



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:17 PM UTC

PDB ID : 6WOO / pdb_00006woo
EMDB ID : EMD-21859
Title : CryoEM structure of yeast 80S ribosome with Met-tRNAⁱMet, eIF5B, and GDP
Authors : Wang, J.; Wang, J.; Puglisi, J.; Fernandez, I.S.
Deposited on : 2020-04-25
Resolution : 2.90 Å(reported)
Based on initial model : 4V8Y

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

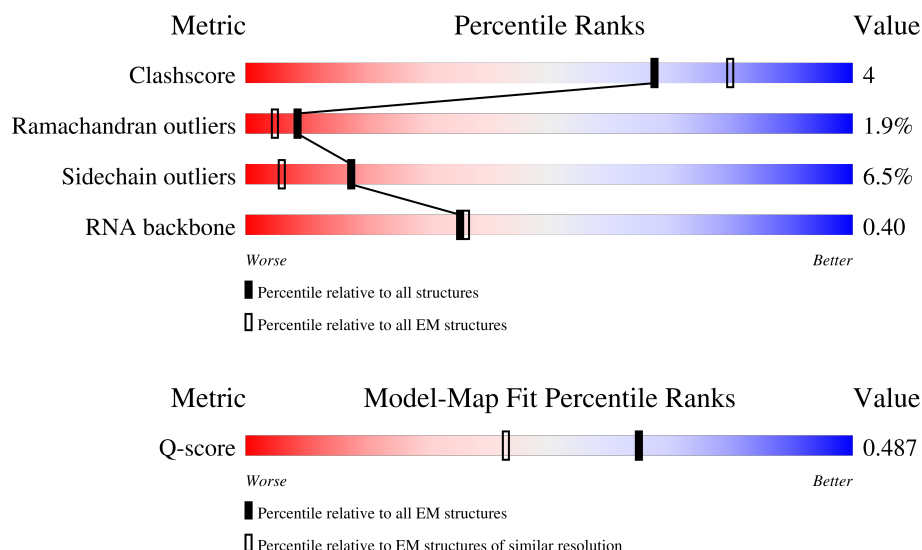
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	5	3271	
2	7	121	
3	8	157	

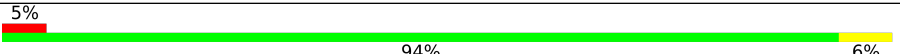
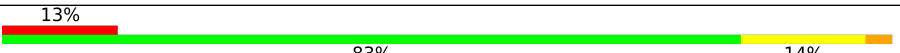
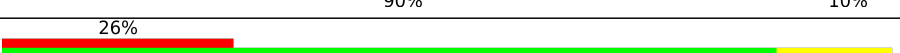
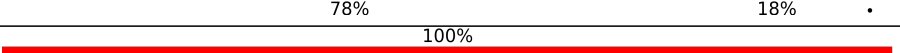
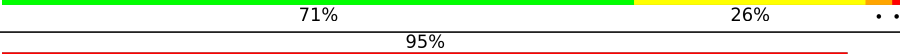
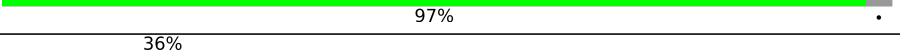
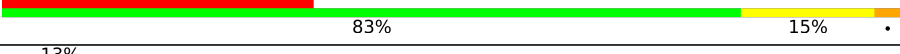
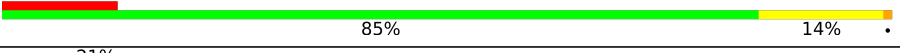
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Mol	Chain	Length	Quality of chain
4	A	249	
5	B	384	
6	C	359	
7	D	295	
8	E	175	
9	F	222	
10	G	233	
11	H	191	
12	I	216	
13	J	168	
14	L	198	
15	M	136	
16	N	202	
17	O	197	
18	P	180	
19	Q	184	
20	R	188	
21	S	169	
22	T	158	
23	U	100	
24	V	132	
25	W	62	
26	X	121	
27	Y	125	
28	Z	134	

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Mol	Chain	Length	Quality of chain
29	a	147	
30	b	57	
31	c	97	
32	d	106	
33	e	122	
34	f	105	
35	g	121	
36	h	116	
37	i	98	
38	j	85	
39	k	76	
40	l	49	
41	m	51	
42	n	23	
43	o	101	
44	p	87	
45	q	217	
46	r	195	
47	K	152	
48	AA	206	
49	BB	214	
50	CC	217	
51	DD	223	
52	EE	257	
53	FF	206	

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Mol	Chain	Length	Quality of chain
54	GG	226	
55	HH	184	
56	II	199	
57	JJ	182	
58	KK	96	
59	LL	145	
60	MM	124	
61	NN	150	
62	OO	127	
63	PP	103	
64	QQ	141	
65	RR	123	
66	SS	136	
67	TT	143	
68	UU	106	
69	VV	87	
70	WW	129	
71	XX	144	
72	YY	134	
73	ZZ	70	
74	aa	97	
75	bb	81	
76	cc	63	
77	dd	53	
78	ee	53	

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Mol	Chain	Length	Quality of chain
79	ff	57	
80	gg	318	
81	2	1796	
82	1	600	
83	3	76	
84	4	6	

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
85	ZN	aa	500	-	-	X	-
87	U6A	3	101	-	X	-	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 211119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3271	Total	C	N	O	P	0	0
			69936	31236	12597	22832	3271		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	249	Total	C	N	O	S	0	0
			1893	1178	384	330	1		

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	384	Total	C	N	O	S	0	0
			3065	1946	582	529	8		

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	359	Total	C	N	O	S	0	0
			2735	1723	520	489	3		

- Molecule 7 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	295	Total	C	N	O	S	0	0
			2370	1498	413	457	2		

- Molecule 8 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1809	1154	324	328	3		

- Molecule 11 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	191	Total	C	N	O	S	0	0
			1524	966	274	280	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	191	GLU	-	insertion	UNP P51401

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	216	Total	C	N	O	S	0	0
			1750	1109	331	303	7		

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 14 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	198	Total	C	N	O		0	0
			1584	988	323	273			

- Molecule 15 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	136	Total	C	N	O	S	0	0
			1054	675	199	178	2		

- Molecule 16 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	202	Total	C	N	O	S	0	0
			1711	1071	359	280	1		

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	180	Total	C	N	O		0	0
			1427	887	284	256			

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	184	Total	C	N	O	S	0	0
			1437	906	289	240	2		

- Molecule 20 is a protein called eL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	169	Total	C	N	O	S	0	0
			1422	916	262	241	3		

- Molecule 22 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	158	Total	C	N	O	S	0	0
			1268	799	245	220	4		

- Molecule 23 is a protein called eL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 24 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	132	Total	C	N	O	S	0	0
			978	614	184	173	7		

- Molecule 25 is a protein called eL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	62	Total	C	N	O	0	0
			513	331	101	81		

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 27 is a protein called uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	125	Total	C	N	O	0	0
			988	622	191	175		

- Molecule 28 is a protein called eL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	134	Total	C	N	O	0	0
			1087	707	201	179		

- Molecule 29 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	147	Total	C	N	O	S	0	0
			1168	746	230	189	3		

- Molecule 30 is a protein called eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	57	Total	C	N	O	0	0
			457	286	99	72		

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	106	Total	C	N	O	S	0	0
			865	550	165	149	1		

- Molecule 33 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	122	Total	C	N	O	S	0	0
			988	626	200	161	1		

- Molecule 34 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	105	Total	C	N	O	S	0	0
			842	534	164	143	1		

- Molecule 35 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	121	Total	C	N	O	S	0	0
			954	592	194	164	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	122	LYS	-	insertion	UNP P87262

- Molecule 36 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	116	Total	C	N	O	S	0	0
			950	603	182	164	1		

- Molecule 37 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	98	Total	C	N	O	S	0	0
			764	477	155	130	2		

- Molecule 38 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	85	Total	C	N	O	S	0	0
			673	410	147	111	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	84	LYS	-	insertion	UNP P49166
j	85	ALA	-	insertion	UNP P49166
j	86	GLN	-	insertion	UNP P49166

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	76	Total	C	N	O	0	0
			607	388	114	105		

- Molecule 40 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	51	Total	C	N	O	S	0	0
			409	253	85	66	5		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			218	133	60	24	1		

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	101	Total	C	N	O	S	0	0
			814	511	165	133	5		

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	87	Total	C	N	O	S	0	0
			668	413	134	115	6		

- Molecule 45 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	195	Total	C	N	O	S	0	0
			1512	968	261	279	4		

- Molecule 47 is a protein called L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	K	147	Total	C	N	O	S	0	0
			735	441	147	147			

- Molecule 48 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	206	Total	C	N	O	S	0	0
			1615	1037	286	290	2		

- Molecule 49 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BB	214	Total	C	N	O	S	0	0
			1716	1086	314	312	4		

- Molecule 50 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	CC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 51 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 52 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	EE	257	Total	C	N	O	S	0	0
			2047	1303	385	356	3		

- Molecule 53 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	FF	201	Total	C	N	O	S	0	0
			1588	996	295	294	3		

- Molecule 54 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	GG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 55 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	HH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 56 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	II	187	Total	C	N	O	S	0	0
			1480	919	296	263	2		

- Molecule 57 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	JJ	182	Total	C	N	O	S	0	0
			1477	933	288	255	1		

- Molecule 58 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	KK	96	Total	C	N	O	S	0	0
			818	530	133	153	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
KK	89	ALA	GLY	conflict	UNP Q08745

- Molecule 59 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LL	145	Total	C	N	O	S	0	0
			1166	746	220	197	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	146	THR	-	insertion	UNP P0CX47

- Molecule 60 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	MM	124	Total	C	N	O	S	0	0
			934	587	165	180	2		

- Molecule 61 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	NN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 62 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	OO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 63 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PP	103	Total	C	N	O	S	0	0
			814	520	149	138	7		

- Molecule 64 is a protein called uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	QQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 65 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	RR	123	Total	C	N	O	S	0	0
			989	619	186	182	2		

- Molecule 66 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	136	Total	C	N	O	S	0	0
			1121	700	223	196	2		

- Molecule 67 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	TT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 68 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	UU	106	Total	C	N	O	S	0	0
			847	535	154	157	1		

- Molecule 69 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	VV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 70 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	WW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 71 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	XX	144	Total	C	N	O	S	0	0
			1123	710	220	190	3		

- Molecule 72 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	YY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 73 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	ZZ	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 74 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	aa	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 75 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 76 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	cc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 77 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	dd	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 78 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	ee	53	Total	C	N	O	S	0	0
			426	268	88	69	1		

- Molecule 79 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	ff	44	Total	C	N	O	S	0	0
			344	216	68	56	4		

- Molecule 80 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	gg	318	Total	C	N	O	S	0	0
			2444	1546	419	471	8		

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	2	1780	Total	C	N	O	P	0	0
			37790	16890	6651	12469	1780		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	677	A	G	conflict	GB 1329886537
2	678	U	A	conflict	GB 1329886537

- Molecule 82 is a protein called eIF5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	600	Total	C	N	O	S	0	0
			4704	2989	801	893	21		

- Molecule 83 is a RNA chain called Met-tRNA-iMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	76	Total	C	N	O	P	0	0
			1630	726	302	526	76		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	17	G	-	insertion	GB 176433

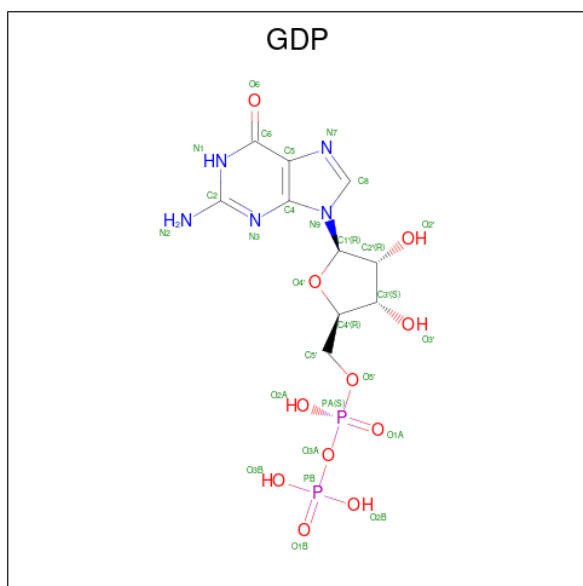
- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	4	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

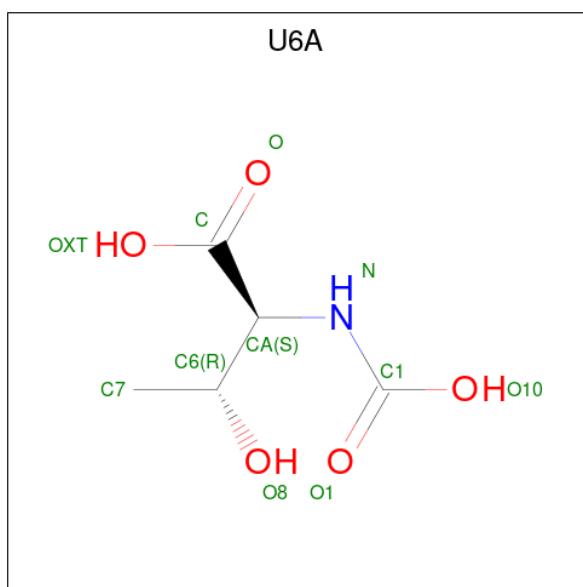
Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	
85	bb	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	

- Molecule 86 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



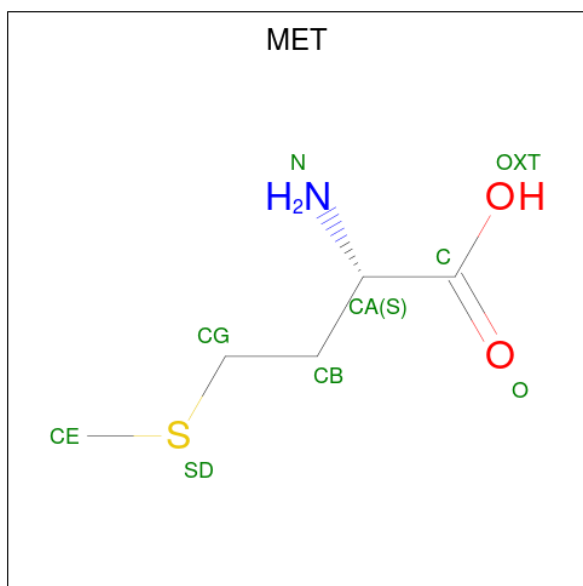
Mol	Chain	Residues	Atoms					AltConf
86	1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 87 is N-carboxy-L-threonine (CCD ID: U6A) (formula: C₅H₉NO₅).



Mol	Chain	Residues	Atoms				AltConf
87	3	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 88 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).

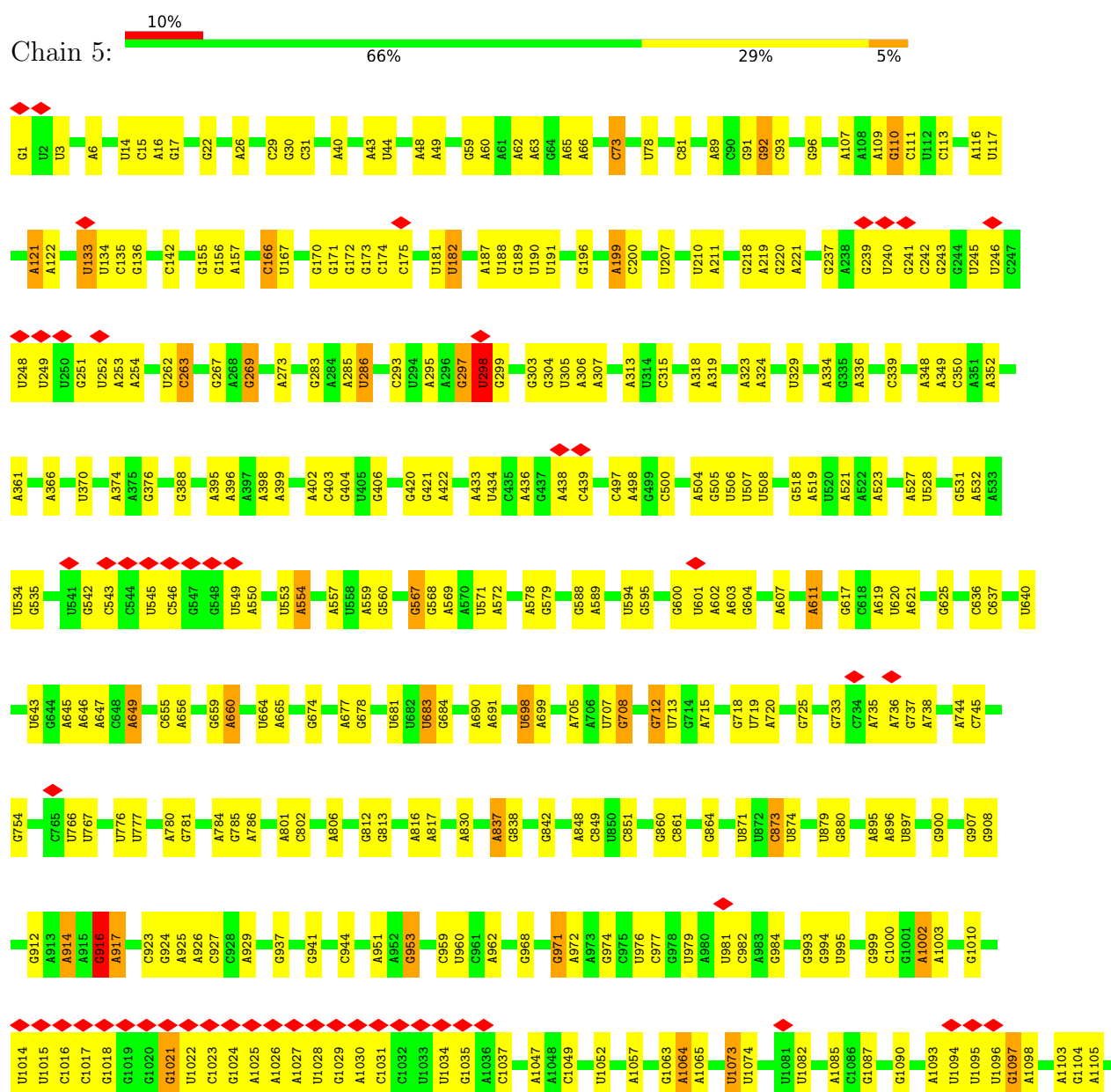


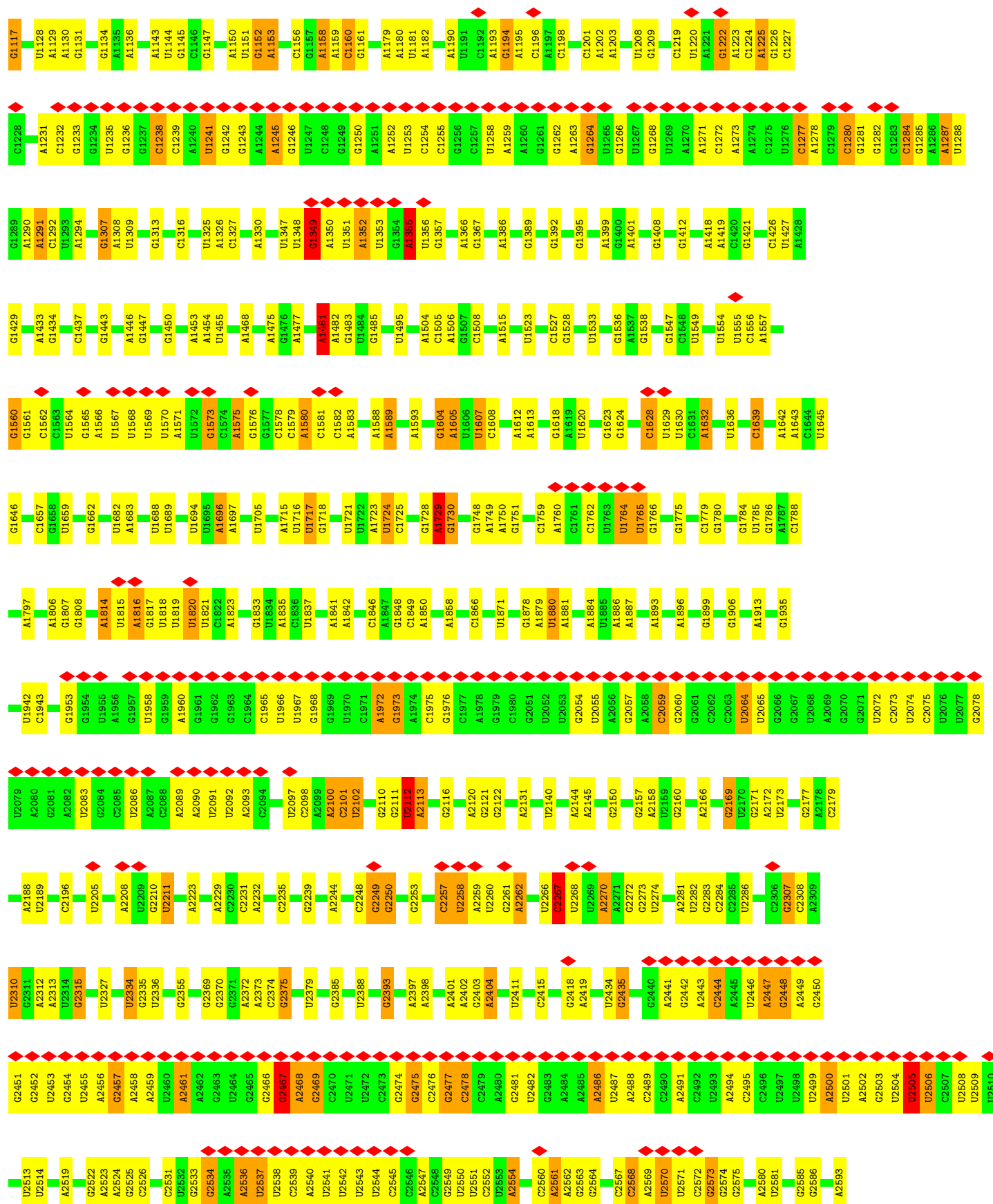
Mol	Chain	Residues	Atoms					AltConf
88	3	1	Total	C	N	O	S	0
			8	5	1	1	1	

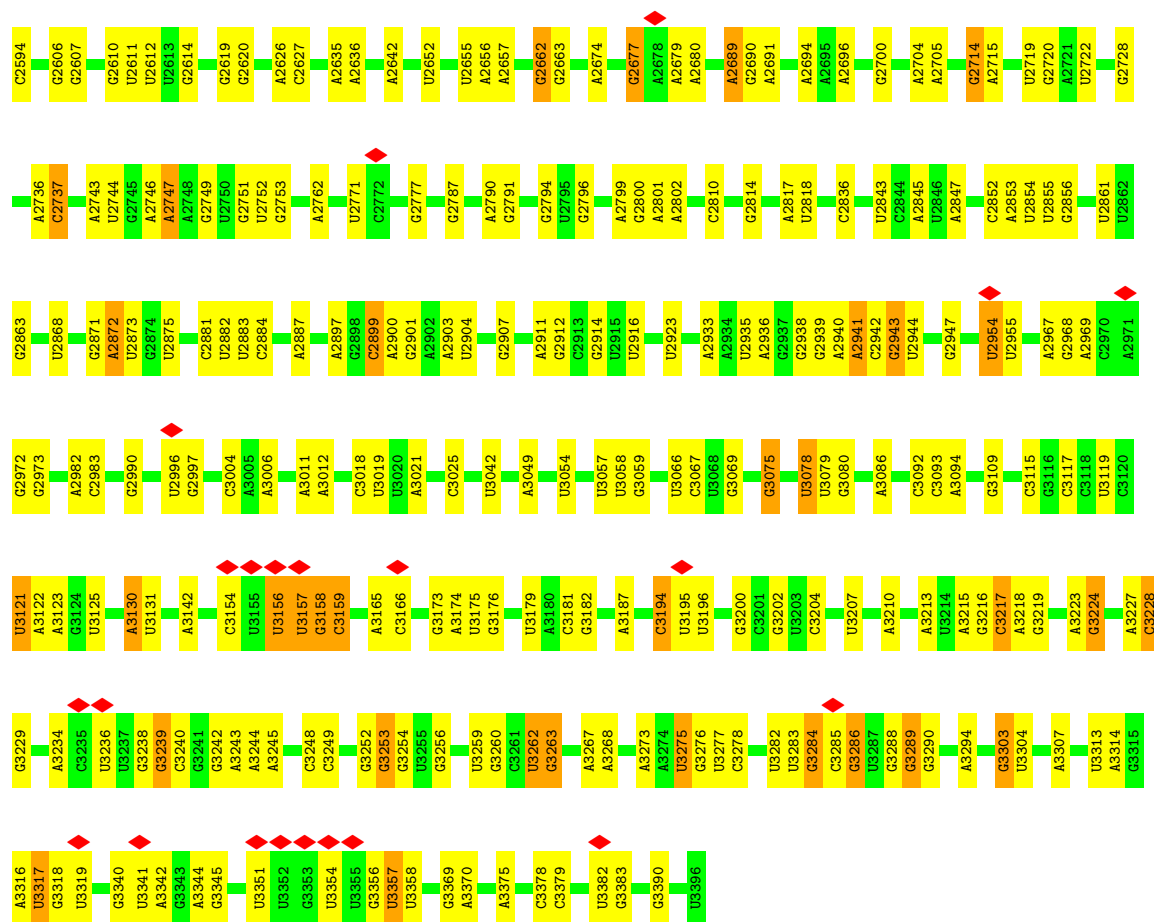
3 Residue-property plots

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

• Molecule 1: 25S ribosomal RNA



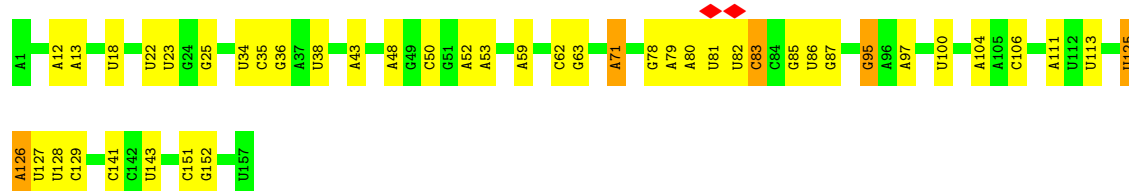




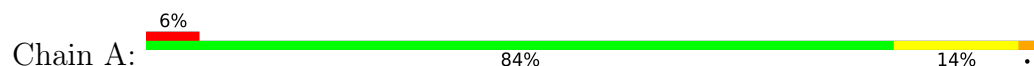
• Molecule 2: 5S ribosomal RNA

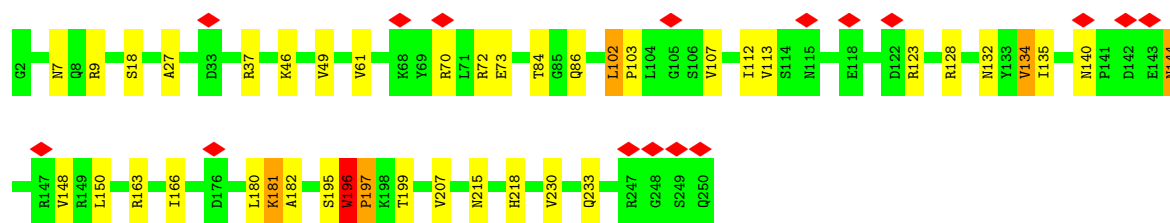


• Molecule 3: 5.8S ribosomal rRNA

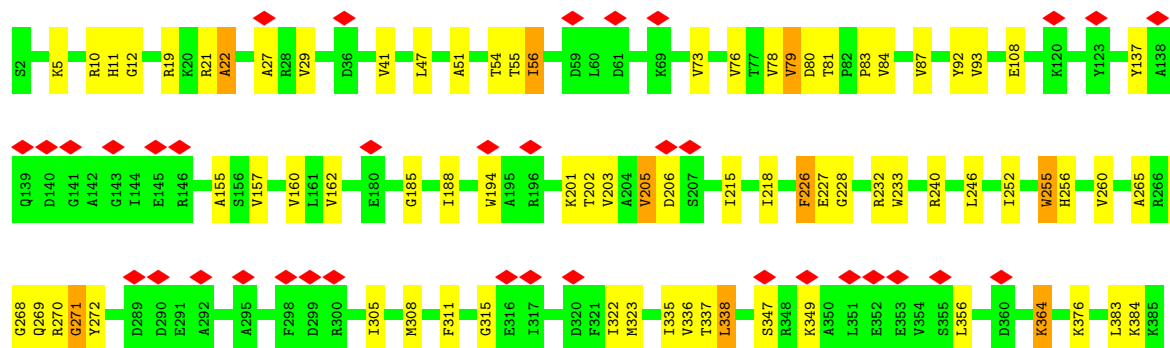
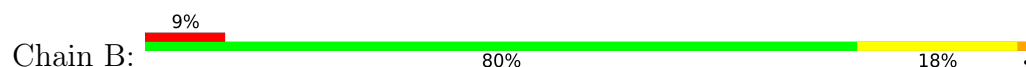


• Molecule 4: uL2

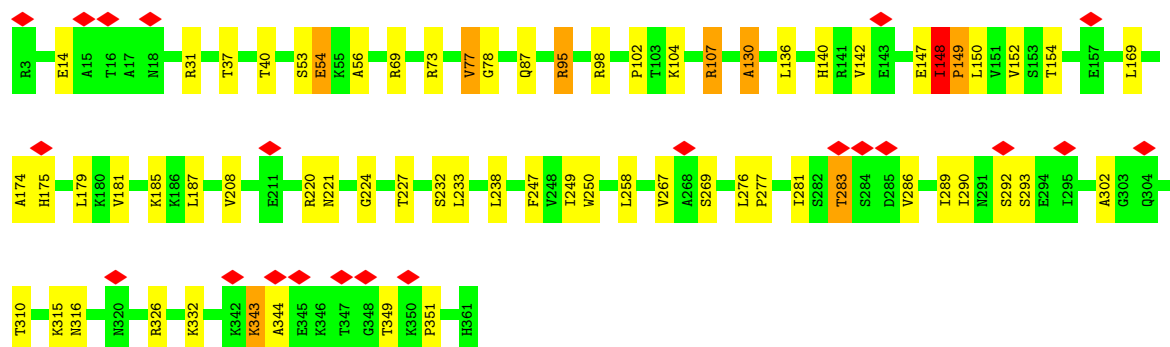
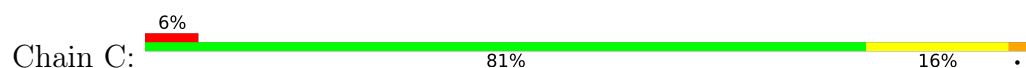




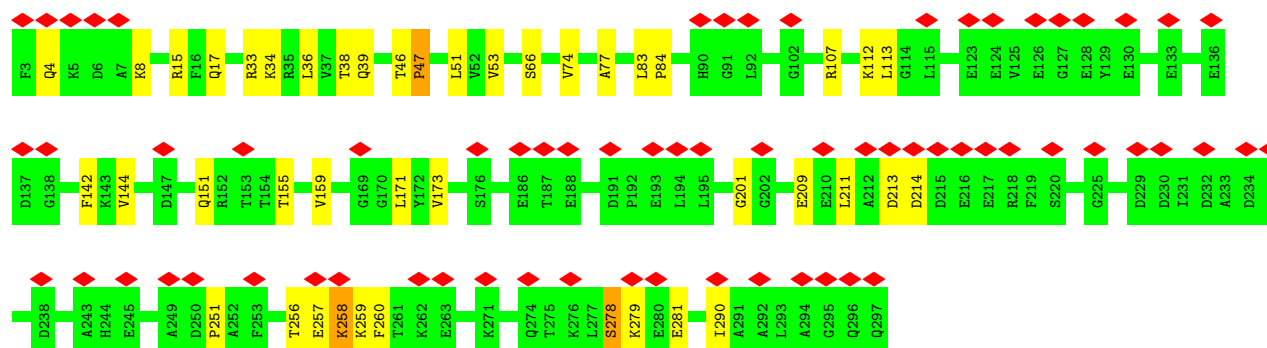
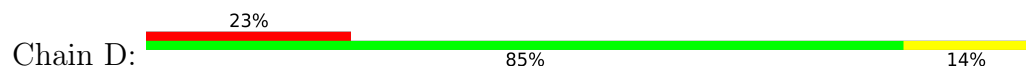
• Molecule 5: uL3



• Molecule 6: uL4

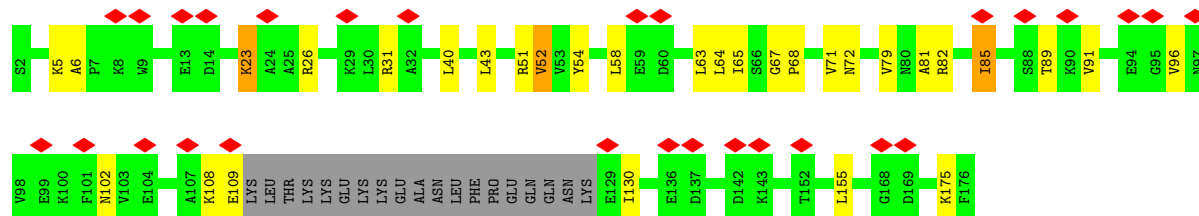


• Molecule 7: uL18



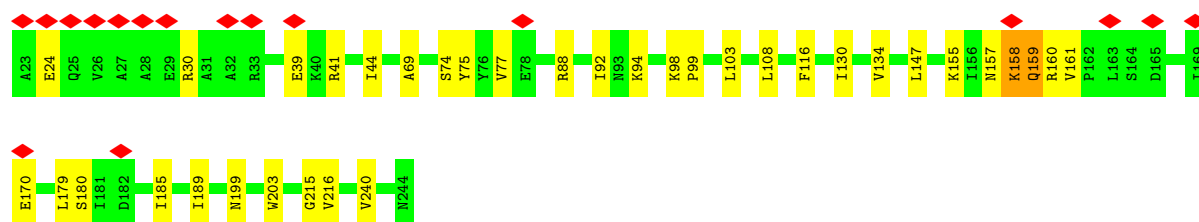
- Molecule 8: eL6

Chain E: 

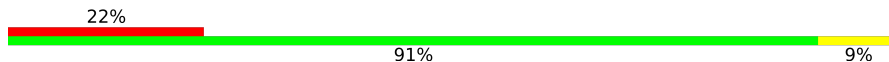


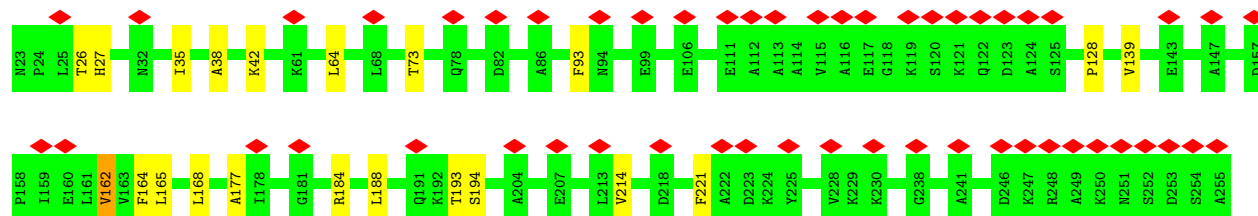
- Molecule 9: uL30

Chain F: 



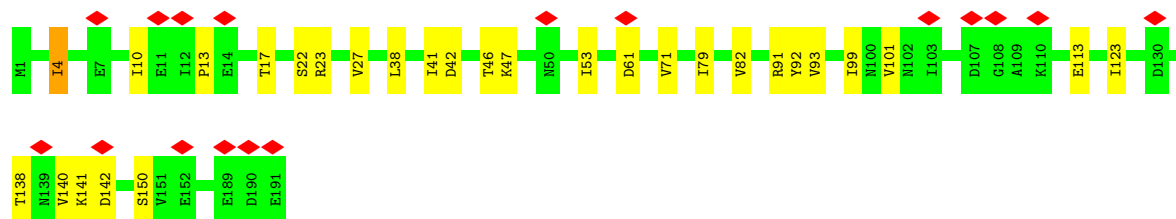
- Molecule 10: eL8

Chain G: 



- Molecule 11: uL6

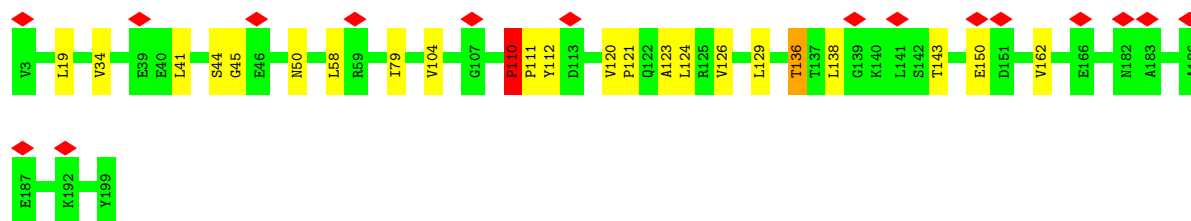
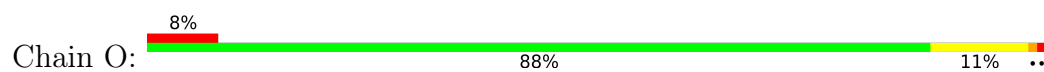
Chain H: 



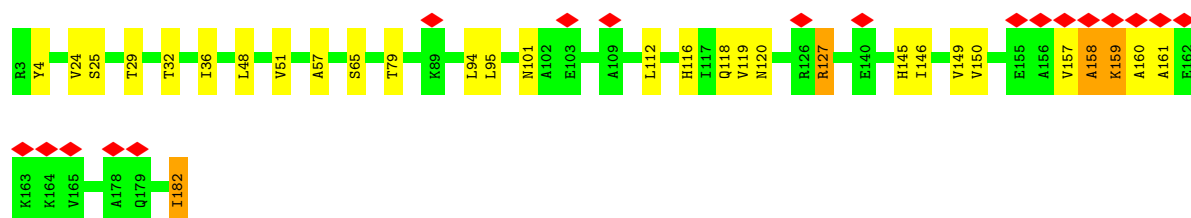
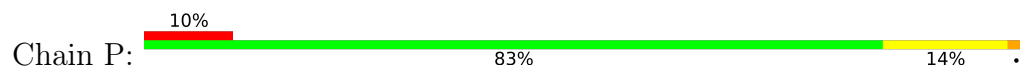
- Molecule 12: uL16

Chain I: 

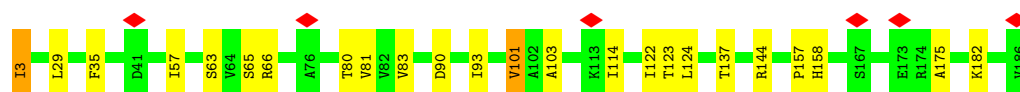
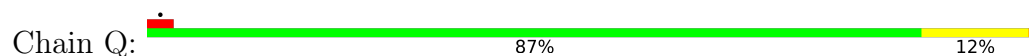




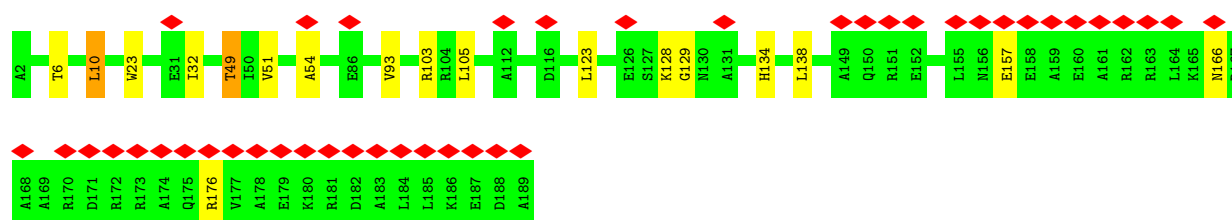
- Molecule 18: uL22



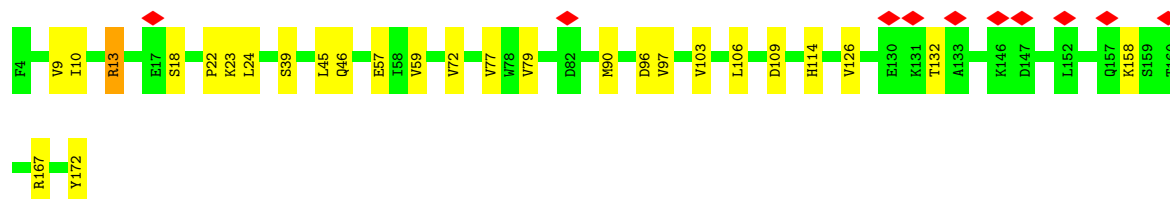
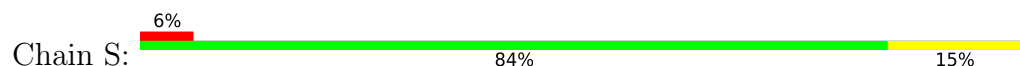
- Molecule 19: eL18



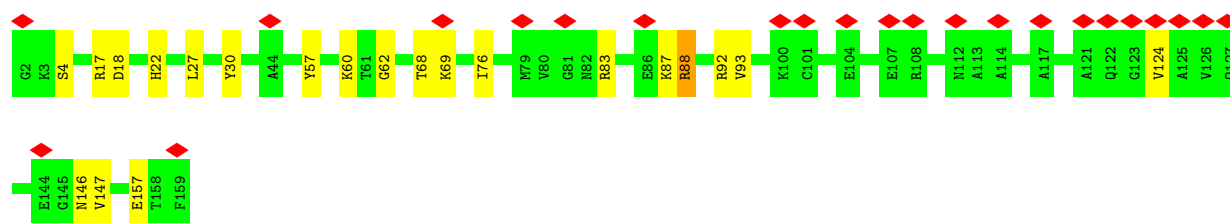
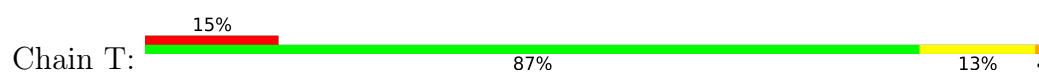
- Molecule 20: eL19



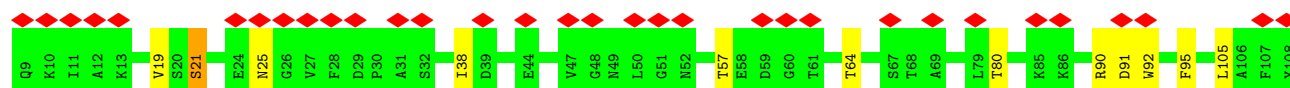
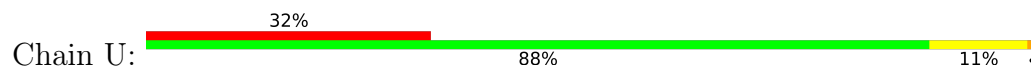
- Molecule 21: eL20



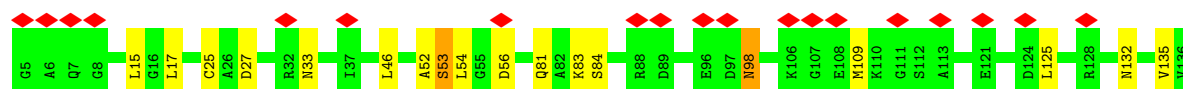
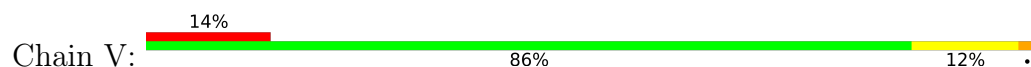
- Molecule 22: eL21



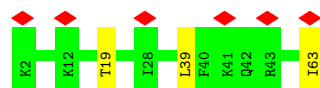
• Molecule 23: eL22



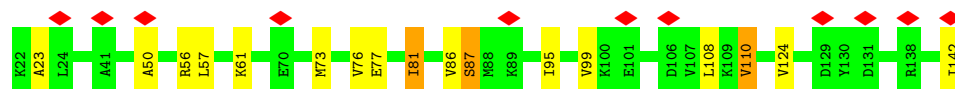
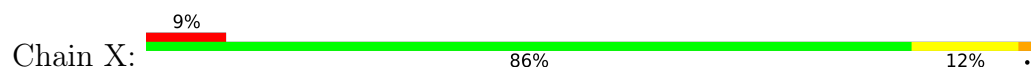
• Molecule 24: uL14



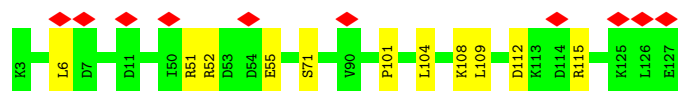
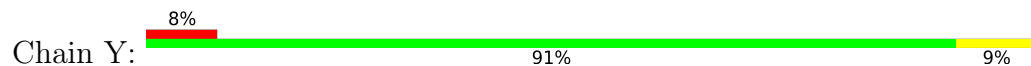
• Molecule 25: eL24



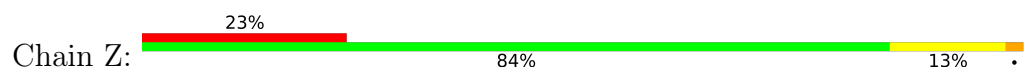
• Molecule 26: uL23

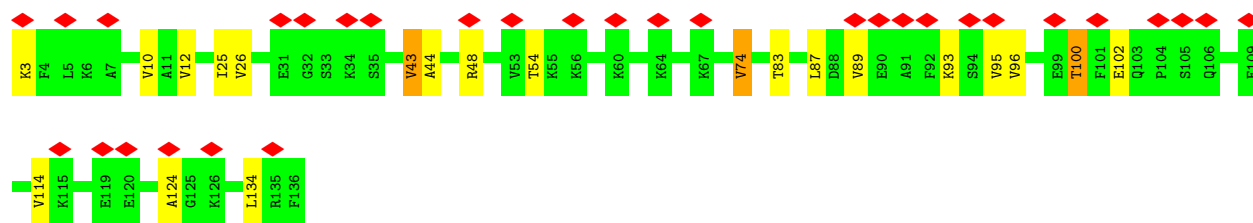


• Molecule 27: uL24

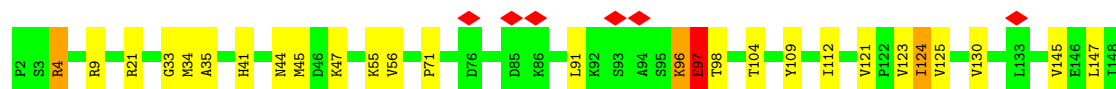
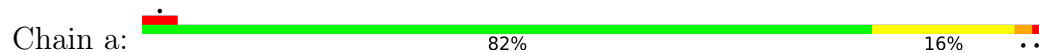


• Molecule 28: eL27

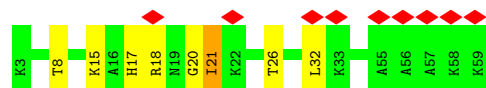
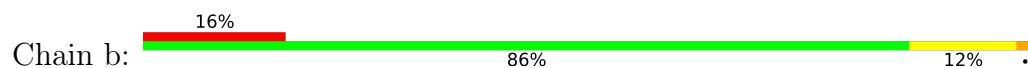




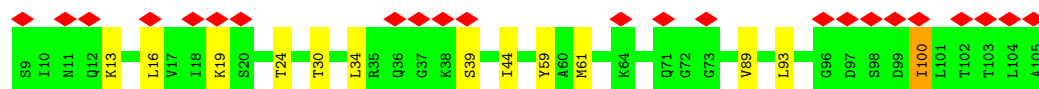
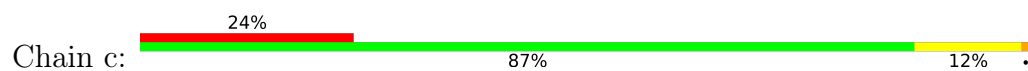
• Molecule 29: uL15



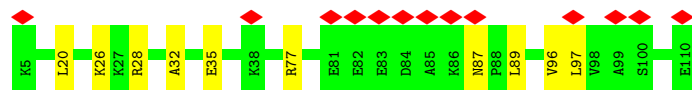
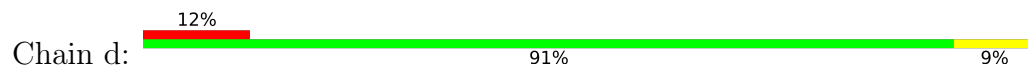
• Molecule 30: eL29



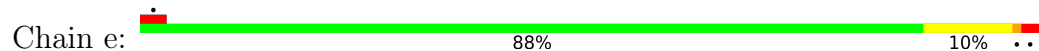
• Molecule 31: eL30



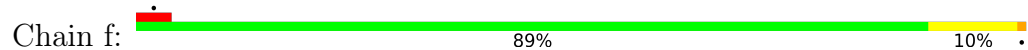
• Molecule 32: eL31

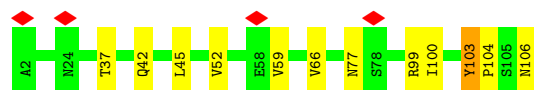


• Molecule 33: eL32

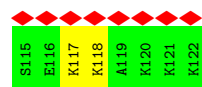
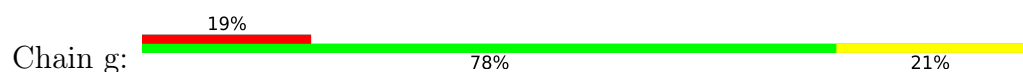


• Molecule 34: eL33





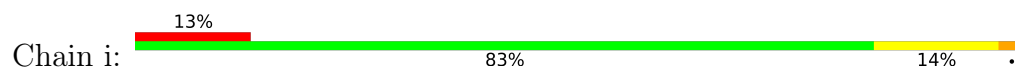
• Molecule 35: eL34



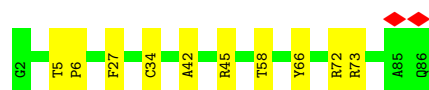
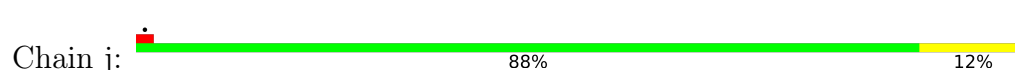
• Molecule 36: uL29



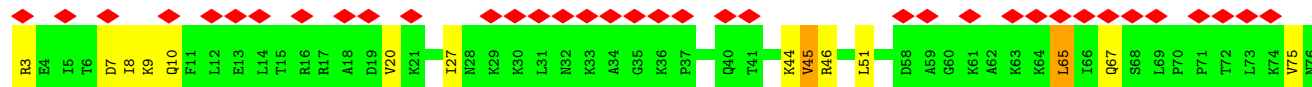
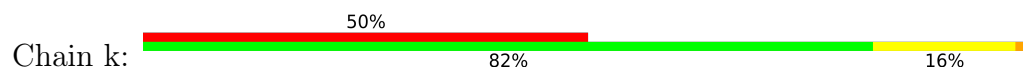
• Molecule 37: eL36



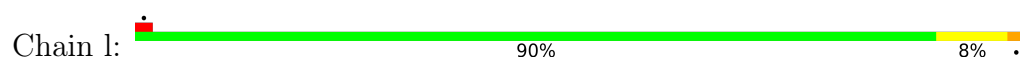
• Molecule 38: eL37



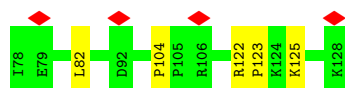
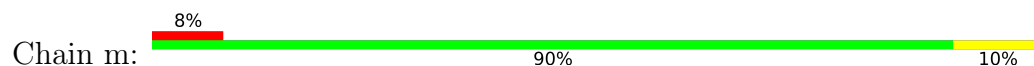
• Molecule 39: eL38



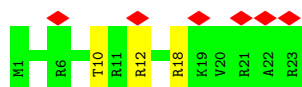
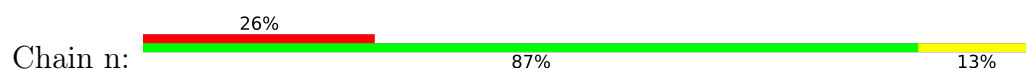
• Molecule 40: eL39



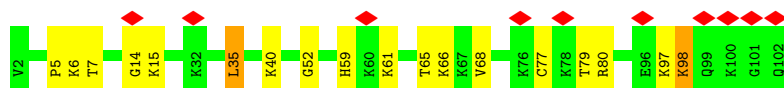
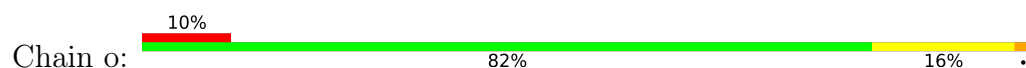
• Molecule 41: eL40



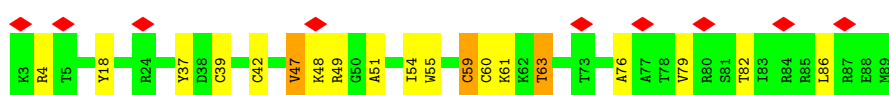
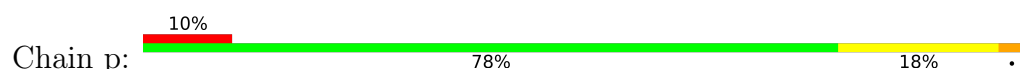
• Molecule 42: eL41



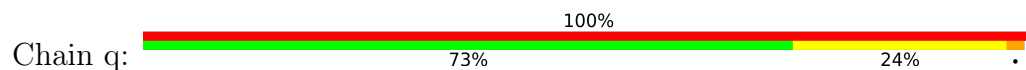
• Molecule 43: eL42



• Molecule 44: eL43

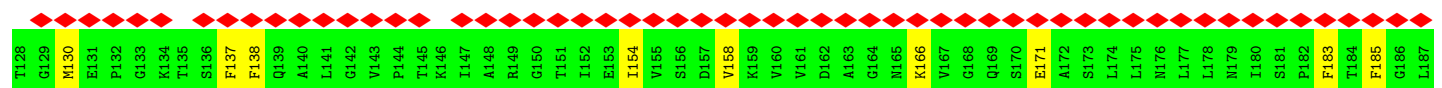
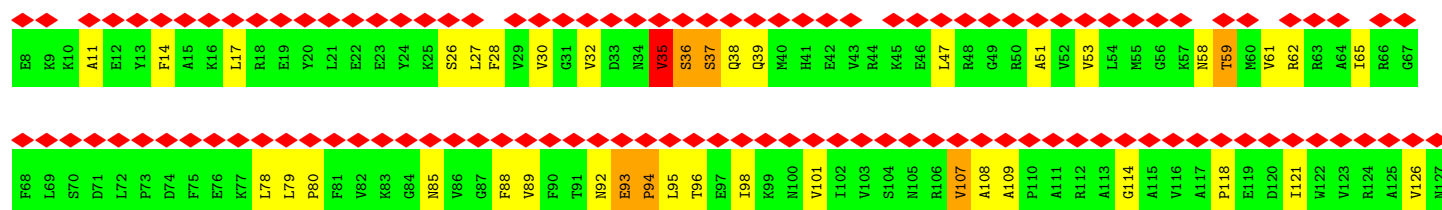


• Molecule 45: uL1

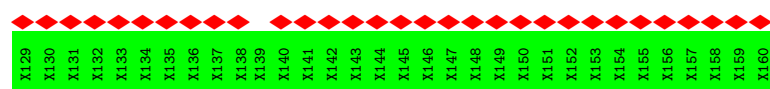
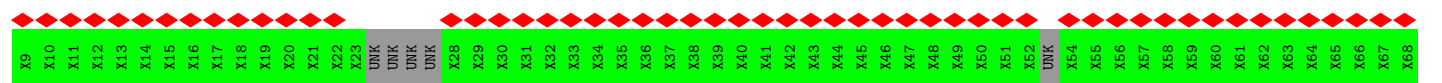




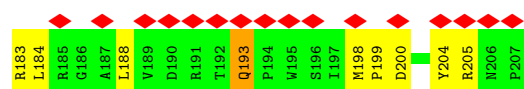
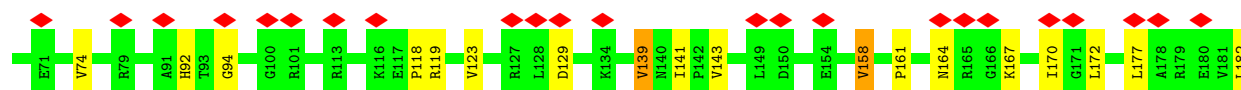
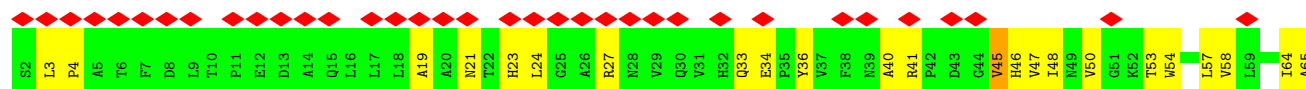
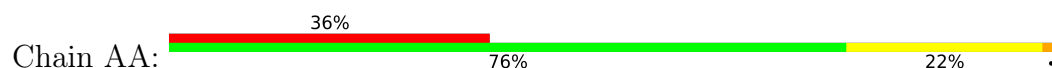
• Molecule 46: uL10



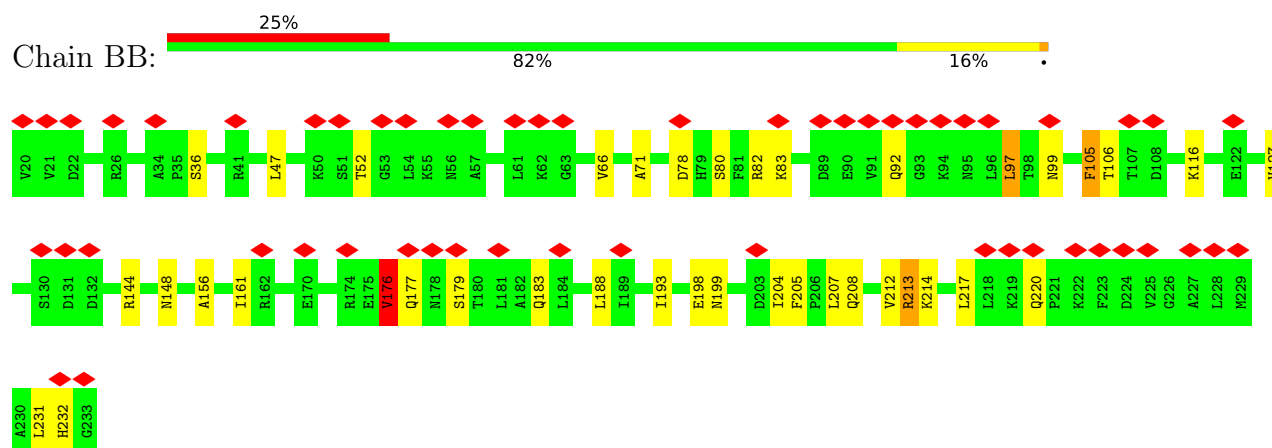
• Molecule 47: L10



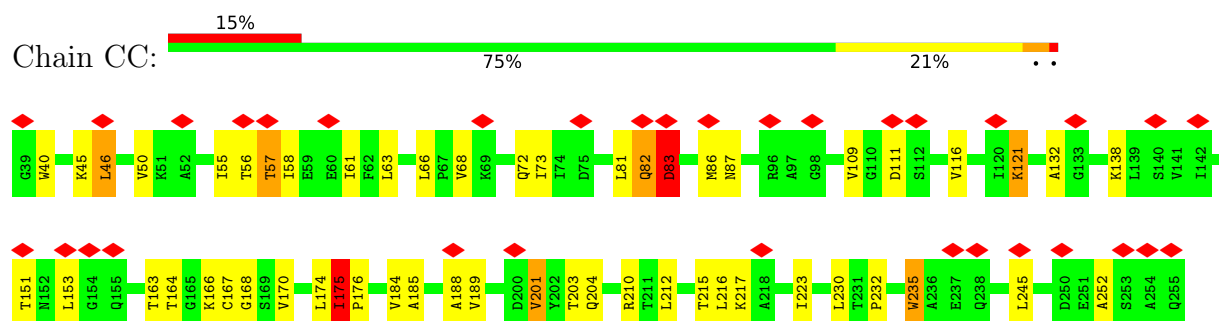
• Molecule 48: uS2



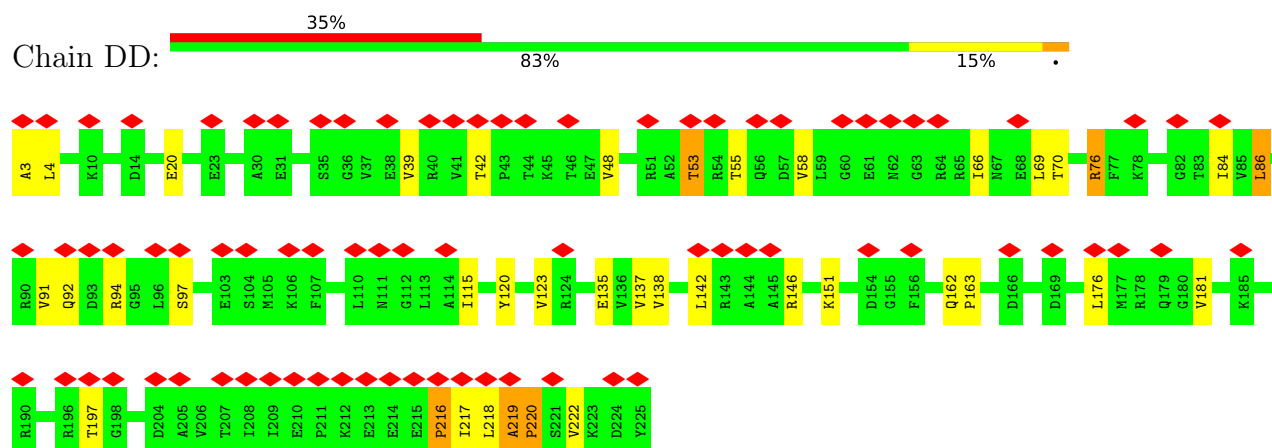
- Molecule 49: eS1



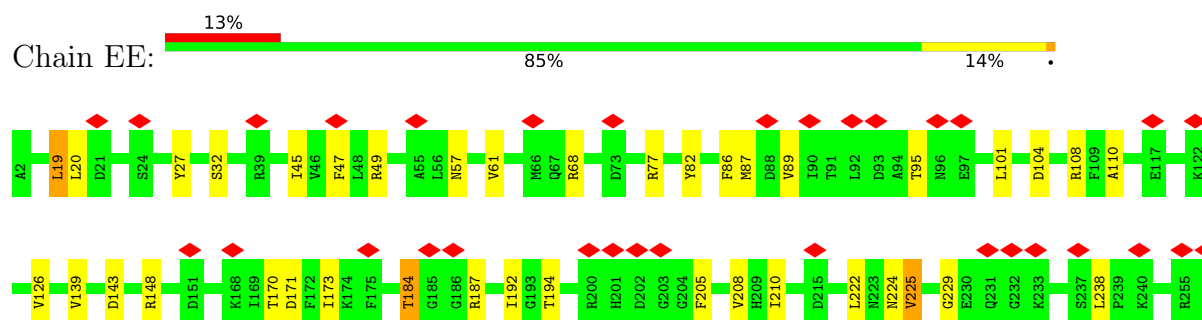
- Molecule 50: uS5



- Molecule 51: uS3

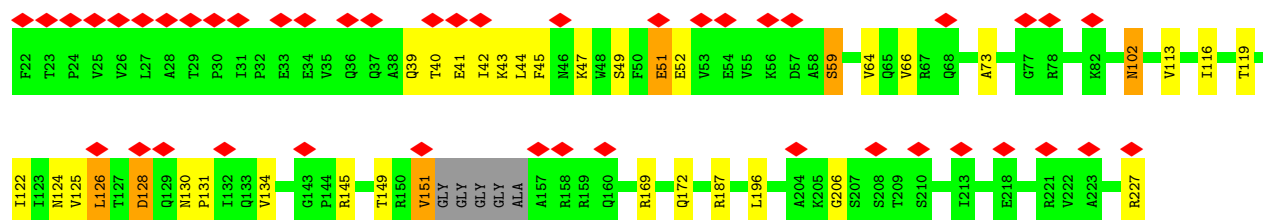
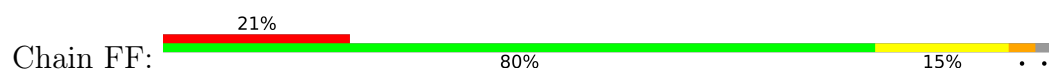


- Molecule 52: eS4

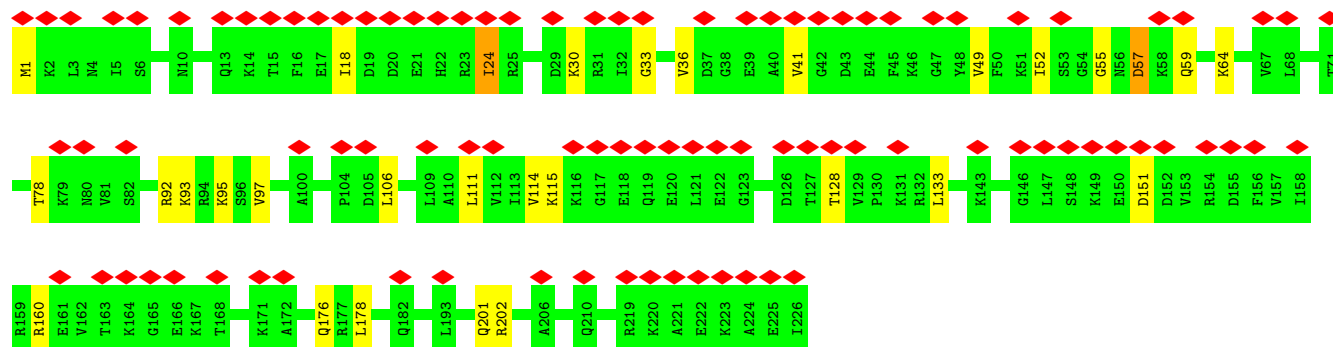
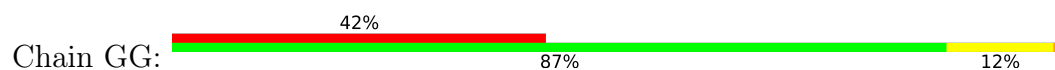




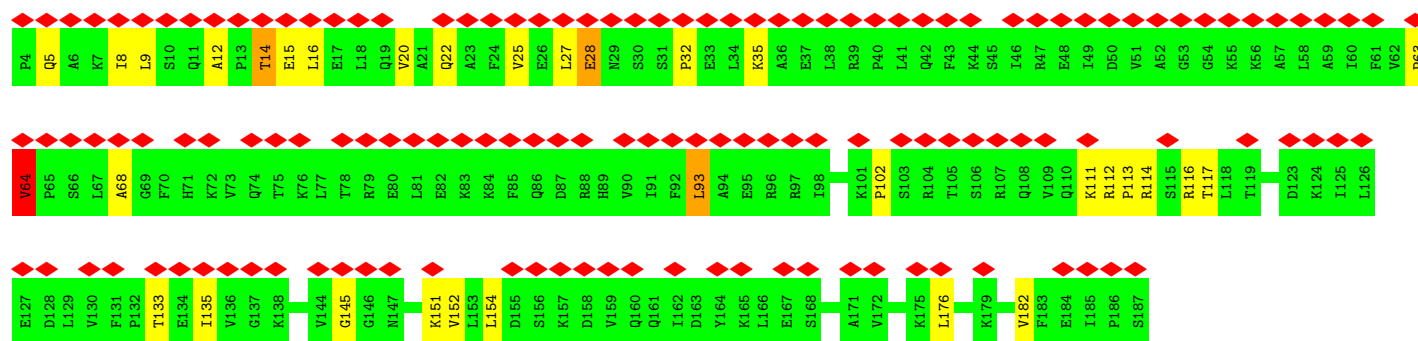
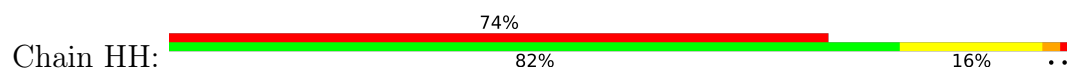
• Molecule 53: uS7



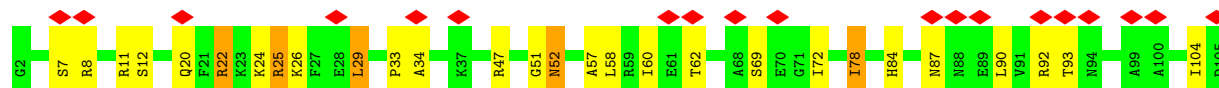
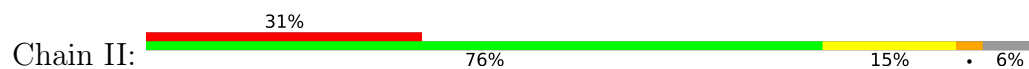
• Molecule 54: eS6

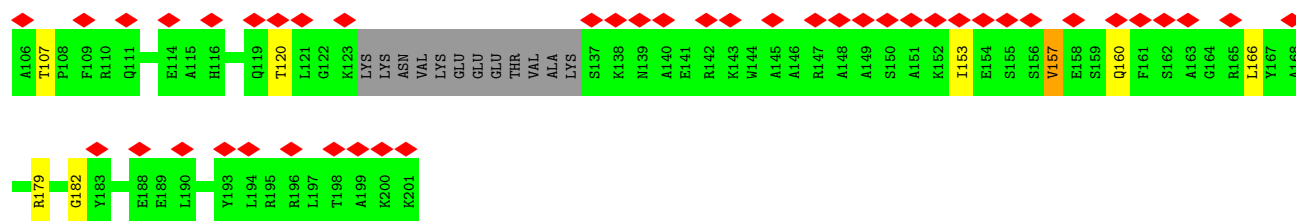


• Molecule 55: eS7

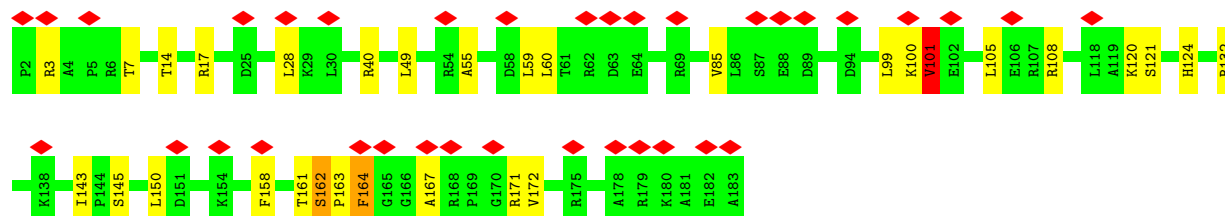
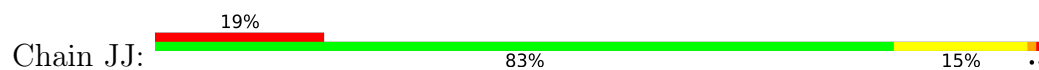


• Molecule 56: eS8

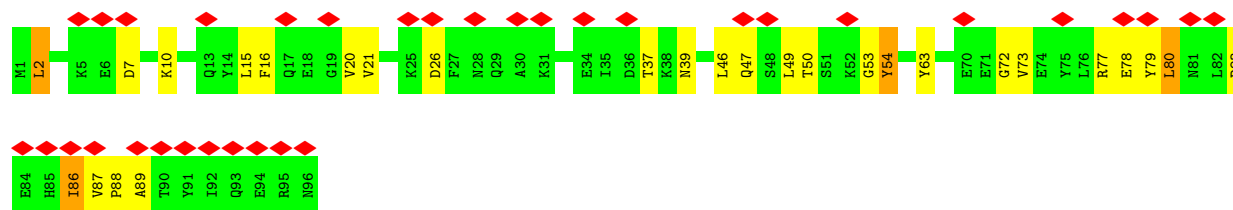
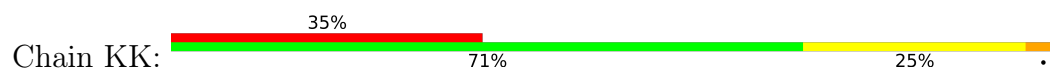




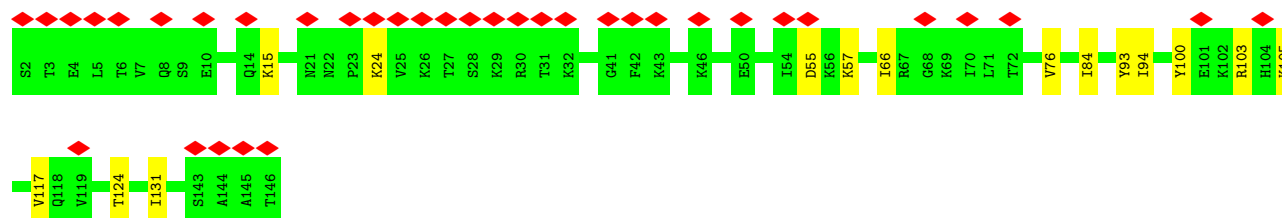
• Molecule 57: uS4



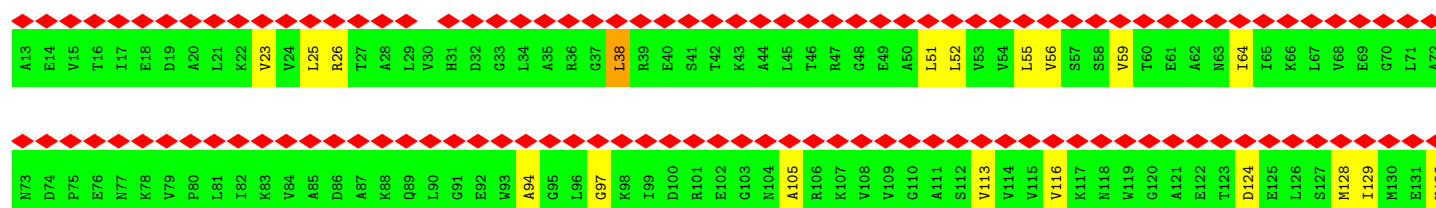
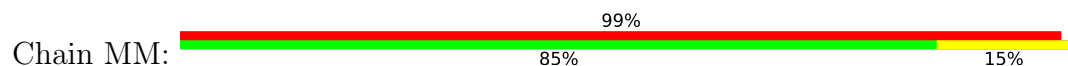
• Molecule 58: eS10

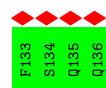


• Molecule 59: uS17

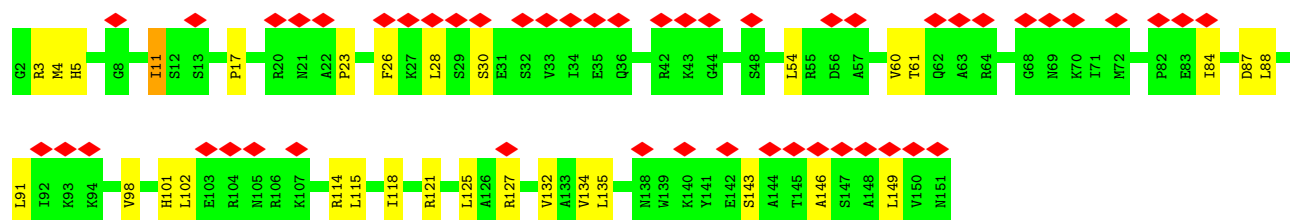
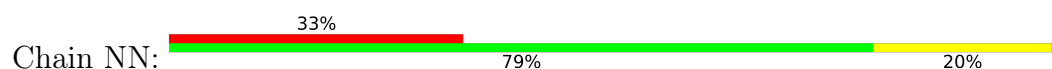


• Molecule 60: eS12

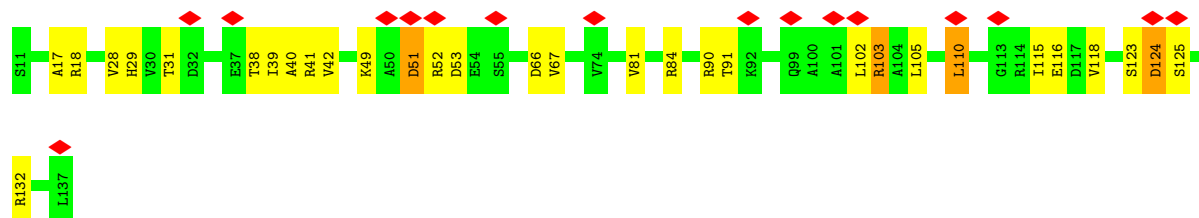
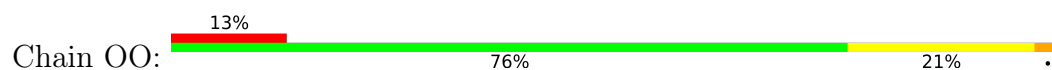




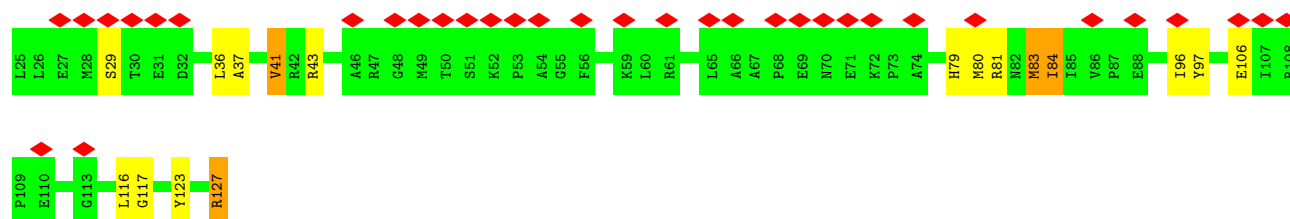
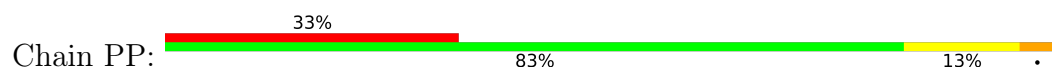
• Molecule 61: uS15



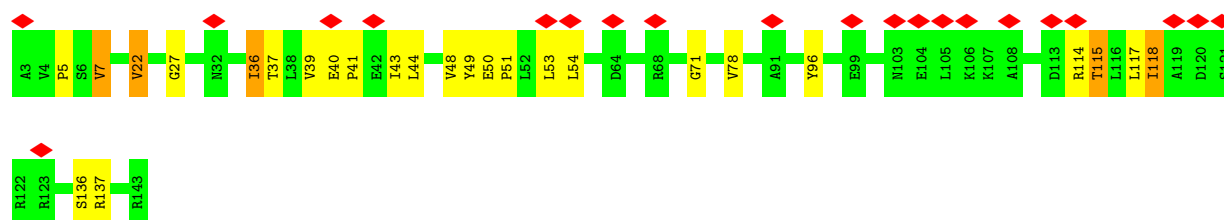
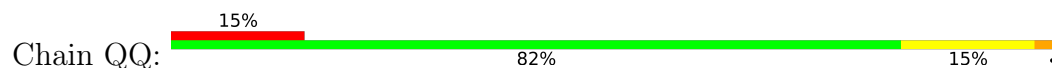
• Molecule 62: uS11



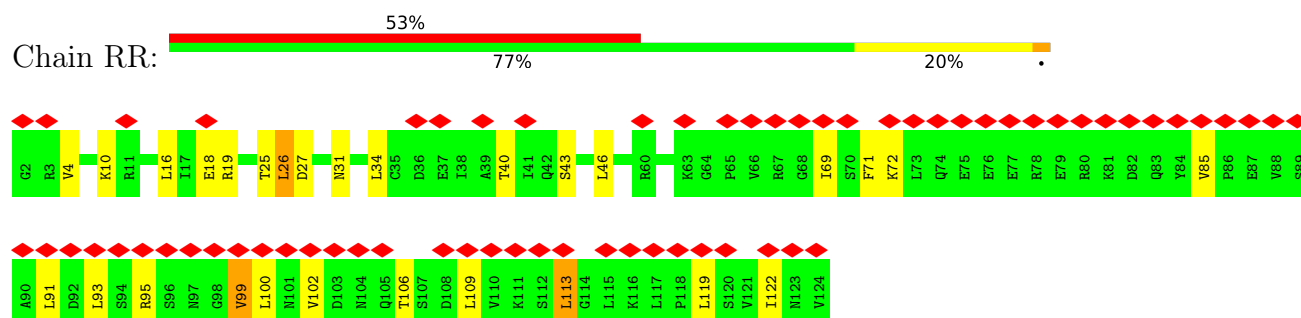
• Molecule 63: uS19



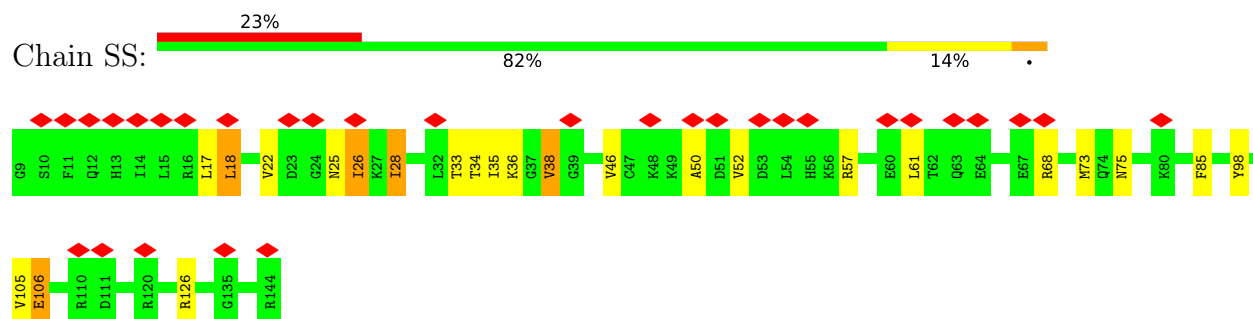
• Molecule 64: uS19



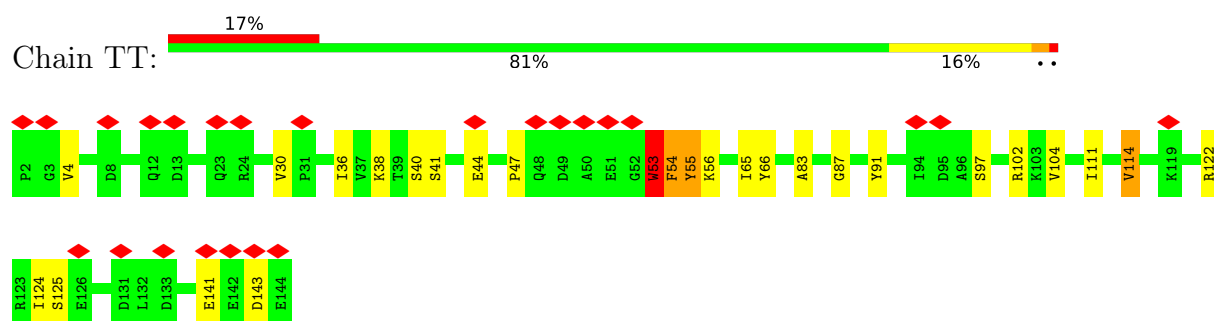
• Molecule 65: eS17



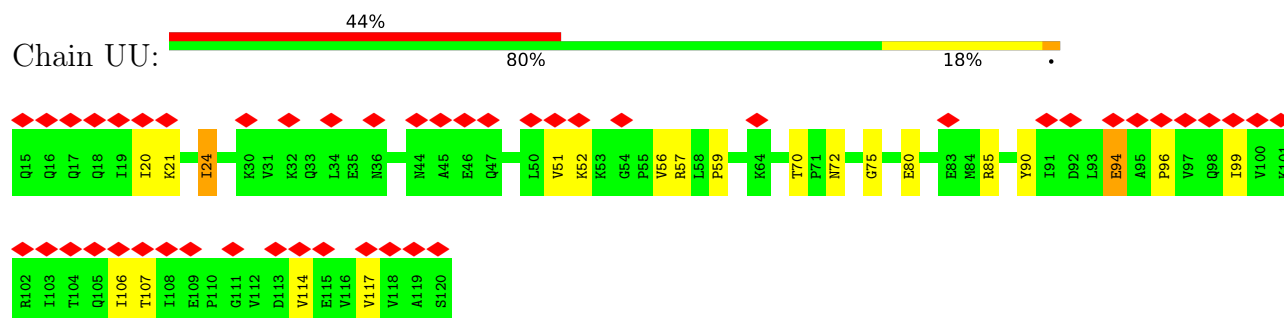
- Molecule 66: uS13



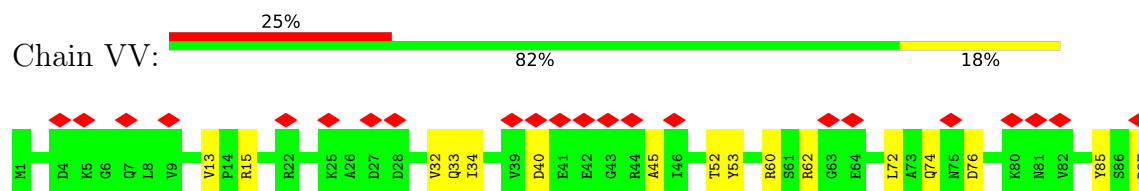
- Molecule 67: eS19



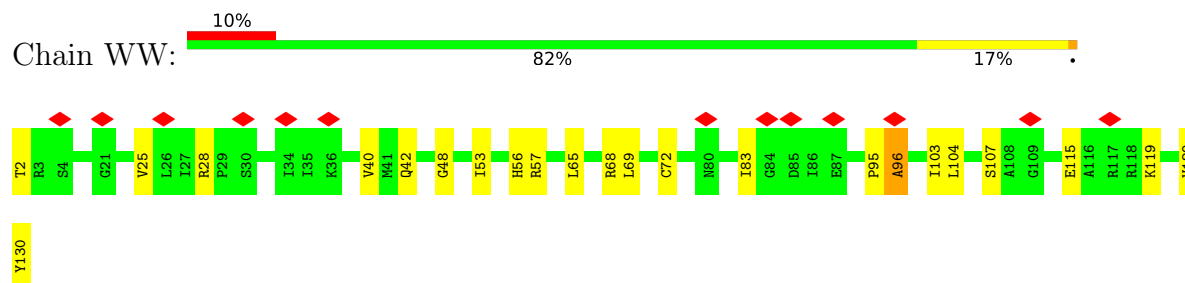
- Molecule 68: uS10



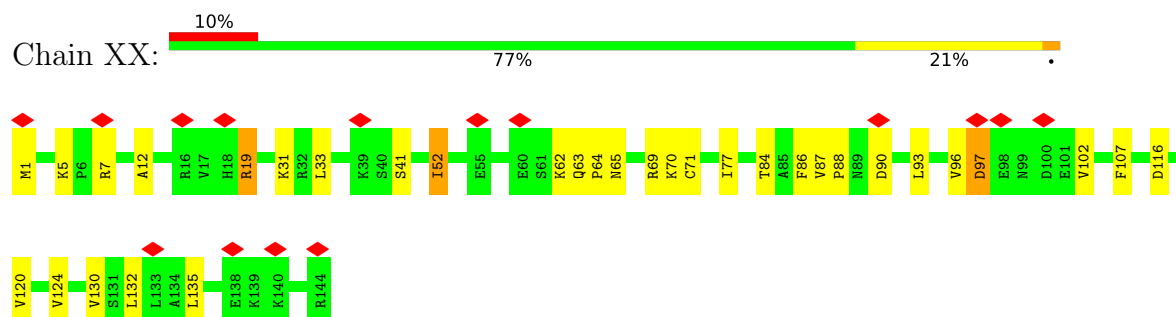
- Molecule 69: eS21



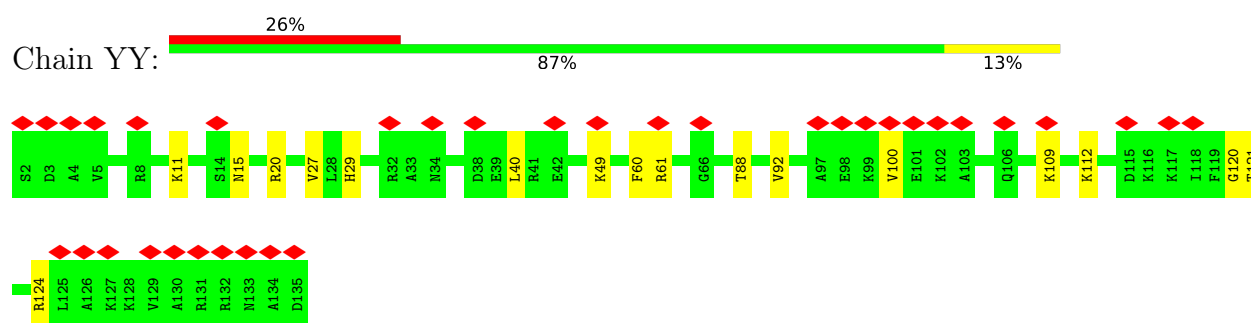
- Molecule 70: uS8



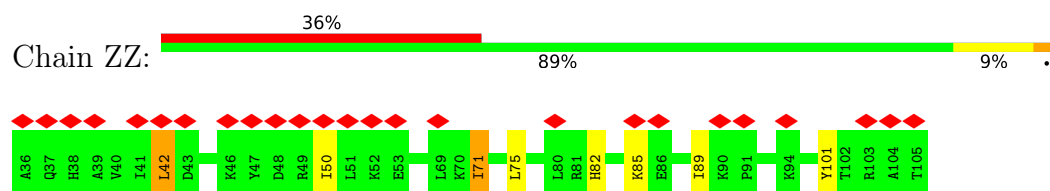
- Molecule 71: uS12



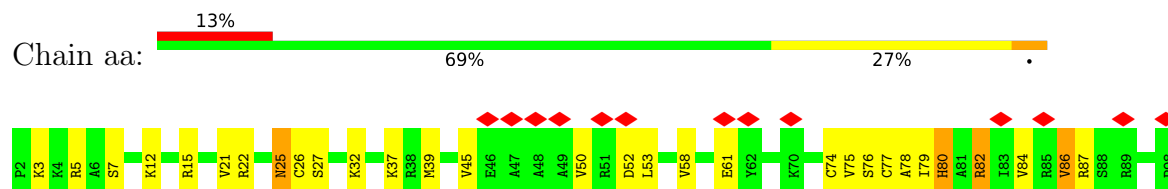
- Molecule 72: eS24



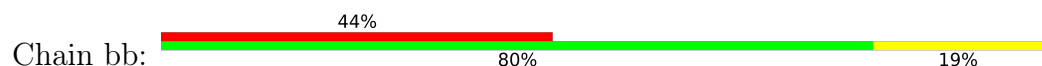
- Molecule 73: eS25

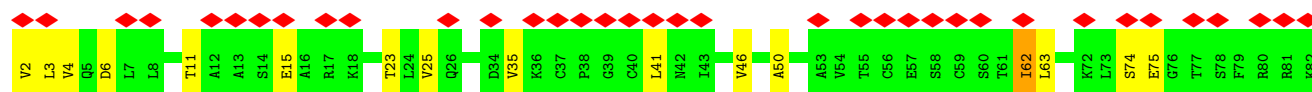


- Molecule 74: eS26

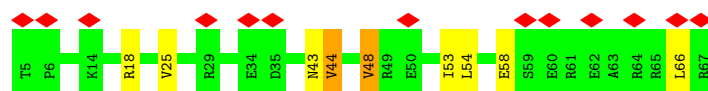
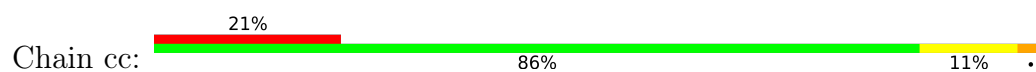


- Molecule 75: eS27

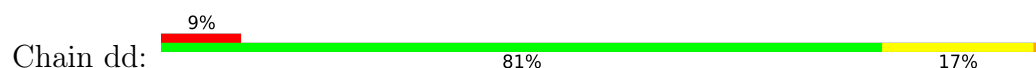




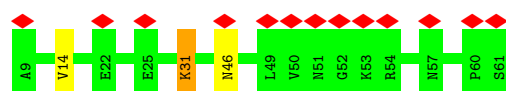
• Molecule 76: eS28



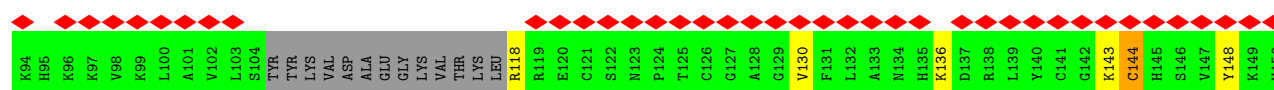
• Molecule 77: uS14



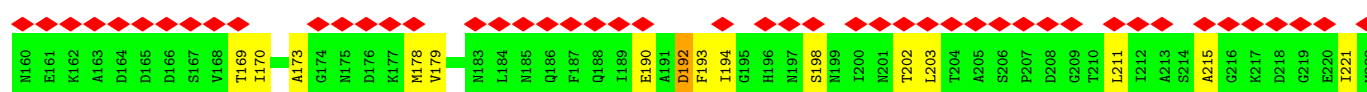
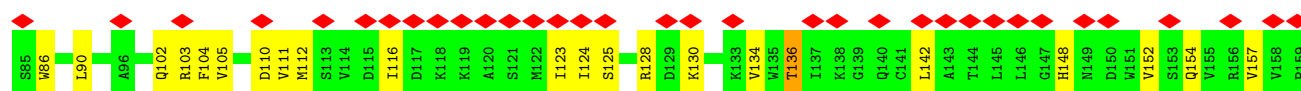
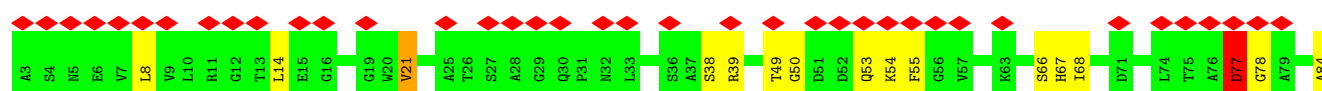
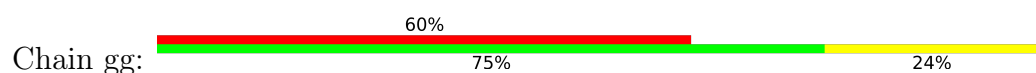
• Molecule 78: eS30

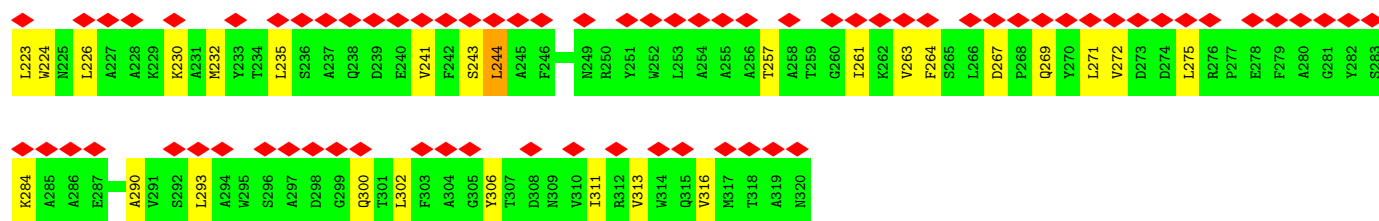


• Molecule 79: eS31

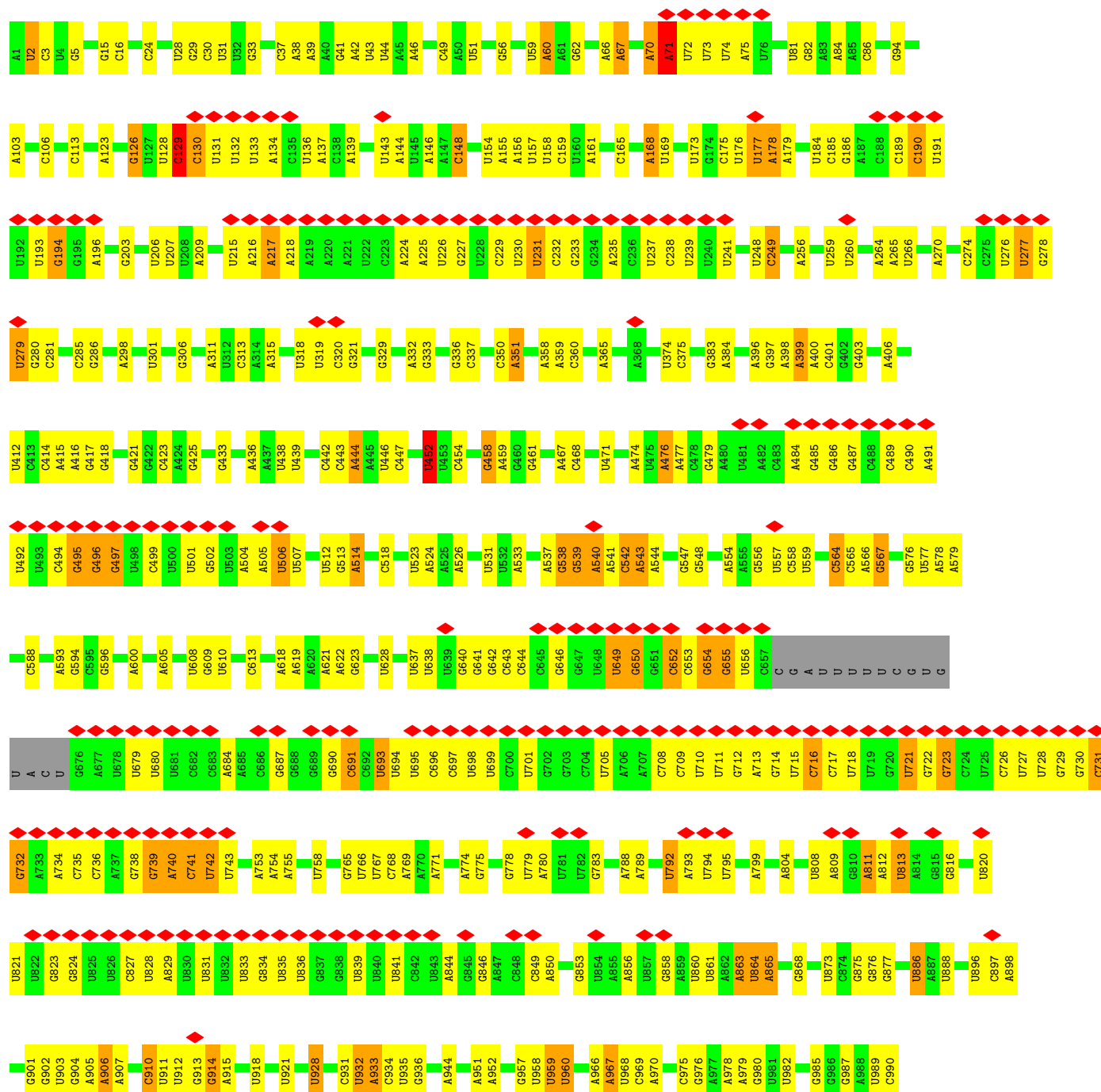


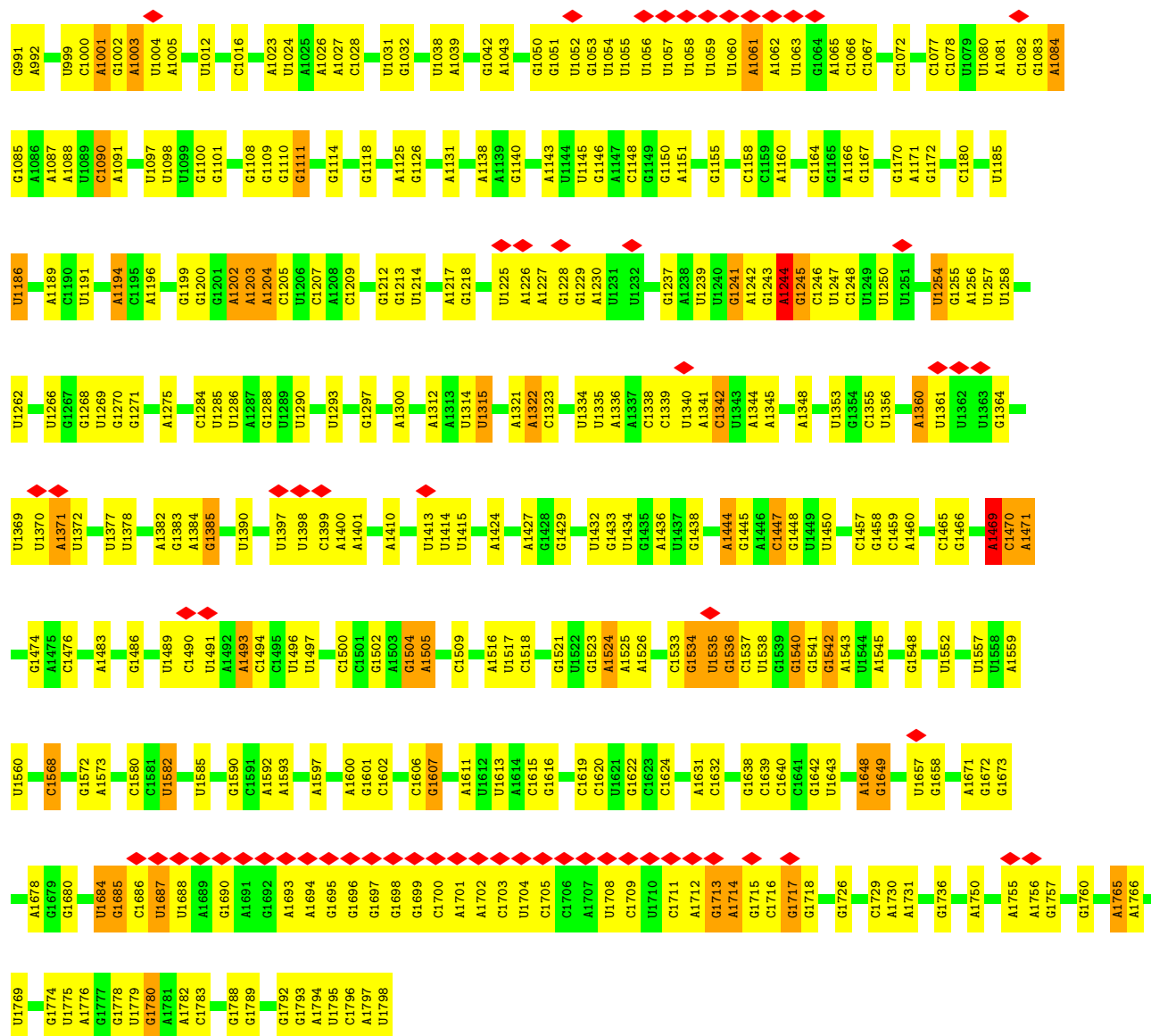
• Molecule 80: RACK1

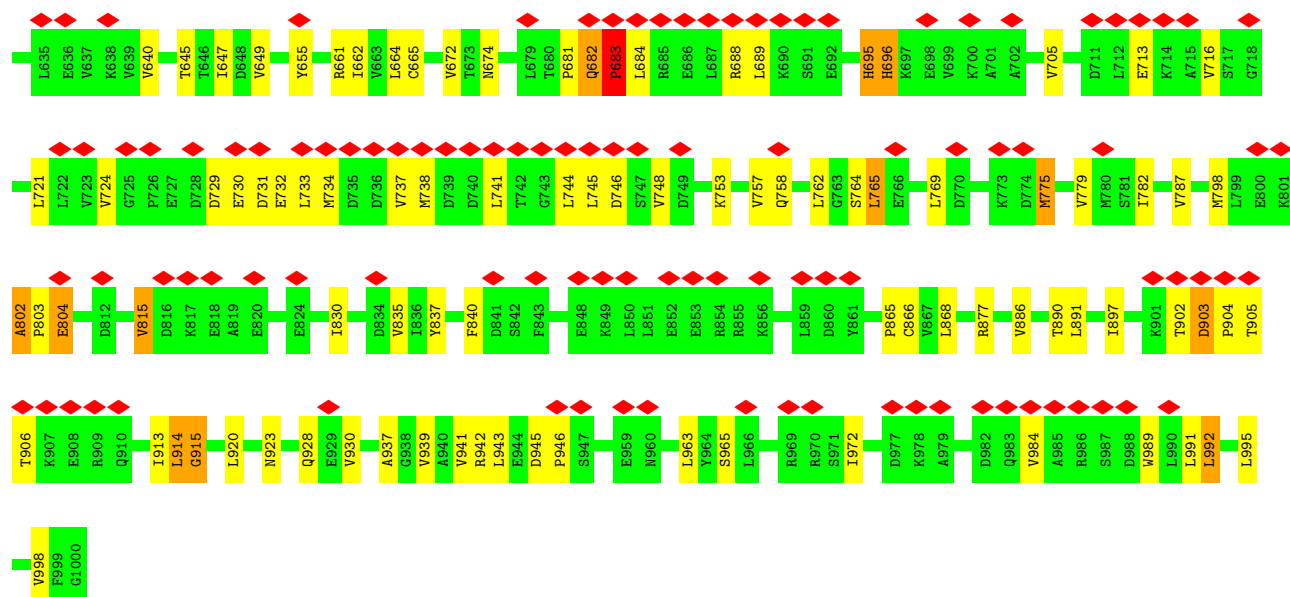




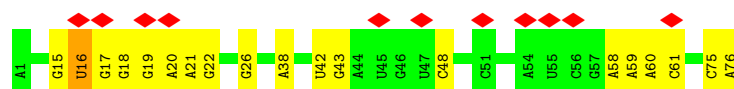
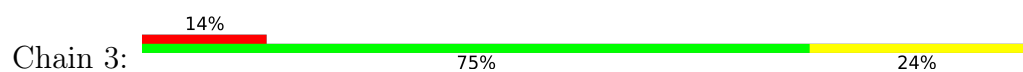
• Molecule 81: 18S ribosomal RNA







- Molecule 83: Met-tRNA-iMet



- Molecule 84: mRNA



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	424.8, 424.8, 424.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.416, 1.416, 1.416	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U6A, GDP

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	5	0.39	0/78264	0.74	51/121981 (0.0%)
2	7	0.38	0/2883	0.70	1/4491 (0.0%)
3	8	0.37	0/3724	0.72	2/5798 (0.0%)
4	A	1.02	0/1927	1.42	0/2589
5	B	1.02	0/3136	1.41	1/4217 (0.0%)
6	C	1.02	0/2787	1.51	5/3773 (0.1%)
7	D	1.02	0/2420	1.52	3/3264 (0.1%)
8	E	1.04	0/1260	1.43	0/1694
9	F	1.00	0/1821	1.54	0/2451
10	G	1.04	0/1841	1.56	0/2486
11	H	1.03	0/1545	1.41	0/2081
12	I	1.00	0/1787	1.41	0/2397
13	J	1.04	0/1365	1.49	0/1831
14	L	1.02	0/1609	1.54	1/2158 (0.0%)
15	M	1.04	0/1069	1.55	0/1439
16	N	0.96	0/1748	1.46	1/2343 (0.0%)
17	O	0.99	0/1585	1.54	1/2128 (0.0%)
18	P	1.01	0/1450	1.48	0/1947
19	Q	1.01	0/1461	1.47	0/1960
20	R	1.03	0/1538	1.61	2/2050 (0.1%)
21	S	0.98	0/1457	1.33	0/1958
22	T	1.01	0/1292	1.40	0/1732
23	U	1.04	0/812	1.45	0/1099
24	V	1.05	0/993	1.38	0/1335
25	W	1.00	0/525	1.40	0/697
26	X	1.02	0/983	1.46	0/1325
27	Y	1.04	0/999	1.47	0/1334
28	Z	1.01	0/1113	1.48	0/1490
29	a	0.98	0/1199	1.38	0/1605
30	b	1.01	0/468	1.53	0/622
31	c	1.07	0/751	1.54	0/1008
32	d	1.03	0/879	1.38	0/1179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	1.01	0/1009	1.50	3/1349 (0.2%)
34	f	1.00	1/860 (0.1%)	1.27	0/1157
35	g	1.05	0/964	1.47	0/1282
36	h	1.02	0/959	1.59	0/1276
37	i	1.03	0/770	1.54	0/1021
38	j	0.98	0/688	1.48	0/912
39	k	1.05	0/613	1.39	0/819
40	l	0.97	0/435	1.37	0/577
41	m	1.01	0/415	1.40	0/551
42	n	0.94	0/219	1.52	0/281
43	o	0.98	0/826	1.39	0/1090
44	p	1.05	0/675	1.55	0/898
45	q	1.10	0/1744	1.48	0/2339
46	r	1.08	0/1538	1.45	0/2079
48	AA	1.03	0/1656	1.48	0/2266
49	BB	1.06	0/1742	1.43	0/2346
50	CC	1.05	0/1665	1.50	3/2263 (0.1%)
51	DD	1.05	0/1759	1.46	2/2368 (0.1%)
52	EE	1.03	0/2088	1.38	0/2811
53	FF	1.05	0/1607	1.50	0/2172
54	GG	1.05	0/1844	1.47	1/2464 (0.0%)
55	HH	1.06	0/1506	1.47	2/2028 (0.1%)
56	II	1.03	0/1505	1.50	2/2010 (0.1%)
57	JJ	1.03	0/1502	1.56	0/2013
58	KK	1.02	0/838	1.41	0/1133
59	LL	1.04	0/1192	1.37	0/1608
60	MM	1.13	0/942	1.46	0/1274
61	NN	1.05	0/1215	1.55	0/1638
62	OO	1.07	0/952	1.53	0/1279
63	PP	1.05	0/831	1.42	0/1117
64	QQ	1.05	0/1125	1.45	0/1510
65	RR	1.04	0/998	1.56	0/1337
66	SS	1.03	0/1140	1.51	0/1532
67	TT	1.04	0/1130	1.58	0/1517
68	UU	1.07	0/857	1.45	1/1158 (0.1%)
69	VV	1.03	0/693	1.41	0/935
70	WW	1.04	0/1038	1.50	0/1395
71	XX	1.02	0/1141	1.39	0/1520
72	YY	1.05	0/1087	1.42	0/1449
73	ZZ	1.05	0/571	1.50	0/768
74	aa	1.04	0/782	1.44	0/1047
75	bb	1.09	0/620	1.41	0/838
76	cc	1.07	0/499	1.39	0/670

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	dd	0.99	0/453	1.45	0/602
78	ee	1.02	0/433	1.37	0/576
79	ff	1.06	0/349	1.40	0/463
80	gg	1.06	0/2495	1.35	0/3392
81	2	0.38	0/42249	0.73	23/65802 (0.0%)
82	1	1.35	36/4776 (0.8%)	1.53	25/6454 (0.4%)
83	3	0.37	0/1823	0.68	0/2842
84	4	0.39	0/147	0.72	0/227
All	All	0.75	37/225656 (0.0%)	1.08	130/330917 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
6	C	0	2
7	D	0	1
9	F	0	2
11	H	0	1
13	J	0	1
17	O	0	1
21	S	0	1
30	b	0	1
33	e	0	1
34	f	0	1
37	i	0	1
39	k	0	1
44	p	0	2
46	r	0	3
49	BB	0	1
50	CC	0	1
51	DD	0	1
52	EE	0	1
53	FF	0	2
54	GG	0	1
55	HH	0	1
56	II	0	3
57	JJ	0	1
58	KK	0	1
59	LL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
64	QQ	0	2
66	SS	0	1
67	TT	0	1
71	XX	0	2
72	YY	0	1
82	1	0	7
All	All	0	48

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	458	VAL	CA-C	-20.21	1.26	1.52
82	1	461	GLU	C-O	-15.54	1.04	1.24
82	1	459	MET	C-O	-13.48	1.06	1.24
82	1	458	VAL	C-O	-12.80	1.05	1.24
82	1	459	MET	CA-CB	-12.59	1.32	1.53
82	1	463	GLU	C-O	-12.56	1.08	1.24
82	1	460	ALA	CA-C	-12.54	1.35	1.52
82	1	462	TYR	CA-C	-12.26	1.36	1.52
82	1	460	ALA	C-O	-11.19	1.09	1.24
82	1	464	LYS	CA-C	-10.55	1.38	1.52
82	1	462	TYR	C-O	-10.24	1.11	1.23
82	1	461	GLU	CA-C	-9.98	1.39	1.52
82	1	465	GLN	N-CA	-9.43	1.34	1.46
82	1	459	MET	N-CA	-8.55	1.34	1.46
82	1	463	GLU	CA-C	-8.40	1.41	1.52
82	1	461	GLU	C-N	-8.24	1.22	1.33
82	1	464	LYS	CA-CB	-8.12	1.39	1.53
82	1	464	LYS	N-CA	-8.05	1.35	1.46
82	1	459	MET	CG-SD	-7.92	1.60	1.80
82	1	463	GLU	CD-OE1	-7.56	1.10	1.25
82	1	462	TYR	CZ-OH	-7.05	1.23	1.38
82	1	465	GLN	CA-C	6.75	1.61	1.52
82	1	457	LYS	C-N	-6.73	1.26	1.34
82	1	462	TYR	CB-CG	-6.69	1.36	1.51
82	1	458	VAL	CA-CB	-6.36	1.46	1.54
82	1	460	ALA	N-CA	-6.33	1.38	1.46
82	1	459	MET	CA-C	-6.00	1.44	1.52
82	1	462	TYR	N-CA	-5.80	1.38	1.45
82	1	465	GLN	CA-CB	-5.67	1.43	1.53
82	1	459	MET	SD-CE	-5.56	1.65	1.79
82	1	463	GLU	CG-CD	-5.38	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	467	PHE	C-O	-5.30	1.17	1.24
82	1	465	GLN	C-O	-5.21	1.17	1.24
82	1	458	VAL	C-N	-5.14	1.26	1.33
34	f	37	THR	N-CA	5.10	1.49	1.46
82	1	463	GLU	CA-CB	-5.08	1.44	1.53
82	1	468	ASP	CA-C	5.00	1.59	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1607	U	C2'-C3'-O3'	12.05	127.58	109.50
82	1	464	LYS	N-CA-C	11.71	135.74	110.80
82	1	462	TYR	CA-C-O	-10.19	108.06	118.97
82	1	469	VAL	CA-C-N	10.12	132.49	119.84
82	1	469	VAL	C-N-CA	10.12	132.49	119.84
82	1	463	GLU	CB-CG-CD	-9.49	96.46	112.60
1	5	1352	A	C2'-C3'-O3'	9.48	123.72	109.50
82	1	463	GLU	CB-CA-C	-9.11	92.30	110.42
82	1	461	GLU	N-CA-CB	-8.98	95.31	110.49
1	5	3194	C	C4'-C3'-O3'	8.49	122.14	109.40
82	1	461	GLU	N-CA-C	8.36	128.60	110.80
1	5	2662	G	C2'-C3'-O3'	8.31	126.16	113.70
81	2	177	U	C2'-C3'-O3'	8.24	121.86	109.50
1	5	297	G	C2'-C3'-O3'	8.11	121.67	109.50
82	1	460	ALA	CA-C-N	8.11	137.03	121.54
82	1	460	ALA	C-N-CA	8.11	137.03	121.54
1	5	567	G	C2'-C3'-O3'	8.03	125.74	113.70
1	5	1560	G	C4'-C3'-O3'	7.95	121.32	109.40
81	2	564	C	C4'-C3'-O3'	7.82	121.13	109.40
1	5	1064	A	C2'-C3'-O3'	7.64	120.96	109.50
1	5	3078	U	C4'-C3'-O3'	7.63	120.84	109.40
81	2	1244	A	C4'-C3'-O3'	7.50	120.64	109.40
1	5	2570	U	C4'-C3'-O3'	7.48	120.62	109.40
1	5	2500	A	C4'-C3'-O3'	7.47	120.61	109.40
1	5	1307	G	C2'-C3'-O3'	7.46	120.69	109.50
1	5	873	C	C4'-C3'-O3'	7.33	123.99	113.00
1	5	2112	U	C4'-C3'-O3'	7.33	120.39	109.40
1	5	3239	G	C2'-C3'-O3'	7.19	124.49	113.70
81	2	1084	A	C2'-C3'-O3'	7.11	124.37	113.70
81	2	279	U	C2'-C3'-O3'	7.01	120.02	109.50
1	5	3303	G	C4'-C3'-O3'	7.00	119.89	109.40
1	5	2064	U	C2'-C3'-O3'	6.95	119.92	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2505	U	C4'-C3'-O3'	6.85	119.67	109.40
82	1	458	VAL	CG1-CB-CG2	-6.84	95.76	110.80
82	1	458	VAL	CA-C-O	-6.83	110.58	119.53
6	C	77	VAL	CA-C-N	6.79	126.56	120.10
6	C	77	VAL	C-N-CA	6.79	126.56	120.10
3	8	125	U	C2'-C3'-O3'	6.75	119.63	109.50
1	5	298	U	C2'-C3'-O3'	6.72	119.59	109.50
81	2	1493	A	C2'-C3'-O3'	6.61	119.42	109.50
1	5	133	U	C4'-C3'-O3'	6.60	119.29	109.40
1	5	2941	A	C2'-C3'-O3'	6.54	119.31	109.50
68	UU	75	GLY	CA-C-O	-6.53	117.97	122.22
82	1	465	GLN	N-CA-CB	-6.49	99.53	110.49
1	5	1284	C	C2'-C3'-O3'	6.44	123.36	113.70
82	1	461	GLU	CA-C-N	6.36	132.55	122.11
82	1	461	GLU	C-N-CA	6.36	132.55	122.11
82	1	459	MET	CA-C-N	6.34	133.65	121.54
82	1	459	MET	C-N-CA	6.34	133.65	121.54
81	2	277	U	C4'-C3'-O3'	6.31	118.87	109.40
1	5	3357	U	C2'-C3'-O3'	6.20	123.00	113.70
1	5	1816	A	C2'-C3'-O3'	6.17	118.76	109.50
81	2	1447	C	C4'-C3'-O3'	6.09	118.53	109.40
33	e	122	PRO	CA-C-N	6.08	132.63	121.70
33	e	122	PRO	C-N-CA	6.08	132.63	121.70
82	1	462	TYR	CB-CA-C	-6.04	98.93	109.07
1	5	1241	U	C4'-C3'-O3'	6.02	118.42	109.40
1	5	2561	A	C4'-C3'-O3'	5.99	118.39	109.40
1	5	659	G	C2'-C3'-O3'	-5.99	104.72	113.70
1	5	166	C	C2'-C3'-O3'	5.97	122.65	113.70
81	2	1090	C	C4'-C3'-O3'	5.95	118.33	109.40
81	2	906	A	C4'-C3'-O3'	-5.92	104.11	113.00
81	2	1360	A	C2'-C3'-O3'	5.92	122.58	113.70
54	GG	55	GLY	CA-C-O	-5.92	118.05	122.37
81	2	721	U	C4'-C3'-O3'	5.87	118.20	109.40
81	2	129	C	C3'-C2'-O2'	5.84	119.46	110.70
82	1	462	TYR	CA-C-N	5.77	132.56	121.54
82	1	462	TYR	C-N-CA	5.77	132.56	121.54
81	2	910	C	C2'-C3'-O3'	5.70	122.24	113.70
17	O	45	GLY	CA-C-O	-5.69	118.31	122.23
82	1	462	TYR	O-C-N	5.67	129.35	122.48
82	1	463	GLU	CA-C-N	5.66	132.36	121.54
82	1	463	GLU	C-N-CA	5.66	132.36	121.54
1	5	1729	A	C4'-C3'-O3'	5.66	121.49	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	HH	68	ALA	CA-C-N	5.63	126.23	119.98
55	HH	68	ALA	C-N-CA	5.63	126.23	119.98
1	5	3228	C	C2'-C3'-O3'	5.60	117.90	109.50
81	2	129	C	C2'-C3'-O3'	5.56	122.05	113.70
1	5	2267	C	N1-C1'-C2'	5.54	120.32	112.00
1	5	1481	A	C2'-C3'-O3'	5.53	117.80	109.50
50	CC	83	ASP	CB-CA-C	5.53	120.60	110.10
5	B	271	GLY	CA-C-O	-5.52	117.44	122.24
1	5	1241	U	C2'-C3'-O3'	5.52	117.78	109.50
6	C	343	LYS	CB-CA-C	5.51	121.38	110.42
1	5	3054	U	C4'-C3'-O3'	-5.50	104.75	113.00
82	1	463	GLU	N-CA-C	5.49	122.50	110.80
81	2	1268	G	C4'-C3'-O3'	-5.48	104.78	113.00
6	C	78	GLY	CA-C-N	5.45	125.15	119.92
6	C	78	GLY	C-N-CA	5.45	125.15	119.92
7	D	201	GLY	CA-C-N	5.43	126.12	120.03
7	D	201	GLY	C-N-CA	5.43	126.12	120.03
1	5	1284	C	C3'-C2'-O2'	5.43	118.84	110.70
1	5	91	G	C2'-C3'-O3'	5.42	121.83	113.70
1	5	3284	G	C4'-C3'-O3'	5.42	117.53	109.40
50	CC	46	LEU	CA-C-N	5.42	126.09	120.03
50	CC	46	LEU	C-N-CA	5.42	126.09	120.03
3	8	43	A	C3'-C2'-O2'	5.37	118.75	110.70
1	5	3121	U	C4'-C3'-O3'	5.36	117.44	109.40
1	5	1349	G	C4'-C3'-O3'	5.34	121.02	113.00
1	5	3317	U	C2'-C3'-O3'	5.33	117.49	109.50
81	2	1371	A	C2'-C3'-O3'	5.33	121.69	113.70
1	5	1355	A	C4'-C3'-O3'	5.30	117.35	109.40
1	5	916	G	C4'-C3'-O3'	5.29	120.94	113.00
33	e	121	ASN	CB-CA-C	5.27	120.56	110.17
1	5	1152	G	C2'-C3'-O3'	5.26	117.40	109.50
1	5	2486	A	C2'-C3'-O3'	5.26	117.39	109.50
81	2	71	A	C4'-C3'-O3'	5.25	117.27	109.40
81	2	452	U	N1-C1'-C2'	5.22	119.84	112.00
51	DD	216	PRO	CA-C-N	5.22	131.37	121.97
51	DD	216	PRO	C-N-CA	5.22	131.37	121.97
81	2	1444	A	C2'-C3'-O3'	5.21	121.52	113.70
1	5	1073	U	C1'-C2'-O2'	-5.19	104.02	111.80
1	5	2467	G	C4'-C3'-O3'	5.19	117.18	109.40
1	5	3075	G	C3'-C2'-O2'	5.17	118.46	110.70
1	5	1238	C	C2'-C3'-O3'	5.17	121.46	113.70
7	D	47	PRO	CB-CA-C	5.12	116.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	465	GLN	CA-CB-CG	5.10	124.29	114.10
16	N	177	GLY	CA-C-O	-5.09	118.21	122.33
81	2	1469	A	C4'-C3'-O3'	-5.09	105.36	113.00
1	5	3289	G	C2'-C3'-O3'	5.06	121.29	113.70
14	L	124	ILE	CB-CA-C	5.06	116.70	111.09
20	R	54	ALA	CA-C-N	5.05	127.46	120.49
20	R	54	ALA	C-N-CA	5.05	127.46	120.49
56	II	12	SER	CA-C-N	5.04	127.29	120.38
56	II	12	SER	C-N-CA	5.04	127.29	120.38
1	5	2990	G	C3'-C2'-O2'	5.03	118.25	110.70
81	2	1444	A	C3'-C2'-O2'	5.03	118.25	110.70
2	7	41	G	C4'-C3'-O3'	-5.02	105.47	113.00
81	2	1084	A	C3'-C2'-O2'	5.01	118.21	110.70
1	5	3317	U	C4'-C3'-O3'	5.00	116.91	109.40

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	1	458	VAL	Mainchain
82	1	463	GLU	Mainchain
82	1	683	PRO	Peptide
82	1	802	ALA	Peptide
82	1	903	ASP	Peptide
82	1	914	LEU	Peptide
82	1	915	GLY	Peptide
4	A	196	TRP	Peptide
49	BB	177	GLN	Peptide
6	C	148	ILE	Peptide
6	C	349	THR	Peptide
50	CC	82	GLN	Peptide
7	D	258	LYS	Peptide
51	DD	219	ALA	Peptide
52	EE	19	LEU	Peptide
9	F	157	ASN	Peptide
9	F	215	GLY	Peptide
53	FF	45	PHE	Peptide
53	FF	51	GLU	Peptide
54	GG	57	ASP	Peptide
11	H	22	SER	Peptide
55	HH	64	VAL	Peptide
56	II	107	THR	Peptide

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Mol	Chain	Res	Type	Group
56	II	182	GLY	Peptide
56	II	8	ARG	Peptide
13	J	93	ASP	Peptide
57	JJ	163	PRO	Peptide
58	KK	53	GLY	Peptide
59	LL	15	LYS	Peptide
17	O	110	PRO	Peptide
64	QQ	114	ARG	Peptide
64	QQ	115	THR	Peptide
21	S	22	PRO	Peptide
66	SS	25	ASN	Peptide
67	TT	53	TRP	Peptide
71	XX	62	LYS	Peptide
71	XX	87	VAL	Peptide
72	YY	29	HIS	Peptide
30	b	20	GLY	Peptide
33	e	121	ASN	Peptide
34	f	103	TYR	Peptide
37	i	12	ASN	Peptide
39	k	65	LEU	Peptide
44	p	47	VAL	Peptide
44	p	59	CYS	Peptide
46	r	108	ALA	Peptide
46	r	109	ALA	Peptide
46	r	36	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	69936	0	35154	281	0
2	7	2579	0	1304	9	0
3	8	3333	0	1685	11	0
4	A	1893	0	1959	19	0
5	B	3065	0	3150	42	0
6	C	2735	0	2854	28	0
7	D	2370	0	2320	19	0
8	E	1239	0	1326	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1784	0	1862	19	0
10	G	1809	0	1891	7	0
11	H	1524	0	1587	11	0
12	I	1750	0	1788	13	0
13	J	1344	0	1370	8	0
14	L	1584	0	1658	16	0
15	M	1054	0	1149	11	0
16	N	1711	0	1766	19	0
17	O	1555	0	1659	8	0
18	P	1427	0	1470	19	0
19	Q	1437	0	1540	15	0
20	R	1521	0	1617	6	0
21	S	1422	0	1463	14	0
22	T	1268	0	1312	11	0
23	U	796	0	812	5	0
24	V	978	0	1025	6	0
25	W	513	0	539	0	0
26	X	968	0	1036	8	0
27	Y	988	0	1076	5	0
28	Z	1087	0	1150	7	0
29	a	1168	0	1210	15	0
30	b	457	0	486	4	0
31	c	743	0	797	4	0
32	d	865	0	917	4	0
33	e	988	0	1054	12	0
34	f	842	0	869	3	0
35	g	954	0	1039	9	0
36	h	950	0	1055	4	0
37	i	764	0	841	10	0
38	j	673	0	677	7	0
39	k	607	0	677	12	0
40	l	428	0	464	2	0
41	m	409	0	444	4	0
42	n	218	0	266	3	0
43	o	814	0	881	3	0
44	p	668	0	711	10	0
45	q	1718	0	1810	19	0
46	r	1512	0	1546	29	0
47	K	735	0	178	0	0
48	AA	1615	0	1631	29	0
49	BB	1716	0	1786	16	0
50	CC	1635	0	1723	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	DD	1734	0	1817	14	0
52	EE	2047	0	2132	17	0
53	FF	1588	0	1657	14	0
54	GG	1820	0	1918	18	0
55	HH	1481	0	1572	14	0
56	II	1480	0	1512	14	0
57	JJ	1477	0	1559	13	0
58	KK	818	0	806	12	0
59	LL	1166	0	1232	7	0
60	MM	934	0	975	11	0
61	NN	1192	0	1255	15	0
62	OO	941	0	979	16	0
63	PP	814	0	850	12	0
64	QQ	1105	0	1166	13	0
65	RR	989	0	1052	16	0
66	SS	1121	0	1148	16	0
67	TT	1112	0	1124	13	0
68	UU	847	0	911	10	0
69	VV	684	0	672	6	0
70	WW	1021	0	1060	12	0
71	XX	1123	0	1203	15	0
72	YY	1073	0	1132	11	0
73	ZZ	563	0	603	6	0
74	aa	769	0	816	14	0
75	bb	610	0	633	6	0
76	cc	497	0	535	5	0
77	dd	443	0	433	5	0
78	ee	426	0	472	4	0
79	ff	344	0	360	2	0
80	gg	2444	0	2399	37	0
81	2	37790	0	19024	231	0
82	1	4704	0	4839	116	0
83	3	1630	0	824	3	0
84	4	131	0	66	0	0
85	aa	1	0	0	2	0
85	bb	1	0	0	0	0
85	ff	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
86	1	28	0	12	0	0
87	3	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	3	8	0	8	0	0
All	All	211119	0	157340	1327	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 (1327) 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)
82:1:423:ASP:OD1	82:1:429:ASN:HA	1.06	1.24
82:1:423:ASP:OD1	82:1:429:ASN:CA	2.01	1.09
82:1:464:LYS:H	82:1:464:LYS:HD2	1.29	0.98
82:1:565:TYR:CE1	82:1:581:LEU:HD13	1.99	0.98
82:1:423:ASP:CG	82:1:429:ASN:HA	1.92	0.94
74:aa:74:CYS:HG	85:aa:500:ZN:ZN	0.55	0.88
82:1:565:TYR:CD1	82:1:581:LEU:HD13	2.10	0.86
82:1:463:GLU:HB2	82:1:464:LYS:HD2	1.55	0.85
82:1:446:TYR:OH	82:1:470:PRO:O	1.95	0.84
6:C:343:LYS:HB3	6:C:344:ALA:HA	1.59	0.84
81:2:976:G:H1	81:2:1023:A:HO2'	1.24	0.82
82:1:565:TYR:CE1	82:1:581:LEU:CD1	2.63	0.82
5:B:84:VAL:HG12	5:B:162:VAL:HG22	1.60	0.80
5:B:232:ARG:NH1	5:B:267:ALA:HA	1.97	0.79
54:GG:202:ARG:NH2	81:2:126:G:N7	2.32	0.77
4:A:27:ALA:O	4:A:128:ARG:NH2	2.17	0.77
2:7:28:C:OP1	13:J:137:ARG:NH1	2.18	0.77
81:2:1339:C:O2'	81:2:1341:A:N7	2.20	0.74
67:TT:102:ARG:NH2	81:2:1502:G:N7	2.34	0.74
74:aa:74:CYS:SG	85:aa:500:ZN:ZN	1.72	0.74
82:1:423:ASP:OD2	82:1:430:VAL:N	2.20	0.74
82:1:459:MET:HG3	82:1:459:MET:O	1.87	0.73
48:AA:33:GLN:HB2	48:AA:34:GLU:HA	1.71	0.71
82:1:464:LYS:HD2	82:1:464:LYS:N	2.06	0.71
29:a:104:THR:HG21	29:a:112:ILE:HD11	1.73	0.71
82:1:802:ALA:O	82:1:804:GLU:N	2.21	0.71
80:gg:173:ALA:HB2	80:gg:203:LEU:HG	1.72	0.71
1:5:31:C:OP2	16:N:188:ARG:NH2	2.24	0.71
18:P:29:THR:HG23	18:P:119:VAL:HG11	1.72	0.71
33:e:122:PRO:HA	33:e:123:LYS:HB3	1.72	0.71
80:gg:241:VAL:HG12	80:gg:257:THR:HG22	1.74	0.70
74:aa:26:CYS:HB2	74:aa:77:CYS:SG	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:26:SER:OG	46:r:95:LEU:HD21	1.92	0.69
82:1:464:LYS:H	82:1:464:LYS:CD	1.97	0.69
1:5:2554:A:N6	44:p:61:LYS:O	2.26	0.68
66:SS:46:VAL:HG11	66:SS:73:MET:HG3	1.76	0.67
1:5:2536:A:H3'	1:5:2537:U:H4'	1.75	0.67
82:1:456:THR:O	82:1:465:GLN:OE1	2.12	0.67
81:2:1648:A:O2'	81:2:1649:G:O5'	2.13	0.67
73:ZZ:50:ILE:HD11	73:ZZ:71:ILE:HD13	1.78	0.66
16:N:106:VAL:HG11	16:N:132:VAL:HG21	1.78	0.66
54:GG:33:GLY:N	54:GG:52:ILE:O	2.27	0.66
5:B:19:ARG:HB3	5:B:270:ARG:HG2	1.77	0.66
59:LL:57:LYS:HD3	59:LL:131:ILE:HG23	1.77	0.66
14:L:47:ALA:HB3	14:L:48:PRO:HD3	1.78	0.65
1:5:2969:A:N7	4:A:215:ASN:ND2	2.45	0.65
5:B:226:PHE:O	5:B:232:ARG:NH2	2.28	0.65
28:Z:26:VAL:HG11	28:Z:96:VAL:HB	1.79	0.65
5:B:252:ILE:HG21	5:B:260:VAL:HG22	1.78	0.65
1:5:2267:C:H2'	1:5:2267:C:O2	1.96	0.64
81:2:155:A:O2'	82:1:688:ARG:NH2	2.30	0.64
1:5:1455:U:H1'	32:d:26:LYS:HE2	1.79	0.64
3:8:83:C:N3	27:Y:52:ARG:NH2	2.46	0.64
49:BB:71:ALA:HB2	49:BB:80:SER:HA	1.80	0.64
1:5:674:G:OP1	6:C:31:ARG:NH1	2.30	0.64
46:r:93:GLU:HB3	46:r:94:PRO:HD3	1.80	0.64
50:CC:45:LYS:HB2	50:CC:252:ALA:HB1	1.79	0.64
55:HH:111:LYS:HB2	81:2:811:A:N7	2.13	0.64
81:2:1202:A:H2'	81:2:1203:A:H5'	1.79	0.64
75:bb:62:ILE:O	75:bb:74:SER:OG	2.12	0.63
1:5:2404:A:N7	1:5:2872:A:N6	2.47	0.63
1:5:2284:C:O2	82:1:942:ARG:NH1	2.31	0.63
6:C:283:THR:HG23	6:C:289:ILE:HD11	1.81	0.63
82:1:449:ILE:HA	82:1:452:ILE:HG22	1.81	0.63
33:e:122:PRO:HA	33:e:123:LYS:CB	2.29	0.63
82:1:565:TYR:CE1	82:1:581:LEU:HB2	2.34	0.63
59:LL:103:ARG:NH1	81:2:306:G:OP1	2.31	0.62
81:2:732:G:O2'	81:2:735:C:N4	2.32	0.62
1:5:837:A:OP2	44:p:4:ARG:NH1	2.32	0.62
1:5:3156:U:O2'	1:5:3157:U:O4'	2.17	0.62
61:NN:4:MET:HB2	81:2:967:A:OP1	1.99	0.62
1:5:1156:C:OP2	9:F:94:LYS:NZ	2.33	0.62
53:FF:151:VAL:HG11	76:cc:66:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:cc:44:VAL:HG12	76:cc:54:LEU:HD21	1.81	0.62
1:5:1259:A:O2'	1:5:1280:C:O2'	2.16	0.62
45:q:17:LEU:HD22	45:q:172:VAL:HG22	1.81	0.62
54:GG:64:LYS:HB2	54:GG:97:VAL:HG11	1.81	0.62
39:k:8:ILE:CG1	39:k:9:LYS:HA	2.29	0.62
1:5:361:A:O3'	38:j:45:ARG:NH2	2.33	0.62
10:G:93:PHE:HB3	10:G:188:LEU:HD11	1.81	0.62
50:CC:170:VAL:HG11	50:CC:215:THR:HA	1.81	0.62
81:2:471:U:O2'	81:2:769:A:N3	2.28	0.62
1:5:188:U:O2'	1:5:207:U:O2	2.18	0.61
53:FF:44:LEU:HD22	53:FF:49:SER:HA	1.82	0.61
81:2:1585:U:H3	81:2:1611:A:H2	1.49	0.61
81:2:609:G:N3	81:2:609:G:H2'	2.16	0.61
8:E:89:THR:HG21	15:M:115:PHE:HB2	1.83	0.61
4:A:102:LEU:HD12	4:A:107:VAL:HG22	1.83	0.61
46:r:30:VAL:HG12	46:r:89:VAL:HG11	1.82	0.61
82:1:423:ASP:CG	82:1:430:VAL:N	2.58	0.60
50:CC:86:MET:HG2	50:CC:216:LEU:HD11	1.83	0.60
62:OO:40:ALA:HB3	62:OO:67:VAL:HG23	1.83	0.60
48:AA:184:LEU:HD21	69:VV:45:ALA:HB3	1.82	0.60
80:gg:293:LEU:HD22	80:gg:302:LEU:HD12	1.82	0.60
1:5:617:G:OP1	8:E:108:LYS:NZ	2.35	0.60
1:5:3275:U:O2'	34:f:99:ARG:NH1	2.34	0.60
1:5:1481:A:O2'	1:5:1858:A:N3	2.30	0.60
45:q:35:GLN:HG2	45:q:166:ALA:HB2	1.83	0.60
81:2:452:U:O2	81:2:452:U:H2'	2.00	0.60
1:5:1429:G:OP2	6:C:107:ARG:NH1	2.35	0.60
55:HH:133:THR:HG21	55:HH:154:LEU:HD22	1.82	0.60
64:QQ:36:ILE:HD12	64:QQ:49:TYR:HE1	1.67	0.59
82:1:423:ASP:CG	82:1:430:VAL:H	2.09	0.59
73:ZZ:71:ILE:HG22	73:ZZ:75:LEU:HD23	1.84	0.59
82:1:423:ASP:OD2	82:1:429:ASN:C	2.45	0.59
48:AA:23:HIS:ND1	48:AA:48:ILE:HB	2.16	0.59
54:GG:59:GLN:NE2	81:2:417:G:O2'	2.34	0.59
7:D:113:LEU:HD13	7:D:142:PHE:CE2	2.37	0.59
1:5:1639:C:OP2	35:g:74:ARG:NH1	2.36	0.59
51:DD:162:GLN:N	51:DD:163:PRO:HD2	2.17	0.59
81:2:654:G:N2	81:2:655:G:O6	2.36	0.59
82:1:423:ASP:CG	82:1:429:ASN:CA	2.66	0.59
83:3:15:G:H2'	83:3:16:U:N3	2.17	0.59
7:D:113:LEU:HD13	7:D:142:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:90:MET:HE1	21:S:114:HIS:CE1	2.37	0.59
48:AA:65:ALA:HB1	48:AA:184:LEU:HD22	1.85	0.59
11:H:92:TYR:HB2	11:H:142:ASP:HB3	1.84	0.59
49:BB:156:ALA:HB3	49:BB:161:ILE:HD11	1.85	0.59
5:B:51:ALA:HB3	5:B:78:VAL:HG23	1.84	0.59
82:1:757:VAL:HG21	82:1:769:LEU:HD21	1.85	0.59
1:5:2836:C:H5	1:5:2852:C:H42	1.51	0.58
1:5:107:A:O2'	1:5:324:A:N3	2.36	0.58
7:D:83:LEU:N	7:D:84:PRO:HD2	2.17	0.58
46:r:32:VAL:HG21	46:r:35:VAL:HG13	1.85	0.58
17:O:50:ASN:ND2	17:O:136:THR:OG1	2.36	0.58
22:T:17:ARG:HG2	22:T:22:HIS:HA	1.84	0.58
46:r:37:SER:HA	46:r:38:GLN:HB3	1.86	0.58
48:AA:19:ALA:HB2	65:RR:99:VAL:HG22	1.85	0.58
54:GG:160:ARG:NH1	81:2:67:A:OP1	2.33	0.58
9:F:98:LYS:HB3	9:F:99:PRO:HD3	1.85	0.58
82:1:541:ILE:O	82:1:544:ASN:ND2	2.36	0.58
1:5:736:A:C5	1:5:737:G:H1'	2.39	0.58
9:F:44:ILE:HD12	9:F:180:SER:HB2	1.86	0.58
55:HH:9:LEU:HD23	55:HH:12:ALA:HB2	1.86	0.58
82:1:413:HIS:HA	82:1:510:GLN:HB3	1.85	0.58
21:S:77:VAL:HG12	21:S:126:VAL:HG13	1.85	0.58
71:XX:1:MET:HB2	81:2:1101:G:N7	2.19	0.58
81:2:1535:U:O2'	81:2:1536:G:N2	2.37	0.58
46:r:27:LEU:HD13	46:r:78:LEU:HD21	1.86	0.58
49:BB:204:ILE:O	81:2:1065:A:O2'	2.22	0.58
73:ZZ:89:ILE:HG23	73:ZZ:101:TYR:HB3	1.86	0.58
1:5:286:U:O2'	16:N:179:LYS:O	2.22	0.57
48:AA:50:VAL:HG23	65:RR:109:LEU:HD11	1.85	0.57
1:5:2467:G:H2'	1:5:2468:A:C5	2.40	0.57
1:5:81:C:HO2'	1:5:683:U:HO2'	1.52	0.57
80:gg:86:TRP:HB2	80:gg:110:ASP:HB3	1.86	0.57
82:1:625:MET:SD	82:1:625:MET:N	2.77	0.57
1:5:2567:C:N4	1:5:2573:G:O6	2.37	0.57
46:r:28:PHE:CD1	46:r:98:ILE:HD12	2.39	0.57
82:1:524:PRO:HG3	82:1:620:MET:HE1	1.86	0.57
1:5:1748:G:H4'	39:k:3:ARG:NE	2.18	0.57
71:XX:69:ARG:NH2	81:2:567:G:N7	2.52	0.57
46:r:191:GLN:HA	46:r:200:PRO:HA	1.85	0.57
62:OO:51:ASP:C	62:OO:53:ASP:H	2.13	0.57
62:OO:90:ARG:NH1	81:2:902:G:OP1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:gg:103:ARG:NH1	81:2:1342:C:OP1	2.37	0.57
81:2:903:U:O2'	81:2:905:A:N7	2.32	0.57
70:WW:69:LEU:HD11	70:WW:72:CYS:HB2	1.87	0.57
82:1:421:LEU:HD13	82:1:597:THR:HG21	1.87	0.57
1:5:1427:U:OP2	29:a:4:ARG:NH2	2.37	0.57
54:GG:18:ILE:HD11	54:GG:24:ILE:HG23	1.86	0.57
1:5:293:C:O2'	37:i:76:ARG:O	2.22	0.56
66:SS:36:LYS:HG2	66:SS:105:VAL:HG21	1.87	0.56
80:gg:136:THR:HG23	80:gg:142:LEU:HD11	1.87	0.56
5:B:269:GLN:NE2	5:B:271:GLY:O	2.37	0.56
74:aa:22:ARG:NH1	74:aa:27:SER:O	2.38	0.56
64:QQ:44:LEU:HB3	64:QQ:78:VAL:HG11	1.86	0.56
81:2:495:G:H2'	81:2:496:G:C8	2.40	0.56
4:A:112:ILE:HB	44:p:79:VAL:HG23	1.86	0.56
52:EE:192:ILE:HD13	52:EE:238:LEU:HD22	1.88	0.56
1:5:1268:G:H1'	1:5:1273:A:H61	1.71	0.56
5:B:268:GLY:O	5:B:270:ARG:NH1	2.38	0.56
1:5:2393:G:O2'	1:5:2982:A:N6	2.38	0.56
39:k:8:ILE:HG12	39:k:9:LYS:HA	1.88	0.56
82:1:498:ILE:HD11	82:1:612:LEU:HD11	1.88	0.56
1:5:2468:A:C8	1:5:2478:C:H4'	2.41	0.56
1:5:2435:G:OP1	16:N:20:ARG:NH1	2.39	0.56
80:gg:261:ILE:HB	80:gg:275:LEU:HB2	1.86	0.56
54:GG:49:VAL:HG13	54:GG:114:VAL:HG23	1.88	0.56
1:5:1724:U:H1'	1:5:1725:C:C6	2.40	0.55
33:e:100:ILE:O	33:e:105:ARG:NH1	2.38	0.55
54:GG:57:ASP:HA	54:GG:106:LEU:HA	1.88	0.55
81:2:504:A:H2'	81:2:506:U:O2	2.06	0.55
29:a:96:LYS:O	29:a:97:GLU:HB3	2.05	0.55
82:1:423:ASP:OD1	82:1:423:ASP:O	2.24	0.55
1:5:640:U:OP1	29:a:21:ARG:NH2	2.40	0.55
1:5:1208:U:H2'	1:5:1208:U:O2	2.05	0.55
1:5:3379:C:H4'	5:B:315:GLY:HA2	1.89	0.55
8:E:43:LEU:HD21	8:E:85:ILE:HD11	1.87	0.55
68:UU:56:VAL:HB	68:UU:90:TYR:HB3	1.88	0.55
72:YY:40:LEU:HD13	72:YY:60:PHE:CZ	2.42	0.55
8:E:40:LEU:HB2	8:E:52:VAL:HG12	1.88	0.55
71:XX:88:PRO:HD2	71:XX:132:LEU:HD13	1.88	0.55
34:f:42:GLN:HA	34:f:45:LEU:HD13	1.87	0.55
80:gg:112:MET:SD	80:gg:128:ARG:NE	2.80	0.55
1:5:63:A:H5''	16:N:174:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1245:A:N7	1:5:1271:A:O2'	2.33	0.55
15:M:15:VAL:HG22	15:M:65:LEU:HD11	1.88	0.55
82:1:422:LEU:HD22	82:1:474:VAL:HG21	1.89	0.55
62:OO:41:ARG:NH1	81:2:896:U:O2	2.39	0.55
81:2:741:C:O2'	81:2:742:U:O4'	2.25	0.55
82:1:503:ILE:HD11	82:1:532:ILE:HA	1.89	0.55
82:1:598:SER:O	82:1:602:GLY:N	2.39	0.54
1:5:1748:G:H4'	39:k:3:ARG:CD	2.38	0.54
71:XX:130:VAL:HG23	71:XX:135:LEU:HD11	1.89	0.54
74:aa:15:ARG:HG2	81:2:936:G:O6	2.07	0.54
81:2:406:A:O2'	81:2:1671:A:N3	2.34	0.54
82:1:930:VAL:HG21	82:1:939:VAL:HG21	1.89	0.54
1:5:1477:A:OP1	1:5:3075:G:O2'	2.24	0.54
52:EE:47:PHE:CE1	52:EE:101:LEU:HD21	2.42	0.54
81:2:1502:G:O2'	81:2:1504:G:N2	2.30	0.54
82:1:469:VAL:C	82:1:471:GLY:H	2.15	0.54
5:B:27:ALA:HB1	5:B:218:ILE:HG22	1.89	0.54
22:T:57:TYR:OH	22:T:87:LYS:HD2	2.07	0.54
58:KK:47:GLN:HA	58:KK:50:THR:HG22	1.90	0.54
61:NN:4:MET:HE2	61:NN:121:ARG:HG3	1.90	0.54
20:R:32:ILE:HD11	20:R:49:THR:HG22	1.89	0.54
61:NN:91:LEU:HD12	61:NN:125:LEU:HD12	1.88	0.54
82:1:565:TYR:CD1	82:1:581:LEU:CD1	2.85	0.54
45:q:41:TYR:HA	45:q:163:LEU:HD13	1.90	0.54
53:FF:102:ASN:N	81:2:1166:A:OP1	2.41	0.54
57:JJ:124:HIS:ND1	81:2:477:A:O2'	2.41	0.54
82:1:775:MET:HG3	82:1:840:PHE:CE1	2.43	0.54
1:5:1628:C:OP1	1:5:1814:A:N6	2.41	0.54
17:O:143:THR:HG21	17:O:150:GLU:HB2	1.90	0.54
50:CC:188:ALA:HB1	50:CC:212:LEU:HD11	1.90	0.54
82:1:753:LYS:HA	82:1:798:MET:HE2	1.89	0.54
1:5:838:G:O6	44:p:4:ARG:NH2	2.41	0.54
1:5:1764:U:H2'	1:5:1765:U:O4'	2.08	0.54
4:A:196:TRP:CE3	4:A:197:PRO:HD3	2.43	0.54
15:M:37:GLU:CD	21:S:72:VAL:HG21	2.33	0.54
53:FF:119:THR:HG21	53:FF:196:LEU:HD23	1.90	0.54
59:LL:94:ILE:HD12	71:XX:12:ALA:HB1	1.90	0.54
67:TT:66:TYR:HA	67:TT:124:ILE:HG13	1.89	0.54
81:2:1016:C:O2	81:2:1016:C:O4'	2.23	0.54
7:D:34:LYS:HA	22:T:27:LEU:HD11	1.90	0.53
70:WW:53:ILE:HD13	75:bb:25:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:gg:202:THR:HG21	80:gg:243:SER:HA	1.90	0.53
82:1:682:GLN:HB2	82:1:683:PRO:HD3	1.91	0.53
1:5:3253:G:H4'	1:5:3253:G:OP1	2.08	0.53
16:N:48:ALA:HA	16:N:133:ILE:HD11	1.90	0.53
80:gg:290:ALA:HA	80:gg:306:TYR:HA	1.90	0.53
82:1:544:ASN:N	82:1:544:ASN:HD22	2.05	0.53
82:1:734:MET:HE3	82:1:738:MET:HG2	1.90	0.53
1:5:1632:A:OP1	28:Z:48:ARG:NH2	2.37	0.53
5:B:92:TYR:HB2	5:B:157:VAL:HB	1.91	0.53
15:M:57:ALA:HB2	21:S:97:VAL:HG21	1.89	0.53
46:r:35:VAL:HB	46:r:36:SER:HA	1.90	0.53
81:2:365:A:OP1	81:2:758:U:O2'	2.19	0.53
1:5:1749:A:OP2	39:k:3:ARG:NH2	2.41	0.53
1:5:3234:A:N1	1:5:3253:G:O6	2.41	0.53
26:X:50:ALA:HB1	36:h:66:VAL:HG21	1.90	0.53
57:JJ:85:VAL:HG12	57:JJ:99:LEU:HD11	1.91	0.53
6:C:208:VAL:HG21	6:C:250:TRP:CE3	2.44	0.53
64:QQ:7:VAL:HG13	64:QQ:22:VAL:HG13	1.89	0.53
73:ZZ:42:LEU:HD22	73:ZZ:75:LEU:HD22	1.91	0.53
48:AA:23:HIS:CD2	48:AA:50:VAL:HG22	2.44	0.53
82:1:995:LEU:HA	82:1:998:VAL:HG22	1.91	0.53
5:B:233:TRP:CD1	5:B:265:ALA:HB1	2.44	0.53
46:r:47:LEU:HB3	46:r:51:ALA:HB3	1.91	0.53
37:i:4:LYS:HA	37:i:12:ASN:HB3	1.91	0.53
65:RR:31:ASN:HA	65:RR:34:LEU:HD12	1.91	0.53
82:1:565:TYR:CZ	82:1:581:LEU:HB2	2.43	0.53
1:5:1134:G:O2'	1:5:2642:A:N3	2.39	0.53
33:e:121:ASN:CG	33:e:122:PRO:HD3	2.34	0.53
56:II:34:ALA:HB1	56:II:58:LEU:HD21	1.90	0.53
67:TT:38:LYS:HA	67:TT:47:PRO:HD3	1.91	0.53
69:VV:32:VAL:HG22	69:VV:60:ARG:HD2	1.90	0.53
74:aa:32:LYS:NZ	81:2:932:U:O2	2.42	0.53
78:ee:46:ASN:HD21	81:2:502:G:H4'	1.74	0.53
18:P:36:ILE:CD1	18:P:95:LEU:HD11	2.39	0.52
54:GG:59:GLN:H	81:2:154:U:H4'	1.74	0.52
80:gg:221:ILE:HG23	80:gg:244:LEU:HD21	1.91	0.52
81:2:81:U:H2'	81:2:82:G:O4'	2.09	0.52
81:2:588:C:O2	81:2:588:C:O4'	2.27	0.52
6:C:233:LEU:HG	6:C:238:LEU:HD11	1.91	0.52
7:D:107:ARG:HG3	7:D:251:PRO:HG3	1.90	0.52
59:LL:93:TYR:HB2	59:LL:100:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:NN:54:LEU:HB3	61:NN:60:VAL:HB	1.89	0.52
67:TT:124:ILE:HG22	67:TT:125:SER:O	2.08	0.52
68:UU:117:VAL:HG13	68:UU:117:VAL:O	2.09	0.52
80:gg:211:LEU:HD22	80:gg:232:MET:HE1	1.90	0.52
13:J:110:ILE:HD11	13:J:122:ILE:HG22	1.90	0.52
50:CC:185:ALA:HB2	50:CC:203:THR:HG21	1.91	0.52
80:gg:263:VAL:HG23	80:gg:272:VAL:HB	1.90	0.52
1:5:1618:G:O2'	3:8:126:A:N1	2.43	0.52
1:5:2940:A:O2'	5:B:256:HIS:O	2.28	0.52
55:HH:113:PRO:HG2	55:HH:116:ARG:HD2	1.91	0.52
72:YY:109:LYS:NZ	81:2:458:G:OP1	2.35	0.52
82:1:688:ARG:NE	82:1:688:ARG:HA	2.24	0.52
1:5:912:G:N7	4:A:9:ARG:NH2	2.58	0.52
18:P:36:ILE:HD11	18:P:95:LEU:HD11	1.91	0.52
19:Q:83:VAL:O	19:Q:103:ALA:HA	2.10	0.52
50:CC:232:PRO:HA	50:CC:235:TRP:CG	2.44	0.52
81:2:1713:G:H3'	81:2:1714:A:H5''	1.91	0.52
1:5:1366:A:C2	1:5:1367:G:C4	2.97	0.52
1:5:2267:C:O2	1:5:2267:C:C2'	2.58	0.52
16:N:44:ARG:NH1	16:N:120:TRP:O	2.43	0.52
19:Q:63:SER:OG	19:Q:90:ASP:HB2	2.08	0.52
65:RR:109:LEU:HD12	65:RR:113:LEU:HD21	1.90	0.52
81:2:990:C:O2	81:2:990:C:O4'	2.27	0.52
1:5:900:G:H1'	1:5:1589:A:N6	2.23	0.52
1:5:2457:G:N2	1:5:2461:A:OP1	2.42	0.52
8:E:31:ARG:NH2	8:E:81:ALA:O	2.41	0.52
52:EE:184:THR:N	52:EE:224:ASN:O	2.41	0.52
81:2:70:A:N1	81:2:71:A:N6	2.57	0.52
81:2:540:A:O2'	81:2:541:A:H4'	2.09	0.52
82:1:466:THR:O	82:1:466:THR:OG1	2.24	0.52
1:5:860:G:C5	4:A:181:LYS:HB2	2.45	0.52
65:RR:19:ARG:O	65:RR:72:LYS:NZ	2.43	0.52
1:5:553:U:H2'	1:5:554:A:H5'	1.91	0.52
1:5:1203:A:N3	1:5:2855:U:O2'	2.37	0.52
17:O:110:PRO:O	17:O:112:TYR:N	2.43	0.52
53:FF:59:SER:HA	76:cc:53:ILE:HB	1.91	0.52
9:F:158:LYS:O	9:F:159:GLN:C	2.52	0.52
11:H:10:ILE:HB	11:H:53:ILE:HG13	1.92	0.52
18:P:29:THR:HA	18:P:32:THR:HG22	1.92	0.52
49:BB:148:ASN:O	81:2:1067:C:O2'	2.28	0.52
82:1:411:LEU:HB3	82:1:486:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1426:C:H4'	6:C:40:THR:HG23	1.91	0.51
1:5:1528:G:O2'	1:5:1588:A:N3	2.43	0.51
21:S:77:VAL:HG21	21:S:106:LEU:HD22	1.92	0.51
23:U:19:VAL:HG12	23:U:105:LEU:HD12	1.92	0.51
28:Z:25:ILE:HA	28:Z:43:VAL:HG12	1.92	0.51
58:KK:87:VAL:N	58:KK:88:PRO:HD2	2.25	0.51
74:aa:45:VAL:HG21	74:aa:53:LEU:CD2	2.39	0.51
81:2:980:G:H4'	81:2:1776:A:H4'	1.92	0.51
82:1:915:GLY:HA2	82:1:943:LEU:HB3	1.92	0.51
14:L:59:ARG:NH1	14:L:66:ASN:O	2.43	0.51
19:Q:80:THR:HG23	19:Q:137:THR:HG22	1.92	0.51
82:1:769:LEU:HD11	82:1:782:ILE:HD12	1.92	0.51
11:H:38:LEU:HD13	11:H:71:VAL:HG23	1.92	0.51
37:i:47:ILE:HA	37:i:48:ALA:HB2	1.91	0.51
39:k:44:LYS:HB3	39:k:51:LEU:HD11	1.92	0.51
81:2:60:A:N3	81:2:60:A:H2'	2.26	0.51
1:5:2444:C:O2	1:5:2444:C:C2'	2.57	0.51
26:X:99:VAL:HG11	26:X:124:VAL:HG11	1.92	0.51
27:Y:101:PRO:HA	27:Y:104:LEU:HD12	1.92	0.51
81:2:1533:C:H3'	81:2:1534:G:C8	2.45	0.51
1:5:698:U:H2'	1:5:699:A:O4'	2.10	0.51
35:g:54:ILE:HD11	35:g:78:GLY:HA2	1.91	0.51
81:2:538:G:H1'	81:2:539:G:C2	2.45	0.51
82:1:815:VAL:HG11	82:1:830:ILE:HG21	1.92	0.51
82:1:972:ILE:HG12	82:1:992:LEU:HD21	1.92	0.51
1:5:1219:C:O4'	1:5:1222:G:O2'	2.26	0.51
1:5:1721:U:O4	20:R:128:LYS:NZ	2.43	0.51
39:k:20:VAL:HG21	39:k:45:VAL:HG12	1.93	0.51
56:II:33:PRO:HB3	81:2:329:G:O2'	2.10	0.51
57:JJ:143:ILE:HG22	57:JJ:145:SER:H	1.75	0.51
60:MM:25:LEU:HD13	60:MM:116:VAL:HG22	1.91	0.51
66:SS:36:LYS:HG3	81:2:1568:C:OP1	2.10	0.51
1:5:1784:G:H2'	1:5:1785:U:O4'	2.11	0.51
51:DD:70:THR:HA	51:DD:86:LEU:HD12	1.91	0.51
81:2:224:A:H2'	81:2:225:A:C8	2.45	0.51
1:5:3119:U:H4'	41:m:104:PRO:HG2	1.93	0.51
20:R:105:LEU:HD23	20:R:138:LEU:HD23	1.93	0.51
52:EE:126:VAL:HG13	52:EE:139:VAL:HG23	1.93	0.51
52:EE:148:ARG:NH1	54:GG:201:GLN:OE1	2.44	0.51
61:NN:132:VAL:HG13	61:NN:134:VAL:HG23	1.91	0.51
81:2:442:C:O2	81:2:444:A:N6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:728:U:O2	81:2:728:U:O4'	2.29	0.51
81:2:1056:U:H2'	81:2:1061:A:N7	2.26	0.51
3:8:95:G:OP2	38:j:72:ARG:NH1	2.42	0.51
16:N:60:VAL:HG22	16:N:134:LEU:HB2	1.93	0.51
27:Y:55:GLU:HB2	27:Y:108:LYS:HB3	1.93	0.51
29:a:71:PRO:HG2	29:a:109:TYR:HA	1.93	0.51
49:BB:105:PHE:CD1	49:BB:213:ARG:HA	2.46	0.51
82:1:410:ILE:HG22	82:1:498:ILE:HB	1.92	0.51
82:1:423:ASP:OD2	82:1:431:GLN:N	2.44	0.51
1:5:1613:A:OP2	39:k:46:ARG:NH2	2.44	0.51
3:8:78:G:H2'	3:8:79:A:O4'	2.11	0.51
21:S:90:MET:HE1	21:S:114:HIS:NE2	2.25	0.51
49:BB:47:LEU:HD21	62:OO:39:ILE:HD11	1.93	0.51
82:1:465:GLN:HB3	82:1:467:PHE:CE1	2.45	0.51
1:5:2743:A:H2'	1:5:2744:U:O4'	2.11	0.50
35:g:113:LYS:O	35:g:117:LYS:HB2	2.11	0.50
36:h:31:LEU:HD12	36:h:47:VAL:HG21	1.92	0.50
46:r:11:ALA:HA	46:r:14:PHE:CD2	2.46	0.50
1:5:1566:A:N3	1:5:1573:G:N2	2.58	0.50
1:5:1717:U:H2'	1:5:1718:G:C8	2.45	0.50
46:r:190:VAL:HG22	46:r:191:GLN:HG3	1.93	0.50
81:2:1081:A:N3	81:2:1081:A:H2'	2.27	0.50
81:2:1288:G:OP1	81:2:1624:C:O2'	2.29	0.50
81:2:1686:C:H2'	81:2:1687:U:H4'	1.93	0.50
38:j:66:TYR:OH	38:j:73:ARG:NH2	2.44	0.50
81:2:1297:G:N2	81:2:1300:A:OP2	2.41	0.50
82:1:765:LEU:HD11	82:1:782:ILE:HG23	1.93	0.50
1:5:433:A:H2'	1:5:434:U:O4'	2.11	0.50
1:5:1136:A:OP2	30:b:8:THR:HG23	2.12	0.50
1:5:2307:G:O2'	1:5:2310:U:OP2	2.29	0.50
66:SS:50:ALA:O	66:SS:68:ARG:NH2	2.44	0.50
1:5:110:G:OP2	14:L:73:ARG:NH1	2.45	0.50
11:H:47:LYS:HA	11:H:53:ILE:HG22	1.93	0.50
71:XX:65:ASN:HD22	71:XX:116:ASP:HB3	1.76	0.50
81:2:888:U:O2'	81:2:989:U:H4'	2.11	0.50
4:A:112:ILE:HD13	4:A:135:ILE:HG12	1.93	0.50
5:B:308:MET:HE1	5:B:376:LYS:HE2	1.94	0.50
12:I:14:ASN:O	12:I:128:ARG:NH2	2.44	0.50
24:V:15:LEU:HD23	24:V:53:SER:HB3	1.93	0.50
29:a:4:ARG:HA	29:a:9:ARG:HG3	1.93	0.50
35:g:51:LEU:HB3	35:g:54:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:EE:86:PHE:CZ	52:EE:87:MET:HE2	2.46	0.50
56:II:22:ARG:HG2	81:2:384:A:H5''	1.94	0.50
1:5:801:A:N6	14:L:19:GLN:OE1	2.45	0.50
1:5:2526:C:OP1	4:A:37:ARG:NH1	2.45	0.50
1:5:3049:A:H4'	5:B:364:LYS:HD2	1.93	0.50
2:7:77:G:H3'	21:S:46:GLN:O	2.12	0.50
6:C:343:LYS:CB	6:C:344:ALA:HA	2.38	0.50
1:5:655:C:H2'	1:5:656:A:C8	2.47	0.50
1:5:999:G:N3	1:5:1002:A:N6	2.60	0.50
1:5:3165:A:H2'	1:5:3166:C:O4'	2.12	0.50
49:BB:127:VAL:HB	49:BB:176:VAL:HG11	1.93	0.50
81:2:539:G:OP1	81:2:540:A:N6	2.44	0.50
81:2:1536:G:H2'	81:2:1536:G:N3	2.27	0.50
82:1:695:HIS:O	82:1:696:HIS:HB2	2.11	0.50
1:5:744:A:OP1	19:Q:66:ARG:NH2	2.45	0.50
1:5:2736:A:H2'	1:5:2737:C:O4'	2.12	0.50
5:B:41:VAL:HA	5:B:185:GLY:HA3	1.94	0.50
7:D:4:GLN:HE21	7:D:4:GLN:HA	1.77	0.50
11:H:92:TYR:HB3	11:H:99:ILE:HD12	1.94	0.50
12:I:85:PHE:CB	12:I:140:THR:HG22	2.42	0.50
36:h:31:LEU:HB3	36:h:44:ILE:HG22	1.92	0.50
52:EE:49:ARG:NH1	81:2:446:U:OP1	2.43	0.50
1:5:1433:A:N3	33:e:27:ARG:NH1	2.60	0.49
48:AA:139:VAL:HG23	48:AA:141:ILE:HD12	1.94	0.49
58:KK:87:VAL:N	58:KK:88:PRO:CD	2.75	0.49
5:B:83:PRO:HB2	5:B:202:THR:HB	1.94	0.49
46:r:79:LEU:HG	46:r:80:PRO:HD3	1.94	0.49
50:CC:87:ASN:HB2	50:CC:212:LEU:HD23	1.92	0.49
77:dd:36:LEU:HB3	77:dd:38:ILE:HG22	1.94	0.49
80:gg:154:GLN:HG3	80:gg:202:THR:HA	1.94	0.49
62:OO:17:ALA:HB3	62:OO:81:VAL:HA	1.94	0.49
1:5:170:G:OP1	14:L:128:ARG:NH1	2.46	0.49
1:5:211:A:OP2	6:C:221:ASN:HB2	2.12	0.49
1:5:2563:G:C6	1:5:2564:G:C2	3.00	0.49
42:n:18:ARG:NH1	81:2:1126:G:OP2	2.46	0.49
63:PP:41:VAL:HG12	63:PP:84:ILE:HD13	1.94	0.49
81:2:15:G:H2'	81:2:16:C:C6	2.47	0.49
81:2:897:C:O4'	81:2:914:G:N1	2.45	0.49
81:2:1254:U:O2	81:2:1254:U:O4'	2.30	0.49
16:N:135:VAL:HG13	16:N:142:ILE:HG12	1.93	0.49
42:n:12:ARG:NH1	81:2:1779:U:O4	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:204:LEU:O	45:q:216:LEU:N	2.46	0.49
66:SS:26:ILE:HB	81:2:1534:G:OP1	2.13	0.49
1:5:1150:A:H2	1:5:2379:U:O2	1.96	0.49
50:CC:82:GLN:HA	50:CC:83:ASP:HB3	1.93	0.49
82:1:503:ILE:HA	82:1:568:ILE:HD11	1.93	0.49
1:5:92:G:OP2	1:5:93:C:H5'	2.12	0.49
5:B:255:TRP:H	5:B:255:TRP:CD1	2.30	0.49
69:VV:85:TYR:CZ	75:bb:6:ASP:HB2	2.47	0.49
82:1:645:THR:HG21	82:1:713:GLU:HA	1.94	0.49
1:5:1231:A:N6	1:5:1277:C:OP2	2.44	0.49
20:R:6:THR:O	20:R:10:LEU:HB2	2.12	0.49
52:EE:173:ILE:HD13	52:EE:229:GLY:HA2	1.95	0.49
81:2:513:G:C8	81:2:514:A:C8	2.99	0.49
1:5:2954:U:O2	1:5:2954:U:O4'	2.31	0.49
55:HH:63:PRO:O	55:HH:64:VAL:HG12	2.12	0.49
78:ee:31:LYS:NZ	81:2:543:A:O2'	2.44	0.49
81:2:641:G:N2	81:2:693:U:O2	2.45	0.49
5:B:78:VAL:HG21	5:B:311:PHE:CZ	2.48	0.49
56:II:179:ARG:NH1	81:2:206:U:O2	2.46	0.49
58:KK:2:LEU:HA	81:2:1257:U:H2'	1.95	0.49
81:2:1684:U:O2	81:2:1717:G:O6	2.30	0.49
1:5:2466:G:N2	45:q:209:SER:O	2.46	0.48
1:5:2488:A:H2'	1:5:2488:A:N3	2.28	0.48
4:A:230:VAL:HG22	4:A:233:GLN:HE21	1.78	0.48
7:D:17:GLN:HE22	22:T:22:HIS:HB2	1.77	0.48
51:DD:216:PRO:O	51:DD:218:LEU:N	2.45	0.48
54:GG:49:VAL:HG12	54:GG:115:LYS:HB3	1.95	0.48
60:MM:38:LEU:HB2	60:MM:64:ILE:O	2.13	0.48
61:NN:88:LEU:HD22	61:NN:135:LEU:HD11	1.95	0.48
81:2:649:U:H2'	81:2:650:G:C8	2.48	0.48
81:2:716:C:N4	81:2:723:G:N3	2.60	0.48
1:5:1232:C:H2'	1:5:1233:G:C8	2.48	0.48
1:5:1575:A:H2'	1:5:1576:G:H8	1.79	0.48
82:1:449:ILE:CG2	82:1:469:VAL:O	2.60	0.48
1:5:712:G:N2	1:5:754:G:O3'	2.46	0.48
1:5:2249:G:H3'	1:5:2250:G:H4'	1.94	0.48
11:H:99:ILE:HG22	11:H:101:VAL:HG23	1.95	0.48
35:g:90:ILE:O	35:g:94:LEU:HB2	2.13	0.48
44:p:76:ALA:HA	44:p:79:VAL:HG12	1.96	0.48
64:QQ:118:ILE:HG21	81:2:1410:A:H5'	1.95	0.48
66:SS:35:ILE:HD12	66:SS:73:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:XX:102:VAL:HG13	71:XX:124:VAL:HG13	1.94	0.48
81:2:265:A:H3'	81:2:266:U:H5'	1.94	0.48
82:1:724:VAL:HG12	82:1:730:GLU:HB2	1.95	0.48
1:5:812:G:C2	1:5:929:A:C2	3.01	0.48
1:5:1395:G:O2'	3:8:18:U:O2	2.31	0.48
1:5:1942:U:H2'	1:5:1943:C:O4'	2.13	0.48
1:5:2611:U:H2'	1:5:2612:U:C6	2.48	0.48
56:II:78:ILE:HG12	56:II:104:ILE:HG22	1.96	0.48
81:2:792:U:H2'	81:2:793:A:O4'	2.14	0.48
82:1:499:LEU:HB3	82:1:527:VAL:HG12	1.94	0.48
82:1:665:CYS:SG	82:1:733:LEU:HB2	2.53	0.48
50:CC:210:ARG:NH1	81:2:5:G:N7	2.62	0.48
80:gg:261:ILE:HD13	80:gg:293:LEU:HD21	1.94	0.48
81:2:1533:C:H3'	81:2:1534:G:H8	1.79	0.48
1:5:1682:U:O4	23:U:90:ARG:NH1	2.46	0.48
1:5:2533:G:H2'	1:5:2534:G:C8	2.49	0.48
5:B:240:ARG:HA	5:B:246:LEU:HD21	1.95	0.48
60:MM:59:VAL:HG21	60:MM:64:ILE:HG22	1.96	0.48
71:XX:71:CYS:SG	71:XX:120:VAL:HG21	2.54	0.48
81:2:1186:U:O2	81:2:1186:U:O4'	2.31	0.48
80:gg:90:LEU:HB2	80:gg:104:PHE:HB2	1.95	0.48
80:gg:264:PHE:HA	80:gg:271:LEU:HA	1.96	0.48
81:2:1204:A:N3	81:2:1204:A:H2'	2.29	0.48
1:5:542:G:H1	1:5:549:U:H3	1.61	0.48
1:5:1190:A:N3	1:5:1190:A:H2'	2.27	0.48
1:5:1412:G:OP1	33:e:105:ARG:NH2	2.47	0.48
1:5:1748:G:H4'	39:k:3:ARG:HD2	1.95	0.48
5:B:56:ILE:HD11	5:B:356:LEU:HD13	1.95	0.48
7:D:278:SER:OG	7:D:279:LYS:N	2.47	0.48
38:j:5:THR:HB	38:j:6:PRO:HD3	1.96	0.48
45:q:159:LEU:HB2	45:q:165:LEU:HD12	1.96	0.48
45:q:183:ILE:O	45:q:187:VAL:HG23	2.14	0.48
63:PP:37:ALA:HB1	63:PP:41:VAL:HG21	1.96	0.48
81:2:1560:U:O4'	81:2:1560:U:O2	2.28	0.48
8:E:89:THR:HG21	15:M:115:PHE:CB	2.44	0.48
9:F:103:LEU:HD23	9:F:108:LEU:HD12	1.96	0.48
11:H:27:VAL:HG12	11:H:82:VAL:HG21	1.95	0.48
14:L:75:PHE:O	14:L:76:THR:HG23	2.14	0.48
70:WW:42:GLN:NE2	70:WW:48:GLY:O	2.47	0.48
81:2:248:U:H3'	81:2:249:C:H5'	1.95	0.48
81:2:1225:U:H2'	81:2:1226:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:737:G:H2'	1:5:738:A:C8	2.49	0.48
3:8:12:A:H1'	18:P:118:GLN:HE22	1.79	0.48
49:BB:217:LEU:HB3	49:BB:220:GLN:HE21	1.78	0.48
58:KK:86:ILE:HB	58:KK:88:PRO:HD2	1.95	0.48
1:5:2157:G:N2	1:5:2177:G:O2'	2.47	0.47
1:5:2211:U:O4'	1:5:2211:U:O2	2.32	0.47
1:5:2447:A:H2'	1:5:2448:G:C8	2.49	0.47
14:L:53:LEU:HD22	14:L:94:GLY:HA2	1.96	0.47
24:V:17:LEU:HB2	24:V:52:ALA:HB3	1.96	0.47
55:HH:25:VAL:HA	55:HH:28:GLU:HB2	1.96	0.47
56:II:84:HIS:CE1	56:II:90:LEU:HD13	2.49	0.47
61:NN:11:ILE:HD11	81:2:864:U:H4'	1.96	0.47
82:1:452:ILE:O	82:1:456:THR:HG22	2.14	0.47
5:B:232:ARG:NH2	5:B:268:GLY:O	2.47	0.47
7:D:39:GLN:NE2	7:D:46:THR:OG1	2.46	0.47
50:CC:176:PRO:HG2	70:WW:96:ALA:HB2	1.96	0.47
50:CC:230:LEU:HD23	70:WW:68:ARG:HA	1.95	0.47
80:gg:128:ARG:C	80:gg:130:LYS:H	2.22	0.47
81:2:652:C:N4	81:2:680:U:O4	2.47	0.47
14:L:177:LYS:HA	37:i:11:LEU:HD21	1.96	0.47
46:r:35:VAL:HB	46:r:36:SER:CA	2.45	0.47
58:KK:54:TYR:HB2	58:KK:72:GLY:HA2	1.95	0.47
72:YY:120:GLY:HA2	81:2:84:A:O3'	2.14	0.47
82:1:865:PRO:HA	82:1:965:SER:OG	2.14	0.47
1:5:1636:U:H4'	28:Z:74:VAL:O	2.14	0.47
1:5:2059:C:H2'	1:5:2060:G:C8	2.49	0.47
10:G:162:VAL:HG23	10:G:165:LEU:HD12	1.96	0.47
57:JJ:17:ARG:NH2	81:2:2:U:O2	2.47	0.47
60:MM:56:VAL:HG21	60:MM:64:ILE:HG21	1.95	0.47
71:XX:70:LYS:HD2	71:XX:93:LEU:HD22	1.96	0.47
82:1:469:VAL:C	82:1:471:GLY:N	2.69	0.47
1:5:63:A:OP1	16:N:169:LYS:NZ	2.48	0.47
1:5:245:U:H2'	1:5:246:U:C6	2.50	0.47
46:r:35:VAL:O	46:r:107:VAL:HG21	2.14	0.47
61:NN:146:ALA:HA	61:NN:149:LEU:HD12	1.97	0.47
72:YY:124:ARG:NH2	81:2:148:C:OP2	2.48	0.47
81:2:1458:G:N3	81:2:1458:G:H2'	2.29	0.47
82:1:464:LYS:HB3	82:1:464:LYS:HE3	1.53	0.47
1:5:269:G:H5''	16:N:14:LYS:HE3	1.96	0.47
1:5:1575:A:H2'	1:5:1576:G:C8	2.49	0.47
5:B:255:TRP:H	5:B:255:TRP:HD1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:213:PHE:N	12:I:214:PRO:HD3	2.29	0.47
33:e:96:ILE:O	33:e:121:ASN:ND2	2.47	0.47
53:FF:126:LEU:HD12	53:FF:126:LEU:O	2.14	0.47
81:2:1788:G:H2'	81:2:1789:G:O4'	2.15	0.47
1:5:553:U:C2'	1:5:554:A:H5'	2.45	0.47
1:5:713:U:O2	1:5:754:G:H4'	2.14	0.47
1:5:2257:C:H2'	1:5:2258:U:H4'	1.97	0.47
10:G:164:PHE:HA	37:i:47:ILE:HD13	1.96	0.47
26:X:76:VAL:HA	26:X:81:ILE:O	2.14	0.47
32:d:77:ARG:HG2	32:d:89:LEU:HD23	1.97	0.47
42:n:12:ARG:NH2	81:2:1778:G:N7	2.63	0.47
48:AA:164:ASN:HA	48:AA:170:ILE:HD11	1.97	0.47
77:dd:10:HIS:HB3	77:dd:11:PRO:HD2	1.97	0.47
81:2:813:U:O2	81:2:813:U:O4'	2.32	0.47
81:2:1170:G:C2	81:2:1171:A:C8	3.03	0.47
81:2:1572:G:H2'	81:2:1572:G:N3	2.30	0.47
82:1:984:VAL:HG21	82:1:989:TRP:CE3	2.49	0.47
46:r:26:SER:HG	46:r:95:LEU:HD21	1.79	0.47
52:EE:222:LEU:HA	52:EE:225:VAL:HB	1.97	0.47
53:FF:145:ARG:HA	53:FF:169:ARG:HD3	1.96	0.47
66:SS:28:ILE:HD11	66:SS:52:VAL:HG21	1.96	0.47
1:5:736:A:C6	1:5:737:G:H1'	2.50	0.47
1:5:2469:G:H4'	45:q:27:ASN:HB3	1.96	0.47
5:B:226:PHE:HA	5:B:269:GLN:HA	1.96	0.47
6:C:290:ILE:HG23	19:Q:35:PHE:CE2	2.50	0.47
45:q:40:ASN:HD21	45:q:196:LYS:HB2	1.80	0.47
57:JJ:143:ILE:HG13	81:2:768:C:C2	2.50	0.47
64:QQ:36:ILE:HD12	64:QQ:49:TYR:CE1	2.49	0.47
81:2:1469:A:H2'	81:2:1470:C:C6	2.49	0.47
81:2:1643:U:O2	81:2:1780:G:N2	2.48	0.47
82:1:467:PHE:CD1	82:1:467:PHE:N	2.83	0.47
1:5:22:G:H5'	38:j:42:ALA:HB1	1.97	0.47
1:5:29:C:H4'	1:5:62:A:H4'	1.96	0.47
1:5:196:G:N1	1:5:199:A:OP2	2.48	0.47
1:5:506:U:H2'	1:5:507:U:O4'	2.15	0.47
6:C:130:ALA:HA	6:C:149:PRO:HD3	1.96	0.47
51:DD:53:THR:HG22	51:DD:91:VAL:HG21	1.96	0.47
51:DD:115:ILE:HG21	51:DD:138:VAL:HG11	1.97	0.47
56:II:69:SER:OG	59:LL:24:LYS:HG3	2.15	0.47
62:OO:42:VAL:HG12	62:OO:67:VAL:HB	1.97	0.47
67:TT:54:PHE:O	67:TT:55:TYR:CG	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1:535:LEU:HD11	82:1:560:GLU:HB3	1.97	0.47
1:5:298:U:OP1	37:i:33:ALA:N	2.47	0.46
1:5:2899:C:O2'	1:5:2901:G:OP2	2.33	0.46
5:B:232:ARG:HG3	5:B:233:TRP:CD1	2.50	0.46
24:V:25:CYS:SG	24:V:27:ASP:OD1	2.73	0.46
63:PP:96:ILE:HD13	63:PP:116:LEU:O	2.15	0.46
66:SS:26:ILE:O	66:SS:57:ARG:NE	2.48	0.46
68:UU:24:ILE:HG22	68:UU:114:VAL:HG12	1.97	0.46
68:UU:72:ASN:ND2	81:2:1429:G:O2'	2.48	0.46
81:2:1672:G:H2'	81:2:1673:G:C8	2.50	0.46
1:5:1254:C:H2'	1:5:1255:C:O4'	2.16	0.46
48:AA:3:LEU:HD23	48:AA:4:PRO:HD2	1.97	0.46
48:AA:41:ARG:HB3	48:AA:45:VAL:HG23	1.97	0.46
50:CC:166:LYS:NZ	50:CC:168:GLY:O	2.49	0.46
56:II:160:GLN:HB3	56:II:166:LEU:HA	1.97	0.46
57:JJ:132:ARG:NH1	81:2:531:U:OP1	2.46	0.46
64:QQ:50:GLU:N	64:QQ:51:PRO:HD2	2.29	0.46
67:TT:97:SER:OG	81:2:1504:G:OP1	2.31	0.46
81:2:51:U:O2'	82:1:695:HIS:NE2	2.47	0.46
81:2:496:G:H3'	81:2:497:G:C5'	2.45	0.46
81:2:1384:A:H2'	81:2:1385:G:O4'	2.15	0.46
1:5:366:A:OP1	6:C:95:ARG:NH1	2.48	0.46
1:5:1287:A:H2'	1:5:1288:U:O4'	2.15	0.46
1:5:1623:G:H2'	1:5:1624:G:O4'	2.16	0.46
1:5:2563:G:H2'	1:5:2564:G:O4'	2.15	0.46
57:JJ:161:THR:HA	57:JJ:167:ALA:HB3	1.96	0.46
80:gg:90:LEU:HD11	80:gg:125:SER:HB3	1.97	0.46
82:1:535:LEU:HD13	82:1:557:VAL:HG13	1.98	0.46
1:5:181:U:H2'	1:5:182:U:O4'	2.14	0.46
1:5:2677:G:N3	1:5:2677:G:H2'	2.30	0.46
1:5:2689:A:N3	1:5:2689:A:H2'	2.31	0.46
7:D:38:THR:HG22	22:T:30:TYR:HB3	1.98	0.46
9:F:170:GLU:HB3	9:F:179:LEU:HA	1.97	0.46
46:r:27:LEU:HD22	46:r:78:LEU:HD11	1.97	0.46
48:AA:183:ARG:HA	48:AA:188:LEU:HB2	1.98	0.46
51:DD:120:TYR:HA	51:DD:123:VAL:HG12	1.98	0.46
54:GG:202:ARG:NH2	81:2:178:A:N1	2.64	0.46
62:OO:123:SER:N	81:2:886:U:O2	2.49	0.46
66:SS:28:ILE:HD12	66:SS:61:LEU:HD21	1.97	0.46
81:2:767:U:O2	81:2:767:U:O4'	2.32	0.46
81:2:1160:A:O2'	81:2:1620:C:N3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:1600:A:O2'	81:2:1602:C:N4	2.48	0.46
1:5:1806:A:H2'	1:5:1807:G:O4'	2.16	0.46
11:H:93:VAL:HG22	41:m:82:LEU:HD22	1.97	0.46
46:r:37:SER:HA	46:r:38:GLN:CB	2.44	0.46
71:XX:86:PHE:CE2	71:XX:88:PRO:HA	2.50	0.46
81:2:129:C:O2'	81:2:130:C:OP1	2.26	0.46
1:5:1145:G:O6	1:5:1158:A:H2	1.99	0.46
1:5:1966:U:H2'	1:5:1967:U:O4'	2.15	0.46
6:C:181:VAL:HG11	6:C:224:GLY:HA3	1.96	0.46
12:I:176:LEU:HD11	12:I:199:PHE:CE1	2.51	0.46
26:X:86:VAL:HG11	26:X:95:ILE:HG12	1.97	0.46
81:2:934:C:C4	81:2:1078:C:H4'	2.50	0.46
2:7:26:C:H2'	2:7:27:A:O4'	2.16	0.46
46:r:17:LEU:HB2	46:r:62:ARG:NH2	2.31	0.46
76:cc:25:VAL:HG11	76:cc:43:ASN:HD22	1.80	0.46
81:2:1148:C:O2'	81:2:1765:A:N1	2.45	0.46
1:5:361:A:N1	1:5:927:C:O2'	2.40	0.46
1:5:2262:A:OP1	81:2:1780:G:C4	2.68	0.46
16:N:183:THR:O	16:N:183:THR:OG1	2.34	0.46
17:O:19:LEU:HD23	17:O:41:LEU:HD21	1.96	0.46
67:TT:87:GLY:C	81:2:1542:G:H5''	2.40	0.46
80:gg:116:ILE:HG13	80:gg:123:ILE:HG22	1.97	0.46
81:2:976:G:N1	81:2:1023:A:O2'	2.37	0.46
1:5:1202:A:N3	1:5:1202:A:H2'	2.31	0.46
2:7:73:C:C2'	2:7:73:C:O2	2.64	0.46
50:CC:46:LEU:HD11	50:CC:66:LEU:HB3	1.97	0.46
56:II:57:ALA:HB1	56:II:60:ILE:HB	1.98	0.46
60:MM:38:LEU:HD22	60:MM:64:ILE:HA	1.96	0.46
81:2:542:C:O2	81:2:542:C:O4'	2.34	0.46
82:1:835:VAL:HG12	82:1:837:TYR:H	1.81	0.46
49:BB:83:LYS:HE3	49:BB:106:THR:HA	1.98	0.46
80:gg:38:SER:OG	80:gg:39:ARG:N	2.49	0.46
81:2:978:A:H2'	81:2:979:A:O4'	2.16	0.46
1:5:211:A:OP1	6:C:220:ARG:HD2	2.15	0.45
19:Q:182:LYS:NZ	29:a:55:LYS:O	2.46	0.45
54:GG:95:LYS:NZ	81:2:159:C:O3'	2.49	0.45
45:q:20:SER:HA	45:q:25:LYS:HB2	1.98	0.45
57:JJ:49:LEU:HD23	57:JJ:101:VAL:HG13	1.98	0.45
81:2:106:C:OP1	81:2:383:G:H5'	2.16	0.45
82:1:485:ASN:HA	82:1:489:ARG:HB2	1.98	0.45
1:5:1326:A:H2'	1:5:1327:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1729:A:H4'	1:5:1730:G:OP2	2.16	0.45
48:AA:92:HIS:HB3	48:AA:182:LEU:HD11	1.99	0.45
50:CC:40:TRP:CE2	50:CC:72:GLN:HB2	2.51	0.45
55:HH:14:THR:OG1	55:HH:15:GLU:N	2.49	0.45
74:aa:75:VAL:O	74:aa:79:ILE:HG12	2.16	0.45
78:ee:14:VAL:HG11	81:2:566:A:N3	2.31	0.45
81:2:1001:A:OP1	83:3:38:A:O2'	2.32	0.45
81:2:1504:G:H3'	81:2:1505:A:C8	2.51	0.45
82:1:449:ILE:HG23	82:1:469:VAL:O	2.17	0.45
82:1:530:ASN:HD22	82:1:531:LYS:HG2	1.81	0.45
82:1:647:ILE:HD12	82:1:664:LEU:HD22	1.98	0.45
1:5:1208:U:O2	1:5:1208:U:C2'	2.64	0.45
1:5:2736:A:OP1	22:T:92:ARG:NH1	2.49	0.45
11:H:91:ARG:NH1	11:H:141:LYS:O	2.47	0.45
18:P:51:VAL:HG23	18:P:57:ALA:HA	1.98	0.45
35:g:90:ILE:HG22	35:g:94:LEU:HD12	1.99	0.45
54:GG:1:MET:SD	54:GG:106:LEU:HB2	2.57	0.45
55:HH:16:LEU:HD23	55:HH:16:LEU:H	1.81	0.45
63:PP:123:TYR:OH	66:SS:126:ARG:NH1	2.46	0.45
68:UU:106:ILE:HG23	68:UU:107:THR:HG23	1.97	0.45
82:1:464:LYS:O	82:1:466:THR:N	2.48	0.45
82:1:920:LEU:CD2	82:1:941:VAL:HG12	2.46	0.45
1:5:2476:C:H2'	1:5:2477:G:H8	1.82	0.45
9:F:77:VAL:HG22	21:S:59:VAL:HA	1.98	0.45
9:F:88:ARG:HB2	9:F:108:LEU:HB3	1.99	0.45
39:k:3:ARG:HD3	39:k:51:LEU:HB3	1.98	0.45
48:AA:23:HIS:HE1	48:AA:53:THR:HG21	1.81	0.45
48:AA:119:ARG:NH1	50:CC:245:LEU:O	2.50	0.45
65:RR:102:VAL:HG13	65:RR:106:THR:HB	1.97	0.45
81:2:129:C:H2'	81:2:130:C:H5'	1.99	0.45
82:1:868:LEU:HB2	82:1:963:LEU:HB2	1.98	0.45
1:5:1976:G:N2	1:5:2055:U:O2'	2.48	0.45
12:I:76:MET:HE1	12:I:138:VAL:HG11	1.98	0.45
17:O:121:PRO:HA	17:O:124:LEU:HD13	1.98	0.45
35:g:81:CYS:SG	35:g:82:ALA:N	2.90	0.45
49:BB:214:LYS:NZ	81:2:886:U:OP1	2.50	0.45
64:QQ:137:ARG:HB2	81:2:1580:C:H4'	1.98	0.45
72:YY:61:ARG:NH2	81:2:523:U:OP1	2.49	0.45
82:1:769:LEU:HD22	82:1:779:VAL:HG21	1.99	0.45
1:5:1:G:H5''	26:X:23:ALA:HB2	1.99	0.45
1:5:549:U:H2'	1:5:550:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1580:A:OP1	4:A:70:ARG:NH2	2.49	0.45
2:7:75:G:O2'	2:7:104:A:N6	2.44	0.45
6:C:102:PRO:O	6:C:104:LYS:NZ	2.47	0.45
6:C:142:VAL:HG11	6:C:247:PHE:CD1	2.52	0.45
16:N:180:PHE:O	16:N:184:LYS:HB2	2.17	0.45
46:r:59:THR:HG22	46:r:62:ARG:HB2	1.99	0.45
60:MM:52:LEU:HB3	60:MM:116:VAL:HB	1.98	0.45
1:5:2722:U:O2'	22:T:88:ARG:O	2.33	0.45
4:A:103:PRO:HA	4:A:163:ARG:HA	1.99	0.45
19:Q:29:LEU:HD11	19:Q:124:LEU:HB2	1.97	0.45
66:SS:57:ARG:HD2	73:ZZ:42:LEU:CD2	2.47	0.45
82:1:458:VAL:O	82:1:458:VAL:HG23	2.15	0.45
82:1:465:GLN:O	82:1:467:PHE:CD1	2.70	0.45
1:5:2312:A:O2'	1:5:2315:G:N3	2.49	0.45
6:C:326:ARG:O	9:F:41:ARG:NH2	2.50	0.45
24:V:81:GLN:O	24:V:98:ASN:ND2	2.44	0.45
46:r:195:ASN:HB2	46:r:196:GLY:HA3	1.99	0.45
48:AA:50:VAL:HA	48:AA:53:THR:HG22	1.97	0.45
81:2:1258:U:O2	81:2:1258:U:O4'	2.34	0.45
82:1:535:LEU:O	82:1:536:TYR:HB3	2.17	0.45
1:5:113:C:C2	1:5:319:A:C2	3.05	0.45
1:5:505:G:H5''	6:C:315:LYS:HA	1.99	0.45
1:5:531:G:H2'	1:5:532:A:C8	2.52	0.45
1:5:2455:U:H2'	1:5:2456:A:C4	2.52	0.45
1:5:2573:G:H2'	1:5:2574:G:C8	2.51	0.45
15:M:38:ILE:HG22	15:M:44:VAL:HG12	1.98	0.45
20:R:23:TRP:HB3	20:R:51:VAL:HG22	1.99	0.45
65:RR:10:LYS:NZ	81:2:1401:A:O3'	2.46	0.45
72:YY:15:ASN:HB3	72:YY:20:ARG:HB2	1.99	0.45
80:gg:152:VAL:HG23	80:gg:152:VAL:O	2.16	0.45
81:2:637:U:O2	81:2:637:U:O4'	2.34	0.45
81:2:1613:U:O2	81:2:1613:U:O5'	2.35	0.45
82:1:529:LEU:HD13	82:1:594:ILE:HG23	1.97	0.45
82:1:734:MET:O	82:1:738:MET:HG3	2.17	0.45
1:5:527:A:H2'	1:5:528:U:O4'	2.17	0.44
1:5:976:U:OP1	19:Q:144:ARG:NH2	2.50	0.44
1:5:1697:A:N6	1:5:1748:G:O2'	2.50	0.44
1:5:2475:G:O5'	1:5:2475:G:H8	2.00	0.44
64:QQ:39:VAL:HG21	64:QQ:48:VAL:HG11	1.98	0.44
65:RR:4:VAL:HG11	81:2:1315:U:O2	2.17	0.44
65:RR:99:VAL:HB	65:RR:100:LEU:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:gg:223:LEU:HB3	80:gg:232:MET:HE3	1.99	0.44
1:5:813:G:O3'	38:j:45:ARG:NH1	2.50	0.44
1:5:2900:A:N3	1:5:3025:C:O2'	2.47	0.44
3:8:71:A:O2'	27:Y:52:ARG:NH2	2.51	0.44
5:B:108:GLU:HB3	5:B:137:TYR:CD1	2.53	0.44
48:AA:23:HIS:CE1	48:AA:53:THR:HG21	2.52	0.44
50:CC:50:VAL:HG12	50:CC:55:ILE:HB	1.98	0.44
64:QQ:50:GLU:O	64:QQ:54:LEU:HD13	2.18	0.44
81:2:1212:G:H21	81:2:1241:G:H1	1.66	0.44
82:1:902:THR:HG23	82:1:904:PRO:HD3	1.99	0.44
1:5:646:A:C2	1:5:2375:G:C2	3.05	0.44
1:5:1721:U:O2'	1:5:1723:A:N7	2.43	0.44
1:5:1785:U:H2'	1:5:1786:G:C8	2.52	0.44
5:B:27:ALA:HB3	5:B:337:THR:HG22	1.99	0.44
13:J:82:ARG:NE	13:J:112:LEU:O	2.47	0.44
48:AA:64:ILE:HD12	48:AA:177:LEU:HD11	1.98	0.44
70:WW:25:VAL:HG13	70:WW:65:LEU:HD11	1.99	0.44
80:gg:124:ILE:HG22	80:gg:134:VAL:HG22	1.98	0.44
80:gg:178:MET:HE1	80:gg:192:ASP:HB2	1.99	0.44
81:2:350:C:H3'	81:2:351:A:H5'	2.00	0.44
81:2:1685:G:H2'	81:2:1686:C:C6	2.52	0.44
1:5:660:A:O2'	1:5:802:C:O2	2.34	0.44
45:q:111:ILE:HD13	45:q:147:LYS:HE2	2.00	0.44
50:CC:167:CYS:SG	50:CC:217:LYS:HD3	2.57	0.44
62:OO:105:LEU:O	62:OO:110:LEU:HB2	2.17	0.44
63:PP:81:ARG:HB3	63:PP:117:GLY:HA3	1.99	0.44
71:XX:19:ARG:NH1	81:2:608:U:O2	2.50	0.44
81:2:156:A:N1	81:2:418:G:O2'	2.41	0.44
82:1:661:ARG:HA	82:1:674:ASN:HA	1.98	0.44
1:5:1447:G:OP1	18:P:65:SER:OG	2.30	0.44
1:5:1556:C:N4	1:5:2169:G:O4'	2.50	0.44
6:C:53:SER:O	6:C:54:GLU:HB2	2.17	0.44
21:S:23:LYS:HA	22:T:146:ASN:HD21	1.82	0.44
39:k:8:ILE:HG13	39:k:9:LYS:HA	1.99	0.44
46:r:61:VAL:O	46:r:65:ILE:HG12	2.17	0.44
70:WW:28:ARG:NH1	81:2:865:A:OP2	2.51	0.44
72:YY:88:THR:O	72:YY:92:VAL:HG23	2.18	0.44
1:5:953:G:C8	1:5:1117:G:C8	3.05	0.44
1:5:1913:A:N3	1:5:2120:A:H2'	2.33	0.44
1:5:2150:G:O2'	1:5:2189:U:OP1	2.27	0.44
1:5:3058:U:OP1	32:d:28:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:130:ILE:HD12	9:F:134:VAL:HG11	2.00	0.44
26:X:110:VAL:HG12	26:X:124:VAL:HG22	1.99	0.44
50:CC:82:GLN:O	50:CC:109:VAL:HA	2.17	0.44
70:WW:107:SER:HA	81:2:804:A:C8	2.53	0.44
72:YY:11:LYS:NZ	81:2:775:G:N7	2.58	0.44
72:YY:121:THR:OG1	81:2:148:C:OP1	2.32	0.44
74:aa:3:LYS:NZ	74:aa:5:ARG:O	2.48	0.44
81:2:414:C:O2'	81:2:417:G:O6	2.31	0.44
82:1:688:ARG:HA	82:1:688:ARG:HE	1.83	0.44
1:5:660:A:N1	1:5:941:G:O2'	2.39	0.44
1:5:1779:C:N4	1:5:2102:U:OP1	2.51	0.44
1:5:2567:C:H2'	1:5:2568:C:H5'	2.00	0.44
54:GG:176:GLN:HG2	81:2:168:A:H5'	1.99	0.44
57:JJ:55:ALA:O	57:JJ:59:LEU:HG	2.17	0.44
65:RR:95:ARG:O	65:RR:99:VAL:HG23	2.17	0.44
67:TT:53:TRP:O	67:TT:56:LYS:N	2.51	0.44
80:gg:124:ILE:HD13	80:gg:170:ILE:HD12	2.00	0.44
80:gg:215:ALA:HB1	80:gg:241:VAL:HG23	1.99	0.44
1:5:504:A:H1'	1:5:611:A:OP1	2.17	0.44
1:5:3234:A:C2	1:5:3254:G:C2	3.06	0.44
14:L:3:ILE:HD13	29:a:45:MET:HE3	1.98	0.44
24:V:109:MET:HE1	24:V:132:ASN:HB2	1.99	0.44
53:FF:187:ARG:NE	81:2:1471:A:OP1	2.46	0.44
58:KK:73:VAL:HG21	58:KK:86:ILE:HD11	2.00	0.44
61:NN:17:PRO:HD3	81:2:959:U:O4'	2.18	0.44
62:OO:124:ASP:CG	81:2:928:U:H1'	2.42	0.44
1:5:1291:A:H2'	1:5:1292:C:O4'	2.18	0.44
1:5:1447:G:N7	18:P:25:SER:OG	2.41	0.44
53:FF:131:PRO:HA	53:FF:134:VAL:HG12	1.99	0.44
55:HH:102:PRO:HD3	55:HH:112:ARG:HD3	2.00	0.44
66:SS:26:ILE:HA	66:SS:57:ARG:HE	1.83	0.44
77:dd:31:ILE:HD11	77:dd:40:ARG:HA	2.00	0.44
1:5:1128:U:OP1	12:I:4:ARG:NH2	2.47	0.43
9:F:75:TYR:CZ	21:S:10:ILE:HD13	2.53	0.43
9:F:92:ILE:HG21	19:Q:3:ILE:N	2.33	0.43
14:L:28:GLN:HE21	16:N:201:ARG:HD3	1.82	0.43
14:L:76:THR:HG22	14:L:101:ARG:O	2.18	0.43
19:Q:101:VAL:HG11	19:Q:114:ILE:HD13	1.99	0.43
23:U:21:SER:O	23:U:25:ASN:ND2	2.50	0.43
31:c:34:LEU:HD23	31:c:59:TYR:HB3	2.00	0.43
34:f:52:VAL:HG21	34:f:99:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:10:ARG:O	35:g:12:PRO:HD3	2.17	0.43
49:BB:116:LYS:NZ	81:2:933:A:O5'	2.51	0.43
50:CC:175:ILE:HD11	50:CC:204:GLN:HB2	1.99	0.43
51:DD:39:VAL:HG22	51:DD:48:VAL:HG12	2.00	0.43
82:1:484:SER:C	82:1:486:LEU:H	2.25	0.43
1:5:860:G:C6	4:A:181:LYS:HB2	2.53	0.43
1:5:1506:A:H1'	1:5:1848:G:C6	2.53	0.43
9:F:160:ARG:HG3	9:F:203:TRP:CG	2.53	0.43
64:QQ:115:THR:O	64:QQ:117:LEU:N	2.49	0.43
67:TT:44:GLU:HG3	81:2:1476:C:H5''	1.99	0.43
81:2:217:A:C2	81:2:844:A:H1'	2.54	0.43
81:2:1003:A:H4'	81:2:1004:U:O5'	2.19	0.43
81:2:1524:A:H2'	81:2:1525:A:C8	2.53	0.43
1:5:1349:G:N7	6:C:302:ALA:HB3	2.34	0.43
1:5:2836:C:O2	1:5:2836:C:O4'	2.35	0.43
1:5:2967:A:N7	1:5:2968:G:H1'	2.33	0.43
5:B:21:ARG:O	5:B:22:ALA:C	2.60	0.43
6:C:175:HIS:O	6:C:179:LEU:HB2	2.17	0.43
6:C:233:LEU:HD12	6:C:233:LEU:HA	1.91	0.43
9:F:147:LEU:HD11	9:F:240:VAL:HG11	1.99	0.43
9:F:160:ARG:HG3	9:F:203:TRP:CD2	2.53	0.43
10:G:139:VAL:HG22	10:G:165:LEU:HD21	2.00	0.43
28:Z:95:VAL:O	28:Z:100:THR:OG1	2.29	0.43
1:5:1447:G:O2'	1:5:2355:G:O6	2.31	0.43
1:5:1505:C:OP1	18:P:127:ARG:HD2	2.18	0.43
1:5:2481:G:H2'	1:5:2482:U:C5	2.54	0.43
5:B:79:VAL:HG21	5:B:338:LEU:HD11	1.99	0.43
6:C:286:VAL:HA	6:C:289:ILE:HD12	2.00	0.43
21:S:79:VAL:HG13	21:S:90:MET:HB2	2.00	0.43
31:c:39:SER:HA	31:c:93:LEU:HA	1.99	0.43
53:FF:116:ILE:HA	53:FF:119:THR:HG22	2.00	0.43
55:HH:135:ILE:HG23	55:HH:152:VAL:HG13	2.00	0.43
62:OO:18:ARG:HD2	81:2:918:U:H4'	2.00	0.43
81:2:51:U:HO2'	82:1:695:HIS:HE2	1.64	0.43
81:2:1241:G:C6	81:2:1242:A:C6	3.06	0.43
1:5:1232:C:OP2	1:5:1264:G:N1	2.50	0.43
1:5:1899:G:O2'	1:5:2334:U:O4	2.26	0.43
1:5:2112:U:H4'	1:5:2113:A:H5'	1.99	0.43
5:B:227:GLU:O	5:B:232:ARG:NH2	2.52	0.43
7:D:107:ARG:CG	7:D:251:PRO:HG3	2.48	0.43
13:J:84:LEU:HD23	13:J:84:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:CC:82:GLN:HA	50:CC:83:ASP:CB	2.49	0.43
71:XX:5:LYS:NZ	81:2:613:C:OP2	2.49	0.43
76:cc:44:VAL:HG11	76:cc:48:VAL:HG11	1.99	0.43
1:5:968:G:N3	30:b:15:LYS:NZ	2.66	0.43
1:5:1225:A:N3	1:5:1225:A:H2'	2.33	0.43
1:5:1389:G:H5'	33:e:99:ASN:O	2.19	0.43
5:B:55:THR:HG23	5:B:73:VAL:HG13	2.01	0.43
9:F:116:PHE:C	9:F:199:ASN:HD21	2.25	0.43
14:L:75:PHE:O	14:L:101:ARG:NH1	2.52	0.43
48:AA:40:ALA:HB2	48:AA:46:HIS:CE1	2.53	0.43
55:HH:151:LYS:HG2	55:HH:182:VAL:HB	2.01	0.43
56:II:25:ARG:HG3	81:2:399:A:O5'	2.19	0.43
63:PP:43:ARG:NH2	81:2:1552:U:OP2	2.52	0.43
75:bb:35:VAL:HG11	75:bb:63:LEU:HD11	2.01	0.43
1:5:916:G:H5'	1:5:917:A:OP1	2.17	0.43
1:5:2882:U:H2'	1:5:2883:U:C6	2.54	0.43
11:H:38:LEU:HD13	11:H:71:VAL:CG2	2.49	0.43
14:L:3:ILE:HD11	29:a:34:MET:HA	2.00	0.43
40:l:24:PRO:HG2	40:l:27:ILE:HD12	2.01	0.43
48:AA:54:TRP:O	48:AA:58:VAL:HG23	2.19	0.43
61:NN:61:THR:HB	81:2:959:U:C6	2.54	0.43
63:PP:79:HIS:HB2	81:2:1241:G:H1'	2.01	0.43
67:TT:91:TYR:HB2	81:2:1590:G:OP1	2.19	0.43
82:1:464:LYS:O	82:1:464:LYS:HG2	2.19	0.43
1:5:976:U:H2'	1:5:977:C:O4'	2.19	0.43
1:5:2282:U:OP1	1:5:2973:G:O2'	2.33	0.43
1:5:2943:G:H2'	1:5:2944:U:O4'	2.19	0.43
3:8:38:U:O2'	36:h:83:LYS:NZ	2.49	0.43
12:I:48:LEU:HD12	12:I:142:ASP:HA	2.01	0.43
29:a:147:LEU:HB3	37:i:7:ILE:HG22	2.01	0.43
43:o:97:LYS:HB2	43:o:98:LYS:HG3	2.00	0.43
46:r:32:VAL:HG21	46:r:35:VAL:CG1	2.48	0.43
48:AA:74:VAL:HG23	48:AA:118:PRO:HB3	2.01	0.43
48:AA:205:ARG:HD2	65:RR:85:VAL:HG23	2.01	0.43
52:EE:77:ARG:HD2	52:EE:82:TYR:CE1	2.54	0.43
55:HH:5:GLN:HE21	55:HH:22:GLN:HG3	1.82	0.43
58:KK:79:TYR:HB3	58:KK:80:LEU:HD23	2.01	0.43
61:NN:114:ARG:O	61:NN:118:ILE:HG12	2.18	0.43
81:2:1110:G:H2'	81:2:1111:G:O4'	2.18	0.43
81:2:1582:U:O2	81:2:1613:U:H5	2.00	0.43
81:2:1592:A:H2'	81:2:1593:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:283:G:O6	1:5:304:G:H1'	2.19	0.43
1:5:744:A:H2'	1:5:745:C:O4'	2.19	0.43
1:5:2746:A:H2'	1:5:2747:A:O4'	2.18	0.43
1:5:3217:C:N3	18:P:182:ILE:HD12	2.34	0.43
5:B:47:LEU:HD22	5:B:335:ILE:HD11	2.00	0.43
51:DD:55:THR:HA	51:DD:58:VAL:HB	2.01	0.43
56:II:51:GLY:O	56:II:52:ASN:C	2.61	0.43
61:NN:87:ASP:HB3	61:NN:125:LEU:HD11	2.01	0.43
81:2:396:A:H2'	81:2:397:G:O4'	2.19	0.43
81:2:868:G:H1	81:2:960:U:H3	1.65	0.43
81:2:1774:G:H2'	81:2:1775:U:O4'	2.19	0.43
82:1:496:ILE:HD11	82:1:526:VAL:HG23	1.99	0.43
1:5:348:A:N3	1:5:352:A:O2'	2.52	0.43
1:5:1347:U:H2'	1:5:1355:A:H61	1.83	0.43
5:B:227:GLU:O	5:B:232:ARG:CZ	2.67	0.43
8:E:58:LEU:HD21	8:E:64:LEU:HB2	2.00	0.43
16:N:94:TYR:CE2	16:N:96:ARG:HB2	2.54	0.43
18:P:119:VAL:HG13	18:P:146:ILE:HG12	2.01	0.43
23:U:90:ARG:C	23:U:92:TRP:H	2.27	0.43
46:r:35:VAL:HB	46:r:37:SER:N	2.33	0.43
52:EE:45:ILE:HD13	52:EE:61:VAL:HG21	2.01	0.43
60:MM:97:GLY:O	81:2:1227:A:N6	2.46	0.43
63:PP:41:VAL:CG1	63:PP:84:ILE:HG21	2.49	0.43
74:aa:45:VAL:HG21	74:aa:53:LEU:HD21	1.99	0.43
77:dd:36:LEU:HD23	77:dd:36:LEU:HA	1.93	0.43
81:2:1525:A:H2'	81:2:1526:A:C8	2.54	0.43
82:1:565:TYR:CE1	82:1:581:LEU:HD12	2.51	0.43
17:O:120:VAL:HG23	17:O:123:ALA:HB3	2.00	0.42
21:S:23:LYS:C	22:T:146:ASN:HD21	2.27	0.42
21:S:167:ARG:HD2	21:S:167:ARG:HA	1.93	0.42
45:q:191:VAL:HA	45:q:194:LEU:HB2	2.00	0.42
51:DD:219:ALA:O	51:DD:220:PRO:C	2.62	0.42
52:EE:170:THR:OG1	52:EE:171:ASP:N	2.52	0.42
57:JJ:158:PHE:CD1	57:JJ:164:PHE:HB3	2.54	0.42
61:NN:23:PRO:HG2	61:NN:26:PHE:HB2	2.01	0.42
70:WW:119:LYS:HG2	81:2:687:G:H5''	2.00	0.42
81:2:1244:A:H2'	81:2:1244:A:N3	2.33	0.42
82:1:989:TRP:HA	82:1:992:LEU:HB2	2.01	0.42
1:5:971:G:H2'	1:5:972:A:O4'	2.19	0.42
27:Y:51:ARG:HG2	27:Y:115:ARG:NH1	2.33	0.42
62:OO:29:HIS:CE1	62:OO:31:THR:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:TT:114:VAL:HG13	67:TT:122:ARG:HB3	2.01	0.42
79:ff:143:LYS:O	79:ff:144:CYS:SG	2.77	0.42
80:gg:84:ALA:HB1	80:gg:111:VAL:HG12	2.01	0.42
81:2:1397:U:O2	81:2:1400:A:N7	2.52	0.42
82:1:446:TYR:HH	82:1:470:PRO:C	2.09	0.42
1:5:121:A:C2	10:G:128:PRO:HB3	2.54	0.42
1:5:1063:G:N7	1:5:1097:G:O2'	2.46	0.42
1:5:1973:G:N2	1:5:2059:C:O2	2.52	0.42
1:5:2854:U:OP2	12:I:3:ARG:NH1	2.52	0.42
1:5:2881:C:OP1	5:B:11:HIS:NE2	2.48	0.42
5:B:29:VAL:HG23	5:B:337:THR:HG21	2.00	0.42
8:E:51:ARG:O	8:E:72:ASN:ND2	2.52	0.42
12:I:77:THR:HG22	12:I:82:ARG:HA	2.00	0.42
44:p:49:ARG:HB2	44:p:55:TRP:CZ3	2.54	0.42
45:q:159:LEU:HD11	45:q:163:LEU:HA	2.01	0.42
56:II:47:ARG:NH1	81:2:397:G:OP2	2.52	0.42
58:KK:21:VAL:HG21	58:KK:46:LEU:HD21	2.00	0.42
80:gg:148:HIS:CD2	80:gg:152:VAL:HG12	2.55	0.42
4:A:102:LEU:HD11	4:A:166:ILE:HD11	2.02	0.42
13:J:132:ASN:HD21	13:J:136:ALA:CB	2.32	0.42
15:M:21:VAL:HG12	15:M:65:LEU:HA	2.01	0.42
44:p:37:TYR:HB2	44:p:47:VAL:CG2	2.49	0.42
48:AA:50:VAL:HG23	65:RR:109:LEU:HD21	2.00	0.42
51:DD:151:LYS:NZ	81:2:1424:A:OP2	2.42	0.42
59:LL:105:LYS:NZ	81:2:306:G:OP2	2.49	0.42
61:NN:127:ARG:NH1	81:2:628:U:OP1	2.53	0.42
63:PP:79:HIS:HA	63:PP:97:TYR:HB3	2.00	0.42
64:QQ:5:PRO:HA	64:QQ:96:TYR:CZ	2.54	0.42
74:aa:78:ALA:O	74:aa:82:ARG:HB2	2.20	0.42
80:gg:39:ARG:HA	80:gg:68:ILE:HG23	2.01	0.42
1:5:1021:G:H2'	1:5:1022:U:C6	2.54	0.42
1:5:1506:A:H1'	1:5:1848:G:O6	2.19	0.42
1:5:1604:G:H3'	1:5:1604:G:N3	2.34	0.42
9:F:69:ALA:HB1	9:F:74:SER:O	2.20	0.42
18:P:118:GLN:NE2	18:P:120:ASN:HD21	2.17	0.42
28:Z:26:VAL:HG13	28:Z:93:LYS:HA	2.01	0.42
46:r:30:VAL:HA	46:r:189:VAL:HA	2.00	0.42
46:r:79:LEU:N	46:r:80:PRO:CD	2.82	0.42
81:2:739:G:H3'	81:2:740:A:H5'	2.02	0.42
81:2:999:U:H2'	81:2:1000:C:O4'	2.19	0.42
81:2:1293:U:H5	81:2:1322:A:N1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:1639:C:H2'	81:2:1640:C:O4'	2.19	0.42
82:1:465:GLN:O	82:1:467:PHE:CE1	2.72	0.42
82:1:649:VAL:HG11	82:1:721:LEU:HD13	2.01	0.42
1:5:63:A:N3	1:5:78:U:O2'	2.51	0.42
1:5:784:A:C2	19:Q:93:ILE:HG22	2.55	0.42
1:5:1972:A:C5	1:5:1973:G:H1'	2.54	0.42
1:5:2679:A:C2	13:J:56:THR:HG21	2.54	0.42
1:5:2903:A:H2'	1:5:2904:U:O4'	2.20	0.42
4:A:181:LYS:HB3	44:p:18:TYR:CE1	2.54	0.42
7:D:34:LYS:O	7:D:38:THR:HG23	2.20	0.42
7:D:74:VAL:HG11	7:D:77:ALA:HB2	2.01	0.42
12:I:176:LEU:HD12	12:I:181:TYR:HD1	1.85	0.42
18:P:158:ALA:HA	18:P:159:LYS:C	2.45	0.42
20:R:10:LEU:HD12	20:R:10:LEU:HA	1.90	0.42
29:a:112:ILE:HD12	29:a:125:VAL:HG11	2.01	0.42
45:q:59:PRO:HD2	45:q:153:SER:HA	2.01	0.42
48:AA:36:TYR:CD1	48:AA:161:PRO:HG3	2.55	0.42
50:CC:61:ILE:HG23	50:CC:66:LEU:HB2	2.01	0.42
52:EE:104:ASP:HB2	52:EE:110:ALA:HB2	2.01	0.42
55:HH:114:ARG:HA	55:HH:117:THR:HG23	2.02	0.42
59:LL:84:ILE:HG21	59:LL:117:VAL:HG21	2.00	0.42
63:PP:80:MET:O	63:PP:116:LEU:HD11	2.19	0.42
75:bb:41:LEU:HD23	75:bb:41:LEU:HA	1.88	0.42
77:dd:5:ASN:ND2	81:2:1245:G:OP1	2.53	0.42
80:gg:77:ASP:HA	80:gg:78:GLY:HA3	1.79	0.42
1:5:643:U:O2'	1:5:1153:A:N1	2.49	0.42
1:5:999:G:C6	1:5:1000:C:N4	2.88	0.42
1:5:1887:A:O3'	5:B:228:GLY:HA3	2.19	0.42
1:5:2097:U:H2'	1:5:2098:C:C6	2.54	0.42
1:5:2415:C:H6	1:5:2415:C:O5'	2.02	0.42
7:D:144:VAL:HG21	7:D:171:LEU:HD23	2.01	0.42
8:E:67:GLY:O	8:E:68:PRO:C	2.63	0.42
18:P:160:ALA:HA	18:P:161:ALA:HA	1.79	0.42
48:AA:172:LEU:HD22	65:RR:93:LEU:HD21	2.02	0.42
50:CC:109:VAL:HG11	50:CC:138:LYS:HG2	2.01	0.42
51:DD:66:ILE:O	51:DD:70:THR:OG1	2.33	0.42
55:HH:93:LEU:HD21	55:HH:176:LEU:HD13	2.02	0.42
56:II:153:ILE:HG21	56:II:157:VAL:HB	2.00	0.42
71:XX:96:VAL:O	71:XX:97:ASP:HB2	2.20	0.42
80:gg:178:MET:HE1	80:gg:192:ASP:CB	2.49	0.42
80:gg:179:VAL:HB	80:gg:193:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:901:G:C6	81:2:902:G:C6	3.08	0.42
81:2:1189:A:N3	81:2:1194:A:O2'	2.51	0.42
1:5:2196:C:O2'	1:5:2270:A:H1'	2.20	0.42
7:D:47:PRO:HB2	7:D:66:SER:OG	2.20	0.42
12:I:138:VAL:HG11	12:I:148:VAL:HG13	2.02	0.42
16:N:11:GLN:HA	16:N:19:LEU:HD11	2.02	0.42
19:Q:122:ILE:HG22	19:Q:123:THR:O	2.19	0.42
31:c:13:LYS:HB3	31:c:100:ILE:HG13	2.00	0.42
52:EE:208:VAL:HG13	52:EE:210:ILE:HD11	2.02	0.42
82:1:411:LEU:HD12	82:1:514:SER:HB3	2.02	0.42
82:1:753:LYS:HD3	82:1:802:ALA:HB2	2.02	0.42
1:5:607:A:OP1	8:E:23:LYS:HA	2.20	0.42
1:5:649:A:OP2	1:5:2868:U:O2'	2.38	0.42
1:5:1819:U:H2'	1:5:1820:U:C5'	2.49	0.42
1:5:2100:A:H5'	1:5:2101:C:OP2	2.20	0.42
1:5:3165:A:C2	1:5:3286:G:C2	3.08	0.42
8:E:54:TYR:CE1	8:E:63:LEU:HD22	2.55	0.42
8:E:91:VAL:HG12	8:E:155:LEU:HD21	2.02	0.42
10:G:177:ALA:HA	10:G:221:PHE:CD2	2.54	0.42
15:M:128:ARG:HA	15:M:131:VAL:HG22	2.01	0.42
32:d:20:LEU:HD11	32:d:32:ALA:HB2	2.00	0.42
45:q:29:LEU:HD22	45:q:171:ASN:HD22	1.84	0.42
68:UU:59:PRO:HA	81:2:1382:A:H5'	2.02	0.42
81:2:968:U:H2'	81:2:969:C:O4'	2.19	0.42
81:2:1060:U:O2	81:2:1060:U:O4'	2.38	0.42
82:1:439:THR:HG21	82:1:477:THR:HB	2.02	0.42
1:5:1696:A:H2'	1:5:1697:A:C8	2.55	0.42
6:C:54:GLU:O	6:C:56:ALA:N	2.53	0.42
15:M:8:LYS:HB3	15:M:9:ALA:HA	2.01	0.42
29:a:35:ALA:O	29:a:41:HIS:ND1	2.50	0.42
44:p:54:ILE:HG23	44:p:63:THR:CG2	2.50	0.42
48:AA:33:GLN:O	69:VV:87:ARG:NH1	2.53	0.42
58:KK:86:ILE:C	58:KK:88:PRO:HD2	2.45	0.42
67:TT:83:ALA:HB2	81:2:1525:A:H4'	2.01	0.42
70:WW:40:VAL:HG11	70:WW:103:ILE:HD12	2.02	0.42
73:ZZ:82:HIS:HA	73:ZZ:85:LYS:HE3	2.02	0.42
78:ee:31:LYS:N	81:2:476:A:OP1	2.53	0.42
81:2:690:G:C5	81:2:691:C:N3	2.87	0.42
81:2:1054:U:H2'	81:2:1055:U:O4'	2.20	0.42
83:3:15:G:H2'	83:3:16:U:C2	2.55	0.42
7:D:38:THR:HG22	22:T:30:TYR:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:114:ARG:NH1	16:N:151:ILE:O	2.53	0.41
48:AA:21:ASN:HA	48:AA:24:LEU:HG	2.01	0.41
56:II:26:LYS:O	56:II:29:LEU:HB2	2.20	0.41
63:PP:127:ARG:NH1	81:2:1180:C:O2'	2.51	0.41
72:YY:27:VAL:HG21	72:YY:40:LEU:HD21	2.01	0.41
81:2:808:U:H2'	81:2:809:A:C4	2.55	0.41
81:2:1729:C:H2'	81:2:1730:A:O4'	2.19	0.41
1:5:273:A:H1'	37:i:78:GLY:HA2	2.02	0.41
1:5:1194:G:C6	1:5:1195:A:C6	3.08	0.41
1:5:2700:G:O2'	1:5:2705:A:N1	2.48	0.41
1:5:3223:A:H2'	1:5:3224:G:O4'	2.20	0.41
19:Q:157:PRO:HA	19:Q:158:HIS:HA	1.84	0.41
29:a:44:ASN:O	29:a:47:LYS:O	2.38	0.41
44:p:42:CYS:SG	44:p:60:CYS:SG	3.19	0.41
45:q:203:SER:HA	45:q:217:TYR:HB2	2.01	0.41
49:BB:179:SER:HA	49:BB:183:GLN:HB2	2.02	0.41
54:GG:52:ILE:HA	54:GG:111:LEU:HD23	2.03	0.41
82:1:425:ILE:HG22	82:1:447:PHE:CZ	2.55	0.41
82:1:565:TYR:HE1	82:1:581:LEU:CD1	2.24	0.41
1:5:242:C:H2'	1:5:243:G:H8	1.84	0.41
5:B:93:VAL:HG22	5:B:155:ALA:H	1.86	0.41
10:G:168:LEU:HA	37:i:43:LEU:HD11	2.02	0.41
18:P:116:HIS:HB3	18:P:149:VAL:HB	2.03	0.41
29:a:123:VAL:O	29:a:124:ILE:C	2.63	0.41
40:l:32:ASN:O	40:l:33:ASN:C	2.63	0.41
45:q:157:PHE:C	45:q:165:LEU:HD11	2.46	0.41
46:r:130:MET:HE1	46:r:138:PHE:HZ	1.84	0.41
53:FF:124:ASN:HA	53:FF:128:ASP:HA	2.01	0.41
57:JJ:143:ILE:HG13	81:2:768:C:N1	2.36	0.41
79:ff:118:ARG:NH1	79:ff:130:VAL:O	2.53	0.41
81:2:1338:C:H1'	81:2:1410:A:C4	2.55	0.41
81:2:1471:A:N3	81:2:1474:G:O2'	2.47	0.41
81:2:1606:C:H2'	81:2:1607:G:C8	2.55	0.41
1:5:73:C:C2	14:L:59:ARG:HD3	2.56	0.41
1:5:303:G:C2	1:5:313:A:C2	3.08	0.41
1:5:500:C:H5''	8:E:82:ARG:HG3	2.03	0.41
1:5:3158:G:O2'	1:5:3159:C:O5'	2.36	0.41
3:8:13:A:O2'	18:P:120:ASN:HB3	2.21	0.41
17:O:79:ILE:HG21	17:O:138:LEU:HD11	2.03	0.41
43:o:35:LEU:HA	43:o:40:LYS:HG2	2.01	0.41
46:r:183:PHE:CE2	46:r:185:PHE:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:EE:19:LEU:HD13	81:2:788:A:C4	2.55	0.41
62:OO:29:HIS:CE1	62:OO:38:THR:HG23	2.56	0.41
80:gg:53:GLN:O	80:gg:55:PHE:N	2.53	0.41
1:5:388:G:N2	18:P:101:ASN:OD1	2.47	0.41
1:5:497:C:H2'	1:5:498:A:O4'	2.21	0.41
1:5:2836:C:H5	1:5:2852:C:N4	2.17	0.41
5:B:347:SER:C	5:B:349:LYS:H	2.29	0.41
7:D:39:GLN:NE2	7:D:46:THR:O	2.53	0.41
15:M:32:LEU:HD11	15:M:94:TRP:CD1	2.55	0.41
24:V:53:SER:O	24:V:56:ASP:HB2	2.20	0.41
38:j:27:PHE:HA	38:j:34:CYS:HA	2.02	0.41
48:AA:198:MET:C	48:AA:200:ASP:H	2.29	0.41
51:DD:3:ALA:HA	51:DD:4:LEU:HA	1.84	0.41
62:OO:102:LEU:O	62:OO:103:ARG:HB3	2.21	0.41
80:gg:50:GLY:HA2	80:gg:55:PHE:CD1	2.56	0.41
81:2:1125:A:C5	81:2:1126:G:H1'	2.55	0.41
82:1:682:GLN:CB	82:1:683:PRO:HD3	2.49	0.41
82:1:744:LEU:HD13	82:1:762:LEU:HD21	2.02	0.41
82:1:745:LEU:HB2	82:1:748:VAL:HG11	2.01	0.41
82:1:897:ILE:HG22	82:1:914:LEU:HD13	2.02	0.41
1:5:267:G:OP2	1:5:318:A:N6	2.54	0.41
1:5:625:G:N2	1:5:1401:A:OP1	2.45	0.41
1:5:2714:G:H8	1:5:2751:G:H2'	1.86	0.41
14:L:4:SER:OG	14:L:5:LYS:N	2.51	0.41
26:X:61:LYS:O	26:X:87:SER:OG	2.37	0.41
29:a:130:VAL:HG11	29:a:145:VAL:HG11	2.02	0.41
30:b:17:HIS:NE2	30:b:21:ILE:HD12	2.35	0.41
35:g:19:LYS:HD3	35:g:19:LYS:HA	1.96	0.41
50:CC:121:LYS:HD3	50:CC:132:ALA:HB1	2.02	0.41
51:DD:76:ARG:NH2	58:KK:63:TYR:CD2	2.88	0.41
64:QQ:71:GLY:HA2	81:2:1483:A:H4'	2.03	0.41
80:gg:300:GLN:O	80:gg:316:VAL:HG12	2.21	0.41
81:2:37:C:H2'	81:2:38:A:O4'	2.21	0.41
81:2:86:C:O2'	81:2:168:A:N1	2.47	0.41
81:2:190:C:O4'	81:2:194:G:N2	2.53	0.41
81:2:229:C:O2'	81:2:231:U:O4	2.34	0.41
82:1:503:ILE:HG23	82:1:529:LEU:HG	2.02	0.41
1:5:262:U:H2'	1:5:263:C:O4'	2.21	0.41
1:5:601:U:H2'	1:5:602:A:O4'	2.20	0.41
1:5:1504:A:N1	1:5:1515:A:O2'	2.40	0.41
1:5:2369:G:H2'	1:5:2370:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3018:C:C4	1:5:3019:U:C4	3.08	0.41
6:C:77:VAL:HG23	6:C:87:GLN:O	2.21	0.41
6:C:258:LEU:HD23	6:C:258:LEU:HA	1.92	0.41
9:F:185:ILE:O	9:F:189:ILE:HG22	2.20	0.41
39:k:20:VAL:HG21	39:k:45:VAL:CG1	2.51	0.41
45:q:198:TRP:N	45:q:199:GLN:HA	2.36	0.41
68:UU:57:ARG:HD2	81:2:1382:A:N3	2.36	0.41
69:VV:53:TYR:CZ	69:VV:72:LEU:HB3	2.55	0.41
71:XX:63:GLN:N	71:XX:64:PRO:HD2	2.34	0.41
81:2:876:G:H1'	81:2:944:A:O4'	2.21	0.41
81:2:1213:G:O2'	81:2:1244:A:N6	2.43	0.41
82:1:446:TYR:OH	82:1:470:PRO:C	2.61	0.41
1:5:1468:A:N1	1:5:1880:U:O2'	2.51	0.41
1:5:2610:G:H2'	1:5:2611:U:O4'	2.20	0.41
1:5:2611:U:H2'	1:5:2612:U:H6	1.85	0.41
1:5:3277:U:O2	1:5:3277:U:O4'	2.36	0.41
2:7:98:C:OP1	21:S:39:SER:HB2	2.21	0.41
4:A:134:VAL:HG23	4:A:150:LEU:HD23	2.03	0.41
5:B:81:THR:OG1	5:B:205:VAL:HG21	2.21	0.41
12:I:89:VAL:HG22	12:I:136:PHE:CE1	2.56	0.41
52:EE:27:TYR:O	81:2:446:U:O2'	2.35	0.41
54:GG:1:MET:HE2	54:GG:1:MET:HB2	1.99	0.41
60:MM:26:ARG:NH2	60:MM:94:ALA:HA	2.36	0.41
60:MM:59:VAL:HG11	60:MM:64:ILE:HG22	2.02	0.41
81:2:1145:U:H2'	81:2:1146:G:O4'	2.20	0.41
1:5:549:U:H2'	1:5:550:A:H8	1.86	0.41
1:5:2505:U:H4'	1:5:2506:U:OP1	2.21	0.41
6:C:276:LEU:HD23	6:C:277:PRO:HD2	2.03	0.41
19:Q:65:SER:HA	19:Q:93:ILE:HD13	2.02	0.41
31:c:30:THR:HG21	31:c:89:VAL:HG11	2.03	0.41
37:i:95:ALA:HA	37:i:99:ARG:HG2	2.03	0.41
43:o:77:CYS:SG	43:o:79:THR:HG22	2.60	0.41
46:r:35:VAL:CB	46:r:36:SER:HA	2.50	0.41
49:BB:144:ARG:HB2	49:BB:208:GLN:HB3	2.03	0.41
53:FF:122:ILE:HA	53:FF:125:VAL:HG12	2.03	0.41
60:MM:56:VAL:HG11	60:MM:64:ILE:CG2	2.51	0.41
64:QQ:40:GLU:HB3	64:QQ:41:PRO:HD3	2.02	0.41
66:SS:105:VAL:HG23	66:SS:106:GLU:H	1.86	0.41
74:aa:25:ASN:OD1	74:aa:25:ASN:N	2.54	0.41
80:gg:14:LEU:HB2	80:gg:311:ILE:HB	2.03	0.41
81:2:512:U:O2	81:2:512:U:H3'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:538:G:O2'	81:2:539:G:O5'	2.35	0.41
81:2:959:U:O2	81:2:959:U:H2'	2.20	0.41
82:1:758:GLN:HG2	82:1:787:VAL:HG22	2.03	0.41
1:5:914:A:C8	4:A:199:THR:HG21	2.56	0.41
1:5:1160:C:C5	1:5:1366:A:H1'	2.55	0.41
1:5:1412:G:H5''	33:e:123:LYS:HE2	2.03	0.41
1:5:2179:C:H2'	4:A:132:ASN:HD21	1.86	0.41
1:5:2884:C:O2	1:5:2939:G:C2	2.74	0.41
1:5:2897:A:H5''	41:m:125:LYS:HB2	2.02	0.41
1:5:3066:U:H2'	1:5:3067:C:C6	2.56	0.41
2:7:11:A:N1	2:7:67:G:O2'	2.41	0.41
3:8:141:C:OP1	16:N:109:ARG:NH1	2.54	0.41
4:A:140:ASN:O	4:A:144:ASN:HA	2.20	0.41
5:B:12:GLY:HA3	5:B:233:TRP:HE3	1.86	0.41
6:C:187:LEU:HD23	6:C:187:LEU:HA	1.90	0.41
18:P:120:ASN:HB2	18:P:145:HIS:HB2	2.03	0.41
23:U:80:THR:HG21	23:U:95:PHE:HD2	1.87	0.41
33:e:20:HIS:CG	33:e:42:VAL:HG21	2.56	0.41
54:GG:30:LYS:HD3	54:GG:36:VAL:HG22	2.03	0.41
61:NN:98:VAL:HG23	61:NN:115:LEU:HD13	2.02	0.41
62:OO:81:VAL:HG11	62:OO:102:LEU:HD13	2.03	0.41
65:RR:18:GLU:HA	65:RR:71:PHE:HB3	2.03	0.41
66:SS:18:LEU:HD12	66:SS:18:LEU:O	2.21	0.41
66:SS:33:THR:HA	66:SS:38:VAL:HG23	2.03	0.41
68:UU:96:PRO:HD2	68:UU:99:ILE:HD13	2.03	0.41
74:aa:80:HIS:O	74:aa:82:ARG:NH2	2.54	0.41
82:1:469:VAL:O	82:1:471:GLY:N	2.53	0.41
82:1:565:TYR:O	82:1:569:GLN:HB2	2.21	0.41
1:5:16:A:H62	3:8:143:U:H3	1.69	0.40
1:5:664:U:H2'	1:5:665:A:C8	2.56	0.40
1:5:2172:A:H2'	1:5:2173:U:O4'	2.22	0.40
5:B:383:LEU:HA	5:B:384:LYS:HA	1.87	0.40
19:Q:29:LEU:HD21	19:Q:124:LEU:HB2	2.03	0.40
28:Z:44:ALA:HB1	28:Z:114:VAL:HG11	2.03	0.40
41:m:122:ARG:NH1	41:m:123:PRO:O	2.54	0.40
50:CC:81:LEU:HD22	50:CC:109:VAL:HG12	2.04	0.40
52:EE:104:ASP:N	52:EE:108:ARG:O	2.50	0.40
58:KK:7:ASP:HA	58:KK:10:LYS:HD2	2.02	0.40
63:PP:83:MET:HE3	63:PP:83:MET:HA	2.01	0.40
66:SS:22:VAL:HG12	66:SS:34:THR:OG1	2.22	0.40
70:WW:107:SER:HA	81:2:804:A:N7	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:705:U:O4	81:2:731:C:H5''	2.21	0.40
81:2:863:A:O2'	81:2:864:U:OP1	2.39	0.40
81:2:1171:A:H2'	81:2:1172:G:C8	2.57	0.40
81:2:1540:G:C6	81:2:1541:G:C4	3.09	0.40
82:1:535:LEU:HD12	82:1:561:PHE:CE1	2.56	0.40
1:5:951:A:OP1	30:b:18:ARG:NH1	2.48	0.40
1:5:1604:G:H4'	1:5:1835:A:H4'	2.03	0.40
1:5:2912:G:N1	1:5:3130:A:C8	2.89	0.40
7:D:290:ILE:HG13	12:I:206:LEU:HD21	2.03	0.40
17:O:44:SER:OG	17:O:129:LEU:HD11	2.21	0.40
18:P:48:LEU:HA	18:P:51:VAL:HG12	2.03	0.40
33:e:121:ASN:CB	33:e:122:PRO:HD3	2.51	0.40
49:BB:97:LEU:HD13	49:BB:232:HIS:NE2	2.37	0.40
53:FF:73:ALA:HB3	53:FF:113:VAL:HG23	2.02	0.40
68:UU:85:ARG:NH2	81:2:1334:U:O3'	2.52	0.40
69:VV:15:ARG:HH12	69:VV:33:GLN:HB2	1.85	0.40
70:WW:95:PRO:HD3	70:WW:130:TYR:CE2	2.56	0.40
81:2:957:G:C6	81:2:958:U:C5	3.08	0.40
81:2:1275:A:C6	81:2:1438:G:C5	3.09	0.40
82:1:565:TYR:OH	82:1:581:LEU:HB2	2.20	0.40
82:1:662:ILE:HD12	82:1:664:LEU:HD11	2.03	0.40
1:5:607:A:OP1	8:E:26:ARG:NH2	2.46	0.40
1:5:2635:A:H4'	1:5:2636:A:O5'	2.21	0.40
5:B:47:LEU:HD23	5:B:47:LEU:HA	1.93	0.40
9:F:155:LYS:HG2	9:F:158:LYS:HA	2.03	0.40
49:BB:82:ARG:NH2	49:BB:188:LEU:O	2.54	0.40
50:CC:68:VAL:HG23	50:CC:73:ILE:HD12	2.04	0.40
51:DD:20:GLU:OE2	51:DD:76:ARG:NH2	2.54	0.40
53:FF:39:GLN:C	53:FF:41:GLU:H	2.30	0.40
57:JJ:7:THR:CG2	81:2:758:U:H5''	2.51	0.40
60:MM:56:VAL:HG11	60:MM:64:ILE:HG23	2.03	0.40
62:OO:51:ASP:C	62:OO:53:ASP:N	2.78	0.40
65:RR:25:THR:O	65:RR:27:ASP:N	2.54	0.40
75:bb:46:VAL:HG11	75:bb:63:LEU:HD12	2.03	0.40
81:2:94:G:O2'	81:2:459:A:O2'	2.15	0.40
81:2:374:U:H2'	81:2:375:C:O4'	2.22	0.40
81:2:1000:C:O4'	81:2:1000:C:O2	2.39	0.40
82:1:625:MET:O	82:1:626:TYR:HB2	2.21	0.40
1:5:707:U:H2'	1:5:708:G:H5''	2.04	0.40
2:7:28:C:O3'	13:J:135:GLY:HA2	2.22	0.40
11:H:38:LEU:O	11:H:41:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:22:VAL:HG13	16:N:199:LEU:CD1	2.51	0.40
15:M:40:ASP:C	15:M:42:LYS:H	2.28	0.40
33:e:109:LEU:HD11	33:e:122:PRO:HB2	2.04	0.40
45:q:26:ARG:HG3	45:q:210:MET:HE2	2.03	0.40
48:AA:33:GLN:N	48:AA:34:GLU:HB2	2.35	0.40
71:XX:52:ILE:HD11	71:XX:77:ILE:HD11	2.04	0.40
72:YY:109:LYS:HA	72:YY:112:LYS:HG2	2.04	0.40
81:2:1334:U:H2'	81:2:1335:U:O4'	2.22	0.40
1:5:1129:A:H2'	1:5:1130:A:C8	2.57	0.40
1:5:1604:G:H2'	1:5:1605:A:O4'	2.22	0.40
1:5:2680:A:C6	13:J:57:PHE:HB3	2.56	0.40
1:5:3262:U:H3'	1:5:3263:G:H5''	2.04	0.40
2:7:8:G:OP1	7:D:33:ARG:NH1	2.54	0.40
22:T:62:GLY:HA3	22:T:76:ILE:HD13	2.03	0.40
26:X:73:MET:HE2	26:X:142:ILE:C	2.46	0.40
49:BB:36:SER:HB3	49:BB:231:LEU:O	2.22	0.40
50:CC:174:LEU:O	50:CC:175:ILE:C	2.64	0.40
57:JJ:105:LEU:HD23	57:JJ:108:ARG:HD2	2.04	0.40
65:RR:106:THR:HA	65:RR:109:LEU:HB3	2.02	0.40
67:TT:66:TYR:HA	67:TT:124:ILE:CG1	2.51	0.40
68:UU:21:LYS:HA	68:UU:94:GLU:HA	2.04	0.40
74:aa:79:ILE:HA	74:aa:84:VAL:HG21	2.04	0.40
81:2:28:U:H2'	81:2:29:G:H8	1.87	0.40
82:1:902:THR:OG1	82:1:903:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	247/249 (99%)	223 (90%)	17 (7%)	7 (3%)	4 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	382/384 (100%)	325 (85%)	54 (14%)	3 (1%)	16	44
6	C	357/359 (99%)	287 (80%)	54 (15%)	16 (4%)	2	8
7	D	293/295 (99%)	266 (91%)	24 (8%)	3 (1%)	12	39
8	E	152/175 (87%)	142 (93%)	8 (5%)	2 (1%)	9	32
9	F	220/222 (99%)	194 (88%)	22 (10%)	4 (2%)	6	25
10	G	231/233 (99%)	210 (91%)	19 (8%)	2 (1%)	14	41
11	H	189/191 (99%)	165 (87%)	21 (11%)	3 (2%)	7	27
12	I	214/216 (99%)	191 (89%)	18 (8%)	5 (2%)	5	19
13	J	166/168 (99%)	149 (90%)	16 (10%)	1 (1%)	21	51
14	L	196/198 (99%)	173 (88%)	19 (10%)	4 (2%)	6	22
15	M	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	8	28
16	N	200/202 (99%)	183 (92%)	16 (8%)	1 (0%)	24	54
17	O	195/197 (99%)	184 (94%)	9 (5%)	2 (1%)	12	39
18	P	178/180 (99%)	158 (89%)	18 (10%)	2 (1%)	11	36
19	Q	182/184 (99%)	169 (93%)	12 (7%)	1 (0%)	24	54
20	R	186/188 (99%)	174 (94%)	11 (6%)	1 (0%)	24	54
21	S	167/169 (99%)	152 (91%)	12 (7%)	3 (2%)	6	25
22	T	156/158 (99%)	141 (90%)	13 (8%)	2 (1%)	9	32
23	U	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
24	V	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	8	28
25	W	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
26	X	119/121 (98%)	108 (91%)	10 (8%)	1 (1%)	16	44
27	Y	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
28	Z	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	8	28
29	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	15
30	b	55/57 (96%)	46 (84%)	7 (13%)	2 (4%)	2	11
31	c	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
32	d	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
33	e	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	26
34	f	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	6	23
35	g	119/121 (98%)	106 (89%)	10 (8%)	3 (2%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	h	114/116 (98%)	108 (95%)	5 (4%)	1 (1%)	14	41
37	i	94/98 (96%)	79 (84%)	13 (14%)	2 (2%)	5	21
38	j	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
39	k	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
40	l	47/49 (96%)	39 (83%)	7 (15%)	1 (2%)	5	21
41	m	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
42	n	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
43	o	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	1
44	p	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	12
45	q	213/217 (98%)	163 (76%)	45 (21%)	5 (2%)	5	19
46	r	191/195 (98%)	144 (75%)	41 (22%)	6 (3%)	3	14
48	AA	204/206 (99%)	166 (81%)	31 (15%)	7 (3%)	3	12
49	BB	212/214 (99%)	187 (88%)	23 (11%)	2 (1%)	14	41
50	CC	215/217 (99%)	188 (87%)	21 (10%)	6 (3%)	4	15
51	DD	221/223 (99%)	189 (86%)	26 (12%)	6 (3%)	4	16
52	EE	255/257 (99%)	217 (85%)	33 (13%)	5 (2%)	6	22
53	FF	197/206 (96%)	155 (79%)	36 (18%)	6 (3%)	3	14
54	GG	224/226 (99%)	201 (90%)	22 (10%)	1 (0%)	30	59
55	HH	182/184 (99%)	157 (86%)	22 (12%)	3 (2%)	7	27
56	II	183/199 (92%)	153 (84%)	25 (14%)	5 (3%)	4	16
57	JJ	180/182 (99%)	156 (87%)	17 (9%)	7 (4%)	2	10
58	KK	94/96 (98%)	81 (86%)	10 (11%)	3 (3%)	3	13
59	LL	143/145 (99%)	127 (89%)	15 (10%)	1 (1%)	18	48
60	MM	122/124 (98%)	85 (70%)	34 (28%)	3 (2%)	4	17
61	NN	148/150 (99%)	137 (93%)	7 (5%)	4 (3%)	4	16
62	OO	125/127 (98%)	106 (85%)	16 (13%)	3 (2%)	4	18
63	PP	101/103 (98%)	88 (87%)	12 (12%)	1 (1%)	12	39
64	QQ	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	30
65	RR	119/123 (97%)	99 (83%)	19 (16%)	1 (1%)	16	44
66	SS	134/136 (98%)	116 (87%)	17 (13%)	1 (1%)	18	48
67	TT	141/143 (99%)	128 (91%)	10 (7%)	3 (2%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	UU	104/106 (98%)	94 (90%)	10 (10%)	0	100	100
69	VV	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
70	WW	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	4	18
71	XX	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	5	21
72	YY	132/134 (98%)	119 (90%)	12 (9%)	1 (1%)	16	44
73	ZZ	68/70 (97%)	59 (87%)	8 (12%)	1 (2%)	8	28
74	aa	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	1	5
75	bb	79/81 (98%)	63 (80%)	15 (19%)	1 (1%)	9	32
76	cc	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
77	dd	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
78	ee	51/53 (96%)	44 (86%)	7 (14%)	0	100	100
79	ff	40/57 (70%)	20 (50%)	19 (48%)	1 (2%)	4	17
80	gg	312/318 (98%)	265 (85%)	43 (14%)	4 (1%)	9	32
82	1	598/600 (100%)	476 (80%)	94 (16%)	28 (5%)	2	7
All	All	11802/12025 (98%)	10238 (87%)	1339 (11%)	225 (2%)	8	23

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	181	LYS
4	A	196	TRP
6	C	54	GLU
6	C	148	ILE
6	C	316	ASN
7	D	259	LYS
9	F	158	LYS
11	H	23	ARG
14	L	4	SER
14	L	76	THR
15	M	5	SER
15	M	6	ILE
17	O	110	PRO
17	O	111	PRO
21	S	13	ARG
22	T	18	ASP
30	b	21	ILE
33	e	121	ASN

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Mol	Chain	Res	Type
34	f	103	TYR
37	i	13	LYS
48	AA	158	VAL
51	DD	217	ILE
53	FF	52	GLU
54	GG	151	ASP
56	II	11	ARG
60	MM	113	VAL
62	OO	51	ASP
66	SS	26	ILE
70	WW	96	ALA
73	ZZ	71	ILE
74	aa	86	VAL
82	1	463	GLU
82	1	465	GLN
82	1	684	LEU
82	1	695	HIS
82	1	696	HIS
82	1	923	ASN
4	A	144	ASN
5	B	5	LYS
5	B	22	ALA
6	C	73	ARG
6	C	130	ALA
6	C	140	HIS
9	F	159	GLN
10	G	38	ALA
12	I	111	LEU
12	I	114	GLY
12	I	144	ASN
13	J	94	ARG
21	S	24	LEU
24	V	84	SER
28	Z	124	ALA
29	a	124	ILE
30	b	26	THR
35	g	57	LEU
40	l	33	ASN
43	o	6	LYS
43	o	14	GLY
44	p	39	CYS
44	p	48	LYS

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Mol	Chain	Res	Type
45	q	27	ASN
45	q	40	ASN
45	q	125	GLY
46	r	35	VAL
48	AA	94	GLY
50	CC	57	THR
51	DD	53	THR
52	EE	20	LEU
52	EE	187	ARG
55	HH	145	GLY
56	II	52	ASN
57	JJ	100	LYS
57	JJ	171	ARG
58	KK	83	PRO
62	OO	52	ARG
62	OO	103	ARG
67	TT	53	TRP
67	TT	54	PHE
67	TT	55	TYR
70	WW	56	HIS
71	XX	97	ASP
74	aa	12	LYS
80	gg	77	ASP
82	1	461	GLU
82	1	626	TYR
82	1	640	VAL
82	1	729	ASP
4	A	123	ARG
4	A	180	LEU
4	A	182	ALA
6	C	147	GLU
6	C	149	PRO
6	C	185	LYS
6	C	269	SER
6	C	293	SER
6	C	351	PRO
18	P	4	TYR
19	Q	175	ALA
20	R	129	GLY
29	a	96	LYS
29	a	97	GLU
33	e	123	LYS

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Mol	Chain	Res	Type
34	f	104	PRO
35	g	75	ALA
46	r	94	PRO
48	AA	27	ARG
48	AA	204	TYR
49	BB	176	VAL
50	CC	56	THR
51	DD	97	SER
53	FF	47	LYS
53	FF	102	ASN
56	II	120	THR
57	JJ	121	SER
58	KK	26	ASP
59	LL	55	ASP
60	MM	105	ALA
63	PP	29	SER
72	YY	49	LYS
74	aa	7	SER
79	ff	144	CYS
80	gg	54	LYS
82	1	432	GLY
82	1	466	THR
82	1	496	ILE
82	1	689	LEU
82	1	803	PRO
82	1	945	ASP
5	B	272	TYR
6	C	14	GLU
6	C	292	SER
7	D	260	PHE
8	E	5	LYS
9	F	24	GLU
12	I	112	GLN
18	P	158	ALA
22	T	69	LYS
24	V	53	SER
36	h	84	LYS
43	o	15	LYS
43	o	66	LYS
46	r	118	PRO
48	AA	167	LYS
50	CC	111	ASP

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Mol	Chain	Res	Type
50	CC	175	ILE
51	DD	92	GLN
51	DD	220	PRO
52	EE	205	PHE
53	FF	130	ASN
53	FF	206	GLY
55	HH	64	VAL
56	II	22	ARG
56	II	24	LYS
57	JJ	162	SER
57	JJ	164	PHE
58	KK	89	ALA
60	MM	124	ASP
61	NN	143	SER
70	WW	57	ARG
71	XX	90	ASP
74	aa	61	GLU
80	gg	21	VAL
82	1	460	ALA
82	1	484	SER
82	1	682	GLN
82	1	905	THR
4	A	197	PRO
6	C	174	ALA
6	C	232	SER
7	D	214	ASP
8	E	6	ALA
12	I	19	LYS
14	L	62	THR
14	L	75	PHE
21	S	18	SER
26	X	56	ARG
28	Z	87	LEU
43	o	52	GLY
43	o	65	THR
45	q	2	SER
46	r	58	ASN
50	CC	151	THR
51	DD	94	ARG
53	FF	59	SER
57	JJ	101	VAL
57	JJ	120	LYS

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Mol	Chain	Res	Type
61	NN	3	ARG
61	NN	28	LEU
61	NN	30	SER
74	aa	80	HIS
75	bb	50	ALA
80	gg	269	GLN
82	1	683	PRO
82	1	731	ASP
82	1	937	ALA
82	1	946	PRO
9	F	216	VAL
10	G	42	LYS
11	H	13	PRO
29	a	33	GLY
43	o	7	THR
44	p	51	ALA
46	r	114	GLY
48	AA	193	GLN
48	AA	199	PRO
49	BB	207	LEU
52	EE	32	SER
52	EE	68	ARG
55	HH	32	PRO
64	QQ	136	SER
65	RR	26	LEU
71	XX	41	SER
82	1	490	GLY
16	N	35	VAL
35	g	77	GLY
37	i	49	GLY
46	r	107	VAL
45	q	205	VAL
50	CC	201	VAL
82	1	414	VAL
82	1	470	PRO
11	H	4	ILE
43	o	5	PRO
64	QQ	27	GLY
82	1	681	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	
4	A	191/191 (100%)	175 (92%)	16 (8%)	10	31
5	B	320/320 (100%)	297 (93%)	23 (7%)	13	39
6	C	286/286 (100%)	268 (94%)	18 (6%)	16	45
7	D	244/244 (100%)	226 (93%)	18 (7%)	13	38
8	E	134/152 (88%)	123 (92%)	11 (8%)	10	32
9	F	186/186 (100%)	183 (98%)	3 (2%)	55	83
10	G	189/191 (99%)	179 (95%)	10 (5%)	20	52
11	H	172/172 (100%)	161 (94%)	11 (6%)	16	44
12	I	184/185 (100%)	173 (94%)	11 (6%)	17	47
13	J	146/146 (100%)	139 (95%)	7 (5%)	23	55
14	L	158/158 (100%)	151 (96%)	7 (4%)	25	59
15	M	108/108 (100%)	101 (94%)	7 (6%)	15	44
16	N	174/174 (100%)	168 (97%)	6 (3%)	32	66
17	O	160/160 (100%)	154 (96%)	6 (4%)	29	64
18	P	145/145 (100%)	136 (94%)	9 (6%)	16	46
19	Q	150/150 (100%)	146 (97%)	4 (3%)	39	73
20	R	153/153 (100%)	144 (94%)	9 (6%)	18	48
21	S	154/154 (100%)	144 (94%)	10 (6%)	15	44
22	T	135/135 (100%)	126 (93%)	9 (7%)	15	43
23	U	87/87 (100%)	82 (94%)	5 (6%)	18	49
24	V	101/101 (100%)	94 (93%)	7 (7%)	14	41
25	W	54/54 (100%)	51 (94%)	3 (6%)	19	50
26	X	105/105 (100%)	99 (94%)	6 (6%)	18	49
27	Y	109/109 (100%)	105 (96%)	4 (4%)	30	64
28	Z	115/115 (100%)	104 (90%)	11 (10%)	8	26
29	a	118/118 (100%)	112 (95%)	6 (5%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	b	46/46 (100%)	45 (98%)	1 (2%)	45	77
31	c	81/81 (100%)	75 (93%)	6 (7%)	13	38
32	d	93/93 (100%)	89 (96%)	4 (4%)	26	60
33	e	106/106 (100%)	101 (95%)	5 (5%)	23	56
34	f	89/89 (100%)	84 (94%)	5 (6%)	19	50
35	g	103/103 (100%)	91 (88%)	12 (12%)	5	17
36	h	103/103 (100%)	102 (99%)	1 (1%)	68	89
37	i	80/80 (100%)	75 (94%)	5 (6%)	16	45
38	j	69/69 (100%)	68 (99%)	1 (1%)	59	85
39	k	68/68 (100%)	61 (90%)	7 (10%)	7	23
40	l	44/44 (100%)	43 (98%)	1 (2%)	44	76
41	m	46/46 (100%)	46 (100%)	0	100	100
42	n	21/21 (100%)	20 (95%)	1 (5%)	23	55
43	o	87/87 (100%)	81 (93%)	6 (7%)	14	41
44	p	69/69 (100%)	65 (94%)	4 (6%)	18	49
45	q	198/198 (100%)	173 (87%)	25 (13%)	4	14
46	r	165/165 (100%)	146 (88%)	19 (12%)	5	18
48	AA	173/173 (100%)	164 (95%)	9 (5%)	21	52
49	BB	192/192 (100%)	178 (93%)	14 (7%)	13	38
50	CC	176/176 (100%)	161 (92%)	15 (8%)	10	31
51	DD	182/182 (100%)	169 (93%)	13 (7%)	13	40
52	EE	219/219 (100%)	212 (97%)	7 (3%)	34	68
53	FF	173/173 (100%)	161 (93%)	12 (7%)	14	41
54	GG	193/193 (100%)	185 (96%)	8 (4%)	27	61
55	HH	165/165 (100%)	158 (96%)	7 (4%)	26	60
56	II	149/160 (93%)	138 (93%)	11 (7%)	13	38
57	JJ	156/156 (100%)	147 (94%)	9 (6%)	18	49
58	KK	89/89 (100%)	77 (86%)	12 (14%)	4	12
59	LL	130/130 (100%)	127 (98%)	3 (2%)	44	76
60	MM	100/100 (100%)	93 (93%)	7 (7%)	14	40
61	NN	127/127 (100%)	122 (96%)	5 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	OO	96/96 (100%)	84 (88%)	12 (12%)	4	15
63	PP	86/86 (100%)	80 (93%)	6 (7%)	14	40
64	QQ	117/117 (100%)	110 (94%)	7 (6%)	17	47
65	RR	112/112 (100%)	101 (90%)	11 (10%)	7	25
66	SS	120/120 (100%)	112 (93%)	8 (7%)	15	43
67	TT	115/115 (100%)	103 (90%)	12 (10%)	7	23
68	UU	99/99 (100%)	92 (93%)	7 (7%)	13	40
69	VV	74/74 (100%)	67 (90%)	7 (10%)	8	26
70	WW	110/110 (100%)	105 (96%)	5 (4%)	24	58
71	XX	119/119 (100%)	112 (94%)	7 (6%)	18	48
72	YY	112/112 (100%)	111 (99%)	1 (1%)	70	90
73	ZZ	61/61 (100%)	60 (98%)	1 (2%)	55	83
74	aa	83/83 (100%)	72 (87%)	11 (13%)	4	12
75	bb	70/70 (100%)	62 (89%)	8 (11%)	5	18
76	cc	56/56 (100%)	52 (93%)	4 (7%)	13	40
77	dd	47/47 (100%)	43 (92%)	4 (8%)	10	31
78	ee	46/46 (100%)	45 (98%)	1 (2%)	45	77
79	ff	38/49 (78%)	36 (95%)	2 (5%)	20	52
80	gg	261/261 (100%)	238 (91%)	23 (9%)	9	29
82	1	524/524 (100%)	477 (91%)	47 (9%)	9	28
All	All	10116/10159 (100%)	9460 (94%)	656 (6%)	17	44

All (656) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	7	ASN
4	A	18	SER
4	A	46	LYS
4	A	49	VAL
4	A	61	VAL
4	A	72	ARG
4	A	73	GLU
4	A	84	THR
4	A	86	GLN
4	A	102	LEU

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Mol	Chain	Res	Type
4	A	113	VAL
4	A	134	VAL
4	A	148	VAL
4	A	195	SER
4	A	207	VAL
4	A	218	HIS
5	B	10	ARG
5	B	54	THR
5	B	56	ILE
5	B	76	VAL
5	B	79	VAL
5	B	80	ASP
5	B	87	VAL
5	B	160	VAL
5	B	188	ILE
5	B	194	TRP
5	B	201	LYS
5	B	203	VAL
5	B	205	VAL
5	B	206	ASP
5	B	215	ILE
5	B	226	PHE
5	B	255	TRP
5	B	305	ILE
5	B	322	ILE
5	B	323	MET
5	B	336	VAL
5	B	338	LEU
5	B	364	LYS
6	C	37	THR
6	C	69	ARG
6	C	95	ARG
6	C	98	ARG
6	C	107	ARG
6	C	136	LEU
6	C	148	ILE
6	C	150	LEU
6	C	152	VAL
6	C	154	THR
6	C	169	LEU
6	C	227	THR
6	C	249	ILE

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Mol	Chain	Res	Type
6	C	267	VAL
6	C	281	ILE
6	C	283	THR
6	C	310	THR
6	C	332	LYS
7	D	8	LYS
7	D	15	ARG
7	D	36	LEU
7	D	51	LEU
7	D	53	VAL
7	D	112	LYS
7	D	151	GLN
7	D	155	THR
7	D	159	VAL
7	D	173	VAL
7	D	209	GLU
7	D	211	LEU
7	D	213	ASP
7	D	256	THR
7	D	257	GLU
7	D	258	LYS
7	D	278	SER
7	D	281	GLU
8	E	23	LYS
8	E	52	VAL
8	E	65	ILE
8	E	71	VAL
8	E	79	VAL
8	E	85	ILE
8	E	96	VAL
8	E	102	ASN
8	E	109	GLU
8	E	130	ILE
8	E	175	LYS
9	F	30	ARG
9	F	39	GLU
9	F	161	VAL
10	G	26	THR
10	G	27	HIS
10	G	35	ILE
10	G	64	LEU
10	G	73	THR

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Mol	Chain	Res	Type
10	G	162	VAL
10	G	184	ARG
10	G	193	THR
10	G	194	SER
10	G	214	VAL
11	H	4	ILE
11	H	17	THR
11	H	42	ASP
11	H	46	THR
11	H	61	ASP
11	H	79	ILE
11	H	113	GLU
11	H	123	ILE
11	H	138	THR
11	H	140	VAL
11	H	150	SER
12	I	48	LEU
12	I	55	ASN
12	I	73	ASN
12	I	90	ARG
12	I	91	VAL
12	I	112	GLN
12	I	129	VAL
12	I	153	ARG
12	I	180	GLU
12	I	182	LEU
12	I	197	VAL
13	J	7	ASN
13	J	18	VAL
13	J	21	ILE
13	J	107	ASP
13	J	108	GLU
13	J	142	LYS
13	J	172	LEU
14	L	58	VAL
14	L	59	ARG
14	L	69	VAL
14	L	92	THR
14	L	124	ILE
14	L	136	GLU
14	L	152	THR
15	M	8	LYS

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Mol	Chain	Res	Type
15	M	28	SER
15	M	38	ILE
15	M	47	ASP
15	M	63	VAL
15	M	66	THR
15	M	68	LEU
16	N	9	GLU
16	N	60	VAL
16	N	64	VAL
16	N	65	ARG
16	N	117	ASN
16	N	132	VAL
17	O	34	VAL
17	O	58	LEU
17	O	104	VAL
17	O	126	VAL
17	O	136	THR
17	O	162	VAL
18	P	24	VAL
18	P	79	THR
18	P	94	LEU
18	P	112	LEU
18	P	127	ARG
18	P	150	VAL
18	P	157	VAL
18	P	159	LYS
18	P	182	ILE
19	Q	3	ILE
19	Q	57	ILE
19	Q	81	VAL
19	Q	101	VAL
20	R	10	LEU
20	R	49	THR
20	R	93	VAL
20	R	103	ARG
20	R	123	LEU
20	R	134	HIS
20	R	157	GLU
20	R	166	ASN
20	R	176	ARG
21	S	9	VAL
21	S	13	ARG

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Mol	Chain	Res	Type
21	S	45	LEU
21	S	57	GLU
21	S	96	ASP
21	S	103	VAL
21	S	109	ASP
21	S	132	THR
21	S	158	LYS
21	S	172	TYR
22	T	4	SER
22	T	60	LYS
22	T	68	THR
22	T	83	ARG
22	T	88	ARG
22	T	93	VAL
22	T	124	VAL
22	T	147	VAL
22	T	157	GLU
23	U	21	SER
23	U	38	ILE
23	U	57	THR
23	U	64	THR
23	U	91	ASP
24	V	33	ASN
24	V	46	LEU
24	V	54	LEU
24	V	83	LYS
24	V	98	ASN
24	V	125	LEU
24	V	135	VAL
25	W	19	THR
25	W	39	LEU
25	W	63	ILE
26	X	57	LEU
26	X	77	GLU
26	X	81	ILE
26	X	87	SER
26	X	108	LEU
26	X	110	VAL
27	Y	6	LEU
27	Y	71	SER
27	Y	109	LEU
27	Y	112	ASP

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Mol	Chain	Res	Type
28	Z	3	LYS
28	Z	10	VAL
28	Z	12	VAL
28	Z	43	VAL
28	Z	54	THR
28	Z	74	VAL
28	Z	83	THR
28	Z	89	VAL
28	Z	100	THR
28	Z	102	GLU
28	Z	134	LEU
29	a	4	ARG
29	a	56	VAL
29	a	91	LEU
29	a	97	GLU
29	a	98	THR
29	a	121	VAL
30	b	32	LEU
31	c	16	LEU
31	c	19	LYS
31	c	24	THR
31	c	44	ILE
31	c	61	MET
31	c	100	ILE
32	d	35	GLU
32	d	87	ASN
32	d	96	VAL
32	d	97	LEU
33	e	33	ARG
33	e	41	VAL
33	e	90	LYS
33	e	123	LYS
33	e	126	LEU
34	f	59	VAL
34	f	66	VAL
34	f	77	ASN
34	f	100	ILE
34	f	106	ASN
35	g	5	VAL
35	g	6	THR
35	g	20	ILE
35	g	24	LYS

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Mol	Chain	Res	Type
35	g	40	THR
35	g	62	TYR
35	g	66	SER
35	g	71	THR
35	g	79	SER
35	g	80	ARG
35	g	94	LEU
35	g	118	LYS
36	h	118	ILE
37	i	17	VAL
37	i	37	THR
37	i	47	ILE
37	i	74	LYS
37	i	76	ARG
38	j	58	THR
39	k	7	ASP
39	k	10	GLN
39	k	27	ILE
39	k	45	VAL
39	k	65	LEU
39	k	67	GLN
39	k	75	VAL
40	l	23	LEU
42	n	10	THR
43	o	35	LEU
43	o	59	HIS
43	o	61	LYS
43	o	68	VAL
43	o	80	ARG
43	o	98	LYS
44	p	59	CYS
44	p	63	THR
44	p	82	THR
44	p	86	LEU
45	q	12	HIS
45	q	16	LEU
45	q	23	THR
45	q	32	VAL
45	q	36	VAL
45	q	55	LEU
45	q	70	ASP
45	q	75	ASP

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Mol	Chain	Res	Type
45	q	90	LEU
45	q	95	LYS
45	q	103	LEU
45	q	128	LEU
45	q	133	LYS
45	q	134	PHE
45	q	136	THR
45	q	140	HIS
45	q	142	ASP
45	q	150	ASP
45	q	173	GLU
45	q	189	PHE
45	q	190	PHE
45	q	196	LYS
45	q	197	ASN
45	q	205	VAL
45	q	216	LEU
46	r	35	VAL
46	r	37	SER
46	r	39	GLN
46	r	53	VAL
46	r	59	THR
46	r	85	ASN
46	r	88	PHE
46	r	92	ASN
46	r	93	GLU
46	r	96	THR
46	r	101	VAL
46	r	121	ILE
46	r	126	VAL
46	r	137	PHE
46	r	154	ILE
46	r	158	VAL
46	r	166	LYS
46	r	171	GLU
46	r	199	PHE
48	AA	45	VAL
48	AA	47	VAL
48	AA	57	LEU
48	AA	123	VAL
48	AA	129	ASP
48	AA	139	VAL

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Mol	Chain	Res	Type
48	AA	143	VAL
48	AA	158	VAL
48	AA	193	GLN
49	BB	52	THR
49	BB	66	VAL
49	BB	78	ASP
49	BB	92	GLN
49	BB	97	LEU
49	BB	99	ASN
49	BB	105	PHE
49	BB	176	VAL
49	BB	193	ILE
49	BB	198	GLU
49	BB	199	ASN
49	BB	205	PHE
49	BB	212	VAL
49	BB	213	ARG
50	CC	57	THR
50	CC	58	ILE
50	CC	63	LEU
50	CC	83	ASP
50	CC	116	VAL
50	CC	121	LYS
50	CC	153	LEU
50	CC	163	THR
50	CC	164	THR
50	CC	175	ILE
50	CC	184	VAL
50	CC	189	VAL
50	CC	201	VAL
50	CC	223	ILE
50	CC	235	TRP
51	DD	42	THR
51	DD	69	LEU
51	DD	76	ARG
51	DD	84	ILE
51	DD	86	LEU
51	DD	135	GLU
51	DD	137	VAL
51	DD	142	LEU
51	DD	146	ARG
51	DD	176	LEU

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Mol	Chain	Res	Type
51	DD	181	VAL
51	DD	197	THR
51	DD	222	VAL
52	EE	57	ASN
52	EE	89	VAL
52	EE	95	THR
52	EE	143	ASP
52	EE	184	THR
52	EE	194	THR
52	EE	225	VAL
53	FF	40	THR
53	FF	42	ILE
53	FF	43	LYS
53	FF	51	GLU
53	FF	64	VAL
53	FF	66	VAL
53	FF	126	LEU
53	FF	128	ASP
53	FF	149	THR
53	FF	151	VAL
53	FF	172	GLN
53	FF	227	ARG
54	GG	24	ILE
54	GG	41	VAL
54	GG	78	THR
54	GG	92	ARG
54	GG	93	LYS
54	GG	128	THR
54	GG	133	LEU
54	GG	178	LEU
55	HH	8	ILE
55	HH	14	THR
55	HH	20	VAL
55	HH	27	LEU
55	HH	28	GLU
55	HH	35	LYS
55	HH	93	LEU
56	II	7	SER
56	II	20	GLN
56	II	25	ARG
56	II	29	LEU
56	II	62	THR

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Mol	Chain	Res	Type
56	II	72	ILE
56	II	78	ILE
56	II	87	ASN
56	II	92	ARG
56	II	93	THR
56	II	157	VAL
57	JJ	3	ARG
57	JJ	14	THR
57	JJ	28	LEU
57	JJ	40	ARG
57	JJ	60	LEU
57	JJ	101	VAL
57	JJ	150	LEU
57	JJ	162	SER
57	JJ	172	VAL
58	KK	2	LEU
58	KK	15	LEU
58	KK	16	PHE
58	KK	20	VAL
58	KK	37	THR
58	KK	39	ASN
58	KK	49	LEU
58	KK	54	TYR
58	KK	77	ARG
58	KK	78	GLU
58	KK	80	LEU
58	KK	86	ILE
59	LL	66	ILE
59	LL	76	VAL
59	LL	124	THR
60	MM	23	VAL
60	MM	38	LEU
60	MM	51	LEU
60	MM	55	LEU
60	MM	128	MET
60	MM	129	ILE
60	MM	132	HIS
61	NN	5	HIS
61	NN	11	ILE
61	NN	84	ILE
61	NN	101	HIS
61	NN	102	LEU

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Mol	Chain	Res	Type
62	OO	28	VAL
62	OO	49	LYS
62	OO	66	ASP
62	OO	84	ARG
62	OO	91	THR
62	OO	110	LEU
62	OO	115	ILE
62	OO	116	GLU
62	OO	118	VAL
62	OO	124	ASP
62	OO	125	SER
62	OO	132	ARG
63	PP	36	LEU
63	PP	41	VAL
63	PP	83	MET
63	PP	84	ILE
63	PP	106	GLU
63	PP	127	ARG
64	QQ	7	VAL
64	QQ	22	VAL
64	QQ	36	ILE
64	QQ	37	THR
64	QQ	43	ILE
64	QQ	53	LEU
64	QQ	118	ILE
65	RR	16	LEU
65	RR	26	LEU
65	RR	40	THR
65	RR	43	SER
65	RR	46	LEU
65	RR	69	ILE
65	RR	91	LEU
65	RR	99	VAL
65	RR	113	LEU
65	RR	119	LEU
65	RR	122	ILE
66	SS	17	LEU
66	SS	18	LEU
66	SS	28	ILE
66	SS	38	VAL
66	SS	75	ASN
66	SS	85	PHE

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Mol	Chain	Res	Type
66	SS	98	TYR
66	SS	106	GLU
67	TT	4	VAL
67	TT	30	VAL
67	TT	36	ILE
67	TT	40	SER
67	TT	41	SER
67	TT	53	TRP
67	TT	65	ILE
67	TT	104	VAL
67	TT	111	ILE
67	TT	114	VAL
67	TT	141	GLU
67	TT	143	ASP
68	UU	20	ILE
68	UU	24	ILE
68	UU	51	VAL
68	UU	52	LYS
68	UU	70	THR
68	UU	80	GLU
68	UU	94	GLU
69	VV	13	VAL
69	VV	34	ILE
69	VV	40	ASP
69	VV	52	THR
69	VV	62	ARG
69	VV	74	GLN
69	VV	76	ASP
70	WW	2	THR
70	WW	83	ILE
70	WW	104	LEU
70	WW	115	GLU
70	WW	129	VAL
71	XX	7	ARG
71	XX	19	ARG
71	XX	31	LYS
71	XX	33	LEU
71	XX	52	ILE
71	XX	84	THR
71	XX	107	PHE
72	YY	100	VAL
73	ZZ	42	LEU

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Mol	Chain	Res	Type
74	aa	21	VAL
74	aa	25	ASN
74	aa	37	LYS
74	aa	39	MET
74	aa	50	VAL
74	aa	52	ASP
74	aa	58	VAL
74	aa	76	SER
74	aa	82	ARG
74	aa	86	VAL
74	aa	87	ARG
75	bb	2	VAL
75	bb	3	LEU
75	bb	4	VAL
75	bb	11	THR
75	bb	15	GLU
75	bb	23	THR
75	bb	62	ILE
75	bb	75	GLU
76	cc	18	ARG
76	cc	44	VAL
76	cc	48	VAL
76	cc	58	GLU
77	dd	23	VAL
77	dd	24	CYS
77	dd	40	ARG
77	dd	53	ASN
78	ee	31	LYS
79	ff	136	LYS
79	ff	148	TYR
80	gg	8	LEU
80	gg	21	VAL
80	gg	49	THR
80	gg	66	SER
80	gg	67	HIS
80	gg	77	ASP
80	gg	102	GLN
80	gg	105	VAL
80	gg	136	THR
80	gg	157	VAL
80	gg	169	THR
80	gg	190	GLU

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Mol	Chain	Res	Type
80	gg	192	ASP
80	gg	194	ILE
80	gg	198	SER
80	gg	224	TRP
80	gg	226	LEU
80	gg	230	LYS
80	gg	235	LEU
80	gg	244	LEU
80	gg	267	ASP
80	gg	284	LYS
80	gg	313	VAL
82	1	411	LEU
82	1	415	ASP
82	1	419	THR
82	1	438	ILE
82	1	458	VAL
82	1	464	LYS
82	1	465	GLN
82	1	466	THR
82	1	468	ASP
82	1	469	VAL
82	1	492	SER
82	1	503	ILE
82	1	507	LEU
82	1	527	VAL
82	1	532	ILE
82	1	536	TYR
82	1	544	ASN
82	1	581	LEU
82	1	582	TYR
82	1	597	THR
82	1	621	SER
82	1	622	LYS
82	1	625	MET
82	1	630	VAL
82	1	655	TYR
82	1	672	VAL
82	1	705	VAL
82	1	716	VAL
82	1	732	GLU
82	1	737	VAL
82	1	741	LEU

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Mol	Chain	Res	Type
82	1	746	ASP
82	1	764	SER
82	1	765	LEU
82	1	775	MET
82	1	804	GLU
82	1	815	VAL
82	1	866	CYS
82	1	877	ARG
82	1	886	VAL
82	1	890	THR
82	1	891	LEU
82	1	906	THR
82	1	913	ILE
82	1	928	GLN
82	1	991	LEU
82	1	992	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	86	GLN
4	A	97	ASN
4	A	132	ASN
4	A	233	GLN
5	B	165	GLN
6	C	59	GLN
6	C	92	ASN
6	C	213	ASN
7	D	4	GLN
7	D	17	GLN
7	D	32	GLN
7	D	39	GLN
7	D	40	HIS
7	D	90	HIS
8	E	97	ASN
8	E	167	ASN
9	F	93	ASN
9	F	194	HIS
9	F	225	GLN
10	G	154	ASN
10	G	239	ASN

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Mol	Chain	Res	Type
10	G	251	ASN
11	H	100	ASN
11	H	156	GLN
12	I	12	GLN
12	I	14	ASN
12	I	112	GLN
12	I	133	GLN
13	J	39	GLN
13	J	132	ASN
13	J	150	ASN
14	L	25	HIS
14	L	28	GLN
14	L	120	GLN
14	L	137	GLN
15	M	41	GLN
15	M	62	GLN
16	N	34	ASN
16	N	123	GLN
16	N	149	ASN
16	N	156	HIS
17	O	26	GLN
17	O	50	ASN
18	P	55	GLN
18	P	118	GLN
18	P	120	ASN
20	R	3	ASN
20	R	7	GLN
20	R	166	ASN
21	S	8	GLN
21	S	63	GLN
21	S	138	GLN
21	S	142	GLN
22	T	5	HIS
22	T	103	GLN
22	T	122	GLN
22	T	131	GLN
22	T	146	ASN
23	U	25	ASN
23	U	49	ASN
23	U	88	GLN
24	V	33	ASN
25	W	59	HIS

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Mol	Chain	Res	Type
26	X	91	ASN
26	X	137	ASN
27	Y	42	GLN
28	Z	76	ASN
28	Z	106	GLN
29	a	25	HIS
29	a	44	ASN
29	a	49	HIS
29	a	74	ASN
30	b	6	ASN
30	b	10	HIS
30	b	12	GLN
32	d	57	GLN
32	d	87	ASN
33	e	20	HIS
33	e	31	ASN
34	f	26	ASN
35	g	34	HIS
35	g	52	GLN
35	g	61	GLN
35	g	98	GLN
35	g	108	GLN
36	h	62	GLN
36	h	68	GLN
36	h	113	GLN
38	j	30	GLN
38	j	48	ASN
38	j	69	HIS
38	j	79	GLN
39	k	28	ASN
40	l	19	GLN
40	l	43	ASN
45	q	35	GLN
45	q	57	ASN
45	q	94	ASN
45	q	96	ASN
45	q	171	ASN
45	q	182	GLN
46	r	38	GLN
46	r	58	ASN
46	r	100	ASN
48	AA	15	GLN

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Mol	Chain	Res	Type
48	AA	46	HIS
48	AA	83	GLN
48	AA	131	GLN
48	AA	140	ASN
49	BB	92	GLN
49	BB	99	ASN
49	BB	199	ASN
50	CC	113	ASN
50	CC	152	ASN
51	DD	22	ASN
51	DD	67	ASN
51	DD	92	GLN
51	DD	162	GLN
51	DD	165	ASN
52	EE	50	ASN
52	EE	96	ASN
52	EE	98	ASN
52	EE	209	HIS
52	EE	216	ASN
52	EE	258	GLN
53	FF	65	GLN
53	FF	68	GLN
53	FF	88	GLN
53	FF	105	ASN
53	FF	141	ASN
54	GG	34	GLN
54	GG	59	GLN
54	GG	185	GLN
54	GG	189	HIS
55	HH	5	GLN
55	HH	110	GLN
56	II	32	GLN
56	II	84	HIS
56	II	119	GLN
58	KK	12	HIS
58	KK	62	GLN
58	KK	93	GLN
58	KK	96	ASN
59	LL	8	GLN
59	LL	127	GLN
60	MM	118	ASN
60	MM	132	HIS

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Mol	Chain	Res	Type
61	NN	5	HIS
61	NN	62	GLN
62	OO	29	HIS
64	QQ	8	GLN
64	QQ	83	GLN
64	QQ	94	GLN
64	QQ	100	GLN
64	QQ	103	ASN
64	QQ	139	GLN
65	RR	97	ASN
66	SS	25	ASN
66	SS	89	GLN
66	SS	136	GLN
68	UU	49	ASN
69	VV	3	ASN
70	WW	12	ASN
70	WW	15	ASN
70	WW	16	ASN
70	WW	42	GLN
70	WW	70	ASN
72	YY	34	ASN
72	YY	110	GLN
73	ZZ	95	HIS
75	bb	51	GLN
76	cc	27	GLN
78	ee	46	ASN
80	gg	102	GLN
80	gg	149	ASN
82	1	427	GLN
82	1	440	GLN
82	1	465	GLN
82	1	530	ASN
82	1	543	ASN
82	1	544	ASN
82	1	575	GLN
82	1	587	ASN
82	1	617	GLN
82	1	653	ASN
82	1	696	HIS
82	1	821	GLN
82	1	838	HIS
82	1	928	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3250/3271 (99%)	798 (24%)	76 (2%)
2	7	120/121 (99%)	21 (17%)	0
3	8	156/157 (99%)	34 (21%)	2 (1%)
81	2	1770/1796 (98%)	559 (31%)	32 (1%)
83	3	75/76 (98%)	17 (22%)	0
84	4	5/6 (83%)	0	0
All	All	5376/5427 (99%)	1429 (26%)	110 (2%)

All (1429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	3	U
1	5	6	A
1	5	14	U
1	5	15	C
1	5	17	G
1	5	26	A
1	5	30	G
1	5	40	A
1	5	43	A
1	5	44	U
1	5	48	A
1	5	49	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	73	C
1	5	89	A
1	5	92	G
1	5	96	G
1	5	109	A
1	5	110	G
1	5	111	C
1	5	116	A
1	5	117	U
1	5	121	A
1	5	122	A
1	5	134	U
1	5	135	C
1	5	136	G

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Mol	Chain	Res	Type
1	5	142	C
1	5	155	G
1	5	156	G
1	5	157	A
1	5	167	U
1	5	171	G
1	5	172	G
1	5	173	G
1	5	174	C
1	5	175	C
1	5	182	U
1	5	187	A
1	5	189	G
1	5	190	U
1	5	191	U
1	5	199	A
1	5	200	C
1	5	210	U
1	5	218	G
1	5	219	A
1	5	220	G
1	5	221	A
1	5	237	G
1	5	239	G
1	5	240	U
1	5	241	G
1	5	248	U
1	5	249	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	254	A
1	5	263	C
1	5	269	G
1	5	285	A
1	5	286	U
1	5	295	A
1	5	298	U
1	5	299	G
1	5	305	U
1	5	306	A
1	5	307	A

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Mol	Chain	Res	Type
1	5	315	C
1	5	323	A
1	5	329	U
1	5	334	A
1	5	336	A
1	5	339	C
1	5	349	A
1	5	350	C
1	5	370	U
1	5	374	A
1	5	376	G
1	5	395	A
1	5	396	A
1	5	398	A
1	5	399	A
1	5	402	A
1	5	403	C
1	5	404	G
1	5	420	G
1	5	421	G
1	5	422	A
1	5	436	A
1	5	438	A
1	5	439	C
1	5	508	U
1	5	518	G
1	5	519	A
1	5	521	A
1	5	523	A
1	5	534	U
1	5	535	G
1	5	543	C
1	5	545	U
1	5	546	C
1	5	554	A
1	5	557	A
1	5	559	A
1	5	560	G
1	5	568	G
1	5	569	A
1	5	571	U
1	5	572	A

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Mol	Chain	Res	Type
1	5	578	A
1	5	579	G
1	5	588	G
1	5	589	A
1	5	594	U
1	5	595	G
1	5	600	G
1	5	603	A
1	5	604	G
1	5	611	A
1	5	619	A
1	5	620	U
1	5	621	A
1	5	636	C
1	5	637	C
1	5	645	A
1	5	647	A
1	5	649	A
1	5	660	A
1	5	677	A
1	5	678	G
1	5	681	U
1	5	683	U
1	5	684	G
1	5	690	A
1	5	691	A
1	5	698	U
1	5	705	A
1	5	708	G
1	5	712	G
1	5	715	A
1	5	718	G
1	5	719	U
1	5	720	A
1	5	725	G
1	5	733	G
1	5	735	A
1	5	767	U
1	5	776	U
1	5	777	U
1	5	780	A
1	5	781	G

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Mol	Chain	Res	Type
1	5	785	G
1	5	786	A
1	5	806	A
1	5	817	A
1	5	830	A
1	5	837	A
1	5	842	G
1	5	848	A
1	5	849	C
1	5	851	C
1	5	861	C
1	5	864	G
1	5	871	U
1	5	874	U
1	5	879	U
1	5	880	G
1	5	895	A
1	5	896	A
1	5	897	U
1	5	907	G
1	5	908	G
1	5	914	A
1	5	916	G
1	5	917	A
1	5	923	C
1	5	924	G
1	5	925	A
1	5	926	A
1	5	937	G
1	5	944	C
1	5	953	G
1	5	959	C
1	5	960	U
1	5	962	A
1	5	971	G
1	5	974	G
1	5	979	U
1	5	981	U
1	5	982	C
1	5	984	G
1	5	993	G
1	5	994	G

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Mol	Chain	Res	Type
1	5	995	U
1	5	1002	A
1	5	1003	A
1	5	1010	G
1	5	1014	U
1	5	1015	U
1	5	1016	C
1	5	1017	C
1	5	1018	G
1	5	1021	G
1	5	1023	C
1	5	1024	G
1	5	1025	A
1	5	1026	A
1	5	1027	A
1	5	1028	U
1	5	1029	G
1	5	1030	A
1	5	1031	C
1	5	1034	U
1	5	1035	G
1	5	1037	C
1	5	1047	A
1	5	1049	C
1	5	1052	U
1	5	1057	A
1	5	1064	A
1	5	1065	A
1	5	1074	U
1	5	1082	U
1	5	1085	A
1	5	1087	G
1	5	1090	G
1	5	1093	A
1	5	1094	U
1	5	1095	U
1	5	1096	U
1	5	1098	A
1	5	1103	A
1	5	1104	G
1	5	1105	A
1	5	1117	G

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Mol	Chain	Res	Type
1	5	1131	G
1	5	1143	A
1	5	1144	U
1	5	1147	G
1	5	1151	U
1	5	1152	G
1	5	1153	A
1	5	1158	A
1	5	1159	A
1	5	1161	G
1	5	1179	A
1	5	1180	A
1	5	1181	U
1	5	1182	A
1	5	1193	A
1	5	1194	G
1	5	1196	C
1	5	1198	C
1	5	1201	C
1	5	1209	G
1	5	1220	U
1	5	1222	G
1	5	1223	A
1	5	1224	C
1	5	1225	A
1	5	1226	G
1	5	1227	C
1	5	1235	U
1	5	1236	G
1	5	1239	C
1	5	1241	U
1	5	1242	G
1	5	1243	G
1	5	1245	A
1	5	1246	G
1	5	1250	G
1	5	1252	A
1	5	1253	U
1	5	1258	U
1	5	1262	G
1	5	1263	A
1	5	1264	G

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Mol	Chain	Res	Type
1	5	1266	G
1	5	1272	C
1	5	1277	C
1	5	1278	A
1	5	1280	C
1	5	1281	G
1	5	1282	G
1	5	1285	G
1	5	1287	A
1	5	1290	A
1	5	1291	A
1	5	1294	A
1	5	1307	G
1	5	1308	A
1	5	1309	U
1	5	1313	G
1	5	1316	C
1	5	1325	U
1	5	1330	A
1	5	1348	U
1	5	1350	A
1	5	1351	U
1	5	1352	A
1	5	1353	U
1	5	1355	A
1	5	1356	U
1	5	1357	G
1	5	1386	A
1	5	1392	G
1	5	1399	A
1	5	1408	G
1	5	1418	A
1	5	1419	A
1	5	1421	G
1	5	1434	G
1	5	1437	C
1	5	1443	G
1	5	1446	A
1	5	1450	G
1	5	1453	A
1	5	1454	A
1	5	1475	A

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Mol	Chain	Res	Type
1	5	1481	A
1	5	1482	A
1	5	1483	G
1	5	1485	G
1	5	1495	U
1	5	1508	C
1	5	1523	U
1	5	1527	C
1	5	1533	U
1	5	1536	G
1	5	1538	G
1	5	1547	G
1	5	1549	U
1	5	1554	U
1	5	1555	U
1	5	1557	A
1	5	1560	G
1	5	1561	G
1	5	1562	C
1	5	1564	U
1	5	1565	G
1	5	1567	U
1	5	1568	U
1	5	1569	U
1	5	1570	U
1	5	1571	A
1	5	1573	G
1	5	1575	A
1	5	1578	C
1	5	1579	C
1	5	1580	A
1	5	1581	C
1	5	1582	C
1	5	1583	A
1	5	1589	A
1	5	1593	A
1	5	1604	G
1	5	1605	A
1	5	1607	U
1	5	1608	C
1	5	1612	A
1	5	1620	U

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Mol	Chain	Res	Type
1	5	1628	C
1	5	1629	U
1	5	1630	U
1	5	1632	A
1	5	1639	C
1	5	1642	A
1	5	1643	A
1	5	1645	U
1	5	1646	G
1	5	1657	C
1	5	1659	U
1	5	1662	G
1	5	1683	A
1	5	1688	U
1	5	1689	U
1	5	1694	U
1	5	1696	A
1	5	1705	U
1	5	1715	A
1	5	1716	U
1	5	1717	U
1	5	1724	U
1	5	1728	G
1	5	1729	A
1	5	1730	G
1	5	1750	A
1	5	1751	G
1	5	1759	C
1	5	1760	A
1	5	1762	C
1	5	1764	U
1	5	1765	U
1	5	1766	G
1	5	1775	G
1	5	1780	G
1	5	1788	C
1	5	1797	A
1	5	1808	G
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	1817	G

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Mol	Chain	Res	Type
1	5	1818	U
1	5	1820	U
1	5	1821	U
1	5	1823	A
1	5	1833	G
1	5	1837	U
1	5	1842	A
1	5	1846	C
1	5	1849	C
1	5	1850	A
1	5	1866	C
1	5	1871	U
1	5	1878	G
1	5	1879	A
1	5	1880	U
1	5	1881	A
1	5	1884	A
1	5	1886	A
1	5	1893	A
1	5	1896	A
1	5	1906	G
1	5	1935	G
1	5	1953	G
1	5	1958	U
1	5	1960	A
1	5	1965	C
1	5	1968	G
1	5	1972	A
1	5	1973	G
1	5	1975	C
1	5	2054	G
1	5	2057	G
1	5	2059	C
1	5	2064	U
1	5	2065	U
1	5	2073	C
1	5	2074	U
1	5	2075	C
1	5	2078	G
1	5	2083	U
1	5	2086	U
1	5	2089	A

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Mol	Chain	Res	Type
1	5	2090	A
1	5	2091	U
1	5	2092	U
1	5	2093	A
1	5	2100	A
1	5	2101	C
1	5	2102	U
1	5	2110	G
1	5	2111	G
1	5	2112	U
1	5	2113	A
1	5	2116	G
1	5	2121	G
1	5	2122	G
1	5	2131	A
1	5	2140	U
1	5	2144	A
1	5	2145	A
1	5	2158	A
1	5	2160	G
1	5	2166	A
1	5	2169	G
1	5	2171	G
1	5	2188	A
1	5	2205	U
1	5	2208	A
1	5	2210	G
1	5	2211	U
1	5	2223	A
1	5	2229	A
1	5	2231	C
1	5	2232	A
1	5	2235	C
1	5	2239	G
1	5	2244	A
1	5	2249	G
1	5	2250	G
1	5	2253	G
1	5	2257	C
1	5	2258	U
1	5	2259	A
1	5	2260	U

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Mol	Chain	Res	Type
1	5	2261	G
1	5	2262	A
1	5	2266	U
1	5	2267	C
1	5	2268	U
1	5	2270	A
1	5	2272	G
1	5	2273	G
1	5	2274	U
1	5	2281	A
1	5	2283	G
1	5	2286	U
1	5	2307	G
1	5	2308	C
1	5	2310	U
1	5	2313	A
1	5	2315	G
1	5	2327	U
1	5	2334	U
1	5	2335	G
1	5	2336	U
1	5	2372	A
1	5	2373	A
1	5	2374	C
1	5	2375	G
1	5	2385	G
1	5	2388	U
1	5	2393	G
1	5	2397	A
1	5	2398	A
1	5	2401	A
1	5	2402	A
1	5	2403	G
1	5	2404	A
1	5	2411	U
1	5	2418	G
1	5	2419	A
1	5	2434	U
1	5	2435	G
1	5	2441	A
1	5	2442	G
1	5	2443	A

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Mol	Chain	Res	Type
1	5	2444	C
1	5	2446	U
1	5	2447	A
1	5	2448	G
1	5	2449	A
1	5	2450	G
1	5	2451	G
1	5	2452	G
1	5	2453	U
1	5	2454	G
1	5	2457	G
1	5	2458	A
1	5	2459	A
1	5	2461	A
1	5	2467	G
1	5	2468	A
1	5	2469	G
1	5	2474	G
1	5	2475	G
1	5	2477	G
1	5	2478	C
1	5	2486	A
1	5	2487	U
1	5	2489	C
1	5	2491	A
1	5	2494	A
1	5	2495	C
1	5	2499	U
1	5	2500	A
1	5	2501	U
1	5	2502	A
1	5	2503	G
1	5	2504	U
1	5	2505	U
1	5	2506	U
1	5	2508	U
1	5	2509	U
1	5	2513	U
1	5	2514	U
1	5	2519	A
1	5	2522	G
1	5	2523	A

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Mol	Chain	Res	Type
1	5	2524	A
1	5	2525	G
1	5	2531	C
1	5	2534	G
1	5	2536	A
1	5	2537	U
1	5	2538	U
1	5	2539	C
1	5	2540	A
1	5	2541	U
1	5	2542	U
1	5	2543	U
1	5	2544	U
1	5	2545	C
1	5	2547	A
1	5	2549	G
1	5	2550	U
1	5	2551	U
1	5	2552	C
1	5	2554	A
1	5	2560	C
1	5	2561	A
1	5	2562	A
1	5	2568	C
1	5	2569	A
1	5	2570	U
1	5	2571	U
1	5	2572	C
1	5	2573	G
1	5	2575	G
1	5	2580	A
1	5	2581	U
1	5	2585	G
1	5	2586	G
1	5	2593	A
1	5	2594	C
1	5	2606	G
1	5	2607	G
1	5	2614	G
1	5	2619	G
1	5	2620	G
1	5	2626	A

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Mol	Chain	Res	Type
1	5	2627	C
1	5	2652	U
1	5	2655	U
1	5	2656	A
1	5	2657	A
1	5	2662	G
1	5	2663	G
1	5	2674	A
1	5	2677	G
1	5	2689	A
1	5	2690	G
1	5	2691	A
1	5	2694	A
1	5	2696	A
1	5	2704	A
1	5	2714	G
1	5	2715	A
1	5	2719	U
1	5	2720	G
1	5	2728	G
1	5	2737	C
1	5	2747	A
1	5	2749	G
1	5	2752	U
1	5	2753	G
1	5	2762	A
1	5	2771	U
1	5	2777	G
1	5	2787	G
1	5	2790	A
1	5	2791	G
1	5	2794	G
1	5	2796	G
1	5	2799	A
1	5	2800	G
1	5	2801	A
1	5	2802	A
1	5	2810	C
1	5	2814	G
1	5	2817	A
1	5	2818	U
1	5	2843	U

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Mol	Chain	Res	Type
1	5	2845	A
1	5	2847	A
1	5	2853	A
1	5	2856	G
1	5	2861	U
1	5	2863	G
1	5	2871	G
1	5	2872	A
1	5	2873	U
1	5	2875	U
1	5	2887	A
1	5	2899	C
1	5	2907	G
1	5	2911	A
1	5	2914	G
1	5	2916	U
1	5	2923	U
1	5	2933	A
1	5	2935	U
1	5	2936	A
1	5	2938	G
1	5	2941	A
1	5	2942	C
1	5	2943	G
1	5	2947	G
1	5	2954	U
1	5	2955	U
1	5	2972	G
1	5	2983	C
1	5	2996	U
1	5	2997	G
1	5	3004	C
1	5	3006	A
1	5	3011	A
1	5	3012	A
1	5	3021	A
1	5	3042	U
1	5	3059	G
1	5	3069	G
1	5	3078	U
1	5	3079	U
1	5	3080	G

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Mol	Chain	Res	Type
1	5	3086	A
1	5	3092	C
1	5	3093	C
1	5	3094	A
1	5	3109	G
1	5	3115	C
1	5	3117	C
1	5	3122	A
1	5	3123	A
1	5	3125	U
1	5	3130	A
1	5	3131	U
1	5	3142	A
1	5	3154	C
1	5	3156	U
1	5	3157	U
1	5	3158	G
1	5	3159	C
1	5	3173	G
1	5	3174	A
1	5	3175	U
1	5	3176	G
1	5	3179	U
1	5	3181	C
1	5	3182	G
1	5	3187	A
1	5	3194	C
1	5	3195	U
1	5	3196	U
1	5	3200	G
1	5	3202	G
1	5	3204	C
1	5	3207	U
1	5	3210	A
1	5	3213	A
1	5	3215	A
1	5	3216	G
1	5	3217	C
1	5	3218	A
1	5	3219	G
1	5	3224	G
1	5	3227	A

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Mol	Chain	Res	Type
1	5	3229	G
1	5	3236	U
1	5	3238	G
1	5	3239	G
1	5	3240	C
1	5	3243	A
1	5	3244	A
1	5	3245	A
1	5	3248	C
1	5	3249	C
1	5	3252	G
1	5	3253	G
1	5	3256	G
1	5	3259	U
1	5	3260	G
1	5	3262	U
1	5	3263	G
1	5	3267	A
1	5	3268	A
1	5	3273	A
1	5	3275	U
1	5	3276	G
1	5	3278	C
1	5	3282	U
1	5	3283	U
1	5	3284	G
1	5	3285	C
1	5	3286	G
1	5	3288	G
1	5	3290	G
1	5	3294	A
1	5	3304	U
1	5	3307	A
1	5	3313	U
1	5	3314	A
1	5	3316	A
1	5	3317	U
1	5	3318	G
1	5	3319	U
1	5	3341	U
1	5	3342	A
1	5	3344	A

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Mol	Chain	Res	Type
1	5	3345	G
1	5	3351	U
1	5	3354	U
1	5	3356	G
1	5	3358	U
1	5	3369	G
1	5	3370	A
1	5	3375	A
1	5	3378	C
1	5	3382	U
1	5	3383	G
1	5	3390	G
2	7	7	G
2	7	18	C
2	7	22	A
2	7	27	A
2	7	38	U
2	7	40	C
2	7	42	A
2	7	43	U
2	7	54	U
2	7	55	A
2	7	65	G
2	7	70	U
2	7	74	C
2	7	76	A
2	7	84	A
2	7	88	G
2	7	93	C
2	7	99	G
2	7	102	A
2	7	112	G
2	7	121	U
3	8	23	U
3	8	25	G
3	8	34	U
3	8	35	C
3	8	36	G
3	8	48	A
3	8	50	C
3	8	52	A
3	8	53	A

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Mol	Chain	Res	Type
3	8	59	A
3	8	62	C
3	8	63	G
3	8	71	A
3	8	80	A
3	8	81	U
3	8	82	U
3	8	83	C
3	8	85	G
3	8	86	U
3	8	87	G
3	8	95	G
3	8	97	A
3	8	100	U
3	8	104	A
3	8	106	C
3	8	111	A
3	8	113	U
3	8	125	U
3	8	126	A
3	8	127	U
3	8	128	U
3	8	129	C
3	8	151	C
3	8	152	G
81	2	2	U
81	2	3	C
81	2	24	C
81	2	30	C
81	2	31	U
81	2	33	G
81	2	39	A
81	2	41	G
81	2	42	A
81	2	43	U
81	2	44	U
81	2	46	A
81	2	49	C
81	2	56	G
81	2	59	U
81	2	60	A
81	2	62	G

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Mol	Chain	Res	Type
81	2	66	A
81	2	67	A
81	2	70	A
81	2	71	A
81	2	72	U
81	2	73	U
81	2	74	U
81	2	75	A
81	2	103	A
81	2	113	C
81	2	123	A
81	2	126	G
81	2	128	U
81	2	129	C
81	2	130	C
81	2	131	U
81	2	132	U
81	2	133	U
81	2	134	A
81	2	136	U
81	2	137	A
81	2	139	A
81	2	143	U
81	2	144	A
81	2	146	A
81	2	148	C
81	2	157	U
81	2	158	U
81	2	161	A
81	2	165	C
81	2	168	A
81	2	169	U
81	2	173	U
81	2	175	C
81	2	176	U
81	2	177	U
81	2	178	A
81	2	179	A
81	2	184	U
81	2	185	C
81	2	186	G
81	2	189	C

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Mol	Chain	Res	Type
81	2	190	C
81	2	191	U
81	2	193	U
81	2	194	G
81	2	196	A
81	2	203	G
81	2	207	U
81	2	209	A
81	2	215	U
81	2	216	A
81	2	217	A
81	2	218	A
81	2	226	U
81	2	227	G
81	2	230	U
81	2	231	U
81	2	232	C
81	2	233	G
81	2	235	A
81	2	237	U
81	2	238	C
81	2	239	U
81	2	241	U
81	2	249	C
81	2	256	A
81	2	259	U
81	2	260	U
81	2	264	A
81	2	270	A
81	2	274	C
81	2	276	U
81	2	277	U
81	2	278	G
81	2	279	U
81	2	280	G
81	2	281	C
81	2	286	G
81	2	298	A
81	2	301	U
81	2	311	A
81	2	313	C
81	2	315	A

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Mol	Chain	Res	Type
81	2	319	U
81	2	320	C
81	2	321	G
81	2	332	A
81	2	333	G
81	2	336	G
81	2	337	C
81	2	351	A
81	2	358	A
81	2	359	A
81	2	360	C
81	2	398	A
81	2	399	A
81	2	400	A
81	2	401	C
81	2	403	G
81	2	412	U
81	2	415	A
81	2	416	A
81	2	421	G
81	2	423	C
81	2	425	G
81	2	433	G
81	2	436	A
81	2	438	U
81	2	439	U
81	2	443	C
81	2	444	A
81	2	447	C
81	2	452	U
81	2	454	C
81	2	458	G
81	2	461	G
81	2	467	A
81	2	468	C
81	2	474	A
81	2	476	A
81	2	479	G
81	2	484	A
81	2	485	G
81	2	486	G
81	2	487	G

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Mol	Chain	Res	Type
81	2	489	C
81	2	490	C
81	2	491	A
81	2	492	U
81	2	494	C
81	2	495	G
81	2	496	G
81	2	497	G
81	2	499	C
81	2	501	U
81	2	505	A
81	2	506	U
81	2	507	U
81	2	514	A
81	2	518	C
81	2	524	A
81	2	526	A
81	2	533	A
81	2	537	A
81	2	539	G
81	2	540	A
81	2	542	C
81	2	543	A
81	2	544	A
81	2	547	G
81	2	548	G
81	2	554	A
81	2	556	G
81	2	557	U
81	2	558	C
81	2	559	U
81	2	564	C
81	2	565	C
81	2	567	G
81	2	576	G
81	2	577	U
81	2	578	A
81	2	579	A
81	2	593	A
81	2	594	G
81	2	596	G
81	2	600	A

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Mol	Chain	Res	Type
81	2	605	A
81	2	610	U
81	2	618	A
81	2	619	A
81	2	621	A
81	2	622	A
81	2	623	G
81	2	638	U
81	2	640	G
81	2	642	G
81	2	643	C
81	2	644	C
81	2	646	G
81	2	649	U
81	2	650	G
81	2	652	C
81	2	653	C
81	2	654	G
81	2	655	G
81	2	656	U
81	2	679	U
81	2	684	A
81	2	691	C
81	2	693	U
81	2	694	U
81	2	695	U
81	2	696	C
81	2	697	C
81	2	698	U
81	2	699	U
81	2	701	U
81	2	708	C
81	2	709	C
81	2	710	U
81	2	711	U
81	2	712	G
81	2	713	A
81	2	714	G
81	2	715	U
81	2	716	C
81	2	717	C
81	2	718	U

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Mol	Chain	Res	Type
81	2	721	U
81	2	722	G
81	2	723	G
81	2	726	C
81	2	727	U
81	2	729	G
81	2	730	G
81	2	731	C
81	2	732	G
81	2	734	A
81	2	736	C
81	2	738	G
81	2	739	G
81	2	740	A
81	2	741	C
81	2	742	U
81	2	743	U
81	2	753	A
81	2	754	A
81	2	755	A
81	2	765	G
81	2	766	U
81	2	771	A
81	2	774	A
81	2	778	G
81	2	779	U
81	2	780	A
81	2	783	G
81	2	789	A
81	2	792	U
81	2	794	U
81	2	795	U
81	2	799	A
81	2	811	A
81	2	812	A
81	2	813	U
81	2	816	G
81	2	820	U
81	2	821	U
81	2	823	G
81	2	824	G
81	2	827	C

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Mol	Chain	Res	Type
81	2	828	U
81	2	829	A
81	2	831	U
81	2	833	U
81	2	834	G
81	2	835	U
81	2	836	U
81	2	839	U
81	2	841	U
81	2	846	G
81	2	849	C
81	2	850	A
81	2	853	G
81	2	856	A
81	2	858	G
81	2	860	U
81	2	861	U
81	2	863	A
81	2	864	U
81	2	865	A
81	2	873	U
81	2	875	G
81	2	877	G
81	2	886	U
81	2	898	A
81	2	904	G
81	2	906	A
81	2	907	A
81	2	911	U
81	2	912	U
81	2	913	G
81	2	914	G
81	2	915	A
81	2	921	U
81	2	928	U
81	2	931	C
81	2	932	U
81	2	933	A
81	2	935	U
81	2	951	A
81	2	952	A
81	2	959	U

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Mol	Chain	Res	Type
81	2	960	U
81	2	966	A
81	2	967	A
81	2	970	A
81	2	975	C
81	2	982	U
81	2	985	G
81	2	987	G
81	2	991	G
81	2	992	A
81	2	1001	A
81	2	1002	G
81	2	1003	A
81	2	1005	A
81	2	1012	U
81	2	1024	U
81	2	1026	A
81	2	1027	A
81	2	1028	C
81	2	1031	U
81	2	1032	G
81	2	1038	U
81	2	1039	A
81	2	1042	G
81	2	1043	A
81	2	1050	G
81	2	1051	G
81	2	1052	U
81	2	1053	G
81	2	1057	U
81	2	1058	U
81	2	1059	U
81	2	1061	A
81	2	1062	A
81	2	1063	U
81	2	1066	C
81	2	1072	C
81	2	1077	C
81	2	1080	U
81	2	1082	C
81	2	1083	G
81	2	1085	G

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Mol	Chain	Res	Type
81	2	1087	A
81	2	1088	A
81	2	1090	C
81	2	1091	A
81	2	1097	U
81	2	1098	U
81	2	1100	G
81	2	1108	G
81	2	1109	G
81	2	1111	G
81	2	1114	G
81	2	1118	G
81	2	1131	A
81	2	1138	A
81	2	1140	G
81	2	1143	A
81	2	1150	G
81	2	1151	A
81	2	1155	G
81	2	1158	C
81	2	1164	G
81	2	1167	G
81	2	1185	U
81	2	1186	U
81	2	1191	U
81	2	1194	A
81	2	1196	A
81	2	1199	G
81	2	1200	G
81	2	1202	A
81	2	1203	A
81	2	1204	A
81	2	1205	C
81	2	1207	C
81	2	1209	C
81	2	1214	U
81	2	1217	A
81	2	1218	G
81	2	1228	G
81	2	1229	G
81	2	1230	A
81	2	1237	G

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Mol	Chain	Res	Type
81	2	1239	U
81	2	1241	G
81	2	1243	G
81	2	1244	A
81	2	1245	G
81	2	1246	C
81	2	1247	U
81	2	1248	C
81	2	1250	U
81	2	1254	U
81	2	1255	G
81	2	1256	A
81	2	1262	U
81	2	1266	U
81	2	1269	U
81	2	1270	G
81	2	1271	G
81	2	1284	C
81	2	1285	U
81	2	1286	U
81	2	1290	U
81	2	1312	A
81	2	1314	U
81	2	1315	U
81	2	1321	A
81	2	1322	A
81	2	1323	C
81	2	1336	A
81	2	1340	U
81	2	1342	C
81	2	1344	A
81	2	1345	A
81	2	1348	A
81	2	1353	U
81	2	1355	C
81	2	1356	U
81	2	1361	U
81	2	1364	G
81	2	1369	U
81	2	1370	U
81	2	1371	A
81	2	1372	U

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Mol	Chain	Res	Type
81	2	1377	U
81	2	1378	U
81	2	1383	G
81	2	1385	G
81	2	1390	U
81	2	1398	U
81	2	1399	C
81	2	1413	U
81	2	1415	U
81	2	1427	A
81	2	1432	U
81	2	1433	G
81	2	1434	U
81	2	1436	A
81	2	1444	A
81	2	1445	G
81	2	1448	G
81	2	1450	U
81	2	1459	C
81	2	1460	A
81	2	1465	C
81	2	1466	G
81	2	1469	A
81	2	1470	C
81	2	1471	A
81	2	1486	G
81	2	1489	U
81	2	1490	C
81	2	1491	U
81	2	1494	C
81	2	1496	U
81	2	1497	U
81	2	1500	C
81	2	1504	G
81	2	1505	A
81	2	1509	C
81	2	1516	A
81	2	1517	U
81	2	1518	C
81	2	1521	G
81	2	1523	G
81	2	1524	A

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Mol	Chain	Res	Type
81	2	1534	G
81	2	1535	U
81	2	1536	G
81	2	1537	C
81	2	1538	U
81	2	1540	G
81	2	1543	A
81	2	1545	A
81	2	1548	G
81	2	1557	U
81	2	1559	A
81	2	1568	C
81	2	1573	A
81	2	1582	U
81	2	1597	A
81	2	1601	G
81	2	1607	G
81	2	1615	C
81	2	1616	G
81	2	1619	C
81	2	1622	G
81	2	1631	A
81	2	1632	C
81	2	1638	G
81	2	1642	G
81	2	1648	A
81	2	1649	G
81	2	1657	U
81	2	1658	G
81	2	1678	A
81	2	1680	G
81	2	1684	U
81	2	1685	G
81	2	1687	U
81	2	1688	U
81	2	1690	G
81	2	1693	A
81	2	1694	A
81	2	1695	G
81	2	1696	G
81	2	1697	G
81	2	1698	G

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Mol	Chain	Res	Type
81	2	1699	G
81	2	1700	C
81	2	1701	A
81	2	1702	A
81	2	1703	C
81	2	1704	U
81	2	1705	C
81	2	1708	U
81	2	1709	C
81	2	1711	C
81	2	1712	A
81	2	1713	G
81	2	1714	A
81	2	1715	G
81	2	1716	C
81	2	1717	G
81	2	1718	G
81	2	1726	G
81	2	1731	A
81	2	1736	G
81	2	1750	A
81	2	1755	A
81	2	1756	A
81	2	1757	G
81	2	1760	G
81	2	1765	A
81	2	1766	A
81	2	1769	U
81	2	1780	G
81	2	1782	A
81	2	1783	C
81	2	1792	G
81	2	1793	G
81	2	1794	A
81	2	1795	U
81	2	1796	C
81	2	1797	A
81	2	1798	U
83	3	16	U
83	3	17	G
83	3	18	G
83	3	19	G

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Mol	Chain	Res	Type
83	3	20	A
83	3	21	A
83	3	22	G
83	3	26	G
83	3	42	U
83	3	43	G
83	3	48	C
83	3	58	A
83	3	59	A
83	3	60	A
83	3	61	C
83	3	75	C
83	3	76	A

All (110) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	133	U
1	5	166	C
1	5	173	G
1	5	249	U
1	5	297	G
1	5	298	U
1	5	406	G
1	5	518	G
1	5	567	G
1	5	588	G
1	5	594	U
1	5	718	G
1	5	766	U
1	5	816	A
1	5	873	C
1	5	896	A
1	5	916	G
1	5	993	G
1	5	1016	C
1	5	1064	A
1	5	1073	U
1	5	1097	G
1	5	1160	C
1	5	1181	U
1	5	1222	G

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Mol	Chain	Res	Type
1	5	1223	A
1	5	1238	C
1	5	1241	U
1	5	1284	C
1	5	1307	G
1	5	1349	G
1	5	1352	A
1	5	1355	A
1	5	1560	G
1	5	1568	U
1	5	1607	U
1	5	1729	A
1	5	1816	A
1	5	1841	A
1	5	2064	U
1	5	2072	U
1	5	2110	G
1	5	2112	U
1	5	2116	G
1	5	2248	C
1	5	2453	U
1	5	2467	G
1	5	2477	G
1	5	2486	A
1	5	2500	A
1	5	2505	U
1	5	2561	A
1	5	2570	U
1	5	2571	U
1	5	2585	G
1	5	2662	G
1	5	2911	A
1	5	2941	A
1	5	2996	U
1	5	3057	U
1	5	3078	U
1	5	3093	C
1	5	3121	U
1	5	3194	C
1	5	3217	C
1	5	3228	C
1	5	3239	G

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Mol	Chain	Res	Type
1	5	3242	G
1	5	3259	U
1	5	3267	A
1	5	3284	G
1	5	3289	G
1	5	3303	G
1	5	3317	U
1	5	3340	G
1	5	3357	U
3	8	22	U
3	8	125	U
81	2	67	A
81	2	71	A
81	2	129	C
81	2	177	U
81	2	217	A
81	2	277	U
81	2	279	U
81	2	280	G
81	2	285	C
81	2	318	U
81	2	399	A
81	2	538	G
81	2	564	C
81	2	695	U
81	2	721	U
81	2	829	A
81	2	863	A
81	2	910	C
81	2	1084	A
81	2	1108	G
81	2	1244	A
81	2	1344	A
81	2	1360	A
81	2	1371	A
81	2	1414	U
81	2	1444	A
81	2	1447	C
81	2	1457	C
81	2	1493	A
81	2	1542	G
81	2	1615	C

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Mol	Chain	Res	Type
81	2	1755	A

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	MET	3	102	83	6,7,8	0.48	0	2,7,9	1.44	0
87	U6A	3	101	83	9,9,10	1.69	2 (22%)	10,11,13	2.60	1 (10%)
86	GDP	1	1101	-	29,30,30	1.15	3 (10%)	45,47,47	1.87	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	MET	3	102	83	-	1/5/6/8	-
87	U6A	3	101	83	-	10/11/11/12	-
86	GDP	1	1101	-	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3	101	U6A	O1-C1	3.32	1.36	1.22
86	1	1101	GDP	C5-C4	3.01	1.47	1.38
87	3	101	U6A	CA-N	2.80	1.49	1.45
86	1	1101	GDP	C6-N1	-2.44	1.34	1.38
86	1	1101	GDP	C5-N7	-2.19	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	3	101	U6A	O1-C1-N	7.63	145.02	125.32
86	1	1101	GDP	C5-C4-N3	-6.25	118.44	128.39
86	1	1101	GDP	C2-N3-C4	5.12	121.13	112.30
86	1	1101	GDP	N9-C4-N3	4.49	134.94	125.95
86	1	1101	GDP	C6-C5-N7	3.42	136.51	130.29
86	1	1101	GDP	C4-C5-N7	-2.89	106.08	110.67
86	1	1101	GDP	C8-N7-C5	2.22	108.22	104.26
86	1	1101	GDP	C3'-C2'-C1'	2.05	105.35	101.46

There are no chirality outliers.

All (14) torsion outliers are listed below:

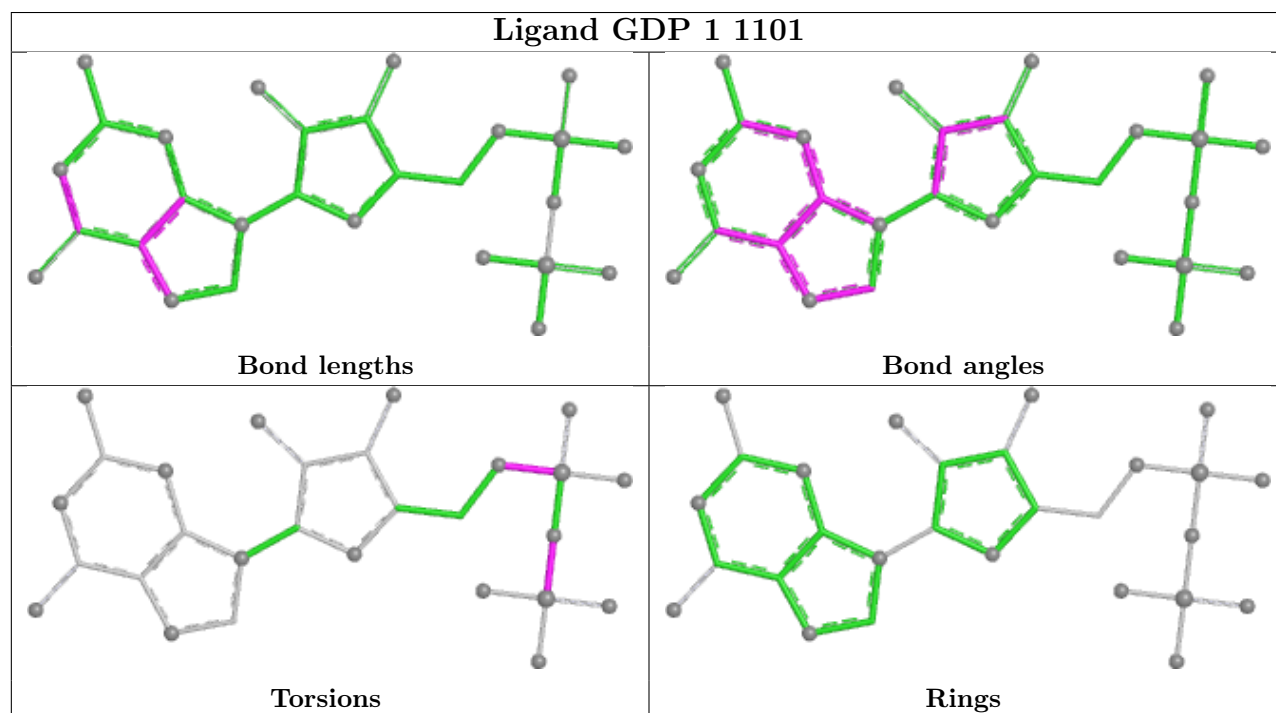
Mol	Chain	Res	Type	Atoms
86	1	1101	GDP	PA-O3A-PB-O2B
86	1	1101	GDP	C5'-O5'-PA-O1A
87	3	101	U6A	O1-C1-N-CA
87	3	101	U6A	C7-C6-CA-C
87	3	101	U6A	O8-C6-CA-C
87	3	101	U6A	C7-C6-CA-N
87	3	101	U6A	O8-C6-CA-N
87	3	101	U6A	OXT-C-CA-N
87	3	101	U6A	C-CA-N-C1
87	3	101	U6A	O-C-CA-N
88	3	102	MET	CB-CG-SD-CE
87	3	101	U6A	OXT-C-CA-C6
87	3	101	U6A	O-C-CA-C6
86	1	1101	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	18
81	2	11
80	gg	2
45	q	1
37	i	1
65	RR	1

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Mol	Chain	Number of breaks
46	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1980:C	O3'	2051:G	P	18.54
1	5	2083:U	O3'	2084:G	P	11.15
1	5	1954:G	O3'	1955:U	P	7.40
1	5	439:C	O3'	495:G	P	7.21
1	2	856:A	O3'	857:U	P	7.17
1	2	1015:U	O3'	1016:C	P	7.16
1	q	215:ARG	C	216:LEU	N	7.12
1	5	2084:G	O3'	2085:C	P	6.55
1	2	134:A	O3'	135:C	P	6.49
1	2	1039:A	O3'	1040:G	P	6.18
1	2	861:U	O3'	862:A	P	6.08
1	5	2081:G	O3'	2082:A	P	6.07
1	5	547:G	O3'	548:G	P	5.67
1	gg	163:ALA	C	164:ASP	N	5.57
1	2	1014:G	O3'	1015:U	P	5.51
1	5	1576:G	O3'	1577:G	P	5.41
1	5	17:G	O3'	18:G	P	4.72
1	5	2506:U	O3'	2507:C	P	4.70
1	i	34:SER	C	35:ASN	N	4.56
1	5	2093:A	O3'	2094:C	P	4.48
1	5	2439:A	O3'	2440:G	P	4.43
1	2	239:U	O3'	240:U	P	4.17
1	RR	99:VAL	C	100:LEU	N	4.13
1	r	115:ALA	C	116:VAL	N	3.89
1	2	1091:A	O3'	1092:A	P	3.88
1	5	2531:C	O3'	2532:U	P	3.87
1	5	2532:U	O3'	2533:G	P	3.77
1	5	1228:C	O3'	1229:G	P	3.64
1	5	1955:U	O3'	1956:A	P	3.51
1	2	240:U	O3'	241:U	P	3.35
1	2	643:C	O3'	644:C	P	3.35
1	2	811:A	O3'	812:A	P	3.34
1	gg	185:ASN	C	186:GLN	N	3.33
1	5	2748:A	O3'	2749:G	P	3.23
1	5	2548:C	O3'	2549:G	P	3.22

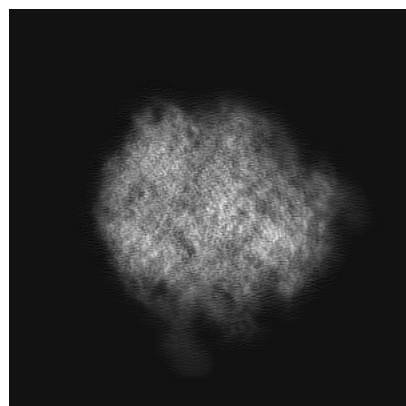
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21859. These allow visual inspection of the internal detail of the map and identification of artifacts.

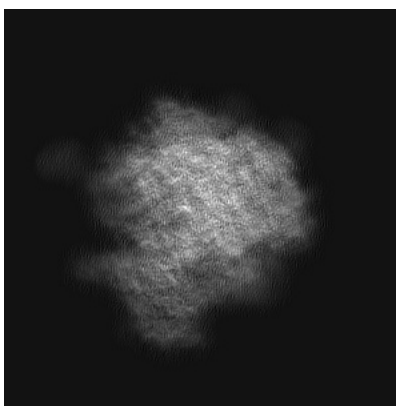
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

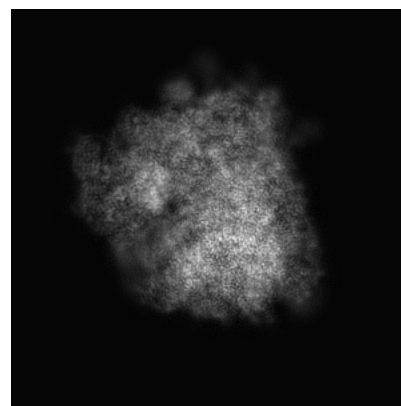
6.1.1 Primary map



X

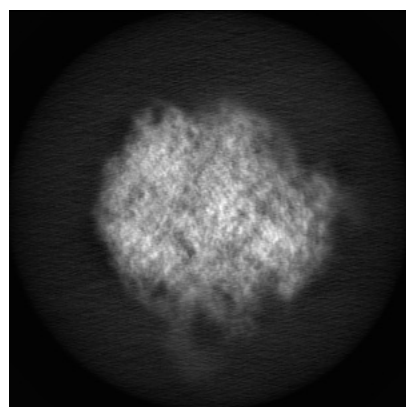


Y

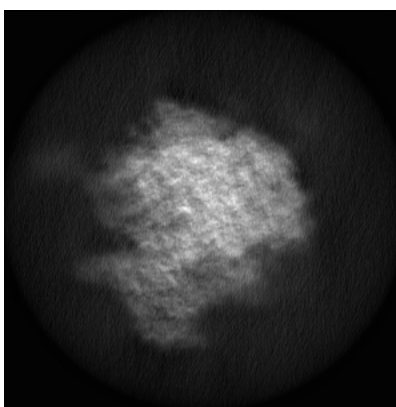


Z

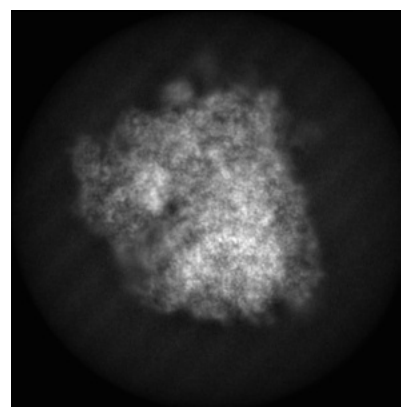
6.1.2 Raw map



X



Y

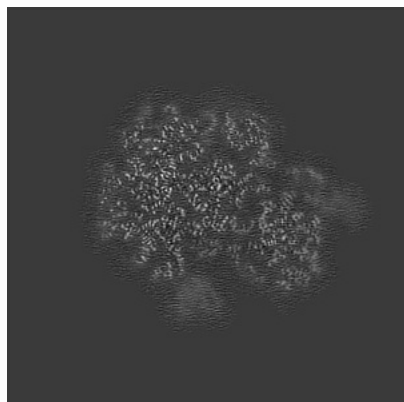


Z

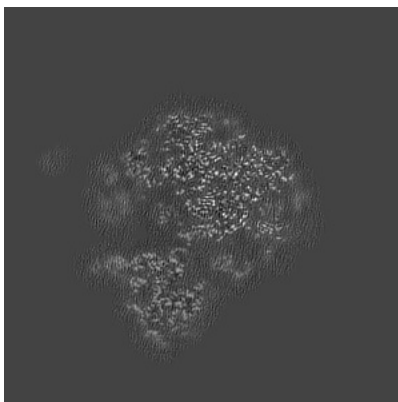
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

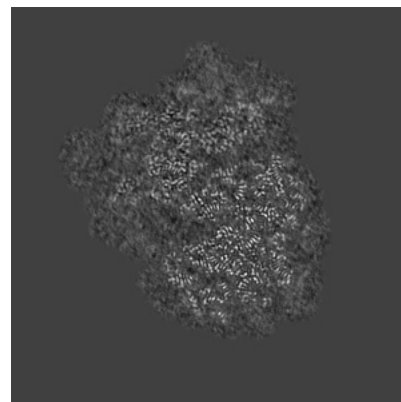
6.2.1 Primary map



X Index: 150

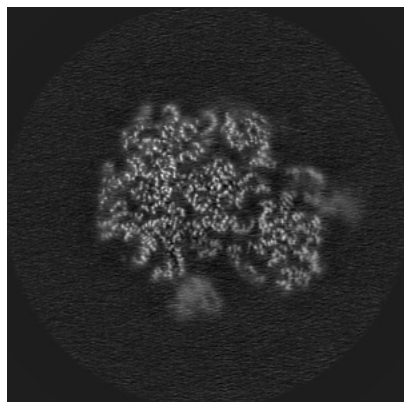


Y Index: 150

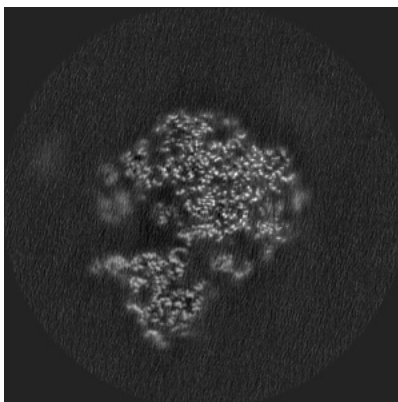


Z Index: 150

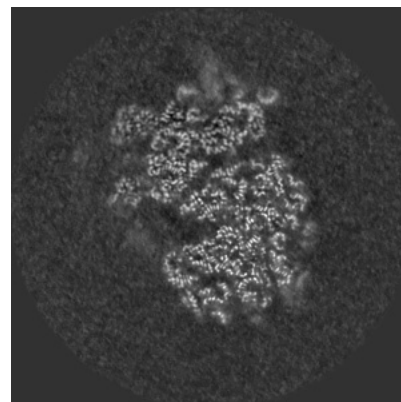
6.2.2 Raw map



X Index: 150



Y Index: 150

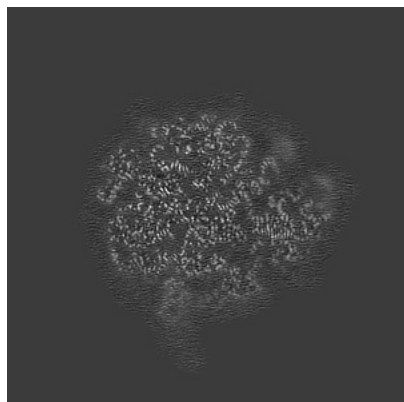


Z Index: 150

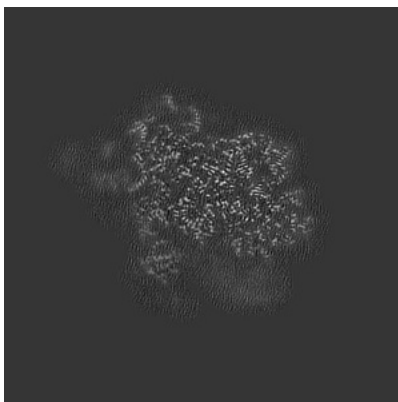
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

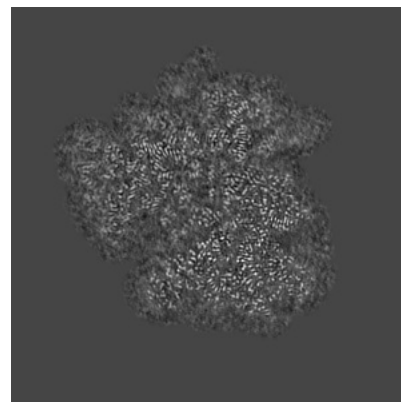
6.3.1 Primary map



X Index: 172

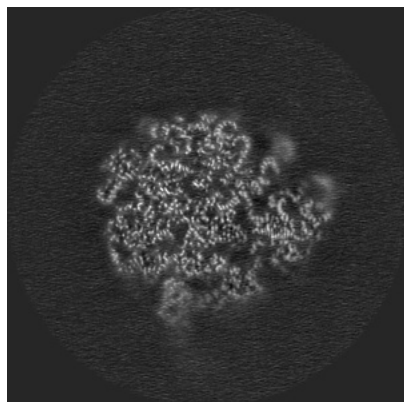


Y Index: 117

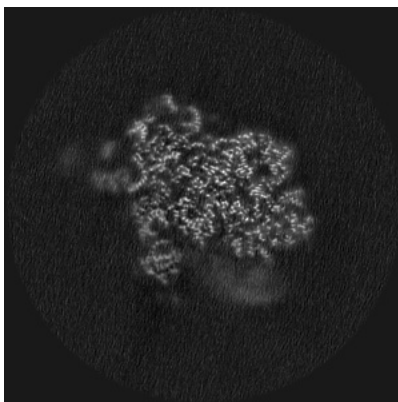


Z Index: 132

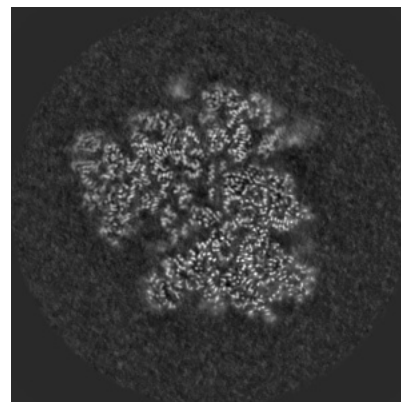
6.3.2 Raw map



X Index: 172



Y Index: 117

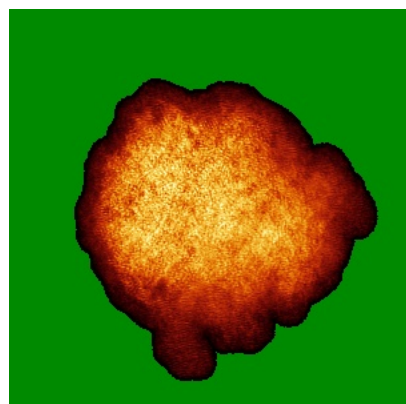


Z Index: 132

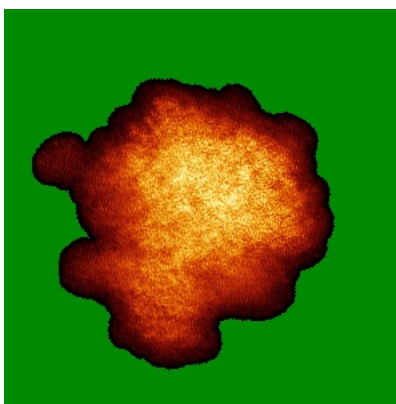
The images above show the largest variance slices of the map in three orthogonal directions.

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

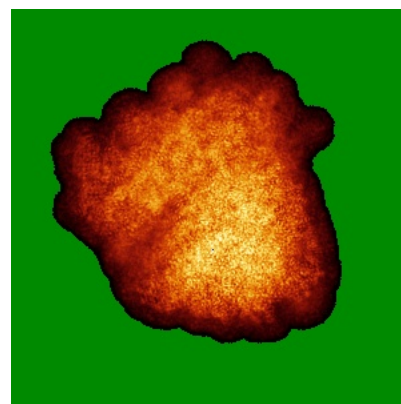
6.4.1 Primary map



X

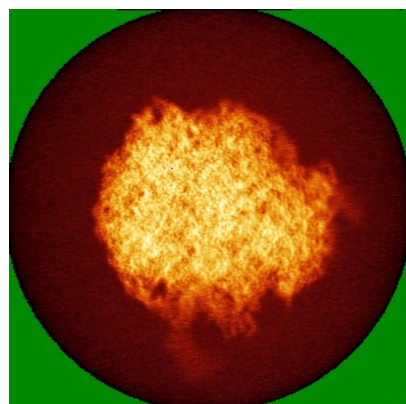


Y

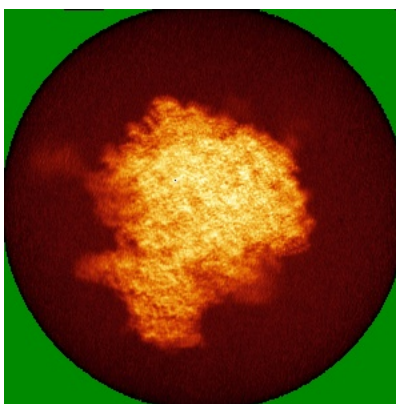


Z

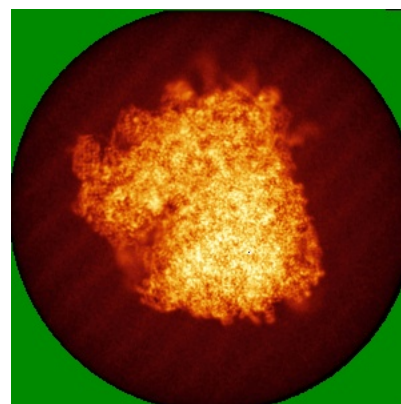
6.4.2 Raw map



X



Y

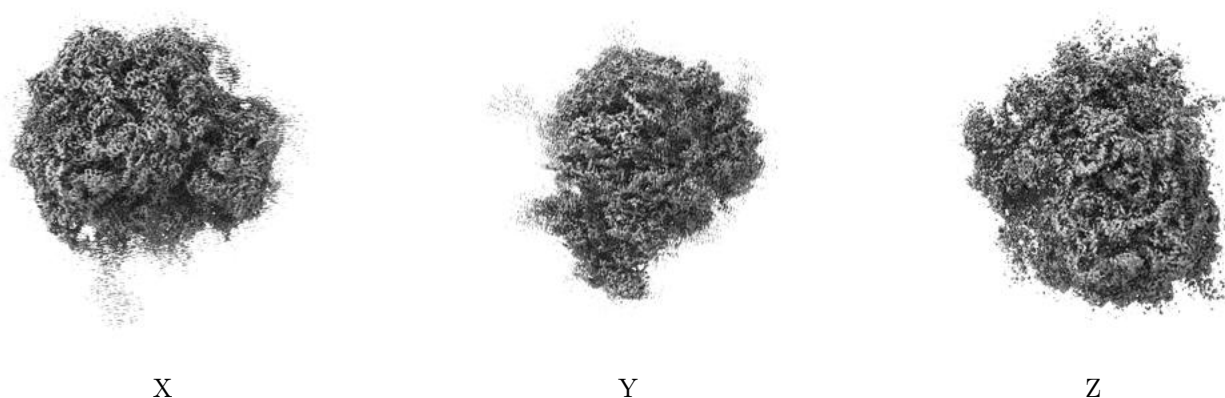


Z

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 0.042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

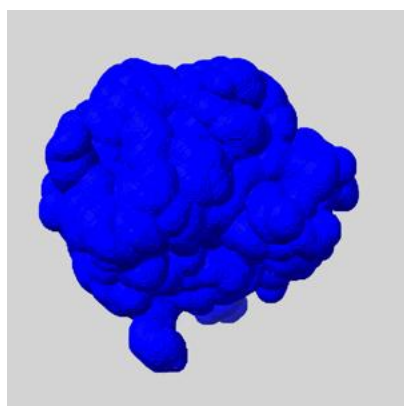
6.6 Mask visualisation [i](#)

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

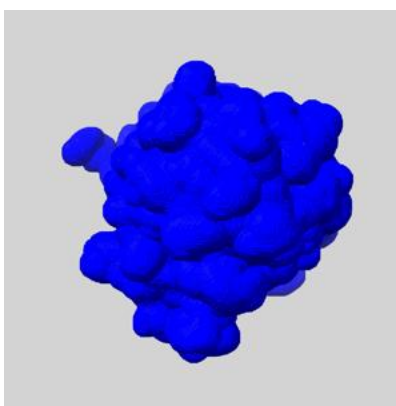
A mask typically either:

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

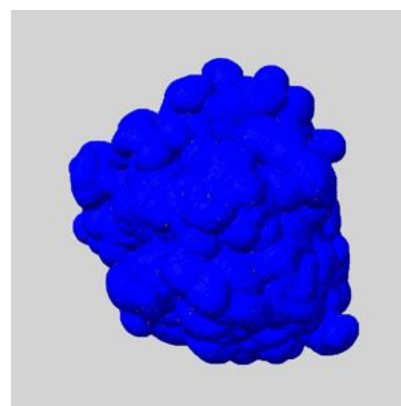
6.6.1 emd_21859_msk_1.map [i](#)



X



Y

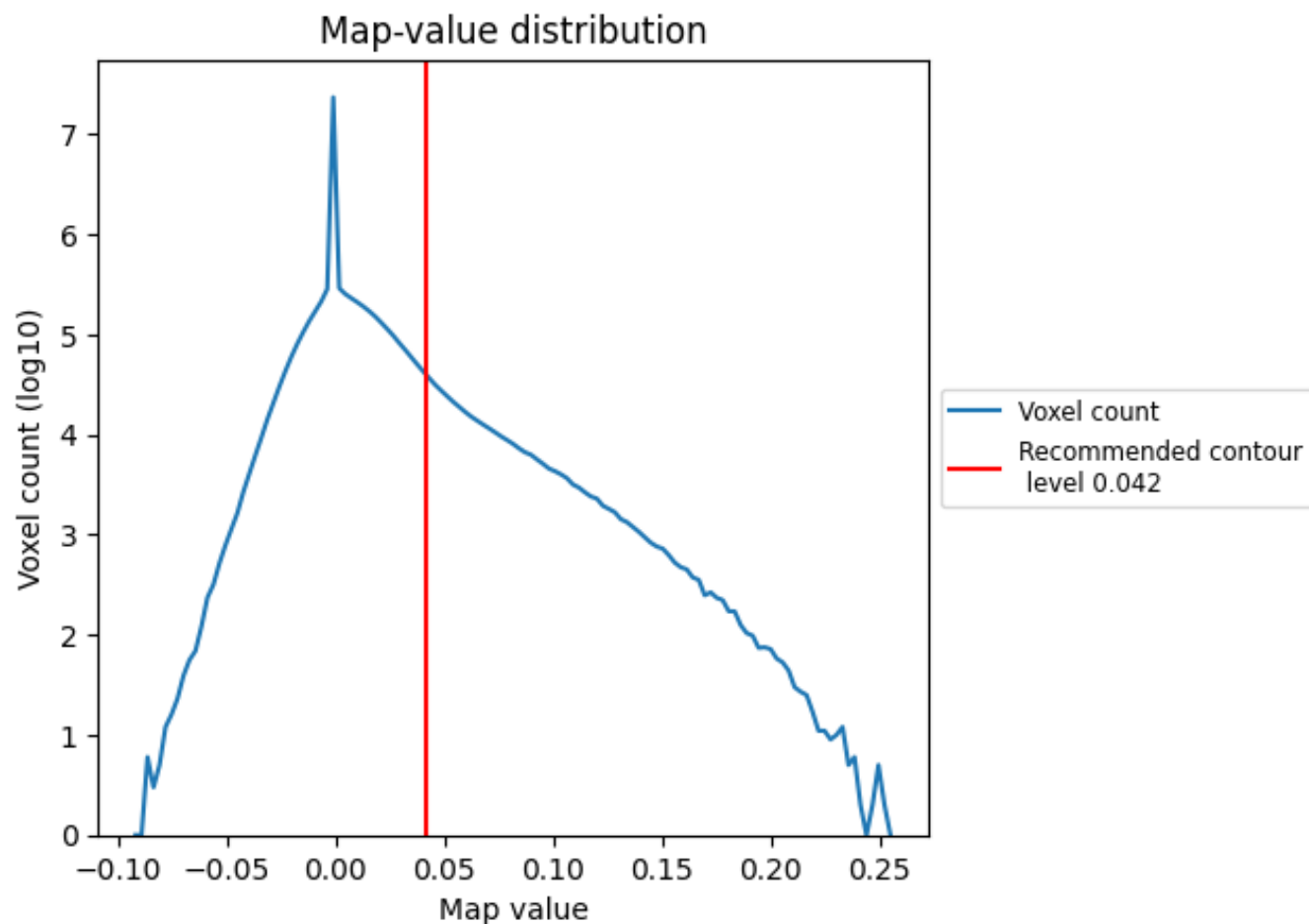


Z

7 Map analysis [i](#)

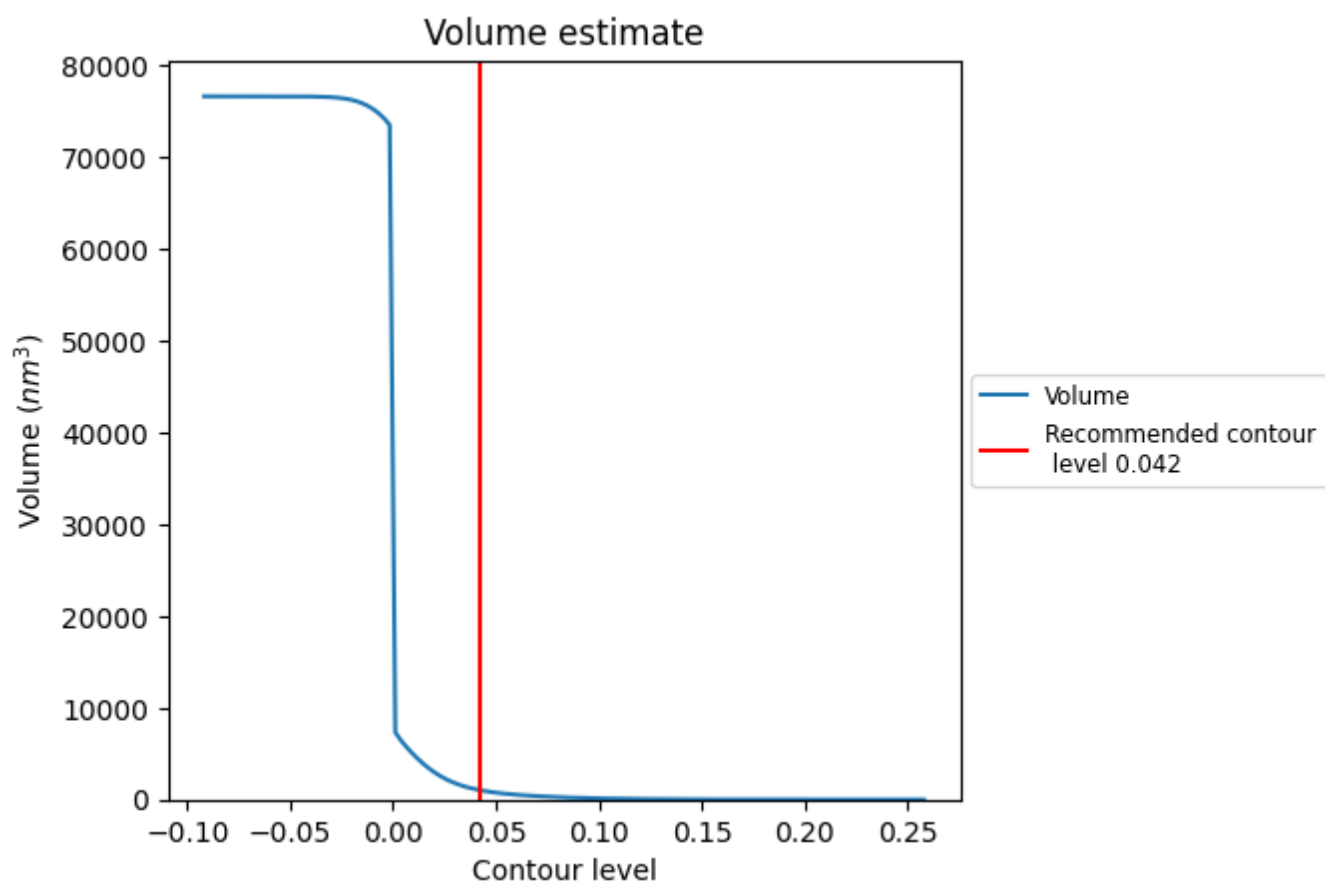
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

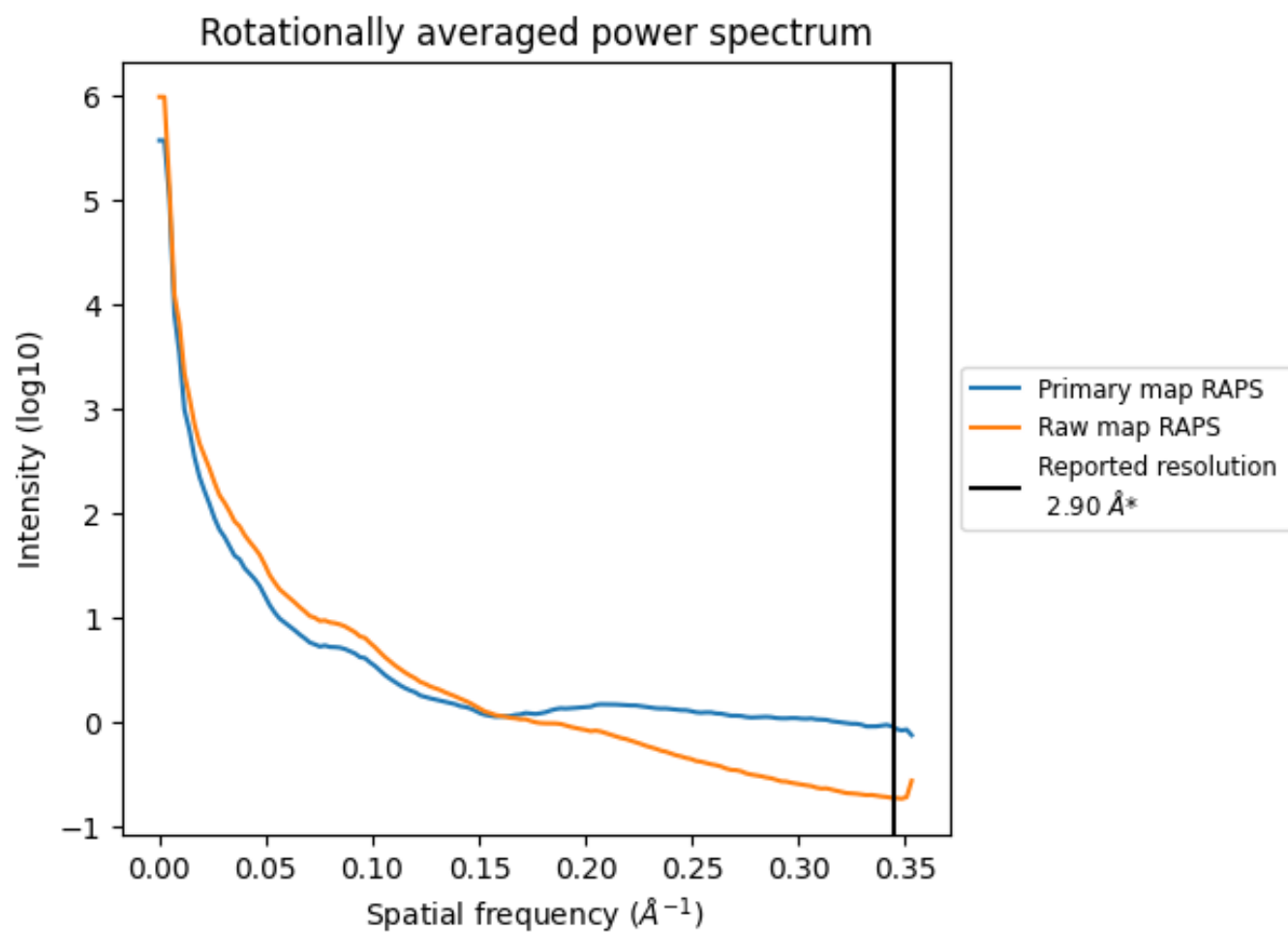
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1033 nm³; this corresponds to an approximate mass of 933 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 ⓘ

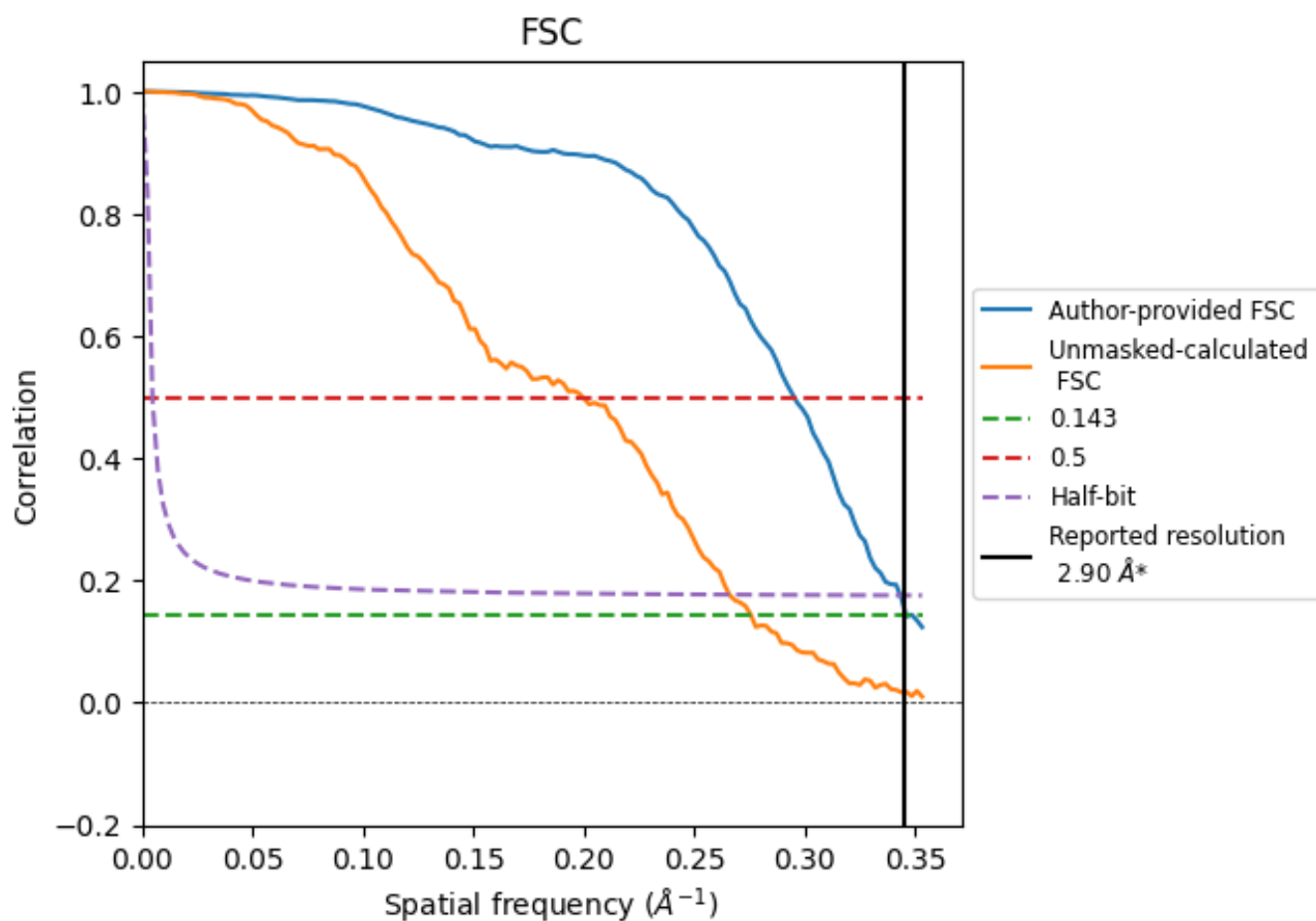


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

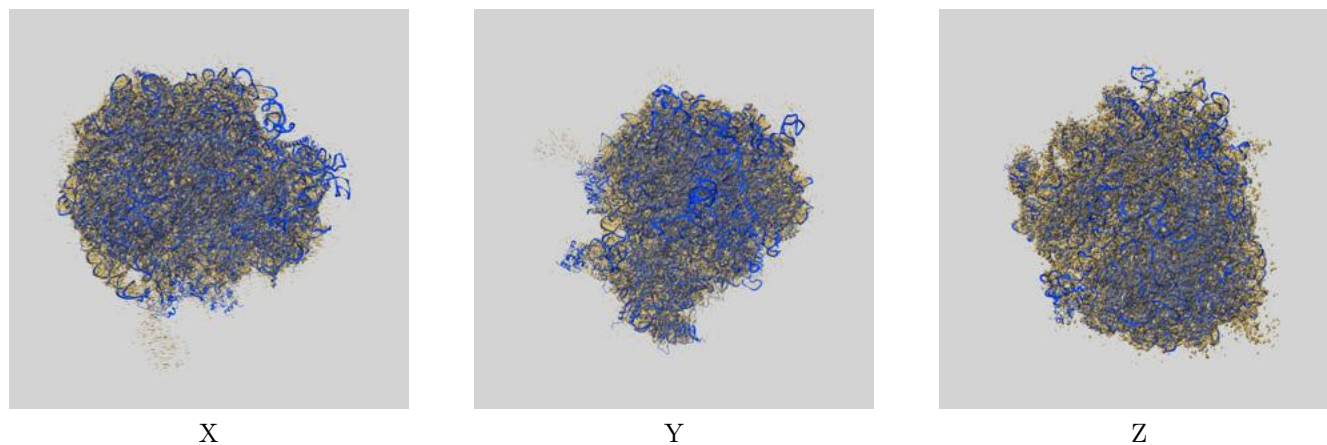
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.39	2.91
Unmasked-calculated*	3.63	5.02	3.76

*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 3.63 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

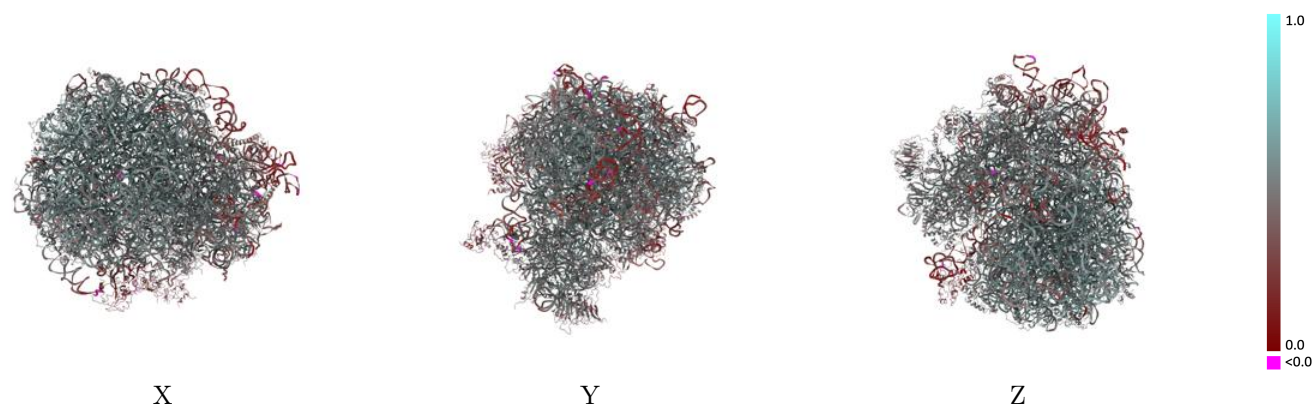
This section contains information regarding the fit between EMDB map EMD-21859 and PDB model 6WOO. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



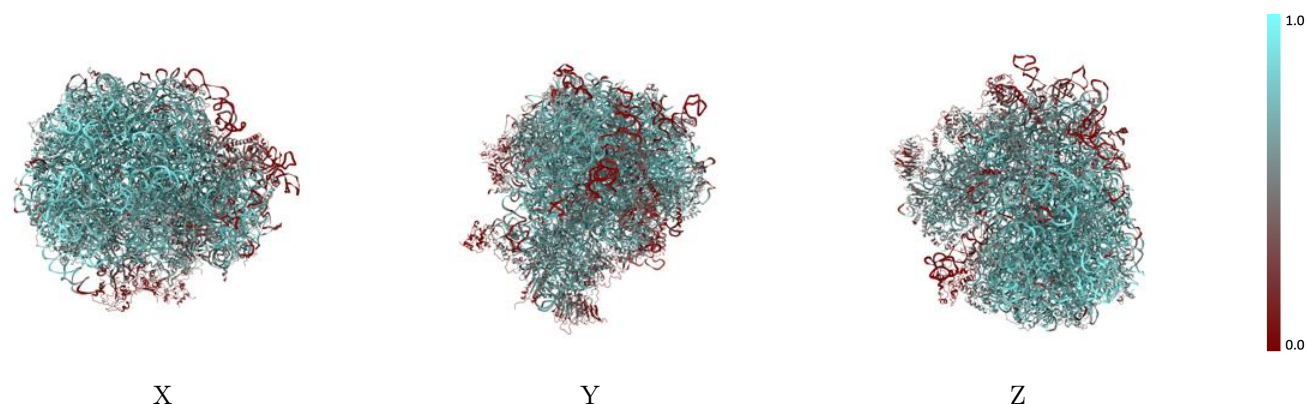
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



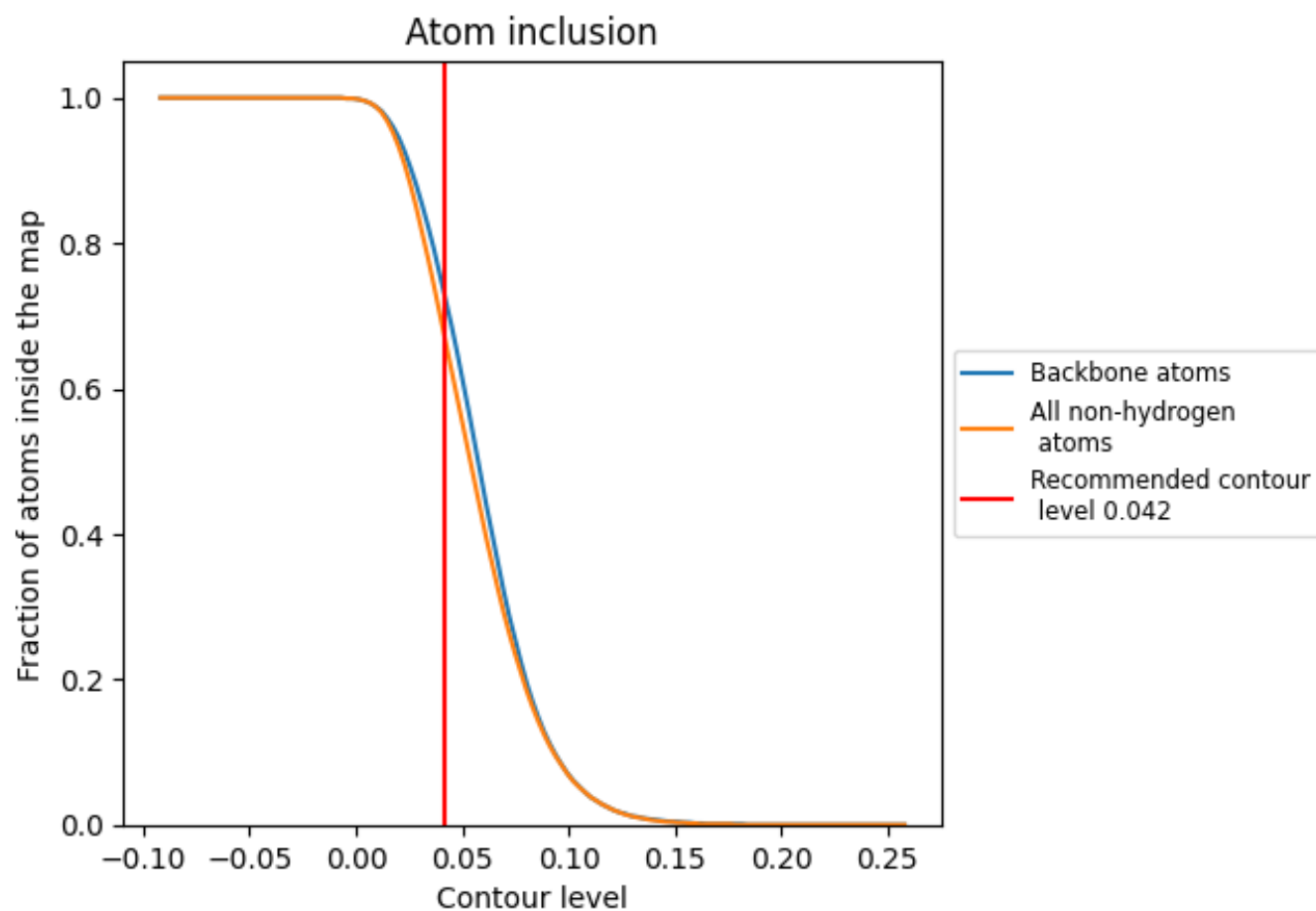
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.042).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4870
1	 0.5100	 0.4650
2	 0.7060	 0.4640
3	 0.6180	 0.4540
4	 0.8170	 0.5400
5	 0.7780	 0.5030
7	 0.8310	 0.5330
8	 0.8590	 0.5460
A	 0.7070	 0.5420
AA	 0.4640	 0.4490
B	 0.6680	 0.5200
BB	 0.5380	 0.4660
C	 0.7030	 0.5290
CC	 0.5750	 0.4890
D	 0.5690	 0.4800
DD	 0.4780	 0.4570
E	 0.6100	 0.4800
EE	 0.6250	 0.5100
F	 0.6770	 0.5210
FF	 0.5530	 0.4630
G	 0.5660	 0.4780
GG	 0.4580	 0.4370
H	 0.6370	 0.5020
HH	 0.2820	 0.4220
I	 0.6610	 0.5220
II	 0.5190	 0.4780
J	 0.4790	 0.4670
JJ	 0.6030	 0.4770
K	 0.0530	 0.2380
KK	 0.4480	 0.4130
L	 0.6680	 0.5220
LL	 0.5460	 0.4990
M	 0.6290	 0.5010
MM	 0.0540	 0.2660
N	 0.7630	 0.5580



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Chain	Atom inclusion	Q-score
NN	0.5070	0.4820
O	0.6800	0.5310
OO	0.6100	0.4860
P	0.6890	0.5270
PP	0.5440	0.4390
Q	0.7210	0.5410
QQ	0.5830	0.4990
R	0.5730	0.4900
RR	0.4140	0.4480
S	0.6740	0.5260
SS	0.5680	0.4960
T	0.6450	0.5250
TT	0.5740	0.4920
U	0.4850	0.4440
UU	0.4310	0.4500
V	0.6590	0.5440
VV	0.5060	0.4740
W	0.6400	0.5310
WW	0.6100	0.5140
X	0.6390	0.5150
XX	0.6380	0.5260
Y	0.6740	0.5300
YY	0.5110	0.4650
Z	0.5630	0.4800
ZZ	0.5010	0.4620
a	0.7640	0.5600
aa	0.6530	0.4900
b	0.6290	0.5090
bb	0.4340	0.4650
c	0.5530	0.4570
cc	0.5430	0.4810
d	0.6260	0.5090
dd	0.6700	0.5000
e	0.7180	0.5390
ee	0.5340	0.4690
f	0.7230	0.5520
ff	0.1370	0.3230
g	0.5840	0.4980
gg	0.3410	0.4240
h	0.6540	0.5170
i	0.6220	0.4850
j	0.7760	0.5620

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Chain	Atom inclusion	Q-score
k	 0.4500	 0.4400
l	 0.7300	 0.5520
m	 0.6770	 0.5280
n	 0.6400	 0.5120
o	 0.6680	 0.5240
p	 0.6440	 0.5060
q	 0.0230	 0.2450
r	 0.0940	 0.2690