



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:00 PM UTC

PDB ID : 5LZZ / pdb_00005lzz
EMDB ID : EMD-4137
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l (combined)
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.47 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

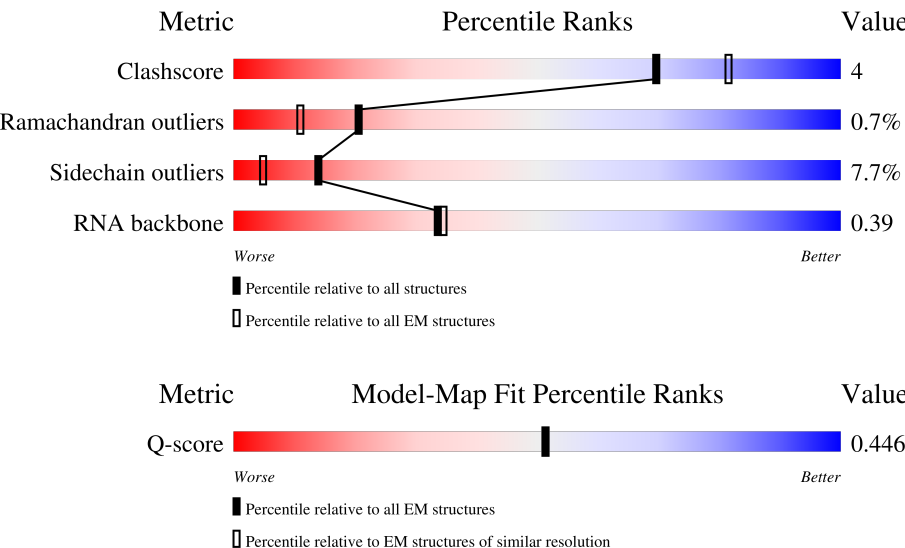
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.47 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.



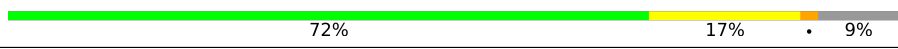
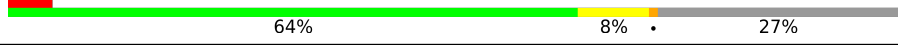
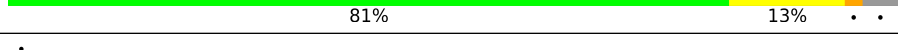
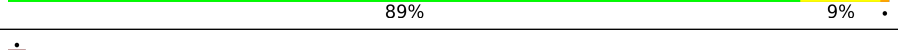
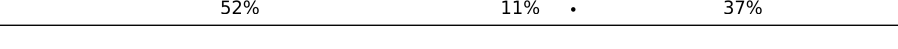
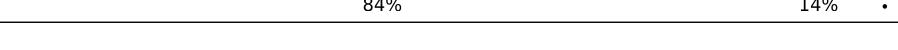
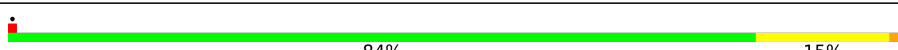
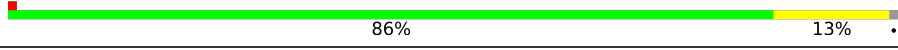
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	A	257	 76% 19% . .
2	B	403	 78% 18% . .
3	C	425	 70% 13% . 15%

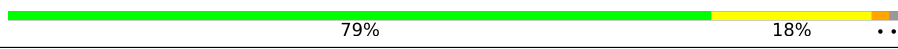
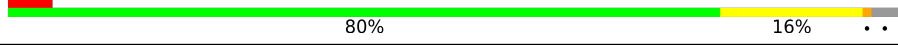
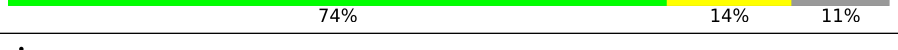
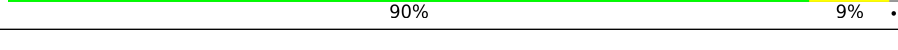
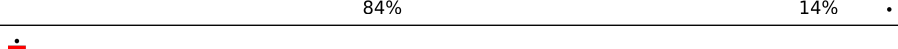
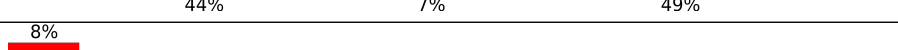
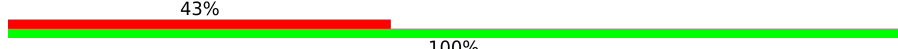
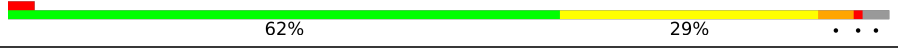
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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	7	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	8	
86	ii	403	
87	jj	710	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	ff	200	-	-	X	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called 60S ribosomal protein L7a,eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	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 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	7	Total	C	N	O	0	0
			49	31	8	10		

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 53 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 58 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 60 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	II	206	Total	C	N	O	S	0	0
			1686	1058	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 61 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
61	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 62 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 64 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	141	Total	C	N	O	S	0	0
			1097	688	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 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 74 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 78 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 79 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 84 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	8	Total	C	N	O	P	0	0
			169	76	29	56	8		

- Molecule 86 is a protein called Protein pelota homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	372	Total	C	N	O	S	0	0
			2947	1844	528	559	16		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	221	MET	LEU	variant	UNP Q9BRX2
ii	386	GLY	-	expression tag	UNP Q9BRX2
ii	387	SER	-	expression tag	UNP Q9BRX2
ii	388	GLU	-	expression tag	UNP Q9BRX2
ii	389	ASN	-	expression tag	UNP Q9BRX2
ii	390	LEU	-	expression tag	UNP Q9BRX2
ii	391	TYR	-	expression tag	UNP Q9BRX2
ii	392	PHE	-	expression tag	UNP Q9BRX2
ii	393	GLN	-	expression tag	UNP Q9BRX2
ii	394	GLY	-	expression tag	UNP Q9BRX2
ii	395	ALA	-	expression tag	UNP Q9BRX2
ii	396	HIS	-	expression tag	UNP Q9BRX2
ii	397	HIS	-	expression tag	UNP Q9BRX2
ii	398	HIS	-	expression tag	UNP Q9BRX2
ii	399	HIS	-	expression tag	UNP Q9BRX2
ii	400	HIS	-	expression tag	UNP Q9BRX2
ii	401	HIS	-	expression tag	UNP Q9BRX2
ii	402	SER	-	expression tag	UNP Q9BRX2
ii	403	THR	-	expression tag	UNP Q9BRX2

- Molecule 87 is a protein called HBS1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	425	Total	C	N	O	S	0	0
			3292	2100	565	609	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450
jj	-23	TYR	-	expression tag	UNP Q9Y450
jj	-22	LYS	-	expression tag	UNP Q9Y450
jj	-21	ASP	-	expression tag	UNP Q9Y450
jj	-20	HIS	-	expression tag	UNP Q9Y450
jj	-19	ASP	-	expression tag	UNP Q9Y450
jj	-18	GLY	-	expression tag	UNP Q9Y450
jj	-17	ASP	-	expression tag	UNP Q9Y450
jj	-16	TYR	-	expression tag	UNP Q9Y450
jj	-15	LYS	-	expression tag	UNP Q9Y450
jj	-14	ASP	-	expression tag	UNP Q9Y450
jj	-13	HIS	-	expression tag	UNP Q9Y450
jj	-12	ASP	-	expression tag	UNP Q9Y450
jj	-11	ILE	-	expression tag	UNP Q9Y450
jj	-10	ASP	-	expression tag	UNP Q9Y450
jj	-9	TYR	-	expression tag	UNP Q9Y450
jj	-8	LYS	-	expression tag	UNP Q9Y450
jj	-7	ASP	-	expression tag	UNP Q9Y450
jj	-6	ASP	-	expression tag	UNP Q9Y450
jj	-5	ASP	-	expression tag	UNP Q9Y450
jj	-4	ASP	-	expression tag	UNP Q9Y450
jj	-3	LYS	-	expression tag	UNP Q9Y450
jj	-2	ALA	-	expression tag	UNP Q9Y450
jj	-1	GLY	-	expression tag	UNP Q9Y450
jj	0	SER	-	expression tag	UNP Q9Y450

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
88	B	1	Total Mg 1 1	0
88	I	1	Total Mg 1 1	0
88	L	1	Total Mg 1 1	0
88	P	1	Total Mg 1 1	0
88	V	1	Total Mg 1 1	0
88	a	1	Total Mg 1 1	0

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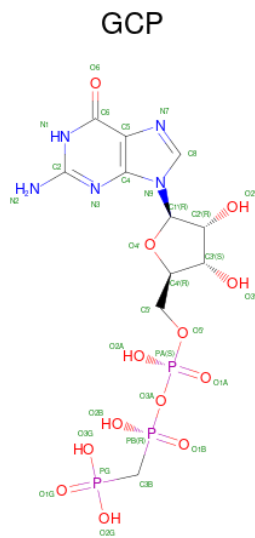
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	e	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	j	1	Total 1	Mg 1	0
88	5	178	Total 178	Mg 178	0
88	7	5	Total 5	Mg 5	0
88	8	5	Total 5	Mg 5	0
88	9	66	Total 66	Mg 66	0
88	jj	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

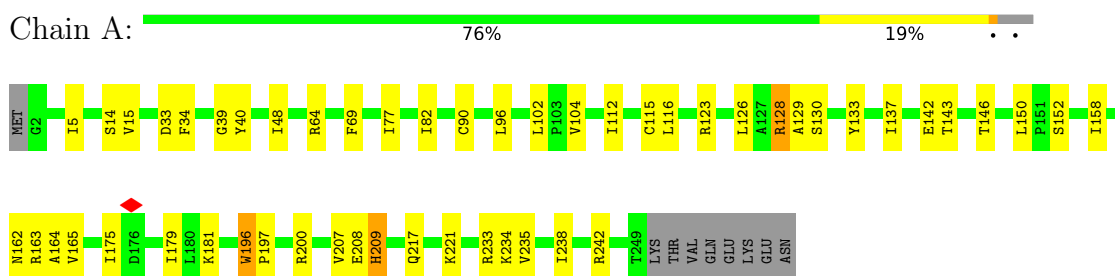


Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

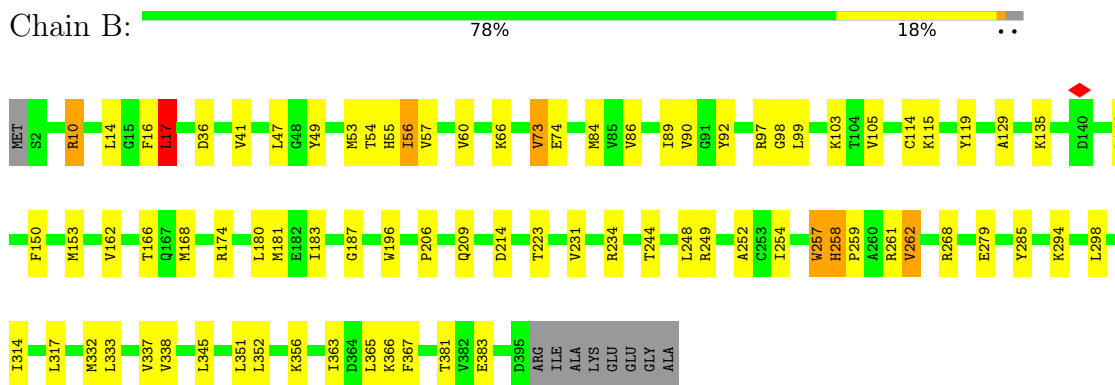
3 Residue-property plots [i](#)

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

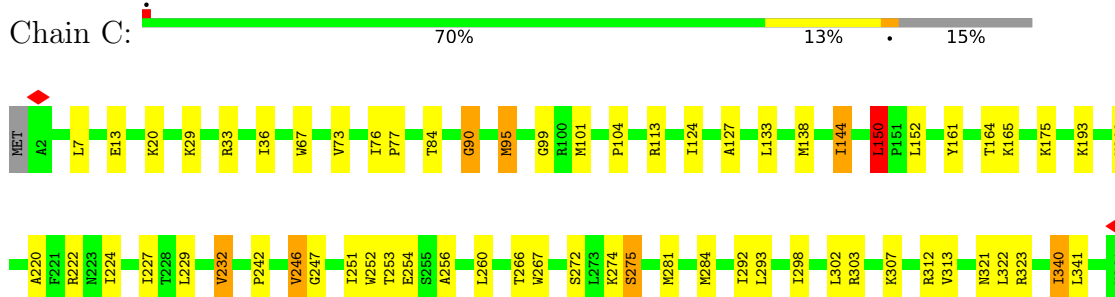
• Molecule 1: uL2

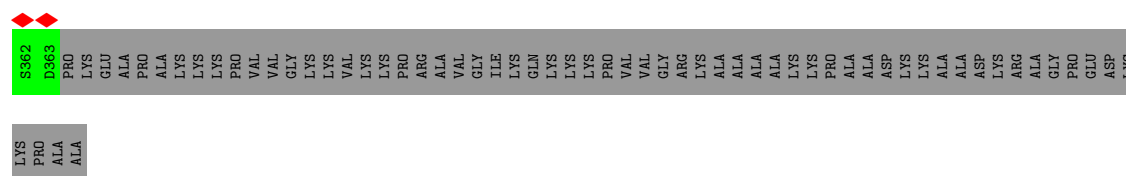


• Molecule 2: uL3

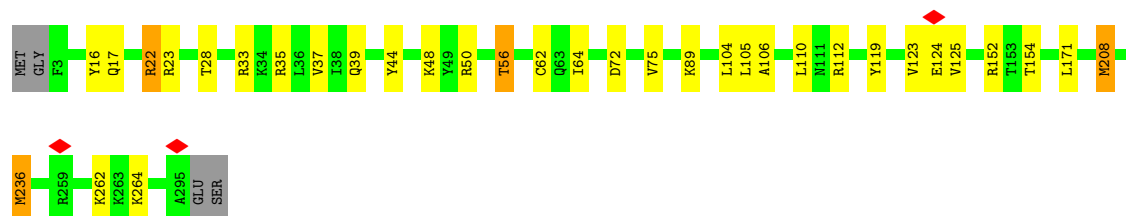
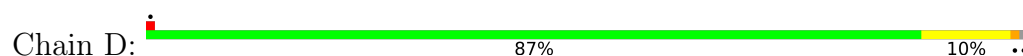


• Molecule 3: uL4

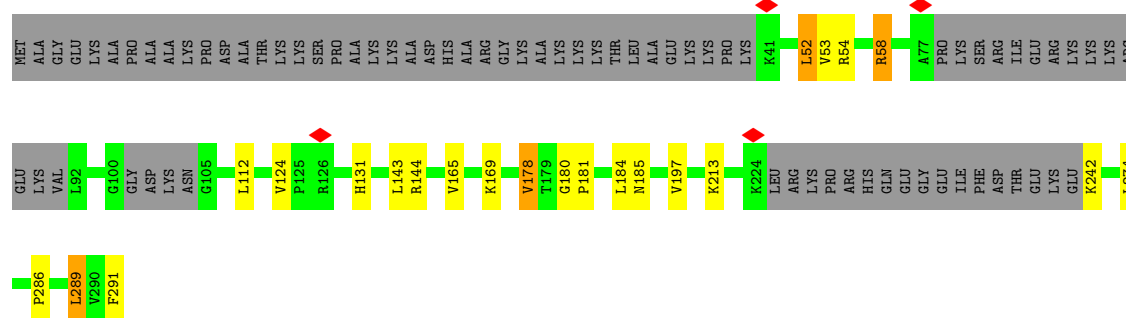




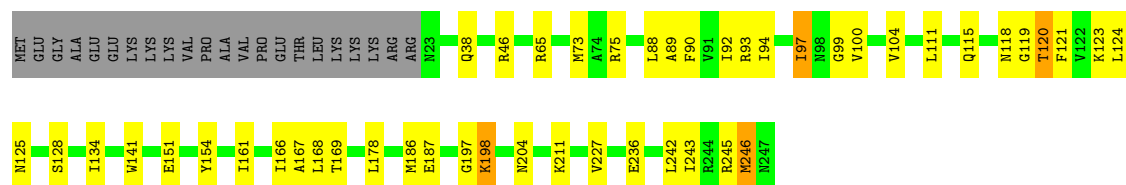
- Molecule 4: 60S ribosomal protein L5



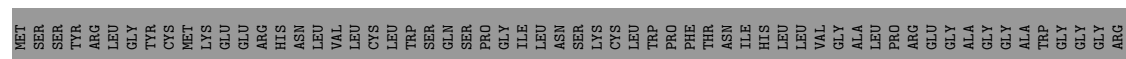
- Molecule 5: 60S ribosomal protein L6

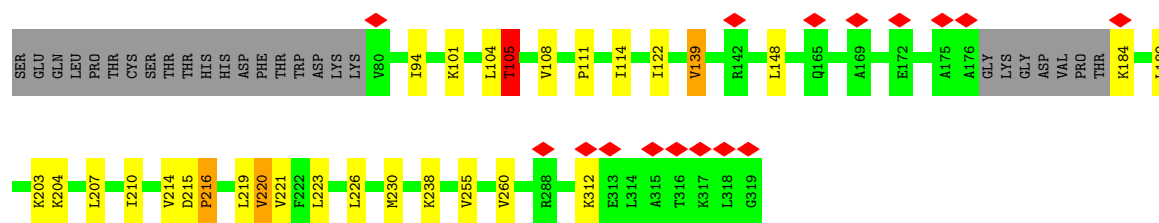


- Molecule 6: uL30

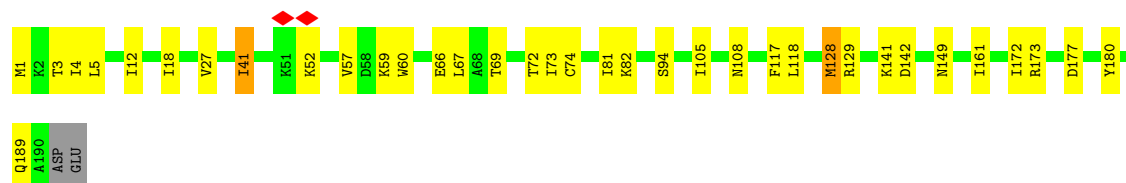
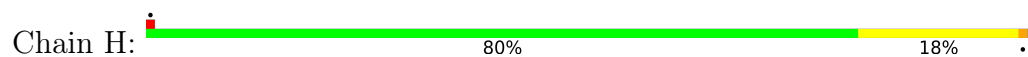


- Molecule 7: 60S ribosomal protein L7a,eL8

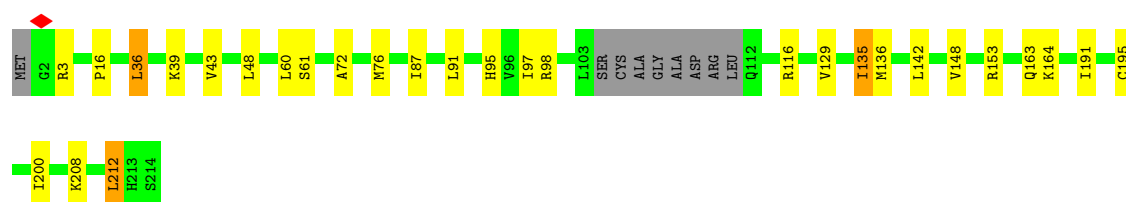
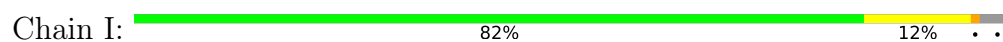




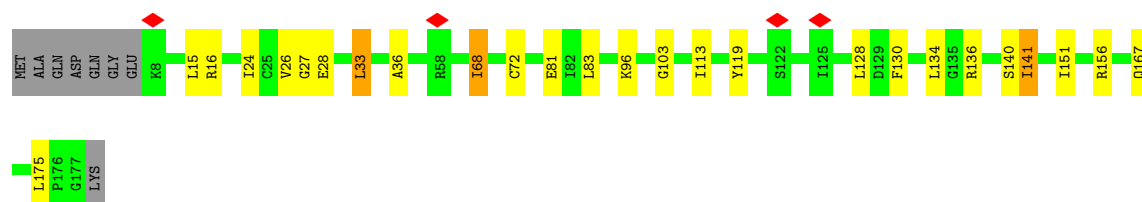
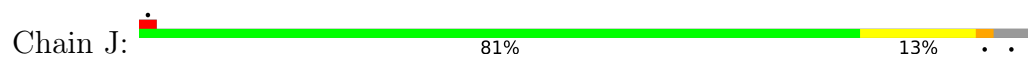
• Molecule 8: uL6



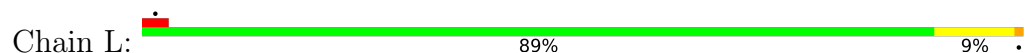
• Molecule 9: Ribosomal protein L10 (Predicted)



• Molecule 10: uL5

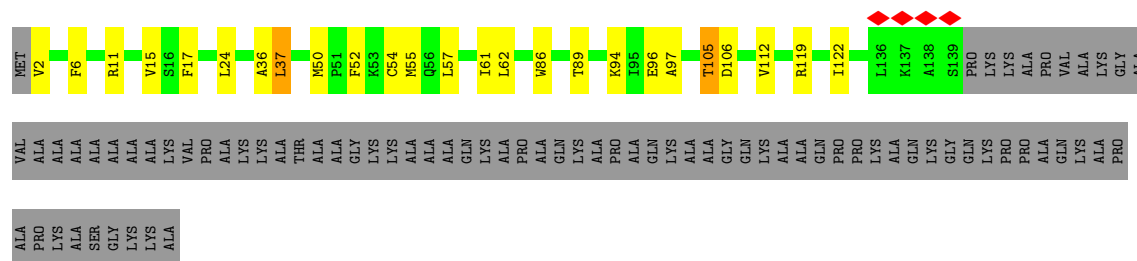


• Molecule 11: eL13



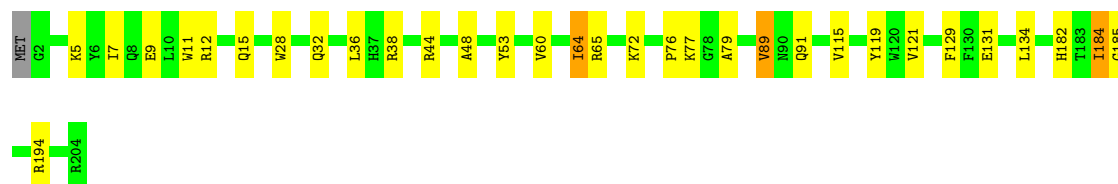
• Molecule 12: eL14





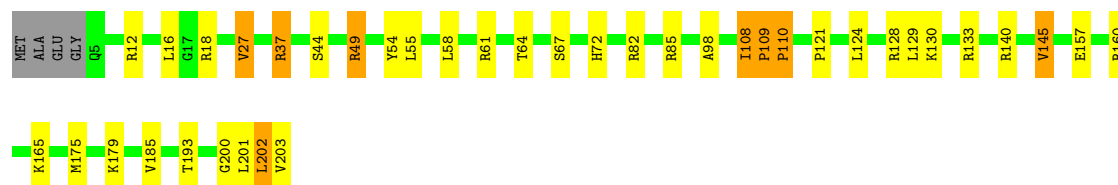
• Molecule 13: Ribosomal protein L15

Chain N: 84% 14% .



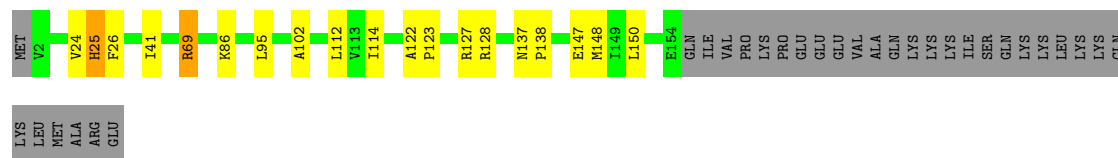
• Molecule 14: uL13

Chain O: 79% 15% . .



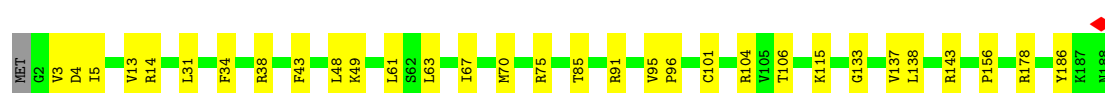
• Molecule 15: uL22

Chain P: 73% 9% . 17%



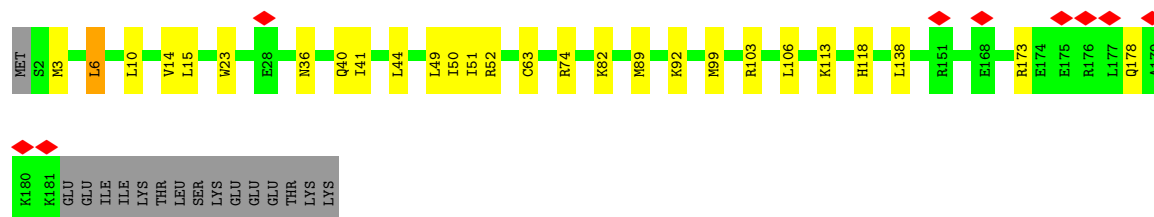
• Molecule 16: eL18

Chain Q: 83% 16% .

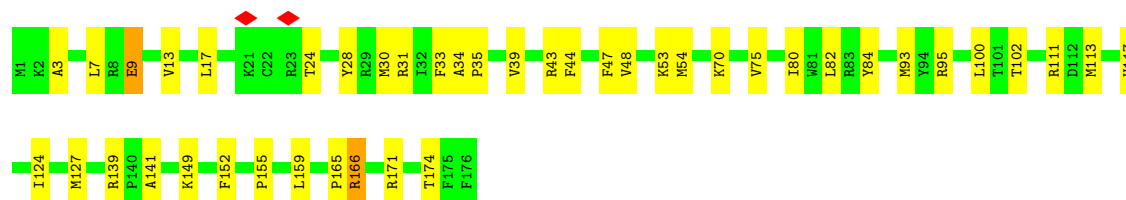
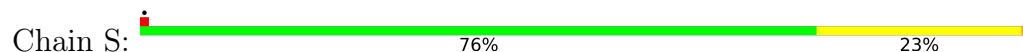


• Molecule 17: eL19

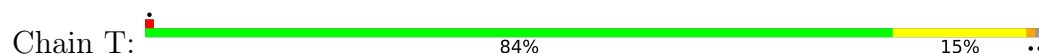
Chain R: 5% 78% 13% . 8%



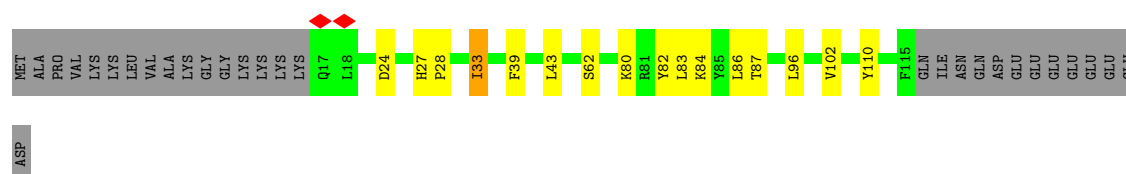
• Molecule 18: eL20



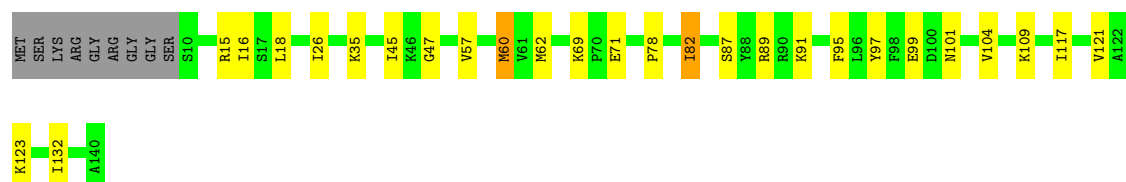
• Molecule 19: eL21



• Molecule 20: eL22



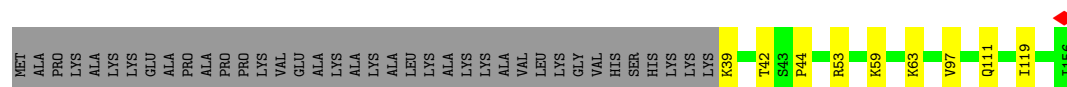
• Molecule 21: uL14



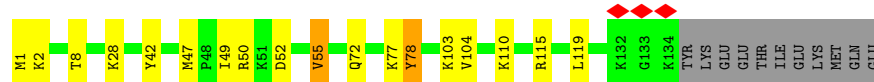
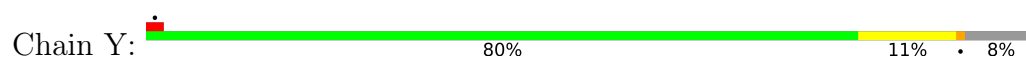
• Molecule 22: eL24



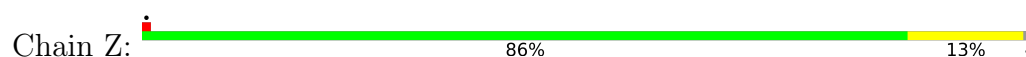
- Molecule 23: uL23



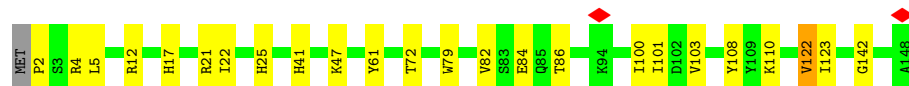
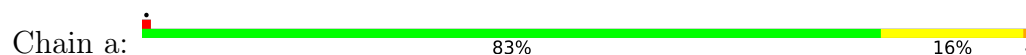
- Molecule 24: uL24



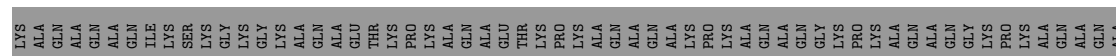
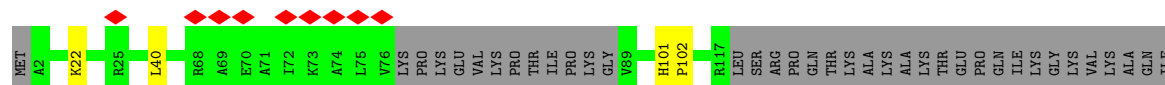
- Molecule 25: 60S ribosomal protein L27



- Molecule 26: uL15



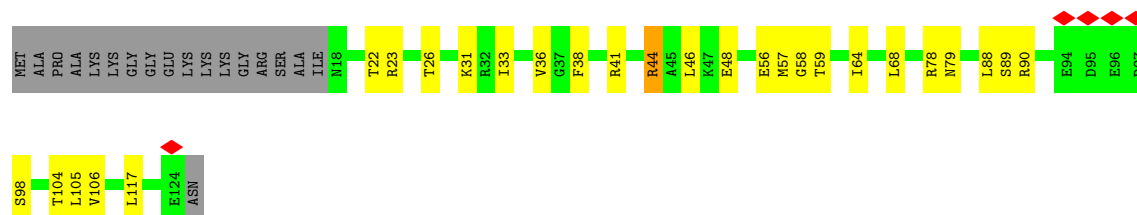
- Molecule 27: eL29



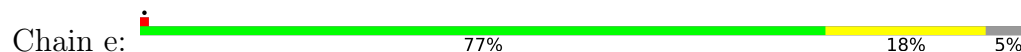
- Molecule 28: eL30



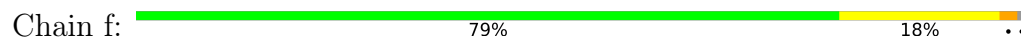
• Molecule 29: eL31



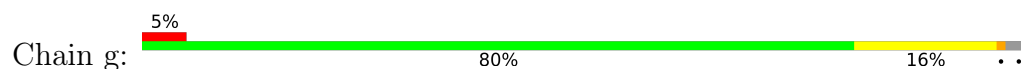
• Molecule 30: eL32



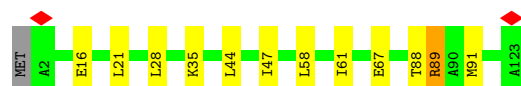
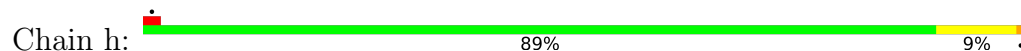
• Molecule 31: eL33



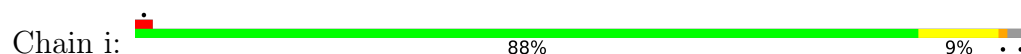
• Molecule 32: eL34

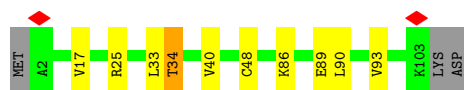


• Molecule 33: uL29



• Molecule 34: 60S ribosomal protein L36

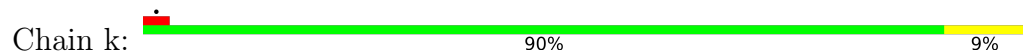




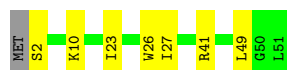
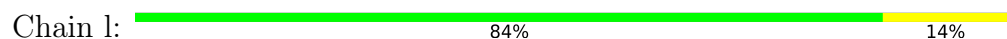
- Molecule 35: Ribosomal protein L37



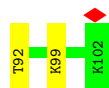
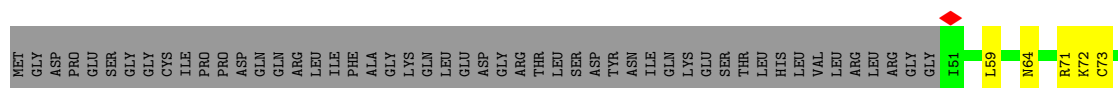
- Molecule 36: eL38



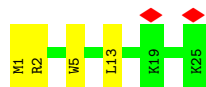
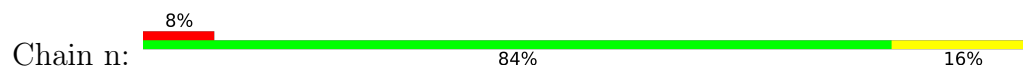
- Molecule 37: eL39



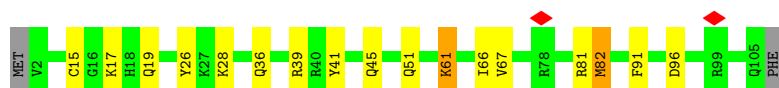
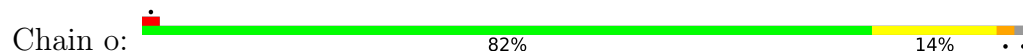
- Molecule 38: eL40



- Molecule 39: eL41



- Molecule 40: eL42



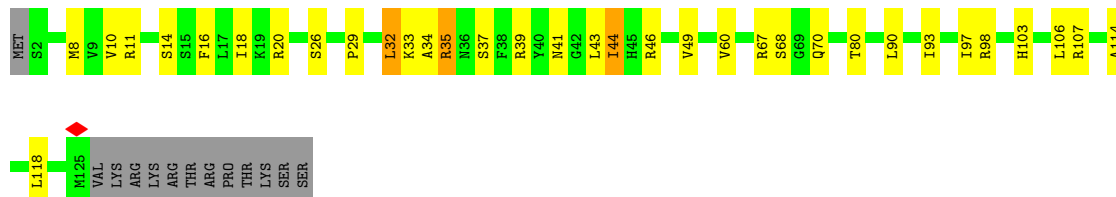
- Molecule 41: eL43

Chain p:  84% 15%

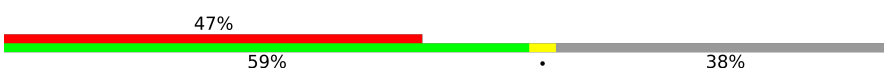


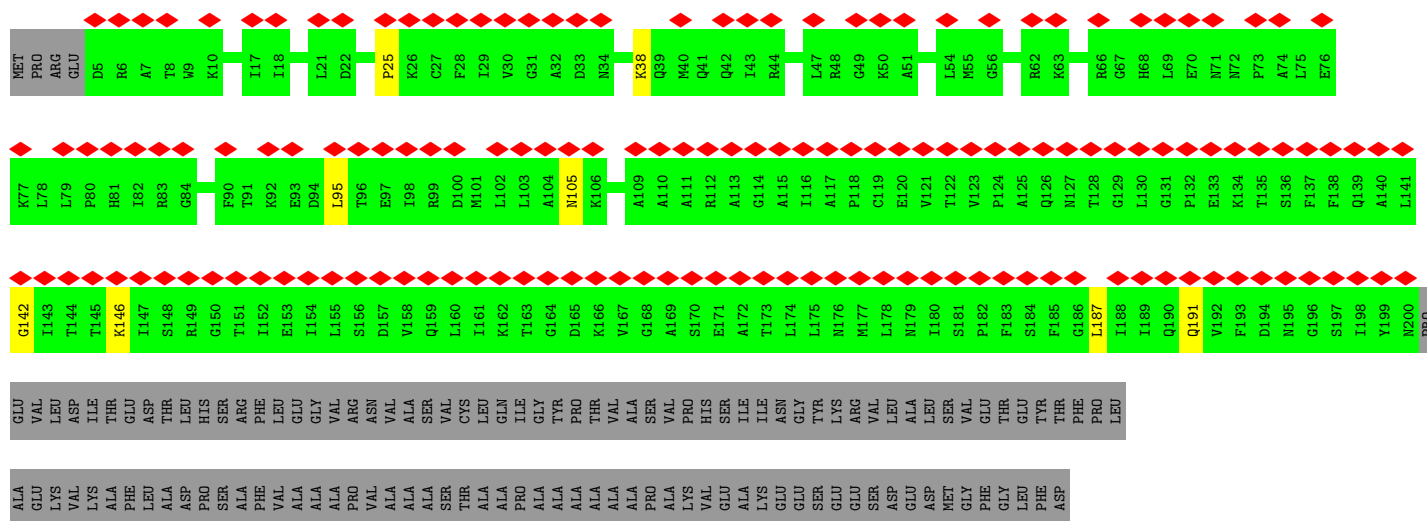
- Molecule 42: eL28

Chain r:  66% 23% 9%



- Molecule 43: uL10

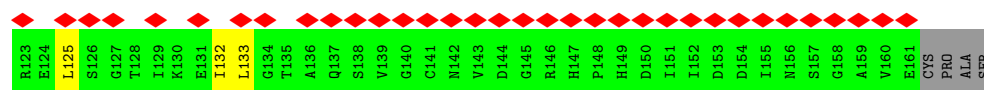
Chain s:  47% 59% 38%



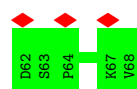
- Molecule 44: uL11

Chain t:  82% 88% 7%

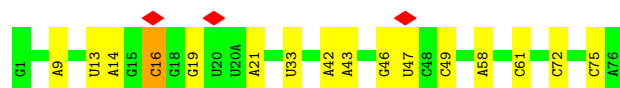




• Molecule 45: Nascent chain



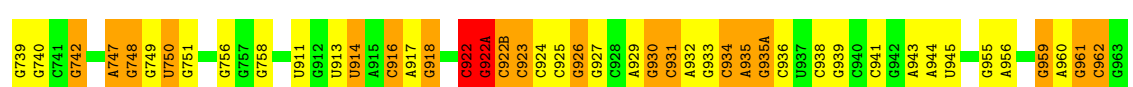
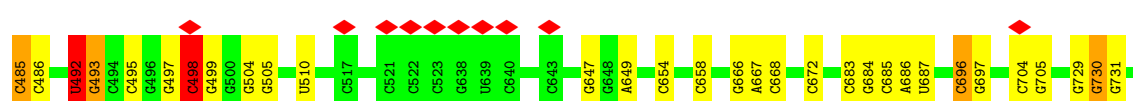
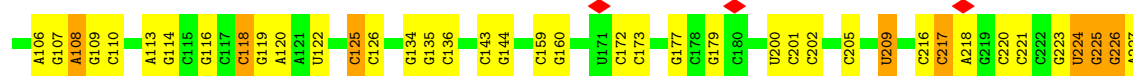
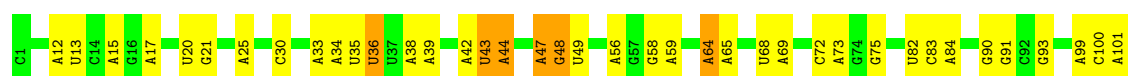
• Molecule 46: P-site tRNA

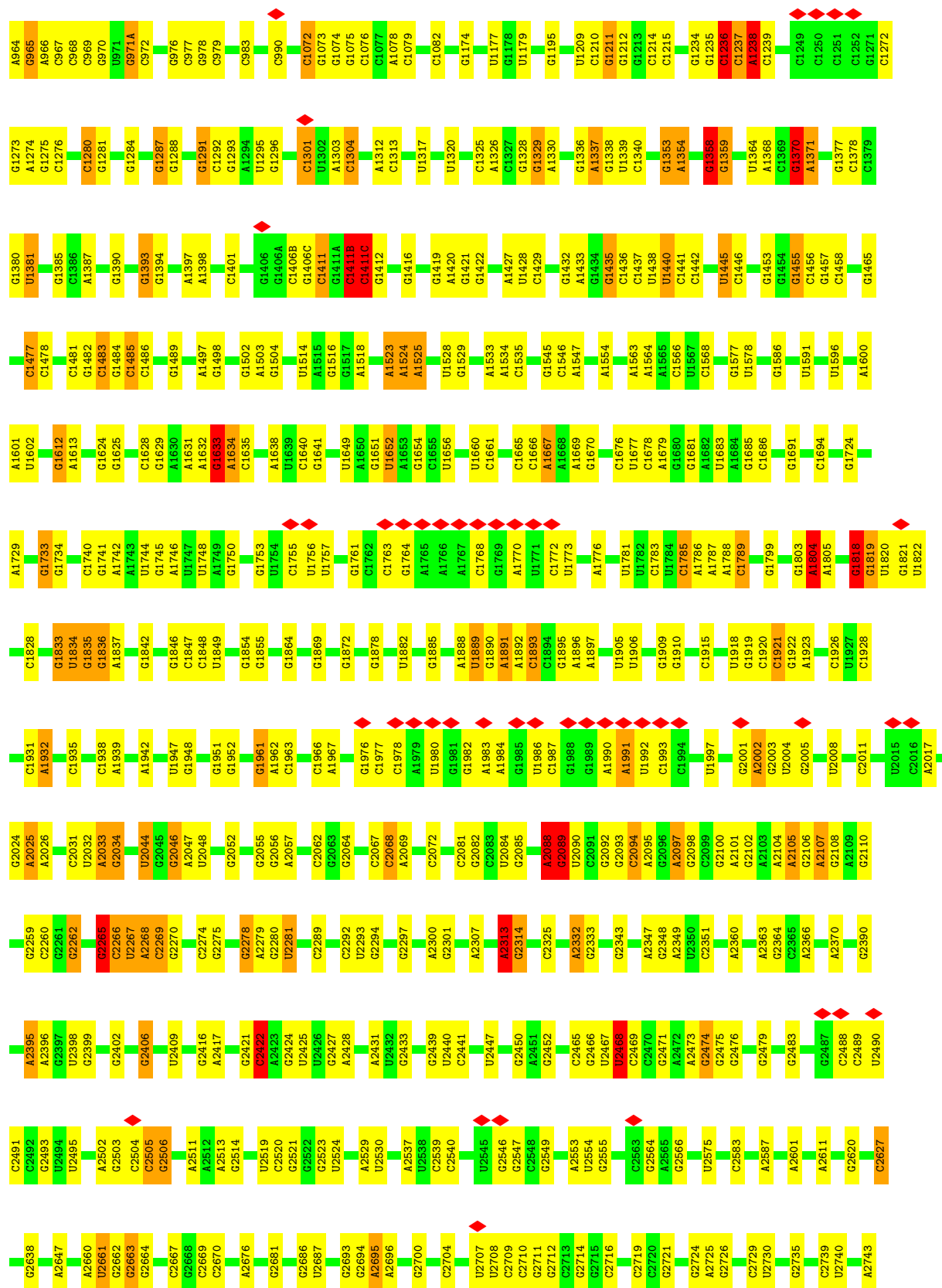


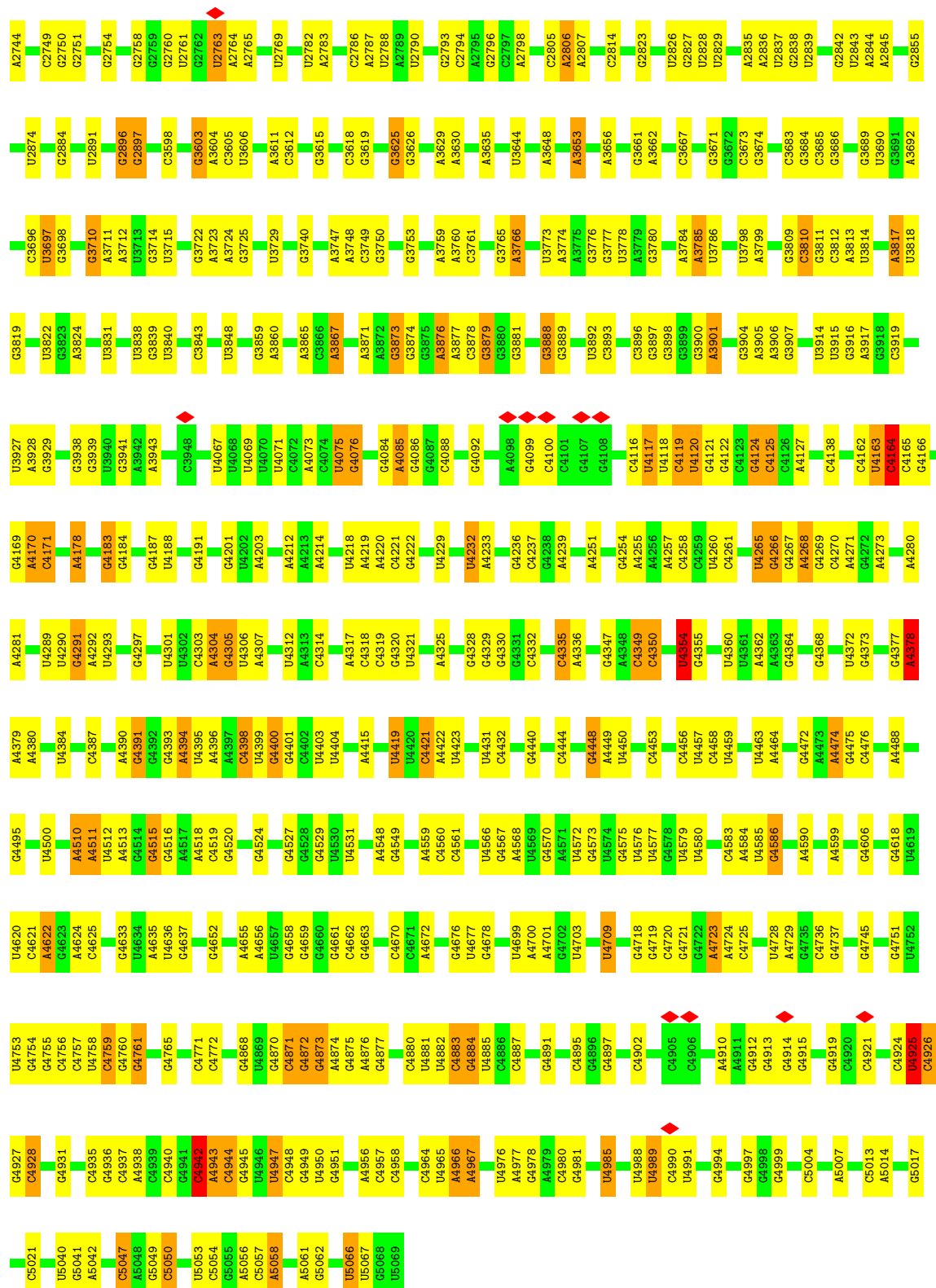
• Molecule 47: E-site tRNA



• Molecule 48: 28S ribosomal RNA

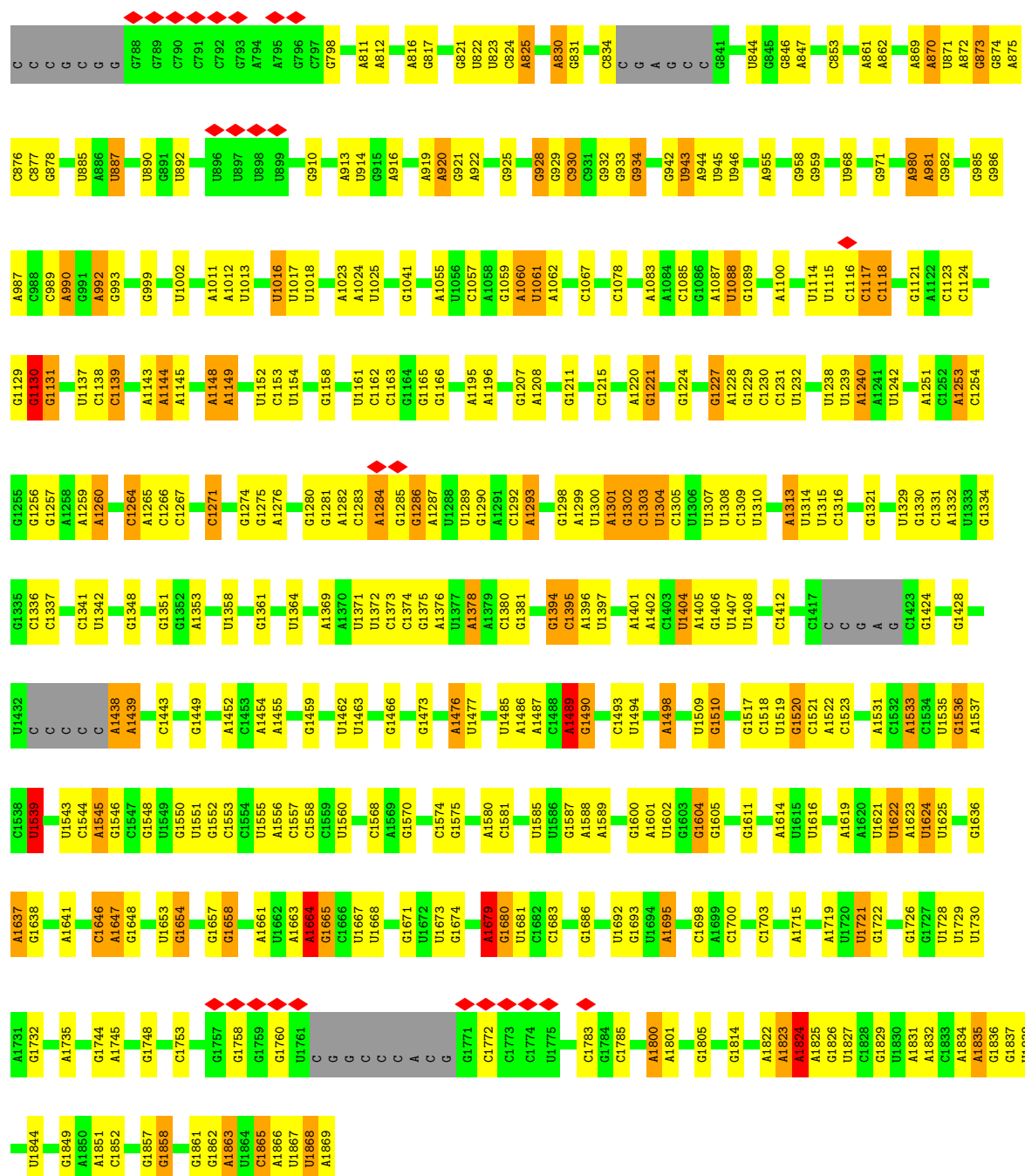






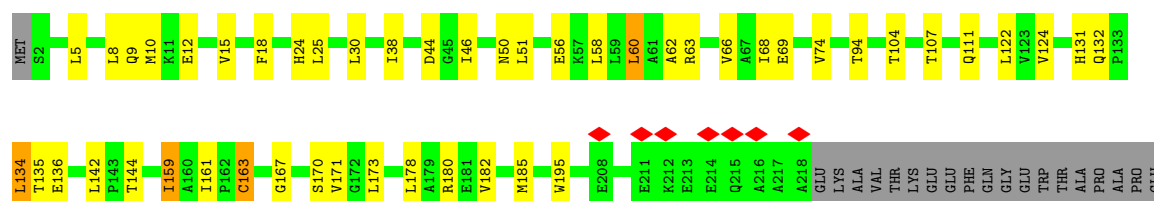
• Molecule 49: 5S ribosomal RNA

Chain 7:



• Molecule 52: uS2

Chain AA: 57% 15% 26%



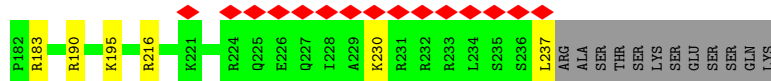
- Molecule 57: uS7

Chain FF:  81% 9% 9%



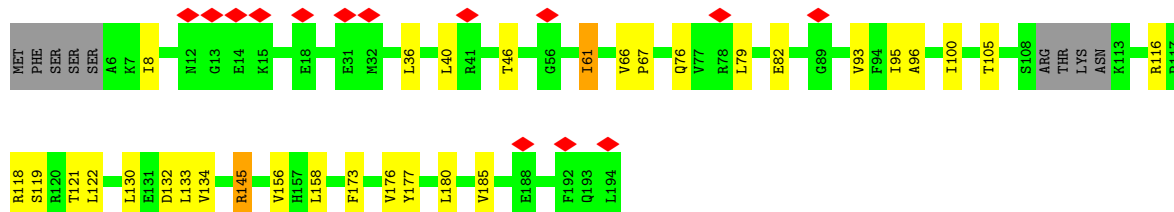
- Molecule 58: 40S ribosomal protein S6

Chain GG:  81% 14% 5%



- Molecule 59: eS7

Chain HH:  79% 15% 5%



- Molecule 60: 40S ribosomal protein S8

Chain II:  81% 17% 5%



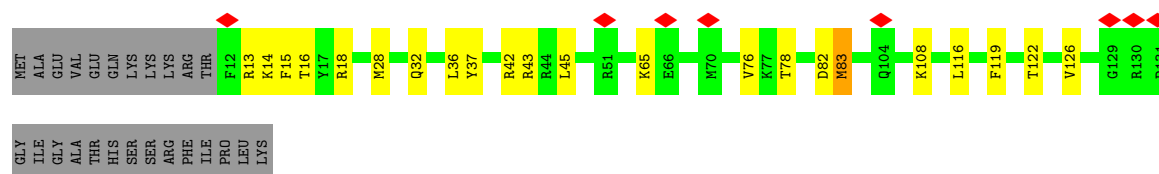
- Molecule 61: Ribosomal protein S9 (Predicted)

Chain JJ:  78% 15% 5%

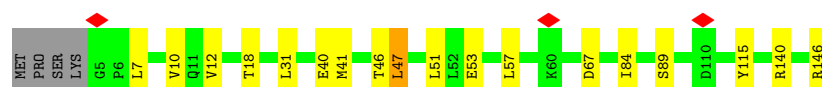
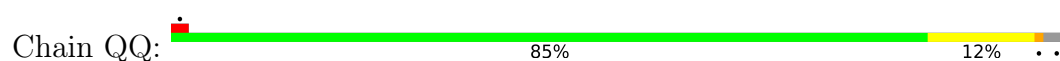




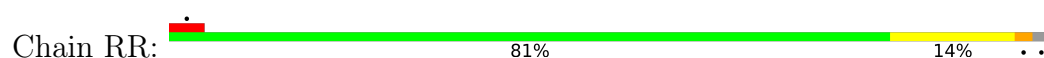
• Molecule 67: uS19



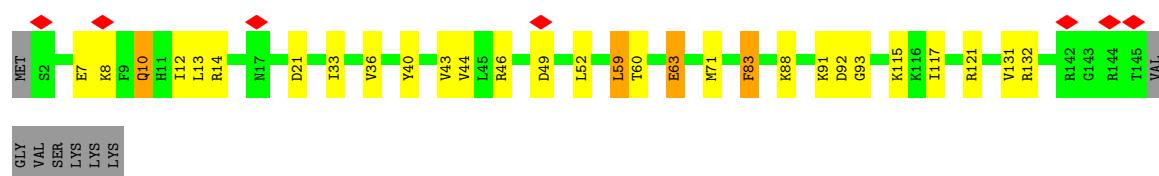
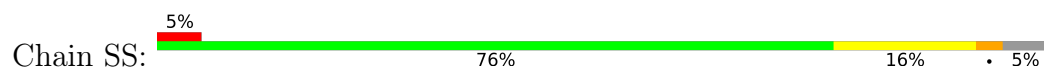
• Molecule 68: uS9



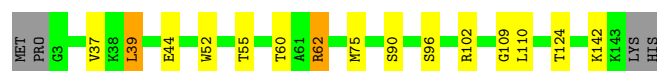
• Molecule 69: eS17



• Molecule 70: uS13

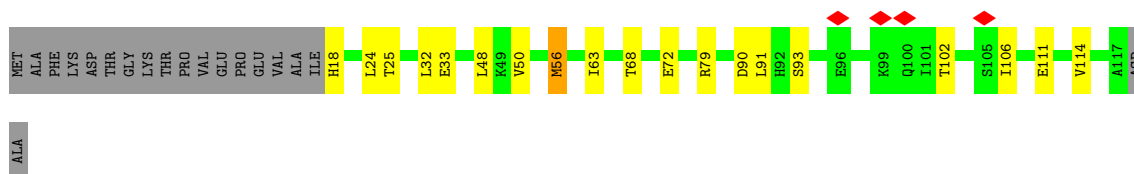


• Molecule 71: eS19



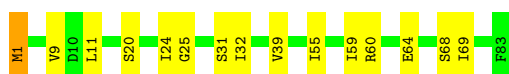
• Molecule 72: uS10





• Molecule 73: eS21

Chain VV: 82% 17%



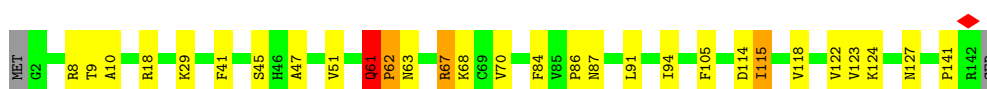
• Molecule 74: uS8

Chain WW: 74% 23%



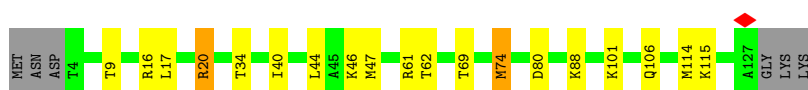
• Molecule 75: uS12

Chain XX: 78% 17%



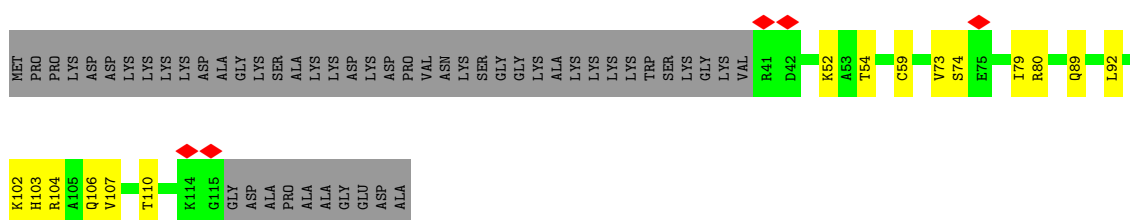
• Molecule 76: 40S ribosomal protein S24

Chain YY: 81% 13% 5%



• Molecule 77: eS25

Chain ZZ: 48% 12% 40%



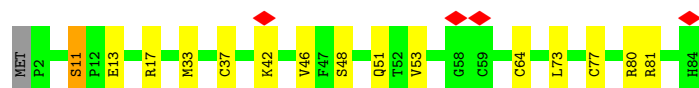
• Molecule 78: eS26

Chain aa: 



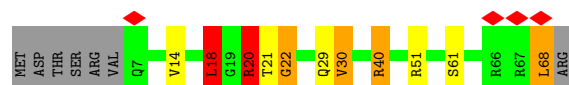
- Molecule 79: 40S ribosomal protein S27

Chain bb: 



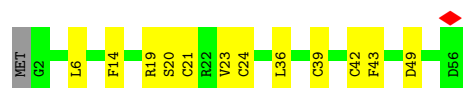
- Molecule 80: eS28

Chain cc: 



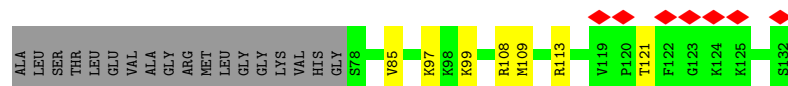
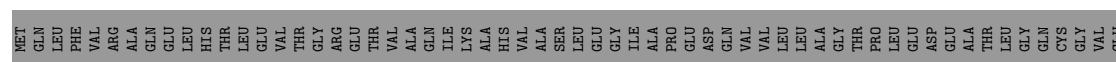
- Molecule 81: uS14

Chain dd: 



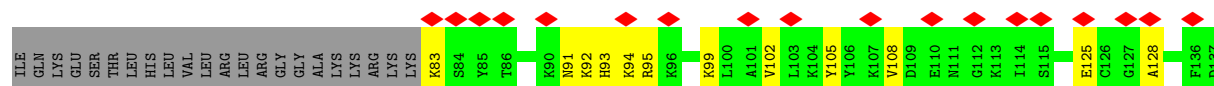
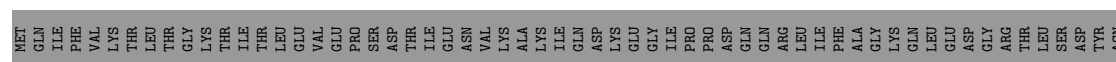
- Molecule 82: eS30

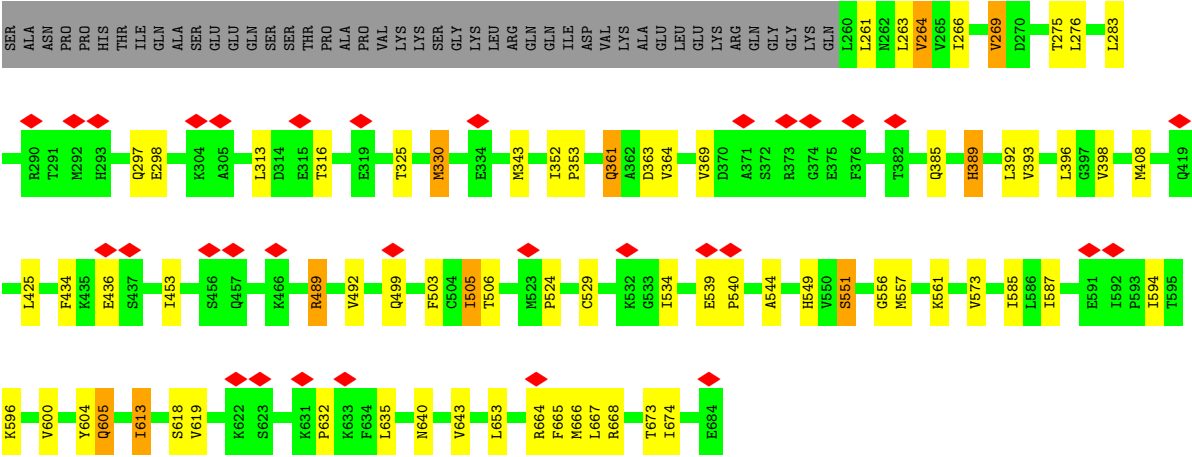
Chain ee: 



- Molecule 83: eS31

Chain ff: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.747	Depositor
Minimum map value	-0.536	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/1936	0.91	4/2596 (0.2%)
2	B	0.65	0/3240	0.88	2/4339 (0.0%)
3	C	0.63	0/2937	0.91	5/3946 (0.1%)
4	D	0.51	0/2437	0.85	1/3264 (0.0%)
5	E	0.53	0/1762	0.81	0/2362
6	F	0.72	0/1911	0.95	3/2549 (0.1%)
7	G	0.56	0/1910	0.87	0/2569
8	H	0.56	0/1535	0.80	0/2063
9	I	0.56	0/1702	0.82	1/2272 (0.0%)
10	J	0.51	0/1385	0.83	0/1852
11	L	0.54	0/1733	0.85	0/2316
12	M	0.57	0/1158	0.87	0/1547
13	N	0.57	0/1746	0.88	1/2338 (0.0%)
14	O	0.62	0/1662	0.91	5/2222 (0.2%)
15	P	0.66	0/1268	0.86	0/1700
16	Q	0.61	0/1539	0.90	1/2054 (0.0%)
17	R	0.56	0/1524	0.87	0/2013
18	S	0.74	0/1501	0.90	2/2012 (0.1%)
19	T	0.54	0/1326	0.81	0/1770
20	U	0.52	0/823	0.78	0/1104
21	V	0.60	0/993	0.86	1/1332 (0.1%)
22	W	0.59	0/873	0.83	0/1158
23	X	0.51	0/984	0.80	0/1323
24	Y	0.57	0/1132	0.85	0/1504
25	Z	0.57	0/1130	0.83	1/1507 (0.1%)
26	a	0.59	0/1191	0.89	1/1590 (0.1%)
27	b	0.51	0/861	0.83	0/1138
28	c	0.54	0/771	0.79	0/1034
29	d	0.61	0/903	0.85	1/1216 (0.1%)
30	e	0.61	0/1071	0.85	0/1429
31	f	0.65	0/895	0.88	0/1198
32	g	0.54	0/916	0.83	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.51	0/1021	0.84	0/1348
34	i	0.58	0/841	0.81	0/1112
35	j	0.58	0/720	0.87	0/952
36	k	0.46	0/575	0.75	0/761
37	l	0.56	0/459	0.83	0/608
38	m	0.67	0/435	0.90	0/575
39	n	0.49	0/240	0.84	0/305
40	o	0.59	0/864	0.82	0/1140
41	p	0.63	0/718	0.88	0/953
42	r	0.66	0/1010	0.93	2/1354 (0.1%)
43	s	0.55	0/1530	0.73	0/2064
44	t	0.59	0/1174	0.82	0/1582
45	1	0.61	0/49	0.97	0/65
46	2	0.37	0/1805	0.72	0/2809
47	3	0.37	0/1777	0.70	0/2763
48	5	0.43	5/84961 (0.0%)	0.83	173/132460 (0.1%)
49	7	0.42	0/2858	0.77	1/4455 (0.0%)
50	8	0.41	0/3581	0.78	4/5577 (0.1%)
51	9	0.42	0/40523	0.82	61/63130 (0.1%)
52	AA	0.57	0/1747	0.88	0/2374
53	BB	0.47	0/1756	0.82	0/2350
54	CC	0.55	0/1753	0.91	1/2369 (0.0%)
55	DD	0.53	0/1796	0.81	0/2417
56	EE	0.50	0/2118	0.84	1/2849 (0.0%)
57	FF	0.48	0/1492	0.87	0/2005
58	GG	0.51	0/1946	0.83	2/2590 (0.1%)
59	HH	0.51	0/1510	0.81	0/2022
60	II	0.54	0/1715	0.83	1/2287 (0.0%)
61	JJ	0.53	0/1550	0.91	2/2069 (0.1%)
62	KK	0.51	0/834	0.84	0/1125
63	LL	0.54	0/1195	0.87	1/1597 (0.1%)
64	MM	0.54	0/918	0.85	0/1233
65	NN	0.55	0/1226	0.91	0/1649
66	OO	0.58	0/1029	0.97	1/1380 (0.1%)
67	PP	0.57	0/1017	0.88	0/1358
68	QQ	0.49	0/1146	0.81	0/1534
69	RR	0.50	0/1082	0.81	0/1452
70	SS	0.52	0/1208	0.86	0/1618
71	TT	0.49	0/1115	0.87	0/1493
72	UU	0.50	0/805	0.87	2/1081 (0.2%)
73	VV	0.56	0/643	0.91	1/860 (0.1%)
74	WW	0.61	0/1051	0.90	0/1406
75	XX	0.59	0/1116	0.89	1/1490 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.47	0/1028	0.79	0/1366
77	ZZ	0.49	0/604	0.87	0/810
78	aa	0.57	0/828	0.89	0/1109
79	bb	0.50	0/665	0.81	0/891
80	cc	0.49	0/490	0.83	0/656
81	dd	0.54	0/470	0.80	0/623
82	ee	0.50	0/447	0.81	0/587
83	ff	0.52	0/567	0.75	0/753
84	gg	0.46	0/2493	0.72	1/3394 (0.0%)
85	hh	0.39	0/188	0.83	0/290
86	ii	0.47	0/2996	0.80	2/4050 (0.0%)
87	jj	0.48	0/3352	0.79	1/4523 (0.0%)
All	All	0.49	5/237792 (0.0%)	0.83	288/348210 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
11	L	0	1
13	N	0	1
31	f	0	1
48	5	0	2
56	EE	0	1
74	WW	0	1
75	XX	0	1
78	aa	0	1
80	cc	0	1
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	922(A)	G	O3'-P	9.08	1.72	1.61
48	5	935	A	C5-C6	-7.20	1.26	1.41
48	5	1411(B)	C	O3'-P	7.03	1.69	1.61
48	5	922	C	O3'-P	5.78	1.68	1.61
48	5	1411(C)	C	O5'-C5'	5.50	1.50	1.42

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	922	C	C2'-C3'-O3'	15.80	137.40	113.70
48	5	481	G	N1-C2-N2	-15.79	68.83	116.20
51	9	1835	A	C2'-C3'-O3'	14.23	130.85	109.50
48	5	1411	C	C2'-C3'-O3'	-13.13	94.00	113.70
48	5	935	A	C5-C6-N6	-12.99	84.72	123.70
48	5	2046	G	C2'-C3'-O3'	11.54	126.80	109.50
48	5	1834	U	C2'-C3'-O3'	10.50	125.24	109.50
48	5	47	A	C4'-C3'-O3'	10.08	124.52	109.40
48	5	385	A	C4'-C3'-O3'	9.89	124.23	109.40
51	9	1664	A	C4'-C3'-O3'	9.62	123.83	109.40
48	5	3697	U	C2'-C3'-O3'	9.25	127.57	113.70
48	5	1411	C	C4'-C3'-O3'	9.23	126.84	113.00
51	9	1394	G	C2'-C3'-O3'	9.12	127.38	113.70
48	5	1455	G	C2'-C3'-O3'	9.05	127.27	113.70
48	5	2474	G	C2'-C3'-O3'	9.00	123.00	109.50
48	5	2695	A	C2'-C3'-O3'	8.92	122.87	109.50
48	5	3888	G	C2'-C3'-O3'	8.82	126.94	113.70
51	9	629	A	C1'-C2'-O2'	-8.60	98.89	111.80
48	5	922	C	O4'-C4'-C3'	-8.40	95.60	104.00
26	a	22	ILE	N-CA-C	-8.38	103.12	110.74
48	5	48	G	C2'-C3'-O3'	8.35	122.02	109.50
51	9	1520	G	C4'-C3'-O3'	8.32	125.48	113.00
51	9	594	A	C4'-C3'-O3'	8.24	121.77	109.40
14	O	110	PRO	N-CA-C	8.19	120.69	110.70
48	5	3619	G	C4'-C3'-O3'	-8.17	100.74	113.00
48	5	1211	G	C2'-C3'-O3'	8.11	125.86	113.70
51	9	434	G	C2'-C3'-O3'	8.05	125.78	113.70
3	C	340	ILE	N-CA-C	-7.91	104.09	111.45
51	9	1130	G	C4'-C3'-O3'	7.89	124.83	113.00
48	5	406	C	C2'-C3'-O3'	7.67	125.21	113.70
48	5	38	A	C4'-C3'-O3'	-7.62	101.57	113.00
48	5	1477	C	C2'-C3'-O3'	7.61	125.11	113.70
51	9	1489	A	C4'-C3'-O3'	7.59	124.39	113.00
51	9	110	U	C2'-C3'-O3'	7.45	124.88	113.70
51	9	1061	U	C2'-C3'-O3'	-7.43	102.56	113.70
48	5	4232	U	C4'-C3'-O3'	7.39	120.48	109.40
48	5	1878	G	C4'-C3'-O3'	-7.38	101.92	113.00
48	5	2266	C	C2'-C3'-O3'	7.37	120.56	109.50
48	5	4119	C	C2'-C3'-O3'	7.37	120.55	109.50
51	9	417	C	C4'-C3'-O3'	-7.35	101.97	113.00
48	5	1485	C	C2'-C3'-O3'	7.34	120.50	109.50
51	9	1253	A	C2'-C3'-O3'	7.31	120.47	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4448	G	C4'-C3'-O3'	7.30	123.95	113.00
48	5	4622	A	C4'-C3'-O3'	-7.27	102.10	113.00
48	5	922	C	C4'-C3'-C2'	-7.20	95.41	102.60
48	5	935	A	N1-C6-N6	-7.16	97.12	118.60
48	5	978	G	C4'-C3'-O3'	7.11	120.07	109.40
48	5	125	C	C2'-C3'-O3'	7.08	124.32	113.70
51	9	870	A	C4'-C3'-O3'	7.07	120.00	109.40
48	5	1428	U	C2'-C3'-O3'	7.06	124.29	113.70
48	5	4947	U	C2'-C3'-O3'	7.05	124.28	113.70
48	5	971(A)	G	C4'-C3'-O3'	7.05	123.58	113.00
51	9	626	G	C4'-C3'-O3'	-6.99	98.91	109.40
48	5	481	G	N3-C2-N2	-6.97	98.98	119.90
51	9	687	C	C2'-C3'-O3'	6.97	119.95	109.50
48	5	4335	C	C4'-C3'-O3'	-6.96	102.55	113.00
51	9	688	U	C2'-C3'-O3'	6.94	119.92	109.50
63	LL	99	TYR	N-CA-C	-6.94	97.94	109.46
48	5	449	C	C2'-C3'-O3'	6.94	119.90	109.50
48	5	3896	C	C2'-C3'-O3'	-6.92	103.31	113.70
51	9	1395	C	C4'-C3'-O3'	6.85	123.28	113.00
48	5	4170	A	C2'-C3'-O3'	6.80	119.71	109.50
48	5	4925	U	C2'-C3'-O3'	6.80	119.70	109.50
16	Q	178	ARG	N-CA-C	6.79	119.54	111.33
48	5	1669	A	C4'-C3'-O3'	-6.75	102.87	113.00
48	5	2034	G	C3'-C2'-O2'	6.75	120.82	110.70
51	9	72	C	C4'-C3'-O3'	6.69	119.44	109.40
48	5	922(A)	G	N9-C1'-C2'	6.67	122.00	112.00
51	9	642	U	C4'-C3'-O3'	6.67	123.00	113.00
48	5	2313	A	C2'-C3'-O3'	6.65	119.48	109.50
48	5	1427	A	C4'-C3'-O3'	-6.64	103.03	113.00
51	9	1679	A	C2'-C3'-O3'	6.64	119.47	109.50
48	5	1370	G	C2'-C3'-O3'	6.64	119.46	109.50
48	5	2068	C	C4'-C3'-O3'	6.62	119.33	109.40
48	5	4559	A	C4'-C3'-O3'	-6.62	103.06	113.00
48	5	4347	G	C4'-C3'-O3'	-6.60	103.10	113.00
48	5	1236	C	C4'-C3'-O3'	6.59	122.89	113.00
48	5	1358	G	C4'-C3'-O3'	6.59	119.28	109.40
58	GG	134	GLY	CA-C-N	6.58	128.07	119.84
58	GG	134	GLY	C-N-CA	6.58	128.07	119.84
51	9	629	A	C3'-C2'-O2'	6.57	124.45	114.60
48	5	4076	G	C4'-C3'-O3'	-6.56	99.56	109.40
48	5	2836	A	C4'-C3'-O3'	-6.54	103.20	113.00
48	5	922	C	N1-C1'-C2'	-6.52	102.22	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4942	C	C4'-C3'-O3'	6.52	119.17	109.40
61	JJ	144	ILE	N-CA-C	6.48	115.12	107.73
48	5	4723	A	N9-C1'-C2'	6.47	121.70	112.00
48	5	2033	A	C4'-C3'-O3'	-6.45	103.32	113.00
48	5	1329	G	C2'-C3'-O3'	6.45	123.37	113.70
48	5	64	A	C4'-C3'-O3'	6.41	119.01	109.40
48	5	4884	G	C2'-C3'-O3'	6.40	123.30	113.70
48	5	935	A	C6-N1-C2	-6.39	99.43	118.60
48	5	90	G	C4'-C3'-O3'	-6.36	103.45	113.00
75	XX	87	ASN	N-CA-C	6.36	118.07	110.19
51	9	1637	A	C2'-C3'-O3'	6.32	118.97	109.50
48	5	4655	A	C4'-C3'-O3'	-6.30	103.55	113.00
48	5	696	C	C2'-C3'-O3'	6.29	118.94	109.50
48	5	492	U	C2'-C3'-O3'	6.28	118.92	109.50
48	5	2468	U	C4'-C3'-O3'	6.28	118.82	109.40
48	5	4378	A	C2'-C3'-O3'	6.27	118.91	109.50
48	5	1291	G	C2'-C3'-O3'	6.27	123.10	113.70
6	F	104	VAL	CB-CA-C	-6.23	103.62	112.22
48	5	4075	U	C4'-C3'-O3'	6.22	118.73	109.40
48	5	2067	C	C4'-C3'-O3'	-6.21	103.69	113.00
51	9	615	C	C1'-C2'-O2'	6.19	117.68	108.40
48	5	498	C	C4'-C3'-O3'	6.17	118.66	109.40
48	5	1428	U	C4'-C3'-O3'	-6.14	103.79	113.00
51	9	1158	G	C1'-C2'-O2'	6.13	117.60	108.40
50	8	94	G	C2'-C3'-O3'	6.13	118.69	109.50
2	B	258	HIS	N-CA-C	6.12	123.35	109.81
48	5	90	G	C2'-C3'-O3'	6.12	122.88	113.70
48	5	1893	C	C2'-C3'-O3'	-6.12	104.52	113.70
51	9	1264	C	C4'-C3'-O3'	6.12	118.58	109.40
51	9	752	G	C2'-C3'-O3'	6.11	118.67	109.50
48	5	1909	G	C1'-C2'-O2'	6.10	117.54	108.40
48	5	959	G	C4'-C3'-O3'	6.08	118.52	109.40
48	5	275	C	C2'-C3'-O3'	6.07	122.80	113.70
42	r	10	VAL	N-CA-C	6.06	116.84	110.72
48	5	2843	U	C4'-C3'-O3'	-6.06	103.91	113.00
48	5	2068	C	C2'-C3'-O3'	6.04	118.56	109.50
48	5	2452	G	C4'-C3'-O3'	-6.01	103.99	113.00
48	5	931	C	C4'-C3'-O3'	-6.00	104.00	113.00
48	5	1891	A	C4'-C3'-O3'	-5.99	104.02	113.00
48	5	2089	G	C2'-C3'-O3'	5.97	118.46	109.50
48	5	2823	G	C3'-C2'-O2'	5.97	119.66	110.70
51	9	642	U	C2'-C3'-O3'	5.97	122.65	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	862	A	C2'-C3'-O3'	-5.94	104.79	113.70
48	5	1238	A	C3'-C2'-O2'	5.93	119.60	110.70
51	9	625	G	C1'-C2'-O2'	-5.93	99.50	108.40
48	5	3873	G	C4'-C3'-O3'	-5.91	104.13	113.00
48	5	4663	G	C3'-C2'-O2'	5.91	119.56	110.70
48	5	4312	U	C4'-C3'-O3'	-5.90	104.15	113.00
48	5	407	A	C4'-C3'-O3'	-5.89	104.16	113.00
48	5	5049	G	C4'-C3'-O3'	5.88	118.22	109.40
32	g	5	LEU	N-CA-C	5.88	117.72	108.96
48	5	1789	C	C2'-C3'-O3'	-5.87	104.90	113.70
48	5	2089	G	C4'-C3'-O3'	5.86	118.19	109.40
48	5	3900	G	C1'-C2'-O2'	5.86	117.19	108.40
48	5	1445	U	C2'-C3'-O3'	5.86	122.49	113.70
25	Z	46	ILE	N-CA-C	5.85	115.25	106.42
48	5	4164	C	C4'-C3'-O3'	-5.82	104.27	113.00
48	5	1336	G	C2'-C3'-O3'	-5.82	104.97	113.70
51	9	1844	U	C4'-C3'-O3'	-5.81	104.28	113.00
48	5	372	A	C4'-C3'-O3'	-5.80	104.30	113.00
48	5	233	U	C4'-C3'-O3'	-5.78	104.33	113.00
51	9	501	C	N1-C1'-C2'	5.77	120.65	112.00
51	9	1353	A	C4'-C3'-O3'	-5.76	104.36	113.00
48	5	2661	U	C2'-C3'-O3'	5.75	118.12	109.50
48	5	3901	A	C4'-C3'-O3'	-5.75	104.38	113.00
51	9	1313	A	C4'-C3'-O3'	5.73	118.00	109.40
51	9	1858	G	C4'-C3'-O3'	-5.73	104.40	113.00
48	5	1818	G	C2'-C3'-O3'	5.73	122.29	113.70
48	5	3876	A	C2'-C3'-O3'	5.72	118.08	109.50
48	5	1072	C	C2'-C3'-O3'	5.71	118.06	109.50
14	O	109	PRO	CA-C-N	5.71	126.26	120.38
14	O	109	PRO	C-N-CA	5.71	126.26	120.38
72	UU	72	GLU	N-CA-C	5.70	118.36	107.75
60	II	82	VAL	CB-CA-C	-5.66	105.12	111.80
48	5	2786	C	C2'-C3'-O3'	-5.65	105.22	113.70
48	5	1411	C	C1'-C2'-O2'	5.65	116.88	108.40
51	9	291	G	C4'-C3'-O3'	-5.64	104.54	113.00
51	9	1329	U	C2'-C3'-O3'	-5.63	105.25	113.70
48	5	3603	G	C4'-C3'-O3'	-5.63	104.56	113.00
48	5	3865	A	C1'-C2'-O2'	5.62	116.84	108.40
51	9	450	C	C4'-C3'-O3'	-5.62	104.57	113.00
48	5	3625	G	C2'-C3'-O3'	5.62	122.13	113.70
48	5	226	G	C4'-C3'-O3'	5.62	117.83	109.40
48	5	4529	G	C4'-C3'-O3'	-5.61	104.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	922	C	C3'-C2'-O2'	5.61	119.11	110.70
48	5	1921	C	C4'-C3'-O3'	5.60	117.80	109.40
1	A	90	CYS	N-CA-C	5.59	116.90	108.46
48	5	2266	C	C4'-C3'-O3'	5.58	117.77	109.40
29	d	38	PHE	N-CA-C	5.57	118.12	111.71
48	5	3749	C	C2'-C3'-O3'	-5.56	105.36	113.70
66	OO	137	SER	N-CA-C	-5.56	104.24	111.02
48	5	1889	U	C1'-C2'-O2'	5.56	116.74	108.40
48	5	3818	U	C2'-C3'-O3'	-5.55	105.38	113.70
61	JJ	86	VAL	N-CA-C	-5.54	106.30	111.45
72	UU	93	SER	N-CA-C	5.54	113.00	108.07
48	5	2406	G	C4'-C3'-O3'	-5.52	104.72	113.00
51	9	553	U	C3'-C2'-O2'	5.51	118.97	110.70
6	F	141	TRP	N-CA-C	5.51	117.17	108.96
50	8	124	U	C4'-C3'-O3'	5.51	117.66	109.40
73	VV	9	VAL	N-CA-C	5.51	116.55	111.81
48	5	2700	G	C4'-C3'-O3'	-5.50	104.74	113.00
3	C	222	ARG	N-CA-C	5.50	119.48	112.34
13	N	185	GLY	N-CA-C	-5.49	103.49	112.83
48	5	2088	A	C2'-C3'-O3'	5.49	117.74	109.50
48	5	4456	C	C3'-C2'-O2'	5.49	118.93	110.70
51	9	532	C	C2'-C3'-O3'	5.49	121.93	113.70
48	5	1633	G	C3'-C2'-O2'	5.48	118.93	110.70
48	5	1835	G	C4'-C3'-O3'	5.48	117.62	109.40
48	5	21	G	C4'-C3'-O3'	5.47	121.21	113.00
48	5	1287	G	C4'-C3'-O3'	5.47	121.20	113.00
48	5	1926	C	C3'-C2'-O2'	5.46	118.89	110.70
48	5	2793	G	C4'-C3'-O3'	-5.46	104.81	113.00
48	5	4239	A	C4'-C3'-O3'	-5.45	104.83	113.00
87	jj	524	PRO	N-CA-C	5.44	117.34	110.70
1	A	196	TRP	CA-C-N	-5.43	113.68	119.98
1	A	196	TRP	C-N-CA	-5.43	113.68	119.98
51	9	1863	A	O4'-C1'-C2'	-5.42	100.38	105.80
48	5	1667	A	C1'-C2'-O2'	5.42	116.52	108.40
14	O	108	ILE	CA-C-N	5.40	125.95	120.38
14	O	108	ILE	C-N-CA	5.40	125.95	120.38
51	9	1868	U	C4'-C3'-O3'	5.40	117.50	109.40
48	5	2427	G	C4'-C3'-O3'	-5.39	104.91	113.00
48	5	1683	U	C4'-C3'-O3'	-5.39	104.92	113.00
51	9	1264	C	C2'-C3'-O3'	-5.39	101.42	109.50
48	5	922(A)	G	P-O3'-C3'	5.39	126.17	119.70
3	C	232	VAL	CB-CA-C	-5.38	105.03	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4354	U	C4'-C3'-O3'	-5.38	104.93	113.00
51	9	1824	A	C4'-C3'-O3'	5.37	117.46	109.40
51	9	160	U	C4'-C3'-O3'	5.37	117.45	109.40
48	5	2044	U	C3'-C2'-O2'	5.34	122.61	114.60
48	5	1804	A	C2'-C3'-O3'	5.34	117.51	109.50
48	5	3848	U	C2'-C3'-O3'	-5.34	105.69	113.70
48	5	3710	G	O4'-C4'-C3'	-5.33	100.77	106.10
84	gg	126	ASP	N-CA-C	-5.33	102.40	110.28
48	5	4384	U	C4'-C3'-O3'	-5.32	105.02	113.00
2	B	259	PRO	N-CA-C	-5.31	101.53	112.47
48	5	3603	G	C2'-C3'-O3'	5.31	121.67	113.70
48	5	1932	A	C4'-C3'-O3'	-5.31	105.04	113.00
48	5	2278	G	C2'-C3'-O3'	5.30	117.46	109.50
48	5	209	U	C4'-C3'-O3'	5.30	117.35	109.40
3	C	150	LEU	CA-C-N	-5.30	113.21	119.84
3	C	150	LEU	C-N-CA	-5.30	113.21	119.84
48	5	4566	U	C2'-C3'-O3'	-5.30	105.75	113.70
48	5	2664	G	C3'-C2'-O2'	5.30	118.65	110.70
51	9	1152	U	C2'-C3'-O3'	-5.29	105.76	113.70
48	5	2281	U	C4'-C3'-O3'	-5.29	105.06	113.00
1	A	137	ILE	CB-CA-C	-5.29	106.42	111.44
51	9	980	A	C4'-C3'-O3'	-5.28	105.08	113.00
51	9	1358	U	C3'-C2'-O2'	5.28	118.62	110.70
48	5	485	C	C3'-C2'-O2'	5.27	118.60	110.70
48	5	930	G	C2'-C3'-O3'	5.27	121.60	113.70
48	5	4364	G	C4'-C3'-O3'	-5.27	105.10	113.00
51	9	665	G	C1'-C2'-O2'	5.26	116.30	108.40
48	5	2265	G	C4'-C3'-O3'	5.25	117.27	109.40
6	F	94	ILE	CB-CA-C	-5.25	105.48	112.46
48	5	3893	C	C4'-C3'-O3'	-5.25	105.13	113.00
51	9	617	G	C1'-C2'-O2'	5.24	116.26	108.40
48	5	1072	C	C4'-C3'-O3'	5.24	117.25	109.40
48	5	4403	U	C4'-C3'-O3'	-5.23	105.15	113.00
48	5	1411	C	C5'-C4'-C3'	5.22	123.84	116.00
48	5	1915	C	C1'-C2'-O2'	-5.22	103.97	111.80
51	9	22	A	C1'-C2'-O2'	5.22	116.23	108.40
48	5	1670	G	C2'-C3'-O3'	-5.21	105.89	113.70
48	5	1921	C	C2'-C3'-O3'	5.21	117.31	109.50
51	9	928	G	C4'-C3'-O3'	-5.21	105.19	113.00
48	5	230	G	C4'-C3'-O3'	-5.19	105.21	113.00
48	5	48	G	C4'-C3'-O3'	5.18	117.18	109.40
51	9	873	G	C2'-C3'-O3'	5.18	117.28	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4076	G	O4'-C4'-C3'	-5.18	100.92	106.10
50	8	91	A	C3'-C2'-O2'	5.18	118.47	110.70
48	5	118	C	C4'-C3'-O3'	-5.17	105.24	113.00
51	9	825	A	C4'-C3'-O3'	-5.17	105.24	113.00
48	5	3871	A	C1'-C2'-O2'	5.17	116.16	108.40
48	5	245	C	C2'-C3'-O3'	5.16	121.45	113.70
48	5	2422	C	C3'-C2'-O2'	5.16	118.44	110.70
54	CC	162	ILE	N-CA-CB	5.16	116.66	110.31
9	I	43	VAL	CB-CA-C	-5.15	104.17	112.16
48	5	959	G	C2'-C3'-O3'	5.15	117.23	109.50
86	ii	46	LYS	CA-C-N	-5.15	116.10	123.10
86	ii	46	LYS	C-N-CA	-5.15	116.10	123.10
48	5	1440	U	C2'-C3'-O3'	5.14	121.41	113.70
48	5	1393	G	C4'-C3'-O3'	-5.13	105.31	113.00
48	5	1788	A	C4'-C3'-O3'	-5.13	105.31	113.00
56	EE	107	GLY	N-CA-C	5.13	120.31	114.67
18	S	139	ARG	CA-C-N	5.12	124.74	119.56
18	S	139	ARG	C-N-CA	5.12	124.74	119.56
49	7	55	A	C3'-C2'-O2'	5.12	118.38	110.70
51	9	1510	G	C1'-C2'-O2'	5.12	116.07	108.40
50	8	69	U	C4'-C3'-O3'	-5.11	105.34	113.00
4	D	236	MET	N-CA-C	5.10	116.53	110.97
48	5	4178	A	C1'-C2'-O2'	5.10	116.05	108.40
51	9	1658	G	C4'-C3'-O3'	-5.10	105.35	113.00
48	5	4676	G	C1'-C2'-O2'	5.09	116.04	108.40
21	V	47	GLY	N-CA-C	5.08	116.77	111.95
48	5	4400	G	C4'-C3'-O3'	-5.08	105.39	113.00
48	5	1411	C	O4'-C4'-C3'	-5.07	98.93	104.00
51	9	394	G	C3'-C2'-O2'	5.07	118.30	110.70
51	9	1539	U	C3'-C2'-O2'	5.05	118.28	110.70
48	5	217	C	C4'-C3'-O3'	5.04	116.96	109.40
51	9	24	C	C4'-C3'-O3'	-5.04	105.45	113.00
51	9	1361	G	C1'-C2'-O2'	5.04	115.95	108.40
51	9	472	C	C4'-C3'-O3'	-5.02	105.47	113.00
48	5	927	G	C4'-C3'-O3'	-5.01	105.48	113.00
42	r	44	ILE	CB-CA-C	-5.01	105.46	112.02

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain

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Mol	Chain	Res	Type	Group
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
3	C	90	GLY	Peptide
56	EE	155	LYS	Peptide
11	L	71	ARG	Peptide
13	N	184	ILE	Peptide
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide
80	cc	20	ARG	Sidechain
31	f	105	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	28	0
2	B	3172	0	3310	35	0
3	C	2883	0	3053	35	0
4	D	2391	0	2424	17	0
5	E	1729	0	1887	11	0
6	F	1875	0	1995	18	0
7	G	1879	0	2027	15	0
8	H	1516	0	1597	24	0
9	I	1664	0	1712	12	0
10	J	1362	0	1399	10	0
11	L	1702	0	1820	9	0
12	M	1137	0	1211	15	0
13	N	1701	0	1749	17	0
14	O	1630	0	1778	23	0
15	P	1242	0	1274	9	0
16	Q	1515	0	1634	15	0
17	R	1508	0	1664	9	0
18	S	1462	0	1508	25	0
19	T	1298	0	1366	12	0
20	U	809	0	833	7	0
21	V	979	0	1039	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	860	0	903	11	0
23	X	967	0	1040	2	0
24	Y	1115	0	1205	7	0
25	Z	1107	0	1182	9	0
26	a	1162	0	1209	18	0
27	b	848	0	920	0	0
28	c	761	0	794	9	0
29	d	888	0	930	15	0
30	e	1053	0	1147	8	0
31	f	876	0	912	8	0
32	g	906	0	1002	7	0
33	h	1013	0	1147	5	0
34	i	830	0	916	5	0
35	j	705	0	738	6	0
36	k	569	0	637	2	0
37	l	447	0	480	5	0
38	m	429	0	466	5	0
39	n	239	0	289	1	0
40	o	851	0	920	10	0
41	p	708	0	756	6	0
42	r	994	0	1051	12	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	2	0
45	1	49	0	51	0	0
46	2	1616	0	824	2	0
47	3	1593	0	811	5	0
48	5	75972	0	38398	352	0
49	7	2558	0	1296	7	0
50	8	3208	0	1629	15	0
51	9	36249	0	18317	277	0
52	AA	1710	0	1708	24	0
53	BB	1729	0	1803	20	0
54	CC	1716	0	1806	14	0
55	DD	1768	0	1866	10	0
56	EE	2076	0	2177	14	0
57	FF	1471	0	1522	8	0
58	GG	1923	0	2089	13	0
59	HH	1488	0	1582	15	0
60	II	1686	0	1772	14	0
61	JJ	1525	0	1640	10	0
62	KK	810	0	836	11	0
63	LL	1175	0	1249	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	MM	908	0	939	21	0
65	NN	1202	0	1289	11	0
66	OO	1016	0	1039	15	0
67	PP	997	0	1045	20	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	9	0
70	SS	1190	0	1249	23	0
71	TT	1097	0	1132	5	0
72	UU	795	0	862	6	0
73	VV	636	0	637	7	0
74	WW	1034	0	1080	15	0
75	XX	1098	0	1167	14	0
76	YY	1011	0	1083	3	0
77	ZZ	598	0	656	4	0
78	aa	814	0	863	10	0
79	bb	651	0	672	5	0
80	cc	488	0	514	17	0
81	dd	459	0	449	9	0
82	ee	443	0	492	0	0
83	ff	555	0	565	65	0
84	gg	2436	0	2393	16	0
85	hh	169	0	86	1	0
86	ii	2947	0	2957	21	0
87	jj	3292	0	3371	33	0
88	5	178	0	0	0	0
88	7	5	0	0	0	0
88	8	5	0	0	0	0
88	9	66	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	2	0
89	g	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	j	1	0	0	0	0
89	m	1	0	0	1	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	32	0	14	1	0
All	All	222005	0	166945	1371	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 4.

All (1371) 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)
86:ii:45:ARG:NH1	86:ii:100:HIS:ND1	1.65	1.41
51:9:1304:U:H5'	83:ff:93:HIS:N	1.13	1.39
48:5:3914:U:O4	48:5:4378:A:N1	1.58	1.35
48:5:922:C:C5'	48:5:922(A):G:H3'	1.59	1.31
51:9:1304:U:C5'	83:ff:93:HIS:N	1.94	1.31
51:9:1302:G:N2	83:ff:93:HIS:CE1	2.01	1.28
51:9:1304:U:H5'	83:ff:92:LYS:C	1.58	1.26
48:5:922:C:H5''	48:5:922(B):C:O5'	1.38	1.23
51:9:1283:C:N4	64:MM:102:LYS:HE3	1.52	1.21
48:5:1411:C:H4'	48:5:1411(C):C:O4'	1.41	1.16
51:9:1283:C:H41	64:MM:102:LYS:HE3	1.00	1.08
51:9:1284:A:N1	64:MM:91:LEU:HD22	1.69	1.07
48:5:922:C:H5'	48:5:922(A):G:C3'	1.85	1.07
51:9:1302:G:H22	83:ff:93:HIS:CE1	1.67	1.06
51:9:1680:G:H1'	80:cc:20:ARG:HH12	1.18	1.03
48:5:922:C:H5''	48:5:922(B):C:P	2.03	0.97
51:9:1282:A:N7	64:MM:102:LYS:NZ	2.12	0.97
51:9:1283:C:H41	64:MM:102:LYS:CE	1.78	0.96
51:9:1290:G:N7	83:ff:95:ARG:NH2	2.14	0.96
48:5:922:C:C5'	48:5:922(B):C:O5'	2.15	0.95
51:9:1292:C:H1'	83:ff:140:TYR:CE2	2.02	0.94
51:9:1309:C:H5'	83:ff:105:TYR:CE1	2.02	0.94
48:5:922:C:H5'	48:5:922(A):G:H3'	0.95	0.93
51:9:1309:C:H5'	83:ff:105:TYR:OH	1.68	0.93
32:g:49:CYS:HG	89:g:201:ZN:ZN	0.63	0.92
51:9:1304:U:H5''	83:ff:93:HIS:HB2	1.50	0.92
51:9:1680:G:O4'	80:cc:20:ARG:NH2	2.02	0.91
51:9:1309:C:H5'	83:ff:105:TYR:CZ	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1302:G:H22	83:ff:93:HIS:HE1	1.19	0.90
51:9:1292:C:H1'	83:ff:140:TYR:CD2	2.06	0.90
51:9:1304:U:C5'	83:ff:93:HIS:CA	2.50	0.90
48:5:922:C:P	48:5:922(B):C:O5'	2.31	0.89
51:9:1302:G:H21	83:ff:93:HIS:CE1	1.85	0.88
48:5:1411:C:O3'	48:5:1411(C):C:C5'	2.21	0.88
51:9:1304:U:H5''	83:ff:93:HIS:CA	2.04	0.88
83:ff:141:CYS:SG	89:ff:200:ZN:ZN	1.62	0.88
51:9:1283:C:N4	64:MM:102:LYS:CE	2.36	0.87
51:9:1292:C:C2	83:ff:140:TYR:CZ	2.62	0.87
51:9:615:C:H2'	51:9:616:A:C8	2.09	0.87
48:5:2031:C:O3'	48:5:2032:U:P	2.33	0.86
55:DD:16:ILE:HD11	81:dd:36:LEU:HD23	1.57	0.86
51:9:1292:C:C1'	83:ff:140:TYR:CE2	2.60	0.85
51:9:1680:G:H1'	80:cc:20:ARG:NH1	1.91	0.84
51:9:1304:U:H5'	83:ff:93:HIS:H	1.35	0.84
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	1.59	0.84
51:9:1284:A:C4	64:MM:91:LEU:HD13	2.12	0.84
48:5:1524:A:N1	48:5:1652:U:O4	2.10	0.84
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.60	0.83
51:9:1680:G:C1'	80:cc:20:ARG:HH12	1.90	0.83
48:5:922:C:C2'	48:5:922(B):C:C2	2.62	0.82
51:9:1304:U:H5''	83:ff:93:HIS:CB	2.07	0.82
48:5:922:C:C5'	48:5:922(A):G:C3'	2.50	0.82
51:9:1309:C:C5'	83:ff:105:TYR:OH	2.28	0.82
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.61	0.81
51:9:628:A:H61	51:9:1332:A:C1'	1.92	0.81
48:5:922:C:H2'	48:5:922(B):C:N3	1.96	0.81
48:5:922:C:H2'	48:5:922(B):C:C2	2.16	0.81
51:9:615:C:O2'	51:9:616:A:O4'	1.97	0.80
51:9:1304:U:H4'	83:ff:91:ASN:O	1.80	0.80
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.63	0.80
51:9:628:A:N6	51:9:1332:A:O4'	2.14	0.80
51:9:1304:U:H5'	83:ff:93:HIS:CA	2.12	0.80
48:5:2395:A:O2'	48:5:2806:A:H1'	1.80	0.80
51:9:1284:A:C2	64:MM:91:LEU:HD22	2.17	0.80
48:5:922:C:O3'	48:5:922(B):C:C6	2.34	0.79
51:9:1309:C:C3'	83:ff:105:TYR:HH	1.95	0.79
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.65	0.79
48:5:1411:C:O3'	48:5:1411(C):C:O5'	2.02	0.78
51:9:1292:C:N1	83:ff:140:TYR:CE2	2.51	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1304:U:O2'	83:ff:91:ASN:OD1	2.01	0.77
67:PP:18:ARG:CD	70:SS:88:LYS:HG2	2.14	0.77
48:5:922:C:C5'	48:5:922(B):C:P	2.72	0.77
48:5:3914:U:C4	48:5:4378:A:N1	2.52	0.77
51:9:1292:C:C2	83:ff:140:TYR:CE1	2.72	0.77
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.67	0.77
16:Q:70:MET:HE1	16:Q:137:VAL:HG21	1.65	0.77
86:ii:45:ARG:HD3	86:ii:94:VAL:HG22	1.67	0.76
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.65	0.76
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.68	0.76
48:5:1411:C:C3'	48:5:1411(C):C:O5'	2.34	0.76
51:9:1304:U:C5'	83:ff:93:HIS:H	1.92	0.76
51:9:615:C:H2'	51:9:616:A:H8	1.48	0.75
51:9:1680:G:C4'	80:cc:20:ARG:NH2	2.49	0.75
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.58	0.75
86:ii:45:ARG:NH1	86:ii:100:HIS:CE1	2.53	0.75
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.68	0.75
3:C:101:MET:SD	3:C:104:PRO:HA	2.26	0.75
80:cc:18:LEU:HB2	80:cc:29:GLN:O	1.87	0.75
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.68	0.74
51:9:1309:C:O3'	83:ff:105:TYR:OH	2.04	0.74
64:MM:36:ARG:HD2	83:ff:102:VAL:CG2	2.17	0.73
48:5:1411:C:O3'	48:5:1411(C):C:H5''	1.88	0.73
51:9:1130:G:H2'	51:9:1130:G:N3	2.01	0.73
9:I:191:ILE:HD11	9:I:212:LEU:HD11	1.70	0.73
40:o:81:ARG:NH2	48:5:4293:U:O2'	2.22	0.73
48:5:3914:U:O4	48:5:4378:A:C2	2.42	0.73
80:cc:21:THR:HG22	80:cc:68:LEU:HD13	1.69	0.72
51:9:1309:C:C3'	83:ff:105:TYR:OH	2.38	0.72
51:9:980:A:H2'	51:9:981:A:C8	2.24	0.71
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.37	0.71
48:5:922:C:O2'	48:5:922(B):C:C2	2.42	0.71
64:MM:36:ARG:HD2	83:ff:102:VAL:HG22	1.72	0.71
51:9:1680:G:C1'	80:cc:20:ARG:NH1	2.51	0.71
51:9:1293:A:O2'	83:ff:138:ARG:NH1	2.24	0.71
87:jj:392:LEU:HD23	87:jj:666:MET:HE2	1.72	0.71
4:D:208:MET:HE1	4:D:236:MET:HE1	1.71	0.70
86:ii:45:ARG:CD	86:ii:94:VAL:HG22	2.21	0.70
48:5:1411:C:C4'	48:5:1411(C):C:O4'	2.32	0.70
51:9:1293:A:O2'	83:ff:138:ARG:CZ	2.40	0.70
48:5:4510:A:O2'	48:5:4511:A:O4'	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1411:C:H3'	48:5:1411(B):C:H3'	1.72	0.69
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.74	0.69
51:9:1292:C:C2	83:ff:140:TYR:CE2	2.80	0.69
51:9:1292:C:N3	83:ff:140:TYR:CE1	2.61	0.69
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.75	0.69
86:ii:45:ARG:HD3	86:ii:94:VAL:CG2	2.22	0.69
15:P:95:LEU:HD12	15:P:148:MET:HE1	1.75	0.69
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.75	0.69
48:5:922:C:O5'	48:5:922(A):G:H3'	1.93	0.69
51:9:628:A:H61	51:9:1332:A:H1'	1.57	0.68
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.76	0.68
18:S:84:TYR:CE1	18:S:93:MET:HE3	2.28	0.68
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.24	0.68
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.33	0.68
84:gg:79:LEU:HD22	84:gg:111:VAL:HG21	1.76	0.67
48:5:738:C:O2'	48:5:738(A):C:O4'	2.10	0.67
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.76	0.67
87:jj:283:LEU:HB3	87:jj:453:ILE:HD11	1.77	0.67
86:ii:45:ARG:HH11	86:ii:100:HIS:CE1	2.10	0.67
52:AA:63:ARG:HG3	52:AA:185:MET:HE1	1.77	0.66
37:l:2:SER:N	48:5:2406:G:N7	2.44	0.66
48:5:3914:U:H3	48:5:4378:A:N6	1.93	0.66
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.28	0.66
51:9:615:C:O2'	51:9:616:A:O5'	2.14	0.66
52:AA:104:THR:O	52:AA:107:THR:HG23	1.97	0.65
48:5:742:G:C2	48:5:922(A):G:C6	2.84	0.65
87:jj:613:ILE:HD12	87:jj:643:VAL:HG21	1.77	0.65
38:m:73:CYS:SG	89:m:200:ZN:ZN	1.85	0.65
48:5:4579:U:H2'	48:5:4580:U:C6	2.31	0.65
48:5:747:A:H4'	48:5:748:G:OP1	1.96	0.65
51:9:1284:A:C2	64:MM:91:LEU:CD2	2.79	0.65
48:5:1818:G:O2'	48:5:1819:G:OP1	2.12	0.65
66:OO:129:ILE:HG21	78:aa:44:ILE:HD13	1.79	0.65
48:5:3914:U:N3	48:5:4378:A:N6	2.45	0.65
40:o:41:TYR:CD1	47:3:75:C:O2	2.50	0.64
48:5:1411:C:H3'	48:5:1411(B):C:C3'	2.26	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.31	0.64
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.79	0.64
51:9:1292:C:N1	83:ff:140:TYR:CZ	2.65	0.64
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.32	0.64
51:9:1407:U:H2'	51:9:1408:U:C6	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.80	0.64
48:5:4942:C:H4'	48:5:4943:A:OP1	1.97	0.64
48:5:1411:C:C5'	48:5:1411(B):C:H2'	2.28	0.64
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.80	0.63
2:B:174:ARG:NH1	48:5:4985:U:O2	2.31	0.63
2:B:92:TYR:HB3	2:B:99:LEU:HD21	1.81	0.63
14:O:72:HIS:N	48:5:4586:G:OP1	2.32	0.63
51:9:446:G:OP2	60:II:47:ARG:NH1	2.32	0.63
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.80	0.62
58:GG:32:MET:HE2	58:GG:63:MET:HG2	1.79	0.62
48:5:922(B):C:O2'	48:5:923:C:O5'	2.17	0.62
24:Y:1:MET:HE2	48:5:1368:A:H1'	1.80	0.62
48:5:922:C:C6	48:5:922(A):G:C6	2.86	0.62
51:9:183:G:O2'	51:9:184:G:O5'	2.17	0.62
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.81	0.62
52:AA:60:LEU:HD13	52:AA:159:ILE:CD1	2.29	0.62
2:B:332:MET:HE1	2:B:365:LEU:HD11	1.81	0.62
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.35	0.62
8:H:4:ILE:HD11	18:S:152:PHE:CD2	2.34	0.61
48:5:2033:A:O2'	48:5:2034:G:O5'	2.10	0.61
51:9:146:G:O2'	51:9:147:A:O5'	2.17	0.61
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.81	0.61
48:5:922:C:C6	48:5:922(A):G:C5	2.88	0.61
51:9:1304:U:P	83:ff:93:HIS:HB2	2.41	0.61
51:9:1309:C:H5'	83:ff:105:TYR:HE1	1.62	0.61
67:PP:18:ARG:NE	70:SS:88:LYS:HD3	2.15	0.61
51:9:1286:G:O6	64:MM:34:GLY:HA3	2.00	0.61
63:LL:37:TYR:CE2	63:LL:51:ILE:HG23	2.34	0.61
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.83	0.61
84:gg:87:LEU:HD21	84:gg:108:VAL:HG11	1.83	0.61
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.82	0.61
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.83	0.61
51:9:1589:A:N3	51:9:1653:U:O2'	2.33	0.61
5:E:52:LEU:HD23	5:E:58:ARG:HA	1.81	0.60
48:5:1370:G:O2'	48:5:1371:A:OP2	2.17	0.60
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.83	0.60
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.83	0.60
48:5:4723:A:H2'	48:5:4724:A:C8	2.36	0.60
51:9:1130:G:O2'	51:9:1131:G:O5'	2.19	0.60
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.82	0.60
48:5:922:C:O5'	48:5:922(A):G:P	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:261:LEU:HD23	87:jj:364:VAL:HG21	1.83	0.60
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.37	0.60
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.34	0.60
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.84	0.60
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.82	0.60
48:5:922:C:O5'	48:5:922(A):G:O5'	2.19	0.60
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.45	0.60
51:9:1292:C:O2	83:ff:140:TYR:CG	2.55	0.60
51:9:1284:A:C8	64:MM:104:VAL:HG21	2.37	0.60
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.84	0.59
51:9:614:C:H1'	51:9:626:G:H21	1.66	0.59
15:P:69:ARG:NH2	48:5:4568:A:N3	2.49	0.59
51:9:1304:U:C5'	83:ff:93:HIS:HB2	2.30	0.59
86:ii:45:ARG:NE	86:ii:94:VAL:HG22	2.17	0.59
86:ii:45:ARG:HH12	86:ii:100:HIS:CG	2.15	0.59
87:jj:534:ILE:HD11	87:jj:544:ALA:HB3	1.84	0.59
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.41	0.59
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.37	0.59
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.83	0.59
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.82	0.59
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.84	0.59
87:jj:263:LEU:HD23	87:jj:264:VAL:N	2.17	0.59
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.35	0.59
4:D:33:ARG:NH1	4:D:72:ASP:OD2	2.36	0.58
12:M:15:VAL:HG22	12:M:50:MET:HE1	1.85	0.58
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.85	0.58
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.35	0.58
28:c:82:GLY:HA2	28:c:91:VAL:HG12	1.85	0.58
10:J:141:ILE:HD11	49:7:55:A:N3	2.17	0.58
48:5:3766:A:N1	51:9:1827:U:O2'	2.30	0.58
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.36	0.58
5:E:124:VAL:HG13	30:e:7:LEU:HD11	1.86	0.58
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	1.84	0.58
48:5:113:A:H2'	48:5:114:G:O4'	2.03	0.58
48:5:964:A:H2'	48:5:965:G:O4'	2.03	0.58
51:9:1129:G:C6	51:9:1130:G:O6	2.56	0.58
59:HH:93:VAL:HG21	59:HH:133:LEU:HD23	1.84	0.58
1:A:48:ILE:HD11	1:A:82:ILE:HG22	1.84	0.58
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.19	0.58
42:r:98:ARG:NH2	48:5:2262:G:OP2	2.37	0.58
48:5:922:C:O3'	48:5:922:C:O5'	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	1.85	0.58
51:9:614:C:H4'	51:9:615:C:H5''	1.86	0.58
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.84	0.58
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.85	0.58
33:h:35:LYS:HA	33:h:44:LEU:HD21	1.85	0.57
48:5:4266:G:N3	48:5:4266:G:H2'	2.19	0.57
2:B:337:VAL:HG21	2:B:345:LEU:HD21	1.85	0.57
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.37	0.57
42:r:26:SER:N	42:r:34:ALA:O	2.38	0.57
48:5:1381:U:H5''	48:5:1381:U:O2	2.03	0.57
86:ii:40:ARG:HB3	86:ii:66:THR:HG22	1.86	0.57
6:F:154:TYR:CE1	6:F:186:MET:HG2	2.39	0.57
67:PP:18:ARG:HE	70:SS:88:LYS:HD3	1.69	0.57
72:UU:48:LEU:HD11	72:UU:91:LEU:HD22	1.86	0.57
18:S:9:GLU:CG	18:S:33:PHE:CE1	2.88	0.57
48:5:922:C:C6	48:5:922:C:H3'	2.39	0.57
51:9:1310:U:OP1	64:MM:36:ARG:NH1	2.38	0.57
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.87	0.57
18:S:80:ILE:HG22	18:S:82:LEU:CD2	2.34	0.57
29:d:36:VAL:HG23	29:d:41:ARG:HG3	1.86	0.57
9:I:91:LEU:HD11	9:I:135:ILE:HG12	1.86	0.57
48:5:2439:G:C6	48:5:2440:U:C4	2.93	0.57
66:OO:75:MET:HE3	66:OO:79:GLN:HE22	1.70	0.57
5:E:185:ASN:ND2	5:E:274:LEU:O	2.38	0.57
48:5:2268:A:H4'	48:5:2269:C:H5'	1.87	0.57
51:9:628:A:N6	51:9:1332:A:C1'	2.67	0.56
42:r:46:ARG:HG2	42:r:70:GLN:HE22	1.70	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
26:a:82:VAL:HG21	26:a:101:ILE:HG12	1.87	0.56
29:d:22:THR:HG22	29:d:89:SER:CB	2.35	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
48:5:3723:A:H2'	48:5:3724:A:C8	2.40	0.56
51:9:1290:G:C5	83:ff:95:ARG:NH2	2.73	0.56
51:9:1304:U:C5'	83:ff:92:LYS:C	2.53	0.56
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.56
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.41	0.56
48:5:1961:G:O2'	48:5:2025:A:N6	2.38	0.56
51:9:1130:G:O2'	51:9:1131:G:P	2.63	0.56
83:ff:141:CYS:HG	89:ff:200:ZN:ZN	0.42	0.56
51:9:363:A:N1	51:9:397:G:O2'	2.36	0.56
51:9:1284:A:C5	64:MM:91:LEU:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:28:PHE:HA	69:RR:55:THR:HG21	1.87	0.56
74:WW:102:ILE:HG22	74:WW:102:ILE:O	2.05	0.56
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.87	0.56
31:f:47:CYS:HB3	31:f:103:VAL:HG12	1.88	0.56
48:5:4977:A:H2'	48:5:4978:G:O4'	2.05	0.56
2:B:89:ILE:CD1	2:B:153:MET:HE1	2.36	0.56
48:5:4515:G:C2	48:5:4516:G:C8	2.94	0.56
48:5:747:A:O2'	48:5:748:G:H3'	2.06	0.56
51:9:1351:G:O2'	51:9:1378:A:N1	2.31	0.56
2:B:57:VAL:HG22	2:B:73:VAL:HG12	1.88	0.55
18:S:53:LYS:NZ	49:7:74:A:O2'	2.39	0.55
51:9:615:C:O2'	51:9:616:A:C5'	2.54	0.55
51:9:1719:A:N6	51:9:1814:G:O2'	2.39	0.55
4:D:35:ARG:HB2	48:5:4325:A:C2	2.41	0.55
5:E:165:VAL:HG12	5:E:178:VAL:HG22	1.88	0.55
51:9:1292:C:C6	83:ff:140:TYR:CZ	2.95	0.55
66:OO:99:ALA:N	66:OO:133:THR:HG22	2.22	0.55
48:5:1411:C:O3'	48:5:1411(C):C:P	2.65	0.55
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.42	0.55
3:C:323:ARG:NH1	48:5:1281:G:C8	2.75	0.55
26:a:86:THR:HG22	48:5:510:U:H5''	1.87	0.55
48:5:922:C:P	48:5:922(B):C:C5'	2.95	0.55
48:5:1074:G:C2	48:5:1238:A:C2	2.95	0.55
52:AA:18:PHE:CD1	52:AA:173:LEU:HD11	2.42	0.55
78:aa:45:VAL:HG11	78:aa:53:ILE:CD1	2.37	0.55
21:V:62:MET:HE1	21:V:78:PRO:HG3	1.89	0.55
48:5:5066:U:H2'	48:5:5067:U:C6	2.42	0.55
53:BB:137:LEU:HB3	53:BB:172:MET:HE3	1.88	0.55
24:Y:77:LYS:O	24:Y:78:TYR:C	2.48	0.55
26:a:41:HIS:HE2	48:5:1681:G:HO2'	1.54	0.55
28:c:29:LEU:HD22	28:c:91:VAL:HG21	1.89	0.55
48:5:1872:G:O2'	48:5:4219:A:N3	2.36	0.55
48:5:2097:A:OP1	48:5:2107:A:N6	2.40	0.55
8:H:180:TYR:HB2	38:m:59:LEU:HD11	1.89	0.55
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.37	0.55
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.40	0.55
51:9:290:U:O2'	51:9:292:A:N7	2.37	0.55
51:9:1139:C:O4'	51:9:1139:C:O2	2.19	0.55
63:LL:4:ILE:HD12	63:LL:56:ILE:HD11	1.87	0.55
81:dd:21:CYS:SG	81:dd:23:VAL:N	2.70	0.55
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:TYR:O	49:7:11:A:N6	2.40	0.54
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.40	0.54
16:Q:70:MET:HE1	16:Q:137:VAL:CG2	2.34	0.54
39:n:2:ARG:O	39:n:5:TRP:N	2.40	0.54
48:5:1325:C:O2	48:5:1325:C:O5'	2.25	0.54
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.42	0.54
48:5:1411:C:C3'	48:5:1411(C):C:P	2.95	0.54
51:9:1680:G:O4'	80:cc:20:ARG:CZ	2.55	0.54
7:G:219:LEU:HD23	13:N:7:ILE:HD11	1.88	0.54
25:Z:41:ALA:HB2	25:Z:77:TYR:CE1	2.43	0.54
40:o:15:CYS:SG	40:o:19:GLN:NE2	2.79	0.54
51:9:1238:U:H2'	51:9:1239:U:O4'	2.08	0.54
2:B:89:ILE:HD13	2:B:153:MET:HE1	1.88	0.54
10:J:15:LEU:HD21	10:J:134:LEU:HD13	1.90	0.54
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.73	0.54
26:a:12:ARG:NH2	48:5:1338:G:OP2	2.41	0.54
48:5:923:C:C5	48:5:926:G:O4'	2.61	0.54
51:9:1622:U:H3	67:PP:122:THR:HG1	1.55	0.54
67:PP:18:ARG:NE	70:SS:88:LYS:HG2	2.22	0.54
87:jj:275:THR:N	90:jj:700:GCP:O1A	2.38	0.54
2:B:252:ALA:HB3	48:5:4457:U:O2	2.08	0.54
51:9:945:U:H2'	51:9:946:U:C6	2.42	0.54
87:jj:330:MET:HE3	87:jj:549:HIS:CD2	2.43	0.54
87:jj:392:LEU:CD2	87:jj:666:MET:HE2	2.37	0.54
14:O:12:ARG:O	18:S:171:ARG:NH2	2.40	0.54
51:9:584:A:C6	51:9:585:C:C4	2.95	0.54
18:S:93:MET:HE1	18:S:117:HIS:NE2	2.22	0.54
48:5:106:A:H2'	48:5:107:G:O4'	2.08	0.54
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.38	0.54
12:M:54:CYS:SG	12:M:55:MET:N	2.80	0.54
51:9:1667:U:H2'	51:9:1668:U:C6	2.43	0.54
65:NN:52:VAL:O	65:NN:53:ILE:C	2.50	0.54
48:5:1411:C:H3'	48:5:1411(C):C:P	2.48	0.54
48:5:2505:C:O2	48:5:2505:C:O4'	2.23	0.54
51:9:666:U:C2	51:9:667:U:C5	2.96	0.54
51:9:1292:C:C5	83:ff:140:TYR:OH	2.61	0.54
53:BB:136:ARG:HB2	53:BB:218:LEU:HD11	1.90	0.54
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.72	0.54
29:d:36:VAL:HG23	29:d:41:ARG:CG	2.37	0.54
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.41	0.53
80:cc:14:VAL:HG13	80:cc:30:VAL:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4260:U:H2'	48:5:4261:C:C6	2.43	0.53
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.89	0.53
55:DD:126:ILE:HD11	55:DD:134:CYS:SG	2.49	0.53
62:KK:35:LEU:HD12	62:KK:40:VAL:HG21	1.90	0.53
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.90	0.53
73:VV:20:SER:HB3	73:VV:59:ILE:HD11	1.90	0.53
75:XX:94:ILE:HD11	75:XX:122:VAL:HG11	1.90	0.53
8:H:128:MET:HE1	8:H:161:ILE:CG2	2.39	0.53
48:5:922(B):C:N3	48:5:923:C:C5	2.77	0.53
51:9:958:G:C6	51:9:959:G:C6	2.96	0.53
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.43	0.53
67:PP:18:ARG:NE	70:SS:88:LYS:CD	2.72	0.53
4:D:22:ARG:HG3	4:D:22:ARG:HH11	1.73	0.53
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.07	0.53
3:C:292:ILE:HG22	3:C:298:ILE:HD12	1.91	0.53
52:AA:63:ARG:HG2	52:AA:185:MET:HE1	1.90	0.53
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	1.89	0.53
51:9:929:G:H2'	51:9:930:C:O4'	2.08	0.53
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.90	0.53
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.38	0.53
51:9:943:U:H2'	51:9:944:A:O4'	2.09	0.53
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.89	0.53
8:H:12:ILE:HG22	8:H:81:ILE:HD11	1.91	0.53
18:S:9:GLU:HG2	18:S:33:PHE:CE1	2.44	0.53
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.44	0.53
36:k:35:LYS:NZ	48:5:2693:G:OP1	2.31	0.53
48:5:1483:C:O2	48:5:1483:C:O4'	2.25	0.53
48:5:4871:C:O4'	48:5:4871:C:O2	2.25	0.53
22:W:3:VAL:HG21	22:W:12:LYS:HE2	1.91	0.53
50:8:47:C:H1'	50:8:61:A:H2'	1.90	0.53
51:9:613:G:H2'	51:9:627:U:C6	2.44	0.53
53:BB:38:MET:HE3	53:BB:185:VAL:HG11	1.91	0.53
56:EE:136:ILE:HG23	56:EE:149:TYR:CE1	2.43	0.53
64:MM:36:ARG:CD	83:ff:102:VAL:HG22	2.37	0.53
74:WW:92:ASN:C	74:WW:92:ASN:HD22	2.17	0.53
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.44	0.52
8:H:1:MET:HG3	18:S:141:ALA:HB2	1.91	0.52
13:N:76:PRO:O	13:N:79:ALA:HB3	2.09	0.52
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.91	0.52
81:dd:21:CYS:SG	81:dd:24:CYS:N	2.78	0.52
11:L:108:GLU:N	11:L:108:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:127:MET:HE1	19:T:155:PRO:HA	1.91	0.52
51:9:1117:C:O2'	51:9:1118:C:O4'	2.26	0.52
53:BB:36:PRO:HG2	53:BB:38:MET:HE2	1.92	0.52
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.91	0.52
48:5:1888:A:N6	48:5:3873:G:O2'	2.43	0.52
51:9:830:A:OP2	51:9:846:G:N2	2.42	0.52
51:9:1550:G:O2'	51:9:1558:C:O2	2.26	0.52
58:GG:157:VAL:HB	58:GG:176:ILE:HD11	1.91	0.52
2:B:49:TYR:CE2	2:B:168:MET:HE1	2.45	0.52
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.91	0.52
20:U:33:ILE:HD12	20:U:96:LEU:HD22	1.91	0.52
40:o:41:TYR:CE1	47:3:75:C:O2	2.62	0.52
48:5:4305:G:C2'	48:5:4305:G:N3	2.73	0.52
6:F:121:PHE:HB2	6:F:204:ASN:OD1	2.10	0.52
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.90	0.52
18:S:82:LEU:HD12	18:S:124:ILE:HG23	1.90	0.52
21:V:60:MET:HE1	21:V:78:PRO:HB2	1.92	0.52
26:a:2:PRO:HG2	26:a:5:LEU:HD12	1.91	0.52
48:5:1411:C:H5'	48:5:1411(B):C:C2'	2.40	0.52
51:9:1292:C:C2	83:ff:140:TYR:CD1	2.98	0.52
51:9:1624:U:O4'	51:9:1624:U:O2	2.27	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.40	0.52
29:d:57:MET:O	29:d:59:THR:N	2.42	0.52
42:r:32:LEU:N	42:r:32:LEU:HD23	2.25	0.52
48:5:3810:C:O4'	48:5:3810:C:O2	2.28	0.52
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.92	0.52
66:OO:99:ALA:H	66:OO:133:THR:HG22	1.75	0.52
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.90	0.52
2:B:254:ILE:HG21	2:B:262:VAL:HB	1.92	0.52
51:9:1143:A:H2'	51:9:1144:A:C8	2.45	0.52
51:9:1373:C:O2'	69:RR:10:LYS:NZ	2.42	0.52
51:9:1438:A:H2'	51:9:1439:A:C8	2.45	0.52
1:A:104:VAL:HG12	1:A:146:THR:HG21	1.91	0.52
14:O:49:ARG:NH2	48:5:1932:A:OP2	2.43	0.52
26:a:2:PRO:CG	26:a:5:LEU:HD12	2.40	0.52
31:f:50:VAL:HG22	31:f:69:VAL:HG12	1.90	0.52
79:bb:33:MET:HE2	79:bb:46:VAL:CG1	2.40	0.52
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.40	0.51
26:a:12:ARG:HD3	48:5:1660:U:H2'	1.91	0.51
29:d:59:THR:OG1	29:d:104:THR:OG1	2.22	0.51
48:5:4989:U:O2	48:5:4989:U:O4'	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.91	0.51
61:JJ:45:ARG:O	61:JJ:49:THR:HG23	2.10	0.51
18:S:3:ALA:O	18:S:111:ARG:NH1	2.43	0.51
48:5:4579:U:O2	48:5:4580:U:C2	2.64	0.51
51:9:1310:U:P	83:ff:105:TYR:OH	2.68	0.51
78:aa:44:ILE:HD12	78:aa:45:VAL:HG13	1.92	0.51
79:bb:33:MET:HE2	79:bb:46:VAL:HG12	1.91	0.51
1:A:48:ILE:HG22	41:p:54:ILE:HD12	1.92	0.51
51:9:501:C:O2	51:9:501:C:C2'	2.59	0.51
51:9:1315:U:O2	51:9:1315:U:O4'	2.28	0.51
1:A:116:LEU:HD13	1:A:164:ALA:HB2	1.93	0.51
29:d:33:ILE:O	29:d:36:VAL:HG22	2.11	0.51
31:f:72:GLY:HA2	31:f:88:PHE:HA	1.91	0.51
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.45	0.51
53:BB:110:MET:HE1	53:BB:140:VAL:HG21	1.92	0.51
2:B:261:ARG:HB2	14:O:64:THR:HG21	1.91	0.51
3:C:76:ILE:HG22	3:C:77:PRO:CD	2.40	0.51
25:Z:53:VAL:CG2	25:Z:62:ILE:HG12	2.41	0.51
86:ii:45:ARG:CD	86:ii:94:VAL:CG2	2.85	0.51
87:jj:619:VAL:HG23	87:jj:632:PRO:HG3	1.93	0.51
24:Y:103:LYS:HE3	48:5:231:U:O2'	2.09	0.51
51:9:1130:G:N3	51:9:1130:G:C2'	2.72	0.51
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.41	0.51
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.92	0.51
3:C:302:LEU:HD22	16:Q:38:ARG:HB3	1.93	0.51
48:5:1528:U:H2'	48:5:1529:G:O4'	2.11	0.51
48:5:4633:G:O2'	48:5:4635:A:OP2	2.17	0.51
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.46	0.51
13:N:28:TRP:O	13:N:32:GLN:NE2	2.42	0.51
19:T:17:ARG:CD	19:T:47:THR:HG23	2.41	0.51
30:e:81:ASN:HA	30:e:111:ILE:HD11	1.93	0.51
48:5:4723:A:C2	48:5:4724:A:C6	2.99	0.51
81:dd:39:CYS:O	81:dd:42:CYS:N	2.43	0.51
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.45	0.51
19:T:62:GLY:HA3	19:T:76:VAL:HG12	1.93	0.51
51:9:1304:U:C5'	83:ff:93:HIS:CB	2.83	0.51
48:5:100:C:O2	48:5:100:C:O4'	2.27	0.50
48:5:2627:C:O4'	48:5:2627:C:O2	2.28	0.50
51:9:501:C:O2	51:9:501:C:H2'	2.10	0.50
51:9:1309:C:C4'	83:ff:105:TYR:OH	2.59	0.50
52:AA:185:MET:HE3	73:VV:39:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:THR:HG22	3:C:220:ALA:O	2.12	0.50
76:YY:20:ARG:CZ	76:YY:74:MET:HE2	2.41	0.50
78:aa:36:ILE:N	78:aa:36:ILE:HD12	2.27	0.50
84:gg:21:ILE:HG22	84:gg:31:ILE:HD11	1.92	0.50
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.44	0.50
20:U:82:TYR:CZ	20:U:86:LEU:HD11	2.46	0.50
26:a:17:HIS:CE1	48:5:1338:G:H2'	2.47	0.50
50:8:137:A:H2'	50:8:138:C:C6	2.46	0.50
51:9:96:C:O2	51:9:473:A:O2'	2.29	0.50
51:9:314:U:O2	51:9:314:U:H2'	2.11	0.50
51:9:1834:A:H2	51:9:1837:G:N1	2.10	0.50
59:HH:176:VAL:HG12	59:HH:180:LEU:HD12	1.93	0.50
2:B:223:THR:HA	2:B:338:VAL:HG22	1.92	0.50
29:d:64:ILE:HG13	29:d:68:LEU:HD23	1.93	0.50
40:o:26:TYR:HB3	40:o:67:VAL:HB	1.93	0.50
51:9:615:C:HO2'	51:9:616:A:C4'	2.20	0.50
51:9:928:G:H2'	51:9:929:G:C8	2.46	0.50
51:9:1292:C:C6	83:ff:140:TYR:OH	2.64	0.50
51:9:1304:U:OP2	83:ff:93:HIS:HB2	2.12	0.50
87:jj:594:ILE:HD11	87:jj:674:ILE:CG2	2.41	0.50
2:B:54:THR:OG1	2:B:55:HIS:N	2.45	0.50
6:F:242:LEU:HD23	6:F:246:MET:HG3	1.93	0.50
48:5:2094:C:O2	48:5:2094:C:O4'	2.29	0.50
48:5:4291:G:H5''	48:5:4291:G:N3	2.26	0.50
51:9:1304:U:OP1	83:ff:92:LYS:HD3	2.10	0.50
30:e:31:ILE:HD11	48:5:2347:A:C4	2.46	0.50
67:PP:83:MET:HB3	67:PP:116:LEU:HD12	1.93	0.50
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.44	0.50
48:5:922:C:P	48:5:922(B):C:P	3.10	0.50
50:8:94:G:H5'	50:8:94:G:C8	2.47	0.50
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.45	0.50
1:A:179:ILE:O	48:5:3653:A:H4'	2.11	0.50
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.46	0.50
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.93	0.50
48:5:4966:A:C2	48:5:4967:A:C2	3.00	0.50
51:9:1679:A:H5''	80:cc:20:ARG:NH2	2.27	0.50
53:BB:136:ARG:HD2	53:BB:138:PHE:CZ	2.47	0.50
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.94	0.50
6:F:119:GLY:O	6:F:120:THR:HG23	2.11	0.49
9:I:191:ILE:CD1	9:I:212:LEU:HD11	2.42	0.49
48:5:1411:C:HO2'	48:5:1411(C):C:H6	1.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1305:C:OP2	83:ff:93:HIS:HA	2.11	0.49
51:9:1309:C:C4'	83:ff:105:TYR:HH	2.25	0.49
48:5:1665:C:H2'	48:5:1666:C:C6	2.47	0.49
48:5:4723:A:C2	48:5:4724:A:C5	3.00	0.49
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.42	0.49
62:KK:64:TRP:CE3	81:dd:23:VAL:HG22	2.47	0.49
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.92	0.49
79:bb:33:MET:HE3	79:bb:73:LEU:HD21	1.94	0.49
8:H:5:LEU:HD22	8:H:60:TRP:CH2	2.47	0.49
48:5:1524:A:H61	48:5:1652:U:H3	1.58	0.49
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.42	0.49
57:FF:119:SER:OG	57:FF:189:ALA:HB1	2.11	0.49
59:HH:116:ARG:NH2	59:HH:121:THR:OG1	2.46	0.49
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.94	0.49
6:F:111:LEU:O	6:F:120:THR:HG21	2.12	0.49
86:ii:175:CYS:HB2	87:jj:316:THR:HG22	1.94	0.49
8:H:69:THR:HA	8:H:72:THR:HG22	1.95	0.49
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.44	0.49
48:5:1237:C:O4'	48:5:1237:C:O2	2.30	0.49
48:5:1786:A:H2'	48:5:1789:C:C5	2.47	0.49
51:9:853:C:O4'	51:9:853:C:O2	2.26	0.49
51:9:1012:A:H2'	51:9:1013:U:O4'	2.12	0.49
51:9:1680:G:H4'	80:cc:20:ARG:NH2	2.28	0.49
53:BB:92:GLN:NE2	53:BB:229:MET:HE1	2.27	0.49
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.43	0.49
7:G:215:ASP:HB3	7:G:216:PRO:HD3	1.93	0.49
33:h:21:LEU:HD21	33:h:58:LEU:HD21	1.94	0.49
31:f:43:LEU:HD22	31:f:76:ARG:HA	1.93	0.49
48:5:224:U:O2	48:5:224:U:O4'	2.27	0.49
51:9:291:G:N3	63:LL:42:LEU:HD13	2.28	0.49
59:HH:145:ARG:HA	74:WW:51:GLU:HB2	1.93	0.49
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.95	0.49
14:O:55:LEU:HD23	14:O:58:LEU:HD12	1.95	0.49
51:9:1489:A:H4'	51:9:1490:G:OP2	2.12	0.49
47:3:75:C:H2'	47:3:76:A:H4'	1.94	0.49
48:5:5047:C:O2'	48:5:5050:C:OP2	2.31	0.49
51:9:434:G:H2'	51:9:435:A:C8	2.47	0.49
7:G:219:LEU:HA	13:N:7:ILE:HD11	1.94	0.48
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.48
70:SS:33:ILE:HD13	70:SS:71:MET:HE1	1.95	0.48
1:A:152:SER:OG	48:5:3661:G:N7	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:57:PRO:HG3	11:L:75:GLY:O	2.13	0.48
48:5:1411:C:H1'	48:5:1411(C):C:C5	2.48	0.48
48:5:2439:G:C5	48:5:2440:U:C5	3.01	0.48
51:9:1614:A:P	67:PP:42:ARG:HH11	2.36	0.48
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	1.95	0.48
78:aa:11:ALA:HB3	78:aa:33:ASP:HB2	1.95	0.48
3:C:224:ILE:CG2	3:C:227:ILE:HD13	2.43	0.48
3:C:224:ILE:HG22	3:C:227:ILE:HD13	1.95	0.48
8:H:3:THR:HB	8:H:67:LEU:HD11	1.95	0.48
48:5:99:A:H2'	48:5:100:C:O2	2.12	0.48
51:9:1304:U:H5'	83:ff:92:LYS:CA	2.38	0.48
58:GG:52:ILE:HG23	58:GG:52:ILE:O	2.13	0.48
2:B:86:VAL:HG13	2:B:162:VAL:HG22	1.95	0.48
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.43	0.48
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.96	0.48
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.95	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.32	0.48
51:9:958:G:N1	51:9:959:G:C6	2.81	0.48
61:JJ:94:LEU:HB2	61:JJ:97:ILE:HD12	1.95	0.48
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.48	0.48
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.96	0.48
18:S:82:LEU:HG	18:S:113:MET:HE2	1.95	0.48
48:5:1667:A:N1	48:5:2281:U:OP2	2.47	0.48
51:9:1144:A:H2'	51:9:1145:A:C8	2.49	0.48
52:AA:62:ALA:O	52:AA:66:VAL:HG23	2.13	0.48
52:AA:68:ILE:HG21	52:AA:74:VAL:HG23	1.96	0.48
74:WW:26:LEU:HD11	74:WW:60:LYS:HB3	1.94	0.48
17:R:10:LEU:O	17:R:14:VAL:HG23	2.14	0.48
28:c:82:GLY:CA	28:c:91:VAL:HG12	2.43	0.48
48:5:1523:A:C8	48:5:1652:U:O4	2.66	0.48
50:8:125:C:O2	50:8:125:C:O4'	2.32	0.48
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.44	0.48
1:A:40:TYR:CE2	48:5:4117:U:C4	3.02	0.48
13:N:119:TYR:CZ	13:N:131:GLU:HB2	2.48	0.48
51:9:1834:A:C2'	51:9:1834:A:N3	2.77	0.48
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.14	0.48
48:5:1411:C:C5'	48:5:1411(C):C:O5'	2.62	0.48
70:SS:121:ARG:HG3	70:SS:131:VAL:CG2	2.43	0.48
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.48
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.94	0.48
40:o:66:ILE:HD13	40:o:91:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1411:C:C5'	48:5:1411(B):C:C2'	2.91	0.48
51:9:664:A:N1	51:9:1163:C:O2	2.47	0.48
51:9:925:G:N2	65:NN:48:SER:OG	2.46	0.48
51:9:1124:C:H5''	53:BB:150:ILE:HD12	1.96	0.48
17:R:23:TRP:CZ3	17:R:51:ILE:HD12	2.49	0.47
84:gg:81:GLY:HA2	84:gg:87:LEU:HD23	1.95	0.47
32:g:91:ILE:O	32:g:92:LYS:C	2.57	0.47
44:t:98:ILE:HG23	44:t:98:ILE:O	2.14	0.47
48:5:1746:A:C2	48:5:1785:C:C2	3.02	0.47
48:5:4724:A:C6	48:5:4725:C:C4	3.02	0.47
56:EE:55:ALA:HB2	56:EE:64:ILE:HD12	1.95	0.47
60:II:3:ILE:HG23	60:II:3:ILE:O	2.14	0.47
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.43	0.47
2:B:317:LEU:HD21	2:B:381:THR:HA	1.96	0.47
9:I:72:ALA:CB	9:I:136:MET:HE1	2.44	0.47
51:9:15:U:H2'	51:9:16:G:O4'	2.14	0.47
51:9:1674:G:H4'	57:FF:77:MET:HE1	1.96	0.47
53:BB:36:PRO:CG	53:BB:38:MET:HE2	2.44	0.47
53:BB:141:GLY:C	53:BB:142:PHE:CD1	2.92	0.47
56:EE:122:LYS:HG2	56:EE:162:ILE:HD11	1.95	0.47
3:C:313:VAL:CG1	6:F:169:THR:HG21	2.43	0.47
4:D:39:GLN:HG2	4:D:48:LYS:HB2	1.96	0.47
14:O:37:ARG:NH2	48:5:4761:G:OP2	2.47	0.47
44:t:81:ILE:HD11	44:t:132:ILE:HG23	1.96	0.47
51:9:604:A:C6	51:9:605:A:N1	2.83	0.47
51:9:980:A:C2	51:9:981:A:C6	3.02	0.47
51:9:1700:C:C2	51:9:1834:A:N6	2.82	0.47
87:jj:393:VAL:HG12	87:jj:398:VAL:HB	1.95	0.47
15:P:137:ASN:HB3	15:P:138:PRO:HD2	1.96	0.47
28:c:74:TYR:CD2	28:c:81:LEU:HG	2.50	0.47
31:f:28:LEU:HD22	31:f:86:ALA:HB2	1.97	0.47
48:5:961:G:C6	48:5:962:C:C4	3.02	0.47
48:5:1854:G:N2	48:5:4394:A:O4'	2.48	0.47
48:5:2307:A:C8	48:5:2332:A:C6	3.03	0.47
48:5:4390:A:H2'	48:5:4391:G:O4'	2.14	0.47
51:9:830:A:C2	51:9:831:G:C8	3.02	0.47
66:OO:99:ALA:O	66:OO:100:THR:C	2.57	0.47
86:ii:40:ARG:CB	86:ii:66:THR:HG22	2.44	0.47
1:A:209:HIS:CE1	1:A:235:VAL:HG11	2.50	0.47
8:H:172:ILE:HB	38:m:64:ASN:HD22	1.79	0.47
14:O:109:PRO:HB2	14:O:110:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3928:A:H2'	48:5:3929:G:O4'	2.15	0.47
80:cc:21:THR:HG22	80:cc:68:LEU:CD1	2.42	0.47
2:B:119:TYR:OH	2:B:129:ALA:N	2.48	0.47
5:E:131:HIS:HB2	48:5:1281:G:C6	2.50	0.47
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.97	0.47
7:G:210:ILE:HG23	7:G:220:VAL:HG11	1.96	0.47
10:J:119:TYR:CD2	70:SS:12:ILE:HD12	2.50	0.47
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.50	0.47
16:Q:4:ASP:OD1	16:Q:4:ASP:N	2.47	0.47
30:e:44:ARG:NH2	48:5:1312:A:O2'	2.48	0.47
42:r:106:LEU:O	42:r:107:ARG:C	2.57	0.47
48:5:2363:A:C2	48:5:3860:A:C4	3.03	0.47
48:5:3648:A:C4	48:5:3785:A:C6	3.02	0.47
48:5:4289:U:H2'	48:5:4290:U:C6	2.49	0.47
48:5:4966:A:H2'	48:5:4967:A:C8	2.49	0.47
51:9:183:G:N3	51:9:183:G:C2'	2.76	0.47
51:9:824:C:H2'	51:9:825:A:O4'	2.14	0.47
51:9:1364:U:O4'	51:9:1364:U:O2	2.30	0.47
52:AA:131:HIS:O	52:AA:135:THR:HG23	2.15	0.47
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.44	0.47
62:KK:93:THR:HG23	62:KK:94:LEU:HD12	1.97	0.47
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HG13	1.96	0.47
87:jj:396:LEU:C	87:jj:396:LEU:HD23	2.40	0.47
87:jj:492:VAL:HG23	87:jj:505:ILE:HG23	1.97	0.47
1:A:207:VAL:HG23	1:A:208:GLU:HG3	1.97	0.47
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.97	0.47
10:J:26:VAL:HG21	10:J:33:LEU:HA	1.97	0.47
42:r:16:PHE:CE2	42:r:43:LEU:HD11	2.48	0.47
48:5:740:G:O6	48:5:922:C:N3	2.48	0.47
48:5:4658:G:C5	48:5:4659:G:N7	2.83	0.47
51:9:163:U:OP2	58:GG:87:ARG:NH2	2.48	0.47
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.78	0.47
75:XX:67:ARG:NH2	75:XX:114:ASP:OD2	2.48	0.47
6:F:92:ILE:HA	6:F:118:ASN:O	2.15	0.47
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.50	0.47
29:d:57:MET:O	29:d:59:THR:OG1	2.28	0.47
48:5:1320:U:O2'	48:5:1891:A:N1	2.37	0.47
51:9:1404:U:C6	72:UU:56:MET:HE2	2.50	0.47
66:OO:151:LEU:HD23	85:hh:42:C:H2'	1.97	0.47
24:Y:42:TYR:CG	24:Y:119:LEU:HD23	2.50	0.47
48:5:1665:C:H2'	48:5:1666:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:WW:55:ASP:O	74:WW:57:ARG:N	2.48	0.47
74:WW:104:LEU:O	74:WW:104:LEU:HD12	2.15	0.47
3:C:95:MET:SD	3:C:95:MET:N	2.85	0.46
9:I:16:PRO:HA	9:I:95:HIS:CD2	2.49	0.46
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.97	0.46
26:a:61:TYR:N	48:5:4354:U:O4	2.46	0.46
51:9:942:G:H2'	51:9:943:U:C6	2.50	0.46
51:9:1011:A:H2'	51:9:1012:A:O4'	2.15	0.46
61:JJ:66:LYS:HA	61:JJ:71:LEU:HD11	1.96	0.46
66:OO:95:ILE:HD13	66:OO:116:LEU:HG	1.96	0.46
7:G:108:VAL:HA	23:X:44:PRO:O	2.15	0.46
17:R:6:LEU:O	17:R:6:LEU:HD22	2.15	0.46
35:j:63:ARG:NH2	50:8:58:G:N7	2.63	0.46
42:r:32:LEU:HD21	42:r:106:LEU:HD12	1.95	0.46
42:r:37:SER:OG	48:5:2267:U:OP1	2.26	0.46
48:5:1411:C:C4'	48:5:1411(C):C:O5'	2.64	0.46
53:BB:139:CYS:SG	53:BB:168:MET:HE2	2.56	0.46
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.96	0.46
61:JJ:37:LEU:HD21	61:JJ:106:LEU:HD21	1.96	0.46
84:gg:91:ASP:HB2	84:gg:98:THR:HG23	1.97	0.46
22:W:45:ASN:HB3	22:W:48:GLN:HE21	1.80	0.46
48:5:922:C:O5'	48:5:922(A):G:C3'	2.59	0.46
48:5:1328:G:O2'	48:5:2349:A:OP1	2.32	0.46
48:5:3747:A:C2	48:5:3817:A:C5	3.03	0.46
51:9:183:G:O2'	51:9:184:G:O4'	2.33	0.46
51:9:584:A:N6	51:9:585:C:N4	2.62	0.46
51:9:1162:C:H2'	51:9:1163:C:O4'	2.15	0.46
87:jj:489:ARG:NH2	87:jj:573:VAL:O	2.48	0.46
8:H:180:TYR:HB2	38:m:59:LEU:CD1	2.45	0.46
11:L:100:PRO:O	34:i:25:ARG:NH2	2.49	0.46
29:d:57:MET:HE1	29:d:88:LEU:O	2.16	0.46
32:g:15:THR:HG22	32:g:16:ALA:H	1.81	0.46
48:5:4944:C:O2	48:5:4944:C:O4'	2.30	0.46
51:9:1220:A:N6	51:9:1221:G:C6	2.83	0.46
67:PP:18:ARG:C	70:SS:92:ASP:O	2.59	0.46
68:QQ:10:VAL:HG12	68:QQ:12:VAL:HG23	1.96	0.46
87:jj:343:MET:HE2	87:jj:361:GLN:HE22	1.81	0.46
42:r:49:VAL:HG11	42:r:97:ILE:HD11	1.96	0.46
51:9:12:U:H2'	51:9:13:C:C6	2.51	0.46
51:9:1834:A:C2	51:9:1837:G:N1	2.83	0.46
67:PP:16:THR:OG1	70:SS:91:LYS:O	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:128:MET:HE1	8:H:161:ILE:HG21	1.97	0.46
9:I:98:ARG:NH1	48:5:1864:G:OP1	2.49	0.46
48:5:3689:G:C5	48:5:3690:U:C5	3.03	0.46
51:9:1148:A:H4'	51:9:1149:A:O4'	2.15	0.46
51:9:1304:U:C4'	83:ff:91:ASN:O	2.57	0.46
51:9:1517:G:C6	51:9:1518:C:C5	3.03	0.46
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.98	0.46
67:PP:18:ARG:HD3	70:SS:88:LYS:HG2	1.93	0.46
74:WW:42:MET:HE2	74:WW:49:GLU:HA	1.97	0.46
87:jj:266:ILE:HD13	87:jj:393:VAL:HG21	1.98	0.46
87:jj:587:ILE:HD11	87:jj:635:LEU:HD13	1.98	0.46
12:M:50:MET:HE3	12:M:54:CYS:SG	2.55	0.46
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.48	0.46
30:e:103:VAL:O	30:e:108:ARG:NH2	2.49	0.46
48:5:2763:U:O2	48:5:2763:U:O4'	2.33	0.46
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.40	0.46
70:SS:121:ARG:HG3	70:SS:131:VAL:HG21	1.98	0.46
73:VV:24:ILE:HG23	73:VV:31:SER:OG	2.16	0.46
2:B:285:TYR:CD1	2:B:363:ILE:HG12	2.51	0.46
51:9:1857:G:C8	66:OO:146:ARG:NH2	2.84	0.46
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.46	0.46
8:H:41:ILE:HG12	8:H:73:ILE:HD11	1.97	0.46
42:r:41:ASN:HB3	42:r:44:ILE:HD12	1.96	0.46
48:5:976:G:N2	48:5:977:C:C2	2.84	0.46
48:5:1411:C:C4'	48:5:1411(B):C:H2'	2.46	0.46
48:5:1545:G:H2'	48:5:1546:C:C6	2.51	0.46
48:5:1804:A:N6	48:5:1833:G:O4'	2.49	0.46
48:5:2409:U:C4	48:5:2783:A:N1	2.84	0.46
51:9:1680:G:C4'	80:cc:20:ARG:CZ	2.93	0.46
72:UU:63:ILE:HG21	81:dd:43:PHE:CE2	2.51	0.46
87:jj:503:PHE:HE1	87:jj:505:ILE:HD12	1.80	0.46
14:O:121:PRO:HD2	18:S:166:ARG:O	2.16	0.46
48:5:36:U:OP1	48:5:1652:U:O2	2.34	0.46
51:9:614:C:C4'	51:9:615:C:H5''	2.45	0.46
52:AA:167:GLY:O	52:AA:171:VAL:HG23	2.16	0.46
55:DD:161:GLY:O	55:DD:164:VAL:HG12	2.16	0.46
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.97	0.46
12:M:122:ILE:HG22	14:O:185:VAL:HG11	1.98	0.45
15:P:102:ALA:CB	15:P:112:LEU:HD11	2.46	0.45
32:g:97:ILE:HD13	48:5:4120:U:C4	2.51	0.45
51:9:297:A:H4'	56:EE:132:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:30:LEU:HD13	52:AA:38:ILE:CD1	2.46	0.45
60:II:113:TYR:OH	60:II:156:ALA:O	2.33	0.45
26:a:100:ILE:HG12	26:a:123:ILE:HB	1.97	0.45
48:5:922:C:C6	48:5:922:C:C3'	2.98	0.45
51:9:304:C:H3'	51:9:305:U:P	2.56	0.45
51:9:1057:C:O4'	51:9:1057:C:O2	2.33	0.45
66:OO:72:TYR:CE2	66:OO:76:LEU:HD11	2.52	0.45
67:PP:18:ARG:CD	70:SS:88:LYS:CG	2.88	0.45
86:ii:197:ILE:HG23	86:ii:202:VAL:HG21	1.97	0.45
2:B:206:PRO:HD2	2:B:209:GLN:HG3	1.98	0.45
3:C:252:TRP:CH2	3:C:260:LEU:HD11	2.51	0.45
48:5:2292:C:H2'	48:5:2293:U:C6	2.52	0.45
58:GG:63:MET:SD	58:GG:63:MET:N	2.89	0.45
3:C:127:ALA:HA	3:C:246:VAL:HG12	1.99	0.45
13:N:60:VAL:HG21	50:8:141:C:H5''	1.99	0.45
14:O:121:PRO:HA	14:O:124:LEU:HB2	1.97	0.45
26:a:103:VAL:HG12	26:a:108:TYR:HB2	1.97	0.45
35:j:72:ARG:NH2	50:8:94:G:OP2	2.49	0.45
48:5:404:U:C4	48:5:405:U:C4	3.05	0.45
48:5:1600:A:C6	48:5:1638:A:C5	3.05	0.45
51:9:684:G:C8	51:9:920:A:N6	2.84	0.45
53:BB:103:MET:HE1	53:BB:212:VAL:HG23	1.97	0.45
74:WW:11:LEU:HD22	74:WW:72:CYS:SG	2.57	0.45
1:A:208:GLU:HG2	48:5:1629:G:H1	1.81	0.45
3:C:209:VAL:HB	3:C:229:LEU:CD1	2.46	0.45
7:G:219:LEU:HD23	13:N:7:ILE:CD1	2.46	0.45
48:5:1651:G:C2	48:5:1652:U:N3	2.85	0.45
48:5:2468:U:C2	48:5:2506:G:N7	2.84	0.45
48:5:4872:G:H4'	48:5:4873:G:H5''	1.98	0.45
48:5:4978:G:O2'	48:5:4980:C:OP2	2.30	0.45
51:9:62:G:C6	51:9:63:U:C5	3.04	0.45
51:9:1276:A:N6	51:9:1321:G:O2'	2.49	0.45
51:9:1304:U:H5''	83:ff:93:HIS:HA	1.93	0.45
1:A:33:ASP:O	1:A:34:PHE:C	2.60	0.45
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.51	0.45
48:5:2268:A:C4'	48:5:2269:C:H5'	2.46	0.45
51:9:1240:A:C8	51:9:1267:C:O2'	2.66	0.45
53:BB:79:VAL:HG21	53:BB:81:PHE:CZ	2.52	0.45
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.52	0.45
13:N:184:ILE:O	13:N:194:ARG:NH1	2.49	0.45
19:T:108:ARG:HH12	48:5:1836:G:HO2'	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1523:A:N7	48:5:1652:U:C4	2.85	0.45
51:9:427:U:O2	51:9:427:U:O4'	2.34	0.45
51:9:1535:U:H2'	51:9:1535:U:O2	2.16	0.45
57:FF:20:PHE:CD1	57:FF:20:PHE:C	2.93	0.45
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.99	0.45
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.99	0.45
69:RR:38:ILE:HD12	69:RR:39:ALA:HB2	1.99	0.45
21:V:82:ILE:HG12	21:V:121:VAL:HG13	1.98	0.45
34:i:90:LEU:HA	34:i:93:VAL:HG22	1.98	0.45
35:j:17:THR:HG21	35:j:29:LEU:HD21	1.99	0.45
48:5:2758:G:O2'	48:5:2765:A:N3	2.35	0.45
51:9:1551:U:O2	51:9:1551:U:O4'	2.33	0.45
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.98	0.45
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	1.98	0.45
86:ii:313:ILE:N	86:ii:313:ILE:HD13	2.32	0.45
4:D:56:THR:HG22	49:7:27:G:P	2.57	0.45
20:U:84:LYS:HG3	20:U:102:VAL:HG11	1.99	0.45
28:c:91:VAL:O	28:c:91:VAL:HG13	2.16	0.45
31:f:20:ASN:ND2	48:5:1885:G:OP1	2.50	0.45
48:5:100:C:H2'	48:5:101:A:O4'	2.16	0.45
48:5:423:G:H2'	48:5:424:U:O4'	2.16	0.45
48:5:1733:G:C4	48:5:4214:A:C2	3.05	0.45
51:9:183:G:O2'	51:9:183:G:N3	2.49	0.45
51:9:1865:C:O2	78:aa:92:ARG:HB3	2.17	0.45
52:AA:10:MET:HE2	52:AA:15:VAL:HG22	1.99	0.45
63:LL:111:VAL:HG22	63:LL:140:PHE:HB2	1.99	0.45
80:cc:40:ARG:NH1	80:cc:61:SER:OG	2.50	0.45
6:F:197:GLY:O	6:F:198:LYS:C	2.60	0.45
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.99	0.45
32:g:64:LEU:HB3	48:5:2749:C:H4'	1.99	0.45
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	2.17	0.45
51:9:626:G:OP2	51:9:626:G:C8	2.70	0.45
60:II:84:ASN:OD1	60:II:90:LEU:HD12	2.16	0.45
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.98	0.45
68:QQ:57:LEU:HD11	68:QQ:115:TYR:CD2	2.52	0.45
86:ii:69:VAL:HG13	86:ii:83:VAL:HG13	1.99	0.45
86:ii:225:ALA:HB2	86:ii:233:LEU:HD23	1.98	0.45
87:jj:352:ILE:N	87:jj:353:PRO:CD	2.80	0.45
37:l:23:ILE:HG22	50:8:52:A:C2	2.51	0.44
48:5:82:U:H2'	48:5:83:C:O4'	2.17	0.44
48:5:1524:A:N1	48:5:1652:U:C4	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1568:C:OP1	71:TT:96:SER:OG	2.31	0.44
51:9:1823:A:H3'	51:9:1824:A:H5'	1.99	0.44
65:NN:33:VAL:HG21	65:NN:66:VAL:HG11	1.98	0.44
1:A:96:LEU:HD13	41:p:83:ILE:HG23	2.00	0.44
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.52	0.44
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.52	0.44
3:C:302:LEU:HD22	16:Q:38:ARG:CB	2.46	0.44
48:5:4219:A:H2'	48:5:4220:A:C8	2.53	0.44
48:5:4576:U:C4	48:5:4577:U:C4	3.06	0.44
51:9:992:A:C2	51:9:993:G:C8	3.05	0.44
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.44
15:P:25:HIS:O	15:P:26:PHE:C	2.60	0.44
29:d:46:LEU:HD13	29:d:64:ILE:HD13	2.00	0.44
48:5:498:C:O2	48:5:498:C:O4'	2.34	0.44
48:5:1358:G:H4'	48:5:1359:G:OP1	2.18	0.44
48:5:1381:U:O2	48:5:1381:U:O4'	2.34	0.44
48:5:1632:A:H2'	48:5:1632:A:N3	2.32	0.44
51:9:1604:G:C6	51:9:1605:G:C4	3.05	0.44
52:AA:24:HIS:HB3	52:AA:51:LEU:HD21	1.98	0.44
59:HH:130:LEU:HD21	59:HH:156:VAL:HG21	1.98	0.44
84:gg:299:PHE:CD2	84:gg:309:VAL:HG12	2.52	0.44
86:ii:253:LEU:HD22	86:ii:351:VAL:HG21	2.00	0.44
2:B:105:VAL:HG11	2:B:150:PHE:CZ	2.53	0.44
3:C:133:LEU:N	3:C:133:LEU:HD12	2.32	0.44
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.52	0.44
16:Q:156:PRO:O	26:a:47:LYS:O	2.34	0.44
48:5:33:A:C6	48:5:34:A:C6	3.05	0.44
48:5:4269:G:C6	48:5:4270:C:C4	3.05	0.44
48:5:5057:C:H2'	48:5:5058:A:C8	2.52	0.44
51:9:944:A:C5	51:9:945:U:C5	3.04	0.44
56:EE:192:ILE:CD1	56:EE:238:LEU:HD23	2.48	0.44
66:OO:151:LEU:HD13	66:OO:151:LEU:N	2.32	0.44
3:C:13:GLU:HB2	3:C:161:TYR:OH	2.18	0.44
3:C:274:LYS:O	3:C:275:SER:C	2.61	0.44
7:G:214:VAL:HG11	7:G:220:VAL:HG23	1.99	0.44
10:J:151:ILE:HD11	10:J:156:ARG:HG2	1.98	0.44
37:l:41:ARG:NH1	48:5:2431:A:OP1	2.50	0.44
48:5:1411:C:C4	48:5:1411(B):C:C4	3.05	0.44
48:5:1990:A:H3'	48:5:1991:A:H5''	2.00	0.44
48:5:3724:A:N6	48:5:3725:G:C6	2.85	0.44
48:5:4423:U:O2	48:5:4423:U:O4'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1292:C:C2	83:ff:140:TYR:CD2	3.06	0.44
51:9:1292:C:O2	83:ff:140:TYR:CD2	2.71	0.44
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.48	0.44
71:TT:39:LEU:HD11	71:TT:52:TRP:CH2	2.51	0.44
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	1.98	0.44
48:5:914:U:O4	48:5:918:G:N7	2.50	0.44
48:5:1523:A:C2	48:5:1524:A:N7	2.86	0.44
48:5:3648:A:H1'	48:5:3785:A:N6	2.32	0.44
48:5:4510:A:C6	48:5:4511:A:C2	3.06	0.44
48:5:4759:C:O4'	48:5:4759:C:O2	2.34	0.44
51:9:1227:G:C2	51:9:1228:A:C8	3.05	0.44
51:9:1735:A:C4	51:9:1800:A:C2	3.05	0.44
54:CC:199:PRO:O	54:CC:202:THR:OG1	2.29	0.44
70:SS:59:LEU:HD12	70:SS:63:GLU:OE2	2.18	0.44
74:WW:42:MET:HE3	74:WW:50:PHE:CD2	2.52	0.44
2:B:55:HIS:CE1	22:W:16:GLY:HA3	2.53	0.44
48:5:223:G:H4'	48:5:225:G:C8	2.53	0.44
48:5:1848:C:H2'	48:5:1849:U:O4'	2.18	0.44
48:5:3685:C:H2'	48:5:3686:G:O4'	2.18	0.44
60:II:66:SER:HA	60:II:73:THR:HA	2.00	0.44
77:ZZ:73:VAL:HG12	77:ZZ:79:ILE:HD11	2.00	0.44
87:jj:361:GLN:O	87:jj:361:GLN:NE2	2.50	0.44
48:5:922(B):C:C4	48:5:923:C:C5	3.06	0.44
48:5:4928:C:O2	48:5:4928:C:O4'	2.34	0.44
51:9:1260:A:C6	51:9:1619:A:C6	3.06	0.44
78:aa:25:ASN:ND2	78:aa:77:CYS:SG	2.89	0.44
84:gg:14:HIS:CE1	84:gg:35:SER:HB2	2.53	0.44
86:ii:27:TRP:CH2	86:ii:349:LEU:HD22	2.53	0.44
9:I:36:LEU:HD12	9:I:87:ILE:HB	1.99	0.44
11:L:27:ASN:O	11:L:28:GLN:C	2.60	0.44
51:9:1438:A:C2	51:9:1439:A:C6	3.05	0.44
80:cc:21:THR:O	80:cc:22:GLY:O	2.36	0.44
22:W:9:SER:OG	22:W:36:CYS:SG	2.58	0.43
37:l:26:TRP:CZ3	37:l:27:ILE:HD12	2.52	0.43
48:5:356:G:O2'	50:8:25:G:N3	2.51	0.43
48:5:1339:U:H2'	48:5:1340:C:C6	2.52	0.43
48:5:1435:G:O2'	48:5:2105:A:N1	2.46	0.43
48:5:4658:G:C6	48:5:4659:G:C5	3.05	0.43
60:II:31:ARG:NH2	60:II:48:VAL:HG12	2.32	0.43
75:XX:123:VAL:HG12	75:XX:124:LYS:HG3	2.00	0.43
48:5:922:C:O3'	48:5:922(B):C:C5	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1411:C:H1'	48:5:1411(C):C:C6	2.52	0.43
48:5:1889:U:O4	48:5:1939:A:N6	2.51	0.43
48:5:2539:C:H2'	48:5:2540:C:O4'	2.18	0.43
48:5:4583:C:O2'	48:5:4718:G:N2	2.49	0.43
49:7:23:A:N3	49:7:118:C:O2'	2.45	0.43
54:CC:195:LEU:HD23	54:CC:224:THR:HG22	1.99	0.43
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.99	0.43
19:T:12:ARG:NH2	48:5:1789:C:OP2	2.52	0.43
19:T:17:ARG:HD3	19:T:47:THR:HG23	1.98	0.43
21:V:89:ARG:HD2	21:V:95:PHE:CZ	2.54	0.43
22:W:3:VAL:HG23	22:W:3:VAL:O	2.18	0.43
28:c:85:CYS:SG	28:c:94:LEU:HD22	2.57	0.43
4:D:75:VAL:O	4:D:112:ARG:NH1	2.52	0.43
13:N:48:ALA:HB1	13:N:53:TYR:HB3	1.99	0.43
18:S:44:PHE:CZ	18:S:48:VAL:HG21	2.53	0.43
48:5:481(A):C:O2	48:5:481(A):C:O4'	2.36	0.43
48:5:1354:A:N1	48:5:1385:G:O2'	2.41	0.43
48:5:2395:A:O2'	48:5:2806:A:C1'	2.58	0.43
48:5:4169:G:H4'	48:5:4171:C:C2	2.54	0.43
48:5:4268:A:H2'	48:5:4269:G:O4'	2.19	0.43
51:9:916:A:C5	65:NN:73:ARG:HD3	2.52	0.43
51:9:981:A:H2'	51:9:982:G:O4'	2.18	0.43
51:9:1485:U:H2'	51:9:1486:A:O4'	2.18	0.43
51:9:1823:A:C3'	51:9:1824:A:H5'	2.49	0.43
54:CC:124:PHE:O	54:CC:143:CYS:HA	2.19	0.43
69:RR:16:ILE:HG12	69:RR:38:ILE:HD11	1.99	0.43
1:A:69:PHE:HB2	48:5:4125:C:H1'	2.01	0.43
2:B:257:TRP:HB3	48:5:4518:A:OP1	2.19	0.43
5:E:180:GLY:O	5:E:181:PRO:C	2.61	0.43
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.48	0.43
29:d:22:THR:HG22	29:d:89:SER:HB2	1.99	0.43
51:9:563:G:O2'	51:9:564:A:O4'	2.35	0.43
51:9:1271:C:H4'	51:9:1301:A:C8	2.54	0.43
67:PP:28:MET:HE2	67:PP:32:GLN:HG2	2.01	0.43
3:C:138:MET:HG2	3:C:144:ILE:HG22	2.00	0.43
34:i:34:THR:HG21	48:5:276:C:OP2	2.18	0.43
47:3:71:G:N3	48:5:3715:U:O2'	2.49	0.43
48:5:1390:G:N2	48:5:1393:G:OP2	2.52	0.43
48:5:1411:C:HO3'	48:5:1411(C):C:P	2.40	0.43
48:5:1634:A:C6	48:5:1635:C:C4	3.07	0.43
51:9:490:C:O2'	51:9:574:A:N1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:MM:64:LEU:HD13	83:ff:108:VAL:HB	2.01	0.43
67:PP:36:LEU:O	70:SS:88:LYS:HD3	2.19	0.43
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.49	0.43
6:F:168:LEU:HB2	6:F:186:MET:HE1	1.99	0.43
7:G:104:LEU:O	7:G:105:THR:C	2.60	0.43
12:M:97:ALA:HB2	14:O:203:VAL:HB	2.00	0.43
32:g:59:VAL:HG21	32:g:63:VAL:HG11	2.01	0.43
48:5:976:G:N2	48:5:977:C:N3	2.66	0.43
48:5:3656:A:O4'	48:5:3747:A:C2	2.71	0.43
48:5:4758:U:O2	48:5:4758:U:O4'	2.36	0.43
51:9:1334:G:C4	51:9:1498:A:C2	3.06	0.43
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.43
75:XX:9:THR:O	75:XX:10:ALA:C	2.59	0.43
30:e:85:LEU:HD22	30:e:120:ILE:HD13	2.01	0.43
35:j:17:THR:CG2	35:j:29:LEU:HD21	2.48	0.43
48:5:43:U:H2'	48:5:44:A:O5'	2.18	0.43
52:AA:161:ILE:HG22	52:AA:163:CYS:SG	2.59	0.43
54:CC:108:LYS:HB2	54:CC:233:LEU:HD23	2.00	0.43
60:II:36:THR:HG21	60:II:179:PRO:HB2	2.01	0.43
84:gg:111:VAL:HG23	84:gg:122:SER:OG	2.18	0.43
2:B:254:ILE:CG2	2:B:262:VAL:HB	2.49	0.43
3:C:253:THR:O	3:C:256:ALA:N	2.52	0.43
13:N:64:ILE:HD12	13:N:65:ARG:N	2.33	0.43
48:5:2002:A:N3	48:5:2002:A:H2'	2.33	0.43
48:5:2465:C:H2'	48:5:2466:G:O4'	2.19	0.43
48:5:3879:G:O2'	48:5:3881:G:OP2	2.35	0.43
48:5:4966:A:C2	48:5:4967:A:C6	3.07	0.43
50:8:103:A:C8	50:8:104:A:C8	3.07	0.43
51:9:1016:U:OP2	65:NN:14:SER:HA	2.19	0.43
51:9:1129:G:C6	51:9:1130:G:C6	3.07	0.43
51:9:1646:C:C2'	51:9:1647:A:OP2	2.66	0.43
65:NN:45:LEU:HG	65:NN:49:GLN:HB2	2.01	0.43
67:PP:119:PHE:CE1	70:SS:117:ILE:HD12	2.54	0.43
79:bb:53:VAL:HG23	79:bb:53:VAL:O	2.19	0.43
87:jj:529:CYS:SG	87:jj:556:GLY:N	2.92	0.43
2:B:47:LEU:HD13	2:B:181:MET:SD	2.59	0.43
12:M:37:LEU:HD23	18:S:100:LEU:HD21	2.00	0.43
48:5:35:U:O2'	48:5:1525:A:N1	2.52	0.43
48:5:1236:C:O2'	48:5:1238:A:OP1	2.37	0.43
48:5:4305:G:N3	48:5:4305:G:H2'	2.33	0.43
51:9:35:C:O2	51:9:520:A:N1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:126:G:O4'	58:GG:195:LYS:HB3	2.18	0.43
51:9:1123:C:C4	51:9:1124:C:C5	3.07	0.43
51:9:1680:G:H4'	80:cc:20:ARG:CZ	2.47	0.43
52:AA:24:HIS:CB	52:AA:51:LEU:HD21	2.49	0.43
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.01	0.43
4:D:56:THR:HG21	49:7:26:C:H5''	2.01	0.42
15:P:69:ARG:NH1	48:5:4980:C:N3	2.66	0.42
20:U:84:LYS:HA	20:U:87:THR:HG22	1.99	0.42
21:V:117:ILE:HD11	21:V:132:ILE:HG23	2.00	0.42
26:a:25:HIS:ND1	48:5:1338:G:N7	2.67	0.42
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.54	0.42
48:5:740:G:N1	48:5:922:C:O2	2.52	0.42
48:5:1236:C:O2'	48:5:1237:C:O5'	2.33	0.42
51:9:1304:U:P	83:ff:93:HIS:CB	3.05	0.42
57:FF:87:LEU:HD21	68:QQ:47:LEU:HD22	2.00	0.42
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	2.00	0.42
59:HH:134:VAL:HG12	59:HH:173:PHE:CD2	2.54	0.42
1:A:142:GLU:O	1:A:143:THR:OG1	2.36	0.42
13:N:115:VAL:HG22	13:N:134:LEU:HD21	2.00	0.42
24:Y:52:ASP:HB2	24:Y:110:LYS:HG3	2.01	0.42
33:h:44:LEU:O	33:h:47:ILE:HG22	2.19	0.42
51:9:1018:U:H5''	65:NN:71:ILE:HD12	2.01	0.42
51:9:1292:C:O2	83:ff:140:TYR:CD1	2.72	0.42
65:NN:3:ARG:HB2	65:NN:6:ALA:HB3	2.01	0.42
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.59	0.42
69:RR:119:VAL:HG13	69:RR:119:VAL:O	2.19	0.42
84:gg:15:ASN:O	84:gg:305:ASN:ND2	2.51	0.42
25:Z:12:LEU:HB2	25:Z:81:MET:HB3	2.01	0.42
32:g:9:ARG:HG3	32:g:34:TYR:CZ	2.54	0.42
36:k:35:LYS:HG2	36:k:44:THR:HG22	2.00	0.42
41:p:39:CYS:HB3	41:p:42:CYS:SG	2.59	0.42
48:5:3723:A:C2	48:5:3724:A:C6	3.07	0.42
52:AA:51:LEU:HG	69:RR:105:MET:HE1	2.01	0.42
67:PP:18:ARG:HA	70:SS:93:GLY:CA	2.49	0.42
70:SS:40:TYR:O	70:SS:44:VAL:HG23	2.19	0.42
13:N:5:LYS:HG2	34:i:40:VAL:HG11	2.02	0.42
18:S:28:TYR:CD2	18:S:54:MET:HE1	2.53	0.42
25:Z:42:LEU:HD23	25:Z:43:VAL:N	2.34	0.42
25:Z:75:TYR:CG	25:Z:80:LEU:HD21	2.54	0.42
28:c:29:LEU:HD23	28:c:94:LEU:HD13	2.00	0.42
33:h:88:THR:O	33:h:91:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:35:ARG:NH1	48:5:2265:G:OP1	2.52	0.42
48:5:1818:G:H2'	48:5:1820:U:OP2	2.18	0.42
48:5:5007:A:N7	48:5:5042:A:O2'	2.35	0.42
49:7:14:C:C4	49:7:66:G:N2	2.88	0.42
50:8:92:U:H2'	50:8:93:C:O4'	2.20	0.42
50:8:152:U:H2'	50:8:153:C:O4'	2.19	0.42
51:9:1231:C:H2'	51:9:1232:U:O4'	2.19	0.42
51:9:1533:A:C2	51:9:1604:G:H4'	2.55	0.42
58:GG:63:MET:HA	58:GG:98:ARG:O	2.20	0.42
61:JJ:84:ILE:O	61:JJ:108:ARG:NH1	2.52	0.42
76:YY:62:THR:HA	76:YY:69:THR:HG22	2.01	0.42
1:A:181:LYS:HB2	48:5:1577:G:C5	2.55	0.42
21:V:87:SER:HA	21:V:97:TYR:HB3	2.01	0.42
40:o:61:LYS:HD2	48:5:4372:U:OP2	2.19	0.42
48:5:113:A:C2	48:5:278:G:C4	3.08	0.42
51:9:293:C:O2'	51:9:294:U:H3'	2.19	0.42
51:9:380:G:OP2	60:II:181:GLN:NE2	2.51	0.42
51:9:1228:A:H2'	51:9:1229:G:C8	2.54	0.42
51:9:1406:G:O2'	51:9:1443:C:N3	2.53	0.42
58:GG:5:ILE:CD1	58:GG:16:ILE:HD13	2.48	0.42
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	2.02	0.42
74:WW:111:MET:HE3	74:WW:116:ALA:HA	2.02	0.42
2:B:14:LEU:HD23	2:B:17:LEU:HD23	2.00	0.42
3:C:323:ARG:NE	48:5:976:G:H21	2.16	0.42
11:L:57:PRO:HG3	11:L:75:GLY:C	2.44	0.42
24:Y:47:MET:HE2	24:Y:115:ARG:HD3	2.00	0.42
26:a:72:THR:HG22	26:a:110:LYS:HB3	2.02	0.42
29:d:33:ILE:HD11	29:d:41:ARG:CB	2.47	0.42
48:5:108:A:N1	48:5:333:U:O2'	2.47	0.42
48:5:2729:C:H2'	48:5:2730:U:O4'	2.19	0.42
51:9:384:U:O4	60:II:5:ARG:NH2	2.51	0.42
51:9:444:G:N2	51:9:446:G:H3'	2.34	0.42
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	2.01	0.42
60:II:38:ILE:HD11	60:II:81:VAL:HG23	2.01	0.42
87:jj:363:ASP:O	87:jj:398:VAL:HG13	2.19	0.42
26:a:82:VAL:CG2	26:a:101:ILE:HG23	2.50	0.42
48:5:1337:A:C2	48:5:2349:A:C2	3.08	0.42
48:5:4349:C:H3'	48:5:4350:C:H5'	2.01	0.42
48:5:4621:C:C2	48:5:4622:A:C8	3.08	0.42
48:5:4709:U:O2	48:5:4709:U:H2'	2.20	0.42
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:111:PHE:HB3	69:RR:114:LEU:HD21	2.02	0.42
73:VV:1:MET:SD	73:VV:1:MET:N	2.72	0.42
74:WW:79:PHE:O	74:WW:125:ILE:HG22	2.19	0.42
75:XX:61:GLN:O	75:XX:63:ASN:N	2.53	0.42
75:XX:141:PRO:HB3	87:jj:561:LYS:HG2	2.01	0.42
8:H:94:SER:HB3	8:H:142:ASP:HB3	2.00	0.42
8:H:128:MET:HE1	8:H:161:ILE:HG23	2.01	0.42
11:L:106:SER:HB3	34:i:17:VAL:HG11	2.01	0.42
15:P:41:ILE:HD12	15:P:150:LEU:CD1	2.49	0.42
29:d:36:VAL:HG11	29:d:44:ARG:HG2	2.01	0.42
48:5:492:U:O2'	48:5:493:G:P	2.78	0.42
48:5:686:A:N3	48:5:686:A:H2'	2.35	0.42
48:5:4398:C:C4	48:5:4399:U:C5	3.08	0.42
51:9:31:U:O2'	51:9:643:A:N1	2.53	0.42
51:9:1374:C:H2'	51:9:1375:G:O4'	2.20	0.42
51:9:1452:A:C6	51:9:1476:A:C6	3.08	0.42
52:AA:5:LEU:CD2	52:AA:8:LEU:HD12	2.48	0.42
54:CC:85:SER:OG	73:VV:25:GLY:O	2.34	0.42
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.01	0.42
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.35	0.42
72:UU:102:THR:HG21	72:UU:114:VAL:HG21	2.02	0.42
84:gg:21:ILE:CG2	84:gg:31:ILE:HD11	2.50	0.42
84:gg:32:LEU:HD12	84:gg:42:MET:HA	2.02	0.42
87:jj:539:GLU:N	87:jj:540:PRO:CD	2.83	0.42
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.55	0.42
48:5:433:A:C2	48:5:3867:A:H4'	2.55	0.42
48:5:916:C:O2	48:5:916:C:O4'	2.36	0.42
48:5:1895:G:C6	48:5:1896:A:C4	3.08	0.42
48:5:3611:A:C6	48:5:3612:C:C4	3.08	0.42
48:5:4320:G:H2'	48:5:4321:U:O4'	2.19	0.42
51:9:1024:A:H2'	51:9:1025:U:O4'	2.19	0.42
54:CC:260:VAL:HG23	54:CC:260:VAL:O	2.19	0.42
59:HH:177:TYR:CD2	59:HH:185:VAL:HG21	2.55	0.42
60:II:79:ILE:HG22	60:II:103:LEU:HB2	2.01	0.42
1:A:129:ALA:O	1:A:130:SER:C	2.63	0.42
2:B:41:VAL:HA	2:B:187:GLY:HA3	2.01	0.42
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.53	0.42
8:H:189:GLN:N	8:H:189:GLN:OE1	2.53	0.42
13:N:12:ARG:NH1	48:5:308:G:O6	2.53	0.42
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.53	0.42
26:a:79:TRP:CZ2	26:a:122:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.42
48:5:1748:U:C2	48:5:1783:C:C2	3.07	0.42
48:5:1846:G:H2'	48:5:1847:C:C6	2.55	0.42
48:5:1905:U:H2'	48:5:1906:U:O4'	2.20	0.42
51:9:666:U:O4'	51:9:1088:U:C2	2.73	0.42
51:9:682:U:OP2	75:XX:8:ARG:HD3	2.20	0.42
51:9:1088:U:H4'	51:9:1089:G:OP2	2.20	0.42
51:9:1604:G:C6	51:9:1605:G:C5	3.08	0.42
72:UU:24:LEU:HB3	72:UU:32:LEU:HD11	2.02	0.42
74:WW:102:ILE:HB	74:WW:113:HIS:HB3	2.02	0.42
87:jj:266:ILE:CD1	87:jj:393:VAL:HG21	2.50	0.42
3:C:101:MET:CE	48:5:2343:G:C4	3.03	0.41
5:E:53:VAL:O	5:E:54:ARG:C	2.62	0.41
7:G:189:LEU:HD22	7:G:255:VAL:HG12	2.02	0.41
14:O:108:ILE:HG22	14:O:157:GLU:OE1	2.20	0.41
40:o:39:ARG:NH2	48:5:4362:A:O2'	2.51	0.41
48:5:3683:C:H4'	48:5:3684:G:OP2	2.20	0.41
48:5:4236:G:H4'	48:5:4328:G:O2'	2.20	0.41
51:9:89:C:H2'	51:9:90:G:O4'	2.20	0.41
51:9:955:A:N1	51:9:968:U:O2'	2.45	0.41
51:9:981:A:H2'	51:9:982:G:C8	2.55	0.41
51:9:1680:G:H2'	51:9:1681:U:C6	2.55	0.41
51:9:1865:C:OP1	78:aa:87:ARG:NH2	2.53	0.41
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.55	0.41
57:FF:87:LEU:HD22	68:QQ:46:THR:OG1	2.19	0.41
62:KK:39:ASN:O	62:KK:40:VAL:C	2.63	0.41
75:XX:68:LYS:CG	75:XX:91:LEU:HD22	2.50	0.41
87:jj:668:ARG:HB3	87:jj:673:THR:HA	2.01	0.41
6:F:75:ARG:NE	48:5:730:G:OP2	2.44	0.41
14:O:44:SER:HB3	14:O:129:LEU:HD11	2.02	0.41
14:O:133:ARG:CZ	48:5:1928:C:C4	3.03	0.41
15:P:122:ALA:HB1	15:P:123:PRO:HD2	2.02	0.41
16:Q:106:THR:HG21	48:5:1353:G:H3'	2.01	0.41
20:U:39:PHE:CZ	20:U:43:LEU:HD11	2.55	0.41
22:W:3:VAL:HG21	22:W:12:LYS:HE3	2.02	0.41
22:W:26:GLY:O	22:W:27:LYS:C	2.62	0.41
37:l:10:LYS:NZ	48:5:2782:U:OP2	2.52	0.41
41:p:46:LYS:O	41:p:57:CYS:HA	2.20	0.41
48:5:2693:G:C6	48:5:2694:G:N1	2.88	0.41
51:9:180:G:C6	51:9:181:A:N1	2.88	0.41
51:9:1657:G:C6	51:9:1658:G:C5	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XX:51:VAL:HG13	75:XX:70:VAL:CG1	2.50	0.41
84:gg:86:THR:HG22	84:gg:102:VAL:HG22	2.02	0.41
86:ii:208:ALA:HB1	86:ii:245:ALA:HB2	2.01	0.41
11:L:76:PHE:CD2	11:L:117:LEU:HD11	2.55	0.41
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.88	0.41
16:Q:48:LEU:O	16:Q:49:LYS:C	2.62	0.41
19:T:17:ARG:HD2	19:T:47:THR:HG23	2.02	0.41
20:U:27:HIS:N	20:U:28:PRO:HD2	2.34	0.41
28:c:50:ASN:OD1	28:c:76:GLY:C	2.63	0.41
48:5:318:A:C2	48:5:4360:U:C2	3.09	0.41
48:5:1301:C:O2	48:5:1301:C:O4'	2.34	0.41
48:5:1546:C:N3	48:5:1612:G:O6	2.54	0.41
48:5:2370:A:N1	48:5:2390:G:O2'	2.39	0.41
51:9:155:G:H4'	58:GG:15:LEU:HD12	2.02	0.41
51:9:932:G:H2'	51:9:934:G:OP2	2.20	0.41
51:9:1336:C:H2'	51:9:1337:C:O4'	2.20	0.41
51:9:1380:C:H2'	51:9:1381:G:O4'	2.20	0.41
51:9:1545:A:H2'	51:9:1546:G:C8	2.55	0.41
51:9:1653:U:H2'	51:9:1654:G:C8	2.55	0.41
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.36	0.41
63:LL:76:VAL:HB	63:LL:125:ILE:HD13	2.01	0.41
69:RR:5:ARG:HG2	69:RR:9:VAL:HG11	2.02	0.41
77:ZZ:103:HIS:O	77:ZZ:104:ARG:C	2.62	0.41
86:ii:161:ALA:HB2	86:ii:196:HIS:CD2	2.56	0.41
87:jj:604:TYR:O	87:jj:605:GLN:C	2.62	0.41
87:jj:665:PHE:CE2	87:jj:667:LEU:HD11	2.56	0.41
3:C:340:ILE:HG21	5:E:52:LEU:HD12	2.02	0.41
9:I:60:LEU:HG	9:I:129:VAL:HG21	2.02	0.41
12:M:94:LYS:NZ	48:5:4872:G:OP2	2.50	0.41
40:o:45:GLN:HE22	40:o:51:GLN:HA	1.85	0.41
51:9:1661:A:OP1	81:dd:19:ARG:NH2	2.53	0.41
54:CC:70:VAL:HG22	54:CC:75:ILE:CG2	2.50	0.41
84:gg:78:ALA:O	84:gg:90:TRP:N	2.53	0.41
86:ii:17:THR:HG21	86:ii:109:GLN:HE21	1.85	0.41
3:C:67:TRP:CE3	3:C:73:VAL:HG21	2.56	0.41
12:M:105:THR:HG22	12:M:106:ASP:H	1.85	0.41
29:d:88:LEU:CD1	29:d:106:VAL:HG22	2.51	0.41
48:5:2896:G:H5''	48:5:2897:G:OP2	2.21	0.41
48:5:3629:A:O2'	51:9:1721:U:O2	2.29	0.41
48:5:3714:G:H2'	48:5:3715:U:O4'	2.21	0.41
51:9:1539:U:OP1	71:TT:44:GLU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1857:G:OP2	66:OO:146:ARG:HG3	2.19	0.41
75:XX:67:ARG:HG2	75:XX:115:ILE:HG23	2.03	0.41
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.50	0.41
10:J:24:ILE:HG21	10:J:36:ALA:HB1	2.02	0.41
10:J:103:GLY:O	10:J:134:LEU:HD12	2.20	0.41
13:N:38:ARG:NH1	50:8:142:U:OP2	2.44	0.41
21:V:99:GLU:HB3	22:W:24:THR:HG23	2.03	0.41
38:m:99:LYS:HG3	48:5:4474:A:H5'	2.02	0.41
48:5:444:G:N2	48:5:1304:C:C2	2.89	0.41
48:5:1524:A:N6	48:5:1652:U:N3	2.59	0.41
48:5:2409:U:C5	48:5:2783:A:N1	2.89	0.41
48:5:2750:G:H2'	48:5:2751:G:O4'	2.20	0.41
48:5:4183:G:N3	48:5:4183:G:H2'	2.36	0.41
48:5:4880:C:O2	48:5:4880:C:O4'	2.39	0.41
51:9:92:A:C6	51:9:446:G:C6	3.08	0.41
51:9:1834:A:N3	51:9:1834:A:H2'	2.36	0.41
78:aa:53:ILE:O	78:aa:57:SER:N	2.54	0.41
17:R:92:LYS:NZ	48:5:2667:C:O2	2.48	0.41
17:R:173:ARG:NH2	51:9:910:G:OP2	2.54	0.41
48:5:68:U:H2'	48:5:69:A:O4'	2.21	0.41
48:5:4303:C:O2'	48:5:4304:A:H2'	2.21	0.41
50:8:64:U:C2	50:8:65:A:C8	3.08	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.68	0.41
51:9:1059:G:C6	51:9:1060:A:C2	3.09	0.41
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.49	0.41
51:9:1661:A:C8	81:dd:14:PHE:CD1	3.09	0.41
51:9:1673:U:H2'	51:9:1674:G:O4'	2.21	0.41
51:9:1857:G:C2'	51:9:1858:G:O5'	2.68	0.41
53:BB:74:LEU:HD21	53:BB:86:LEU:HD11	2.02	0.41
54:CC:233:LEU:O	54:CC:234:GLY:C	2.63	0.41
63:LL:55:TYR:CD1	63:LL:55:TYR:C	2.97	0.41
3:C:152:LEU:HD23	3:C:251:ILE:HG12	2.01	0.41
8:H:117:PHE:CE2	8:H:118:LEU:HD23	2.56	0.41
28:c:104:ILE:HG23	28:c:105:ILE:HG23	2.02	0.41
48:5:2313:A:O2'	48:5:2314:G:OP1	2.28	0.41
48:5:2523:G:C6	48:5:2524:U:C4	3.08	0.41
48:5:4085:A:C6	48:5:4164:C:C5	3.08	0.41
48:5:4458:C:H2'	48:5:4459:U:C6	2.55	0.41
51:9:666:U:N3	51:9:667:U:C5	2.88	0.41
51:9:1284:A:N3	64:MM:91:LEU:HD13	2.34	0.41
1:A:39:GLY:HA3	7:G:94:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG23	1:A:162:ASN:ND2	2.36	0.41
2:B:10:ARG:NH1	2:B:14:LEU:HG	2.36	0.41
3:C:313:VAL:HG11	6:F:169:THR:HG21	2.03	0.41
4:D:17:GLN:O	48:5:4265:U:N3	2.53	0.41
6:F:93:ARG:NH2	6:F:97:ILE:HD12	2.36	0.41
6:F:167:ALA:O	6:F:169:THR:HG23	2.21	0.41
8:H:5:LEU:HD22	8:H:60:TRP:CZ3	2.56	0.41
40:o:82:MET:N	40:o:82:MET:SD	2.94	0.41
48:5:934:C:O4'	48:5:935(A):G:O4'	2.38	0.41
48:5:2519:U:H1'	48:5:2520:C:C6	2.55	0.41
48:5:4518:A:H8	48:5:4518:A:OP2	2.04	0.41
48:5:4662:C:O2'	48:5:5004:C:OP1	2.28	0.41
50:8:71:A:C2	50:8:88:A:H1'	2.55	0.41
51:9:372:U:OP1	63:LL:136:LYS:NZ	2.50	0.41
51:9:816:A:C6	51:9:817:G:C4	3.09	0.41
51:9:989:C:O4'	51:9:990:A:C2	2.74	0.41
51:9:1692:U:H2'	51:9:1693:G:C8	2.56	0.41
62:KK:65:ARG:NH2	81:dd:20:SER:OG	2.54	0.41
67:PP:18:ARG:NE	70:SS:88:LYS:CG	2.84	0.41
75:XX:41:PHE:CE1	75:XX:47:ALA:HB3	2.56	0.41
87:jj:506:THR:HG22	87:jj:551:SER:HB3	2.01	0.41
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.51	0.41
3:C:150:LEU:O	3:C:152:LEU:N	2.54	0.41
3:C:266:THR:OG1	3:C:267:TRP:N	2.54	0.41
8:H:41:ILE:CG2	8:H:73:ILE:HD11	2.50	0.41
9:I:48:LEU:C	9:I:48:LEU:HD13	2.47	0.41
41:p:32:SER:OG	41:p:33:GLN:N	2.54	0.41
48:5:106:A:H1'	48:5:336:A:N3	2.36	0.41
48:5:1744:U:H2'	48:5:1745:G:O4'	2.21	0.41
48:5:2088:A:O2'	48:5:2089:G:OP2	2.31	0.41
48:5:4303:C:O2	48:5:4303:C:O4'	2.39	0.41
48:5:4624:A:H2'	48:5:4625:C:O4'	2.21	0.41
51:9:398:A:H5'	51:9:398:A:C8	2.56	0.41
58:GG:16:ILE:HD12	58:GG:16:ILE:N	2.35	0.41
79:bb:11:SER:OG	79:bb:13:GLU:HG2	2.20	0.41
87:jj:266:ILE:HG23	87:jj:389:HIS:HB3	2.02	0.41
87:jj:330:MET:HE2	87:jj:343:MET:SD	2.61	0.41
1:A:15:VAL:HG21	48:5:1628:C:H5''	2.03	0.40
2:B:36:ASP:OD1	2:B:36:ASP:N	2.53	0.40
2:B:257:TRP:CD1	2:B:257:TRP:C	3.00	0.40
6:F:161:ILE:HB	6:F:166:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:122:ILE:HD13	48:5:4163:U:H1'	2.03	0.40
10:J:140:SER:O	10:J:141:ILE:C	2.64	0.40
12:M:6:PHE:O	12:M:11:ARG:NE	2.52	0.40
18:S:9:GLU:OE2	18:S:31:ARG:NH2	2.54	0.40
19:T:83:LYS:HD2	19:T:85:LEU:HD21	2.04	0.40
48:5:750:U:H2'	48:5:751:G:O4'	2.21	0.40
48:5:914:U:O4	48:5:918:G:C8	2.74	0.40
48:5:2805:C:N4	48:5:2806:A:N6	2.69	0.40
48:5:4419:U:OP1	48:5:4421:C:N4	2.54	0.40
48:5:4925:U:H4'	48:5:4926:C:H5'	2.03	0.40
51:9:1536:G:H2'	51:9:1537:A:C8	2.56	0.40
69:RR:99:ASP:O	69:RR:102:THR:OG1	2.38	0.40
77:ZZ:102:LYS:HB2	77:ZZ:107:VAL:HG12	2.03	0.40
2:B:57:VAL:HB	2:B:367:PHE:HB3	2.04	0.40
4:D:106:ALA:CB	4:D:171:LEU:HD13	2.51	0.40
17:R:23:TRP:CE3	17:R:51:ILE:HD12	2.56	0.40
17:R:118:HIS:ND1	48:5:2663:G:OP1	2.52	0.40
35:j:31:LYS:O	35:j:33:THR:HG23	2.20	0.40
48:5:4966:A:C2	48:5:4967:A:N1	2.89	0.40
51:9:846:G:H2'	56:EE:19:MET:HE2	2.03	0.40
51:9:958:G:H2'	51:9:959:G:O4'	2.22	0.40
53:BB:66:VAL:HG22	53:BB:87:ILE:CG2	2.51	0.40
55:DD:72:VAL:HG23	62:KK:20:VAL:CG2	2.51	0.40
59:HH:66:VAL:N	59:HH:67:PRO:CD	2.84	0.40
67:PP:18:ARG:HD2	70:SS:88:LYS:CG	2.51	0.40
84:gg:207:CYS:CB	84:gg:221:LEU:HD11	2.51	0.40
3:C:242:PRO:HB2	48:5:2297:G:H4'	2.03	0.40
9:I:61:SER:OG	48:5:4431:U:OP1	2.31	0.40
19:T:64:VAL:HG13	19:T:72:VAL:HB	2.04	0.40
20:U:80:LYS:HD3	20:U:110:TYR:CE2	2.57	0.40
35:j:39:TYR:N	35:j:40:PRO:CD	2.84	0.40
41:p:59:SER:OG	41:p:60:CYS:N	2.54	0.40
48:5:1411:C:H5'	48:5:1411(B):C:O3'	2.21	0.40
48:5:1942:A:N3	48:5:4432:C:O2'	2.49	0.40
48:5:2473:A:C2	48:5:2506:G:C2	3.09	0.40
48:5:4187:G:H2'	48:5:4188:U:O4'	2.21	0.40
48:5:4399:U:H2'	48:5:4400:G:O4'	2.21	0.40
51:9:614:C:O2	51:9:614:C:C2'	2.69	0.40
51:9:986:G:H2'	51:9:987:A:O4'	2.21	0.40
51:9:1614:A:OP2	67:PP:42:ARG:NH1	2.53	0.40
51:9:1695:A:N1	51:9:1832:A:O2'	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:69:GLU:HB3	54:CC:270:THR:HG21	2.03	0.40
84:gg:207:CYS:HB3	84:gg:221:LEU:HD11	2.03	0.40
1:A:196:TRP:O	1:A:197:PRO:C	2.63	0.40
3:C:33:ARG:HD2	3:C:36:ILE:HD12	2.03	0.40
3:C:209:VAL:HB	3:C:229:LEU:HD13	2.04	0.40
3:C:321:ASN:OD1	48:5:1280:C:O2'	2.40	0.40
18:S:30:MET:HE1	18:S:47:PHE:CB	2.51	0.40
42:r:93:ILE:HD13	42:r:114:ALA:HB2	2.04	0.40
48:5:922:C:N1	48:5:922(A):G:C6	2.90	0.40
48:5:1685:G:C5	48:5:1686:C:C4	3.09	0.40
48:5:2268:A:C3'	48:5:2269:C:H5'	2.52	0.40
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.45	0.40
51:9:1546:G:H5'	68:QQ:18:THR:HG21	2.04	0.40
51:9:1646:C:O2'	51:9:1647:A:OP2	2.36	0.40
51:9:1664:A:H4'	51:9:1665:G:OP1	2.21	0.40
52:AA:5:LEU:HD23	52:AA:8:LEU:HD12	2.03	0.40
70:SS:10:GLN:HA	70:SS:10:GLN:HE21	1.86	0.40
74:WW:7:LEU:O	74:WW:11:LEU:HG	2.22	0.40
5:E:184:LEU:O	48:5:4883:C:N4	2.55	0.40
12:M:112:VAL:CG1	14:O:201:LEU:HD11	2.50	0.40
13:N:91:GLN:NE2	48:5:4178:A:OP2	2.54	0.40
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	2.03	0.40
21:V:82:ILE:HD12	21:V:104:VAL:HG13	2.02	0.40
30:e:16:ARG:HD3	30:e:20:PHE:CE1	2.56	0.40
33:h:58:LEU:HA	33:h:61:ILE:HD12	2.02	0.40
48:5:2081:C:H2'	48:5:2082:G:O4'	2.20	0.40
48:5:4124:G:O2'	48:5:4125:C:OP1	2.32	0.40
53:BB:107:ARG:NH1	66:OO:133:THR:O	2.54	0.40
63:LL:4:ILE:CD1	63:LL:56:ILE:HD11	2.49	0.40
64:MM:22:LEU:HD13	64:MM:22:LEU:C	2.46	0.40
84:gg:174:VAL:HB	84:gg:188:HIS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	220 (89%)	24 (10%)	2 (1%)	16	49
2	B	392/403 (97%)	355 (91%)	35 (9%)	2 (0%)	24	58
3	C	360/425 (85%)	332 (92%)	23 (6%)	5 (1%)	9	38
4	D	291/297 (98%)	278 (96%)	10 (3%)	3 (1%)	12	44
5	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
6	F	223/247 (90%)	204 (92%)	16 (7%)	3 (1%)	9	39
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	14	47
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	177 (88%)	23 (11%)	1 (0%)	24	58
10	J	168/178 (94%)	157 (94%)	9 (5%)	2 (1%)	10	41
11	L	208/211 (99%)	193 (93%)	14 (7%)	1 (0%)	24	58
12	M	136/218 (62%)	125 (92%)	11 (8%)	0	100	100
13	N	201/204 (98%)	181 (90%)	19 (10%)	1 (0%)	24	58
14	O	197/203 (97%)	183 (93%)	13 (7%)	1 (0%)	24	58
15	P	151/184 (82%)	140 (93%)	9 (6%)	2 (1%)	9	39
16	Q	185/188 (98%)	168 (91%)	16 (9%)	1 (0%)	24	58
17	R	178/196 (91%)	171 (96%)	6 (3%)	1 (1%)	21	53
18	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	7	34
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	9 (9%)	2 (2%)	5	31
21	V	129/140 (92%)	113 (88%)	16 (12%)	0	100	100
22	W	102/157 (65%)	93 (91%)	8 (8%)	1 (1%)	12	44
23	X	116/156 (74%)	109 (94%)	6 (5%)	1 (1%)	14	47
24	Y	132/145 (91%)	126 (96%)	5 (4%)	1 (1%)	16	49
25	Z	133/136 (98%)	123 (92%)	8 (6%)	2 (2%)	8	37
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	12	44
28	c	96/115 (84%)	89 (93%)	7 (7%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	12	44
30	e	126/135 (93%)	121 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	32
32	g	112/117 (96%)	103 (92%)	8 (7%)	1 (1%)	14	47
33	h	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16	49
34	i	100/105 (95%)	92 (92%)	8 (8%)	0	100	100
35	j	84/97 (87%)	74 (88%)	9 (11%)	1 (1%)	10	41
36	k	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8	37
37	l	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
38	m	50/102 (49%)	46 (92%)	4 (8%)	0	100	100
39	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
40	o	102/106 (96%)	92 (90%)	9 (9%)	1 (1%)	12	44
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	11	42
42	r	122/137 (89%)	104 (85%)	14 (12%)	4 (3%)	3	23
43	s	194/318 (61%)	174 (90%)	18 (9%)	2 (1%)	12	44
44	t	151/165 (92%)	134 (89%)	15 (10%)	2 (1%)	9	39
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	195 (91%)	19 (9%)	1 (0%)	24	58
53	BB	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
54	CC	219/293 (75%)	202 (92%)	16 (7%)	1 (0%)	24	58
55	DD	226/243 (93%)	206 (91%)	18 (8%)	2 (1%)	14	47
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	168 (93%)	10 (6%)	3 (2%)	7	34
58	GG	235/249 (94%)	217 (92%)	17 (7%)	1 (0%)	30	62
59	HH	181/194 (93%)	168 (93%)	13 (7%)	0	100	100
60	II	204/208 (98%)	191 (94%)	11 (5%)	2 (1%)	12	44
61	JJ	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	6 (6%)	3 (3%)	3	24
63	LL	139/158 (88%)	124 (89%)	14 (10%)	1 (1%)	18	51
64	MM	115/132 (87%)	99 (86%)	16 (14%)	0	100	100
65	NN	147/151 (97%)	134 (91%)	13 (9%)	0	100	100
66	OO	134/168 (80%)	120 (90%)	13 (10%)	1 (1%)	18	51
67	PP	118/145 (81%)	103 (87%)	14 (12%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/135 (96%)	115 (88%)	14 (11%)	1 (1%)	16	49
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	131 (94%)	7 (5%)	1 (1%)	18	51
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	9 (7%)	2 (2%)	7	36
75	XX	139/143 (97%)	124 (89%)	12 (9%)	3 (2%)	5	30
76	YY	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	88 (89%)	9 (9%)	2 (2%)	6	32
79	bb	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	10	41
80	cc	60/69 (87%)	55 (92%)	3 (5%)	2 (3%)	3	23
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	5 (8%)	1 (2%)	8	37
84	gg	311/317 (98%)	284 (91%)	24 (8%)	3 (1%)	12	44
86	ii	370/403 (92%)	343 (93%)	26 (7%)	1 (0%)	36	67
87	jj	423/710 (60%)	381 (90%)	38 (9%)	4 (1%)	14	47
All	All	12317/14495 (85%)	11302 (92%)	923 (8%)	92 (1%)	20	51

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	236	GLU
18	S	155	PRO
31	f	107	PRO
75	XX	62	PRO
87	jj	605	GLN
1	A	217	GLN
11	L	63	THR
13	N	89	VAL
14	O	200	GLY
20	U	24	ASP
20	U	62	SER

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Mol	Chain	Res	Type
22	W	27	LYS
29	d	58	GLY
33	h	89	ARG
42	r	11	ARG
42	r	68	SER
43	s	142	GLY
44	t	125	LEU
66	OO	20	GLN
75	XX	61	GLN
75	XX	86	PRO
84	gg	224	GLY
87	jj	269	VAL
1	A	14	SER
3	C	275	SER
6	F	99	GLY
7	G	105	THR
10	J	141	ILE
15	P	25	HIS
18	S	166	ARG
31	f	106	TYR
35	j	59	THR
42	r	33	LYS
52	AA	159	ILE
78	aa	47	ALA
80	cc	22	GLY
87	jj	596	LYS
2	B	17	LEU
4	D	44	TYR
16	Q	14	ARG
17	R	3	MET
25	Z	90	PRO
25	Z	91	LEU
55	DD	93	THR
57	FF	21	GLY
57	FF	63	LYS
60	II	123	ARG
62	KK	64	TRP
67	PP	82	ASP
74	WW	78	ARG
78	aa	26	CYS
86	ii	12	ASN
3	C	254	GLU

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Mol	Chain	Res	Type
4	D	119	TYR
6	F	125	ASN
24	Y	78	TYR
36	k	20	ALA
40	o	96	ASP
43	s	25	PRO
44	t	54	LYS
57	FF	43	GLU
62	KK	30	PRO
63	LL	66	VAL
71	TT	109	GLY
80	cc	18	LEU
83	ff	128	ALA
7	G	216	PRO
18	S	165	PRO
27	b	102	PRO
41	p	51	ALA
69	RR	119	VAL
74	WW	29	PRO
79	bb	51	GLN
87	jj	618	SER
10	J	68	ILE
58	GG	135	PRO
3	C	90	GLY
3	C	99	GLY
4	D	125	VAL
15	P	114	ILE
23	X	119	ILE
32	g	48	VAL
55	DD	48	ILE
62	KK	40	VAL
2	B	98	GLY
3	C	247	GLY
9	I	135	ILE
54	CC	171	GLY
84	gg	13	GLY
42	r	29	PRO
60	II	3	ILE
84	gg	243	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	177 (93%)	13 (7%)	14	41
2	B	342/348 (98%)	310 (91%)	32 (9%)	8	31
3	C	302/347 (87%)	282 (93%)	20 (7%)	15	42
4	D	247/250 (99%)	235 (95%)	12 (5%)	22	49
5	E	190/251 (76%)	178 (94%)	12 (6%)	16	43
6	F	196/215 (91%)	177 (90%)	19 (10%)	8	30
7	G	200/272 (74%)	186 (93%)	14 (7%)	14	40
8	H	169/171 (99%)	155 (92%)	14 (8%)	10	35
9	I	175/181 (97%)	161 (92%)	14 (8%)	11	36
10	J	143/149 (96%)	132 (92%)	11 (8%)	12	37
11	L	175/176 (99%)	165 (94%)	10 (6%)	18	45
12	M	117/161 (73%)	109 (93%)	8 (7%)	14	41
13	N	171/172 (99%)	162 (95%)	9 (5%)	20	47
14	O	171/173 (99%)	155 (91%)	16 (9%)	8	31
15	P	134/163 (82%)	129 (96%)	5 (4%)	30	56
16	Q	164/165 (99%)	151 (92%)	13 (8%)	11	36
17	R	159/175 (91%)	143 (90%)	16 (10%)	7	28
18	S	157/157 (100%)	144 (92%)	13 (8%)	10	35
19	T	139/140 (99%)	128 (92%)	11 (8%)	11	36
20	U	89/114 (78%)	87 (98%)	2 (2%)	45	65
21	V	101/107 (94%)	88 (87%)	13 (13%)	4	21
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	100 (94%)	6 (6%)	18	45
24	Y	124/135 (92%)	117 (94%)	7 (6%)	19	46
25	Z	117/118 (99%)	113 (97%)	4 (3%)	32	58
26	a	119/120 (99%)	116 (98%)	3 (2%)	42	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	84/184 (46%)	81 (96%)	3 (4%)	31	57
28	c	84/98 (86%)	77 (92%)	7 (8%)	10	35
29	d	98/110 (89%)	86 (88%)	12 (12%)	5	22
30	e	114/121 (94%)	103 (90%)	11 (10%)	8	30
31	f	88/89 (99%)	81 (92%)	7 (8%)	11	36
32	g	98/100 (98%)	90 (92%)	8 (8%)	10	35
33	h	109/110 (99%)	105 (96%)	4 (4%)	30	56
34	i	86/89 (97%)	81 (94%)	5 (6%)	18	45
35	j	73/80 (91%)	68 (93%)	5 (7%)	14	41
36	k	64/65 (98%)	61 (95%)	3 (5%)	23	50
37	l	47/48 (98%)	46 (98%)	1 (2%)	47	66
38	m	48/90 (53%)	45 (94%)	3 (6%)	16	43
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	35
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	47
41	p	74/75 (99%)	71 (96%)	3 (4%)	27	53
42	r	108/121 (89%)	95 (88%)	13 (12%)	5	23
43	s	164/258 (64%)	158 (96%)	6 (4%)	30	56
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	59
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	161 (89%)	19 (11%)	6	27
53	BB	194/231 (84%)	174 (90%)	20 (10%)	7	28
54	CC	187/225 (83%)	172 (92%)	15 (8%)	11	36
55	DD	190/202 (94%)	172 (90%)	18 (10%)	8	31
56	EE	224/225 (100%)	208 (93%)	16 (7%)	13	39
57	FF	158/170 (93%)	151 (96%)	7 (4%)	25	51
58	GG	207/218 (95%)	187 (90%)	20 (10%)	8	30
59	HH	165/174 (95%)	151 (92%)	14 (8%)	10	34
60	II	178/180 (99%)	166 (93%)	12 (7%)	15	41
61	JJ	161/168 (96%)	142 (88%)	19 (12%)	5	23
62	KK	87/136 (64%)	82 (94%)	5 (6%)	18	45
63	LL	130/142 (92%)	112 (86%)	18 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	MM	99/108 (92%)	86 (87%)	13 (13%)	4	20
65	NN	130/131 (99%)	117 (90%)	13 (10%)	7	29
66	OO	106/130 (82%)	99 (93%)	7 (7%)	15	42
67	PP	109/130 (84%)	98 (90%)	11 (10%)	7	28
68	QQ	117/121 (97%)	108 (92%)	9 (8%)	12	37
69	RR	119/121 (98%)	109 (92%)	10 (8%)	10	34
70	SS	125/132 (95%)	109 (87%)	16 (13%)	4	21
71	TT	111/115 (96%)	102 (92%)	9 (8%)	11	35
72	UU	92/107 (86%)	83 (90%)	9 (10%)	7	30
73	VV	67/67 (100%)	63 (94%)	4 (6%)	17	44
74	WW	112/113 (99%)	102 (91%)	10 (9%)	9	33
75	XX	113/115 (98%)	105 (93%)	8 (7%)	13	39
76	YY	107/112 (96%)	91 (85%)	16 (15%)	3	17
77	ZZ	66/103 (64%)	58 (88%)	8 (12%)	5	22
78	aa	88/98 (90%)	75 (85%)	13 (15%)	3	17
79	bb	75/76 (99%)	66 (88%)	9 (12%)	5	23
80	cc	55/62 (89%)	49 (89%)	6 (11%)	6	26
81	dd	48/49 (98%)	46 (96%)	2 (4%)	26	52
82	ee	46/106 (43%)	39 (85%)	7 (15%)	3	16
83	ff	61/140 (44%)	55 (90%)	6 (10%)	7	30
84	gg	272/275 (99%)	257 (94%)	15 (6%)	19	46
86	ii	326/353 (92%)	310 (95%)	16 (5%)	22	49
87	jj	358/608 (59%)	331 (92%)	27 (8%)	12	38
All	All	10733/12306 (87%)	9907 (92%)	826 (8%)	14	37

All (826) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	123	ARG
1	A	128	ARG
1	A	163	ARG

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	233	ARG
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
2	B	73	VAL
2	B	74	GLU
2	B	90	VAL
2	B	97	ARG
2	B	103	LYS
2	B	115	LYS
2	B	135	LYS
2	B	146	LEU
2	B	214	ASP
2	B	231	VAL
2	B	234	ARG
2	B	244	THR
2	B	248	LEU
2	B	258	HIS
2	B	262	VAL
2	B	268	ARG
2	B	279	GLU
2	B	294	LYS
2	B	298	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	352	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	7	LEU
3	C	20	LYS
3	C	29	LYS

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Mol	Chain	Res	Type
3	C	84	THR
3	C	95	MET
3	C	113	ARG
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	232	VAL
3	C	246	VAL
3	C	272	SER
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
3	C	322	LEU
4	D	22	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	110	LEU
4	D	123	VAL
4	D	124	GLU
4	D	208	MET
4	D	262	LYS
4	D	264	LYS
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	197	VAL
5	E	213	LYS
5	E	242	LYS
5	E	289	LEU
5	E	291	PHE
6	F	38	GLN

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Mol	Chain	Res	Type
6	F	46	ARG
6	F	65	ARG
6	F	73	MET
6	F	88	LEU
6	F	97	ILE
6	F	100	VAL
6	F	115	GLN
6	F	120	THR
6	F	123	LYS
6	F	128	SER
6	F	134	ILE
6	F	151	GLU
6	F	178	LEU
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	245	ARG
6	F	246	MET
7	G	105	THR
7	G	139	VAL
7	G	148	LEU
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	207	LEU
7	G	220	VAL
7	G	221	VAL
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	260	VAL
7	G	312	LYS
8	H	41	ILE
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	82	LYS
8	H	105	ILE
8	H	108	ASN
8	H	128	MET

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Mol	Chain	Res	Type
8	H	129	ARG
8	H	141	LYS
8	H	149	ASN
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	76	MET
9	I	97	ILE
9	I	116	ARG
9	I	142	LEU
9	I	148	VAL
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	195	CYS
9	I	200	ILE
9	I	208	LYS
9	I	212	LEU
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	72	CYS
10	J	81	GLU
10	J	83	LEU
10	J	96	LYS
10	J	113	ILE
10	J	136	ARG
10	J	167	GLN
10	J	175	LEU
11	L	10	LEU
11	L	58	ILE
11	L	59	VAL
11	L	63	THR
11	L	74	ARG
11	L	92	ARG
11	L	106	SER
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG
12	M	2	VAL
12	M	37	LEU
12	M	57	LEU

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Mol	Chain	Res	Type
12	M	61	ILE
12	M	62	LEU
12	M	89	THR
12	M	96	GLU
12	M	105	THR
13	N	9	GLU
13	N	15	GLN
13	N	36	LEU
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	89	VAL
13	N	121	VAL
13	N	182	HIS
14	O	16	LEU
14	O	27	VAL
14	O	37	ARG
14	O	49	ARG
14	O	61	ARG
14	O	67	SER
14	O	82	ARG
14	O	85	ARG
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	24	VAL
15	P	69	ARG
15	P	86	LYS
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	31	LEU
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG

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Mol	Chain	Res	Type
16	Q	91	ARG
16	Q	95	VAL
16	Q	101	CYS
16	Q	115	LYS
16	Q	138	LEU
16	Q	143	ARG
17	R	6	LEU
17	R	15	LEU
17	R	36	ASN
17	R	40	GLN
17	R	41	ILE
17	R	50	ILE
17	R	52	ARG
17	R	63	CYS
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	106	LEU
17	R	113	LYS
17	R	138	LEU
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	13	VAL
18	S	17	LEU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	75	VAL
18	S	95	ARG
18	S	102	THR
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	17	ARG
19	T	33	ILE
19	T	45	MET
19	T	52	MET
19	T	60	LYS
19	T	96	ILE

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Mol	Chain	Res	Type
19	T	117	LYS
19	T	144	ASN
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	83	LEU
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	35	LYS
21	V	45	ILE
21	V	57	VAL
21	V	60	MET
21	V	69	LYS
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	97	VAL
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	28	LYS
24	Y	50	ARG
24	Y	55	VAL
24	Y	72	GLN
24	Y	104	VAL
25	Z	3	LYS
25	Z	11	VAL
25	Z	33	THR
25	Z	83	THR
26	a	4	ARG
26	a	84	GLU
26	a	122	VAL
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS

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Mol	Chain	Res	Type
28	c	23	LYS
28	c	37	MET
28	c	50	ASN
28	c	78	ASN
28	c	81	LEU
28	c	83	THR
28	c	92	CYS
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	56	GLU
29	d	78	ARG
29	d	79	ASN
29	d	90	ARG
29	d	98	SER
29	d	105	LEU
29	d	117	LEU
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	87	VAL
30	e	106	LYS
30	e	128	ARG
31	f	5	LEU
31	f	7	CYS
31	f	23	GLU
31	f	28	LEU
31	f	33	VAL
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	22	LEU
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG

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Mol	Chain	Res	Type
32	g	66	ARG
32	g	90	ARG
32	g	114	GLN
33	h	16	GLU
33	h	28	LEU
33	h	67	GLU
33	h	89	ARG
34	i	33	LEU
34	i	34	THR
34	i	48	CYS
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	13	ASN
35	j	58	THR
35	j	79	ARG
35	j	80	GLU
36	k	37	ARG
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
41	p	62	LYS
41	p	70	THR
42	r	8	MET
42	r	14	SER
42	r	18	ILE
42	r	20	ARG
42	r	32	LEU
42	r	35	ARG
42	r	39	ARG
42	r	60	VAL

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Mol	Chain	Res	Type
42	r	67	ARG
42	r	80	THR
42	r	90	LEU
42	r	103	HIS
42	r	118	LEU
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	72	GLU
44	t	98	ILE
44	t	133	LEU
52	AA	9	GLN
52	AA	12	GLU
52	AA	25	LEU
52	AA	44	ASP
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	122	LEU
52	AA	124	VAL
52	AA	132	GLN
52	AA	134	LEU
52	AA	136	GLU
52	AA	142	LEU
52	AA	163	CYS
52	AA	170	SER
52	AA	178	LEU
53	BB	29	ASP
53	BB	38	MET
53	BB	50	THR
53	BB	63	LYS
53	BB	71	LEU
53	BB	82	ARG
53	BB	83	LYS
53	BB	96	CYS

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Mol	Chain	Res	Type
53	BB	105	LEU
53	BB	125	VAL
53	BB	139	CYS
53	BB	157	GLN
53	BB	175	GLU
53	BB	180	ASP
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
53	BB	231	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	115	GLN
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	139	LEU
54	CC	160	LEU
54	CC	167	ARG
54	CC	188	CYS
54	CC	192	LEU
54	CC	235	ASN
54	CC	244	ILE
54	CC	251	LEU
54	CC	255	LEU
55	DD	28	GLU
55	DD	31	GLU
55	DD	45	ARG
55	DD	51	LEU
55	DD	65	ARG
55	DD	72	VAL
55	DD	126	ILE
55	DD	127	MET
55	DD	134	CYS
55	DD	142	LEU
55	DD	146	ARG
55	DD	160	SER
55	DD	168	VAL
55	DD	170	THR
55	DD	190	LEU

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Mol	Chain	Res	Type
55	DD	206	ASP
55	DD	212	GLU
55	DD	218	LEU
56	EE	6	LYS
56	EE	17	HIS
56	EE	41	CYS
56	EE	42	LEU
56	EE	51	ARG
56	EE	66	MET
56	EE	77	ARG
56	EE	108	ARG
56	EE	115	THR
56	EE	165	GLU
56	EE	171	ASP
56	EE	194	VAL
56	EE	222	LEU
56	EE	232	ASN
56	EE	246	LEU
56	EE	247	THR
57	FF	36	GLN
57	FF	63	LYS
57	FF	88	MET
57	FF	89	THR
57	FF	122	ARG
57	FF	125	SER
57	FF	204	ARG
58	GG	26	THR
58	GG	41	LEU
58	GG	59	GLN
58	GG	63	MET
58	GG	67	VAL
58	GG	72	ARG
58	GG	76	LEU
58	GG	95	LYS
58	GG	103	ASP
58	GG	107	SER
58	GG	108	VAL
58	GG	150	GLU
58	GG	171	THR
58	GG	178	ARG
58	GG	181	THR
58	GG	183	ARG

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Mol	Chain	Res	Type
58	GG	190	ARG
58	GG	216	ARG
58	GG	230	LYS
58	GG	237	LEU
59	HH	8	ILE
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	61	ILE
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	105	THR
59	HH	119	SER
59	HH	132	ASP
59	HH	145	ARG
59	HH	158	LEU
60	II	6	ASP
60	II	10	LYS
60	II	23	LYS
60	II	49	ARG
60	II	59	ARG
60	II	92	ARG
60	II	121	LEU
60	II	130	THR
60	II	161	LEU
60	II	168	GLN
60	II	175	ILE
60	II	178	ARG
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	80	ARG
61	JJ	86	VAL
61	JJ	89	GLU
61	JJ	95	ASP
61	JJ	103	GLU
61	JJ	109	ARG

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Mol	Chain	Res	Type
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	128	VAL
61	JJ	131	ARG
61	JJ	133	ARG
61	JJ	169	ARG
61	JJ	175	ARG
62	KK	1	MET
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	54	THR
63	LL	56	ILE
63	LL	66	VAL
63	LL	69	ARG
63	LL	85	THR
63	LL	108	ASN
63	LL	110	SER
63	LL	111	VAL
63	LL	121	GLN
63	LL	126	VAL
63	LL	132	ARG
63	LL	134	LEU
63	LL	153	LYS
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	45	ARG
64	MM	49	LEU
64	MM	69	CYS
64	MM	76	LEU
64	MM	77	ILE
64	MM	83	LYS
64	MM	85	LEU
64	MM	99	LYS

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Mol	Chain	Res	Type
64	MM	101	ARG
65	NN	27	LYS
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	76	LYS
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
65	NN	134	VAL
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	104	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	45	LEU
67	PP	65	LYS
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	108	LYS
67	PP	126	VAL
68	QQ	7	LEU
68	QQ	31	LEU
68	QQ	40	GLU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	53	GLU
68	QQ	67	ASP
68	QQ	89	SER
68	QQ	140	ARG
69	RR	31	ASN

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Mol	Chain	Res	Type
69	RR	44	LYS
69	RR	49	LYS
69	RR	62	GLN
69	RR	78	ARG
69	RR	97	GLU
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	10	GLN
70	SS	13	LEU
70	SS	14	ARG
70	SS	21	ASP
70	SS	36	VAL
70	SS	46	ARG
70	SS	49	ASP
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	63	GLU
70	SS	83	PHE
70	SS	115	LYS
70	SS	132	ARG
71	TT	37	VAL
71	TT	39	LEU
71	TT	55	THR
71	TT	62	ARG
71	TT	90	SER
71	TT	102	ARG
71	TT	110	LEU
71	TT	124	THR
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	33	GLU
72	UU	56	MET
72	UU	68	THR
72	UU	79	ARG
72	UU	90	ASP
72	UU	106	ILE

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Mol	Chain	Res	Type
72	UU	111	GLU
73	VV	1	MET
73	VV	11	LEU
73	VV	64	GLU
73	VV	68	SER
74	WW	7	LEU
74	WW	18	GLU
74	WW	23	ARG
74	WW	51	GLU
74	WW	52	ILE
74	WW	65	LEU
74	WW	84	LYS
74	WW	92	ASN
74	WW	97	ARG
74	WW	103	VAL
75	XX	18	ARG
75	XX	29	LYS
75	XX	45	SER
75	XX	61	GLN
75	XX	67	ARG
75	XX	105	PHE
75	XX	115	ILE
75	XX	127	ASN
76	YY	9	THR
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	40	ILE
76	YY	44	LEU
76	YY	46	LYS
76	YY	47	MET
76	YY	61	ARG
76	YY	74	MET
76	YY	80	ASP
76	YY	88	LYS
76	YY	101	LYS
76	YY	106	GLN
76	YY	114	MET
76	YY	115	LYS
77	ZZ	52	LYS
77	ZZ	54	THR
77	ZZ	59	CYS

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Mol	Chain	Res	Type
77	ZZ	74	SER
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	106	GLN
78	aa	2	THR
78	aa	12	LYS
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	34	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	55	GLU
78	aa	81	SER
78	aa	96	THR
78	aa	100	ARG
79	bb	11	SER
79	bb	17	ARG
79	bb	37	CYS
79	bb	42	LYS
79	bb	48	SER
79	bb	64	CYS
79	bb	77	CYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	18	LEU
80	cc	20	ARG
80	cc	30	VAL
80	cc	40	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	6	LEU
81	dd	49	ASP
82	ee	85	VAL
82	ee	97	LYS
82	ee	99	LYS
82	ee	108	ARG
82	ee	109	MET
82	ee	113	ARG
82	ee	121	THR

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Mol	Chain	Res	Type
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	125	GLU
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	87	LEU
84	gg	113	PHE
84	gg	149	GLU
84	gg	198	VAL
84	gg	207	CYS
84	gg	258	ILE
84	gg	273	GLU
84	gg	287	THR
84	gg	289	LEU
84	gg	298	LEU
84	gg	305	ASN
84	gg	306	LEU
86	ii	8	ILE
86	ii	40	ARG
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	112	LEU
86	ii	149	ILE
86	ii	170	LYS
86	ii	172	LYS
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	264	VAL
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU

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Mol	Chain	Res	Type
87	jj	313	LEU
87	jj	325	THR
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	551	SER
87	jj	557	MET
87	jj	585	ILE
87	jj	600	VAL
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	140	ASN
1	A	205	ASN
1	A	215	ASN
1	A	217	GLN
2	B	55	HIS
2	B	109	HIS
2	B	204	GLN
2	B	245	HIS
2	B	354	GLN
3	C	187	GLN
3	C	215	ASN
3	C	310	HIS
4	D	17	GLN
4	D	191	ASN
4	D	244	HIS

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Mol	Chain	Res	Type
5	E	194	GLN
6	F	57	HIS
6	F	79	ASN
7	G	135	GLN
7	G	143	GLN
7	G	206	GLN
7	G	259	GLN
7	G	261	ASN
8	H	15	ASN
8	H	98	HIS
9	I	73	ASN
9	I	95	HIS
9	I	123	GLN
9	I	144	ASN
9	I	147	HIS
10	J	97	ASN
11	L	115	GLN
13	N	15	GLN
13	N	86	HIS
14	O	50	ASN
14	O	65	ASN
14	O	96	GLN
14	O	150	GLN
15	P	56	GLN
16	Q	40	ASN
16	Q	57	ASN
16	Q	188	ASN
17	R	34	ASN
17	R	130	ASN
18	S	50	GLN
18	S	125	GLN
18	S	163	HIS
19	T	98	HIS
22	W	30	GLN
22	W	48	GLN
23	X	73	HIS
23	X	93	ASN
23	X	105	ASN
24	Y	18	HIS
24	Y	56	GLN
24	Y	100	HIS
26	a	19	HIS

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Mol	Chain	Res	Type
27	b	10	HIS
27	b	60	ASN
28	c	50	ASN
28	c	73	HIS
29	d	30	HIS
29	d	100	ASN
30	e	92	ASN
31	f	65	ASN
31	f	78	HIS
32	g	110	GLN
33	h	65	GLN
33	h	108	GLN
38	m	91	HIS
40	o	19	GLN
40	o	36	GLN
41	p	56	HIS
42	r	85	ASN
43	s	34	ASN
43	s	126	GLN
43	s	179	ASN
44	t	65	GLN
44	t	95	GLN
52	AA	36	GLN
52	AA	111	GLN
53	BB	92	GLN
53	BB	159	GLN
53	BB	202	GLN
53	BB	208	HIS
54	CC	136	HIS
54	CC	178	HIS
55	DD	145	GLN
56	EE	67	GLN
56	EE	98	ASN
56	EE	188	ASN
56	EE	260	GLN
57	FF	83	ASN
57	FF	95	HIS
57	FF	101	HIS
57	FF	118	ASN
58	GG	13	GLN
58	GG	105	ASN
58	GG	186	GLN

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Mol	Chain	Res	Type
58	GG	187	HIS
59	HH	76	GLN
59	HH	162	GLN
59	HH	168	HIS
60	II	7	ASN
60	II	88	ASN
60	II	146	GLN
60	II	155	ASN
61	JJ	113	GLN
62	KK	28	HIS
62	KK	42	ASN
63	LL	39	ASN
63	LL	65	ASN
64	MM	55	ASN
65	NN	49	GLN
65	NN	90	HIS
66	OO	20	GLN
66	OO	26	ASN
66	OO	79	GLN
66	OO	83	GLN
67	PP	35	GLN
67	PP	98	ASN
68	QQ	35	ASN
69	RR	31	ASN
69	RR	121	GLN
69	RR	127	ASN
70	SS	10	GLN
70	SS	73	ASN
70	SS	135	HIS
73	VV	47	ASN
73	VV	49	GLN
74	WW	92	ASN
75	XX	31	HIS
75	XX	77	ASN
76	YY	85	ASN
78	aa	7	ASN
78	aa	86	ASN
79	bb	26	GLN
79	bb	49	HIS
79	bb	83	GLN
79	bb	84	HIS
81	dd	10	HIS

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Mol	Chain	Res	Type
83	ff	93	HIS
84	gg	64	HIS
84	gg	76	GLN
84	gg	159	ASN
84	gg	196	ASN
84	gg	222	ASN
86	ii	107	ASN
86	ii	188	GLN
86	ii	216	GLN
86	ii	244	HIS
86	ii	358	GLN
87	jj	268	HIS
87	jj	279	HIS
87	jj	361	GLN
87	jj	385	GLN
87	jj	389	HIS
87	jj	473	GLN
87	jj	537	HIS
87	jj	549	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	21 (29%)	1 (1%)
48	5	3511/3543 (99%)	899 (25%)	182 (5%)
49	7	119/120 (99%)	13 (10%)	1 (0%)
50	8	149/156 (95%)	38 (25%)	6 (4%)
51	9	1683/1869 (90%)	444 (26%)	85 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5615/5847 (96%)	1434 (25%)	275 (4%)

All (1434) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	14	A
46	2	16	C
46	2	19	G
46	2	21	A

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Mol	Chain	Res	Type
46	2	42	A
46	2	43	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	58	A
46	2	61	C
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	72	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	17	A
48	5	25	A
48	5	30	C
48	5	36	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G

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Mol	Chain	Res	Type
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	75	G
48	5	84	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	122	U
48	5	125	C
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C

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Mol	Chain	Res	Type
48	5	221	C
48	5	224	U
48	5	225	G
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	236	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	265	C
48	5	266	C
48	5	267	G
48	5	275	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	321	U
48	5	322	C
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	365	U
48	5	386	A
48	5	387	G
48	5	388	A
48	5	399	G
48	5	401	G
48	5	407	A

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Mol	Chain	Res	Type
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	417	G
48	5	418	A
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	647	G
48	5	649	A
48	5	654	C
48	5	658	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	684	G

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Mol	Chain	Res	Type
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	739	G
48	5	742	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	750	U
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	938	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A

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Mol	Chain	Res	Type
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	970	G
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1195	G
48	5	1209	U
48	5	1210	C
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C

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Mol	Chain	Res	Type
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1412	G
48	5	1416	G
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1422	G
48	5	1429	C
48	5	1432	G

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Mol	Chain	Res	Type
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1503	A
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1524	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C

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Mol	Chain	Res	Type
48	5	1568	C
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1649	U
48	5	1652	U
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1676	C
48	5	1677	U
48	5	1678	C
48	5	1679	A
48	5	1691	G
48	5	1694	C
48	5	1724	G
48	5	1729	A
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G

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Mol	Chain	Res	Type
48	5	1768	C
48	5	1770	A
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1785	C
48	5	1787	A
48	5	1799	G
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1890	G
48	5	1892	A
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1938	C
48	5	1948	G
48	5	1951	G
48	5	1952	G
48	5	1961	G

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Mol	Chain	Res	Type
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2017	A
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2044	U
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2068	C
48	5	2069	A
48	5	2072	C
48	5	2084	U
48	5	2085	G
48	5	2089	G

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Mol	Chain	Res	Type
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2274	C
48	5	2275	G
48	5	2279	A
48	5	2280	G
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2325	C
48	5	2332	A
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2366	A

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Mol	Chain	Res	Type
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2402	G
48	5	2416	G
48	5	2417	A
48	5	2421	G
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2476	G
48	5	2479	G
48	5	2483	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2511	A
48	5	2513	A
48	5	2514	G
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2549	G
48	5	2553	A
48	5	2554	U
48	5	2555	G

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Mol	Chain	Res	Type
48	5	2564	G
48	5	2566	G
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2611	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2647	A
48	5	2660	A
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2670	C
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2760	G
48	5	2761	U

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Mol	Chain	Res	Type
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2788	U
48	5	2790	U
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2844	A
48	5	2855	G
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3618	C
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3667	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3692	A

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Mol	Chain	Res	Type
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3759	A
48	5	3760	A
48	5	3761	C
48	5	3765	G
48	5	3766	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3798	U
48	5	3799	A
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3824	A
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3843	C
48	5	3859	G

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Mol	Chain	Res	Type
48	5	3867	A
48	5	3874	G
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3888	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3927	U
48	5	3939	G
48	5	3941	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C

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Mol	Chain	Res	Type
48	5	4127	A
48	5	4138	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A
48	5	4218	U
48	5	4221	C
48	5	4222	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4237	C
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4266	G
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4292	A
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C

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Mol	Chain	Res	Type
48	5	4329	G
48	5	4330	G
48	5	4332	C
48	5	4335	C
48	5	4336	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4368	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4463	U
48	5	4464	A
48	5	4472	G
48	5	4474	A
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U

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Mol	Chain	Res	Type
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4572	U
48	5	4573	G
48	5	4575	G
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4618	G
48	5	4620	U
48	5	4636	U
48	5	4637	G
48	5	4652	G
48	5	4656	A
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4700	A
48	5	4701	A
48	5	4703	U
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G

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Mol	Chain	Res	Type
48	5	4728	U
48	5	4729	A
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4881	U
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4902	C
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4926	C

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Mol	Chain	Res	Type
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4981	G
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4994	G
48	5	4997	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5021	C
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C

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Mol	Chain	Res	Type
48	5	5056	A
48	5	5058	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	22	A
49	7	25	G
49	7	33	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	76	U
49	7	97	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A
50	8	21	C
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	90	C
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C

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Mol	Chain	Res	Type
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	153	C
50	8	156	U
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	64	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A

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Mol	Chain	Res	Type
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	173	A
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	292	A
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G

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Mol	Chain	Res	Type
51	9	309	G
51	9	312	G
51	9	313	A
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	363	A
51	9	364	A
51	9	368	U
51	9	370	G
51	9	372	U
51	9	379	C
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	453	C
51	9	459	C
51	9	460	A
51	9	462	C

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Mol	Chain	Res	Type
51	9	463	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	523	A
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	559	G
51	9	560	A
51	9	562	U
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U

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Mol	Chain	Res	Type
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	631	U
51	9	632	C
51	9	637	U
51	9	642	U
51	9	643	A
51	9	644	G
51	9	646	G
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G

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Mol	Chain	Res	Type
51	9	798	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	844	U
51	9	847	A
51	9	861	A
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	876	C
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	913	A
51	9	914	U
51	9	919	A
51	9	920	A
51	9	921	G
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	971	G
51	9	981	A
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1016	U

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Mol	Chain	Res	Type
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1087	A
51	9	1088	U
51	9	1100	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1137	U
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1230	C

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Mol	Chain	Res	Type
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1280	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1341	C
51	9	1342	U
51	9	1348	G
51	9	1369	A
51	9	1371	U
51	9	1372	U

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Mol	Chain	Res	Type
51	9	1376	A
51	9	1378	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1405	A
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1455	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1487	A
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1498	A
51	9	1509	U
51	9	1510	G
51	9	1519	U
51	9	1520	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A

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Mol	Chain	Res	Type
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1683	C
51	9	1686	G
51	9	1695	A
51	9	1698	C
51	9	1703	C
51	9	1715	A
51	9	1721	U
51	9	1722	G

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Mol	Chain	Res	Type
51	9	1726	G
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1744	G
51	9	1745	A
51	9	1748	G
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1851	A
51	9	1852	C
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (275) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	453	G
48	5	466	A
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G

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Mol	Chain	Res	Type
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1497	A
48	5	1523	A
48	5	1533	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A

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Mol	Chain	Res	Type
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2333	G
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2513	A
48	5	2529	A
48	5	2530	U
48	5	2546	G
48	5	2553	A
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2739	C
48	5	2754	G
48	5	2794	C

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Mol	Chain	Res	Type
48	5	2806	A
48	5	2845	A
48	5	2874	U
48	5	3603	G
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3760	A
48	5	3765	G
48	5	3784	A
48	5	3785	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	3938	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4257	A
48	5	4266	G
48	5	4291	G
48	5	4378	A
48	5	4379	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4510	A
48	5	4527	G

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Mol	Chain	Res	Type
48	5	4572	U
48	5	4699	U
48	5	4719	G
48	5	4753	U
48	5	4756	C
48	5	4872	G
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4944	C
48	5	4947	U
48	5	4965	U
48	5	5013	C
48	5	5047	C
49	7	109	U
50	8	2	G
50	8	51	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	128	U
51	9	141	A
51	9	142	C
51	9	160	U
51	9	182	C
51	9	214	U
51	9	293	C
51	9	312	G
51	9	360	A
51	9	363	A
51	9	369	C
51	9	434	G
51	9	465	A
51	9	492	C
51	9	500	A

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Mol	Chain	Res	Type
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	587	A
51	9	591	U
51	9	594	A
51	9	606	G
51	9	613	G
51	9	615	C
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	875	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1130	G
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1285	G
51	9	1313	A
51	9	1330	G
51	9	1394	G

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Mol	Chain	Res	Type
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1581	C
51	9	1621	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 272 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	$\# Z > 2$
90	GCP	jj	700	88	32,34,34	1.50	7 (21%)	49,54,54	1.73	7 (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
90	GCP	jj	700	88	-	3/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C5-C4	3.35	1.48	1.38
90	jj	700	GCP	PG-O3G	3.08	1.61	1.55
90	jj	700	GCP	PG-O2G	2.90	1.61	1.55
90	jj	700	GCP	PB-O3A	2.57	1.61	1.58
90	jj	700	GCP	PB-O2B	2.23	1.61	1.56
90	jj	700	GCP	C5-N7	-2.23	1.34	1.39
90	jj	700	GCP	C6-N1	-2.21	1.34	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C4-N3	-6.04	118.78	128.39
90	jj	700	GCP	C2-N3-C4	4.87	120.68	112.30
90	jj	700	GCP	N9-C4-N3	4.38	134.71	125.95
90	jj	700	GCP	C6-C5-N7	3.21	136.14	130.29
90	jj	700	GCP	C4-C5-N7	-2.71	106.37	110.67
90	jj	700	GCP	PB-O3A-PA	-2.60	123.88	132.37
90	jj	700	GCP	O6-C6-C5	-2.04	121.14	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O3A

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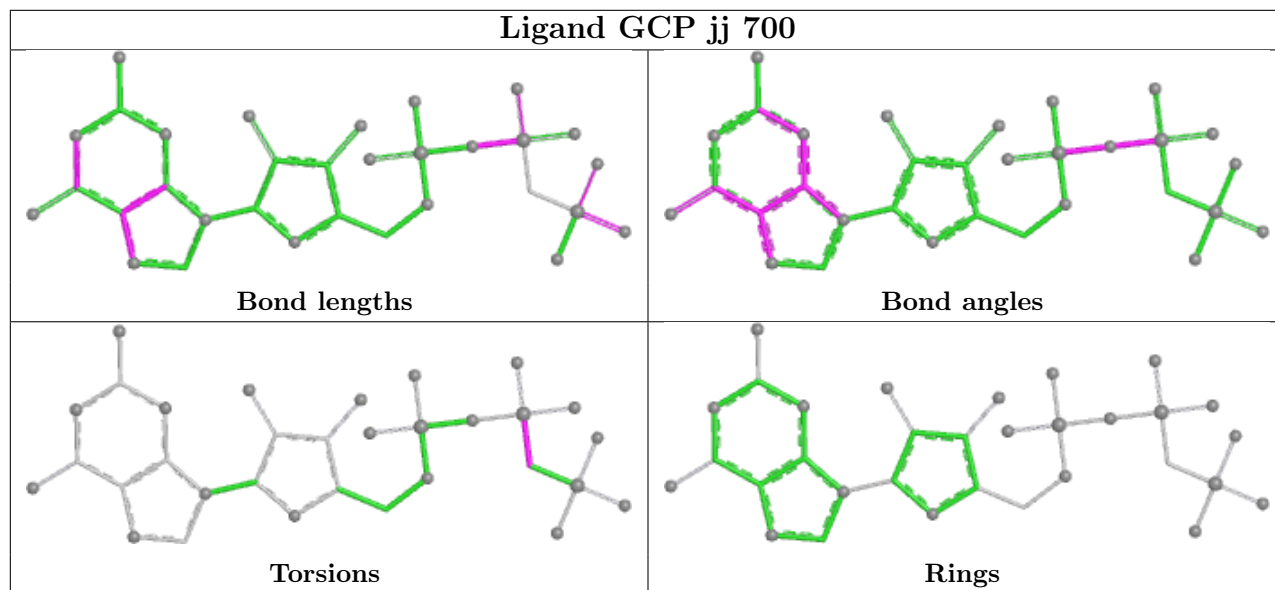
Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	jj	700	GCP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	42
51	9	8
47	3	2
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	40.91
1	5	1252:C	O3'	1271:G	P	36.05
1	5	1405:C	O3'	1406:G	P	23.79
1	5	1219:G	O3'	1233:G	P	22.30
1	5	1406:G	O3'	1406(A):G	P	20.51
1	5	3948:C	O3'	4065:G	P	19.69
1	5	990:C	O3'	1064:G	P	18.04
1	5	523:C	O3'	638:G	P	18.03
1	5	4138:C	O3'	4146:G	P	18.02
1	5	4101:C	O3'	4107:G	P	17.30
1	5	4777:C	O3'	4859:C	P	16.29
1	5	5022:U	O3'	5028:G	P	15.23
1	5	760:G	O3'	904:C	P	14.93
1	5	1696:C	O3'	1720:C	P	14.86
1	5	1364:U	O3'	1368:A	P	14.43
1	5	182:G	O3'	189:G	P	14.08
1	5	1406(C):G	O3'	1411:C	P	13.56
1	5	2901:G	O3'	3597:G	P	13.16
1	5	1411:C	O3'	1411(A):G	P	13.03
1	5	921:C	O3'	922:C	P	12.78
1	5	481:G	O3'	481(A):C	P	12.48
1	5	934:C	O3'	935:A	P	10.82
1	5	970:G	O3'	971:U	P	10.67
1	5	737:C	O3'	738:C	P	9.93
1	5	4729:A	O3'	4735:G	P	9.81
1	5	512:U	O3'	515:C	P	9.70
1	5	971:U	O3'	971(A):G	P	9.68
1	5	1180:C	O3'	1183:C	P	9.47
1	5	500:G	O3'	504:G	P	6.88
1	5	1100:U	O3'	1168:G	P	5.94
1	3	19:G	O3'	20:U	P	5.60
1	5	480:C	O3'	481:G	P	5.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	16:C	O3'	18:U	P	5.24
1	5	4740:G	O3'	4743:G	P	5.13
1	9	322:C	O3'	323:C	P	5.02
1	9	798:G	O3'	799:U	P	4.84
1	5	1239:C	O3'	1244:G	P	4.76
1	2	16:C	O3'	18:G	P	4.39
1	9	304:C	O3'	305:U	P	4.29
1	5	935:A	O3'	935(A):G	P	4.26
1	9	309:G	O3'	310:C	P	4.26
1	5	170:C	O3'	171:U	P	3.83
1	5	738:C	O3'	738(A):C	P	3.67
1	5	1438:U	O3'	1440:U	P	3.47
1	5	4899:G	O3'	4902:C	P	3.40
1	9	902:G	O3'	903:A	P	3.37
1	9	903:A	O3'	904:A	P	3.27
1	9	1295:A	O3'	1296:U	P	3.25
1	5	267:G	O3'	268:G	P	3.08
1	5	5020:G	O3'	5021:C	P	3.05
1	5	751:G	O3'	752:G	P	2.99
1	9	593:C	O3'	594:A	P	2.98
1	5	2031:C	O3'	2032:U	P	2.33

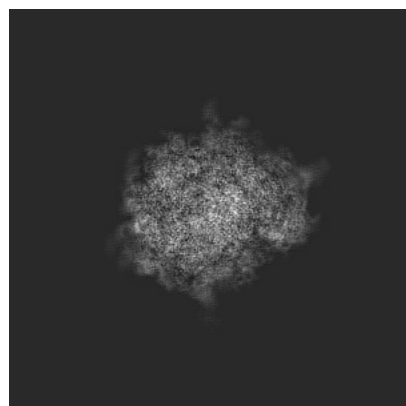
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4137. These allow visual inspection of the internal detail of the map and identification of artifacts.

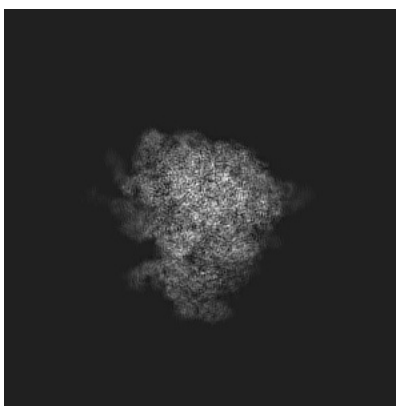
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

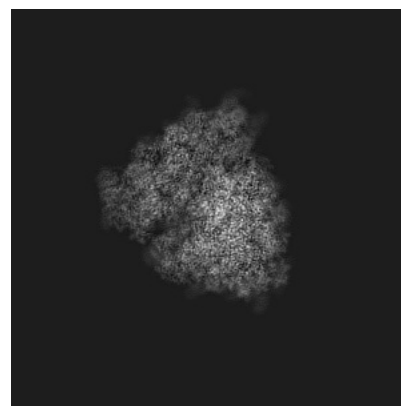
6.1.1 Primary map



X

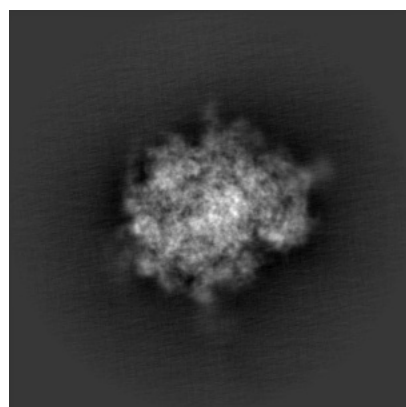


Y

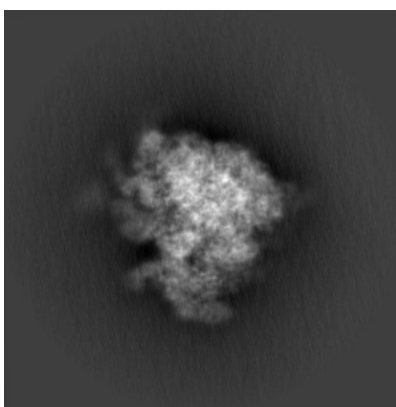


Z

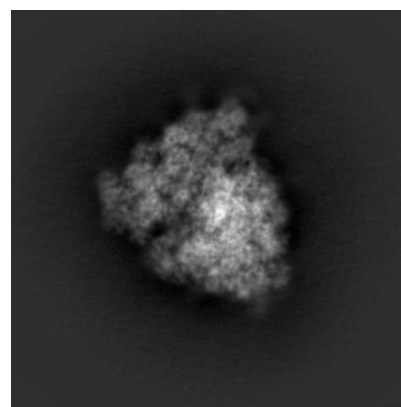
6.1.2 Raw map



X



Y

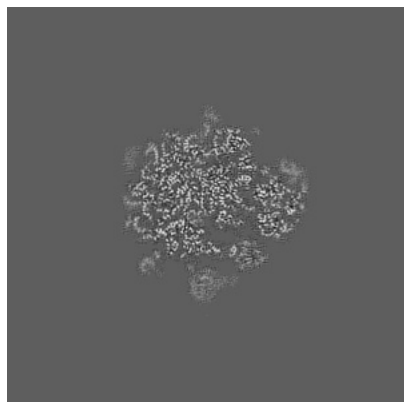


Z

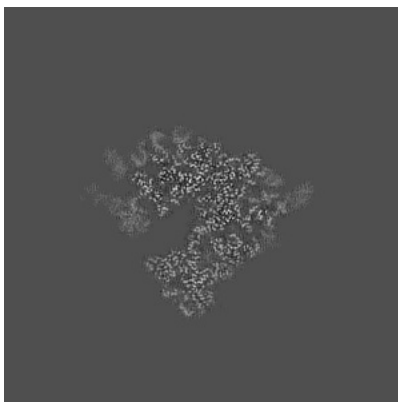
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

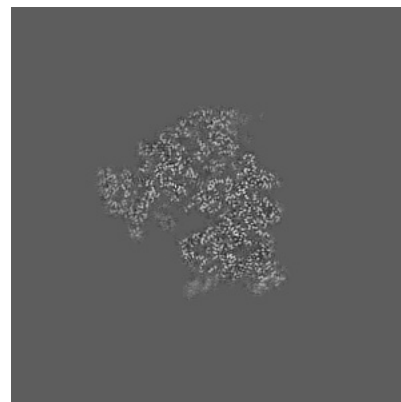
6.2.1 Primary map



X Index: 210

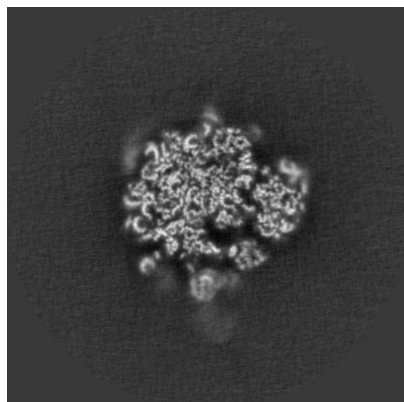


Y Index: 210

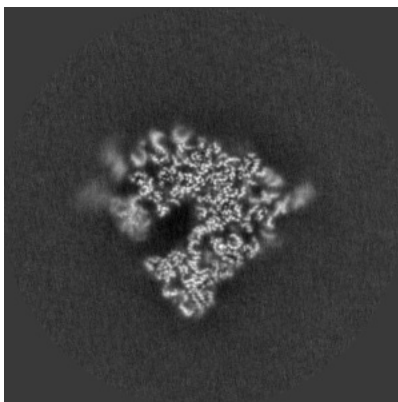


Z Index: 210

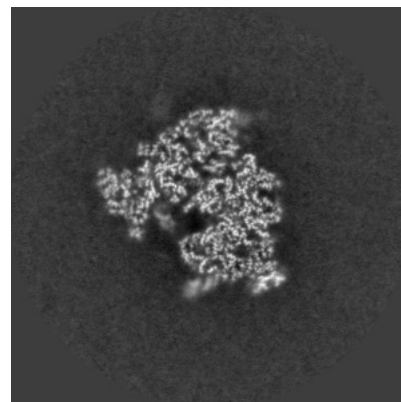
6.2.2 Raw map



X Index: 210



Y Index: 210

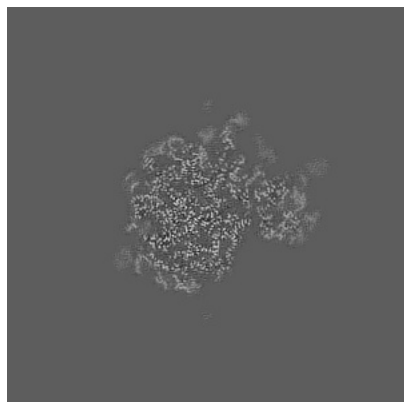


Z Index: 210

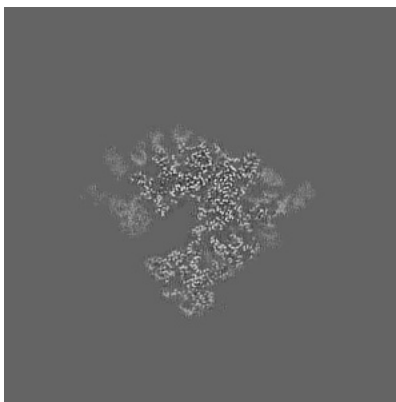
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

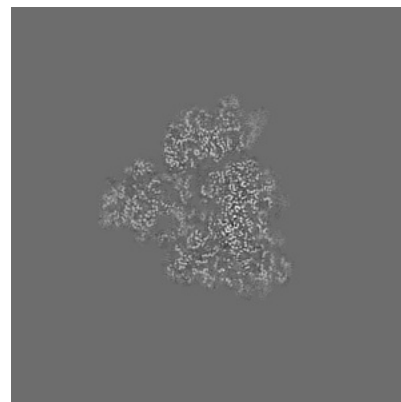
6.3.1 Primary map



X Index: 233

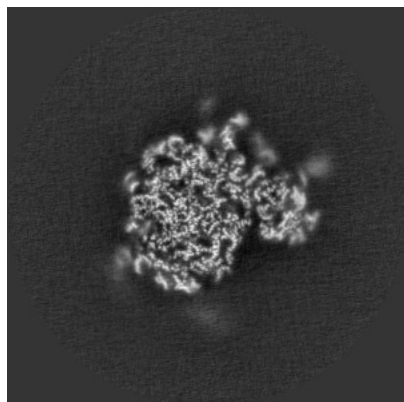


Y Index: 211

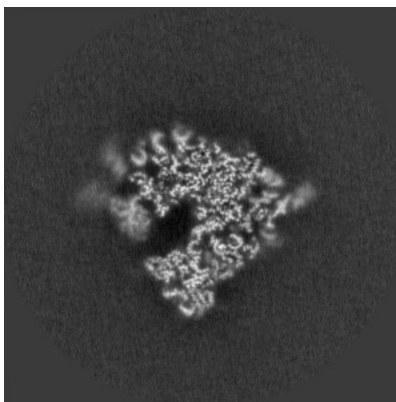


Z Index: 195

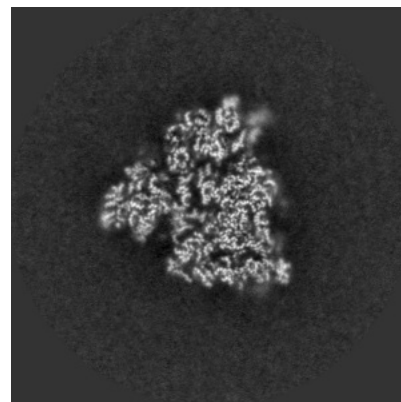
6.3.2 Raw map



X Index: 233



Y Index: 211

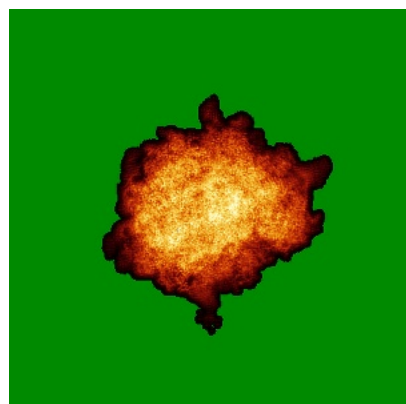


Z Index: 198

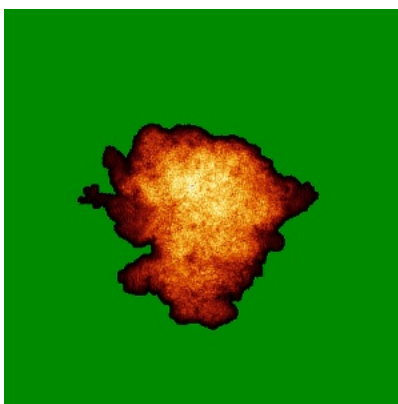
The images above show the largest variance slices of the map in three orthogonal directions.

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

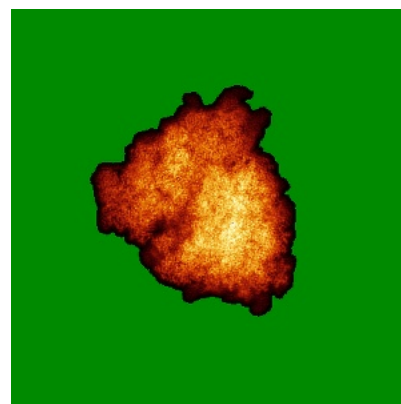
6.4.1 Primary map



X

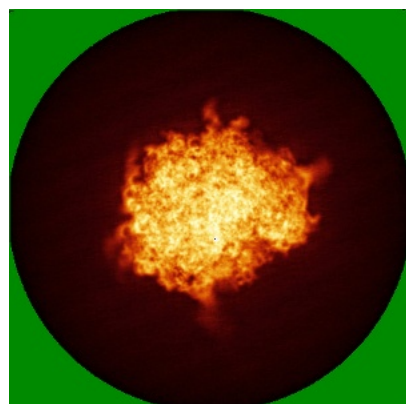


Y

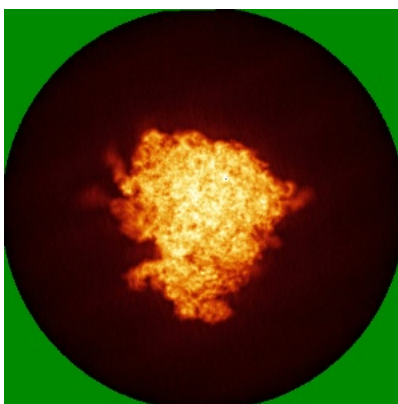


Z

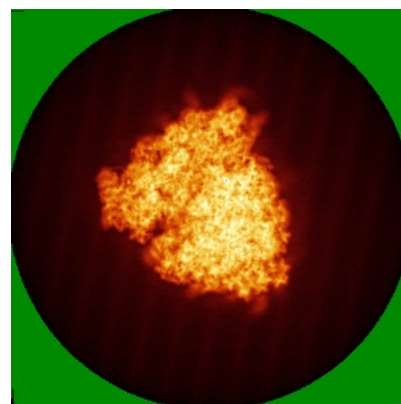
6.4.2 Raw map



X



Y

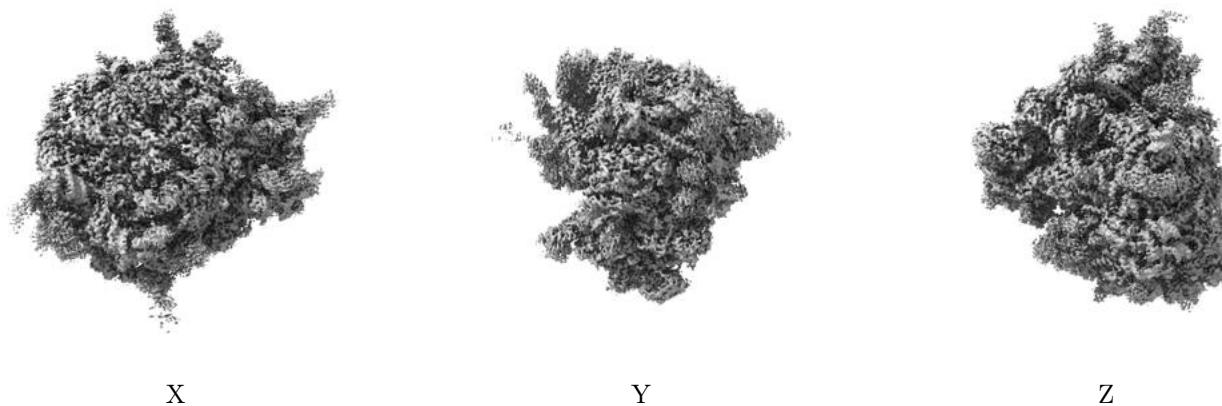


Z

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

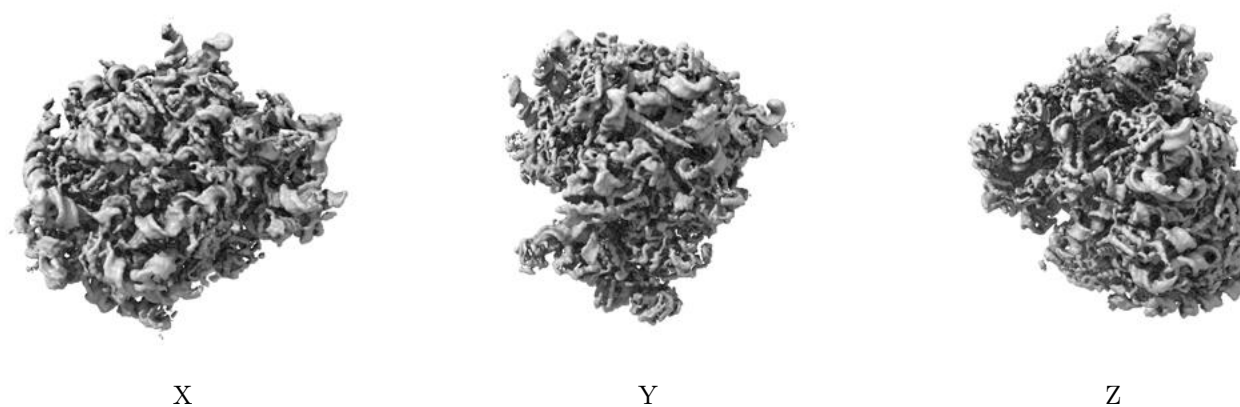
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

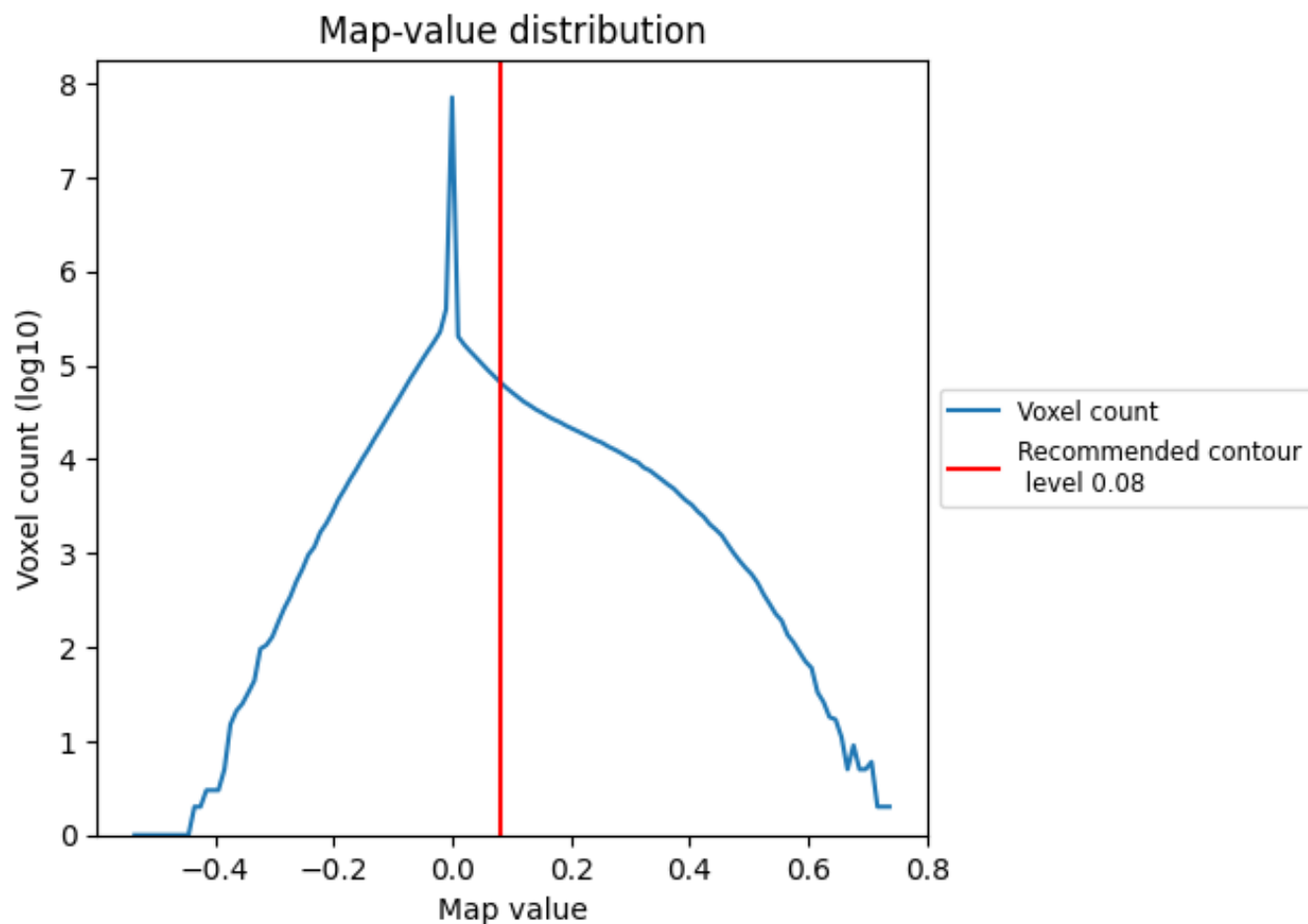
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

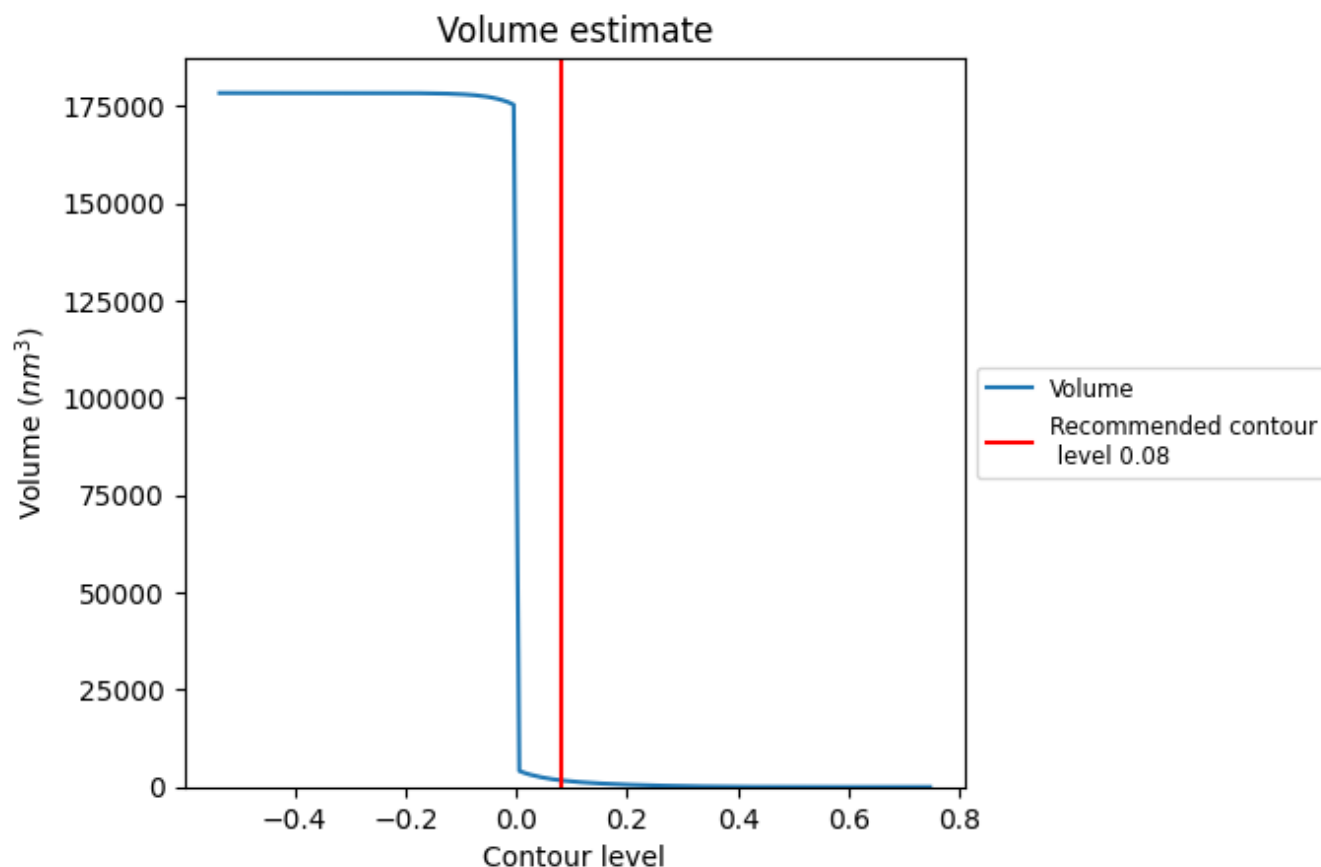
This section contains the results of statistical analysis of the map.

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.

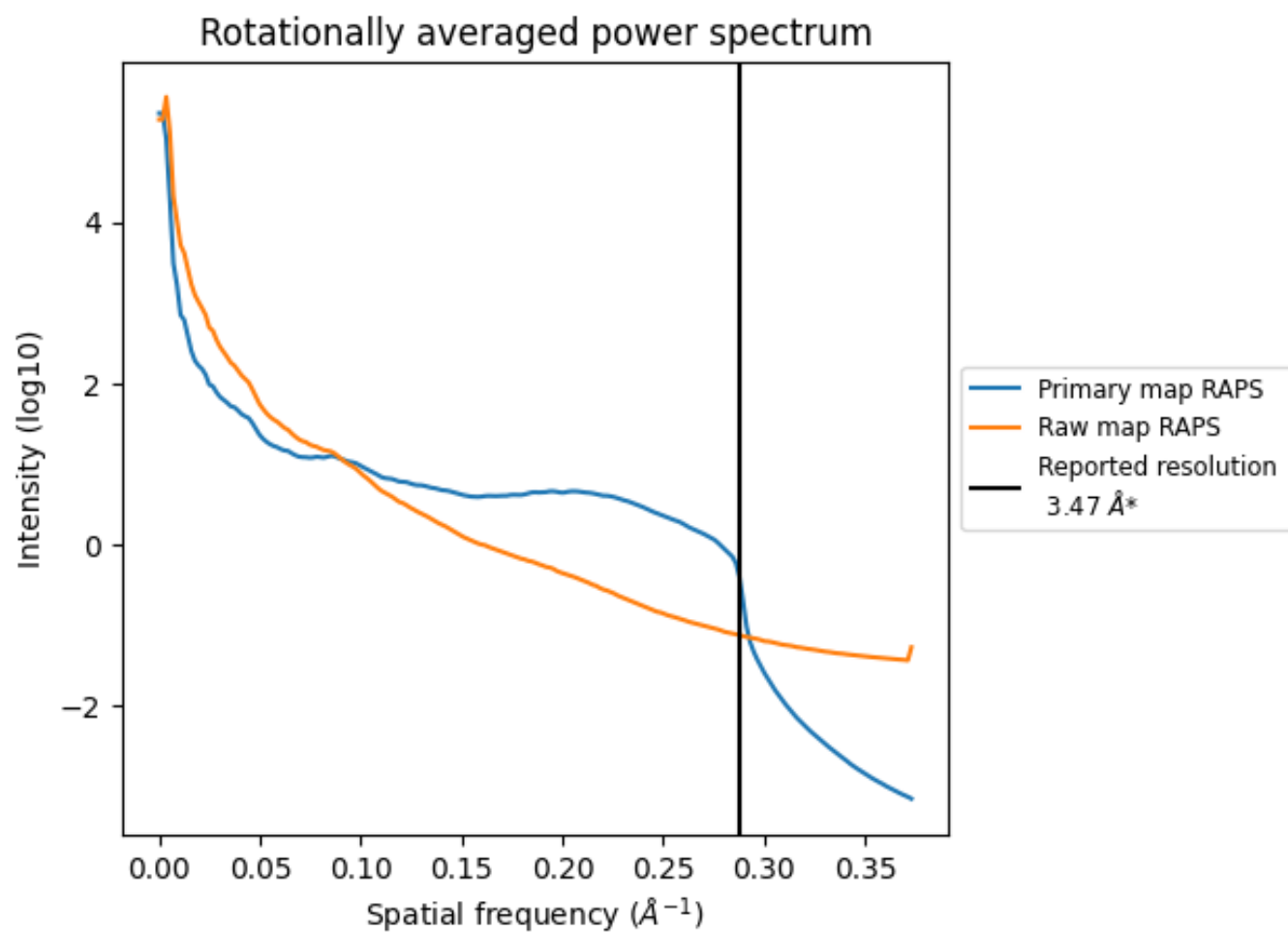
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1722 nm³; this corresponds to an approximate mass of 1556 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 ⓘ

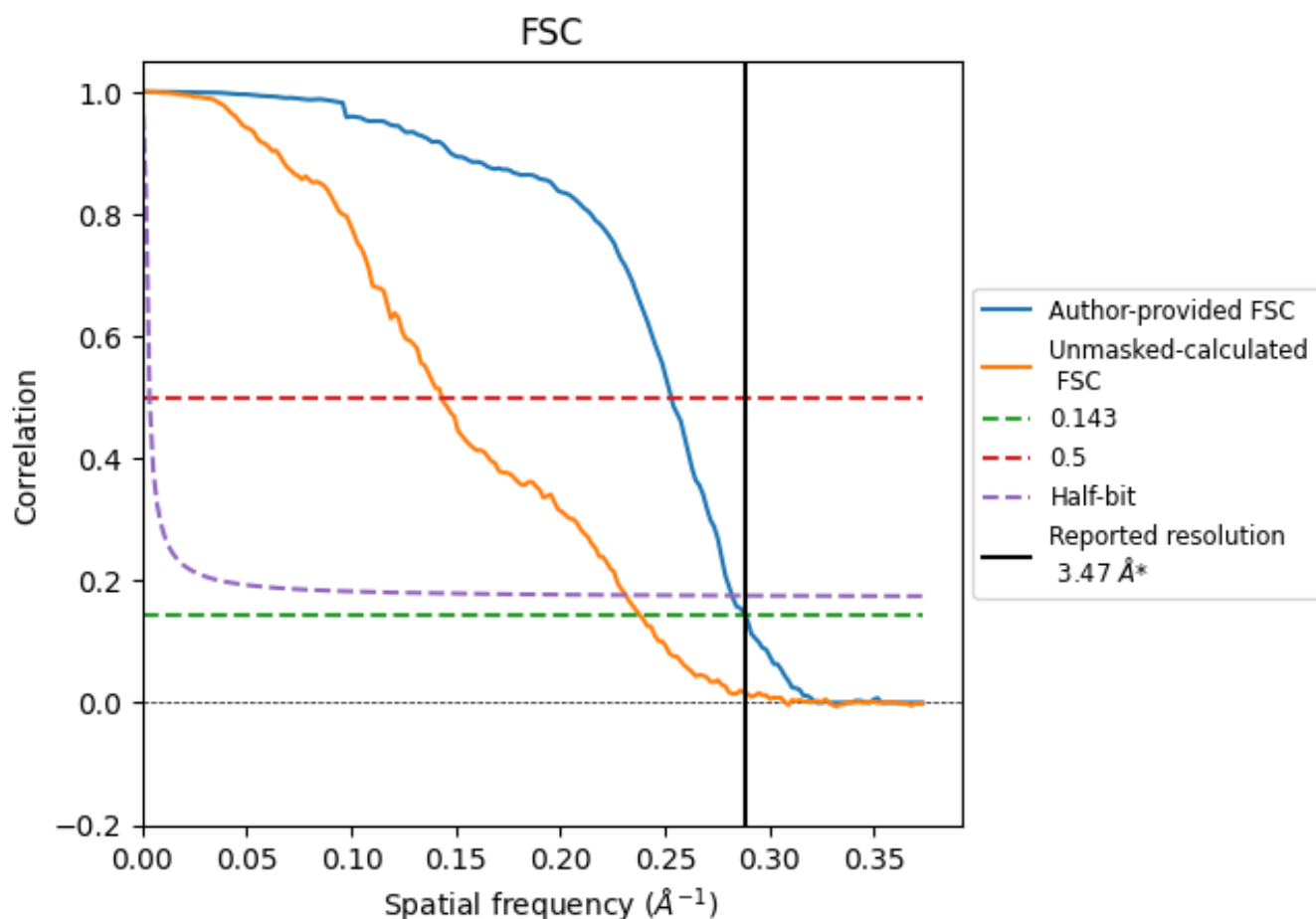


*Reported resolution corresponds to spatial frequency of $0.288 \text{ \AA}^{-1}$

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

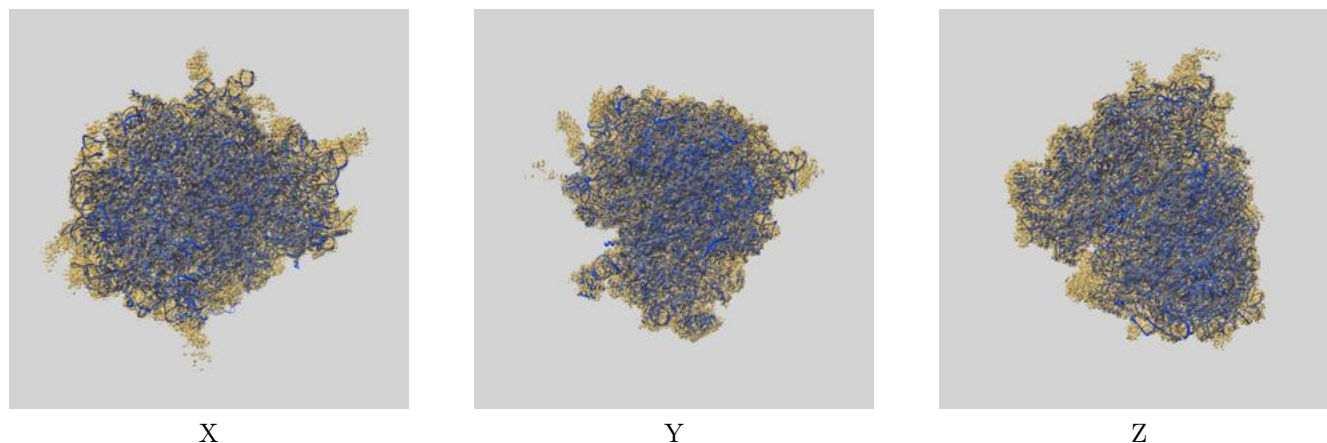
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.95	3.54
Unmasked-calculated*	4.20	6.98	4.32

*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 4.20 differs from the reported value 3.47 by more than 10 %

9 Map-model fit [i](#)

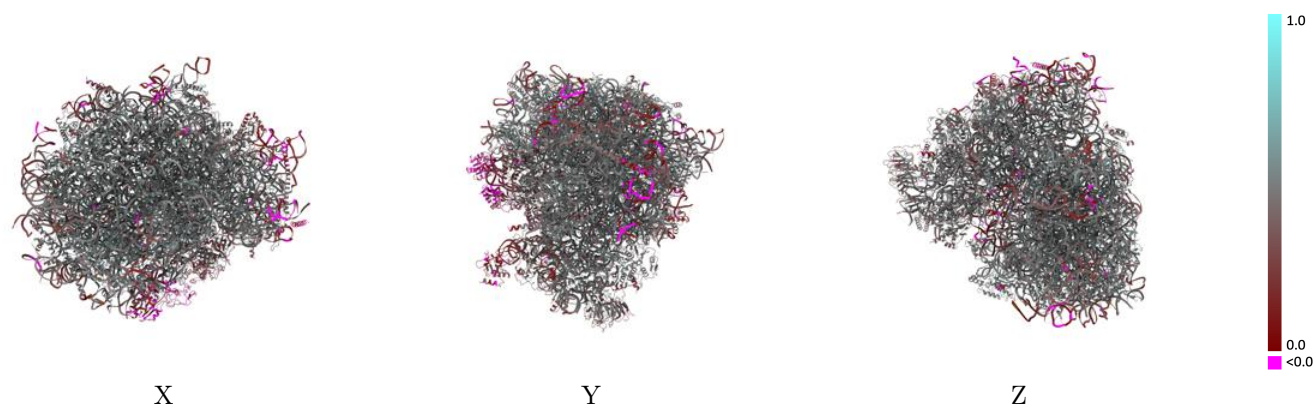
This section contains information regarding the fit between EMDB map EMD-4137 and PDB model 5LZZ. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



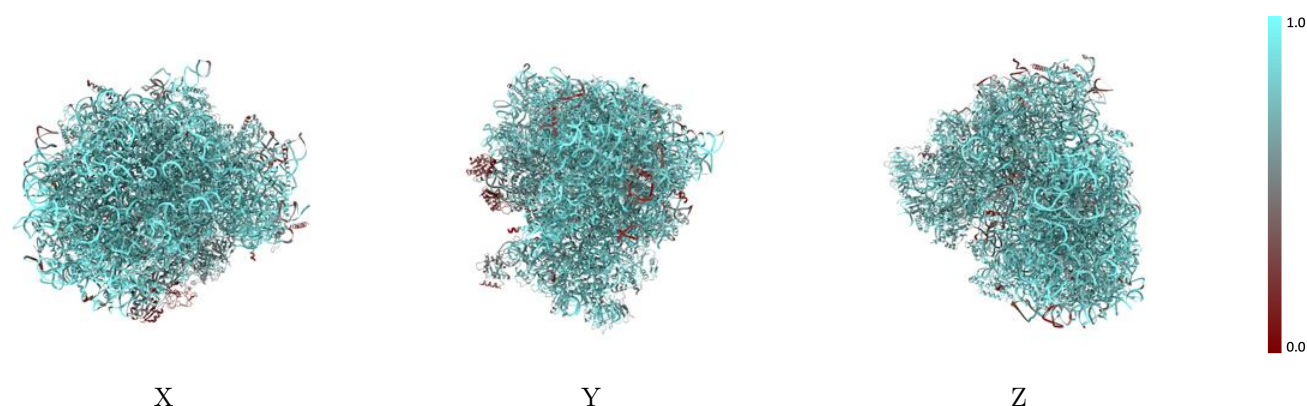
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



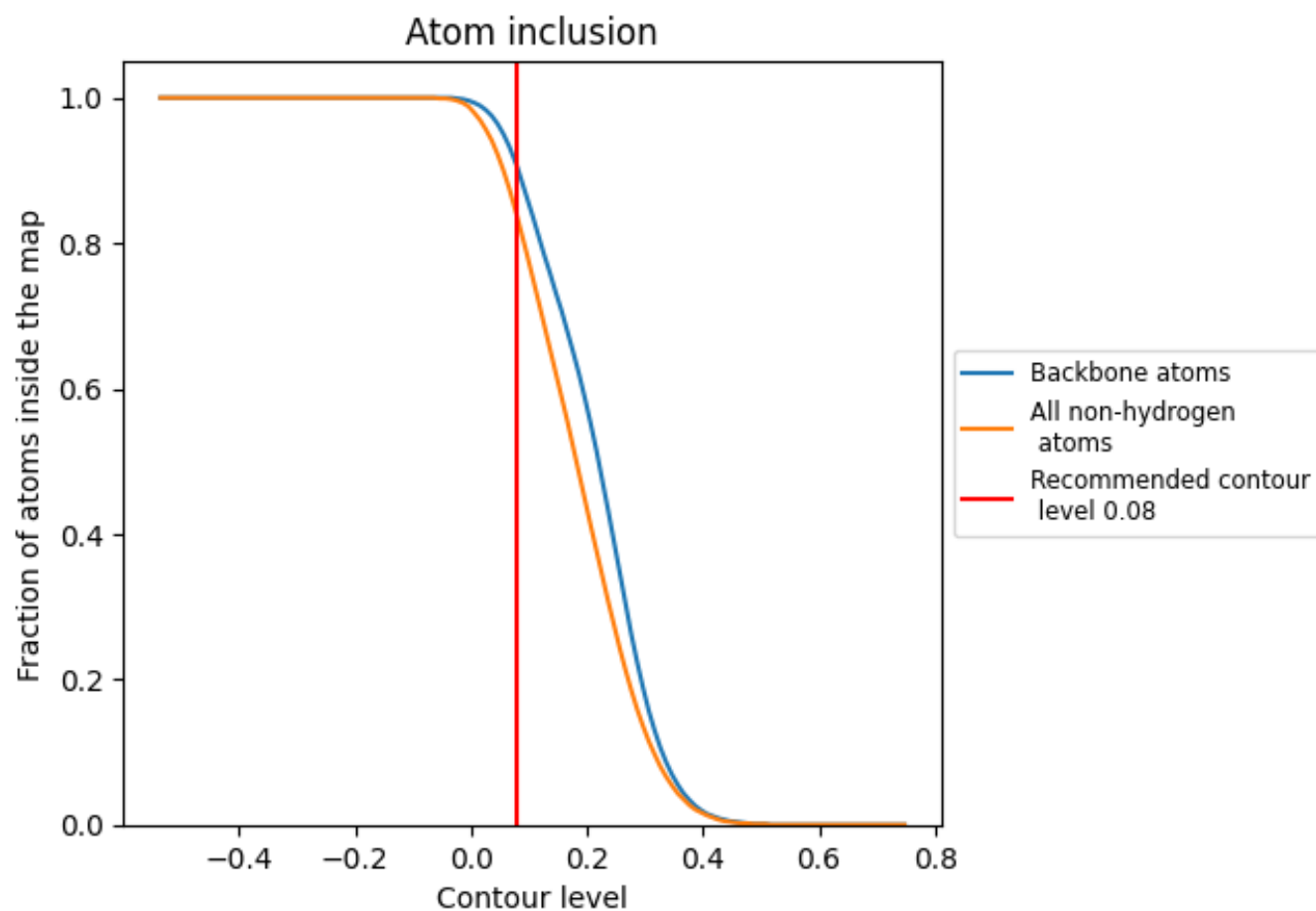
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4460
1	 0.4490	 0.3290
2	 0.8300	 0.4290
3	 0.5840	 0.2260
5	 0.8920	 0.4490
7	 0.9390	 0.4940
8	 0.8980	 0.4490
9	 0.8790	 0.4310
A	 0.8530	 0.5150
AA	 0.7930	 0.4570
B	 0.8560	 0.5110
BB	 0.7820	 0.4670
C	 0.8520	 0.5060
CC	 0.8060	 0.4810
D	 0.8370	 0.4780
DD	 0.7470	 0.4350
E	 0.8450	 0.4890
EE	 0.7990	 0.4750
F	 0.8520	 0.5180
FF	 0.7620	 0.4480
G	 0.7640	 0.4410
GG	 0.7380	 0.3920
H	 0.8260	 0.4940
HH	 0.7000	 0.4040
I	 0.8310	 0.5080
II	 0.7870	 0.4610
J	 0.8210	 0.4720
JJ	 0.8210	 0.4670
KK	 0.7630	 0.4020
L	 0.8150	 0.4760
LL	 0.8000	 0.4810
M	 0.8390	 0.4900
MM	 0.4840	 0.1950
N	 0.8500	 0.5180
NN	 0.8130	 0.4850



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Chain	Atom inclusion	Q-score
O	 0.8500	 0.5100
OO	 0.8140	 0.4840
P	 0.8490	 0.5110
PP	 0.7380	 0.4060
Q	 0.8430	 0.5100
QQ	 0.7960	 0.4620
R	 0.7950	 0.4600
RR	 0.7580	 0.4370
S	 0.8620	 0.5210
SS	 0.7710	 0.4240
T	 0.8210	 0.4920
TT	 0.8100	 0.4360
U	 0.7940	 0.4370
UU	 0.7460	 0.4290
V	 0.8130	 0.5150
VV	 0.8100	 0.4750
W	 0.6790	 0.3720
WW	 0.8440	 0.5080
X	 0.8010	 0.4830
XX	 0.8010	 0.5020
Y	 0.8300	 0.4960
YY	 0.7960	 0.4470
Z	 0.8540	 0.4880
ZZ	 0.7020	 0.3930
a	 0.8460	 0.5160
aa	 0.8080	 0.4770
b	 0.7340	 0.4180
bb	 0.7500	 0.4340
c	 0.7940	 0.4640
cc	 0.7210	 0.4510
d	 0.8100	 0.4820
dd	 0.8460	 0.4950
e	 0.8470	 0.5140
ee	 0.7250	 0.4270
f	 0.8650	 0.5260
ff	 0.5620	 0.2600
g	 0.8120	 0.4920
gg	 0.7550	 0.4020
h	 0.8030	 0.4760
hh	 0.1480	 0.2260
i	 0.8100	 0.4640
ii	 0.6220	 0.3820

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Chain	Atom inclusion	Q-score
j	 0.8680	 0.5140
jj	 0.6420	 0.3630
k	 0.7500	 0.4310
l	 0.8410	 0.4970
m	 0.8490	 0.5040
n	 0.6740	 0.4700
o	 0.8090	 0.5040
p	 0.7980	 0.4900
r	 0.8750	 0.5190
s	 0.2300	 0.0810
t	 0.1440	 0.0370