	1.72	0.53
67:RR:60:ARG:HG2	67:RR:63:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:13:ILE:HA	84:EF:92:ALA:HB2	1.89	0.53
84:EF:341:THR:HG22	84:EF:401:ILE:CG2	2.38	0.53
13:M:5:ARG:HB3	13:M:57:LEU:HD13	1.90	0.53
14:N:6:TYR:HD1	35:i:40:VAL:HG13	1.73	0.53
19:S:30:MET:CE	19:S:32:ILE:HD11	2.39	0.53
44:s:135:THR:HG23	44:s:147:ILE:HG13	1.91	0.53
54:EE:63:LYS:HZ2	74:YY:18:LEU:HD23	1.73	0.53
84:EF:147:GLN:CG	84:EF:235:ILE:HG23	2.39	0.53
85:l:1498:A:O2'	85:l:1499:C:H5'	2.09	0.53
4:C:168:VAL:HG23	4:C:177:TRP:CZ3	2.44	0.53
18:R:136:ARG:N	18:R:136:ARG:HD2	2.24	0.53
25:Y:127:GLN:OE1	25:Y:127:GLN:C	2.52	0.53
36:j:67:LEU:HD22	36:j:67:LEU:N	2.24	0.53
45:t:116:MET:HE2	45:t:131:GLU:OE2	2.09	0.53
61:LL:122:ILE:O	61:LL:122:ILE:HD12	2.09	0.53
84:EF:262:VAL:HG22	84:EF:311:ASN:HB2	1.91	0.53
51:BB:212:VAL:O	51:BB:212:VAL:HG13	2.09	0.53
53:DD:48:ILE:HG21	53:DD:86:LEU:HD12	1.89	0.53
49:9:805:U:H5''	72:WW:83:LEU:HD23	1.91	0.53
80:ee:101:ARG:CZ	80:ee:101:ARG:HA	2.38	0.53
84:EF:218:ARG:HG2	84:EF:236:LEU:HD23	1.91	0.53
84:EF:250:LEU:HD11	84:EF:280:PHE:HE2	1.73	0.53
8:G:103:ASP:OD1	8:G:105:THR:HG23	2.09	0.53
37:k:6:GLU:N	37:k:6:GLU:OE1	2.41	0.53
47:5:3758:U:H2'	47:5:3765:G:H22	1.74	0.53
63:NN:37:ILE:HG23	63:NN:50:ILE:HG21	1.91	0.53
84:EF:22:THR:HG23	84:EF:57:ALA:HB2	1.91	0.53
84:EF:340:PHE:CD2	84:EF:404:MET:HE2	2.44	0.53
10:I:52:MET:HB2	10:I:152:LEU:HD12	1.90	0.53
16:P:67:VAL:O	16:P:80:GLN:OE1	2.26	0.53
16:P:110:ASP:C	16:P:110:ASP:OD1	2.52	0.53
21:U:25:CYS:O	21:U:29:VAL:HG23	2.09	0.53
52:CC:192:LEU:HD23	52:CC:193:VAL:N	2.24	0.53
56:GG:122:PRO:HA	56:GG:126:ASP:OD1	2.09	0.53
5:D:74:ILE:O	5:D:74:ILE:HG23	2.09	0.52
8:G:217:ILE:O	8:G:221:VAL:HG13	2.10	0.52
20:T:68:THR:HG21	47:5:4313:A:O3'	2.09	0.52
21:U:55:ASN:O	21:U:55:ASN:OD1	2.27	0.52
25:Y:98:GLY:C	25:Y:99:ILE:HD12	2.34	0.52
30:d:101:LYS:C	30:d:102:LEU:HD12	2.34	0.52
47:5:1336:G:H2'	47:5:2346:C:H42	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4396:A:N6	47:5:4447:C:O2	2.42	0.52
48:8:75:G:H2'	48:8:76:C:C6	2.44	0.52
51:BB:168:MET:HA	51:BB:197:ILE:HD12	1.90	0.52
74:YY:7:ILE:HD11	74:YY:40:ILE:HD13	1.91	0.52
2:A:44:ILE:HD11	2:A:85:GLY:HA2	1.90	0.52
7:F:59:GLU:O	7:F:63:MET:HG3	2.09	0.52
20:T:91:VAL:CG2	20:T:96:ILE:HD11	2.36	0.52
44:s:75:LEU:CB	44:s:78:LEU:HD22	2.39	0.52
45:t:104:ILE:HB	45:t:143:VAL:HG22	1.91	0.52
53:DD:38:GLU:OE1	53:DD:49:ILE:HD12	2.08	0.52
59:JJ:28:GLU:HG3	59:JJ:43:VAL:HG11	1.91	0.52
84:EF:8:ILE:HG21	84:EF:111:CYS:SG	2.49	0.52
84:EF:10:ILE:HG23	84:EF:10:ILE:O	2.09	0.52
84:EF:13:ILE:HB	84:EF:136:HIS:HB3	1.89	0.52
84:EF:248:LEU:CD1	84:EF:272:LEU:HD12	2.39	0.52
5:D:15:ARG:HH12	47:5:1743:A:H1'	1.75	0.52
5:D:271:MET:HB2	5:D:275:GLN:OE1	2.10	0.52
9:H:105:ILE:HD12	9:H:105:ILE:O	2.10	0.52
22:V:36:ASN:C	22:V:37:LEU:HD12	2.34	0.52
42:p:8:VAL:O	42:p:8:VAL:HG13	2.09	0.52
49:9:1298:G:H5''	65:PP:77:LYS:HD2	1.91	0.52
49:9:1665:G:C5	69:TT:88:MET:HE1	2.44	0.52
54:EE:147:ILE:HD12	54:EE:147:ILE:H	1.74	0.52
60:KK:64:TRP:CE3	79:dd:23:VAL:HG22	2.44	0.52
69:TT:45:LEU:HD23	69:TT:45:LEU:H	1.74	0.52
6:E:165:VAL:HG12	6:E:166:VAL:N	2.25	0.52
15:O:158:GLU:OE1	15:O:158:GLU:HA	2.09	0.52
32:f:10:ILE:HD12	32:f:10:ILE:N	2.25	0.52
41:o:85:ILE:HG22	41:o:86:LYS:N	2.24	0.52
62:MM:33:ARG:CZ	62:MM:91:LEU:HD11	2.39	0.52
3:B:216:MET:HE2	3:B:281:ASN:HA	1.90	0.52
8:G:200:VAL:HG23	8:G:232:VAL:HG21	1.90	0.52
10:I:184:MET:HE3	10:I:190:LEU:HD13	1.91	0.52
24:X:80:PRO:C	24:X:81:LEU:HD12	2.34	0.52
24:X:81:LEU:HD11	24:X:99:ILE:CD1	2.39	0.52
24:X:150:ALA:HB1	24:X:155:ILE:HG23	1.92	0.52
24:X:153:ILE:HD11	24:X:155:ILE:HG22	1.91	0.52
47:5:909:A:C2	47:5:910:G:N7	2.78	0.52
47:5:4896:G:H2'	47:5:4897:G:H8	1.74	0.52
17:Q:19:LYS:HD2	17:Q:20:SER:N	2.24	0.52
23:W:82:ILE:HD12	56:GG:144:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:48:LYS:O	38:l:49:LEU:HD12	2.08	0.52
50:AA:55:TRP:CZ3	50:AA:58:LEU:HD22	2.45	0.52
55:FF:100:ILE:CG2	55:FF:111:VAL:HG11	2.40	0.52
61:LL:86:ILE:C	61:LL:86:ILE:HD12	2.34	0.52
65:PP:69:PRO:C	65:PP:70:MET:HE2	2.34	0.52
84:EF:118:ALA:HB2	84:EF:152:VAL:HG13	1.92	0.52
30:d:22:THR:HG22	30:d:89:SER:HB2	1.90	0.52
31:e:57:ASN:C	31:e:57:ASN:OD1	2.52	0.52
31:e:66:THR:O	31:e:66:THR:HG22	2.09	0.52
47:5:4890:G:C2	47:5:4891:G:C8	2.98	0.52
52:CC:130:ILE:HG23	52:CC:162:ILE:HD11	1.92	0.52
52:CC:193:VAL:HG11	52:CC:240:THR:HA	1.92	0.52
52:CC:196:ILE:N	52:CC:196:ILE:HD12	2.25	0.52
62:MM:38:ALA:O	62:MM:42:LEU:HD13	2.10	0.52
69:TT:85:ASN:HB2	69:TT:88:MET:HB2	1.91	0.52
74:YY:62:THR:HA	74:YY:69:THR:HG22	1.90	0.52
76:aa:53:ILE:C	76:aa:53:ILE:HD12	2.35	0.52
82:gg:79:LEU:CD1	82:gg:120:ILE:HD13	2.39	0.52
84:EF:139:LEU:C	84:EF:143:LEU:HD12	2.35	0.52
2:A:74:GLU:N	2:A:74:GLU:OE1	2.42	0.52
2:A:96:LEU:HD21	42:p:87:LYS:HA	1.91	0.52
6:E:165:VAL:HG13	6:E:180:GLY:CA	2.38	0.52
9:H:161:ILE:HD12	9:H:161:ILE:C	2.33	0.52
30:d:20:VAL:HG23	30:d:20:VAL:O	2.09	0.52
46:3:1:G:C6	46:3:73:A:N1	2.78	0.52
49:9:1462:U:H3'	49:9:1463:U:O4'	2.10	0.52
54:EE:86:PHE:CD1	54:EE:103:TYR:CE1	2.98	0.52
56:GG:32:MET:CE	56:GG:63:MET:HE3	2.37	0.52
49:9:616:A:O2'	80:ee:85:VAL:HG22	2.09	0.52
50:AA:104:THR:O	50:AA:107:THR:HG23	2.09	0.52
53:DD:227:LYS:HE3	82:gg:184:LEU:HD11	1.91	0.52
84:EF:12:VAL:O	84:EF:92:ALA:HB2	2.10	0.52
3:B:231:VAL:HG21	3:B:251:VAL:HG23	1.90	0.52
13:M:99:GLU:C	13:M:99:GLU:OE1	2.53	0.52
17:Q:19:LYS:HE2	47:5:1349:G:H5''	1.91	0.52
27:a:112:LEU:HD23	47:5:1387:A:C6	2.45	0.52
54:EE:222:LEU:HA	54:EE:225:ILE:HD12	1.92	0.52
59:JJ:140:GLN:HG3	74:YY:64:PHE:CZ	2.45	0.52
60:KK:64:TRP:CE3	79:dd:23:VAL:HG13	2.45	0.52
84:EF:124:GLU:HA	84:EF:127:ILE:HG22	1.92	0.52
84:EF:263:PRO:HD3	84:EF:312:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:85:THR:HG23	9:H:86:LEU:HG	1.91	0.51
47:5:4948:C:H3'	47:5:4949:G:H5''	1.91	0.51
49:9:481:C:H2'	49:9:482:G:C1'	2.40	0.51
61:LL:40:ILE:HD11	61:LL:68:ILE:CG1	2.40	0.51
62:MM:17:ALA:C	62:MM:124:ILE:HD11	2.35	0.51
8:G:217:ILE:HG22	8:G:221:VAL:HG13	1.91	0.51
15:O:23:VAL:O	15:O:27:VAL:HG23	2.10	0.51
34:h:44:LEU:O	34:h:47:ILE:HG22	2.11	0.51
44:s:75:LEU:HB3	44:s:78:LEU:HD22	1.91	0.51
85:1:1500:A:H5''	85:1:1501:U:OP1	2.10	0.51
13:M:80:ALA:HB3	13:M:82:ILE:CD1	2.40	0.51
17:Q:19:LYS:NZ	47:5:1349:G:O5'	2.44	0.51
18:R:136:ARG:N	18:R:136:ARG:CD	2.73	0.51
18:R:154:LEU:C	18:R:154:LEU:HD23	2.35	0.51
47:5:271:C:C2	47:5:272:U:C5	2.98	0.51
52:CC:130:ILE:HG22	52:CC:158:ALA:HB1	1.92	0.51
55:FF:103:LEU:N	75:ZZ:66:LYS:HZ1	2.08	0.51
60:KK:3:MET:HE1	60:KK:48:ALA:N	2.24	0.51
75:ZZ:67:LEU:HD13	75:ZZ:68:ILE:N	2.25	0.51
84:EF:17:ASP:OD1	84:EF:71:ILE:HD11	2.10	0.51
33:g:6:THR:HG22	47:5:2400:G:H21	1.76	0.51
44:s:135:THR:HG21	44:s:146:LYS:HA	1.91	0.51
53:DD:48:ILE:CG2	53:DD:86:LEU:HD12	2.40	0.51
57:HH:129:ILE:HD11	57:HH:180:LEU:HD13	1.92	0.51
66:QQ:29:ASN:OD1	66:QQ:31:LEU:HD22	2.11	0.51
74:YY:43:LYS:C	74:YY:43:LYS:HD3	2.35	0.51
83:AT:52:G:H22	83:AT:64:G:H1	1.57	0.51
84:EF:6:THR:HG21	84:EF:237:PRO:HB3	1.92	0.51
84:EF:118:ALA:HB3	84:EF:154:LYS:O	2.10	0.51
84:EF:141:TYR:HB2	84:EF:183:TYR:CE2	2.45	0.51
10:I:184:MET:HG2	10:I:189:ARG:HB2	1.91	0.51
47:5:3616:U:O4'	47:5:3617:G:C6	2.64	0.51
55:FF:158:ALA:CB	55:FF:173:LEU:HD23	2.40	0.51
61:LL:40:ILE:HG12	61:LL:143:LEU:CD1	2.40	0.51
68:SS:71:MET:HE3	68:SS:71:MET:C	2.35	0.51
70:UU:38:ASP:HA	70:UU:41:ARG:HG3	1.92	0.51
84:EF:116:VAL:HG12	84:EF:116:VAL:O	2.10	0.51
84:EF:138:LEU:HD12	84:EF:181:ILE:CD1	2.40	0.51
3:B:223:THR:O	3:B:274:TYR:HA	2.09	0.51
3:B:257:TRP:CD1	3:B:257:TRP:C	2.89	0.51
3:B:389:MET:HE1	47:5:5041:G:C5	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:146:LEU:HD22	47:5:4323:A:H2	1.75	0.51
6:E:144:ARG:HB2	6:E:147:ILE:HG22	1.91	0.51
32:f:63:LYS:N	32:f:63:LYS:HD2	2.25	0.51
47:5:275:C:H4'	47:5:276:C:OP1	2.10	0.51
67:RR:41:ILE:HG21	67:RR:47:ARG:HB2	1.93	0.51
84:EF:11:VAL:HG23	84:EF:90:ILE:O	2.10	0.51
84:EF:49:MET:O	84:EF:49:MET:HE3	2.11	0.51
84:EF:246:LEU:HD23	84:EF:246:LEU:C	2.36	0.51
6:E:206:ILE:O	6:E:209:VAL:HG22	2.11	0.51
6:E:210:LYS:HE3	6:E:210:LYS:O	2.10	0.51
7:F:150:ASN:HD21	47:5:943:A:H62	1.58	0.51
17:Q:125:GLN:O	17:Q:129:ASP:OD1	2.29	0.51
44:s:138:PHE:CB	44:s:145:THR:HG21	2.40	0.51
57:HH:144:ILE:HD13	57:HH:154:ILE:HG13	1.91	0.51
84:EF:214:TRP:HZ3	84:EF:216:VAL:HG13	1.74	0.51
84:EF:281:ALA:HB3	84:EF:336:GLU:OE1	2.11	0.51
4:C:180:ILE:HD12	4:C:227:ILE:HD11	1.91	0.51
5:D:261:VAL:HG12	5:D:263:LYS:H	1.76	0.51
26:Z:46:ILE:HD11	26:Z:48:ARG:O	2.11	0.51
55:FF:103:LEU:HD12	75:ZZ:66:LYS:HZ1	1.74	0.51
80:ee:124:LYS:NZ	85:1:1504:U:P	2.84	0.51
3:B:262:VAL:CG2	47:5:4565:C:O4'	2.59	0.51
8:G:104:LEU:HD12	24:X:42:THR:O	2.10	0.51
14:N:136:ASP:C	14:N:136:ASP:OD1	2.54	0.51
19:S:79:GLY:C	19:S:80:ILE:HD13	2.36	0.51
19:S:125:GLN:OE1	19:S:125:GLN:C	2.53	0.51
25:Y:8:THR:HG23	25:Y:10:ASP:OD1	2.10	0.51
44:s:15:LEU:HA	44:s:18:ILE:HG22	1.92	0.51
47:5:2632:U:C2	47:5:2633:U:C5	2.98	0.51
49:9:1259:A:H1'	49:9:1264:C:H42	1.76	0.51
53:DD:11:PHE:CZ	70:UU:84:ILE:HD11	2.46	0.51
70:UU:35:VAL:HG21	70:UU:110:VAL:HG21	1.91	0.51
78:cc:42:ILE:HD12	78:cc:42:ILE:O	2.10	0.51
84:EF:75:ILE:HG23	84:EF:90:ILE:HG23	1.93	0.51
13:M:106:ASP:C	13:M:106:ASP:OD1	2.53	0.51
14:N:92:LEU:N	14:N:92:LEU:HD12	2.26	0.51
17:Q:13:VAL:HG22	17:Q:13:VAL:O	2.11	0.51
26:Z:46:ILE:HD13	26:Z:68:ILE:HG23	1.92	0.51
42:p:28:LYS:O	42:p:31:ILE:HG13	2.10	0.51
49:9:1360:U:H3'	49:9:1361:G:C8	2.46	0.51
57:HH:144:ILE:HG22	72:WW:52:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:aa:45:VAL:CG2	76:aa:64:LEU:HD13	2.41	0.51
80:ee:101:ARG:HA	80:ee:101:ARG:NE	2.26	0.51
84:EF:116:VAL:HG13	84:EF:123:PHE:CG	2.45	0.51
4:C:62:THR:HG21	4:C:91:ALA:HB1	1.94	0.50
17:Q:42:THR:HA	17:Q:45:GLN:OE1	2.11	0.50
19:S:93:MET:HE3	19:S:93:MET:CA	2.41	0.50
19:S:93:MET:HE3	19:S:94:TYR:N	2.22	0.50
25:Y:79:VAL:HG21	25:Y:98:GLY:HA3	1.93	0.50
28:b:32:LEU:HD23	47:5:1464:C:C5'	2.40	0.50
33:g:5:LEU:H	33:g:5:LEU:HD23	1.76	0.50
49:9:1589:A:O3'	69:TT:82:ARG:HD2	2.11	0.50
71:VV:59:ILE:C	71:VV:59:ILE:HD12	2.36	0.50
81:ff:99:LYS:HB3	81:ff:100:LEU:HD22	1.92	0.50
84:EF:394:LEU:HD22	84:EF:400:ALA:HB3	1.93	0.50
6:E:205:ASP:C	6:E:205:ASP:OD1	2.54	0.50
42:p:31:ILE:HD12	42:p:32:SER:N	2.26	0.50
48:8:108:A:N1	48:8:112:G:C6	2.78	0.50
51:BB:124:HIS:O	51:BB:124:HIS:ND1	2.43	0.50
58:II:23:LYS:HD3	58:II:23:LYS:N	2.26	0.50
72:WW:27:ILE:HD11	72:WW:61:ILE:HG13	1.93	0.50
72:WW:47:ILE:C	72:WW:47:ILE:HD12	2.36	0.50
72:WW:86:LEU:C	72:WW:86:LEU:HD23	2.37	0.50
6:E:247:GLU:OE1	6:E:248:GLN:N	2.44	0.50
15:O:169:ARG:CZ	47:5:4860:G:H5''	2.40	0.50
18:R:3:MET:C	18:R:4:LEU:HD22	2.36	0.50
30:d:64:ILE:HG22	30:d:106:VAL:CG2	2.41	0.50
44:s:55:MET:C	44:s:55:MET:SD	2.94	0.50
47:5:2265:G:H1'	47:5:2266:C:OP1	2.12	0.50
54:EE:103:TYR:CD2	54:EE:182:MET:HE2	2.46	0.50
2:A:115:CYS:SG	2:A:165:VAL:HG12	2.52	0.50
3:B:224:LYS:HD2	3:B:224:LYS:H	1.75	0.50
4:C:146:GLU:N	4:C:146:GLU:OE2	2.45	0.50
19:S:32:ILE:HG21	19:S:40:ALA:HA	1.92	0.50
20:T:94:GLU:OE1	20:T:94:GLU:N	2.44	0.50
21:U:29:VAL:HG11	21:U:68:SER:OG	2.11	0.50
37:k:30:ASP:C	37:k:30:ASP:OD1	2.54	0.50
69:TT:45:LEU:HD23	69:TT:45:LEU:N	2.25	0.50
43:r:81:THR:C	43:r:82:ILE:HD12	2.37	0.50
49:9:1079:C:H4'	49:9:1182:A:H61	1.77	0.50
49:9:1698:C:C5	85:1:1500:A:N6	2.80	0.50
73:XX:115:ILE:HD12	73:XX:118:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:42:PHE:HE2	84:EF:59:VAL:HG22	1.77	0.50
30:d:22:THR:HG22	30:d:89:SER:CB	2.42	0.50
51:BB:110:MET:HE1	51:BB:113:MET:CE	2.41	0.50
54:EE:126:VAL:HG22	54:EE:158:ASP:O	2.12	0.50
57:HH:134:VAL:HG21	57:HH:158:LEU:HD11	1.94	0.50
62:MM:45:ARG:HA	62:MM:45:ARG:NH1	2.26	0.50
84:EF:186:ASP:HB3	84:EF:217:THR:HG23	1.92	0.50
85:1:1502:A:H1'	85:1:1503:A:H62	1.77	0.50
3:B:43:LEU:HD12	3:B:183:ILE:HG21	1.93	0.50
3:B:231:VAL:HG21	3:B:251:VAL:CG2	2.42	0.50
4:C:150:LEU:HD23	4:C:150:LEU:C	2.37	0.50
4:C:152:LEU:HD11	4:C:174:LEU:CD1	2.41	0.50
8:G:199:LEU:CD1	8:G:205:ALA:HB2	2.42	0.50
33:g:59:VAL:HG22	33:g:60:ARG:H	1.75	0.50
42:p:89:LEU:C	42:p:89:LEU:HD13	2.37	0.50
50:AA:76:VAL:HG13	50:AA:123:VAL:CG2	2.42	0.50
51:BB:201:CYS:SG	51:BB:207:LEU:HD13	2.51	0.50
76:aa:44:ILE:HD12	76:aa:45:VAL:HG22	1.94	0.50
78:cc:14:VAL:HG13	78:cc:30:VAL:CG1	2.42	0.50
16:P:119:VAL:HG13	16:P:146:ILE:CD1	2.42	0.50
22:V:71:GLU:N	22:V:71:GLU:OE1	2.45	0.50
28:b:70:GLU:HA	28:b:70:GLU:OE2	2.11	0.50
47:5:48:G:H1'	47:5:49:U:OP2	2.11	0.50
72:WW:10:ALA:HB1	72:WW:27:ILE:HD12	1.93	0.50
3:B:43:LEU:HD12	3:B:183:ILE:HB	1.94	0.50
10:I:183:ASP:C	10:I:183:ASP:OD1	2.54	0.50
11:J:43:LEU:CD1	11:J:82:ILE:HD12	2.42	0.50
15:O:162:GLU:OE1	15:O:162:GLU:HA	2.12	0.50
21:U:112:LEU:HD22	21:U:112:LEU:N	2.26	0.50
46:2:11:C:H2'	46:2:12:U:C6	2.46	0.50
49:9:1665:G:N7	69:TT:88:MET:HE1	2.27	0.50
50:AA:5:LEU:HB2	71:VV:41:LYS:HZ1	1.76	0.50
67:RR:113:SER:C	67:RR:114:LEU:HD22	2.37	0.50
68:SS:5:ILE:HD11	68:SS:9:PHE:CG	2.47	0.50
1:7:39:C:N3	11:J:73:THR:HG22	2.27	0.49
2:A:246:LEU:C	2:A:246:LEU:HD13	2.37	0.49
15:O:145:VAL:HG22	15:O:145:VAL:O	2.12	0.49
18:R:6:LEU:C	18:R:6:LEU:HD23	2.36	0.49
25:Y:121:ARG:NH2	47:5:194:C:O2	2.45	0.49
45:t:106:PHE:HA	45:t:109:ILE:HG22	1.94	0.49
51:BB:218:LEU:N	51:BB:218:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:CC:244:ILE:O	52:CC:247:THR:HG22	2.12	0.49
64:OO:99:ALA:N	64:OO:133:THR:HG22	2.27	0.49
69:TT:29:LYS:HG3	69:TT:29:LYS:O	2.12	0.49
75:ZZ:52:LYS:HE2	75:ZZ:52:LYS:N	2.27	0.49
85:1:1498:A:H2'	85:1:1499:C:H5'	1.93	0.49
5:D:15:ARG:HD3	20:T:19:PHE:HE1	1.77	0.49
6:E:64:MET:HE1	6:E:67:ARG:HD2	1.95	0.49
22:V:39:ILE:HD12	22:V:61:VAL:HG21	1.95	0.49
28:b:32:LEU:HD23	47:5:1464:C:H5''	1.93	0.49
41:o:82:MET:HE1	47:5:4346:U:O4'	2.12	0.49
44:s:35:VAL:HG13	44:s:35:VAL:O	2.12	0.49
44:s:62:ARG:NH2	44:s:83:ARG:HE	2.10	0.49
49:9:532:C:O2'	49:9:533:A:P	2.69	0.49
49:9:1355:C:H2'	49:9:1356:G:O4'	2.11	0.49
52:CC:75:ILE:HG21	52:CC:81:ILE:HD11	1.93	0.49
54:EE:63:LYS:NZ	74:YY:18:LEU:HD23	2.27	0.49
55:FF:102:LEU:HB3	75:ZZ:66:LYS:HE2	1.95	0.49
76:aa:19:GLN:OE1	76:aa:19:GLN:N	2.45	0.49
84:EF:24:THR:HG21	84:EF:60:LEU:HD11	1.94	0.49
9:H:105:ILE:HD12	9:H:105:ILE:C	2.37	0.49
18:R:63:CYS:O	18:R:67:THR:HG23	2.12	0.49
32:f:15:LYS:HB2	32:f:27:LEU:HD21	1.94	0.49
44:s:21:LEU:HD23	44:s:90:PHE:HZ	1.77	0.49
44:s:116:ILE:HD12	44:s:116:ILE:O	2.12	0.49
47:5:4717:A:H2'	47:5:4718:G:O4'	2.12	0.49
54:EE:47:PHE:CE2	54:EE:52:LEU:HD11	2.47	0.49
70:UU:67:LYS:CD	70:UU:67:LYS:C	2.85	0.49
72:WW:22:LYS:HA	72:WW:22:LYS:HE2	1.94	0.49
77:bb:5:LYS:HD3	77:bb:6:ASP:N	2.28	0.49
82:gg:64:HIS:NE2	82:gg:65:PHE:CE2	2.80	0.49
84:EF:16:VAL:HG23	84:EF:71:ILE:HD12	1.94	0.49
84:EF:292:VAL:HG12	84:EF:299:LEU:HD12	1.93	0.49
85:1:1493:G:C2	85:1:1494:C:C4	3.01	0.49
6:E:165:VAL:HG11	6:E:178:VAL:CG2	2.42	0.49
9:H:173:ARG:O	9:H:176:LEU:HD21	2.12	0.49
14:N:138:PHE:CD2	47:5:18:C:H4'	2.47	0.49
19:S:155:PRO:HB2	47:5:4764:A:N7	2.27	0.49
49:9:1337:C:O2'	70:UU:67:LYS:NZ	2.45	0.49
6:E:189:LEU:HD21	6:E:256:VAL:HG21	1.94	0.49
12:L:161:PHE:CD1	12:L:161:PHE:C	2.90	0.49
18:R:160:GLU:HA	18:R:160:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:149:GLU:N	20:T:149:GLU:OE1	2.45	0.49
26:Z:89:ILE:HD11	26:Z:117:LYS:HB3	1.95	0.49
49:9:158:A:H1'	49:9:464:A:N1	2.28	0.49
49:9:465:A:H4'	49:9:466:G:O5'	2.13	0.49
50:AA:5:LEU:HD23	50:AA:8:LEU:HD12	1.95	0.49
58:II:113:TYR:CD1	58:II:121:LEU:HD22	2.47	0.49
68:SS:101:ASN:C	68:SS:101:ASN:OD1	2.55	0.49
82:gg:21:ILE:CG2	82:gg:31:ILE:HD11	2.42	0.49
84:EF:152:VAL:HB	84:EF:192:PRO:HA	1.94	0.49
84:EF:262:VAL:HG13	84:EF:311:ASN:HA	1.95	0.49
5:D:153:THR:HG21	47:5:4323:A:N6	2.26	0.49
6:E:181:PRO:HB3	6:E:261:LEU:HD21	1.94	0.49
6:E:204:ILE:HD12	6:E:204:ILE:O	2.13	0.49
7:F:62:GLN:NE2	47:5:1212:G:H5''	2.28	0.49
9:H:172:ILE:HD13	39:m:64:ASN:HB3	1.94	0.49
14:N:64:ILE:C	14:N:64:ILE:CD1	2.85	0.49
38:l:29:MET:O	38:l:29:MET:SD	2.71	0.49
49:9:1481:G:H4'	70:UU:79:ARG:HH12	1.76	0.49
52:CC:199:PRO:O	52:CC:202:THR:HG23	2.12	0.49
65:PP:133:ILE:HD11	83:AT:41:A:H4'	1.95	0.49
71:VV:70:LEU:HD13	71:VV:70:LEU:C	2.38	0.49
84:EF:155:MET:HE2	84:EF:162:TYR:CD2	2.47	0.49
15:O:141:LEU:C	15:O:141:LEU:HD23	2.36	0.49
33:g:11:LEU:O	33:g:11:LEU:HD13	2.12	0.49
41:o:66:ILE:HD11	41:o:85:ILE:HB	1.94	0.49
41:o:96:ASP:C	41:o:96:ASP:OD1	2.55	0.49
50:AA:76:VAL:HG13	50:AA:123:VAL:HG23	1.95	0.49
57:HH:30:LEU:HD11	57:HH:82:GLU:OE1	2.13	0.49
68:SS:118:ARG:HG2	68:SS:118:ARG:O	2.12	0.49
84:EF:262:VAL:HG13	84:EF:311:ASN:CA	2.43	0.49
84:EF:292:VAL:HG13	84:EF:309:GLY:O	2.13	0.49
84:EF:378:LYS:O	84:EF:379:ILE:HD12	2.12	0.49
2:A:144:LYS:C	2:A:145:LYS:HD2	2.38	0.49
4:C:334:THR:HG21	7:F:50:TYR:OH	2.13	0.49
47:5:4700:A:C2	47:5:4701:A:C8	3.01	0.49
49:9:1143:A:H4'	49:9:1355:C:H42	1.77	0.49
70:UU:81:GLN:O	79:dd:53:ILE:O	2.29	0.49
84:EF:249:PRO:HB3	84:EF:365:THR:HG22	1.94	0.49
9:H:44:GLU:OE1	47:5:4764:A:N3	2.45	0.49
32:f:69:VAL:HG11	47:5:4944:C:O2	2.12	0.49
49:9:1591:C:O2'	55:FF:87:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AA:14:ASP:HB3	50:AA:177:MET:HE1	1.94	0.49
50:AA:121:LEU:HD22	50:AA:122:LEU:H	1.77	0.49
55:FF:160:GLU:OE2	55:FF:160:GLU:HA	2.13	0.49
84:EF:259:ILE:HG23	84:EF:260:GLY:N	2.28	0.49
6:E:285:TYR:CE2	32:f:32:GLY:HA3	2.48	0.49
18:R:28:GLU:O	18:R:32:ILE:HD13	2.13	0.49
20:T:84:ILE:HD11	28:b:21:ILE:CG2	2.36	0.49
25:Y:117:LYS:HD2	25:Y:118:ILE:HG23	1.95	0.49
28:b:65:MET:HE2	28:b:65:MET:HA	1.94	0.49
48:8:71:A:H4'	48:8:72:A:O5'	2.12	0.49
49:9:381:C:H5'	58:II:48:VAL:HG12	1.95	0.49
49:9:562:U:O4	49:9:587:A:N7	2.46	0.49
50:AA:40:LYS:HE2	67:RR:101:ASP:CG	2.37	0.49
58:II:132:GLU:O	58:II:136:ILE:HD12	2.13	0.49
75:ZZ:44:LEU:C	75:ZZ:44:LEU:HD12	2.38	0.49
76:aa:21:ILE:HD12	76:aa:21:ILE:O	2.12	0.49
76:aa:44:ILE:HD12	76:aa:45:VAL:N	2.28	0.49
76:aa:46:GLU:N	76:aa:46:GLU:OE2	2.45	0.49
80:ee:124:LYS:CE	85:1:1504:U:C5	2.91	0.49
84:EF:250:LEU:HD11	84:EF:280:PHE:CE2	2.48	0.49
84:EF:321:ARG:HG3	84:EF:322:ARG:N	2.28	0.49
84:EF:412:VAL:CG2	84:EF:441:VAL:HG13	2.42	0.49
32:f:101:ILE:HD12	32:f:101:ILE:C	2.38	0.48
37:k:69:LEU:HD23	37:k:69:LEU:C	2.37	0.48
40:n:20:MET:HE2	40:n:20:MET:CA	2.43	0.48
44:s:20:LEU:CD1	44:s:54:LEU:HD12	2.43	0.48
47:5:4699:U:H4'	47:5:4700:A:OP1	2.13	0.48
58:II:94:LYS:N	58:II:94:LYS:HD2	2.27	0.48
70:UU:24:LEU:HD12	70:UU:24:LEU:N	2.28	0.48
8:G:159:THR:HG22	8:G:160:LYS:N	2.29	0.48
15:O:113:ASP:C	15:O:113:ASP:OD1	2.56	0.48
18:R:96:MET:HA	18:R:96:MET:HE3	1.94	0.48
30:d:64:ILE:HD12	30:d:64:ILE:O	2.12	0.48
35:i:94:LEU:O	35:i:94:LEU:HD13	2.13	0.48
37:k:60:LEU:HD13	37:k:61:PRO:HD2	1.96	0.48
49:9:1180:C:H3'	49:9:1181:A:C8	2.48	0.48
64:OO:17:LEU:HD13	64:OO:18:GLY:N	2.28	0.48
65:PP:80:LEU:O	65:PP:116:LEU:HD12	2.14	0.48
75:ZZ:44:LEU:HD12	75:ZZ:44:LEU:O	2.13	0.48
84:EF:139:LEU:HD11	84:EF:432:THR:OG1	2.12	0.48
84:EF:303:LEU:HB3	84:EF:304:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:LEU:HD12	3:B:183:ILE:CB	2.44	0.48
4:C:189:MET:HE2	47:5:2333:G:N7	2.29	0.48
7:F:136:GLU:HA	7:F:136:GLU:OE2	2.12	0.48
19:S:130:GLU:OE2	19:S:131:GLU:O	2.32	0.48
19:S:147:ASP:C	19:S:147:ASP:OD1	2.55	0.48
34:h:15:GLU:N	34:h:15:GLU:OE2	2.45	0.48
44:s:66:ARG:CZ	44:s:79:LEU:HD22	2.43	0.48
47:5:3788:C:HO2'	47:5:3789:C:P	2.36	0.48
47:5:4880:C:H2'	47:5:4881:U:O4'	2.13	0.48
49:9:476:A:O2'	49:9:488:U:H4'	2.13	0.48
49:9:934:G:O6	49:9:1008:A:N1	2.46	0.48
49:9:1538:C:O3'	69:TT:45:LEU:HD21	2.13	0.48
52:CC:78:LEU:HD23	52:CC:78:LEU:H	1.78	0.48
55:FF:18:LYS:C	55:FF:19:LEU:HD22	2.38	0.48
81:ff:145:CYS:O	81:ff:145:CYS:SG	2.70	0.48
84:EF:368:ILE:HG21	84:EF:410:MET:CG	2.42	0.48
3:B:43:LEU:HD12	3:B:183:ILE:CG2	2.44	0.48
13:M:105:THR:HG22	13:M:106:ASP:H	1.79	0.48
19:S:115:ALA:HB1	47:5:1925:G:N3	2.27	0.48
41:o:51:GLN:NE2	41:o:55:ILE:HD11	2.28	0.48
47:5:2633:U:C2	47:5:2634:C:C5	3.00	0.48
47:5:4170:A:H1'	47:5:4171:C:OP2	2.12	0.48
53:DD:143:ARG:CG	85:1:1502:A:H4'	2.42	0.48
55:FF:153:LEU:HG	55:FF:189:ALA:HA	1.93	0.48
58:II:23:LYS:H	58:II:23:LYS:CD	2.26	0.48
59:JJ:124:HIS:NE2	80:ee:108:ARG:HD2	2.28	0.48
3:B:261:ARG:HD2	15:O:64:THR:OG1	2.13	0.48
16:P:119:VAL:HG13	16:P:146:ILE:HD11	1.96	0.48
20:T:103:ASP:C	20:T:103:ASP:OD1	2.56	0.48
43:r:28:GLU:HG2	43:r:29:PRO:HD2	1.95	0.48
44:s:116:ILE:HA	44:s:167:VAL:HG23	1.95	0.48
46:2:35:G:N2	85:1:1495:U:O2	2.46	0.48
47:5:351:C:H2'	47:5:352:G:O4'	2.13	0.48
47:5:4132:C:H2'	47:5:4133:C:O4'	2.14	0.48
49:9:933:G:H21	49:9:1000:C:H3'	1.78	0.48
57:HH:85:LYS:HD2	57:HH:85:LYS:C	2.39	0.48
84:EF:196:TRP:HD1	88:EF:502:GTP:H1'	1.78	0.48
6:E:115:MET:CE	47:5:2261:G:H4'	2.43	0.48
8:G:241:ALA:HB2	47:5:6:C:H1'	1.95	0.48
9:H:4:ILE:HB	19:S:144:GLN:HE21	1.78	0.48
9:H:126:VAL:HG11	9:H:161:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:127:GLN:OE1	20:T:129:LYS:O	2.31	0.48
42:p:64:VAL:HG11	42:p:71:TYR:HE1	1.78	0.48
47:5:1990:A:H3'	47:5:1991:A:H5''	1.95	0.48
47:5:2722:G:H2'	47:5:2723:U:O4'	2.13	0.48
53:DD:16:ILE:C	53:DD:16:ILE:HD12	2.39	0.48
57:HH:68:GLN:OE1	57:HH:68:GLN:O	2.32	0.48
58:II:137:LEU:HD13	58:II:137:LEU:C	2.39	0.48
65:PP:124:LYS:CD	65:PP:124:LYS:N	2.77	0.48
84:EF:248:LEU:HD11	84:EF:276:MET:HE1	1.94	0.48
84:EF:340:PHE:HD2	84:EF:404:MET:HE2	1.79	0.48
84:EF:353:ILE:HG23	84:EF:372:PHE:CE1	2.48	0.48
2:A:101:VAL:HG22	2:A:163:ARG:HB3	1.96	0.48
3:B:41:VAL:HG21	3:B:196:TRP:CG	2.48	0.48
13:M:2:VAL:HG23	13:M:2:VAL:O	2.13	0.48
17:Q:8:ASN:OD1	17:Q:9:LYS:N	2.46	0.48
47:5:3896:C:O3'	47:5:3897:G:O4'	2.32	0.48
49:9:1117:C:O2	49:9:1117:C:H2'	2.14	0.48
84:EF:216:VAL:HG21	84:EF:218:ARG:HH11	1.79	0.48
84:EF:368:ILE:HG21	84:EF:410:MET:HG2	1.95	0.48
5:D:210:TYR:O	5:D:214:GLU:HG2	2.13	0.48
14:N:21:PHE:CD1	14:N:21:PHE:C	2.91	0.48
41:o:71:GLU:OE2	41:o:71:GLU:C	2.56	0.48
47:5:4529:G:H2'	47:5:4530:U:O4'	2.14	0.48
49:9:1698:C:N1	85:1:1500:A:C6	2.81	0.48
50:AA:67:ALA:HA	71:VV:50:PHE:CZ	2.48	0.48
61:LL:79:LYS:HB3	61:LL:87:VAL:HG12	1.95	0.48
72:WW:42:MET:HE1	72:WW:48:GLY:C	2.39	0.48
75:ZZ:91:LEU:HD23	75:ZZ:94:LYS:NZ	2.29	0.48
84:EF:118:ALA:HB2	84:EF:152:VAL:CG1	2.43	0.48
2:A:194:ASN:CG	2:A:194:ASN:O	2.57	0.48
7:F:178:LEU:HD11	7:F:206:PHE:CG	2.49	0.48
9:H:41:ILE:HD13	9:H:73:ILE:CG1	2.43	0.48
14:N:123:GLU:OE1	14:N:123:GLU:C	2.56	0.48
16:P:117:ILE:HD13	16:P:148:MET:HB3	1.95	0.48
28:b:92:LYS:O	28:b:96:LEU:HD23	2.14	0.48
47:5:1198:G:H2'	47:5:1199:G:H8	1.79	0.48
49:9:1332:A:N7	49:9:1333:U:C6	2.82	0.48
53:DD:35:SER:O	53:DD:99:ILE:HD11	2.14	0.48
63:NN:84:LEU:HD11	63:NN:89:TYR:HB2	1.95	0.48
78:cc:18:LEU:HD11	78:cc:67:ARG:HH21	1.79	0.48
83:AT:14:A:C6	83:AT:15:G:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:321:ARG:HG3	84:EF:322:ARG:H	1.79	0.48
5:D:33:ARG:O	5:D:37:VAL:HG12	2.14	0.48
16:P:18:ARG:HA	16:P:94:MET:HE2	1.94	0.48
18:R:11:ALA:HB2	18:R:41:ILE:HD11	1.96	0.48
19:S:30:MET:HE2	19:S:32:ILE:HD11	1.96	0.48
20:T:111:GLU:OE2	20:T:111:GLU:C	2.57	0.48
25:Y:121:ARG:HH12	47:5:247:G:H21	1.61	0.48
32:f:26:ALA:C	32:f:27:LEU:HD23	2.39	0.48
38:l:30:LYS:HB2	38:l:33:ASN:HB2	1.96	0.48
39:m:58:GLN:O	39:m:61:GLN:N	2.47	0.48
44:s:65:ILE:HG12	44:s:78:LEU:HD21	1.96	0.48
47:5:3834:C:C2	47:5:3835:C:C5	3.02	0.48
52:CC:195:LEU:C	52:CC:196:ILE:HD12	2.39	0.48
53:DD:76:ARG:CZ	60:KK:66:HIS:HB3	2.44	0.48
53:DD:165:ASN:OD1	53:DD:165:ASN:C	2.57	0.48
82:gg:14:HIS:CD2	82:gg:41:ILE:HD13	2.49	0.48
82:gg:42:MET:SD	82:gg:42:MET:C	2.97	0.48
82:gg:79:LEU:HD22	82:gg:111:VAL:HG21	1.95	0.48
84:EF:77:LEU:HD23	84:EF:90:ILE:CD1	2.44	0.48
84:EF:228:LEU:C	84:EF:228:LEU:HD12	2.39	0.48
3:B:195:ASP:O	3:B:199:GLU:OE1	2.32	0.47
5:D:115:MET:HA	5:D:115:MET:HE3	1.95	0.47
12:L:21:ARG:NH2	14:N:197:THR:HA	2.29	0.47
13:M:35:ARG:HE	13:M:49:ALA:HB1	1.79	0.47
29:c:22:MET:HE2	29:c:22:MET:HA	1.94	0.47
33:g:101:LYS:O	33:g:104:VAL:HG22	2.14	0.47
47:5:759:G:N2	47:5:904:G:H22	2.12	0.47
47:5:1348:U:H2'	47:5:1349:G:H5'	1.95	0.47
47:5:2836:A:C2	47:5:3895:G:H4'	2.49	0.47
47:5:4759:C:O2	47:5:4759:C:O4'	2.32	0.47
49:9:962:A:N1	49:9:1055:A:O2'	2.47	0.47
58:II:194:GLU:OE1	61:LL:10:TYR:CD1	2.67	0.47
62:MM:60:MET:HG2	81:ff:103:LEU:HD11	1.96	0.47
63:NN:99:ARG:HA	63:NN:102:LEU:HD12	1.96	0.47
72:WW:105:THR:HG23	72:WW:105:THR:O	2.14	0.47
74:YY:114:MET:C	74:YY:114:MET:SD	2.97	0.47
84:EF:250:LEU:O	84:EF:365:THR:HG21	2.14	0.47
3:B:365:LEU:HD22	3:B:365:LEU:N	2.29	0.47
9:H:128:MET:N	9:H:128:MET:HE2	2.29	0.47
26:Z:60:LYS:O	26:Z:60:LYS:HD3	2.14	0.47
29:c:32:LYS:HE3	47:5:2675:G:C5	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1873:A:C2	47:5:1874:A:C8	3.02	0.47
49:9:1154:U:O2	49:9:1154:U:O4'	2.32	0.47
54:EE:183:VAL:HG13	54:EE:220:THR:HG21	1.96	0.47
73:XX:65:ALA:HB3	73:XX:67:ARG:CZ	2.43	0.47
9:H:176:LEU:HB3	39:m:60:ALA:CB	2.43	0.47
13:M:135:LEU:HD13	13:M:135:LEU:C	2.40	0.47
18:R:148:ASP:C	18:R:148:ASP:OD1	2.57	0.47
22:V:96:LEU:HD12	22:V:97:TYR:N	2.29	0.47
47:5:1445:U:O2'	47:5:1446:C:P	2.72	0.47
47:5:4884:G:O2'	47:5:4885:U:P	2.71	0.47
49:9:51:U:O2	49:9:488:U:O2	2.32	0.47
50:AA:125:THR:HG22	50:AA:175:TRP:HE1	1.79	0.47
61:LL:122:ILE:HD12	61:LL:122:ILE:C	2.39	0.47
64:OO:143:LYS:HE2	64:OO:143:LYS:HA	1.96	0.47
71:VV:11:LEU:H	71:VV:11:LEU:CD2	2.28	0.47
88:EF:502:GTP:C3'	88:EF:502:GTP:PA	3.03	0.47
4:C:180:ILE:CD1	4:C:227:ILE:HD11	2.44	0.47
6:E:151:THR:HG23	6:E:153:LEU:CD1	2.43	0.47
42:p:29:ILE:HD11	42:p:69:TRP:CG	2.48	0.47
44:s:62:ARG:HA	44:s:65:ILE:HD12	1.96	0.47
44:s:66:ARG:NH2	44:s:79:LEU:HD22	2.30	0.47
44:s:135:THR:HG22	44:s:152:ILE:HG23	1.96	0.47
46:3:69:C:HO2'	46:3:70:U:H6	1.61	0.47
52:CC:81:ILE:HD12	52:CC:81:ILE:N	2.29	0.47
73:XX:72:VAL:HG12	73:XX:73:GLN:N	2.30	0.47
84:EF:147:GLN:HA	84:EF:147:GLN:NE2	2.28	0.47
84:EF:429:MET:O	84:EF:429:MET:HE3	2.14	0.47
2:A:144:LYS:HD3	2:A:144:LYS:N	2.28	0.47
3:B:217:ILE:HD12	3:B:217:ILE:C	2.39	0.47
9:H:18:ILE:HD12	9:H:18:ILE:O	2.14	0.47
12:L:9:ILE:O	12:L:9:ILE:HG23	2.15	0.47
13:M:42:CYS:HG	13:M:77:TRP:CD1	2.33	0.47
15:O:185:VAL:HG12	15:O:185:VAL:O	2.13	0.47
19:S:9:GLU:C	19:S:9:GLU:OE1	2.58	0.47
21:U:34:MET:C	21:U:34:MET:HE2	2.38	0.47
24:X:86:ALA:O	24:X:90:ILE:HG23	2.13	0.47
30:d:64:ILE:HD11	47:5:2373:C:O3'	2.14	0.47
30:d:94:GLU:OE1	30:d:94:GLU:N	2.48	0.47
46:2:38:U:C2	46:2:39:G:C8	3.02	0.47
47:5:261:G:H2'	47:5:262:C:O4'	2.14	0.47
49:9:493:A:C2	49:9:494:C:C5	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AA:18:PHE:HD2	50:AA:51:LEU:HD22	1.79	0.47
55:FF:20:PHE:C	55:FF:20:PHE:CD1	2.92	0.47
64:OO:116:LEU:C	64:OO:116:LEU:HD13	2.39	0.47
84:EF:15:HIS:ND1	84:EF:126:GLY:HA2	2.30	0.47
84:EF:174:VAL:O	84:EF:178:ILE:HB	2.13	0.47
11:J:115:LEU:H	11:J:115:LEU:HD22	1.79	0.47
15:O:122:ALA:HB2	19:S:163:HIS:CD2	2.49	0.47
44:s:20:LEU:HD22	44:s:90:PHE:HB3	1.96	0.47
47:5:2465:C:H2'	47:5:2466:G:O4'	2.13	0.47
49:9:616:A:OP2	73:XX:65:ALA:HB1	2.14	0.47
49:9:1019:C:H2'	49:9:1020:A:O4'	2.14	0.47
51:BB:110:MET:HA	51:BB:110:MET:CE	2.40	0.47
54:EE:126:VAL:HB	54:EE:139:LEU:HD21	1.97	0.47
58:II:101:ILE:HD11	58:II:198:TYR:CZ	2.49	0.47
63:NN:86:GLU:OE1	63:NN:86:GLU:N	2.47	0.47
84:EF:325:VAL:HG23	84:EF:325:VAL:O	2.14	0.47
2:A:143:THR:OG1	2:A:145:LYS:HG2	2.14	0.47
4:C:289:LEU:HD23	4:C:289:LEU:O	2.15	0.47
4:C:309:ILE:HD12	4:C:309:ILE:C	2.39	0.47
7:F:189:LEU:HD21	7:F:207:LEU:HD21	1.96	0.47
8:G:148:LEU:HD22	8:G:271:LEU:HD13	1.97	0.47
9:H:5:LEU:HD23	9:H:6:SER:N	2.30	0.47
9:H:41:ILE:HD13	9:H:73:ILE:HG13	1.96	0.47
12:L:18:TRP:O	12:L:22:VAL:HG23	2.14	0.47
13:M:70:GLN:NE2	47:5:735:G:H4'	2.30	0.47
19:S:99:ASP:OD1	19:S:100:LEU:N	2.48	0.47
20:T:147:GLU:HG2	20:T:148:PRO:HD2	1.95	0.47
47:5:33:A:H3'	47:5:47:A:H61	1.79	0.47
47:5:485:C:O2'	47:5:486:C:P	2.72	0.47
47:5:1447:C:H2'	47:5:1448:G:O4'	2.14	0.47
49:9:352:U:H2'	49:9:353:C:C6	2.50	0.47
49:9:1337:C:H2'	49:9:1338:G:C8	2.49	0.47
50:AA:78:SER:HB2	50:AA:87:VAL:HG11	1.97	0.47
52:CC:233:LEU:HD13	52:CC:233:LEU:C	2.40	0.47
53:DD:150:MET:SD	53:DD:150:MET:N	2.88	0.47
56:GG:121:ILE:O	56:GG:126:ASP:OD1	2.31	0.47
64:OO:97:LEU:HD21	64:OO:112:ALA:HB1	1.95	0.47
67:RR:20:TYR:O	67:RR:24:LEU:HD22	2.14	0.47
75:ZZ:48:VAL:O	75:ZZ:83:LEU:HD22	2.15	0.47
75:ZZ:67:LEU:HD13	75:ZZ:67:LEU:C	2.40	0.47
82:gg:256:ILE:HD11	82:gg:286:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:35:ASP:OD1	84:EF:38:THR:HB	2.14	0.47
84:EF:80:PHE:CE1	84:EF:89:ILE:HD11	2.50	0.47
84:EF:114:LEU:CB	84:EF:150:VAL:HG22	2.40	0.47
84:EF:345:ILE:HG21	84:EF:381:ARG:HG2	1.95	0.47
84:EF:360:VAL:HG22	84:EF:427:ARG:O	2.14	0.47
9:H:181:VAL:O	39:m:59:LEU:HD21	2.13	0.47
11:J:89:VAL:HG13	11:J:114:ASP:OD2	2.15	0.47
21:U:19:LEU:H	21:U:19:LEU:HD12	1.79	0.47
28:b:68:ARG:HH12	47:5:1831:G:P	2.38	0.47
31:e:89:LEU:HD11	43:r:116:ALA:HB1	1.96	0.47
44:s:30:VAL:HG22	44:s:89:VAL:HG23	1.95	0.47
44:s:34:ASN:CG	44:s:34:ASN:O	2.57	0.47
44:s:126:GLN:O	44:s:154:ILE:HD12	2.15	0.47
47:5:4942:C:O2	47:5:4942:C:H2'	2.14	0.47
53:DD:48:ILE:HG23	53:DD:86:LEU:HA	1.96	0.47
54:EE:181:CYS:SG	54:EE:225:ILE:HG23	2.55	0.47
56:GG:63:MET:HE2	56:GG:63:MET:C	2.40	0.47
68:SS:72:GLN:C	68:SS:72:GLN:OE1	2.57	0.47
84:EF:60:LEU:HD13	84:EF:78:TRP:CD1	2.50	0.47
85:1:1498:A:C8	85:1:1499:C:C5	3.03	0.47
7:F:143:TYR:CE2	7:F:236:GLU:HB2	2.49	0.47
18:R:96:MET:HE2	18:R:100:ARG:CZ	2.45	0.47
47:5:1977:C:H42	47:5:1990:A:N6	2.13	0.47
49:9:1757:G:O6	49:9:1775:U:C2	2.68	0.47
64:OO:75:MET:HG2	64:OO:118:ALA:HB2	1.97	0.47
72:WW:93:LEU:HD23	72:WW:93:LEU:O	2.14	0.47
78:cc:42:ILE:C	78:cc:42:ILE:CD1	2.88	0.47
81:ff:91:ASN:C	81:ff:91:ASN:OD1	2.58	0.47
83:AT:1:G:O6	83:AT:73:A:N1	2.48	0.47
3:B:361:GLU:C	3:B:361:GLU:OE1	2.57	0.47
6:E:180:GLY:O	6:E:181:PRO:C	2.58	0.47
16:P:94:MET:HE1	16:P:146:ILE:HB	1.98	0.47
18:R:111:GLU:OE1	18:R:111:GLU:N	2.48	0.47
47:5:4889:G:C6	47:5:4931:G:C6	3.03	0.47
49:9:581:U:H4'	74:YY:66:GLY:HA2	1.97	0.47
49:9:1337:C:H4'	70:UU:67:LYS:NZ	2.30	0.47
49:9:1359:U:C2	49:9:1360:U:C5	3.02	0.47
68:SS:10:GLN:OE1	68:SS:57:GLY:O	2.32	0.47
84:EF:171:VAL:HG22	84:EF:190:PHE:CD2	2.50	0.47
84:EF:342:ALA:CB	84:EF:438:ILE:HA	2.45	0.47
84:EF:363:CYS:O	84:EF:364:HIS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:92:MET:HB2	9:H:179:ILE:HD11	1.97	0.46
14:N:9:GLU:HA	14:N:9:GLU:OE2	2.15	0.46
27:a:117:LEU:HD22	27:a:140:VAL:HG21	1.96	0.46
42:p:10:ILE:HD13	47:5:1554:A:H4'	1.97	0.46
47:5:2695:A:H1'	47:5:2696:A:OP2	2.15	0.46
49:9:561:A:O2'	49:9:562:U:P	2.73	0.46
49:9:1139:C:O2	49:9:1139:C:O4'	2.32	0.46
51:BB:181:LEU:HD23	51:BB:181:LEU:C	2.40	0.46
52:CC:163:VAL:CG1	52:CC:164:PRO:HD2	2.45	0.46
84:EF:433:VAL:O	84:EF:434:ALA:HB2	2.15	0.46
2:A:82:ILE:O	42:p:64:VAL:HG23	2.14	0.46
6:E:113:ARG:HD2	6:E:113:ARG:N	2.30	0.46
19:S:60:GLU:OE2	19:S:60:GLU:C	2.58	0.46
20:T:127:GLN:C	20:T:127:GLN:CD	2.83	0.46
22:V:16:ILE:O	22:V:16:ILE:HD12	2.15	0.46
31:e:99:ILE:N	31:e:99:ILE:HD12	2.30	0.46
42:p:26:VAL:HA	42:p:29:ILE:HG22	1.96	0.46
57:HH:73:GLN:N	57:HH:73:GLN:CD	2.73	0.46
66:QQ:37:ARG:HD3	66:QQ:41:MET:HE1	1.96	0.46
80:ee:79:LEU:O	80:ee:82:VAL:HG23	2.16	0.46
84:EF:30:LYS:HB3	84:EF:202:LEU:HD13	1.96	0.46
84:EF:171:VAL:HG13	84:EF:190:PHE:CD2	2.50	0.46
84:EF:276:MET:HE2	84:EF:328:ASP:HB2	1.97	0.46
3:B:77:THR:HG21	3:B:337:VAL:HG22	1.98	0.46
14:N:146:PRO:HA	14:N:149:GLN:HG2	1.98	0.46
15:O:9:LEU:O	15:O:36:VAL:HG12	2.15	0.46
32:f:27:LEU:C	32:f:28:LEU:HD23	2.41	0.46
33:g:32:TYR:O	33:g:33:LEU:HD22	2.15	0.46
44:s:166:LYS:N	44:s:166:LYS:HD2	2.31	0.46
47:5:1323:A:C2	47:5:3879:G:C2	3.03	0.46
49:9:111:A:H4'	61:LL:69:ARG:HD3	1.96	0.46
49:9:152:U:C2	49:9:167:G:N2	2.83	0.46
51:BB:189:ILE:HB	51:BB:190:PRO:HD3	1.97	0.46
55:FF:76:MET:SD	55:FF:173:LEU:HD21	2.55	0.46
56:GG:7:PHE:CE1	56:GG:9:ALA:HB3	2.51	0.46
56:GG:98:ARG:CD	56:GG:106:LEU:HD21	2.46	0.46
56:GG:215:LYS:HD3	56:GG:215:LYS:N	2.31	0.46
63:NN:33:VAL:O	63:NN:37:ILE:HG13	2.15	0.46
19:S:31:ARG:C	19:S:32:ILE:HD12	2.40	0.46
19:S:80:ILE:HD13	19:S:80:ILE:N	2.31	0.46
47:5:2330:G:H4'	47:5:2331:G:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:115:U:O2'	49:9:381:C:H1'	2.15	0.46
49:9:293:C:O2	49:9:293:C:H2'	2.16	0.46
49:9:316:G:C8	56:GG:183:ARG:NH2	2.84	0.46
49:9:1137:U:O2'	49:9:1138:C:P	2.73	0.46
50:AA:159:ILE:CG2	71:VV:69:ILE:HG21	2.45	0.46
52:CC:185:THR:OG1	52:CC:192:LEU:HD21	2.15	0.46
58:II:78:ILE:HD12	58:II:78:ILE:N	2.30	0.46
84:EF:244:LYS:HE2	84:EF:417:ASP:O	2.16	0.46
2:A:109:GLU:OE2	2:A:136:VAL:HG12	2.15	0.46
4:C:164:THR:HG21	47:5:223:G:H2'	1.96	0.46
5:D:15:ARG:HH22	47:5:1743:A:H1'	1.80	0.46
5:D:63:GLN:HB3	5:D:74:ILE:HD11	1.98	0.46
10:I:184:MET:HE3	10:I:190:LEU:CD1	2.46	0.46
14:N:192:TRP:O	14:N:196:ASN:OD1	2.34	0.46
15:O:102:LEU:HD13	15:O:103:LYS:N	2.30	0.46
19:S:163:HIS:CD2	19:S:163:HIS:N	2.83	0.46
24:X:140:LEU:HD12	24:X:140:LEU:N	2.31	0.46
38:l:30:LYS:NZ	48:8:75:G:P	2.89	0.46
44:s:17:ILE:CG2	44:s:64:ALA:HB1	2.46	0.46
47:5:2886:U:H2'	47:5:2887:U:O4'	2.16	0.46
49:9:918:U:O3'	49:9:919:A:O4'	2.33	0.46
51:BB:137:LEU:HD11	51:BB:176:VAL:HG21	1.97	0.46
57:HH:68:GLN:OE1	57:HH:68:GLN:C	2.58	0.46
70:UU:82:MET:HB2	79:dd:52:PHE:CD1	2.51	0.46
84:EF:242:THR:OG1	84:EF:271:VAL:HG23	2.15	0.46
84:EF:359:PRO:HB2	84:EF:426:VAL:HG12	1.96	0.46
3:B:67:VAL:O	3:B:67:VAL:HG22	2.16	0.46
9:H:55:LEU:HD13	9:H:55:LEU:C	2.41	0.46
49:9:1129:G:H3'	49:9:1130:G:H21	1.80	0.46
49:9:1266:C:N3	49:9:1517:G:N2	2.64	0.46
50:AA:122:LEU:HD23	50:AA:142:LEU:HD22	1.96	0.46
55:FF:157:GLY:HA2	55:FF:188:TYR:HD2	1.80	0.46
58:II:89:GLU:O	58:II:93:THR:HG22	2.16	0.46
64:OO:104:ARG:HB3	64:OO:104:ARG:NH1	2.31	0.46
84:EF:363:CYS:HG	84:EF:410:MET:CE	2.29	0.46
7:F:52:LYS:O	7:F:56:TYR:CD2	2.69	0.46
14:N:7:ILE:HG22	14:N:46:ASP:OD2	2.16	0.46
23:W:93:LYS:HA	23:W:96:GLN:HG3	1.97	0.46
29:c:48:LEU:CD2	29:c:60:ILE:HG21	2.45	0.46
44:s:6:ARG:O	44:s:7:ALA:C	2.59	0.46
44:s:45:MET:HE2	45:t:122:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:272:U:C2	47:5:273:U:C5	3.04	0.46
47:5:4453:C:C2	47:5:4529:G:N2	2.84	0.46
54:EE:80:ILE:HG13	54:EE:81:THR:HG23	1.97	0.46
56:GG:73:VAL:HG12	56:GG:74:ARG:N	2.31	0.46
62:MM:35:ILE:HG23	62:MM:36:ARG:N	2.31	0.46
71:VV:55:ILE:CD1	71:VV:69:ILE:HD11	2.40	0.46
76:aa:21:ILE:HD12	76:aa:21:ILE:C	2.41	0.46
84:EF:42:PHE:CE2	84:EF:59:VAL:HG22	2.50	0.46
84:EF:96:ARG:HA	84:EF:99:ILE:HB	1.98	0.46
84:EF:149:ILE:HD13	84:EF:231:ALA:HB1	1.98	0.46
84:EF:181:ILE:O	84:EF:181:ILE:CG2	2.63	0.46
84:EF:281:ALA:HB2	84:EF:334:PRO:HB2	1.98	0.46
9:H:18:ILE:C	9:H:18:ILE:CD1	2.89	0.46
13:M:39:ASP:C	13:M:39:ASP:OD1	2.59	0.46
22:V:117:ILE:HD12	22:V:117:ILE:N	2.31	0.46
28:b:35:VAL:HG12	28:b:36:ASP:N	2.30	0.46
44:s:55:MET:SD	47:5:1998:A:C4	3.09	0.46
47:5:971(A):G:H4'	47:5:972:C:OP1	2.16	0.46
47:5:1455:G:O2'	47:5:1456:C:P	2.74	0.46
47:5:3625:G:O2'	47:5:3626:G:P	2.73	0.46
49:9:1284:A:N7	62:MM:91:LEU:HD13	2.31	0.46
55:FF:124:ASP:OD1	55:FF:124:ASP:C	2.59	0.46
61:LL:77:VAL:HG13	61:LL:122:ILE:HA	1.98	0.46
66:QQ:72:VAL:HG21	66:QQ:84:ILE:HD11	1.97	0.46
72:WW:26:LEU:C	72:WW:26:LEU:HD13	2.41	0.46
74:YY:48:TYR:CG	74:YY:48:TYR:O	2.69	0.46
84:EF:13:ILE:HD11	84:EF:148:LEU:HD12	1.98	0.46
3:B:261:ARG:H	3:B:261:ARG:HE	1.63	0.46
4:C:80:ARG:NH2	47:5:1646:A:P	2.88	0.46
7:F:97:ILE:HD12	17:Q:2:GLY:O	2.16	0.46
9:H:161:ILE:O	9:H:165:THR:HG22	2.16	0.46
16:P:125:MET:O	16:P:140:MET:HB2	2.16	0.46
22:V:42:VAL:HG22	22:V:55:ALA:HB2	1.97	0.46
49:9:122:G:N3	54:EE:146:THR:HG21	2.30	0.46
49:9:682:U:O2'	72:WW:4:MET:HE2	2.15	0.46
49:9:1405:A:H2'	49:9:1406:G:O4'	2.16	0.46
53:DD:164:VAL:HG22	53:DD:168:VAL:CG2	2.46	0.46
83:AT:52:G:N2	83:AT:64:G:H22	2.14	0.46
84:EF:24:THR:HG21	84:EF:89:ILE:HG21	1.97	0.46
84:EF:256:ILE:HG13	84:EF:258:GLY:H	1.81	0.46
84:EF:341:THR:HG23	84:EF:402:VAL:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:176:LEU:HB3	39:m:60:ALA:HB1	1.98	0.46
11:J:43:LEU:HD13	11:J:82:ILE:HD12	1.98	0.46
26:Z:97:ASN:O	26:Z:100:VAL:HG12	2.16	0.46
30:d:64:ILE:HD12	30:d:64:ILE:C	2.41	0.46
37:k:35:LYS:HB3	37:k:42:LEU:HD21	1.96	0.46
43:r:36:ASN:C	43:r:36:ASN:OD1	2.59	0.46
44:s:135:THR:HG22	44:s:145:THR:HG23	1.98	0.46
47:5:930:G:O2'	47:5:931:C:O4'	2.34	0.46
47:5:1440:U:O2'	47:5:1441:C:P	2.74	0.46
47:5:1485:C:H1'	47:5:1486:C:OP1	2.16	0.46
47:5:2505:C:O2	47:5:2505:C:O4'	2.34	0.46
47:5:4947:U:HO2'	47:5:4948:C:P	2.38	0.46
48:8:14:U:C2'	48:8:15:G:O5'	2.63	0.46
49:9:1231:C:H42	49:9:1527:C:H42	1.63	0.46
49:9:1298:G:N7	49:9:1514:G:H1'	2.30	0.46
49:9:1567:G:H21	49:9:1567:G:P	2.39	0.46
57:HH:53:VAL:HG22	57:HH:54:GLY:H	1.81	0.46
58:II:17:LYS:CD	58:II:17:LYS:H	2.29	0.46
72:WW:10:ALA:HB3	72:WW:34:ILE:HD11	1.97	0.46
74:YY:48:TYR:CE2	74:YY:50:THR:HG21	2.51	0.46
84:EF:162:TYR:CD1	84:EF:207:ASN:HB3	2.51	0.46
84:EF:208:MET:HE2	84:EF:210:TRP:CZ2	2.51	0.46
2:A:107:MET:HE3	2:A:111:THR:HG21	1.98	0.45
3:B:257:TRP:HZ3	47:5:4518:A:HO2'	1.63	0.45
3:B:259:PRO:O	3:B:261:ARG:O	2.34	0.45
7:F:150:ASN:ND2	47:5:943:A:H62	2.14	0.45
20:T:92:ARG:HG2	20:T:94:GLU:OE1	2.15	0.45
46:2:37:A:C2	85:1:1493:G:C6	3.04	0.45
47:5:222:C:H2'	47:5:223:G:O4'	2.15	0.45
47:5:1315:C:N4	47:5:1316:G:O6	2.49	0.45
47:5:2502:G:H4'	47:5:2503:G:OP1	2.16	0.45
49:9:502:C:H5'	54:EE:66:MET:HE1	1.98	0.45
51:BB:137:LEU:HB2	51:BB:172:MET:HE2	1.98	0.45
82:gg:5:MET:CE	82:gg:312:VAL:HG22	2.45	0.45
84:EF:13:ILE:HD11	84:EF:148:LEU:CD1	2.47	0.45
84:EF:42:PHE:CE1	84:EF:58:TRP:HB3	2.50	0.45
84:EF:317:VAL:O	84:EF:320:VAL:O	2.34	0.45
14:N:84:PRO:HA	14:N:87:HIS:ND1	2.31	0.45
20:T:127:GLN:OE1	20:T:129:LYS:N	2.49	0.45
29:c:48:LEU:HD12	29:c:72:HIS:O	2.16	0.45
31:e:26:ASP:OD2	47:5:436:C:H4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1211:G:O2'	47:5:1212:G:P	2.74	0.45
47:5:1484:G:H2'	47:5:1484:G:N3	2.31	0.45
47:5:4151:G:H2'	47:5:4152:G:C8	2.51	0.45
49:9:110:U:O2'	49:9:111:A:P	2.74	0.45
49:9:493:A:C2	49:9:494:C:C6	3.04	0.45
50:AA:76:VAL:C	50:AA:77:ILE:HD12	2.42	0.45
56:GG:153:VAL:O	56:GG:153:VAL:HG12	2.16	0.45
64:OO:116:LEU:HD13	64:OO:116:LEU:O	2.16	0.45
3:B:224:LYS:NZ	47:5:4625:C:OP1	2.49	0.45
16:P:48:LEU:HD11	16:P:91:LEU:CD1	2.46	0.45
32:f:40:GLU:C	32:f:40:GLU:OE1	2.60	0.45
41:o:84:ALA:C	41:o:85:ILE:HD13	2.41	0.45
47:5:125:C:O2'	47:5:126:C:P	2.74	0.45
47:5:4966:A:H2'	47:5:4967:A:C8	2.51	0.45
58:II:87:ASN:OD1	58:II:87:ASN:C	2.59	0.45
84:EF:163:SEP:C	84:EF:210:TRP:CZ2	3.00	0.45
84:EF:363:CYS:H	84:EF:410:MET:HE1	1.81	0.45
19:S:113:MET:CB	19:S:124:ILE:HD11	2.46	0.45
24:X:127:LEU:HD12	24:X:127:LEU:C	2.40	0.45
29:c:45:LEU:CD1	29:c:47:ILE:HD11	2.45	0.45
47:5:253:G:H2'	47:5:254:G:O4'	2.16	0.45
47:5:4880:C:O2	47:5:4880:C:O5'	2.33	0.45
48:8:113:C:H3'	48:8:114:G:H5''	1.98	0.45
52:CC:163:VAL:HG13	52:CC:164:PRO:HD2	1.99	0.45
55:FF:106:GLU:OE1	55:FF:106:GLU:N	2.50	0.45
65:PP:37:TYR:OH	65:PP:45:LEU:HD11	2.16	0.45
66:QQ:72:VAL:CG2	66:QQ:84:ILE:HD11	2.46	0.45
67:RR:61:ILE:HG23	67:RR:74:GLN:HE22	1.81	0.45
67:RR:98:VAL:CG2	67:RR:117:LEU:HD22	2.46	0.45
70:UU:80:PHE:CE1	79:dd:52:PHE:O	2.70	0.45
70:UU:81:GLN:HG2	70:UU:82:MET:N	2.31	0.45
74:YY:46:LYS:HD2	74:YY:47:MET:N	2.31	0.45
2:A:142:GLU:C	2:A:143:THR:HG23	2.41	0.45
7:F:104:VAL:O	7:F:108:LEU:HD23	2.16	0.45
15:O:173:GLN:OE1	15:O:173:GLN:HA	2.17	0.45
31:e:58:ILE:HD12	47:5:2319:C:N3	2.32	0.45
47:5:1348:U:C2'	47:5:1349:G:H5'	2.46	0.45
49:9:528:A:C4	49:9:558:G:N2	2.84	0.45
49:9:962:A:H4'	55:FF:135:ARG:NH2	2.31	0.45
49:9:1093:A:H2'	49:9:1094:C:H6	1.82	0.45
49:9:1360:U:O2	49:9:1379:A:N7	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:GG:68:LEU:HA	56:GG:100:CYS:SG	2.57	0.45
78:cc:17:VAL:O	78:cc:17:VAL:HG13	2.17	0.45
80:ee:95:GLN:OE1	80:ee:95:GLN:N	2.50	0.45
81:ff:94:LYS:HD3	81:ff:94:LYS:N	2.32	0.45
82:gg:22:ALA:O	82:gg:31:ILE:HD12	2.17	0.45
82:gg:258:ILE:HD11	82:gg:268:ASP:OD1	2.16	0.45
2:A:233:ARG:O	2:A:233:ARG:HD3	2.17	0.45
5:D:4:VAL:HG11	47:5:4247:G:H5'	1.99	0.45
17:Q:19:LYS:HE2	47:5:1349:G:P	2.56	0.45
24:X:84:GLU:OE2	24:X:84:GLU:N	2.49	0.45
25:Y:42:TYR:CD1	25:Y:119:LEU:HD21	2.51	0.45
42:p:72:ASN:OD1	42:p:72:ASN:N	2.50	0.45
44:s:62:ARG:CG	44:s:82:ILE:HD12	2.42	0.45
44:s:72:ASN:C	44:s:74:ALA:H	2.25	0.45
44:s:161:ILE:HD11	44:s:167:VAL:HG13	1.99	0.45
47:5:270:U:C2	47:5:271:C:C5	3.05	0.45
47:5:1477:C:O2'	47:5:1478:C:P	2.74	0.45
47:5:1929:A:C2	47:5:1932:A:C8	3.05	0.45
47:5:4691:A:N1	47:5:4700:A:C8	2.85	0.45
49:9:24:C:O2'	49:9:25:A:P	2.73	0.45
49:9:464:A:C2	84:EF:41:LYS:HD2	2.52	0.45
51:BB:56:LYS:HD2	51:BB:56:LYS:C	2.41	0.45
55:FF:123:GLU:HG3	55:FF:140:ASP:HA	1.97	0.45
56:GG:1:MET:HE3	56:GG:109:LEU:HD21	1.99	0.45
59:JJ:137:VAL:O	59:JJ:137:VAL:HG23	2.17	0.45
61:LL:103:GLU:OE1	73:XX:11:ARG:NE	2.49	0.45
8:G:133:ILE:HD11	14:N:22:LEU:HD21	1.98	0.45
8:G:148:LEU:CD2	8:G:271:LEU:HD22	2.47	0.45
15:O:108:ILE:HD11	15:O:113:ASP:HA	1.98	0.45
24:X:95:THR:C	24:X:96:LEU:HD23	2.41	0.45
25:Y:1:MET:HE1	47:5:1368:A:N3	2.31	0.45
27:a:75:LEU:HD22	27:a:117:LEU:HD12	1.98	0.45
35:i:40:VAL:O	35:i:44:ILE:HD13	2.17	0.45
41:o:66:ILE:HD12	41:o:66:ILE:O	2.16	0.45
44:s:32:ALA:HB3	44:s:85:ASN:HB3	1.97	0.45
44:s:160:LEU:HD22	44:s:175:LEU:HD21	1.98	0.45
47:5:4947:U:O2'	47:5:4948:C:P	2.74	0.45
57:HH:61:ILE:HD12	57:HH:93:VAL:HG23	1.99	0.45
60:KK:48:ALA:O	60:KK:52:LEU:HD23	2.17	0.45
64:OO:85:CYS:HB2	64:OO:124:MET:CE	2.47	0.45
67:RR:20:TYR:CZ	67:RR:38:ILE:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:RR:93:GLN:OE1	67:RR:93:GLN:HA	2.17	0.45
72:WW:7:LEU:C	72:WW:7:LEU:HD13	2.42	0.45
75:ZZ:78:LYS:HE3	75:ZZ:78:LYS:HA	1.99	0.45
83:AT:52:G:H22	83:AT:64:G:H22	1.65	0.45
84:EF:155:MET:HE2	84:EF:162:TYR:HD2	1.81	0.45
84:EF:157:SER:HB3	88:EF:502:GTP:C6	2.52	0.45
84:EF:340:PHE:CE1	84:EF:438:ILE:HG23	2.51	0.45
4:C:269:LYS:HE2	47:5:654:C:O3'	2.16	0.45
8:G:130:PRO:HG2	8:G:133:ILE:HD12	1.99	0.45
14:N:137:PRO:O	14:N:152:THR:HG22	2.17	0.45
17:Q:147:GLU:CD	17:Q:147:GLU:H	2.25	0.45
34:h:116:LEU:C	34:h:116:LEU:HD13	2.42	0.45
35:i:58:MET:HE3	35:i:90:LEU:HD13	1.98	0.45
47:5:132:G:H2'	47:5:133:C:O4'	2.17	0.45
49:9:122:G:O2'	54:EE:146:THR:HG22	2.17	0.45
49:9:574:A:H4'	74:YY:89:HIS:CG	2.52	0.45
55:FF:125:SER:OG	55:FF:136:ARG:HB3	2.17	0.45
64:OO:126:ILE:N	64:OO:126:ILE:HD12	2.32	0.45
71:VV:62:MET:HE3	71:VV:64:GLU:OE1	2.16	0.45
72:WW:27:ILE:HG12	72:WW:61:ILE:HB	1.98	0.45
76:aa:71:LEU:N	76:aa:71:LEU:HD12	2.32	0.45
84:EF:278:VAL:HG22	84:EF:287:THR:O	2.17	0.45
84:EF:346:ILE:CD1	84:EF:394:LEU:HD23	2.46	0.45
17:Q:109:ALA:O	17:Q:113:ILE:HG22	2.17	0.45
27:a:63:LEU:C	27:a:63:LEU:HD13	2.42	0.45
28:b:107:ARG:HE	28:b:107:ARG:N	2.15	0.45
32:f:37:ASP:OD1	32:f:37:ASP:N	2.50	0.45
44:s:61:MET:HB3	44:s:82:ILE:HD13	1.99	0.45
47:5:217:C:O2	47:5:217:C:O4'	2.35	0.45
47:5:220:C:C2	47:5:221:C:C5	3.05	0.45
47:5:1630:A:H5''	47:5:1631:A:N7	2.32	0.45
47:5:2104:A:OP1	47:5:2104:A:H3'	2.17	0.45
47:5:2758:G:H2'	47:5:2759:G:C4	2.52	0.45
47:5:4162:C:O2	47:5:4162:C:O4'	2.35	0.45
47:5:4625:C:O5'	47:5:4625:C:H6	2.00	0.45
49:9:381:C:H5'	58:II:48:VAL:CG1	2.47	0.45
49:9:941:C:H4'	51:BB:124:HIS:HD2	1.82	0.45
49:9:1798:C:H2'	49:9:1799:G:O4'	2.15	0.45
52:CC:68:ARG:HG2	52:CC:68:ARG:HH11	1.81	0.45
64:OO:75:MET:SD	78:cc:62:GLU:CD	3.00	0.45
73:XX:128:VAL:HG21	73:XX:141:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:186:ASP:O	84:EF:216:VAL:HA	2.17	0.45
84:EF:216:VAL:HG21	84:EF:218:ARG:NH1	2.32	0.45
84:EF:323:GLY:O	84:EF:366:ALA:HB2	2.16	0.45
3:B:17:LEU:N	3:B:18:PRO:CD	2.80	0.45
7:F:199:HIS:HA	7:F:202:GLU:OE2	2.17	0.45
14:N:36:LEU:HD21	14:N:109:HIS:CG	2.52	0.45
20:T:13:TYR:N	20:T:13:TYR:CD1	2.85	0.45
36:j:58:THR:HG22	36:j:59:THR:N	2.32	0.45
40:n:19:LYS:C	40:n:20:MET:HE2	2.42	0.45
45:t:35:LEU:HD22	45:t:64:ILE:HG21	1.98	0.45
47:5:119:G:H3'	47:5:120:A:H5''	1.98	0.45
48:8:14:U:H2'	48:8:15:G:O5'	2.17	0.45
49:9:887:U:O2	49:9:887:U:O4'	2.35	0.45
54:EE:126:VAL:HG21	54:EE:155:LYS:O	2.17	0.45
67:RR:11:LYS:HD2	67:RR:11:LYS:C	2.42	0.45
73:XX:90:CYS:SG	73:XX:130:LEU:HD11	2.57	0.45
7:F:91:VAL:CG2	7:F:113:LEU:HD11	2.48	0.44
10:I:76:MET:HA	10:I:76:MET:HE3	1.99	0.44
19:S:169:THR:HG23	19:S:170:LYS:H	1.81	0.44
44:s:40:MET:HE3	47:5:1999:A:H62	1.81	0.44
44:s:65:ILE:CD1	44:s:82:ILE:HD11	2.47	0.44
47:5:406:C:HO2'	47:5:407:A:P	2.41	0.44
47:5:504:G:O2'	47:5:505:G:P	2.74	0.44
47:5:1818:G:H4'	47:5:1819:G:OP1	2.15	0.44
47:5:4560:C:O2	47:5:4560:C:O4'	2.35	0.44
49:9:914:U:O2	49:9:914:U:O4'	2.35	0.44
49:9:1218:C:H1'	49:9:1683:C:H42	1.83	0.44
49:9:1388:A:H61	53:DD:161:GLY:HA2	1.82	0.44
49:9:1397:U:O2	49:9:1397:U:O4'	2.35	0.44
60:KK:3:MET:HE1	60:KK:48:ALA:CA	2.48	0.44
70:UU:26:SER:O	70:UU:84:ILE:HD12	2.17	0.44
84:EF:274:PRO:HA	84:EF:289:VAL:O	2.17	0.44
85:1:1499:C:O5'	85:1:1499:C:H6	2.00	0.44
3:B:160:ILE:HD13	3:B:194:LEU:CD2	2.47	0.44
15:O:61:ARG:HA	15:O:70:PRO:HD2	2.00	0.44
20:T:147:GLU:OE1	20:T:148:PRO:O	2.35	0.44
32:f:35:ALA:O	32:f:39:THR:HG23	2.17	0.44
51:BB:62:LEU:HD12	51:BB:65:ARG:HD3	1.98	0.44
51:BB:103:MET:HE3	51:BB:103:MET:O	2.16	0.44
54:EE:129:ILE:HD11	54:EE:155:LYS:C	2.41	0.44
66:QQ:12:VAL:HG11	66:QQ:90:LYS:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:cc:10:LYS:HD2	78:cc:61:SER:HB3	1.98	0.44
84:EF:214:TRP:CZ2	84:EF:231:ALA:HB2	2.53	0.44
3:B:181:MET:SD	3:B:183:ILE:HD13	2.58	0.44
13:M:106:ASP:O	13:M:109:ARG:HG2	2.17	0.44
17:Q:19:LYS:HE2	47:5:1349:G:C5'	2.47	0.44
20:T:40:VAL:CG1	20:T:96:ILE:HG23	2.47	0.44
22:V:131:ARG:CZ	22:V:131:ARG:HA	2.47	0.44
47:5:1483:C:H4'	47:5:1484:G:H5'	1.99	0.44
49:9:387:C:O5'	49:9:387:C:H6	2.01	0.44
49:9:434:G:P	58:II:23:LYS:HZ1	2.41	0.44
49:9:953:C:H2'	49:9:954:U:O4'	2.18	0.44
49:9:1155:U:O3'	72:WW:71:LYS:NZ	2.50	0.44
55:FF:100:ILE:HD11	55:FF:177:LEU:HD12	2.00	0.44
57:HH:53:VAL:HG22	57:HH:54:GLY:N	2.33	0.44
57:HH:144:ILE:CG2	72:WW:52:ILE:HG13	2.46	0.44
64:OO:94:HIS:C	64:OO:95:ILE:HD12	2.42	0.44
81:ff:91:ASN:OD1	81:ff:91:ASN:O	2.35	0.44
84:EF:216:VAL:HG22	84:EF:223:ALA:HB3	1.99	0.44
84:EF:377:GLU:HA	84:EF:390:GLY:H	1.83	0.44
4:C:131:SER:O	4:C:150:LEU:HD21	2.16	0.44
6:E:153:LEU:O	6:E:154:ILE:HD12	2.17	0.44
6:E:213:LYS:CD	6:E:213:LYS:H	2.30	0.44
11:J:119:TYR:HE1	68:SS:12:ILE:HD12	1.80	0.44
29:c:35:LEU:HA	29:c:38:ILE:HG22	1.99	0.44
46:3:31:C:C4	46:3:32:U:C4	3.05	0.44
47:5:4119:C:O2'	47:5:4120:U:P	2.75	0.44
47:5:4453:C:H2'	47:5:4454:G:O4'	2.18	0.44
47:5:4711:C:H2'	47:5:4712:C:O4'	2.18	0.44
49:9:1599:U:O2	49:9:1599:U:O4'	2.35	0.44
54:EE:115:THR:HG23	54:EE:118:GLU:H	1.82	0.44
61:LL:69:ARG:O	61:LL:130:GLU:HB3	2.17	0.44
65:PP:58:LYS:HD2	65:PP:58:LYS:C	2.43	0.44
70:UU:67:LYS:C	70:UU:67:LYS:HD2	2.42	0.44
70:UU:79:ARG:H	70:UU:79:ARG:HD2	1.83	0.44
71:VV:59:ILE:HD13	71:VV:65:SER:HA	1.99	0.44
84:EF:36:LYS:HA	84:EF:39:ILE:HG22	1.99	0.44
3:B:217:ILE:HD12	3:B:218:ASP:N	2.33	0.44
5:D:34:LYS:O	5:D:38:ILE:HG22	2.18	0.44
5:D:115:MET:HE2	5:D:139:PRO:CG	2.47	0.44
5:D:214:GLU:HA	5:D:214:GLU:OE2	2.17	0.44
13:M:103:LYS:O	13:M:104:MET:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:133:ILE:C	14:N:134:LEU:HD22	2.41	0.44
15:O:102:LEU:HD13	15:O:102:LEU:C	2.42	0.44
39:m:89:CYS:SG	39:m:92:THR:HG22	2.58	0.44
44:s:143:ILE:HA	44:s:158:VAL:HG21	1.98	0.44
46:2:23:A:H2'	46:2:24:G:C8	2.52	0.44
47:5:480:C:O2'	47:5:481:G:P	2.75	0.44
49:9:681:U:H4'	73:XX:9:THR:HG22	1.99	0.44
49:9:1415:C:H2'	49:9:1416:C:C6	2.53	0.44
49:9:1462:U:O2	49:9:1462:U:O4'	2.35	0.44
52:CC:69:LEU:CD2	52:CC:273:LEU:HD21	2.47	0.44
52:CC:92:GLU:HA	52:CC:95:ASP:OD2	2.18	0.44
54:EE:18:TRP:HH2	54:EE:31:PRO:HD3	1.82	0.44
56:GG:41:LEU:C	56:GG:41:LEU:HD13	2.43	0.44
58:II:90:LEU:HD22	58:II:90:LEU:H	1.82	0.44
63:NN:71:ILE:H	63:NN:71:ILE:HD12	1.81	0.44
64:OO:75:MET:SD	78:cc:62:GLU:OE2	2.75	0.44
64:OO:132:VAL:O	64:OO:132:VAL:HG23	2.17	0.44
68:SS:5:ILE:O	68:SS:5:ILE:HG23	2.18	0.44
68:SS:8:LYS:HD2	68:SS:8:LYS:O	2.18	0.44
71:VV:59:ILE:HD12	71:VV:60:ARG:N	2.33	0.44
73:XX:60:LYS:O	73:XX:63:ASN:O	2.36	0.44
2:A:247:ARG:HD3	49:9:1069:U:H4'	1.99	0.44
4:C:326:LEU:HD22	4:C:333:LYS:HB2	2.00	0.44
5:D:11:ALA:HB1	47:5:1743:A:H5'	2.00	0.44
6:E:156:LEU:HD11	6:E:198:ILE:HD12	1.99	0.44
9:H:117:PHE:O	9:H:120:GLU:HB2	2.18	0.44
9:H:165:THR:HG23	9:H:165:THR:O	2.17	0.44
10:I:93:PRO:HB2	10:I:125:THR:HG22	2.00	0.44
11:J:22:LEU:HB3	11:J:128:LEU:HD13	2.00	0.44
47:5:520:U:H2'	47:5:521:C:O4'	2.17	0.44
47:5:1347:G:H2'	47:5:1348:U:O4'	2.18	0.44
47:5:3723:A:H2'	47:5:3724:A:C8	2.52	0.44
47:5:4356:G:C2	47:5:4357:G:C8	3.05	0.44
47:5:4691:A:H2'	47:5:4692:A:O4'	2.17	0.44
48:8:108:A:H2'	48:8:109:C:O4'	2.17	0.44
49:9:427:U:O2	49:9:427:U:O4'	2.36	0.44
49:9:1154:U:O2	49:9:1156:U:C2	2.71	0.44
50:AA:107:THR:HG22	50:AA:113:GLN:OE1	2.17	0.44
56:GG:67:VAL:HG22	56:GG:69:THR:HG22	2.00	0.44
56:GG:171:THR:HG23	56:GG:171:THR:O	2.17	0.44
58:II:205:ARG:O	58:II:206:LYS:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:WW:87:GLU:O	72:WW:91:ASN:OD1	2.35	0.44
80:ee:99:LYS:HD2	80:ee:101:ARG:HH22	1.81	0.44
84:EF:10:ILE:HD11	84:EF:113:VAL:HG22	2.00	0.44
84:EF:228:LEU:O	84:EF:232:LEU:HG	2.18	0.44
84:EF:285:VAL:O	84:EF:285:VAL:HG12	2.17	0.44
84:EF:337:ALA:HB3	84:EF:412:VAL:HG22	1.99	0.44
84:EF:413:GLU:HB3	84:EF:421:LEU:HD22	2.00	0.44
5:D:51:MET:HE2	5:D:166:ALA:HB2	1.99	0.44
13:M:113:MET:HE1	47:5:4881:U:C4	2.52	0.44
47:5:934:C:O2	47:5:934:C:O4'	2.36	0.44
47:5:2655:C:C2	47:5:2656:U:C5	3.06	0.44
47:5:2661:U:O3'	47:5:2662:G:H4'	2.18	0.44
49:9:1447:G:OP1	70:UU:29:VAL:HG13	2.17	0.44
56:GG:132:ARG:HB3	56:GG:133:LEU:HD12	2.00	0.44
56:GG:156:TYR:N	56:GG:156:TYR:CD1	2.85	0.44
58:II:139:LYS:HD2	58:II:139:LYS:N	2.32	0.44
75:ZZ:66:LYS:HD3	75:ZZ:67:LEU:N	2.33	0.44
78:cc:14:VAL:HG13	78:cc:30:VAL:HG11	2.00	0.44
82:gg:87:LEU:N	82:gg:87:LEU:HD12	2.32	0.44
83:AT:49:C:H2'	83:AT:60:C:H1'	1.99	0.44
84:EF:138:LEU:HA	84:EF:181:ILE:HG21	2.00	0.44
84:EF:280:PHE:HA	84:EF:325:VAL:O	2.18	0.44
84:EF:323:GLY:O	84:EF:324:ASN:C	2.61	0.44
4:C:150:LEU:HB3	4:C:151:PRO:HD3	1.99	0.44
7:F:236:GLU:OE1	19:S:38:VAL:HG22	2.17	0.44
8:G:223:LEU:HD13	8:G:223:LEU:C	2.42	0.44
16:P:87:SER:O	16:P:91:LEU:HG	2.17	0.44
33:g:63:VAL:O	33:g:63:VAL:HG12	2.18	0.44
37:k:42:LEU:HD23	37:k:42:LEU:C	2.43	0.44
44:s:40:MET:O	44:s:44:ARG:HD2	2.17	0.44
47:5:406:C:H2'	47:5:407:A:O5'	2.18	0.44
47:5:1629:G:C2	47:5:1631:A:C2	3.05	0.44
47:5:4272:G:H3'	47:5:4273:A:H5''	1.99	0.44
49:9:612:U:O4	49:9:629:A:N7	2.51	0.44
49:9:616:A:H4'	80:ee:84:LYS:HZ3	1.80	0.44
49:9:1364:U:O2	49:9:1364:U:O4'	2.36	0.44
53:DD:213:PRO:HD3	67:RR:19:LYS:HG2	1.99	0.44
84:EF:205:SER:OG	84:EF:208:MET:HG3	2.18	0.44
84:EF:253:VAL:HG13	84:EF:263:PRO:CA	2.48	0.44
84:EF:387:LEU:HD23	84:EF:388:GLU:HB2	1.99	0.44
84:EF:411:CYS:O	84:EF:421:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:13:GLY:O	15:O:124:LEU:HD12	2.17	0.44
28:b:63:LYS:HE2	28:b:63:LYS:N	2.33	0.44
31:e:113:GLU:OE1	31:e:113:GLU:O	2.36	0.44
37:k:23:VAL:HG12	37:k:64:LEU:CD1	2.48	0.44
47:5:1915:C:O2	47:5:1915:C:O4'	2.36	0.44
47:5:2845:A:H61	47:5:3843:C:N4	2.16	0.44
47:5:4635:A:H2	47:5:4663:G:H21	1.65	0.44
49:9:142:C:O2	49:9:142:C:O4'	2.35	0.44
64:OO:62:VAL:HG11	64:OO:67:ASP:OD2	2.18	0.44
67:RR:108:LEU:O	67:RR:108:LEU:HD13	2.17	0.44
70:UU:23:THR:C	70:UU:24:LEU:HD12	2.43	0.44
74:YY:29:HIS:NE2	74:YY:69:THR:HG23	2.33	0.44
75:ZZ:75:GLU:O	75:ZZ:75:GLU:OE1	2.36	0.44
84:EF:159:GLU:HA	84:EF:159:GLU:OE1	2.17	0.44
2:A:173:GLY:O	42:p:69:TRP:CH2	2.71	0.43
5:D:109:LEU:O	5:D:113:PHE:HB2	2.18	0.43
8:G:247:VAL:HG22	8:G:248:HIS:N	2.33	0.43
9:H:70:VAL:HG13	9:H:71:ARG:N	2.32	0.43
13:M:62:LEU:H	13:M:62:LEU:HD23	1.83	0.43
14:N:17:ASP:OD1	14:N:18:VAL:N	2.51	0.43
21:U:18:LEU:HD21	21:U:73:THR:CG2	2.48	0.43
28:b:33:LYS:NZ	47:5:4298:A:O3'	2.49	0.43
47:5:1214:C:O2	47:5:1214:C:O4'	2.34	0.43
47:5:1238:A:O2'	47:5:1239:C:P	2.76	0.43
47:5:2883:G:C6	47:5:2884:G:N7	2.86	0.43
49:9:634:A:O2'	80:ee:92:VAL:HG22	2.17	0.43
49:9:1231:C:O4'	49:9:1665:G:C6	2.71	0.43
49:9:1503:C:C2	49:9:1504:U:C5	3.06	0.43
49:9:1826:G:C2	49:9:1827:U:C5	3.06	0.43
54:EE:126:VAL:HG23	54:EE:156:VAL:O	2.18	0.43
55:FF:175:ASP:HA	55:FF:178:ILE:HG22	1.99	0.43
56:GG:124:LEU:N	56:GG:124:LEU:HD12	2.33	0.43
59:JJ:12:THR:HG22	59:JJ:12:THR:O	2.19	0.43
62:MM:67:ALA:CB	81:ff:114:ILE:HD11	2.48	0.43
69:TT:85:ASN:CB	69:TT:88:MET:HB2	2.49	0.43
70:UU:82:MET:HE3	70:UU:82:MET:C	2.42	0.43
78:cc:12:ALA:HB1	78:cc:32:VAL:HG12	2.00	0.43
85:1:1498:A:N7	85:1:1499:C:C4	2.86	0.43
4:C:314:LEU:HD21	47:5:715:G:H4'	1.99	0.43
9:H:72:THR:HG22	47:5:4690:G:O2'	2.19	0.43
9:H:118:LEU:HD21	9:H:177:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:24:LEU:HD11	13:M:86:TRP:CD2	2.53	0.43
27:a:43:ILE:HG23	27:a:44:ASN:N	2.33	0.43
29:c:48:LEU:HD21	29:c:60:ILE:CG2	2.47	0.43
41:o:82:MET:O	41:o:83:LEU:HD12	2.17	0.43
47:5:1575:A:H2'	47:5:1576:G:O4'	2.17	0.43
47:5:1741:G:H3'	47:5:1742:A:C5'	2.48	0.43
47:5:1929:A:N3	47:5:1929:A:H2'	2.33	0.43
47:5:2757:A:H2'	47:5:2758:G:C8	2.53	0.43
47:5:2811:G:H22	47:5:2813:A:H3'	1.82	0.43
49:9:1056:U:H2'	49:9:1057:C:O4'	2.18	0.43
49:9:1239:U:O2'	65:PP:124:LYS:HE3	2.18	0.43
51:BB:39:PHE:CD2	51:BB:74:LEU:HD21	2.54	0.43
63:NN:115:LEU:O	63:NN:115:LEU:HD13	2.17	0.43
84:EF:34:ILE:CG2	84:EF:39:ILE:HD12	2.48	0.43
84:EF:60:LEU:HD22	84:EF:60:LEU:N	2.33	0.43
84:EF:118:ALA:O	84:EF:119:GLY:C	2.60	0.43
84:EF:166:ARG:CD	84:EF:170:ILE:HD12	2.48	0.43
84:EF:226:THR:HG23	84:EF:227:THR:HG23	2.00	0.43
84:EF:412:VAL:HG23	84:EF:441:VAL:CG1	2.47	0.43
4:C:170:LEU:HD13	4:C:170:LEU:C	2.43	0.43
4:C:334:THR:HG22	4:C:337:ARG:HH12	1.83	0.43
5:D:115:MET:N	5:D:115:MET:SD	2.90	0.43
9:H:115:ARG:HG2	9:H:123:ILE:HD12	1.99	0.43
10:I:165:ILE:C	10:I:165:ILE:HD12	2.44	0.43
11:J:89:VAL:HG21	11:J:115:LEU:HD13	2.00	0.43
14:N:64:ILE:HD12	14:N:64:ILE:O	2.18	0.43
19:S:164:LYS:HB3	19:S:165:PRO:HD3	2.00	0.43
38:l:12:PHE:CD2	38:l:13:LEU:HD23	2.53	0.43
46:2:26:G:C2	46:2:27:C:C6	3.07	0.43
47:5:282:C:C2	47:5:306:A:N6	2.86	0.43
47:5:3799:A:H2'	47:5:3800:A:O4'	2.18	0.43
47:5:4260:U:H2'	47:5:4261:C:H6	1.83	0.43
47:5:4964:C:O3'	47:5:4965:U:O4'	2.36	0.43
49:9:442:C:N4	49:9:449:A:H62	2.13	0.43
49:9:682:U:C2'	72:WW:4:MET:HE2	2.47	0.43
49:9:1093:A:H1'	72:WW:9:ASP:OD1	2.18	0.43
51:BB:134:LEU:C	51:BB:135:LEU:HD22	2.43	0.43
56:GG:91:GLU:HA	56:GG:91:GLU:OE2	2.17	0.43
61:LL:40:ILE:HD11	61:LL:68:ILE:HG12	2.00	0.43
75:ZZ:61:GLU:HB3	75:ZZ:65:TYR:CE1	2.53	0.43
81:ff:103:LEU:C	81:ff:103:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:419:PRO:N	84:EF:420:PRO:CD	2.82	0.43
13:M:47:ARG:HG2	19:S:73:LEU:HD13	1.99	0.43
14:N:6:TYR:CE1	35:i:40:VAL:HG13	2.52	0.43
22:V:128:LEU:HD12	22:V:129:TRP:NE1	2.34	0.43
24:X:115:LYS:HE2	24:X:116:LEU:HD22	2.01	0.43
30:d:55:LYS:C	30:d:55:LYS:HD2	2.44	0.43
42:p:64:VAL:HG11	42:p:71:TYR:CE1	2.53	0.43
44:s:20:LEU:HD11	44:s:54:LEU:HD12	2.00	0.43
44:s:116:ILE:CA	44:s:167:VAL:HG23	2.48	0.43
47:5:449:C:C4'	47:5:450:G:OP2	2.66	0.43
47:5:2859:G:C2	47:5:2860:C:C6	3.06	0.43
47:5:3720:G:H22	47:5:3733:A:H2	1.66	0.43
47:5:3921:U:H1'	47:5:4543:G:H21	1.84	0.43
47:5:4479:A:H2'	47:5:4480:A:O4'	2.19	0.43
49:9:558:G:H2'	49:9:559:G:C1'	2.49	0.43
49:9:917:U:H2'	49:9:918:U:C6	2.53	0.43
49:9:1827:U:C2	49:9:1828:C:C5	3.07	0.43
50:AA:40:LYS:O	50:AA:48:ILE:HG22	2.19	0.43
64:OO:78:ALA:HB3	64:OO:118:ALA:HB3	2.00	0.43
65:PP:34:MET:HG2	65:PP:45:LEU:HD12	2.00	0.43
67:RR:108:LEU:HD13	67:RR:108:LEU:C	2.42	0.43
68:SS:39:ARG:HD3	69:TT:45:LEU:HA	2.00	0.43
70:UU:46:LYS:O	70:UU:47:ASN:OD1	2.37	0.43
80:ee:85:VAL:O	80:ee:89:THR:HG23	2.18	0.43
3:B:33:PRO:HA	3:B:351:LEU:HD13	2.01	0.43
3:B:53:MET:HE2	47:5:4627:U:C5	2.53	0.43
3:B:62:ARG:CG	3:B:62:ARG:O	2.66	0.43
8:G:302:ARG:NE	8:G:302:ARG:HA	2.34	0.43
15:O:39:GLU:OE2	15:O:39:GLU:N	2.48	0.43
17:Q:41:SER:O	17:Q:45:GLN:OE1	2.37	0.43
19:S:164:LYS:C	19:S:164:LYS:HD3	2.44	0.43
47:5:3668:C:C2'	47:5:3669:G:O5'	2.66	0.43
47:5:3880:G:H2'	47:5:3881:G:C8	2.53	0.43
47:5:4405:G:N1	47:5:4440:G:H1'	2.33	0.43
49:9:92:A:H61	49:9:444:G:H1'	1.83	0.43
49:9:632:C:C2	49:9:633:C:C5	3.06	0.43
49:9:656:G:H21	49:9:663:C:H5''	1.84	0.43
49:9:1502:C:C2	49:9:1503:C:C5	3.06	0.43
50:AA:5:LEU:HD13	71:VV:41:LYS:NZ	2.33	0.43
53:DD:163:PRO:HB3	53:DD:167:TYR:CE2	2.54	0.43
55:FF:65:GLN:OE1	55:FF:65:GLN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:GG:1:MET:HE2	56:GG:109:LEU:HD21	2.00	0.43
58:II:70:GLU:HB3	58:II:112:TRP:CZ3	2.54	0.43
75:ZZ:58:LEU:HD23	75:ZZ:58:LEU:C	2.44	0.43
78:cc:62:GLU:O	78:cc:62:GLU:HG2	2.18	0.43
84:EF:377:GLU:CG	84:EF:401:ILE:HB	2.48	0.43
2:A:13:GLY:C	2:A:14:SER:HG	2.23	0.43
3:B:292:LEU:HD23	3:B:292:LEU:H	1.84	0.43
7:F:100:VAL:HG12	7:F:138:TYR:HE2	1.84	0.43
8:G:139:VAL:HG12	8:G:140:LEU:N	2.34	0.43
12:L:21:ARG:CZ	14:N:197:THR:HA	2.49	0.43
14:N:191:ALA:O	14:N:195:ARG:HD3	2.19	0.43
19:S:169:THR:HG23	19:S:170:LYS:N	2.33	0.43
22:V:29:ALA:O	22:V:117:ILE:HG23	2.17	0.43
26:Z:89:ILE:HG23	26:Z:91:LEU:HD21	1.97	0.43
30:d:37:GLY:O	30:d:41:ARG:HG3	2.18	0.43
44:s:75:LEU:O	44:s:77:LYS:N	2.51	0.43
44:s:167:VAL:HG12	44:s:168:GLY:N	2.34	0.43
45:t:109:ILE:HG13	45:t:132:ILE:HG21	2.00	0.43
47:5:3702:A:N6	47:5:3750:G:H21	2.17	0.43
47:5:3783:A:N7	47:5:3792:G:C8	2.87	0.43
47:5:4624:A:H2'	47:5:4625:C:O5'	2.19	0.43
49:9:1313:A:H4'	49:9:1314:U:O5'	2.19	0.43
49:9:1520:G:C5'	49:9:1521:C:OP2	2.66	0.43
49:9:1551:U:O2	49:9:1551:U:O4'	2.37	0.43
49:9:1580:A:C8	70:UU:56:MET:HE1	2.53	0.43
52:CC:139:LEU:HD21	52:CC:213:LEU:HD11	2.00	0.43
63:NN:142:GLU:OE1	63:NN:145:THR:HG23	2.18	0.43
68:SS:10:GLN:NE2	68:SS:59:LEU:HD23	2.34	0.43
71:VV:1:MET:SD	71:VV:1:MET:O	2.77	0.43
72:WW:14:ILE:HD12	72:WW:65:LEU:HD12	2.01	0.43
83:AT:66:C:H2'	83:AT:67:A:C1'	2.49	0.43
84:EF:37:ARG:HA	84:EF:40:GLU:HG2	2.01	0.43
84:EF:203:GLU:N	84:EF:203:GLU:OE1	2.51	0.43
5:D:217:ASP:OD1	5:D:217:ASP:N	2.51	0.43
7:F:135:VAL:O	7:F:135:VAL:CG1	2.67	0.43
18:R:28:GLU:HG3	18:R:31:GLU:OE2	2.19	0.43
21:U:63:LEU:HD23	21:U:63:LEU:N	2.33	0.43
31:e:26:ASP:OD1	31:e:27:ARG:N	2.52	0.43
34:h:4:ILE:CD1	34:h:56:ARG:HE	2.32	0.43
34:h:20:GLN:OE1	34:h:20:GLN:HA	2.18	0.43
41:o:82:MET:HE1	47:5:4346:U:C1'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:35:VAL:HG22	44:s:39:GLN:HB2	2.01	0.43
46:2:10:G:HO2'	46:2:11:C:P	2.41	0.43
46:3:65:G:C2	46:3:66:C:C5	3.06	0.43
47:5:369:G:C4	47:5:371:A:OP2	2.72	0.43
47:5:2458:C:H2'	47:5:2459:G:O4'	2.19	0.43
47:5:2470:C:O2	47:5:2470:C:O4'	2.36	0.43
47:5:3685:C:C2	47:5:3686:G:C8	3.07	0.43
47:5:5052:C:H2'	47:5:5053:U:O4'	2.19	0.43
49:9:1:U:O2	49:9:1:U:O4'	2.35	0.43
49:9:962:A:C5'	55:FF:135:ARG:HH22	2.32	0.43
49:9:1336:C:H2'	49:9:1337:C:O4'	2.19	0.43
49:9:1550:G:H3'	49:9:1579:A:H61	1.83	0.43
50:AA:76:VAL:HG12	50:AA:87:VAL:HB	2.00	0.43
50:AA:119:PRO:O	50:AA:142:LEU:HD21	2.19	0.43
52:CC:196:ILE:N	52:CC:196:ILE:CD1	2.81	0.43
54:EE:191:ARG:O	54:EE:192:ILE:HD12	2.18	0.43
55:FF:158:ALA:HB3	55:FF:173:LEU:HD23	2.00	0.43
56:GG:15:LEU:HD23	56:GG:15:LEU:C	2.43	0.43
60:KK:40:VAL:HG23	60:KK:40:VAL:O	2.19	0.43
66:QQ:57:LEU:HD21	66:QQ:115:TYR:CD1	2.54	0.43
74:YY:72:PHE:CD1	74:YY:72:PHE:N	2.86	0.43
82:gg:272:GLN:CD	82:gg:272:GLN:N	2.77	0.43
83:AT:28:G:C2	83:AT:45:G:N2	2.87	0.43
84:EF:340:PHE:O	84:EF:404:MET:N	2.52	0.43
2:A:109:GLU:OE2	2:A:109:GLU:HA	2.18	0.43
8:G:220:VAL:O	8:G:220:VAL:HG12	2.18	0.43
8:G:258:THR:HG23	8:G:259:GLN:N	2.33	0.43
11:J:35:ARG:HD2	11:J:123:ILE:O	2.18	0.43
12:L:150:LEU:HD21	34:h:123:ALA:HA	2.01	0.43
19:S:103:ALA:O	19:S:107:THR:HG23	2.19	0.43
19:S:131:GLU:C	19:S:131:GLU:CD	2.86	0.43
20:T:87:LYS:HE3	47:5:4305:G:H22	1.84	0.43
43:r:31:ASN:C	43:r:31:ASN:OD1	2.62	0.43
44:s:39:GLN:NE2	44:s:107:VAL:HG11	2.34	0.43
44:s:57:LYS:HB3	44:s:60:MET:HB3	2.01	0.43
47:5:2080:U:H2'	47:5:2081:C:C6	2.54	0.43
47:5:2654:C:H2'	47:5:2655:C:C6	2.54	0.43
47:5:3802:U:O2	47:5:3802:U:O4'	2.36	0.43
47:5:3888:G:O2'	47:5:3889:G:P	2.76	0.43
47:5:4597:U:H2'	47:5:4598:C:O4'	2.19	0.43
47:5:4736:C:C2'	47:5:4737:G:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4947:U:C2'	47:5:4948:C:O5'	2.66	0.43
49:9:488:U:P	84:EF:313:LYS:HE3	2.58	0.43
49:9:872:A:C4'	49:9:873:G:OP1	2.67	0.43
51:BB:122:GLU:HA	51:BB:122:GLU:OE2	2.19	0.43
51:BB:198:GLU:C	51:BB:198:GLU:CD	2.87	0.43
64:OO:98:ARG:HH21	64:OO:134:PRO:HG3	1.84	0.43
69:TT:55:THR:OG1	69:TT:56:ARG:NH2	2.52	0.43
72:WW:18:GLU:CA	72:WW:65:LEU:HD11	2.49	0.43
78:cc:46:VAL:HG12	78:cc:47:LYS:N	2.34	0.43
84:EF:355:ALA:HB2	84:EF:375:LEU:HG	1.99	0.43
84:EF:360:VAL:HG21	84:EF:427:ARG:CZ	2.49	0.43
2:A:173:GLY:O	42:p:69:TRP:HH2	2.02	0.43
3:B:53:MET:SD	3:B:77:THR:HG22	2.59	0.43
3:B:61:ASP:O	3:B:61:ASP:OD1	2.37	0.43
3:B:258:HIS:CE1	47:5:4517:A:O3'	2.72	0.43
4:C:361:LYS:O	4:C:361:LYS:HD3	2.19	0.43
7:F:174:ILE:CD1	7:F:189:LEU:HD13	2.48	0.43
10:I:126:VAL:HG12	10:I:127:ALA:N	2.33	0.43
12:L:164:GLU:HG3	27:a:100:ILE:HG21	2.01	0.43
15:O:79:ILE:CG2	15:O:138:LEU:HD21	2.49	0.43
16:P:64:ASN:HD22	16:P:64:ASN:H	1.65	0.43
17:Q:175:GLU:OE2	27:a:50:PRO:O	2.36	0.43
19:S:104:GLY:O	19:S:108:GLN:HG2	2.18	0.43
22:V:104:VAL:HG21	22:V:112:MET:SD	2.59	0.43
24:X:82:THR:HG22	24:X:155:ILE:CD1	2.47	0.43
43:r:6:GLN:O	43:r:10:VAL:HG12	2.18	0.43
44:s:61:MET:HE2	44:s:82:ILE:CG2	2.48	0.43
45:t:133:LEU:HD13	45:t:150:ASP:HB3	2.00	0.43
47:5:308:G:H4'	47:5:309:C:OP1	2.18	0.43
47:5:1544:G:N1	47:5:1616:U:C2	2.87	0.43
47:5:2657:G:H2'	47:5:2658:G:C5	2.54	0.43
47:5:2685:C:H3'	47:5:2686:G:H5''	2.01	0.43
48:8:15:G:O2'	48:8:16:G:O4'	2.32	0.43
48:8:74:U:O2'	48:8:75:G:H3'	2.19	0.43
49:9:597:G:C6	49:9:640:A:N6	2.87	0.43
51:BB:106:THR:HG22	51:BB:108:ASP:H	1.83	0.43
53:DD:76:ARG:HH22	60:KK:67:PHE:C	2.27	0.43
61:LL:80:MET:HE2	61:LL:122:ILE:CG2	2.49	0.43
66:QQ:32:ILE:HG12	66:QQ:68:ILE:HD12	2.00	0.43
67:RR:24:LEU:HD22	67:RR:24:LEU:H	1.83	0.43
68:SS:72:GLN:OE1	68:SS:72:GLN:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:UU:82:MET:HB2	79:dd:52:PHE:HD1	1.84	0.43
76:aa:18:VAL:HG22	76:aa:19:GLN:N	2.34	0.43
4:C:358:LEU:C	4:C:358:LEU:HD13	2.44	0.43
6:E:142:LYS:NZ	47:5:712:C:OP1	2.52	0.43
9:H:12:ILE:HD12	9:H:12:ILE:C	2.43	0.43
10:I:54:SER:HB2	10:I:135:ILE:HD11	2.01	0.43
10:I:190:LEU:HD23	10:I:197:VAL:HG21	2.01	0.43
11:J:38:LYS:HG2	11:J:123:ILE:HD11	2.01	0.43
17:Q:3:VAL:HG12	17:Q:5:ILE:CD1	2.49	0.43
23:W:2:LYS:HE2	23:W:2:LYS:N	2.34	0.43
29:c:32:LYS:HE3	47:5:2675:G:C8	2.53	0.43
29:c:62:TYR:O	29:c:66:LEU:HD23	2.19	0.43
35:i:50:PHE:HB2	35:i:55:ARG:HD3	2.00	0.43
36:j:58:THR:HG22	36:j:59:THR:H	1.83	0.43
47:5:199:G:C4	47:5:201:C:C5	3.07	0.43
47:5:2638:G:H22	47:5:2697:A:N6	2.12	0.43
47:5:2740:U:O2	47:5:2740:U:O4'	2.37	0.43
47:5:4414:A:H2'	47:5:4422:A:C6	2.54	0.43
48:8:41:A:H61	48:8:102:G:C2'	2.32	0.43
49:9:653:A:H2'	49:9:654:A:O4'	2.19	0.43
49:9:662:G:H4'	49:9:663:C:OP1	2.19	0.43
55:FF:72:LEU:HD13	55:FF:72:LEU:C	2.43	0.43
56:GG:63:MET:HE2	56:GG:64:LYS:CA	2.49	0.43
57:HH:144:ILE:HD11	57:HH:152:ARG:HB3	2.00	0.43
64:OO:23:GLU:O	64:OO:23:GLU:CD	2.62	0.43
74:YY:17:LEU:H	74:YY:17:LEU:HD22	1.84	0.43
84:EF:162:TYR:HB3	84:EF:208:MET:HG2	2.00	0.43
85:1:1498:A:C5	85:1:1499:C:C2	3.07	0.43
2:A:112:ILE:HG21	42:p:79:VAL:HG21	2.01	0.42
8:G:195:THR:HG23	47:5:151:G:O6	2.18	0.42
14:N:89:VAL:HG23	14:N:90:ASN:N	2.33	0.42
27:a:84:GLU:N	27:a:84:GLU:OE2	2.52	0.42
47:5:6:C:C2	47:5:7:C:C5	3.07	0.42
47:5:433:A:H2	47:5:3866:C:HO2'	1.65	0.42
47:5:2448:G:H2'	47:5:2449:A:C8	2.54	0.42
47:5:4263:C:H2'	47:5:4264:G:O4'	2.19	0.42
49:9:688:U:H1'	49:9:689:U:OP2	2.19	0.42
49:9:853:C:O2	49:9:853:C:O4'	2.35	0.42
54:EE:18:TRP:CZ2	54:EE:43:PRO:HD3	2.54	0.42
59:JJ:144:ILE:HG22	59:JJ:146:SER:H	1.84	0.42
75:ZZ:91:LEU:HD23	75:ZZ:94:LYS:HZ1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:20:LYS:CG	84:EF:115:ILE:HG21	2.49	0.42
2:A:204:MET:SD	47:5:1631:A:C2	3.13	0.42
3:B:292:LEU:HD23	3:B:292:LEU:N	2.34	0.42
6:E:284:VAL:HG13	6:E:289:LEU:HD13	2.01	0.42
17:Q:90:VAL:HB	27:a:80:THR:HG21	2.02	0.42
27:a:82:VAL:HG12	27:a:83:SER:N	2.34	0.42
29:c:32:LYS:NZ	47:5:2658:G:C6	2.86	0.42
30:d:105:LEU:HD13	30:d:105:LEU:C	2.44	0.42
31:e:94:SER:C	31:e:95:TYR:HD1	2.27	0.42
38:l:23:ILE:HG22	48:8:52:A:C4	2.54	0.42
47:5:1920:C:H3'	47:5:1921:C:H5''	2.00	0.42
47:5:2673:G:H4'	47:5:2675:G:C8	2.54	0.42
47:5:4254:G:N3	47:5:4254:G:H2'	2.34	0.42
49:9:1580:A:H5'	70:UU:56:MET:HE3	2.01	0.42
49:9:1620:A:N3	49:9:1620:A:H2'	2.34	0.42
50:AA:46:ILE:HG22	50:AA:47:TYR:N	2.34	0.42
57:HH:118:ARG:O	57:HH:121:THR:HG22	2.20	0.42
58:II:43:ILE:HD11	58:II:60:LEU:HD11	2.00	0.42
59:JJ:35:TYR:HD1	59:JJ:112:THR:HG21	1.84	0.42
62:MM:117:GLU:HG2	62:MM:117:GLU:O	2.18	0.42
63:NN:35:GLU:C	63:NN:35:GLU:OE1	2.62	0.42
63:NN:127:ARG:HG3	63:NN:128:TYR:N	2.34	0.42
65:PP:70:MET:HE2	65:PP:70:MET:N	2.34	0.42
68:SS:43:VAL:HG21	68:SS:83:PHE:CZ	2.53	0.42
74:YY:49:LYS:HD3	74:YY:49:LYS:N	2.33	0.42
82:gg:256:ILE:HD11	82:gg:286:CYS:CB	2.48	0.42
84:EF:429:MET:O	84:EF:429:MET:CG	2.66	0.42
85:1:1498:A:C6	85:1:1499:C:C2	3.07	0.42
2:A:204:MET:HE1	47:5:1631:A:N1	2.34	0.42
5:D:213:GLU:OE1	5:D:214:GLU:OE2	2.37	0.42
6:E:155:ILE:HD11	6:E:160:HIS:HB2	2.01	0.42
13:M:70:GLN:HE21	47:5:735:G:H5''	1.83	0.42
18:R:137:ILE:HD13	18:R:137:ILE:N	2.34	0.42
23:W:2:LYS:HE2	23:W:2:LYS:H	1.85	0.42
25:Y:7:VAL:HG12	25:Y:8:THR:N	2.35	0.42
25:Y:88:GLU:OE2	25:Y:88:GLU:HA	2.19	0.42
42:p:31:ILE:HD12	42:p:31:ILE:C	2.45	0.42
47:5:13:U:O2	47:5:13:U:O4'	2.38	0.42
47:5:1237:C:O2	47:5:1237:C:O4'	2.36	0.42
47:5:2309:G:O6	47:5:2330:G:C2	2.72	0.42
47:5:2381:A:H1'	47:5:2383:C:P	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:3832:U:H2'	47:5:3833:C:H6	1.84	0.42
48:8:85:U:O2	48:8:85:U:O4'	2.37	0.42
49:9:803:C:H2'	49:9:804:U:O4'	2.19	0.42
49:9:1132:C:H3'	49:9:1133:A:H5''	2.01	0.42
49:9:1415:C:O2'	69:TT:128:GLN:NE2	2.52	0.42
49:9:1689:C:C2	49:9:1690:U:C5	3.08	0.42
64:OO:90:ILE:HD13	64:OO:90:ILE:N	2.34	0.42
65:PP:107:ILE:O	65:PP:107:ILE:CG1	2.67	0.42
69:TT:75:MET:HA	69:TT:75:MET:HE3	2.00	0.42
78:cc:44:ARG:NH1	78:cc:63:ARG:HB3	2.34	0.42
78:cc:55:VAL:C	78:cc:56:LEU:HD22	2.44	0.42
2:A:175:ILE:HD12	2:A:176:ASP:OD1	2.19	0.42
8:G:104:LEU:HD11	47:5:4086:G:C2	2.54	0.42
18:R:134:ASN:OD1	18:R:137:ILE:HG12	2.19	0.42
19:S:30:MET:HE1	19:S:47:PHE:HB2	2.01	0.42
30:d:87:ARG:HH11	30:d:122:VAL:HG21	1.85	0.42
34:h:51:ARG:O	34:h:54:ILE:HG12	2.20	0.42
44:s:17:ILE:HG21	44:s:64:ALA:CB	2.48	0.42
44:s:101:MET:HG3	44:s:102:LEU:N	2.33	0.42
47:5:1330:A:C2	47:5:2357:G:C5	3.08	0.42
47:5:1933:G:H2'	47:5:1934:A:C8	2.54	0.42
47:5:2104:A:H3'	47:5:2104:A:N3	2.34	0.42
47:5:3668:C:H2'	47:5:3669:G:O5'	2.19	0.42
49:9:77:A:H1'	56:GG:176:ILE:HD12	2.01	0.42
49:9:317:C:H41	56:GG:183:ARG:NH1	2.17	0.42
49:9:1560:U:C2	49:9:1575:G:O6	2.70	0.42
50:AA:121:LEU:HD22	50:AA:122:LEU:N	2.34	0.42
52:CC:66:LEU:HD23	52:CC:66:LEU:H	1.83	0.42
58:II:143:LYS:HD2	58:II:143:LYS:C	2.44	0.42
63:NN:92:ILE:HG23	63:NN:141:TYR:HE2	1.84	0.42
65:PP:57:LEU:HD13	65:PP:57:LEU:C	2.44	0.42
82:gg:127:LYS:O	82:gg:128:THR:HG23	2.19	0.42
84:EF:61:ASP:OD2	84:EF:72:THR:HA	2.18	0.42
84:EF:408:LYS:HG3	84:EF:409:PRO:HD2	2.02	0.42
84:EF:413:GLU:HA	84:EF:441:VAL:HG21	2.01	0.42
84:EF:441:VAL:HG11	84:EF:443:LYS:HE2	2.01	0.42
2:A:77:ILE:HD12	2:A:77:ILE:H	1.84	0.42
8:G:226:LEU:HD23	8:G:226:LEU:O	2.19	0.42
9:H:92:MET:CE	9:H:161:ILE:HD11	2.44	0.42
11:J:38:LYS:HD3	11:J:42:GLN:OE1	2.20	0.42
18:R:4:LEU:HD12	18:R:32:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:154:ILE:C	20:T:154:ILE:CD1	2.93	0.42
46:2:25:C:C4	46:2:26:G:C8	3.07	0.42
47:5:56:A:H2'	47:5:57:G:C8	2.53	0.42
47:5:1197:C:H3'	47:5:1198:G:C8	2.55	0.42
47:5:4119:C:O2	47:5:4119:C:O4'	2.38	0.42
48:8:111:U:O2	48:8:111:U:O4'	2.38	0.42
49:9:210:U:C2	49:9:211:G:C8	3.07	0.42
49:9:379:C:H2'	49:9:380:G:O4'	2.19	0.42
49:9:612:U:H3	49:9:629:A:H62	1.68	0.42
49:9:1332:A:C2	49:9:1500:G:C4	3.07	0.42
49:9:1553:C:O2'	49:9:1554:C:C6	2.70	0.42
49:9:1866:A:H62	76:aa:84:VAL:HG22	1.84	0.42
52:CC:61:LEU:HD22	52:CC:61:LEU:N	2.35	0.42
52:CC:192:LEU:HD23	52:CC:192:LEU:C	2.44	0.42
75:ZZ:62:VAL:HA	75:ZZ:65:TYR:CD2	2.55	0.42
83:AT:22:G:H2'	83:AT:23:A:O4'	2.19	0.42
5:D:109:LEU:HD11	5:D:142:PHE:CE2	2.54	0.42
6:E:261:LEU:N	6:E:262:PRO:HD2	2.35	0.42
10:I:26:VAL:HG12	10:I:122:PRO:HB3	2.01	0.42
10:I:48:LEU:HD13	10:I:49:CYS:N	2.35	0.42
11:J:113:ILE:H	11:J:113:ILE:HD12	1.84	0.42
14:N:157:LYS:HD2	47:5:56:A:H4'	2.01	0.42
14:N:199:GLN:OE1	14:N:199:GLN:HA	2.20	0.42
15:O:142:ALA:HA	15:O:145:VAL:HG12	2.00	0.42
18:R:96:MET:SD	47:5:2667:C:O4'	2.77	0.42
33:g:11:LEU:HD12	33:g:18:ASN:HB2	2.02	0.42
47:5:696:C:C4'	47:5:697:G:OP2	2.67	0.42
47:5:977:C:H2'	47:5:978:G:C8	2.55	0.42
47:5:1306:C:H2'	47:5:1307:A:H8	1.84	0.42
47:5:1484:G:O3'	47:5:1485:C:H3'	2.19	0.42
47:5:3695:U:H2'	47:5:3696:C:O4'	2.20	0.42
47:5:4124:G:H1'	47:5:4125:C:OP1	2.19	0.42
47:5:4266:G:N3	47:5:4266:G:H2'	2.34	0.42
50:AA:58:LEU:HD23	50:AA:58:LEU:C	2.45	0.42
55:FF:40:ALA:HB1	55:FF:45:TYR:CG	2.54	0.42
63:NN:87:ASP:OD1	63:NN:87:ASP:N	2.53	0.42
75:ZZ:69:THR:O	75:ZZ:73:VAL:HG23	2.19	0.42
84:EF:303:LEU:HB3	84:EF:304:PRO:CD	2.50	0.42
84:EF:370:CYS:HB3	84:EF:404:MET:SD	2.59	0.42
2:A:101:VAL:HG23	2:A:165:VAL:N	2.35	0.42
5:D:106:ALA:CB	5:D:171:LEU:HD23	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:26:VAL:HG12	10:I:122:PRO:CB	2.50	0.42
15:O:21:ALA:HA	15:O:87:MET:HE3	2.01	0.42
16:P:106:GLY:C	16:P:107:LEU:HD12	2.45	0.42
20:T:156:TYR:CD1	20:T:157:GLU:N	2.88	0.42
22:V:35:LYS:HE2	22:V:35:LYS:HA	2.02	0.42
24:X:81:LEU:HD12	24:X:81:LEU:N	2.35	0.42
27:a:4:ARG:CG	27:a:5:LEU:HD22	2.50	0.42
27:a:61:TYR:CE1	47:5:294:G:C8	3.08	0.42
44:s:13:TYR:O	44:s:17:ILE:HG22	2.19	0.42
46:2:10:G:O2'	46:2:11:C:P	2.77	0.42
47:5:383:A:H2'	47:5:384:A:O4'	2.20	0.42
47:5:3867:A:H2'	47:5:3868:G:O4'	2.20	0.42
47:5:4578:G:C6	47:5:4726:G:O6	2.72	0.42
47:5:4955:A:O3'	47:5:4956:A:O4'	2.38	0.42
49:9:928:G:H2'	49:9:929:G:C8	2.55	0.42
49:9:976:G:H1'	64:OO:50:LYS:HD3	2.01	0.42
49:9:1055:A:N6	49:9:1064:C:N4	2.68	0.42
49:9:1116:C:O2	49:9:1116:C:H2'	2.18	0.42
49:9:1574:C:H3'	49:9:1575:G:H5''	2.01	0.42
52:CC:70:VAL:HG21	52:CC:93:ILE:HG23	2.01	0.42
54:EE:42:LEU:HD23	54:EE:42:LEU:C	2.45	0.42
54:EE:48:LEU:HD23	54:EE:61:VAL:HG13	2.01	0.42
55:FF:112:LEU:HD23	55:FF:112:LEU:C	2.45	0.42
61:LL:98:LYS:HG3	61:LL:99:TYR:CD1	2.55	0.42
63:NN:26:LEU:HD13	63:NN:26:LEU:C	2.45	0.42
67:RR:23:ARG:HA	82:gg:194:TYR:CE2	2.54	0.42
71:VV:71:ARG:NH2	77:bb:4:ALA:HB2	2.35	0.42
79:dd:43:PHE:HZ	79:dd:52:PHE:CE2	2.38	0.42
84:EF:253:VAL:HG13	84:EF:263:PRO:HA	2.01	0.42
84:EF:264:VAL:HG22	84:EF:309:GLY:CA	2.49	0.42
84:EF:349:HIS:CD2	84:EF:353:ILE:HG13	2.53	0.42
1:7:61:G:H4'	5:D:271:MET:CE	2.48	0.42
7:F:193:ILE:HD13	7:F:193:ILE:N	2.35	0.42
8:G:201:GLU:C	8:G:201:GLU:OE1	2.63	0.42
9:H:35:ARG:NH1	9:H:35:ARG:HB2	2.34	0.42
15:O:169:ARG:CZ	47:5:4860:G:C5'	2.98	0.42
17:Q:63:LEU:O	17:Q:67:ILE:HG13	2.19	0.42
18:R:60:ARG:O	18:R:64:ARG:HG3	2.20	0.42
18:R:136:ARG:CD	18:R:136:ARG:H	2.32	0.42
38:l:30:LYS:HZ1	48:8:75:G:H8	1.66	0.42
40:n:2:ARG:HD3	49:9:1842:C:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:114:ALA:O	43:r:118:LEU:HD23	2.20	0.42
47:5:1450:C:O2'	47:5:2104:A:H1'	2.19	0.42
47:5:2358:G:H2'	47:5:2359:U:O4'	2.19	0.42
47:5:2397:G:O2'	47:5:2398:U:H3'	2.20	0.42
47:5:3807:A:C2	47:5:3808:C:C4	3.07	0.42
47:5:3829:G:C2	47:5:3830:A:C8	3.07	0.42
47:5:4867:G:O6	47:5:4868:G:O6	2.38	0.42
49:9:383:G:H21	61:LL:133:PRO:HG3	1.84	0.42
49:9:636:C:H5''	80:ee:95:GLN:NE2	2.35	0.42
49:9:1054:G:C6	49:9:1055:A:N7	2.88	0.42
49:9:1101:U:H2'	49:9:1102:G:H8	1.85	0.42
54:EE:86:PHE:CD1	54:EE:103:TYR:CZ	3.08	0.42
54:EE:86:PHE:CZ	54:EE:87:MET:HE3	2.55	0.42
54:EE:146:THR:HG23	54:EE:146:THR:O	2.20	0.42
57:HH:68:GLN:OE1	57:HH:72:PHE:HB2	2.20	0.42
58:II:206:LYS:C	58:II:206:LYS:HD2	2.44	0.42
63:NN:16:LEU:HD21	63:NN:65:PHE:CE2	2.53	0.42
65:PP:124:LYS:H	65:PP:124:LYS:HD2	1.85	0.42
68:SS:118:ARG:CZ	68:SS:118:ARG:HB3	2.50	0.42
73:XX:131:LEU:HD12	73:XX:132:ALA:N	2.34	0.42
84:EF:201:MET:HA	84:EF:228:LEU:HD23	2.02	0.42
2:A:180:LEU:HD11	42:p:18:TYR:CD2	2.55	0.42
2:A:245:ARG:NH2	47:5:3656:A:H4'	2.35	0.42
4:C:227:ILE:HD12	4:C:227:ILE:N	2.35	0.42
7:F:178:LEU:HD11	7:F:206:PHE:CB	2.50	0.42
10:I:121:LYS:HD2	10:I:121:LYS:N	2.35	0.42
15:O:23:VAL:HG13	15:O:33:VAL:HG11	2.01	0.42
23:W:32:LEU:O	23:W:32:LEU:HD13	2.20	0.42
26:Z:46:ILE:HD13	26:Z:68:ILE:HG22	2.00	0.42
42:p:76:ALA:O	42:p:79:VAL:HG12	2.19	0.42
46:2:48:C:C4	46:2:59:U:C6	3.08	0.42
47:5:1325:C:O2	47:5:1325:C:O4'	2.38	0.42
47:5:4194:U:O2	47:5:4194:U:H2'	2.20	0.42
47:5:4448:G:H4'	47:5:4449:A:OP2	2.20	0.42
48:8:13:G:C4	48:8:14:U:H5	2.38	0.42
49:9:149:A:C5	49:9:150:A:C8	3.08	0.42
49:9:442:C:C4	49:9:452:G:N2	2.88	0.42
49:9:913:A:P	57:HH:99:ARG:NH1	2.93	0.42
50:AA:131:HIS:ND1	50:AA:132:GLN:N	2.68	0.42
52:CC:83:LEU:HD23	52:CC:83:LEU:C	2.44	0.42
54:EE:92:ILE:CG2	74:YY:17:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:EE:207:VAL:HG22	54:EE:208:VAL:N	2.35	0.42
56:GG:76:LEU:HD21	56:GG:92:ARG:HB3	2.02	0.42
57:HH:40:LEU:HD21	57:HH:79:LEU:HD21	2.02	0.42
59:JJ:113:GLN:O	59:JJ:117:LEU:HD13	2.20	0.42
72:WW:7:LEU:HD12	72:WW:74:VAL:CG2	2.49	0.42
82:gg:23:THR:HG22	82:gg:31:ILE:HD13	2.01	0.42
82:gg:256:ILE:HD12	82:gg:256:ILE:N	2.35	0.42
84:EF:6:THR:HG21	84:EF:237:PRO:CB	2.50	0.42
84:EF:155:MET:SD	84:EF:193:ILE:N	2.92	0.42
84:EF:280:PHE:CZ	84:EF:326:ALA:HB2	2.55	0.42
1:7:83:A:H4'	7:F:223:THR:HB	2.02	0.42
2:A:102:LEU:C	2:A:102:LEU:HD12	2.45	0.42
3:B:220:ILE:HG12	3:B:278:THR:HG23	2.01	0.42
4:C:65:GLU:OE1	4:C:65:GLU:N	2.53	0.42
15:O:16:LEU:C	15:O:16:LEU:HD12	2.45	0.42
20:T:129:LYS:HE3	47:5:1836:G:C4'	2.50	0.42
23:W:94:ARG:NE	23:W:94:ARG:HA	2.34	0.42
32:f:87:LYS:HZ1	47:5:1903:G:H5''	1.85	0.42
33:g:59:VAL:HG22	33:g:60:ARG:N	2.35	0.42
33:g:107:LEU:O	33:g:107:LEU:HD13	2.19	0.42
44:s:189:ILE:HD11	44:s:191:GLN:O	2.19	0.42
47:5:977:C:H2'	47:5:978:G:O4'	2.20	0.42
47:5:1349:G:H2'	47:5:1350:C:O4'	2.20	0.42
47:5:1831:G:H2'	47:5:1832:C:O4'	2.20	0.42
47:5:2079:G:H2'	47:5:2080:U:C6	2.55	0.42
47:5:4132:C:H2'	47:5:4133:C:C6	2.55	0.42
47:5:4525:C:C4	47:5:4526:U:O4	2.73	0.42
49:9:42:A:C2	49:9:43:U:C2	3.07	0.42
49:9:483:C:H2'	49:9:484:A:O4'	2.20	0.42
49:9:1018:U:H5''	63:NN:71:ILE:HD13	2.01	0.42
49:9:1298:G:N3	49:9:1298:G:H2'	2.34	0.42
49:9:1799:G:HO2'	49:9:1800:A:H8	1.67	0.42
58:II:59:ARG:O	58:II:60:LEU:HD12	2.19	0.42
58:II:110:ARG:HG2	58:II:110:ARG:HH11	1.85	0.42
62:MM:92:CYS:O	62:MM:94:ILE:HD12	2.19	0.42
64:OO:61:LYS:HA	64:OO:61:LYS:HE3	2.01	0.42
73:XX:13:LEU:N	73:XX:13:LEU:HD23	2.34	0.42
77:bb:5:LYS:HD3	77:bb:5:LYS:C	2.45	0.42
81:ff:125:GLU:C	81:ff:125:GLU:CD	2.88	0.42
83:AT:48:C:H3'	83:AT:49:C:C5'	2.50	0.42
85:1:1499:C:H5''	85:1:1500:A:P	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:100:VAL:HG12	7:F:138:TYR:CE2	2.55	0.41
9:H:57:VAL:HG23	9:H:70:VAL:HG23	2.02	0.41
10:I:148:VAL:O	10:I:152:LEU:HD23	2.19	0.41
11:J:18:ARG:HB2	11:J:133:VAL:HG12	2.02	0.41
12:L:178:ALA:HB1	27:a:146:LEU:HD21	2.01	0.41
14:N:92:LEU:N	14:N:92:LEU:CD1	2.83	0.41
17:Q:138:LEU:C	17:Q:139:LEU:HD22	2.45	0.41
18:R:39:GLN:OE1	18:R:39:GLN:HA	2.20	0.41
20:T:157:GLU:C	20:T:157:GLU:OE1	2.63	0.41
24:X:87:MET:O	24:X:90:ILE:HG13	2.19	0.41
36:j:67:LEU:HD21	48:8:41:A:H5'	2.02	0.41
44:s:55:MET:SD	44:s:56:GLY:N	2.93	0.41
44:s:143:ILE:HG22	44:s:154:ILE:CG2	2.48	0.41
47:5:232:G:C2	47:5:383:A:C2	3.08	0.41
47:5:758:G:H2'	47:5:759:G:O4'	2.20	0.41
47:5:1198:G:H2'	47:5:1199:G:C8	2.55	0.41
47:5:1971:C:N3	47:5:1972:G:N7	2.67	0.41
47:5:2016:C:O2	47:5:2016:C:H2'	2.20	0.41
47:5:3614:G:C6	47:5:3617:G:C2	3.08	0.41
47:5:3873:G:H2'	47:5:3874:G:C8	2.55	0.41
49:9:164:A:O2'	49:9:165:G:O4'	2.35	0.41
49:9:552:G:H4'	80:ee:112:ASN:CG	2.44	0.41
49:9:570:C:O3'	74:YY:36:PRO:HA	2.20	0.41
49:9:1101:U:H2'	49:9:1102:G:C8	2.55	0.41
49:9:1154:U:H5	52:CC:192:LEU:HD22	1.84	0.41
49:9:1501:C:C2	49:9:1502:C:C5	3.07	0.41
49:9:1620:A:H1'	49:9:1624:U:OP2	2.19	0.41
51:BB:137:LEU:HD22	51:BB:215:VAL:HG22	2.01	0.41
54:EE:221:ARG:H	54:EE:221:ARG:HD2	1.85	0.41
55:FF:20:PHE:C	55:FF:20:PHE:HD1	2.28	0.41
67:RR:15:VAL:HA	67:RR:18:GLU:OE1	2.19	0.41
6:E:168:LEU:HD11	6:E:179:THR:OG1	2.20	0.41
8:G:151:LEU:HD13	8:G:271:LEU:HD12	2.02	0.41
11:J:113:ILE:HG12	11:J:119:TYR:HB2	2.01	0.41
14:N:53:TYR:CD1	14:N:54:LYS:N	2.88	0.41
14:N:161:MET:HE2	14:N:161:MET:HB3	1.82	0.41
18:R:76:MET:HE3	18:R:76:MET:HB3	1.97	0.41
19:S:82:LEU:HD11	19:S:109:CYS:SG	2.60	0.41
22:V:48:ARG:HG2	22:V:49:LEU:N	2.35	0.41
25:Y:67:ILE:HD12	25:Y:67:ILE:N	2.35	0.41
28:b:25:ARG:HH12	47:5:1845:U:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:57:ASN:ND2	47:5:1899:G:O2'	2.53	0.41
33:g:23:SER:OG	33:g:33:LEU:HD23	2.21	0.41
47:5:964:A:H2'	47:5:965:G:O4'	2.20	0.41
47:5:2520:C:O2	47:5:2640:G:N2	2.53	0.41
47:5:4251:A:H2'	47:5:4252:C:O4'	2.20	0.41
49:9:154:U:H3'	49:9:155:G:H5''	2.02	0.41
49:9:502:C:C5'	54:EE:66:MET:HE1	2.50	0.41
49:9:1262:C:H3'	49:9:1263:U:C6	2.55	0.41
49:9:1306:U:C2'	49:9:1307:U:O5'	2.69	0.41
51:BB:106:THR:HG23	64:OO:130:GLU:OE1	2.19	0.41
51:BB:150:ILE:HD13	67:RR:129:LYS:HB2	2.01	0.41
54:EE:55:ALA:HB3	54:EE:61:VAL:HG22	2.02	0.41
56:GG:16:ILE:HD12	56:GG:16:ILE:N	2.35	0.41
69:TT:128:GLN:CD	69:TT:128:GLN:C	2.88	0.41
74:YY:10:ARG:CZ	74:YY:10:ARG:HA	2.50	0.41
80:ee:112:ASN:HA	80:ee:116:VAL:HG12	2.01	0.41
82:gg:206:LEU:HD23	82:gg:206:LEU:H	1.85	0.41
84:EF:179:LYS:HA	84:EF:183:TYR:O	2.19	0.41
84:EF:361:LEU:HD11	84:EF:363:CYS:SG	2.60	0.41
3:B:160:ILE:HD13	3:B:194:LEU:HD21	2.02	0.41
5:D:146:LEU:HD21	5:D:159:VAL:CG1	2.50	0.41
11:J:24:ILE:HD12	11:J:40:LEU:HG	2.02	0.41
14:N:21:PHE:CD1	14:N:21:PHE:O	2.73	0.41
17:Q:113:ILE:HD11	17:Q:118:GLY:HA3	2.03	0.41
22:V:27:ASN:O	22:V:27:ASN:OD1	2.37	0.41
25:Y:11:ARG:HD2	47:5:229:G:H5''	2.03	0.41
32:f:63:LYS:N	32:f:63:LYS:CD	2.83	0.41
40:n:20:MET:HE2	40:n:20:MET:HA	2.02	0.41
44:s:92:LYS:O	44:s:92:LYS:HG2	2.18	0.41
47:5:169:G:N2	47:5:267:G:C2	2.89	0.41
47:5:922(B):C:H3'	47:5:923:C:H5''	2.02	0.41
47:5:1369:C:OP2	47:5:1370:G:C3'	2.68	0.41
47:5:1633:G:C5'	47:5:1634:A:OP1	2.68	0.41
47:5:4371:G:H1'	47:5:4372:U:C6	2.56	0.41
47:5:4410:G:C6	47:5:4433:G:C6	3.08	0.41
47:5:4527:G:H22	47:5:4556:U:H2'	1.84	0.41
47:5:4592:C:H2'	47:5:4593:C:C6	2.56	0.41
48:8:51:U:O2	48:8:51:U:H2'	2.19	0.41
49:9:530:U:H2'	49:9:531:A:C1'	2.51	0.41
49:9:1262:C:H2'	49:9:1263:U:O4'	2.20	0.41
49:9:1502:C:N3	49:9:1503:C:C5	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:1614:A:OP2	65:PP:39:ALA:HB1	2.20	0.41
50:AA:200:ASP:OD2	67:RR:86:PRO:HG2	2.20	0.41
51:BB:91:VAL:HG13	51:BB:95:ASN:O	2.21	0.41
59:JJ:58:ARG:O	59:JJ:62:THR:HG23	2.20	0.41
70:UU:35:VAL:CG2	70:UU:110:VAL:HG21	2.49	0.41
71:VV:71:ARG:CZ	77:bb:4:ALA:HB2	2.51	0.41
79:dd:31:ILE:HD11	79:dd:40:ARG:HB3	2.02	0.41
83:AT:53:G:O2'	83:AT:54:U:H5'	2.20	0.41
83:AT:66:C:H2'	83:AT:67:A:O4'	2.20	0.41
1:7:42:A:C5	1:7:43:U:C5	3.09	0.41
4:C:113:ARG:HD2	47:5:1508:A:OP1	2.20	0.41
4:C:251:ILE:HD12	4:C:251:ILE:N	2.36	0.41
5:D:214:GLU:OE2	5:D:214:GLU:CA	2.68	0.41
8:G:296:GLY:O	8:G:300:VAL:HG23	2.20	0.41
11:J:85:LYS:HG3	11:J:115:LEU:HD12	2.01	0.41
19:S:82:LEU:HD12	19:S:113:MET:HE2	2.01	0.41
23:W:37:GLU:O	23:W:41:LEU:HD23	2.20	0.41
24:X:83:THR:HG22	24:X:84:GLU:OE2	2.19	0.41
28:b:62:ALA:HB3	28:b:63:LYS:HE2	2.02	0.41
28:b:108:ALA:O	28:b:112:ILE:HG22	2.20	0.41
29:c:30:GLY:HA3	47:5:2675:G:O6	2.20	0.41
32:f:69:VAL:HG11	47:5:4944:C:H1'	2.03	0.41
36:j:18:LEU:HD22	36:j:18:LEU:H	1.86	0.41
44:s:29:ILE:O	44:s:189:ILE:HA	2.20	0.41
44:s:55:MET:CB	44:s:87:GLY:HA3	2.49	0.41
44:s:190:GLN:C	44:s:191:GLN:HG2	2.45	0.41
47:5:77:U:C4	47:5:78:U:C5	3.08	0.41
47:5:4188:U:H2'	47:5:4189:U:C6	2.56	0.41
47:5:4659:G:H2'	47:5:4660:G:O4'	2.21	0.41
47:5:4964:C:H4'	47:5:4965:U:OP1	2.21	0.41
49:9:824:C:H2'	49:9:825:A:O4'	2.20	0.41
49:9:1332:A:N1	49:9:1500:G:C4	2.89	0.41
50:AA:122:LEU:HD21	50:AA:142:LEU:HD13	2.01	0.41
53:DD:49:ILE:HG23	53:DD:89:GLU:HG2	2.02	0.41
56:GG:26:THR:HG22	56:GG:36:VAL:HG11	2.02	0.41
60:KK:29:MET:SD	60:KK:31:LYS:O	2.78	0.41
61:LL:112:HIS:C	61:LL:112:HIS:ND1	2.77	0.41
66:QQ:107:GLU:C	66:QQ:107:GLU:CD	2.88	0.41
67:RR:119:VAL:O	67:RR:119:VAL:HG13	2.20	0.41
73:XX:36:LEU:O	73:XX:36:LEU:HD23	2.21	0.41
79:dd:31:ILE:HG12	79:dd:38:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:EF:7:HIS:CD2	84:EF:294:MET:HE1	2.55	0.41
84:EF:259:ILE:HG21	84:EF:311:ASN:HB2	2.02	0.41
84:EF:361:LEU:HD12	84:EF:362:ASP:N	2.35	0.41
84:EF:418:TYR:N	84:EF:418:TYR:CD1	2.89	0.41
3:B:72:VAL:HG23	3:B:74:GLU:OE1	2.21	0.41
15:O:27:VAL:HG12	15:O:98:ALA:HB1	2.02	0.41
15:O:110:PRO:N	15:O:111:PRO:CD	2.84	0.41
21:U:64:GLU:CD	21:U:64:GLU:C	2.88	0.41
22:V:40:ILE:HD11	47:5:3799:A:N9	2.35	0.41
29:c:77:ASN:OD1	29:c:77:ASN:C	2.63	0.41
34:h:64:THR:O	34:h:67:GLU:HG3	2.21	0.41
35:i:94:LEU:HD13	35:i:94:LEU:C	2.45	0.41
36:j:82:THR:HB	48:8:94:G:H21	1.85	0.41
41:o:88:CYS:HA	47:5:4230:C:OP2	2.20	0.41
44:s:6:ARG:HH22	47:5:1957:U:H2'	1.86	0.41
47:5:1273:G:H2'	47:5:1274:A:O4'	2.19	0.41
47:5:1820:C:C4	47:5:1822:U:H1'	2.56	0.41
47:5:4318:C:H3'	47:5:4319:C:H5''	2.01	0.41
49:9:445:A:H2'	49:9:446:G:O4'	2.20	0.41
49:9:1261:C:C6	49:9:1619:A:N1	2.89	0.41
49:9:1337:C:H4'	70:UU:67:LYS:HZ3	1.86	0.41
49:9:1622:U:H3'	49:9:1623:A:C5'	2.50	0.41
53:DD:162:ASP:N	53:DD:163:PRO:CD	2.83	0.41
54:EE:195:ILE:H	54:EE:195:ILE:CD1	2.29	0.41
55:FF:135:ARG:NH2	64:OO:66:ARG:HD3	2.36	0.41
58:II:13:LYS:HD2	61:LL:137:THR:HG21	2.02	0.41
61:LL:80:MET:HE2	61:LL:122:ILE:HG23	2.02	0.41
64:OO:75:MET:HE1	64:OO:76:LEU:CD2	2.50	0.41
65:PP:84:ILE:N	65:PP:84:ILE:HD12	2.34	0.41
67:RR:98:VAL:HG21	67:RR:117:LEU:HD22	2.01	0.41
70:UU:82:MET:HE3	70:UU:82:MET:O	2.21	0.41
75:ZZ:76:ARG:NH1	75:ZZ:76:ARG:HB2	2.36	0.41
83:AT:45:G:H2'	83:AT:46:G:C8	2.55	0.41
84:EF:387:LEU:HD23	84:EF:387:LEU:C	2.45	0.41
2:A:96:LEU:HD23	2:A:96:LEU:O	2.20	0.41
2:A:196:TRP:HB3	2:A:197:PRO:HD3	2.02	0.41
2:A:235:VAL:HG12	2:A:236:GLY:N	2.36	0.41
9:H:12:ILE:HD11	9:H:53:LYS:HA	2.01	0.41
16:P:64:ASN:HD22	16:P:64:ASN:N	2.18	0.41
17:Q:138:LEU:HD21	47:5:1427:A:N1	2.36	0.41
20:T:75:VAL:O	20:T:75:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:13:TYR:N	33:g:13:TYR:CD1	2.89	0.41
43:r:5:LEU:O	43:r:9:VAL:HG12	2.20	0.41
47:5:1511:U:C2	47:5:1512:G:C8	3.08	0.41
47:5:1669:A:H1'	47:5:1852:U:O2'	2.20	0.41
47:5:4075:U:C4'	47:5:4076:G:OP1	2.68	0.41
47:5:4922:C:H2'	47:5:4923:C:C6	2.55	0.41
49:9:386:C:H4'	58:II:6:ASP:O	2.20	0.41
49:9:501:C:H2'	49:9:502:C:H5''	2.03	0.41
49:9:1239:U:H4'	65:PP:124:LYS:HE3	2.02	0.41
50:AA:140:VAL:HG12	50:AA:141:ASN:N	2.35	0.41
50:AA:174:MET:HA	50:AA:174:MET:CE	2.47	0.41
52:CC:75:ILE:HG21	52:CC:81:ILE:CD1	2.50	0.41
52:CC:137:VAL:C	52:CC:162:ILE:HD13	2.45	0.41
56:GG:147:LEU:HD12	56:GG:153:VAL:HG13	2.02	0.41
58:II:123:ARG:O	58:II:124:LYS:C	2.64	0.41
58:II:143:LYS:HD2	58:II:143:LYS:O	2.21	0.41
60:KK:93:THR:HG23	60:KK:94:LEU:HD12	2.02	0.41
67:RR:99:ASP:OD1	67:RR:100:PRO:HD2	2.21	0.41
73:XX:61:GLN:CB	73:XX:62:PRO:HD2	2.50	0.41
73:XX:77:ASN:CB	73:XX:79:LYS:HE3	2.51	0.41
75:ZZ:51:ASP:CG	75:ZZ:52:LYS:N	2.78	0.41
84:EF:248:LEU:O	84:EF:326:ALA:HB3	2.20	0.41
2:A:144:LYS:N	2:A:144:LYS:CD	2.84	0.41
3:B:309:LEU:HD22	3:B:309:LEU:N	2.35	0.41
9:H:152:GLU:OE2	9:H:152:GLU:HA	2.20	0.41
18:R:16:ARG:HG2	18:R:16:ARG:HH11	1.85	0.41
32:f:94:ALA:HB3	47:5:1308:C:O2	2.21	0.41
33:g:100:GLN:O	33:g:104:VAL:HG13	2.21	0.41
46:2:59:U:C2'	46:2:60:C:H5'	2.51	0.41
47:5:1323:A:H2'	47:5:1324:A:O4'	2.19	0.41
47:5:1332:C:H2'	47:5:1333:A:H8	1.85	0.41
47:5:1444:G:H2'	47:5:1445:U:C5	2.56	0.41
47:5:1455:G:H4'	47:5:1456:C:OP1	2.20	0.41
47:5:1579:C:C2	47:5:1580:C:C5	3.08	0.41
47:5:1670:G:O2'	47:5:1853:G:H4'	2.21	0.41
47:5:1948:G:H2'	47:5:1949:U:O4'	2.21	0.41
47:5:1990:A:C2'	47:5:1991:A:OP1	2.69	0.41
47:5:2546:G:H4'	47:5:2547:G:OP1	2.20	0.41
47:5:3719:A:C4	47:5:3720:G:C8	3.08	0.41
47:5:4396:A:N6	47:5:4447:C:C2	2.89	0.41
49:9:910:G:H2'	49:9:911:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:929:G:H2'	49:9:930:C:O4'	2.21	0.41
49:9:942:G:H2'	49:9:943:U:N1	2.35	0.41
51:BB:39:PHE:CE2	51:BB:74:LEU:HD21	2.55	0.41
51:BB:193:ILE:HD13	51:BB:193:ILE:N	2.35	0.41
56:GG:63:MET:HE2	56:GG:64:LYS:C	2.45	0.41
57:HH:193:GLN:HB3	57:HH:194:LEU:HD23	2.03	0.41
64:OO:96:LYS:HG2	64:OO:132:VAL:HG11	2.03	0.41
71:VV:49:GLN:O	71:VV:50:PHE:CD1	2.73	0.41
80:ee:124:LYS:HE2	85:1:1504:U:C5	2.52	0.41
2:A:90:CYS:SG	2:A:101:VAL:CG1	3.09	0.41
6:E:113:ARG:NH1	6:E:113:ARG:HA	2.35	0.41
9:H:94:SER:HA	9:H:179:ILE:HA	2.03	0.41
11:J:113:ILE:CG1	11:J:119:TYR:HB2	2.50	0.41
13:M:31:ILE:N	13:M:31:ILE:HD13	2.36	0.41
18:R:119:MET:O	18:R:123:LEU:HD23	2.20	0.41
25:Y:117:LYS:HD2	25:Y:118:ILE:N	2.36	0.41
27:a:43:ILE:HG23	47:5:1682:A:O2'	2.19	0.41
29:c:32:LYS:O	29:c:36:LYS:HG3	2.21	0.41
30:d:64:ILE:HG22	30:d:106:VAL:HG21	2.03	0.41
44:s:141:LEU:HD11	44:s:160:LEU:HA	2.03	0.41
47:5:731:G:C6	47:5:932:A:C4	3.09	0.41
47:5:1932:A:C2'	47:5:1933:G:O5'	2.69	0.41
47:5:2102:G:H2'	47:5:2103:A:O4'	2.19	0.41
47:5:3692:A:C5	47:5:3693:U:C6	3.08	0.41
47:5:3788:C:O2	47:5:3788:C:H2'	2.20	0.41
47:5:4313:A:H3'	47:5:4314:C:H5''	2.03	0.41
47:5:4625:C:O5'	47:5:4625:C:C6	2.74	0.41
49:9:55:U:O2	49:9:55:U:O4'	2.38	0.41
49:9:1624:U:O2	49:9:1624:U:O4'	2.37	0.41
50:AA:198:MET:CE	67:RR:89:SER:HB3	2.50	0.41
53:DD:76:ARG:CZ	60:KK:22:VAL:HB	2.50	0.41
54:EE:126:VAL:HG12	54:EE:139:LEU:HD11	2.02	0.41
58:II:161:LEU:HD13	58:II:195:LEU:HD23	2.02	0.41
68:SS:10:GLN:O	68:SS:10:GLN:HG2	2.21	0.41
82:gg:59:LEU:HD22	82:gg:59:LEU:N	2.35	0.41
84:EF:42:PHE:HE1	84:EF:58:TRP:HB3	1.84	0.41
84:EF:105:GLY:O	84:EF:109:ALA:HB2	2.21	0.41
84:EF:153:ASN:O	84:EF:154:LYS:C	2.62	0.41
3:B:299:ILE:HD12	3:B:299:ILE:N	2.36	0.41
4:C:165:LYS:O	4:C:168:VAL:HG12	2.20	0.41
6:E:206:ILE:HD12	6:E:206:ILE:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:86:PRO:HG3	7:F:143:TYR:CE2	2.56	0.41
7:F:88:LEU:HD21	7:F:121:PHE:HD2	1.86	0.41
8:G:216:PRO:HG2	8:G:219:LEU:HD12	2.03	0.41
10:I:165:ILE:HD12	10:I:165:ILE:O	2.21	0.41
10:I:167:ILE:O	10:I:167:ILE:HG23	2.19	0.41
11:J:111:GLU:HB3	11:J:125:ILE:HD11	2.01	0.41
12:L:58:ILE:HG23	12:L:70:VAL:HG11	2.02	0.41
12:L:161:PHE:CZ	27:a:105:ARG:NH2	2.88	0.41
13:M:129:LYS:HA	13:M:132:ARG:HG2	2.03	0.41
15:O:56:ALA:O	15:O:60:LYS:HG3	2.20	0.41
20:T:84:ILE:N	20:T:84:ILE:HD12	2.36	0.41
22:V:88:TYR:CE2	22:V:124:GLU:OE1	2.73	0.41
24:X:140:LEU:HD12	24:X:140:LEU:H	1.86	0.41
35:i:45:ARG:HD2	35:i:50:PHE:CE1	2.56	0.41
37:k:25:ILE:HG23	37:k:34:PHE:HE1	1.85	0.41
37:k:35:LYS:HZ1	47:5:2696:A:H62	1.67	0.41
44:s:116:ILE:C	44:s:116:ILE:CD1	2.93	0.41
44:s:145:THR:OG1	44:s:152:ILE:HG22	2.21	0.41
46:2:21:A:C5	46:2:48:C:C4	3.09	0.41
46:3:30:G:C6	46:3:41:A:C6	3.09	0.41
46:3:74:C:O2	46:3:74:C:H2'	2.21	0.41
47:5:134:G:H4'	47:5:135:G:O5'	2.21	0.41
47:5:686:A:H2'	47:5:686:A:N3	2.35	0.41
47:5:929:A:C6	47:5:930:G:C6	3.09	0.41
47:5:1084:C:H2'	47:5:1085:C:C6	2.56	0.41
47:5:2034:G:C4	47:5:2035:C:C5	3.08	0.41
47:5:2643:G:O6	47:5:2692:U:O4	2.39	0.41
47:5:2805:C:H2'	47:5:2806:A:O4'	2.21	0.41
47:5:4541:G:N1	47:5:4545:G:C6	2.89	0.41
47:5:4948:C:H3'	47:5:4949:G:C5'	2.50	0.41
49:9:356:C:O2	49:9:356:C:C2'	2.69	0.41
49:9:436:G:P	49:9:471:G:O2'	2.79	0.41
49:9:529:A:C4	49:9:530:U:C5	3.08	0.41
49:9:933:G:H22	76:aa:19:GLN:HE22	1.67	0.41
49:9:1120:U:H3'	49:9:1121:G:H5''	2.02	0.41
49:9:1438:A:H2'	49:9:1439:A:C8	2.55	0.41
49:9:1517:G:O2'	49:9:1518:C:H5'	2.20	0.41
49:9:1649:U:OP1	66:QQ:128:GLU:OE2	2.38	0.41
51:BB:127:VAL:HG13	51:BB:176:VAL:HG11	2.01	0.41
51:BB:137:LEU:CD2	51:BB:215:VAL:HG13	2.51	0.41
51:BB:143:THR:HG1	51:BB:205:TYR:HE1	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:CC:121:ARG:HD3	52:CC:122:THR:N	2.36	0.41
53:DD:143:ARG:NH1	85:1:1503:A:C4	2.83	0.41
53:DD:146:ARG:NH2	85:1:1500:A:H4'	2.36	0.41
56:GG:68:LEU:HD22	56:GG:68:LEU:N	2.35	0.41
56:GG:123:GLY:C	56:GG:124:LEU:HD12	2.46	0.41
57:HH:39:GLN:OE1	57:HH:75:ILE:HG21	2.21	0.41
61:LL:68:ILE:HG13	61:LL:143:LEU:HD11	2.03	0.41
63:NN:31:ASP:C	63:NN:31:ASP:OD1	2.64	0.41
70:UU:27:ARG:NH1	79:dd:51:GLY:HA3	2.36	0.41
70:UU:38:ASP:HA	70:UU:41:ARG:CG	2.50	0.41
71:VV:55:ILE:HD11	71:VV:69:ILE:CD1	2.42	0.41
72:WW:14:ILE:CD1	72:WW:65:LEU:HD12	2.51	0.41
72:WW:71:LYS:HE2	72:WW:71:LYS:HB2	1.90	0.41
73:XX:130:LEU:HD12	73:XX:130:LEU:O	2.21	0.41
75:ZZ:48:VAL:C	75:ZZ:83:LEU:HD22	2.46	0.41
75:ZZ:66:LYS:C	75:ZZ:66:LYS:CD	2.93	0.41
82:gg:275:ILE:HG22	82:gg:275:ILE:O	2.21	0.41
84:EF:228:LEU:O	84:EF:231:ALA:HB3	2.20	0.41
84:EF:281:ALA:HB3	84:EF:282:PRO:HD3	2.03	0.41
3:B:347:LEU:N	3:B:347:LEU:HD12	2.36	0.41
4:C:33:ARG:O	4:C:37:VAL:HG23	2.21	0.41
5:D:118:ILE:HD12	5:D:118:ILE:H	1.85	0.41
8:G:173:LYS:HD2	8:G:173:LYS:C	2.45	0.41
15:O:50:ASN:ND2	15:O:136:ALA:HB3	2.36	0.41
20:T:5:LYS:HD2	47:5:4302:U:H4'	2.04	0.41
25:Y:2:LYS:HA	47:5:243:A:H5'	2.02	0.41
39:m:71:ARG:HE	39:m:96:ARG:HD3	1.85	0.41
42:p:82:ALA:O	42:p:86:LEU:HD22	2.21	0.41
44:s:128:THR:HG22	44:s:178:LEU:HD21	2.03	0.41
44:s:198:ILE:N	44:s:198:ILE:HD12	2.36	0.41
45:t:123:ARG:HG3	45:t:124:GLU:H	1.84	0.41
46:3:69:C:O2'	46:3:70:U:H6	2.04	0.41
47:5:12:A:H4'	47:5:13:U:OP1	2.21	0.41
47:5:2656:U:C4	47:5:2657:G:C6	3.08	0.41
47:5:3720:G:C2	47:5:3721:U:C6	3.09	0.41
47:5:4099:G:H22	47:5:4109:G:H22	1.69	0.41
47:5:4400:G:C6	47:5:4401:G:C8	3.09	0.41
47:5:4440:G:C4	47:5:4441:A:C8	3.09	0.41
47:5:4618:G:C2	47:5:4619:U:C5	3.09	0.41
47:5:4735:G:O2'	47:5:4736:C:P	2.79	0.41
48:8:67:U:C2	48:8:68:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:72:C:C4'	49:9:73:C:OP1	2.69	0.41
49:9:426:A:C5	49:9:427:U:C2	3.09	0.41
49:9:453:C:C2'	49:9:454:U:H5'	2.51	0.41
49:9:615:C:O2'	80:ee:84:LYS:NZ	2.52	0.41
49:9:1664:A:C4'	49:9:1665:G:OP1	2.69	0.41
52:CC:177:PRO:HD3	71:VV:9:VAL:HG21	2.03	0.41
53:DD:146:ARG:HH12	85:1:1500:A:HO2'	1.68	0.41
58:II:194:GLU:OE1	61:LL:10:TYR:CE1	2.73	0.41
62:MM:52:LEU:HD21	62:MM:62:VAL:HG23	2.02	0.41
67:RR:21:TYR:CE1	67:RR:61:ILE:HG21	2.56	0.41
73:XX:85:VAL:HG23	73:XX:85:VAL:O	2.20	0.41
84:EF:69:ARG:HG3	84:EF:71:ILE:N	2.36	0.41
84:EF:88:THR:HG23	84:EF:88:THR:O	2.19	0.41
84:EF:155:MET:HE3	84:EF:208:MET:CE	2.47	0.41
84:EF:193:ILE:HG22	84:EF:200:ASN:O	2.21	0.41
84:EF:193:ILE:HD13	84:EF:228:LEU:HD22	2.02	0.41
84:EF:249:PRO:HG2	84:EF:266:ARG:HH11	1.86	0.41
84:EF:413:GLU:HG2	84:EF:418:TYR:CE1	2.56	0.41
1:7:62:U:H3'	1:7:63:C:C5'	2.51	0.40
3:B:389:MET:HE3	3:B:389:MET:CA	2.49	0.40
4:C:232:VAL:HG23	4:C:233:THR:HG23	2.02	0.40
4:C:269:LYS:CE	47:5:654:C:O3'	2.68	0.40
4:C:323:ARG:NH2	47:5:976:G:H21	2.19	0.40
7:F:120:THR:HG22	7:F:121:PHE:N	2.37	0.40
7:F:242:LEU:HD21	7:F:246:MET:SD	2.61	0.40
11:J:40:LEU:O	11:J:44:THR:HG23	2.21	0.40
12:L:6:ASN:HA	27:a:48:TYR:CD2	2.57	0.40
13:M:36:ALA:HB2	13:M:52:PHE:CZ	2.56	0.40
16:P:36:ILE:HD12	16:P:44:ALA:HB1	2.03	0.40
17:Q:128:LEU:HD23	17:Q:128:LEU:C	2.46	0.40
20:T:84:ILE:HD12	20:T:84:ILE:H	1.86	0.40
23:W:82:ILE:HG12	56:GG:131:ARG:HE	1.86	0.40
26:Z:60:LYS:HD3	26:Z:60:LYS:C	2.46	0.40
43:r:73:PRO:HA	43:r:76:SER:HB3	2.02	0.40
44:s:161:ILE:HG12	44:s:167:VAL:HA	2.02	0.40
44:s:161:ILE:N	44:s:161:ILE:HD12	2.35	0.40
46:3:1:G:C2	46:3:73:A:C2	3.09	0.40
47:5:704:C:O2	47:5:704:C:H2'	2.21	0.40
47:5:3888:G:HO2'	47:5:3889:G:P	2.44	0.40
47:5:4553:A:H2'	47:5:4554:G:O4'	2.22	0.40
49:9:687:C:O2	49:9:687:C:H2'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:933:G:N2	76:aa:19:GLN:HE22	2.19	0.40
49:9:1300:U:O2	49:9:1300:U:O4'	2.38	0.40
49:9:1865:C:O2	49:9:1865:C:O4'	2.38	0.40
51:BB:123:ALA:HB3	51:BB:168:MET:HE3	2.03	0.40
55:FF:102:LEU:C	75:ZZ:66:LYS:HE3	2.45	0.40
57:HH:144:ILE:HG22	72:WW:52:ILE:CG1	2.51	0.40
58:II:46:VAL:O	58:II:53:LYS:HA	2.21	0.40
69:TT:112:MET:CE	69:TT:130:ASP:HB2	2.51	0.40
84:EF:253:VAL:HG22	84:EF:263:PRO:HA	2.03	0.40
2:A:209:HIS:NE2	2:A:235:VAL:HG11	2.37	0.40
4:C:57:LEU:H	4:C:57:LEU:HD22	1.86	0.40
4:C:335:MET:HE1	7:F:57:HIS:CG	2.57	0.40
6:E:115:MET:HE1	47:5:2261:G:C5'	2.51	0.40
8:G:133:ILE:HD11	14:N:22:LEU:CD2	2.50	0.40
8:G:196:VAL:HG21	8:G:254:THR:CG2	2.51	0.40
19:S:164:LYS:HD3	19:S:165:PRO:N	2.35	0.40
20:T:93:ILE:HA	20:T:96:ILE:HD13	2.03	0.40
29:c:65:MET:HE3	29:c:65:MET:HB3	1.99	0.40
30:d:42:ALA:HB3	30:d:43:PRO:HD3	2.02	0.40
31:e:11:LYS:HE2	31:e:11:LYS:HA	2.02	0.40
40:n:10:MET:HE2	40:n:10:MET:HA	2.03	0.40
47:5:269:G:C4	47:5:270:U:C5	3.09	0.40
47:5:1370:G:H5'	47:5:1372:A:O4'	2.21	0.40
47:5:1472:C:C2	47:5:1473:U:C5	3.09	0.40
47:5:1646:A:H2'	47:5:1647:U:C6	2.57	0.40
47:5:2844:A:O2'	47:5:4631:G:H4'	2.22	0.40
47:5:3693:U:C2	47:5:3694:U:C5	3.09	0.40
49:9:452:G:H2'	49:9:453:C:O4'	2.21	0.40
49:9:1154:U:C5	52:CC:192:LEU:HD22	2.56	0.40
49:9:1781:A:H2'	49:9:1782:G:C8	2.57	0.40
50:AA:30:LEU:HB2	50:AA:47:TYR:CE2	2.56	0.40
54:EE:103:TYR:CD2	54:EE:189:LEU:HD11	2.55	0.40
57:HH:99:ARG:HB3	57:HH:99:ARG:HH11	1.85	0.40
68:SS:101:ASN:OD1	68:SS:101:ASN:O	2.39	0.40
73:XX:61:GLN:O	73:XX:63:ASN:N	2.54	0.40
79:dd:43:PHE:CD1	79:dd:43:PHE:C	2.99	0.40
81:ff:92:LYS:O	81:ff:94:LYS:HD3	2.21	0.40
83:AT:19:U:C2	83:AT:58:A:N3	2.89	0.40
83:AT:51:G:H22	83:AT:65:G:H1	1.70	0.40
84:EF:66:GLU:HG3	84:EF:73:ILE:HD12	2.03	0.40
3:B:367:PHE:CG	23:W:1:MET:HE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:314:LEU:O	8:G:317:LYS:HG2	2.21	0.40
11:J:42:GLN:OE1	11:J:42:GLN:N	2.54	0.40
12:L:42:ARG:HH22	47:5:106:A:H5''	1.87	0.40
17:Q:91:ARG:CB	27:a:76:ASP:OD1	2.69	0.40
17:Q:97:LYS:C	17:Q:98:LEU:HD23	2.46	0.40
19:S:82:LEU:HB2	19:S:93:MET:HB2	2.04	0.40
29:c:47:ILE:HD13	29:c:94:LEU:HD22	2.04	0.40
44:s:39:GLN:HE22	44:s:107:VAL:HG11	1.86	0.40
44:s:53:VAL:HG22	44:s:89:VAL:HG22	2.03	0.40
44:s:119:CYS:C	44:s:183:PHE:CZ	2.99	0.40
47:5:243:A:H2'	47:5:244:G:O4'	2.21	0.40
47:5:1817:U:C2	47:5:1823:G:C2	3.10	0.40
47:5:2016:C:C2	47:5:2017:A:C8	3.10	0.40
47:5:2676:A:H2'	47:5:2677:G:O4'	2.20	0.40
47:5:2768:C:H5'	47:5:2769:U:P	2.61	0.40
47:5:4458:C:H2'	47:5:4459:U:C6	2.56	0.40
47:5:5050:C:C2	47:5:5051:C:C5	3.09	0.40
50:AA:68:ILE:HG21	50:AA:74:VAL:CG2	2.51	0.40
50:AA:176:TRP:CD1	50:AA:199:PRO:HA	2.56	0.40
51:BB:103:MET:HG3	51:BB:188:LEU:HD11	2.02	0.40
55:FF:76:MET:HB3	55:FF:89:THR:HG22	2.02	0.40
59:JJ:29:LEU:HD21	80:ee:111:TYR:HA	2.02	0.40
61:LL:132:ARG:O	61:LL:134:LEU:HD22	2.20	0.40
64:OO:47:LEU:H	64:OO:47:LEU:HD22	1.86	0.40
69:TT:75:MET:N	69:TT:75:MET:SD	2.93	0.40
72:WW:34:ILE:CG2	72:WW:35:VAL:N	2.84	0.40
73:XX:71:ARG:CZ	73:XX:80:LYS:HB3	2.51	0.40
77:bb:79:PHE:CD1	77:bb:79:PHE:C	2.99	0.40
84:EF:161:PRO:C	84:EF:162:TYR:CD1	2.99	0.40
84:EF:325:VAL:O	84:EF:325:VAL:CG2	2.69	0.40
2:A:107:MET:HE1	2:A:113:VAL:CG1	2.51	0.40
2:A:189:TYR:CD2	2:A:196:TRP:HB2	2.56	0.40
3:B:41:VAL:HG21	3:B:196:TRP:CD1	2.57	0.40
3:B:389:MET:HE1	47:5:5041:G:C6	2.57	0.40
4:C:10:VAL:HG12	4:C:11:TYR:N	2.36	0.40
4:C:312:ARG:HH12	47:5:2274:C:H5''	1.86	0.40
8:G:94:ILE:HD12	8:G:94:ILE:N	2.36	0.40
9:H:44:GLU:OE2	13:M:3:PHE:HE2	2.03	0.40
12:L:110:LEU:O	12:L:110:LEU:HD23	2.21	0.40
15:O:113:ASP:OD1	15:O:114:LYS:N	2.54	0.40
22:V:45:ILE:C	22:V:45:ILE:CD1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:81:LEU:O	27:a:81:LEU:HD23	2.21	0.40
46:2:16:U:H2'	46:2:16:U:O2	2.20	0.40
47:5:756:G:C6	47:5:908:G:C6	3.09	0.40
47:5:1850:A:C6	47:5:1851:G:C6	3.09	0.40
47:5:1920:C:H4'	47:5:1921:C:OP2	2.22	0.40
47:5:4120:U:O2	47:5:4120:U:H2'	2.21	0.40
47:5:4349:C:H4'	47:5:4350:C:OP2	2.21	0.40
49:9:464:A:C6	84:EF:41:LYS:HD3	2.56	0.40
49:9:495:U:O3'	49:9:496:C:O4'	2.40	0.40
49:9:682:U:H2'	72:WW:4:MET:HE2	2.03	0.40
49:9:799:U:C5	49:9:867:G:N1	2.90	0.40
49:9:1401:A:H2'	49:9:1402:A:C8	2.56	0.40
50:AA:132:GLN:HB3	50:AA:133:PRO:HD3	2.03	0.40
55:FF:164:ARG:HA	55:FF:164:ARG:NE	2.37	0.40
57:HH:154:ILE:HD12	57:HH:154:ILE:N	2.37	0.40
63:NN:66:VAL:HG13	63:NN:67:THR:N	2.37	0.40
63:NN:80:LEU:HD22	63:NN:80:LEU:N	2.36	0.40
66:QQ:41:MET:C	66:QQ:41:MET:HE2	2.46	0.40
68:SS:8:LYS:HD2	68:SS:8:LYS:C	2.46	0.40
69:TT:142:LYS:HD3	69:TT:142:LYS:O	2.21	0.40
75:ZZ:58:LEU:HG	75:ZZ:62:VAL:HG21	2.02	0.40
77:bb:74:THR:HG22	77:bb:75:GLU:N	2.36	0.40
78:cc:58:LEU:N	78:cc:58:LEU:HD12	2.37	0.40
84:EF:152:VAL:HG11	84:EF:166:ARG:NH1	2.36	0.40
84:EF:264:VAL:HG22	84:EF:309:GLY:HA2	2.04	0.40
1:7:65:G:H2'	1:7:66:G:O4'	2.22	0.40
4:C:74:ALA:O	4:C:75:ARG:HG2	2.22	0.40
5:D:4:VAL:HG11	47:5:4247:G:C5'	2.50	0.40
7:F:143:TYR:CD1	7:F:143:TYR:N	2.86	0.40
7:F:196:VAL:HG23	7:F:196:VAL:O	2.21	0.40
12:L:21:ARG:CZ	12:L:21:ARG:O	2.70	0.40
12:L:121:ARG:O	12:L:121:ARG:HD3	2.21	0.40
18:R:154:LEU:HD21	18:R:158:GLN:NE2	2.36	0.40
19:S:99:ASP:OD2	19:S:105:ALA:N	2.55	0.40
20:T:158:PHE:C	20:T:158:PHE:CD1	3.00	0.40
22:V:18:LEU:HD23	22:V:18:LEU:N	2.35	0.40
35:i:34:THR:HG22	35:i:35:LYS:N	2.36	0.40
44:s:75:LEU:C	44:s:77:LYS:H	2.29	0.40
47:5:1986:U:H2'	47:5:2007:G:O6	2.21	0.40
47:5:2330:G:O3'	47:5:2331:G:O4'	2.40	0.40
47:5:2332:A:H4'	47:5:2333:G:OP1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:2423:A:H2'	47:5:2424:G:O4'	2.21	0.40
47:5:3651:A:H2'	47:5:3652:A:O4'	2.22	0.40
47:5:3807:A:C6	47:5:3808:C:N4	2.89	0.40
47:5:4873:G:H3'	47:5:4874:A:H5''	2.02	0.40
47:5:4925:U:H1'	47:5:4926:C:P	2.62	0.40
47:5:4926:C:H3'	47:5:4926:C:O2	2.21	0.40
47:5:4948:C:H2'	47:5:4949:G:N2	2.37	0.40
47:5:5051:C:H2'	47:5:5052:C:C6	2.56	0.40
49:9:1055:A:H2'	49:9:1056:U:C6	2.57	0.40
49:9:1464:C:OP2	67:RR:63:ARG:NH2	2.55	0.40
49:9:1573:G:H2'	49:9:1574:C:Cl'	2.52	0.40
51:BB:188:LEU:CD2	51:BB:212:VAL:HG11	2.51	0.40
52:CC:267:GLN:NE2	71:VV:50:PHE:HE2	2.19	0.40
54:EE:68:ARG:O	54:EE:68:ARG:NH1	2.54	0.40
55:FF:127:ARG:HD2	55:FF:135:ARG:O	2.21	0.40
58:II:48:VAL:HG12	58:II:49:ARG:H	1.86	0.40
60:KK:29:MET:SD	60:KK:29:MET:C	3.04	0.40
65:PP:16:THR:O	65:PP:16:THR:HG23	2.21	0.40
68:SS:5:ILE:HD12	75:ZZ:49:LEU:HD12	2.03	0.40
72:WW:69:LEU:HD13	72:WW:70:ASN:N	2.36	0.40
72:WW:75:ILE:O	72:WW:75:ILE:HG23	2.21	0.40
73:XX:61:GLN:HB3	73:XX:62:PRO:CD	2.52	0.40
82:gg:264:LYS:O	82:gg:265:ILE:HG23	2.22	0.40
83:AT:45:G:H2'	83:AT:46:G:O4'	2.22	0.40
84:EF:191:VAL:HG21	84:EF:231:ALA:CB	2.52	0.40
84:EF:280:PHE:N	84:EF:280:PHE:CD1	2.89	0.40
84:EF:337:ALA:CB	84:EF:412:VAL:HG22	2.51	0.40
84:EF:340:PHE:CD1	84:EF:341:THR:N	2.89	0.40
84:EF:346:ILE:HD12	84:EF:433:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
3	B	392/394 (100%)	377 (96%)	15 (4%)	0	100	100
4	C	360/362 (99%)	350 (97%)	10 (3%)	0	100	100
5	D	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
6	E	208/216 (96%)	204 (98%)	4 (2%)	0	100	100
7	F	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
8	G	229/240 (95%)	223 (97%)	6 (3%)	0	100	100
9	H	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
10	I	201/213 (94%)	196 (98%)	5 (2%)	0	100	100
11	J	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
12	L	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
13	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
14	N	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
15	O	197/199 (99%)	187 (95%)	10 (5%)	0	100	100
16	P	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
17	Q	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
18	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
19	S	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
20	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
21	U	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
22	V	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
23	W	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
24	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
25	Y	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
26	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
27	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
28	b	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
29	c	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
30	d	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
31	e	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
32	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
33	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
35	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
36	j	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
37	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
38	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
39	m	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
40	n	23/25 (92%)	23 (100%)	0	0	100	100
41	o	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
42	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
43	r	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	s	194/196 (99%)	157 (81%)	35 (18%)	2 (1%)	12	45
45	t	133/153 (87%)	121 (91%)	11 (8%)	1 (1%)	16	50
50	AA	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
51	BB	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
52	CC	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
53	DD	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
54	EE	260/262 (99%)	252 (97%)	8 (3%)	0	100	100
55	FF	181/191 (95%)	171 (94%)	10 (6%)	0	100	100
56	GG	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
57	HH	181/189 (96%)	175 (97%)	6 (3%)	0	100	100
58	II	204/206 (99%)	187 (92%)	17 (8%)	0	100	100
59	JJ	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
60	KK	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
61	LL	139/151 (92%)	133 (96%)	6 (4%)	0	100	100
62	MM	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
63	NN	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
64	OO	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
65	PP	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
66	QQ	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
67	RR	130/132 (98%)	128 (98%)	2 (2%)	0	100	100
68	SS	142/144 (99%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	TT	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
70	UU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
71	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
72	WW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
73	XX	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	18	53
74	YY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
75	ZZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
76	aa	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
77	bb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
78	cc	60/62 (97%)	60 (100%)	0	0	100	100
79	dd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
80	ee	55/57 (96%)	55 (100%)	0	0	100	100
81	ff	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
82	gg	311/313 (99%)	301 (97%)	10 (3%)	0	100	100
84	EF	438/441 (99%)	384 (88%)	53 (12%)	1 (0%)	43	76
All	All	11958/12186 (98%)	11487 (96%)	466 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
73	XX	62	PRO
44	s	76	GLU
44	s	195	ASN
84	EF	160	PRO
45	t	54	LYS

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	A	190/190 (100%)	188 (99%)	2 (1%)	65	83
3	B	342/342 (100%)	340 (99%)	2 (1%)	78	88
4	C	302/302 (100%)	302 (100%)	0	100	100
5	D	247/247 (100%)	247 (100%)	0	100	100
6	E	190/190 (100%)	188 (99%)	2 (1%)	65	83
7	F	196/196 (100%)	191 (97%)	5 (3%)	40	72
8	G	200/205 (98%)	198 (99%)	2 (1%)	68	84
9	H	169/169 (100%)	169 (100%)	0	100	100
10	I	175/180 (97%)	172 (98%)	3 (2%)	53	78
11	J	143/143 (100%)	142 (99%)	1 (1%)	76	86
12	L	175/175 (100%)	172 (98%)	3 (2%)	53	78
13	M	117/117 (100%)	115 (98%)	2 (2%)	53	78
14	N	171/171 (100%)	168 (98%)	3 (2%)	51	77
15	O	171/171 (100%)	167 (98%)	4 (2%)	44	74
16	P	134/134 (100%)	132 (98%)	2 (2%)	57	80
17	Q	164/164 (100%)	161 (98%)	3 (2%)	51	77
18	R	158/159 (99%)	155 (98%)	3 (2%)	50	76
19	S	156/157 (99%)	152 (97%)	4 (3%)	40	72
20	T	139/139 (100%)	137 (99%)	2 (1%)	59	80
21	U	89/89 (100%)	89 (100%)	0	100	100
22	V	106/106 (100%)	106 (100%)	0	100	100
23	W	86/86 (100%)	85 (99%)	1 (1%)	63	82
24	X	106/106 (100%)	103 (97%)	3 (3%)	38	70
25	Y	124/124 (100%)	123 (99%)	1 (1%)	73	86
26	Z	117/117 (100%)	117 (100%)	0	100	100
27	a	119/119 (100%)	117 (98%)	2 (2%)	53	78
28	b	84/84 (100%)	83 (99%)	1 (1%)	63	82
29	c	84/84 (100%)	84 (100%)	0	100	100
30	d	98/98 (100%)	97 (99%)	1 (1%)	68	84
31	e	114/114 (100%)	111 (97%)	3 (3%)	40	72
32	f	88/88 (100%)	86 (98%)	2 (2%)	44	74
33	g	98/98 (100%)	95 (97%)	3 (3%)	35	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	h	109/109 (100%)	108 (99%)	1 (1%)	70	85
35	i	86/86 (100%)	86 (100%)	0	100	100
36	j	73/73 (100%)	73 (100%)	0	100	100
37	k	64/64 (100%)	63 (98%)	1 (2%)	55	79
38	l	47/47 (100%)	46 (98%)	1 (2%)	47	75
39	m	48/48 (100%)	48 (100%)	0	100	100
40	n	24/24 (100%)	24 (100%)	0	100	100
41	o	92/92 (100%)	91 (99%)	1 (1%)	65	83
42	p	74/74 (100%)	71 (96%)	3 (4%)	27	61
43	r	108/108 (100%)	107 (99%)	1 (1%)	70	85
44	s	164/164 (100%)	156 (95%)	8 (5%)	22	56
45	t	110/126 (87%)	110 (100%)	0	100	100
50	AA	180/181 (99%)	177 (98%)	3 (2%)	53	78
51	BB	194/194 (100%)	192 (99%)	2 (1%)	68	84
52	CC	187/187 (100%)	187 (100%)	0	100	100
53	DD	190/190 (100%)	190 (100%)	0	100	100
54	EE	224/224 (100%)	223 (100%)	1 (0%)	84	90
55	FF	158/161 (98%)	157 (99%)	1 (1%)	78	88
56	GG	206/207 (100%)	203 (98%)	3 (2%)	57	80
57	HH	165/169 (98%)	163 (99%)	2 (1%)	63	82
58	II	178/178 (100%)	168 (94%)	10 (6%)	19	52
59	JJ	161/161 (100%)	158 (98%)	3 (2%)	50	76
60	KK	87/87 (100%)	87 (100%)	0	100	100
61	LL	130/136 (96%)	127 (98%)	3 (2%)	44	74
62	MM	99/99 (100%)	98 (99%)	1 (1%)	68	84
63	NN	130/130 (100%)	129 (99%)	1 (1%)	73	86
64	OO	106/106 (100%)	105 (99%)	1 (1%)	70	85
65	PP	115/115 (100%)	114 (99%)	1 (1%)	70	85
66	QQ	117/117 (100%)	115 (98%)	2 (2%)	53	78
67	RR	119/119 (100%)	117 (98%)	2 (2%)	53	78
68	SS	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	TT	110/111 (99%)	110 (100%)	0	100	100
70	UU	92/92 (100%)	90 (98%)	2 (2%)	45	74
71	VV	67/67 (100%)	66 (98%)	1 (2%)	57	80
72	WW	112/112 (100%)	110 (98%)	2 (2%)	51	77
73	XX	113/113 (100%)	113 (100%)	0	100	100
74	YY	107/107 (100%)	103 (96%)	4 (4%)	30	64
75	ZZ	66/66 (100%)	66 (100%)	0	100	100
76	aa	88/88 (100%)	85 (97%)	3 (3%)	32	66
77	bb	75/75 (100%)	75 (100%)	0	100	100
78	cc	55/55 (100%)	54 (98%)	1 (2%)	51	77
79	dd	48/48 (100%)	48 (100%)	0	100	100
80	ee	47/47 (100%)	46 (98%)	1 (2%)	47	75
81	ff	61/61 (100%)	61 (100%)	0	100	100
82	gg	272/272 (100%)	271 (100%)	1 (0%)	84	90
84	EF	365/366 (100%)	345 (94%)	20 (6%)	19	53
All	All	10400/10445 (100%)	10253 (99%)	147 (1%)	57	80

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	135	THR
2	A	175	ILE
3	B	240	LEU
3	B	261	ARG
6	E	156	LEU
6	E	198	ILE
7	F	49	ILE
7	F	59	GLU
7	F	62	GLN
7	F	162	ASN
7	F	204	ASN
8	G	212	HIS
8	G	310	LYS
10	I	36	LEU
10	I	71	CYS
10	I	115	MET
11	J	42	GLN

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Mol	Chain	Res	Type
12	L	10	LEU
12	L	184	MET
12	L	204	GLU
13	M	30	VAL
13	M	43	THR
14	N	24	ARG
14	N	33	LEU
14	N	161	MET
15	O	5	GLN
15	O	55	LEU
15	O	61	ARG
15	O	182	GLU
16	P	64	ASN
16	P	80	GLN
17	Q	19	LYS
17	Q	21	GLN
17	Q	67	ILE
18	R	12	SER
18	R	28	GLU
18	R	111	GLU
19	S	68	PHE
19	S	77	ASN
19	S	80	ILE
19	S	160	ARG
20	T	94	GLU
20	T	143	THR
23	W	32	LEU
24	X	71	LEU
24	X	82	THR
24	X	116	LEU
25	Y	29	ILE
27	a	5	LEU
27	a	72	THR
28	b	101	HIS
30	d	26	THR
31	e	7	LEU
31	e	32	LYS
31	e	78	LEU
32	f	18	LEU
32	f	47	CYS
33	g	13	TYR
33	g	49	CYS

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Mol	Chain	Res	Type
33	g	107	LEU
34	h	4	ILE
37	k	31	ASN
38	l	19	GLN
41	o	104	ILE
42	p	10	ILE
42	p	48	LYS
42	p	69	TRP
43	r	22	LYS
44	s	24	TYR
44	s	72	ASN
44	s	75	LEU
44	s	82	ILE
44	s	135	THR
44	s	163	THR
44	s	184	SER
44	s	189	ILE
50	AA	10	MET
50	AA	36	GLN
50	AA	121	LEU
51	BB	96	CYS
51	BB	124	HIS
54	EE	160	ILE
55	FF	171	GLU
56	GG	63	MET
56	GG	82	SER
56	GG	145	PHE
57	HH	36	LEU
57	HH	93	VAL
58	II	27	TYR
58	II	46	VAL
58	II	48	VAL
58	II	80	ASP
58	II	82	VAL
58	II	95	THR
58	II	137	LEU
58	II	139	LYS
58	II	154	LYS
58	II	159	SER
59	JJ	28	GLU
59	JJ	40	LYS
59	JJ	92	MET

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Mol	Chain	Res	Type
61	LL	4	ILE
61	LL	42	LEU
61	LL	146	THR
62	MM	94	ILE
63	NN	14	SER
64	OO	124	MET
65	PP	108	LYS
66	QQ	114	GLN
66	QQ	116	ASP
67	RR	7	LYS
67	RR	99	ASP
70	UU	80	PHE
70	UU	91	LEU
71	VV	64	GLU
72	WW	9	ASP
72	WW	42	MET
74	YY	17	LEU
74	YY	25	ILE
74	YY	58	PHE
74	YY	84	LYS
76	aa	3	LYS
76	aa	44	ILE
76	aa	77	CYS
78	cc	62	GLU
80	ee	121	THR
82	gg	196	ASN
84	EF	51	LYS
84	EF	64	LYS
84	EF	98	PHE
84	EF	139	LEU
84	EF	155	MET
84	EF	171	VAL
84	EF	178	ILE
84	EF	266	ARG
84	EF	272	LEU
84	EF	273	LYS
84	EF	280	PHE
84	EF	283	VAL
84	EF	303	LEU
84	EF	340	PHE
84	EF	361	LEU
84	EF	372	PHE

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Mol	Chain	Res	Type
84	EF	395	LYS
84	EF	410	MET
84	EF	421	LEU
84	EF	442	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	83	HIS
3	B	258	HIS
4	C	278	ASN
5	D	198	HIS
7	F	55	HIS
7	F	171	ASN
7	F	240	ASN
8	G	117	GLN
8	G	143	GLN
8	G	147	GLN
8	G	194	ASN
8	G	206	GLN
9	H	163	GLN
10	I	51	HIS
10	I	59	GLN
11	J	23	ASN
11	J	71	HIS
13	M	66	HIS
15	O	63	ASN
15	O	143	HIS
16	P	64	ASN
16	P	80	GLN
18	R	141	HIS
18	R	158	GLN
19	S	117	HIS
20	T	70	HIS
21	U	41	GLN
23	W	30	GLN
23	W	59	HIS
25	Y	20	ASN
25	Y	56	GLN
27	a	14	HIS
27	a	62	HIS
30	d	34	HIS

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Mol	Chain	Res	Type
30	d	100	ASN
35	i	36	HIS
43	r	103	HIS
44	s	41	GLN
44	s	72	ASN
45	t	103	ASN
50	AA	81	ASN
50	AA	84	GLN
50	AA	111	GLN
50	AA	215	GLN
51	BB	101	HIS
51	BB	177	GLN
53	DD	101	GLN
54	EE	188	ASN
55	FF	79	HIS
55	FF	82	ASN
57	HH	165	ASN
60	KK	73	ASN
61	LL	100	ASN
61	LL	106	HIS
62	MM	48	HIS
62	MM	73	GLN
63	NN	5	HIS
64	OO	79	GLN
66	QQ	142	GLN
67	RR	56	HIS
69	TT	128	GLN
71	VV	82	ASN
78	cc	29	GLN
81	ff	91	ASN
82	gg	14	HIS
82	gg	117	ASN
84	EF	26	HIS
84	EF	108	GLN
84	EF	348	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	7	118/119 (99%)	14 (11%)	0
46	2	73/75 (97%)	19 (26%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	3	72/75 (96%)	12 (16%)	0
47	5	3518/3543 (99%)	734 (20%)	73 (2%)
48	8	149/156 (95%)	30 (20%)	1 (0%)
49	9	1681/1697 (99%)	341 (20%)	20 (1%)
83	AT	67/76 (88%)	24 (35%)	2 (2%)
85	1	14/15 (93%)	6 (42%)	3 (21%)
All	All	5692/5756 (98%)	1180 (20%)	100 (1%)

All (1180) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	7	7	G
1	7	22	A
1	7	25	G
1	7	33	U
1	7	53	U
1	7	54	A
1	7	61	G
1	7	62	U
1	7	63	C
1	7	64	G
1	7	85	G
1	7	97	G
1	7	100	A
1	7	110	G
46	2	8	U
46	2	11	C
46	2	12	U
46	2	13	C
46	2	16	U
46	2	19	U
46	2	20	U
46	2	21	A
46	2	46	G
46	2	47	C
46	2	48	C
46	2	49	C
46	2	59	U
46	2	60	C
46	2	63	C
46	2	67	A
46	2	74	C

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Mol	Chain	Res	Type
46	2	75	C
46	2	76	A
46	3	7	G
46	3	13	C
46	3	16	U
46	3	21	A
46	3	34	A
46	3	35	G
46	3	49	C
46	3	58	A
46	3	63	C
46	3	69	C
46	3	70	U
46	3	76	A
47	5	12	A
47	5	13	U
47	5	25	A
47	5	35	U
47	5	39	A
47	5	42	A
47	5	48	G
47	5	49	U
47	5	59	A
47	5	64	A
47	5	65	A
47	5	66	A
47	5	73	A
47	5	74	G
47	5	75	G
47	5	91	G
47	5	93	G
47	5	104	G
47	5	109	G
47	5	118	C
47	5	119	G
47	5	120	A
47	5	126	C
47	5	134	G
47	5	135	G
47	5	136	C
47	5	143	C
47	5	144	G

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Mol	Chain	Res	Type
47	5	146	G
47	5	159	C
47	5	172	C
47	5	173	C
47	5	182	G
47	5	200	U
47	5	201	C
47	5	209	U
47	5	216	C
47	5	218	A
47	5	220	C
47	5	224	U
47	5	227	A
47	5	233	U
47	5	234	G
47	5	245	C
47	5	246	G
47	5	262	C
47	5	264	C
47	5	265	C
47	5	266	C
47	5	276	C
47	5	280	G
47	5	281	U
47	5	297	U
47	5	306	A
47	5	309	C
47	5	310	G
47	5	315	G
47	5	316	U
47	5	322	C
47	5	334	A
47	5	336	A
47	5	340	C
47	5	350	C
47	5	357	U
47	5	363	A
47	5	373	G
47	5	386	A
47	5	387	G
47	5	399	G
47	5	407	A

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Mol	Chain	Res	Type
47	5	409	G
47	5	410	A
47	5	412	G
47	5	413	G
47	5	414	C
47	5	431	G
47	5	432	U
47	5	440	U
47	5	446	C
47	5	449	C
47	5	450	G
47	5	452	A
47	5	453	G
47	5	454	U
47	5	455	C
47	5	459	C
47	5	464	G
47	5	467	U
47	5	468	U
47	5	469	C
47	5	481	G
47	5	481(A)	C
47	5	482	G
47	5	483	G
47	5	486	C
47	5	492	U
47	5	493	G
47	5	498	C
47	5	499	G
47	5	505	G
47	5	510	U
47	5	647	G
47	5	658	C
47	5	667	A
47	5	672	C
47	5	682	G
47	5	683	C
47	5	684	G
47	5	685	C
47	5	687	U
47	5	696	C
47	5	697	G

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Mol	Chain	Res	Type
47	5	704	C
47	5	705	G
47	5	708	G
47	5	722	G
47	5	730	G
47	5	731	G
47	5	738	C
47	5	738(A)	C
47	5	739	G
47	5	742	G
47	5	747	A
47	5	748	G
47	5	749	G
47	5	758	G
47	5	908	G
47	5	913	U
47	5	914	U
47	5	917	A
47	5	918	G
47	5	923	C
47	5	925	C
47	5	926	G
47	5	929	A
47	5	930	G
47	5	931	C
47	5	932	A
47	5	933	G
47	5	934	C
47	5	935	A
47	5	935(A)	G
47	5	936	C
47	5	939	G
47	5	941	C
47	5	943	A
47	5	944	A
47	5	945	U
47	5	956	A
47	5	959	G
47	5	960	A
47	5	961	G
47	5	967	C
47	5	969	C

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Mol	Chain	Res	Type
47	5	972	C
47	5	979	C
47	5	983	C
47	5	990	C
47	5	1072	C
47	5	1073	G
47	5	1075	G
47	5	1076	C
47	5	1179	U
47	5	1187	G
47	5	1195	G
47	5	1200	G
47	5	1204	C
47	5	1211	G
47	5	1212	G
47	5	1214	C
47	5	1215	C
47	5	1216	C
47	5	1234	G
47	5	1235	G
47	5	1236	C
47	5	1237	C
47	5	1238	A
47	5	1239	C
47	5	1272	C
47	5	1273	G
47	5	1274	A
47	5	1276	C
47	5	1277	G
47	5	1281	G
47	5	1284	G
47	5	1287	G
47	5	1288	G
47	5	1292	C
47	5	1293	G
47	5	1294	A
47	5	1295	C
47	5	1296	G
47	5	1297	U
47	5	1301	C
47	5	1303	A
47	5	1304	C

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Mol	Chain	Res	Type
47	5	1325	C
47	5	1326	A
47	5	1330	A
47	5	1349	G
47	5	1354	A
47	5	1358	G
47	5	1359	G
47	5	1371	A
47	5	1377	G
47	5	1380	G
47	5	1381	U
47	5	1387	A
47	5	1394	G
47	5	1397	A
47	5	1398	A
47	5	1415	G
47	5	1419	G
47	5	1420	A
47	5	1421	G
47	5	1429	C
47	5	1438	U
47	5	1440	U
47	5	1441	C
47	5	1445	U
47	5	1446	C
47	5	1456	C
47	5	1457	G
47	5	1458	C
47	5	1478	C
47	5	1482	G
47	5	1483	C
47	5	1484	G
47	5	1486	C
47	5	1493	G
47	5	1497	A
47	5	1498	G
47	5	1502	G
47	5	1504	G
47	5	1516	G
47	5	1518	A
47	5	1523	A
47	5	1534	A

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Mol	Chain	Res	Type
47	5	1547	A
47	5	1563	A
47	5	1564	A
47	5	1566	C
47	5	1574	G
47	5	1578	U
47	5	1591	U
47	5	1596	U
47	5	1602	U
47	5	1612	G
47	5	1613	A
47	5	1624	G
47	5	1625	G
47	5	1631	A
47	5	1633	G
47	5	1634	A
47	5	1638	A
47	5	1640	C
47	5	1641	G
47	5	1646	A
47	5	1654	G
47	5	1661	C
47	5	1676	C
47	5	1691	G
47	5	1724	G
47	5	1729	A
47	5	1734	G
47	5	1741	G
47	5	1742	A
47	5	1746	A
47	5	1750	G
47	5	1754	U
47	5	1756	U
47	5	1761	G
47	5	1764	G
47	5	1768	C
47	5	1772	C
47	5	1773	U
47	5	1776	A
47	5	1777	C
47	5	1781	U
47	5	1787	A

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Mol	Chain	Res	Type
47	5	1799	G
47	5	1804	A
47	5	1805	A
47	5	1819	G
47	5	1821	G
47	5	1822	U
47	5	1828	C
47	5	1834	U
47	5	1835	G
47	5	1836	G
47	5	1837	A
47	5	1842	G
47	5	1855	G
47	5	1869	G
47	5	1883	G
47	5	1890	G
47	5	1893	C
47	5	1897	A
47	5	1899	G
47	5	1910	G
47	5	1916	G
47	5	1918	U
47	5	1919	G
47	5	1920	C
47	5	1921	C
47	5	1922	G
47	5	1923	A
47	5	1930	U
47	5	1931	C
47	5	1933	G
47	5	1939	A
47	5	1945	G
47	5	1947	U
47	5	1951	G
47	5	1952	G
47	5	1959	U
47	5	1960	A
47	5	1961	G
47	5	1962	A
47	5	1964	A
47	5	1975	G
47	5	1976	G

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Mol	Chain	Res	Type
47	5	1977	C
47	5	1978	C
47	5	1979	A
47	5	1980	U
47	5	1982	G
47	5	1984	A
47	5	1986	U
47	5	1987	C
47	5	1991	A
47	5	1997	U
47	5	2001	G
47	5	2002	A
47	5	2003	G
47	5	2004	U
47	5	2008	U
47	5	2025	A
47	5	2026	A
47	5	2047	A
47	5	2048	U
47	5	2055	G
47	5	2056	G
47	5	2062	C
47	5	2064	G
47	5	2069	A
47	5	2084	C
47	5	2085	G
47	5	2089	G
47	5	2090	U
47	5	2092	G
47	5	2093	A
47	5	2094	C
47	5	2095	A
47	5	2097	U
47	5	2098	G
47	5	2100	G
47	5	2101	A
47	5	2102	G
47	5	2103	A
47	5	2104	A
47	5	2105	A
47	5	2107	C
47	5	2108	G

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Mol	Chain	Res	Type
47	5	2259	G
47	5	2260	C
47	5	2262	G
47	5	2266	C
47	5	2267	U
47	5	2268	A
47	5	2269	C
47	5	2270	G
47	5	2274	C
47	5	2289	C
47	5	2300	A
47	5	2301	G
47	5	2306	G
47	5	2313	A
47	5	2314	G
47	5	2316	G
47	5	2322	G
47	5	2331	G
47	5	2333	G
47	5	2345	G
47	5	2348	G
47	5	2351	C
47	5	2395	A
47	5	2396	A
47	5	2398	U
47	5	2399	G
47	5	2402	G
47	5	2416	G
47	5	2417	A
47	5	2422	C
47	5	2425	U
47	5	2433	G
47	5	2463	G
47	5	2471	G
47	5	2475	G
47	5	2485	U
47	5	2487	G
47	5	2488	C
47	5	2489	C
47	5	2490	U
47	5	2491	C
47	5	2495	U

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Mol	Chain	Res	Type
47	5	2503	G
47	5	2504	C
47	5	2505	C
47	5	2506	G
47	5	2513	A
47	5	2518	G
47	5	2529	A
47	5	2530	U
47	5	2537	A
47	5	2546	G
47	5	2547	G
47	5	2549	G
47	5	2552	G
47	5	2553	A
47	5	2572	C
47	5	2582	A
47	5	2583	C
47	5	2586	G
47	5	2587	A
47	5	2589	C
47	5	2601	A
47	5	2620	G
47	5	2627	C
47	5	2653	C
47	5	2658	G
47	5	2661	U
47	5	2662	G
47	5	2669	C
47	5	2676	A
47	5	2686	G
47	5	2687	U
47	5	2695	A
47	5	2696	A
47	5	2705	G
47	5	2707	U
47	5	2708	U
47	5	2710	C
47	5	2711	G
47	5	2712	G
47	5	2716	C
47	5	2724	G
47	5	2725	A

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Mol	Chain	Res	Type
47	5	2726	G
47	5	2735	G
47	5	2740	U
47	5	2743	A
47	5	2753	G
47	5	2754	G
47	5	2759	G
47	5	2760	G
47	5	2761	U
47	5	2763	U
47	5	2764	A
47	5	2769	U
47	5	2772	C
47	5	2787	A
47	5	2788	U
47	5	2789	A
47	5	2790	U
47	5	2796	G
47	5	2807	A
47	5	2811	G
47	5	2814	C
47	5	2826	U
47	5	2827	G
47	5	2828	U
47	5	2842	G
47	5	2855	G
47	5	2880	U
47	5	2897	G
47	5	2898	G
47	5	3598	C
47	5	3604	A
47	5	3605	C
47	5	3615	G
47	5	3625	G
47	5	3626	G
47	5	3635	A
47	5	3644	U
47	5	3646	A
47	5	3653	A
47	5	3662	A
47	5	3669	G
47	5	3672	G

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Mol	Chain	Res	Type
47	5	3673	C
47	5	3674	G
47	5	3692	A
47	5	3696	C
47	5	3711	A
47	5	3712	A
47	5	3748	A
47	5	3753	G
47	5	3759	A
47	5	3760	A
47	5	3763	A
47	5	3772	U
47	5	3773	U
47	5	3774	A
47	5	3776	G
47	5	3777	G
47	5	3783	A
47	5	3784	A
47	5	3786	U
47	5	3787	G
47	5	3789	C
47	5	3798	U
47	5	3808	C
47	5	3810	C
47	5	3817	A
47	5	3819	G
47	5	3831	U
47	5	3838	U
47	5	3839	G
47	5	3840	U
47	5	3867	A
47	5	3876	A
47	5	3877	A
47	5	3878	C
47	5	3879	G
47	5	3889	G
47	5	3892	U
47	5	3897	G
47	5	3898	G
47	5	3901	A
47	5	3905	A
47	5	3906	A

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Mol	Chain	Res	Type
47	5	3907	G
47	5	3915	U
47	5	3916	G
47	5	3917	A
47	5	3939	G
47	5	3942	A
47	5	3943	A
47	5	4069	U
47	5	4073	A
47	5	4076	G
47	5	4077	A
47	5	4085	A
47	5	4086	G
47	5	4088	C
47	5	4092	G
47	5	4116	C
47	5	4119	C
47	5	4120	U
47	5	4122	G
47	5	4125	C
47	5	4127	A
47	5	4128	A
47	5	4133	C
47	5	4158	C
47	5	4162	C
47	5	4163	U
47	5	4166	G
47	5	4170	A
47	5	4171	C
47	5	4183	G
47	5	4184	G
47	5	4191	G
47	5	4203	A
47	5	4212	A
47	5	4213	A
47	5	4222	G
47	5	4225	G
47	5	4229	U
47	5	4232	U
47	5	4233	A
47	5	4243	C
47	5	4251	A

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Mol	Chain	Res	Type
47	5	4254	G
47	5	4258	C
47	5	4266	G
47	5	4268	A
47	5	4271	A
47	5	4273	A
47	5	4281	A
47	5	4290	U
47	5	4291	G
47	5	4297	G
47	5	4303	C
47	5	4304	A
47	5	4305	G
47	5	4306	U
47	5	4314	C
47	5	4317	A
47	5	4318	C
47	5	4319	C
47	5	4329	G
47	5	4330	G
47	5	4336	A
47	5	4339	A
47	5	4349	C
47	5	4350	C
47	5	4354	U
47	5	4355	G
47	5	4373	G
47	5	4376	A
47	5	4377	G
47	5	4378	A
47	5	4380	A
47	5	4387	C
47	5	4393	G
47	5	4394	A
47	5	4395	U
47	5	4401	G
47	5	4419	U
47	5	4421	C
47	5	4422	A
47	5	4436	U
47	5	4437	U
47	5	4440	G

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Mol	Chain	Res	Type
47	5	4444	C
47	5	4448	G
47	5	4449	A
47	5	4453	C
47	5	4464	A
47	5	4466	C
47	5	4471	U
47	5	4475	G
47	5	4476	C
47	5	4488	A
47	5	4500	U
47	5	4510	A
47	5	4512	U
47	5	4513	A
47	5	4518	A
47	5	4519	C
47	5	4520	G
47	5	4522	G
47	5	4524	G
47	5	4528	G
47	5	4531	U
47	5	4548	A
47	5	4549	G
47	5	4560	C
47	5	4565	C
47	5	4567	G
47	5	4573	G
47	5	4575	G
47	5	4584	A
47	5	4586	G
47	5	4590	A
47	5	4599	A
47	5	4627	U
47	5	4636	U
47	5	4637	G
47	5	4656	A
47	5	4657	U
47	5	4670	C
47	5	4671	C
47	5	4672	A
47	5	4677	U
47	5	4694	G

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Mol	Chain	Res	Type
47	5	4695	C
47	5	4709	U
47	5	4719	G
47	5	4720	C
47	5	4721	G
47	5	4736	C
47	5	4737	G
47	5	4745	G
47	5	4750	G
47	5	4751	G
47	5	4752	U
47	5	4754	G
47	5	4756	C
47	5	4757	C
47	5	4759	C
47	5	4761	G
47	5	4765	G
47	5	4771	C
47	5	4772	C
47	5	4870	G
47	5	4872	G
47	5	4873	G
47	5	4875	G
47	5	4876	U
47	5	4877	G
47	5	4881	U
47	5	4882	U
47	5	4883	C
47	5	4885	U
47	5	4895	C
47	5	4902	C
47	5	4910	A
47	5	4914	C
47	5	4915	G
47	5	4919	G
47	5	4921	C
47	5	4924	C
47	5	4925	U
47	5	4926	C
47	5	4927	G
47	5	4928	C
47	5	4931	G

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Mol	Chain	Res	Type
47	5	4934	A
47	5	4937	C
47	5	4943	A
47	5	4944	C
47	5	4948	C
47	5	4950	U
47	5	4951	G
47	5	4955	A
47	5	4956	A
47	5	4957	C
47	5	4958	C
47	5	4959	U
47	5	4960	G
47	5	4964	C
47	5	4965	U
47	5	4966	A
47	5	4976	U
47	5	4988	U
47	5	4989	U
47	5	4990	C
47	5	4991	U
47	5	5006	U
47	5	5007	A
47	5	5014	A
47	5	5017	G
47	5	5040	U
47	5	5041	G
47	5	5047	C
47	5	5050	C
47	5	5053	U
47	5	5054	C
47	5	5061	A
47	5	5062	G
47	5	5067	U
48	8	2	G
48	8	15	G
48	8	23	C
48	8	34	U
48	8	35	C
48	8	39	G
48	8	59	A
48	8	62	A

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Mol	Chain	Res	Type
48	8	63	U
48	8	75	G
48	8	77	A
48	8	79	G
48	8	87	G
48	8	94	G
48	8	95	A
48	8	103	A
48	8	105	C
48	8	108	A
48	8	109	C
48	8	110	U
48	8	111	U
48	8	112	G
48	8	114	G
48	8	123	U
48	8	125	C
48	8	126	C
48	8	127	U
48	8	137	A
48	8	150	C
48	8	153	C
49	9	3	C
49	9	4	C
49	9	8	U
49	9	25	A
49	9	26	U
49	9	33	G
49	9	41	G
49	9	42	A
49	9	44	U
49	9	46	A
49	9	56	G
49	9	62	G
49	9	65	C
49	9	67	C
49	9	68	A
49	9	69	C
49	9	71	G
49	9	73	C
49	9	74	G
49	9	75	G

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Mol	Chain	Res	Type
49	9	77	A
49	9	79	A
49	9	103	A
49	9	111	A
49	9	113	G
49	9	114	G
49	9	115	U
49	9	116	U
49	9	124	U
49	9	126	G
49	9	127	C
49	9	143	U
49	9	147	A
49	9	155	G
49	9	158	A
49	9	163	U
49	9	168	C
49	9	180	G
49	9	182	C
49	9	183	G
49	9	184	G
49	9	188	C
49	9	189	U
49	9	192	C
49	9	215	G
49	9	289	G
49	9	291	G
49	9	294	U
49	9	302	A
49	9	303	C
49	9	306	C
49	9	307	G
49	9	308	G
49	9	309	G
49	9	312	G
49	9	314	U
49	9	318	A
49	9	319	C
49	9	322	C
49	9	330	G
49	9	335	G
49	9	347	G

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Mol	Chain	Res	Type
49	9	355	G
49	9	362	C
49	9	364	A
49	9	368	U
49	9	370	G
49	9	381	C
49	9	383	G
49	9	385	G
49	9	386	C
49	9	398	A
49	9	399	C
49	9	400	C
49	9	407	G
49	9	408	A
49	9	409	C
49	9	417	C
49	9	418	A
49	9	421	G
49	9	438	G
49	9	448	A
49	9	450	C
49	9	452	G
49	9	453	C
49	9	454	U
49	9	464	A
49	9	465	A
49	9	466	G
49	9	471	G
49	9	472	C
49	9	473	A
49	9	474	G
49	9	476	A
49	9	482	G
49	9	483	C
49	9	487	U
49	9	492	C
49	9	493	A
49	9	496	C
49	9	500	A
49	9	516	A
49	9	525	A
49	9	528	A

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Mol	Chain	Res	Type
49	9	530	U
49	9	531	A
49	9	532	C
49	9	533	A
49	9	547	G
49	9	548	C
49	9	549	C
49	9	550	C
49	9	551	U
49	9	554	A
49	9	555	A
49	9	556	U
49	9	559	G
49	9	561	A
49	9	562	U
49	9	570	C
49	9	571	U
49	9	576	A
49	9	583	A
49	9	587	A
49	9	588	G
49	9	590	A
49	9	591	U
49	9	592	C
49	9	600	G
49	9	604	A
49	9	606	G
49	9	608	C
49	9	614	C
49	9	617	G
49	9	620	G
49	9	627	U
49	9	628	A
49	9	643	A
49	9	644	G
49	9	660	C
49	9	666	U
49	9	668	A
49	9	669	A
49	9	671	A
49	9	672	A
49	9	673	G

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Mol	Chain	Res	Type
49	9	689	U
49	9	752	G
49	9	753	C
49	9	754	G
49	9	811	A
49	9	821	G
49	9	822	U
49	9	830	A
49	9	834	C
49	9	844	U
49	9	847	A
49	9	852	G
49	9	853	C
49	9	859	G
49	9	860	G
49	9	867	G
49	9	868	G
49	9	870	A
49	9	871	U
49	9	872	A
49	9	873	G
49	9	874	G
49	9	875	A
49	9	878	G
49	9	887	U
49	9	890	U
49	9	891	G
49	9	913	A
49	9	914	U
49	9	919	A
49	9	920	A
49	9	930	C
49	9	933	G
49	9	934	G
49	9	955	A
49	9	970	G
49	9	971	G
49	9	981	A
49	9	990	A
49	9	992	A
49	9	1002	U
49	9	1023	A

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Mol	Chain	Res	Type
49	9	1045	U
49	9	1058	A
49	9	1062	A
49	9	1083	A
49	9	1085	C
49	9	1086	G
49	9	1100	A
49	9	1115	U
49	9	1116	C
49	9	1117	C
49	9	1118	C
49	9	1119	A
49	9	1121	G
49	9	1133	A
49	9	1138	C
49	9	1139	C
49	9	1148	A
49	9	1149	A
49	9	1153	C
49	9	1154	U
49	9	1155	U
49	9	1156	U
49	9	1161	U
49	9	1164	G
49	9	1181	A
49	9	1195	A
49	9	1203	G
49	9	1208	A
49	9	1215	C
49	9	1216	C
49	9	1221	G
49	9	1224	G
49	9	1240	A
49	9	1242	U
49	9	1251	A
49	9	1253	A
49	9	1254	C
49	9	1256	G
49	9	1257	G
49	9	1259	A
49	9	1264	C
49	9	1265	A

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Mol	Chain	Res	Type
49	9	1274	G
49	9	1275	G
49	9	1281	G
49	9	1282	A
49	9	1284	A
49	9	1285	G
49	9	1286	G
49	9	1293	A
49	9	1294	G
49	9	1295	A
49	9	1298	G
49	9	1301	A
49	9	1302	G
49	9	1303	C
49	9	1307	U
49	9	1308	U
49	9	1313	A
49	9	1314	U
49	9	1333	U
49	9	1337	C
49	9	1342	U
49	9	1371	U
49	9	1372	U
49	9	1378	A
49	9	1395	C
49	9	1396	A
49	9	1397	U
49	9	1402	A
49	9	1406	G
49	9	1409	A
49	9	1428	G
49	9	1439	A
49	9	1442	U
49	9	1447	G
49	9	1449	G
49	9	1454	A
49	9	1462	U
49	9	1463	U
49	9	1466	G
49	9	1473	G
49	9	1475	G
49	9	1476	A

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Mol	Chain	Res	Type
49	9	1477	U
49	9	1481	G
49	9	1489	A
49	9	1490	G
49	9	1494	U
49	9	1495	G
49	9	1498	A
49	9	1507	G
49	9	1520	G
49	9	1521	C
49	9	1522	A
49	9	1533	A
49	9	1535	U
49	9	1536	G
49	9	1544	C
49	9	1548	G
49	9	1552	G
49	9	1554	C
49	9	1555	U
49	9	1556	A
49	9	1557	C
49	9	1570	G
49	9	1574	C
49	9	1575	G
49	9	1579	A
49	9	1580	A
49	9	1585	U
49	9	1587	G
49	9	1588	A
49	9	1601	A
49	9	1604	G
49	9	1606	G
49	9	1621	U
49	9	1623	A
49	9	1638	G
49	9	1648	G
49	9	1649	U
49	9	1654	G
49	9	1665	G
49	9	1680	G
49	9	1682	C
49	9	1683	C

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Mol	Chain	Res	Type
49	9	1698	C
49	9	1699	A
49	9	1706	G
49	9	1715	A
49	9	1721	U
49	9	1722	G
49	9	1726	G
49	9	1730	U
49	9	1744	G
49	9	1748	G
49	9	1753	C
49	9	1756	C
49	9	1783	C
49	9	1784	G
49	9	1785	C
49	9	1823	A
49	9	1824	A
49	9	1829	G
49	9	1836	G
49	9	1838	U
49	9	1849	G
49	9	1851	A
49	9	1852	C
49	9	1861	G
49	9	1862	G
49	9	1863	A
49	9	1865	C
83	AT	8	U
83	AT	13	C
83	AT	16	U
83	AT	17	G
83	AT	18	G
83	AT	19	U
83	AT	20	U
83	AT	21	A
83	AT	22	G
83	AT	24	G
83	AT	39	G
83	AT	40	C
83	AT	43	G
83	AT	45	G
83	AT	48	C

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Mol	Chain	Res	Type
83	AT	49	C
83	AT	50	C
83	AT	53	G
83	AT	54	U
83	AT	57	A
83	AT	58	A
83	AT	61	C
83	AT	67	A
83	AT	76	A
85	1	1496	A
85	1	1500	A
85	1	1501	U
85	1	1502	A
85	1	1503	A
85	1	1504	U

All (100) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	2	10	G
47	5	12	A
47	5	48	G
47	5	125	C
47	5	134	G
47	5	217	C
47	5	226	G
47	5	245	C
47	5	275	C
47	5	385	A
47	5	406	C
47	5	449	C
47	5	480	C
47	5	485	C
47	5	492	U
47	5	504	G
47	5	696	C
47	5	729	G
47	5	916	C
47	5	930	G
47	5	935(A)	G
47	5	959	G
47	5	971(A)	G

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Mol	Chain	Res	Type
47	5	1072	C
47	5	1211	G
47	5	1236	C
47	5	1238	A
47	5	1291	G
47	5	1329	G
47	5	1370	G
47	5	1440	U
47	5	1445	U
47	5	1455	G
47	5	1477	C
47	5	1485	C
47	5	1633	G
47	5	1804	A
47	5	1818	G
47	5	1834	U
47	5	1835	G
47	5	1921	C
47	5	1979	A
47	5	1983	A
47	5	2025	A
47	5	2046	G
47	5	2068	C
47	5	2089	G
47	5	2104	A
47	5	2265	G
47	5	2266	C
47	5	2330	G
47	5	2398	U
47	5	2502	G
47	5	2546	G
47	5	2661	U
47	5	2695	A
47	5	3625	G
47	5	3673	C
47	5	3788	C
47	5	3888	G
47	5	3896	C
47	5	4075	U
47	5	4119	C
47	5	4124	G
47	5	4170	A

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Mol	Chain	Res	Type
47	5	4232	U
47	5	4448	G
47	5	4719	G
47	5	4884	G
47	5	4925	U
47	5	4936	G
47	5	4942	C
47	5	4947	U
47	5	4964	C
48	8	124	U
49	9	2	A
49	9	24	C
49	9	72	C
49	9	110	U
49	9	126	G
49	9	465	A
49	9	532	C
49	9	553	U
49	9	555	A
49	9	561	A
49	9	688	U
49	9	752	G
49	9	870	A
49	9	872	A
49	9	1137	U
49	9	1253	A
49	9	1395	C
49	9	1489	A
49	9	1664	A
49	9	1679	A
83	AT	7	G
83	AT	17	G
85	1	1499	C
85	1	1501	U
85	1	1503	A

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

1 non-standard protein/DNA/RNA residue is 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
84	SEP	EF	163	84	8,9,10	1.60	1 (12%)	7,12,14	1.40	1 (14%)

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
84	SEP	EF	163	84	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	EF	163	SEP	P-O1P	3.52	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	EF	163	SEP	OG-CB-CA	2.97	111.04	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	EF	163	SEP	C-CA-CB-OG
84	EF	163	SEP	CB-OG-P-O1P
84	EF	163	SEP	CB-OG-P-O2P
84	EF	163	SEP	CB-OG-P-O3P
84	EF	163	SEP	CA-CB-OG-P
84	EF	163	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	EF	163	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 285 ligands modelled in this entry, 284 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
88	GTP	EF	502	-	33,34,34	1.28	4 (12%)	50,54,54	1.93	14 (28%)

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	GTP	EF	502	-	-	6/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	EF	502	GTP	PB-O3A	3.02	1.62	1.59
88	EF	502	GTP	C5-C4	2.76	1.46	1.38
88	EF	502	GTP	C6-N1	-2.62	1.34	1.38
88	EF	502	GTP	C4-N9	-2.57	1.31	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	EF	502	GTP	C5-C4-N3	-4.67	120.95	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	EF	502	GTP	C2-N3-C4	4.21	119.55	112.30
88	EF	502	GTP	C2'-C3'-C4'	4.06	110.46	102.61
88	EF	502	GTP	C6-C5-N7	3.85	137.30	130.29
88	EF	502	GTP	N9-C4-N3	3.51	132.97	125.95
88	EF	502	GTP	C2'-C1'-N9	-3.44	103.68	113.25
88	EF	502	GTP	O3A-PA-O1A	-2.85	102.14	110.70
88	EF	502	GTP	C4-C5-N7	-2.57	106.60	110.67
88	EF	502	GTP	O2A-PA-O3A	-2.50	100.53	107.27
88	EF	502	GTP	O2A-PA-O1A	2.32	123.23	112.44
88	EF	502	GTP	C8-N9-C4	2.27	110.27	106.03
88	EF	502	GTP	O4'-C1'-C2'	2.26	111.45	106.62
88	EF	502	GTP	O5'-C5'-C4'	2.13	116.26	108.99
88	EF	502	GTP	N9-C8-N7	-2.09	109.53	113.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	EF	502	GTP	PB-O3B-PG-O2G
88	EF	502	GTP	C5'-O5'-PA-O3A
88	EF	502	GTP	C4'-C5'-O5'-PA
88	EF	502	GTP	C5'-O5'-PA-O1A
88	EF	502	GTP	O4'-C4'-C5'-O5'
88	EF	502	GTP	PB-O3B-PG-O3G

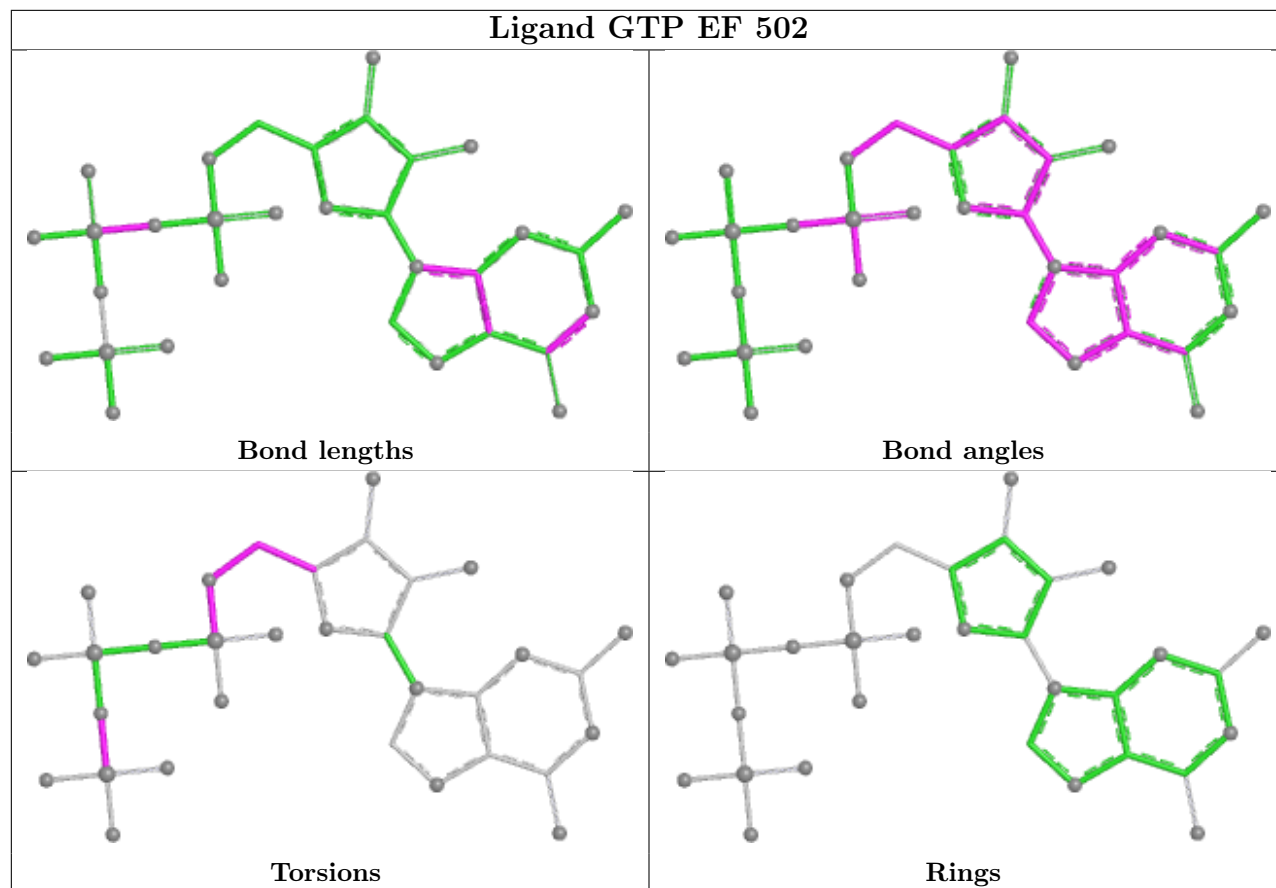
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	EF	502	GTP	3	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	5	29
49	9	17
6	E	3
46	3	2
23	W	1
28	b	1
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.57
1	W	63:GLN	C	79:GLN	N	41.48
1	b	76:VAL	C	89:VAL	N	36.97
1	5	1252:C	O3'	1271:G	P	36.50
1	E	77:ALA	C	92:LEU	N	30.05
1	5	1219:G	O3'	1233:G	P	20.97
1	5	3948:C	O3'	4065:G	P	19.19
1	9	130:G	O3'	141:A	P	18.73
1	9	697:G	O3'	729:C	P	18.59
1	9	1761:U	O3'	1771:G	P	17.89
1	5	1406(C):G	O3'	1411:C	P	17.55
1	5	990:C	O3'	1064:G	P	17.52
1	5	523:C	O3'	638:G	P	17.48
1	9	834:C	O3'	841:G	P	17.42
1	9	756:C	O3'	788:G	P	17.40
1	5	4138:C	O3'	4146:G	P	17.36
1	5	4101:C	O3'	4107:G	P	17.28
1	9	323:C	O3'	329:G	P	17.28
1	5	4777:C	O3'	4859:C	P	16.37
1	9	1417:C	O3'	1423:C	P	16.34
1	5	760:G	O3'	904:G	P	15.67
1	5	1696:C	O3'	1720:C	P	15.51
1	5	5022:U	O3'	5028:G	P	14.07
1	5	1364:U	O3'	1368:A	P	13.41
1	5	2901:G	O3'	3597:G	P	13.14
1	5	182:G	O3'	189:G	P	12.15
1	5	4729:A	O3'	4735:G	P	10.41
1	5	1180:C	O3'	1183:C	P	9.49
1	9	225:G	O3'	287:U	P	7.66
1	9	736:C	O3'	743:U	P	7.59
1	5	512:U	O3'	515:C	P	7.55
1	E	224:LYS	C	242:LYS	N	7.31
1	9	745:C	O3'	749:U	P	6.94
1	3	19:U	O3'	20:U	P	6.33
1	5	1957:U	O3'	1958:A	P	6.23
1	9	689:U	O3'	690:G	P	5.45
1	5	500:G	O3'	504:G	P	5.38
1	5	1239:C	O3'	1244:G	P	5.35
1	2	16:U	O3'	18:G	P	5.31
1	5	1100:U	O3'	1168:G	P	5.30
1	3	16:U	O3'	18:G	P	4.83
1	9	322:C	O3'	323:C	P	4.81
1	5	4740:G	O3'	4743:G	P	4.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	1432:U	O3'	1438:A	P	4.11
1	E	100:GLY	C	105:GLY	N	4.07
1	9	304:C	O3'	305:U	P	3.99
1	9	798:G	O3'	799:U	P	3.85
1	5	170:C	O3'	171:U	P	3.64
1	9	903:A	O3'	904:A	P	3.32
1	5	4899:G	O3'	4902:C	P	3.31
1	9	886:A	O3'	887:U	P	3.30
1	5	5020:G	O3'	5021:C	P	3.21
1	5	267:G	O3'	268:G	P	3.08
1	5	1438:U	O3'	1440:U	P	2.97

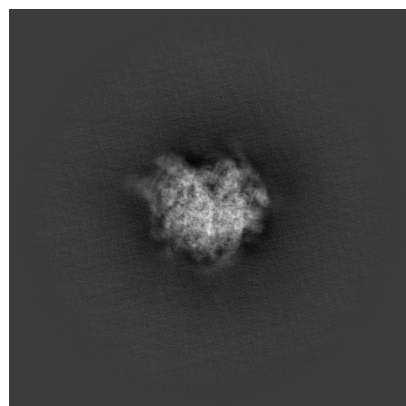
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72171. These allow visual inspection of the internal detail of the map and identification of artifacts.

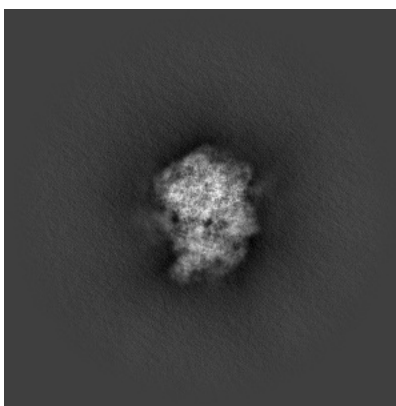
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

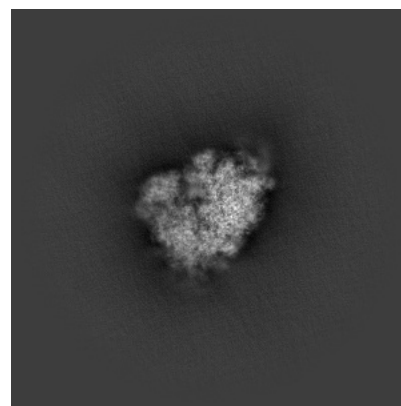
6.1.1 Primary map



X

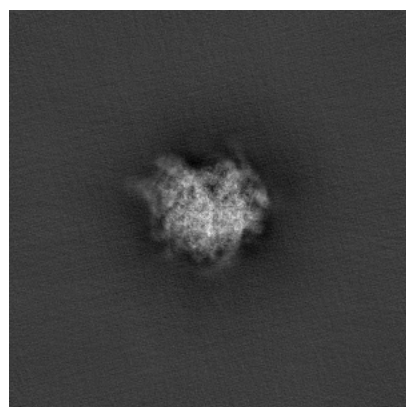


Y

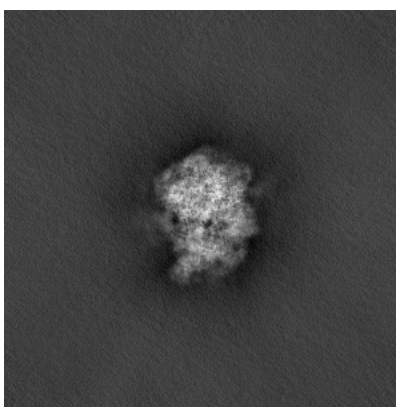


Z

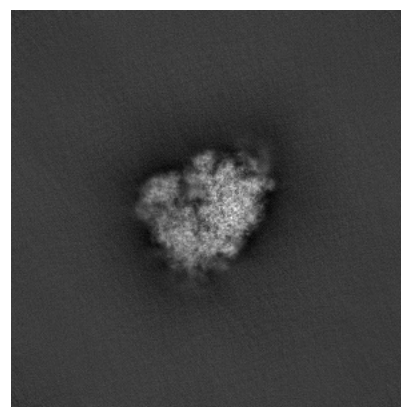
6.1.2 Raw map



X



Y

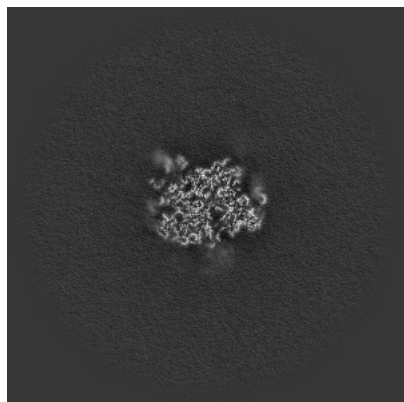


Z

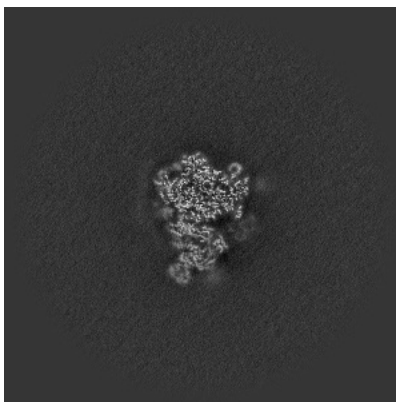
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

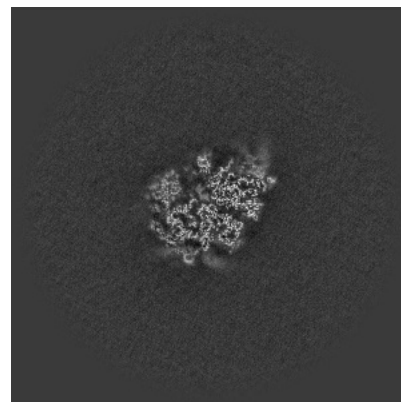
6.2.1 Primary map



X Index: 256

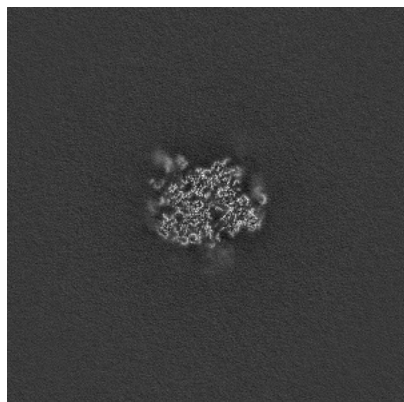


Y Index: 256

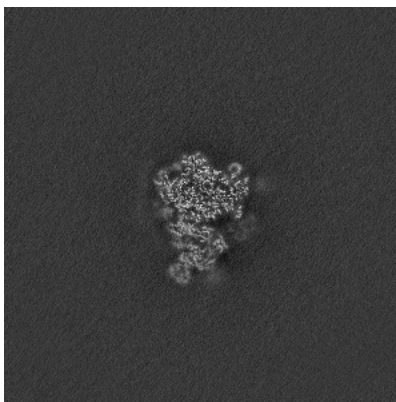


Z Index: 256

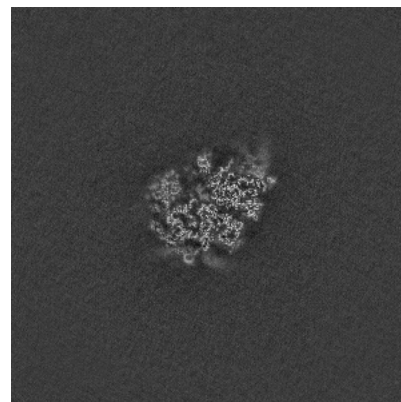
6.2.2 Raw map



X Index: 256



Y Index: 256

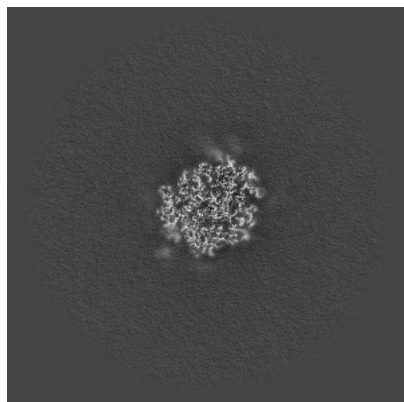


Z Index: 256

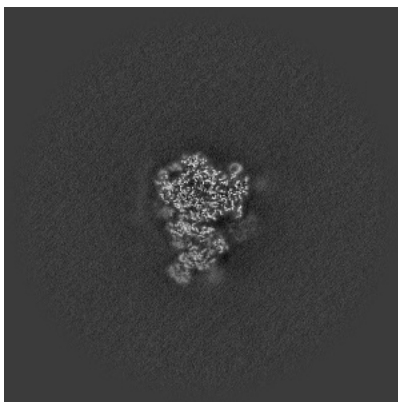
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

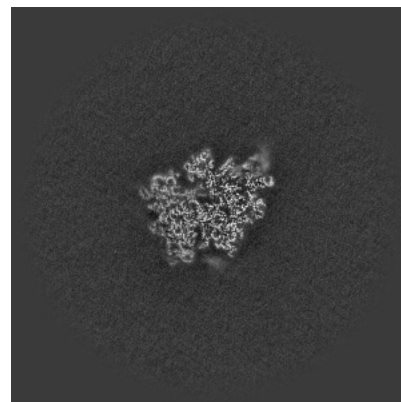
6.3.1 Primary map



X Index: 282

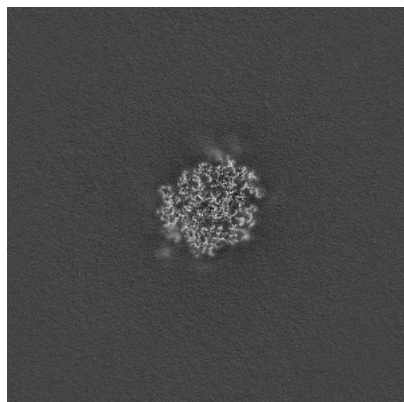


Y Index: 255

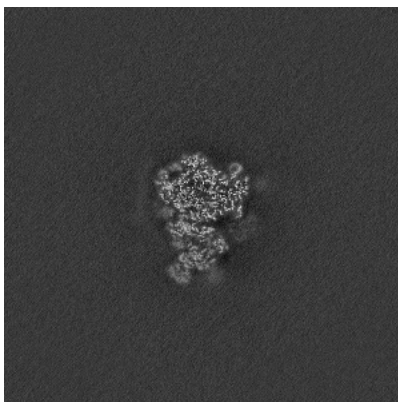


Z Index: 251

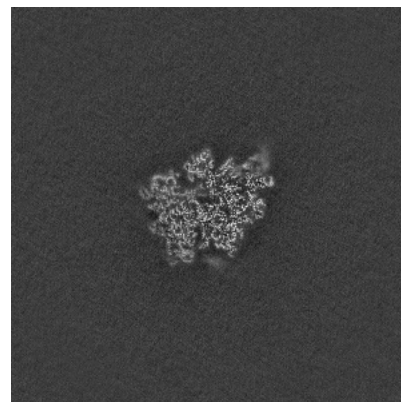
6.3.2 Raw map



X Index: 282



Y Index: 255

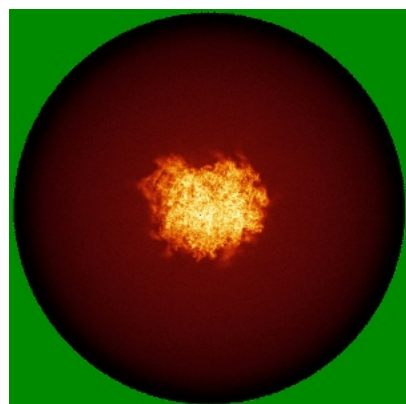


Z Index: 251

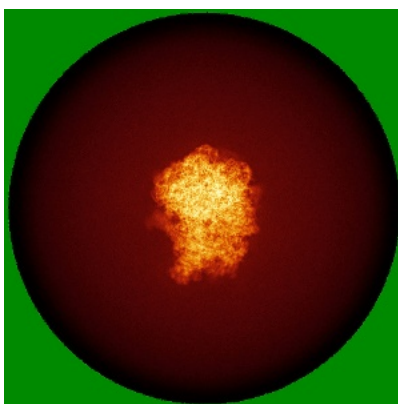
The images above show the largest variance slices of the map in three orthogonal directions.

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

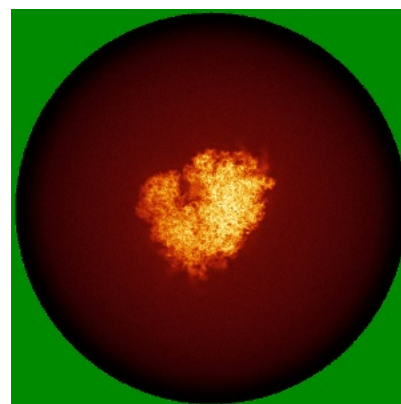
6.4.1 Primary map



X

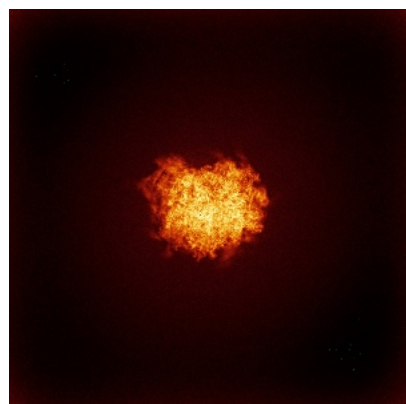


Y

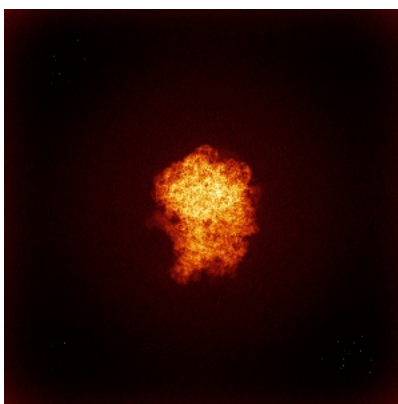


Z

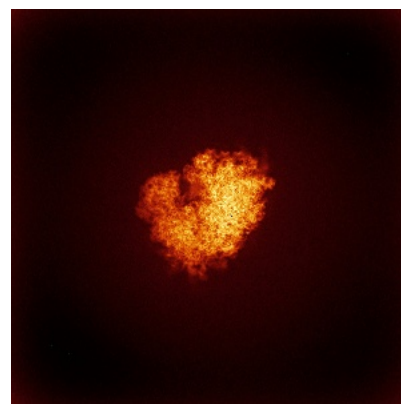
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



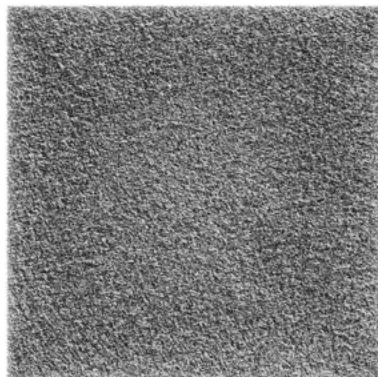
Y



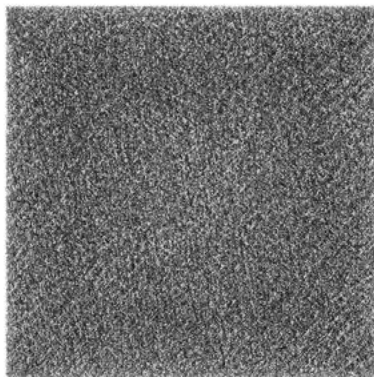
Z

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

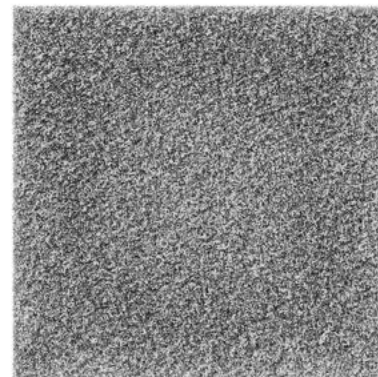
6.5.2 Raw map



X



Y



Z

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

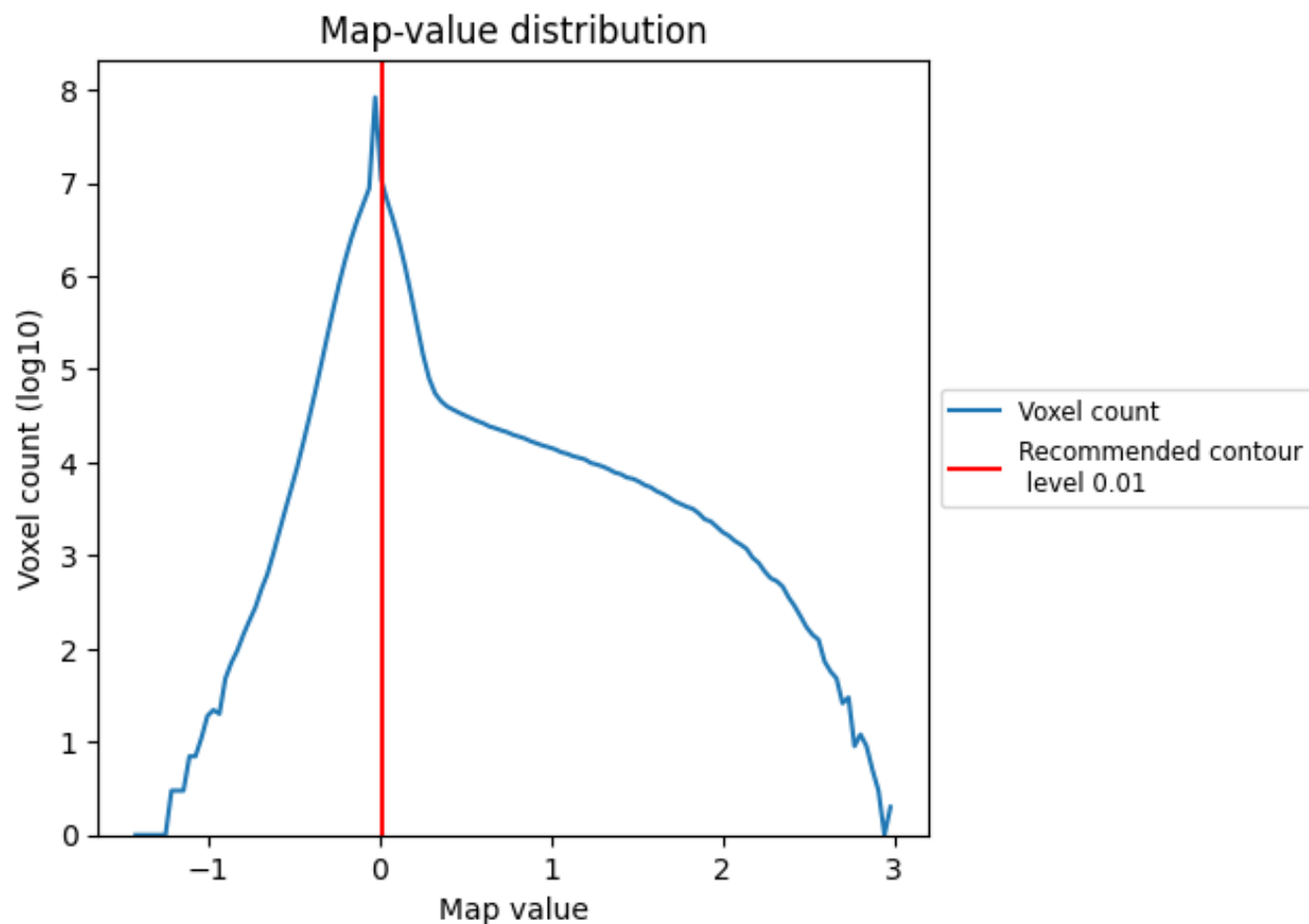
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

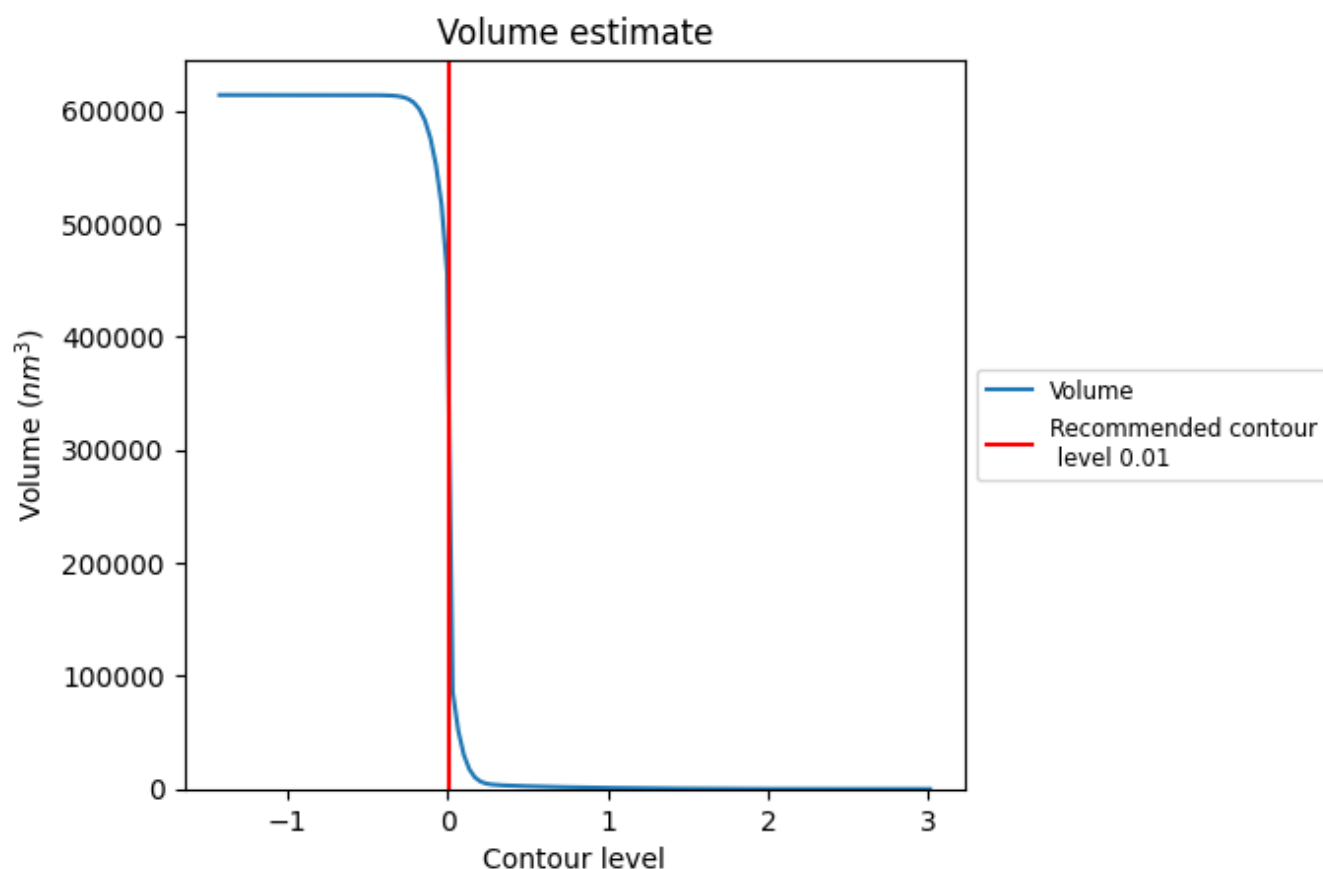
This section contains the results of statistical analysis of the map.

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.

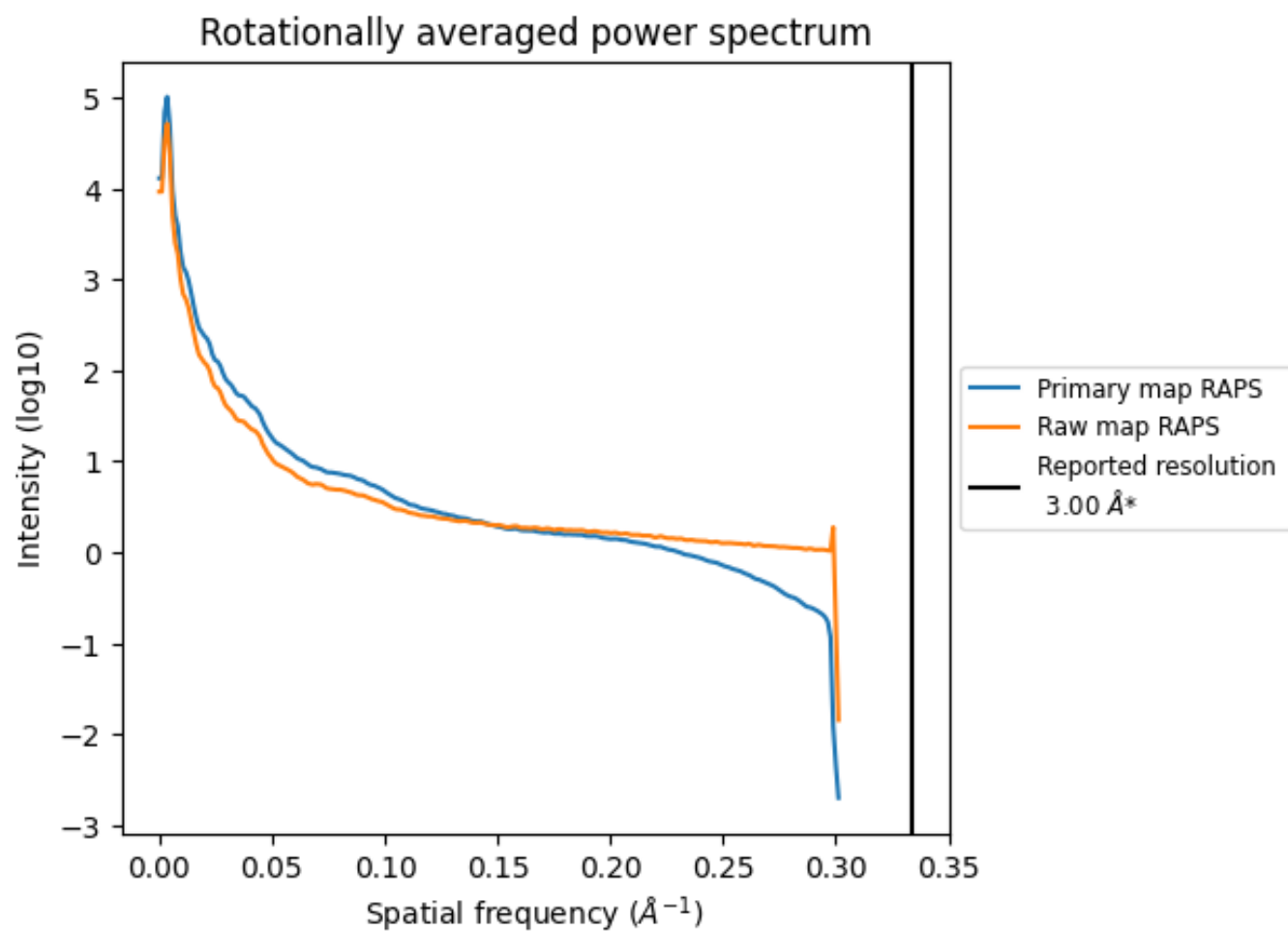
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331465 nm^3 ; this corresponds to an approximate mass of 299421 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 ⓘ

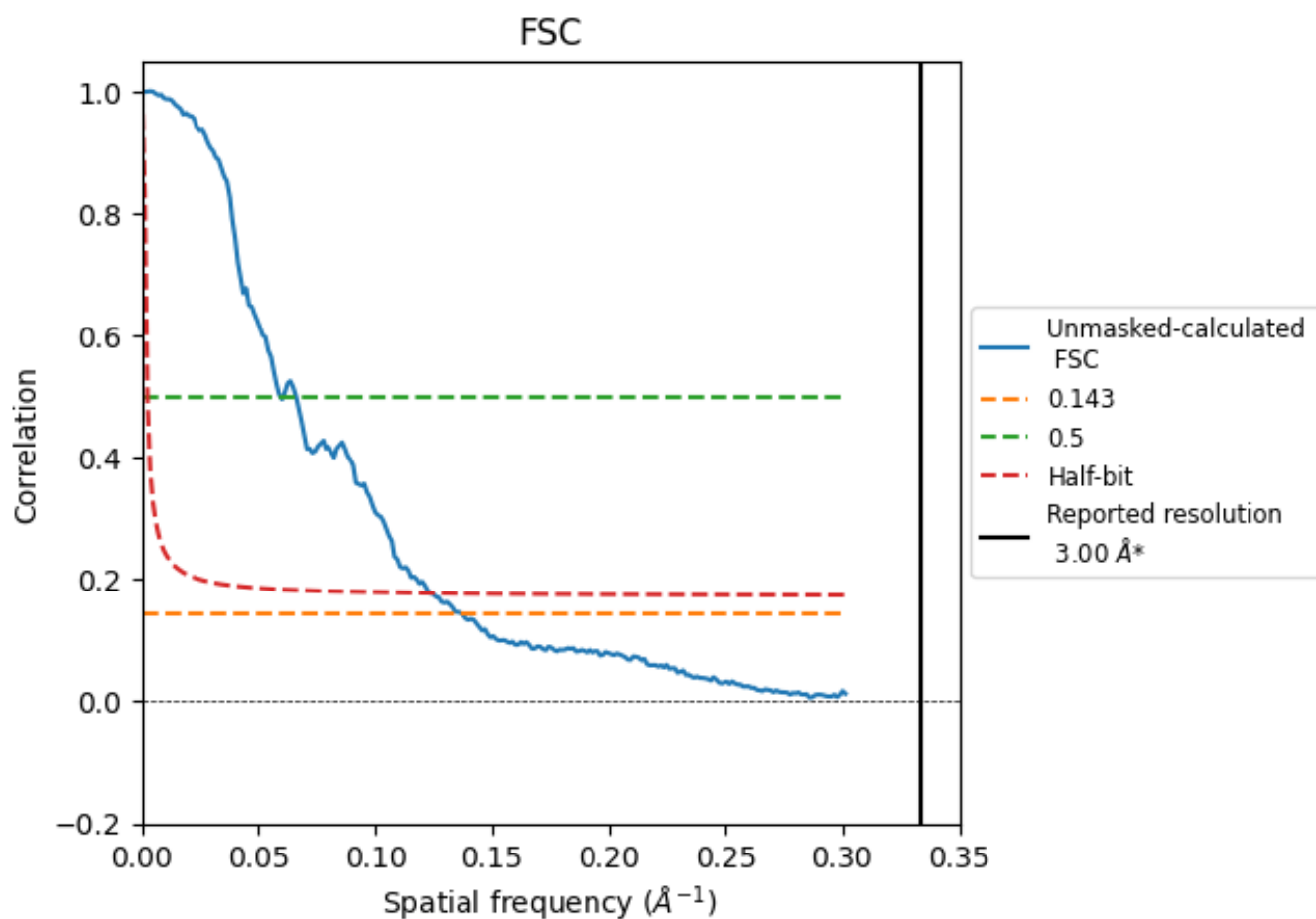


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

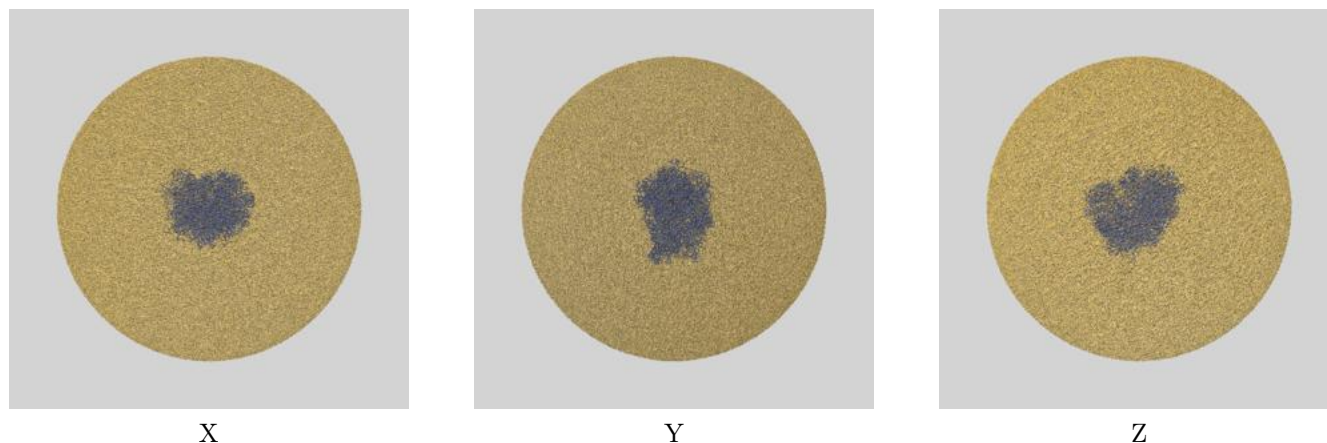
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.30	16.89	8.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.30 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

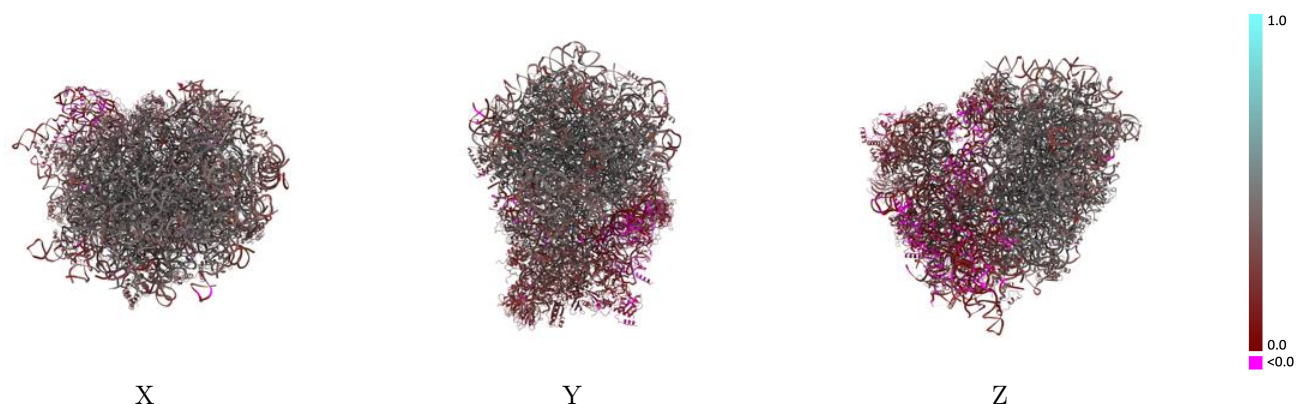
This section contains information regarding the fit between EMDB map EMD-72171 and PDB model 9Q2P. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



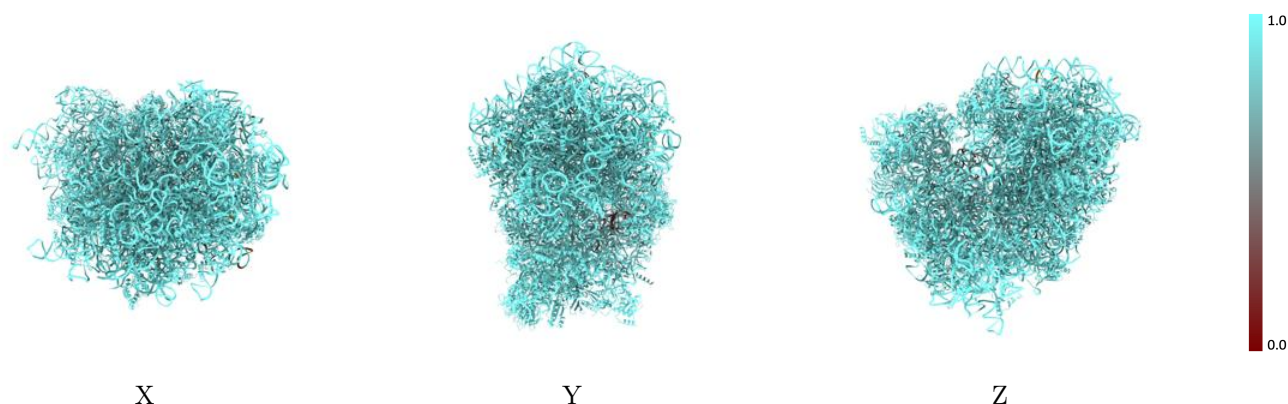
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



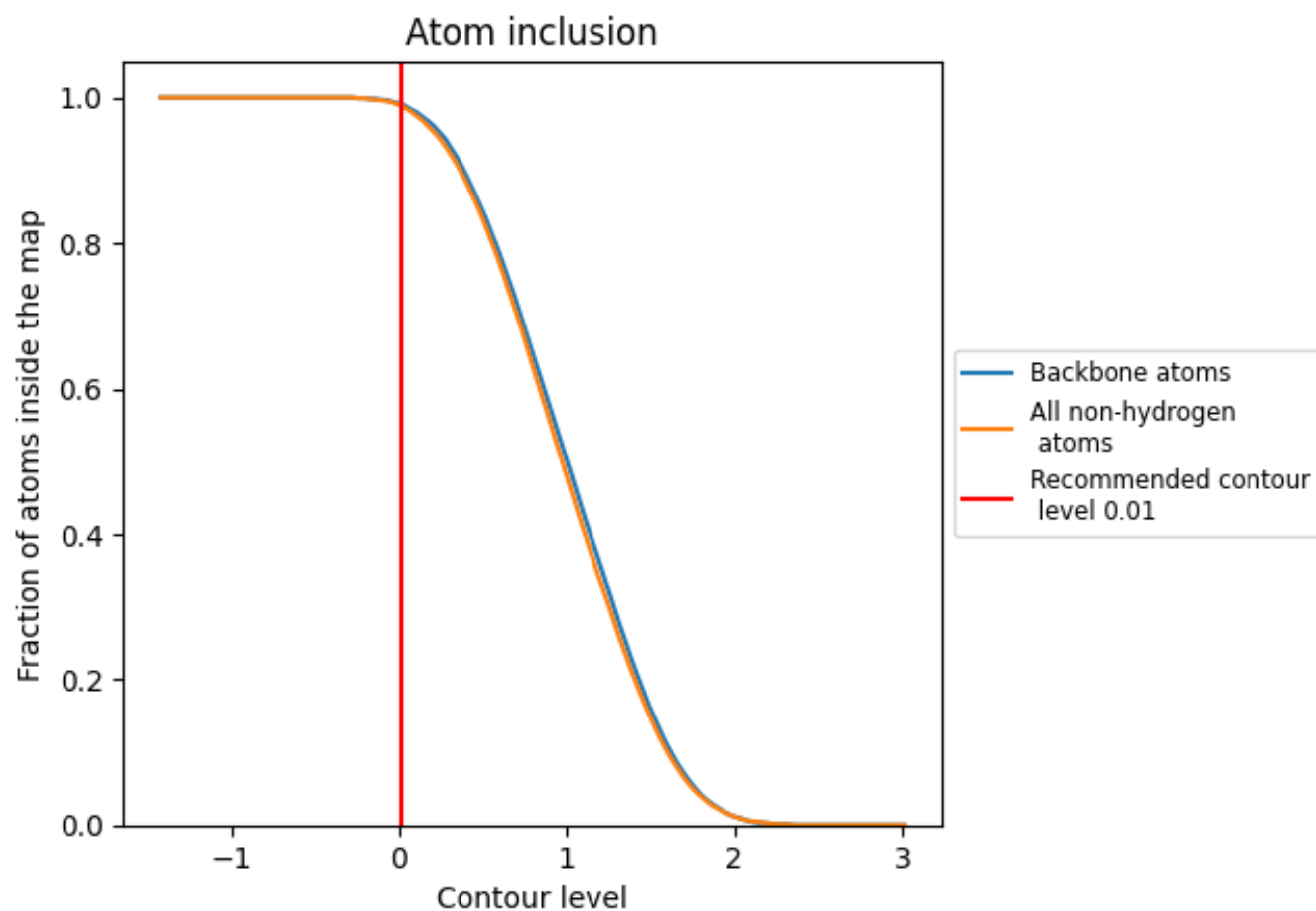
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.3490
1	 0.9970	 0.3070
2	 0.9990	 0.3620
3	 0.9090	 0.1070
5	 0.9990	 0.3990
7	 1.0000	 0.4210
8	 1.0000	 0.4080
9	 0.9980	 0.2820
A	 0.9980	 0.4530
AA	 0.9950	 0.3070
AT	 0.5660	 0.0780
B	 0.9980	 0.4450
BB	 0.9890	 0.3410
C	 0.9990	 0.4400
CC	 0.9940	 0.3610
D	 1.0000	 0.3850
DD	 0.9880	 0.2570
E	 0.9980	 0.4120
EE	 0.9480	 0.0550
EF	 0.8540	 0.2070
F	 0.9960	 0.4350
FF	 0.9960	 0.2770
G	 0.9980	 0.3740
GG	 0.9450	 0.0950
H	 0.9910	 0.4150
HH	 0.9850	 0.2980
I	 0.9940	 0.4430
II	 0.9990	 0.4040
J	 0.9990	 0.3640
JJ	 0.9780	 0.0920
KK	 1.0000	 0.2060
L	 0.9960	 0.4070
LL	 0.9900	 0.2930
M	 0.9990	 0.4100
MM	 0.9960	 0.1150























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Chain	Atom inclusion	Q-score
N	 0.9980	 0.4430
NN	 0.9910	 0.3760
O	 0.9970	 0.4420
OO	 0.9970	 0.3540
P	 1.0000	 0.4450
PP	 0.9890	 0.2530
Q	 0.9970	 0.4480
QQ	 0.9970	 0.2640
R	 0.9970	 0.4020
RR	 0.9930	 0.2750
S	 0.9970	 0.4510
SS	 0.9990	 0.2550
T	 0.9980	 0.4340
TT	 1.0000	 0.2520
U	 1.0000	 0.3700
UU	 0.9970	 0.2400
V	 0.9920	 0.4310
VV	 0.9940	 0.3420
W	 0.9900	 0.3140
WW	 0.9970	 0.3800
X	 1.0000	 0.4350
XX	 0.9600	 0.2110
Y	 0.9990	 0.4270
YY	 0.9730	 0.0730
Z	 1.0000	 0.4010
ZZ	 0.9970	 0.2500
a	 0.9960	 0.4480
aa	 0.9950	 0.3760
b	 0.9950	 0.3720
bb	 0.9970	 0.3420
c	 0.9890	 0.4040
cc	 0.9920	 0.2970
d	 0.9990	 0.4350
dd	 0.9980	 0.2610
e	 1.0000	 0.4670
ee	 0.9570	 0.1090
f	 0.9960	 0.4670
ff	 0.9910	 0.1270
g	 0.9990	 0.4270
gg	 0.9970	 0.2180
h	 0.9960	 0.4040
i	 1.0000	 0.4070

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Chain	Atom inclusion	Q-score
j	 1.0000	 0.4520
k	 0.9960	 0.3870
l	 0.9930	 0.4060
m	 0.9880	 0.4360
n	 0.9950	 0.4340
o	 0.9980	 0.4380
p	 0.9940	 0.4280
r	 0.9970	 0.4480
s	 0.9960	 0.2050
t	 0.9520	 0.0320