Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:50 PM EST

PDB ID	:	7UCJ
EMDB ID	:	EMD-26444
Title	:	Mammalian 80S translation initiation complex with mRNA and Harringtonine
Authors	:	Yang, R.; Arango, D.; Sturgill, D.; Oberdoerffer, S.
Deposited on	:	2022-03-16
Resolution	:	3.10 Å(reported)

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

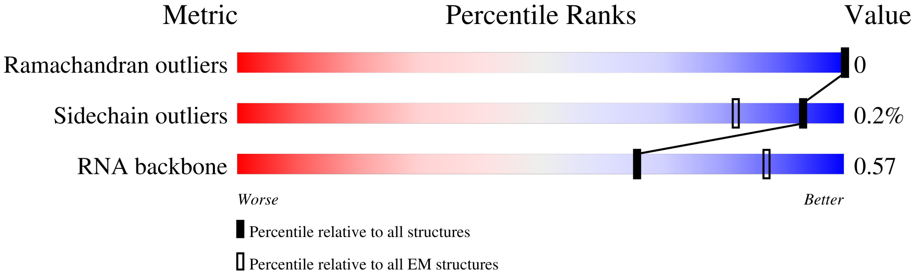
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

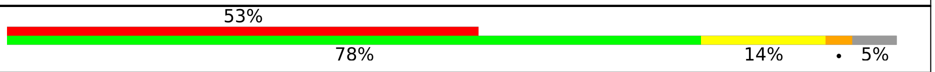
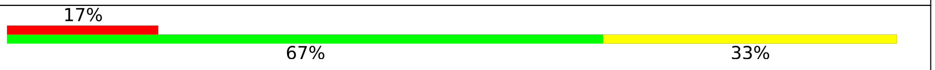
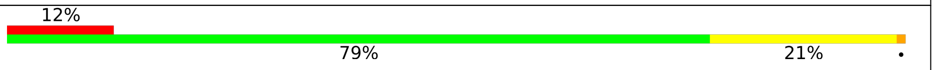
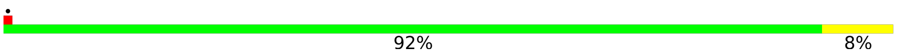
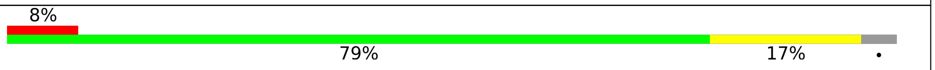
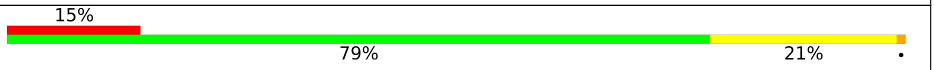
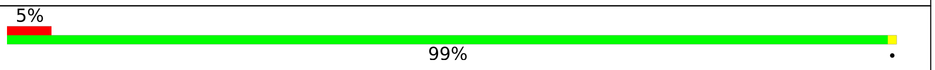
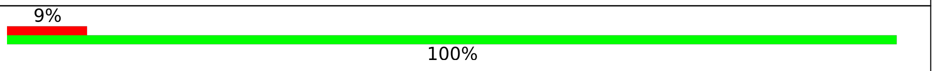
The reported resolution of this entry is 3.10 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2	76	
2	1	6	
3	5	3499	
4	7	120	
5	8	156	
6	9	1698	
7	A	248	
8	B	394	

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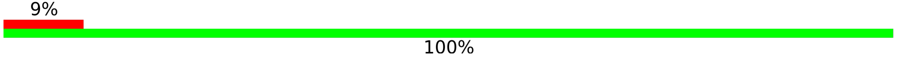
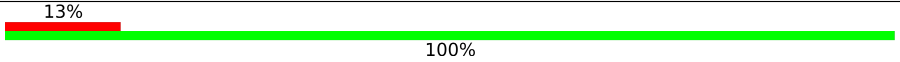
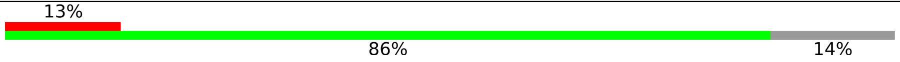
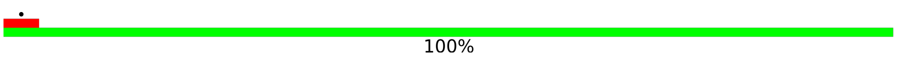
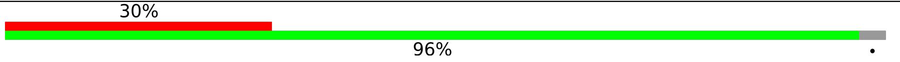
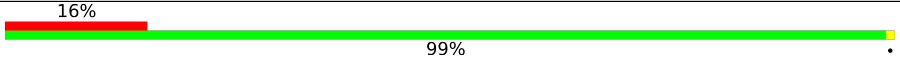
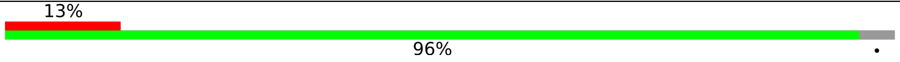
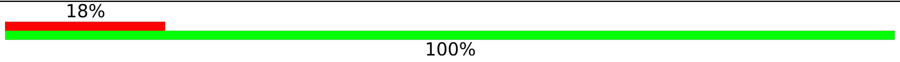
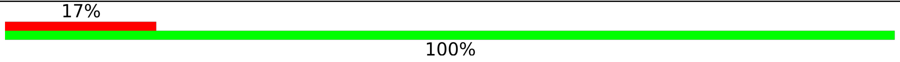
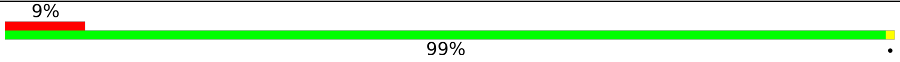
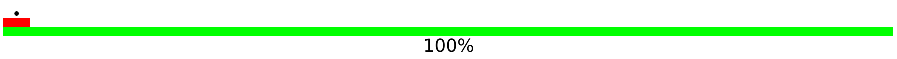
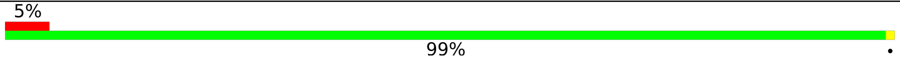
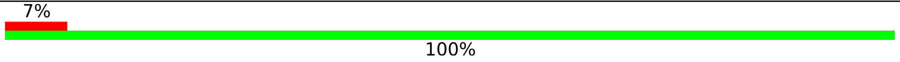
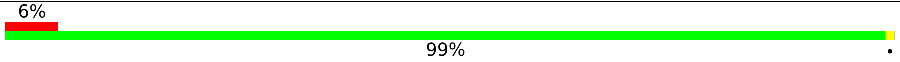
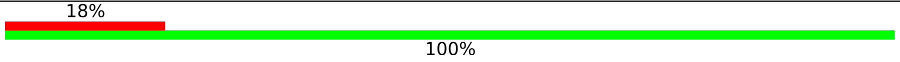
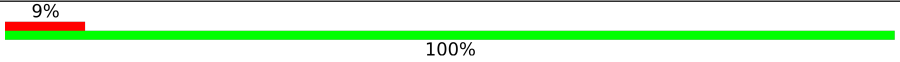
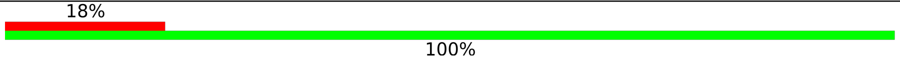
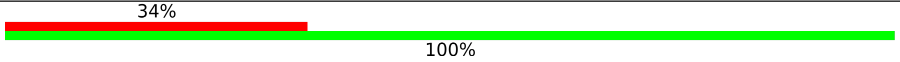
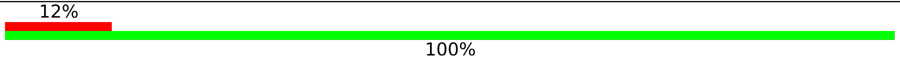
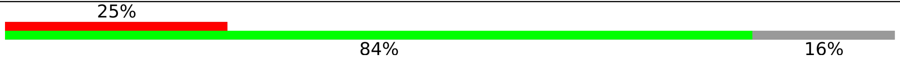
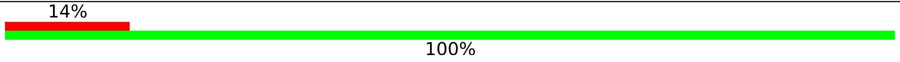
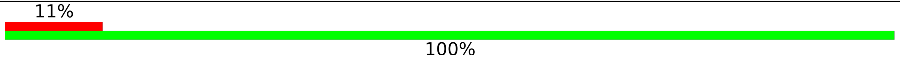
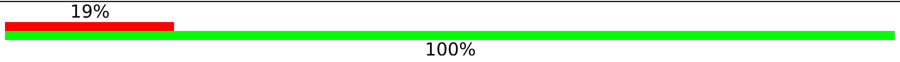
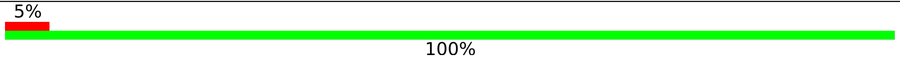
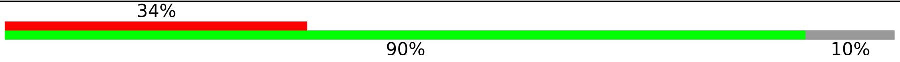
Mol	Chain	Length	Quality of chain
9	C	360	
10	D	291	
11	E	250	
12	F	225	
13	G	233	
14	H	190	
15	I	213	
16	J	169	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	98	
27	V	130	
28	W	95	
29	X	118	
30	Y	134	
31	Z	135	
32	a	147	
33	b	116	

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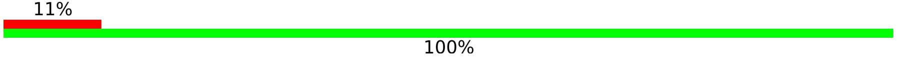
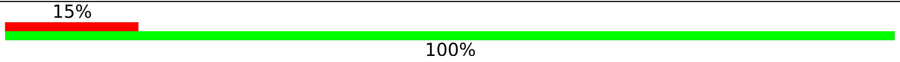
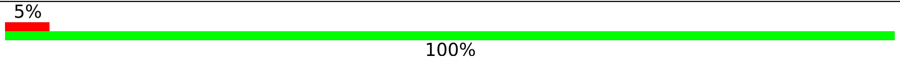
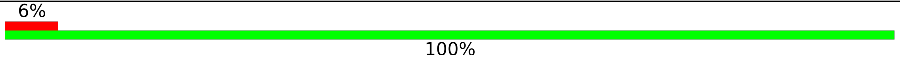
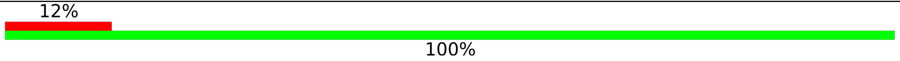
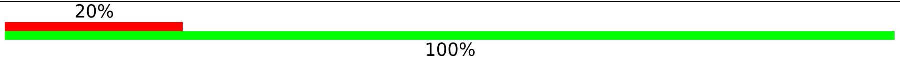
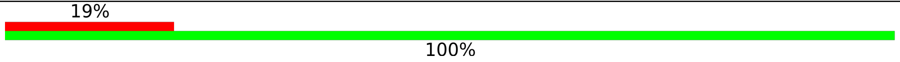
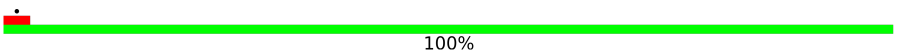
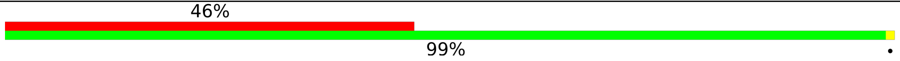
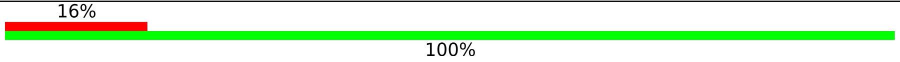
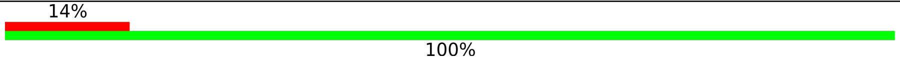
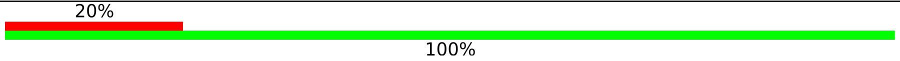
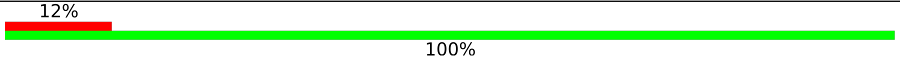
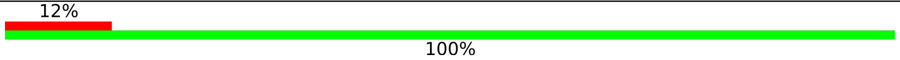
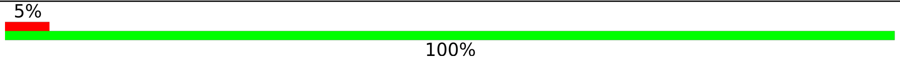
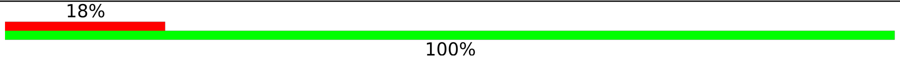
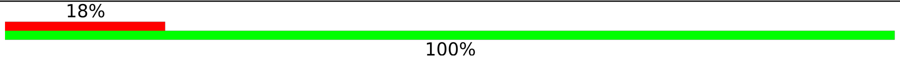
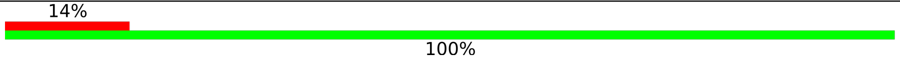
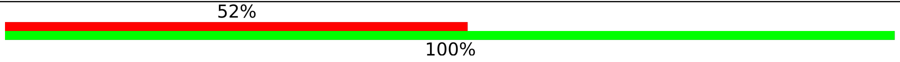
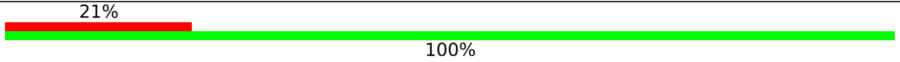
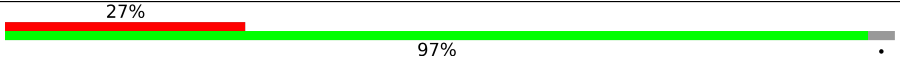
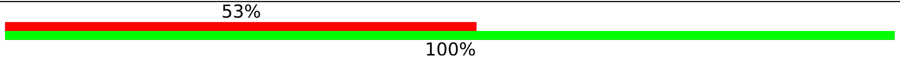
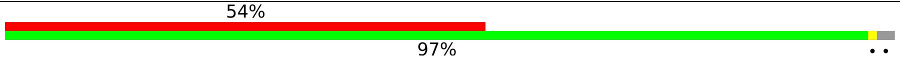
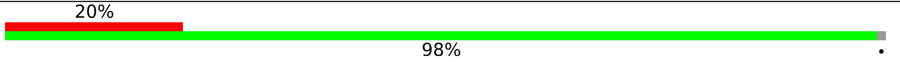
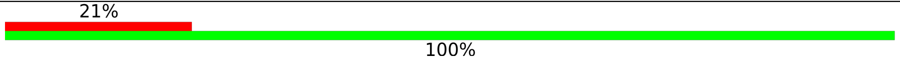
Mol	Chain	Length	Quality of chain
34	c	95	
35	d	107	
36	e	128	
37	f	109	
38	g	114	
39	h	122	
40	i	102	
41	j	86	
42	k	69	
43	l	50	
44	m	51	
45	n	25	
46	o	103	
47	p	91	
48	r	124	
49	AA	217	
50	BB	211	
51	CC	221	
52	DD	227	
53	EE	262	
54	FF	191	
55	GG	237	
56	HH	189	
57	II	206	
58	JJ	185	

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Mol	Chain	Length	Quality of chain
59	KK	96	67% 100%
60	LL	151	12% 95% 5%
61	NN	149	13% 100%
62	OO	136	15% 100%
63	PP	120	55% 99% •
64	QQ	142	35% 100%
65	RR	132	55% 100%
66	SS	144	37% 99% •
67	TT	141	37% 100%
68	UU	100	61% 99% •
69	VV	83	28% 100%
70	WW	129	9% 100%
71	XX	141	13% 100%
72	YY	124	28% 100%
73	ZZ	75	48% 100%
74	Aa	101	17% 100%
75	Bb	83	31% 100%
76	Cc	62	42% 95% 5%
77	Dd	55	22% 100%
78	Ee	55	38% 100%
79	Gg	313	73% 99% •

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 208732 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 P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	72	1552	694	289	498	71	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	6	130	58	25	41	6	0	0

- Molecule 3 is a RNA chain called 28s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	3499	75142	33527	13732	24384	3499	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	7	120	2558	1141	456	842	119	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	8	150	3192	1424	561	1057	150	0	0

- Molecule 6 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	9	1698	36291	16217	6509	11868	1697	0	0

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

- Molecule 8 is a protein called 60S ribosomal protein L3.

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

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	360	2870	1806	575	475	14	0	0

- Molecule 10 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	291	2381	1506	436	425	14	0	0

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	215	1720	1109	327	281	3	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7.

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

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	226	1830	1167	353	306	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein L10.

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

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	169	1353	855	252	240	6	0	0

- Molecule 17 is a protein called 60S ribosomal protein L13.

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

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	98	800	514	139	145	2	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	130	973	615	183	170	5	0	0

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	80	654	412	130	109	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L23a.

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

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called 60S ribosomal protein L29.

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

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	95	738	467	131	134	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

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

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	m	51	420	261	88	65	6	0	0

- Molecule 45 is a protein called eL41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	103	842	528	172	136	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

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

- Molecule 49 is a protein called 40S_SA_C domain-containing protein.

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

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BB	211	1715	1088	307	306	14	0	0

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	73	MET	VAL	conflict	UNP G1TUT9
CC	101	SER	ALA	conflict	UNP G1TUT9
CC	119	GLY	ALA	conflict	UNP G1TUT9
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	215	MET	LEU	conflict	UNP G1TUT9
CC	227	ARG	TRP	conflict	UNP G1TUT9

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DD	227	Total 1760	C 1121	N 317	O 315	S 7	0	0

- Molecule 53 is a protein called 40S ribosomal protein S4.

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

- Molecule 54 is a protein called Ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S6.

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

- Molecule 56 is a protein called 40S ribosomal protein S7.

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

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	II	203	Total 1668	C 1047	N 328	O 288	S 5	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 58 is a protein called 40S ribosomal protein S9.

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

- Molecule 59 is a protein called 40S ribosomal protein S10.

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

- Molecule 60 is a protein called 40S ribosomal protein S11.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14.

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

- Molecule 63 is a protein called 40S ribosomal protein S15.

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

- Molecule 64 is a protein called 40S ribosomal protein S16.

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

- Molecule 65 is a protein called 40S ribosomal protein S17.

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

- Molecule 66 is a protein called 40S ribosomal protein S18.

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

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	TT	141	1097	688	211	195	3	0	0

- Molecule 68 is a protein called 40S ribosomal protein S20.

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

- Molecule 69 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 70 is a protein called 40S ribosomal protein S15a.

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

- Molecule 71 is a protein called 40S ribosomal protein S23.

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

- Molecule 72 is a protein called 40S ribosomal protein S24.

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

- Molecule 73 is a protein called 40S ribosomal protein S25.

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

- Molecule 74 is a protein called eS26.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 75 is a protein called 40S ribosomal protein S27.

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

- Molecule 76 is a protein called 40S ribosomal protein S28.

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

- Molecule 77 is a protein called 40S ribosomal protein S29.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

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

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
80	5	196	196	196	0
80	7	7	7	7	0
80	8	7	7	7	0
80	9	77	77	77	0
80	A	1	1	1	0
80	I	1	1	1	0

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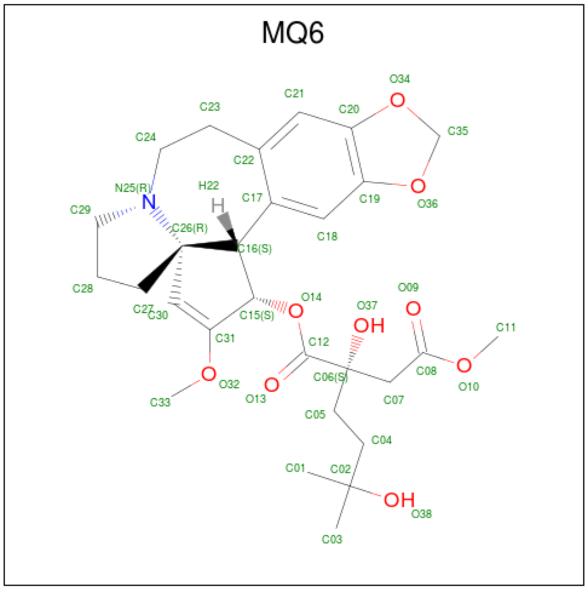
Mol	Chain	Residues	Atoms	AltConf
80	N	1	Total Mg 1 1	0
80	P	1	Total Mg 1 1	0
80	V	1	Total Mg 1 1	0
80	a	1	Total Mg 1 1	0
80	g	1	Total Mg 1 1	0
80	FF	1	Total Mg 1 1	0
80	TT	1	Total Mg 1 1	0

- Molecule 81 is Harringtonine (three-letter code: MQ6) (formula: $C_{28}H_{37}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
81	5	1	Total C N O 38 28 1 9	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
82	g	1	Total Zn 1 1	0

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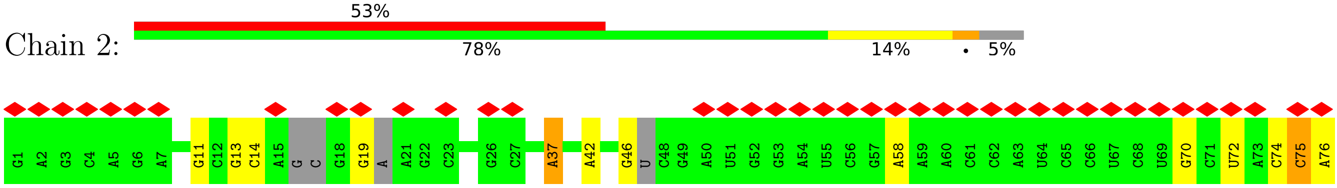
Mol	Chain	Residues	Atoms		AltConf
82	j	1	Total 1	Zn 1	0
82	m	1	Total 1	Zn 1	0
82	o	1	Total 1	Zn 1	0
82	p	1	Total 1	Zn 1	0
82	Aa	1	Total 1	Zn 1	0
82	Dd	1	Total 1	Zn 1	0

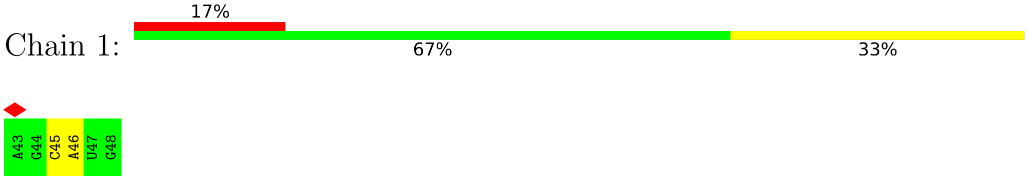
3 Residue-property plots ⓘ

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.

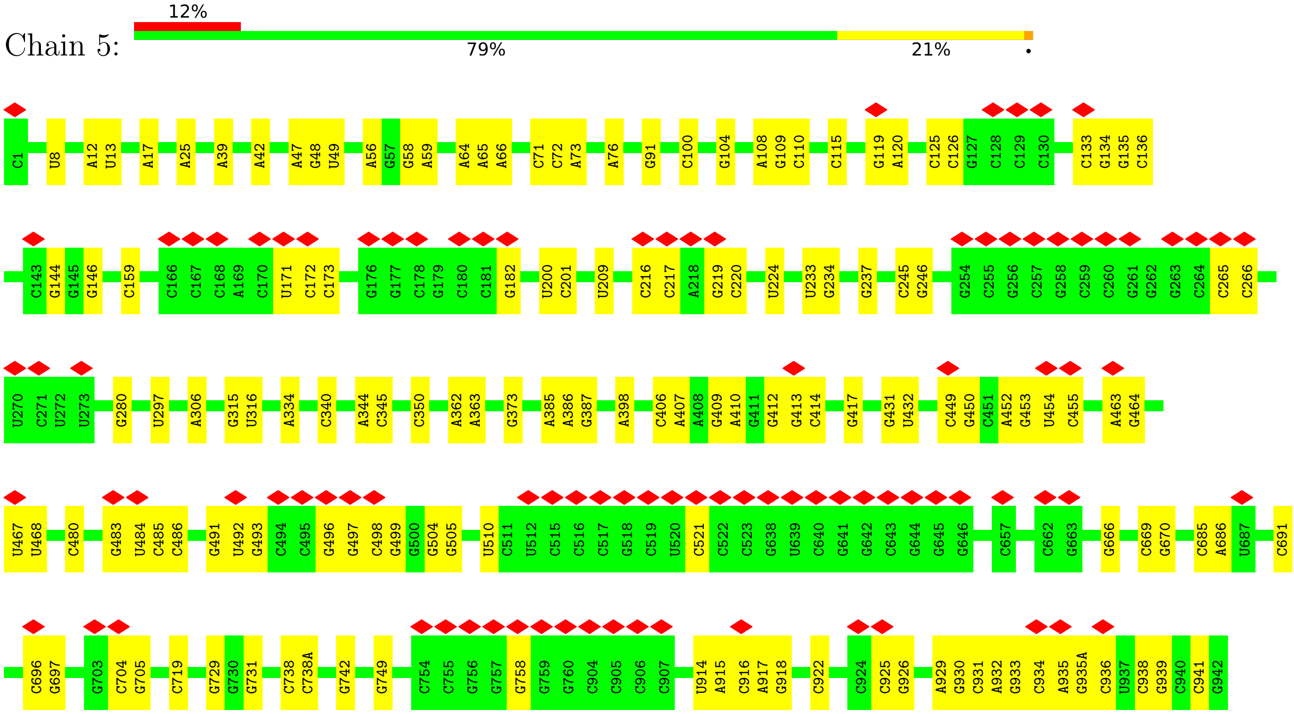
- Molecule 1: P-site tRNA

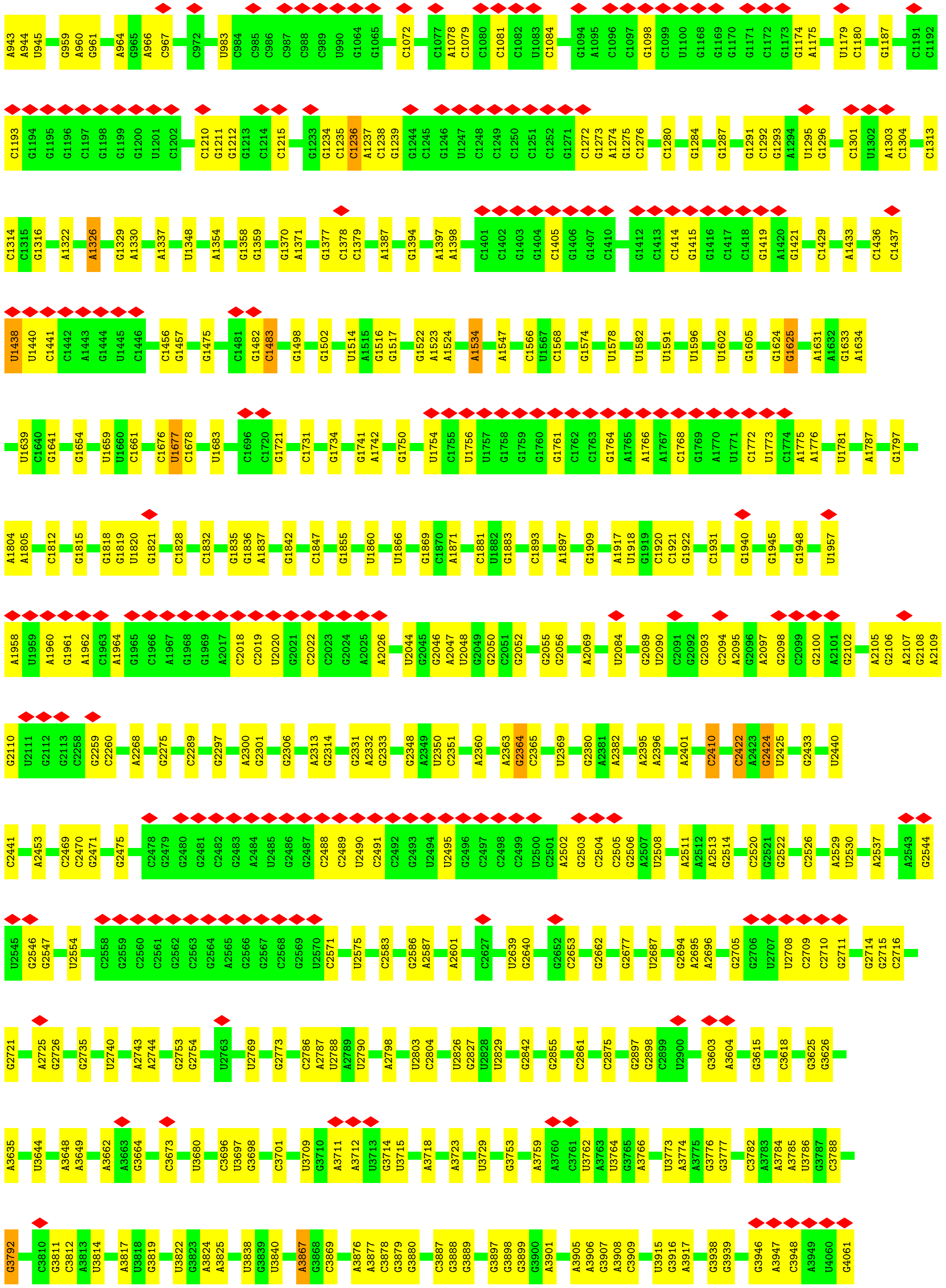


- Molecule 2: mRNA



- Molecule 3: 28s rRNA




A943 A944 U945 G959 A960 G961 A964 G965 A966 C967 C972 U983 C984 G985 C986 C987 C988 C989 U990 G1064 G1065 C1072 C1077 A1078 C1079 C1080 C1081 C1082 U1083 C1084 G1094 A1095 C1096 C1097 G1098 C1099 U1100 G1168 G1169 G1170 G1171 C1172 G1173 G1174 A1175 U1179 C1180 G1187 C1191 C1192
C1193 G1194 G1195 G1196 C1197 G1198 G1199 G1200 U1201 C1202 C1210 G1211 G1212 G1213 C1214 C1215 G1233 G1234 C1235 C1236 A1237 C1238 G1239 G1244 C1245 G1246 U1247 C1248 C1249 C1250 C1251 C1252 G1271 C1272 G1273 A1274 G1275 C1276 C1280 G1284 G1287 G1291 C1292 G1293 A1294 U1295 G1296 C1301 U1302 A1303 C1304 C1313
C1314 C1315 G1316 A1322 A1326 G1329 A1330 A1337 U1348 A1354 G1358 G1359 G1370 A1371 G1377 C1378 C1379 A1387 G1394 A1397 A1398 C1401 C1402 G1403 G1404 C1405 G1406 G1407 C1410 G1412 C1413 C1414 G1415 G1416 C1417 C1418 G1419 A1420 G1421 C1429 A1433 C1436 C1437
U1438 U1440 C1441 C1442 A1443 G1444 U1445 C1446 C1456 G1457 G1475 C1481 G1482 C1483 G1498 G1502 U1514 A1515 G1516 G1517 G1522 A1523 A1524 A1534 A1547 C1566 U1567 C1568 G1574 U1578 U1582 U1591 U1596 U1602 G1605 G1624 G1625 A1631 A1632 G1633 A1634
U1639 C1640 G1641 G1654 U1659 U1660 C1661 C1676 U1677 C1678 U1683 C1696 C1720 G1721 C1731 G1734 G1741 A1742 G1750 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 C1774 A1775 A1776 U1781 A1787 G1797
A1804 A1805 C1812 G1815 G1818 G1819 U1820 G1821 C1828 C1832 G1835 G1836 A1837 G1842 C1847 G1855 U1860 U1866 G1869 C1870 A1871 C1881 U1882 G1883 C1893 A1897 G1909 A1917 U1918 G1919 C1920 C1921 G1922 C1931 G1940 G1945 G1948 U1957
A1958 U1959 A1960 G1961 A1962 C1963 A1964 G1965 C1966 A1967 G1968 G1969 A2017 C2018 C2019 U2020 G2021 C2022 C2023 G2024 A2025 A2026 U2044 G2045 G2046 A2047 U2048 G2049 C2050 C2051 G2052 G2055 G2056 A2069 U2084 G2089 U2090 C2091 G2092 G2093 C2094 A2095 G2096 A2097 G2098 C2099 G2100 A2101 G2102 A2105 G2106 A2107 G2108 A2109
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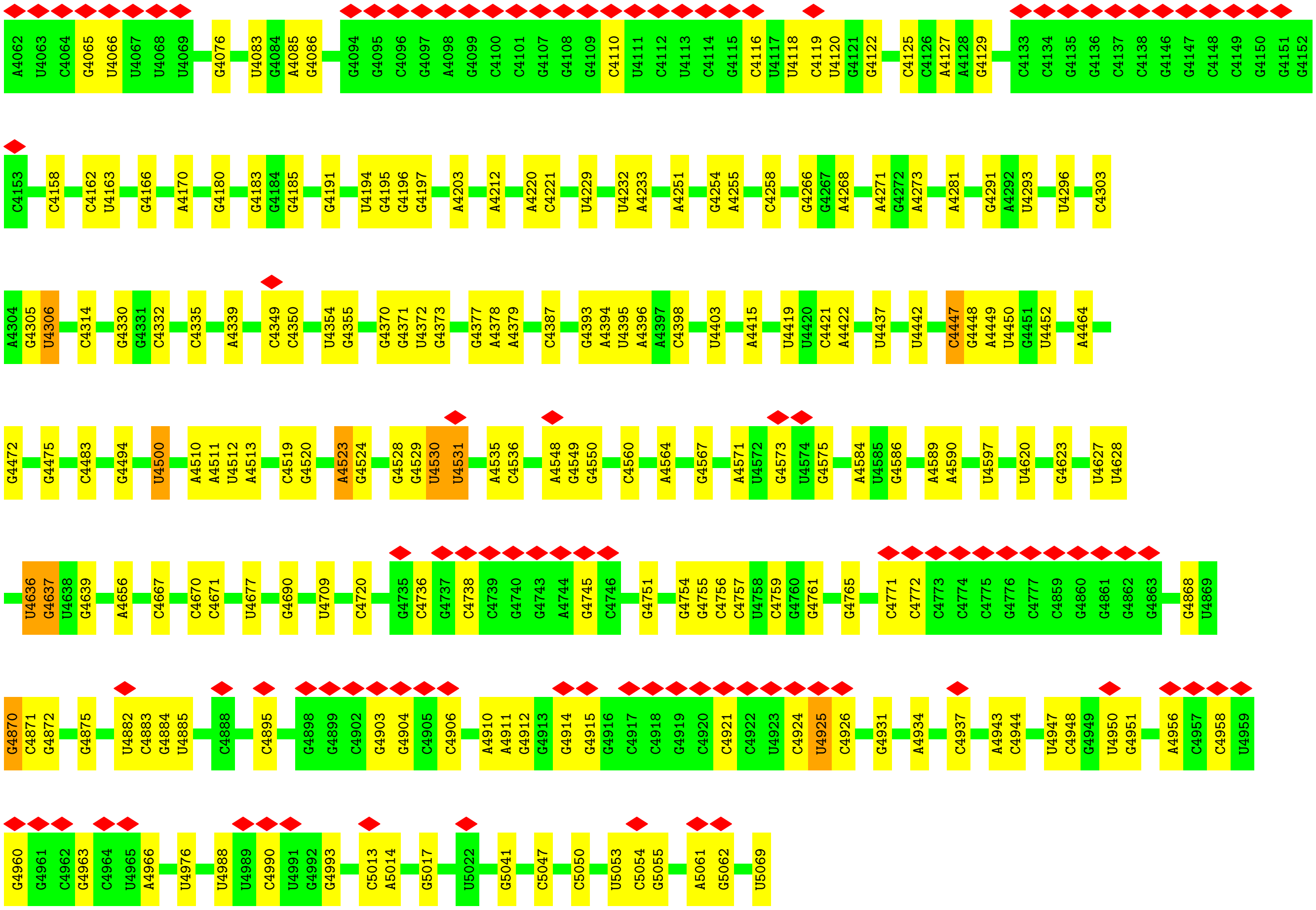
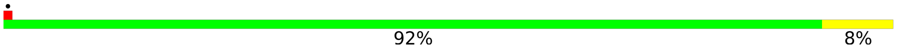
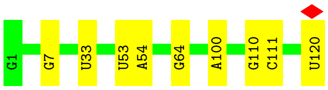


- Molecule 4: 5S rRNA

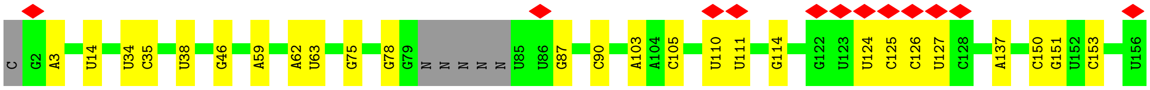
Chain 7:





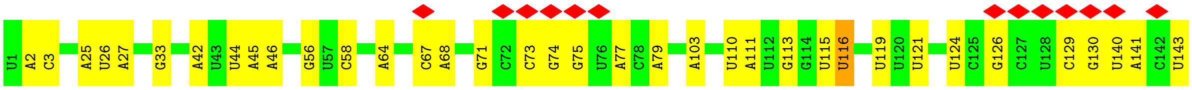
- Molecule 5: 5.8S rRNA

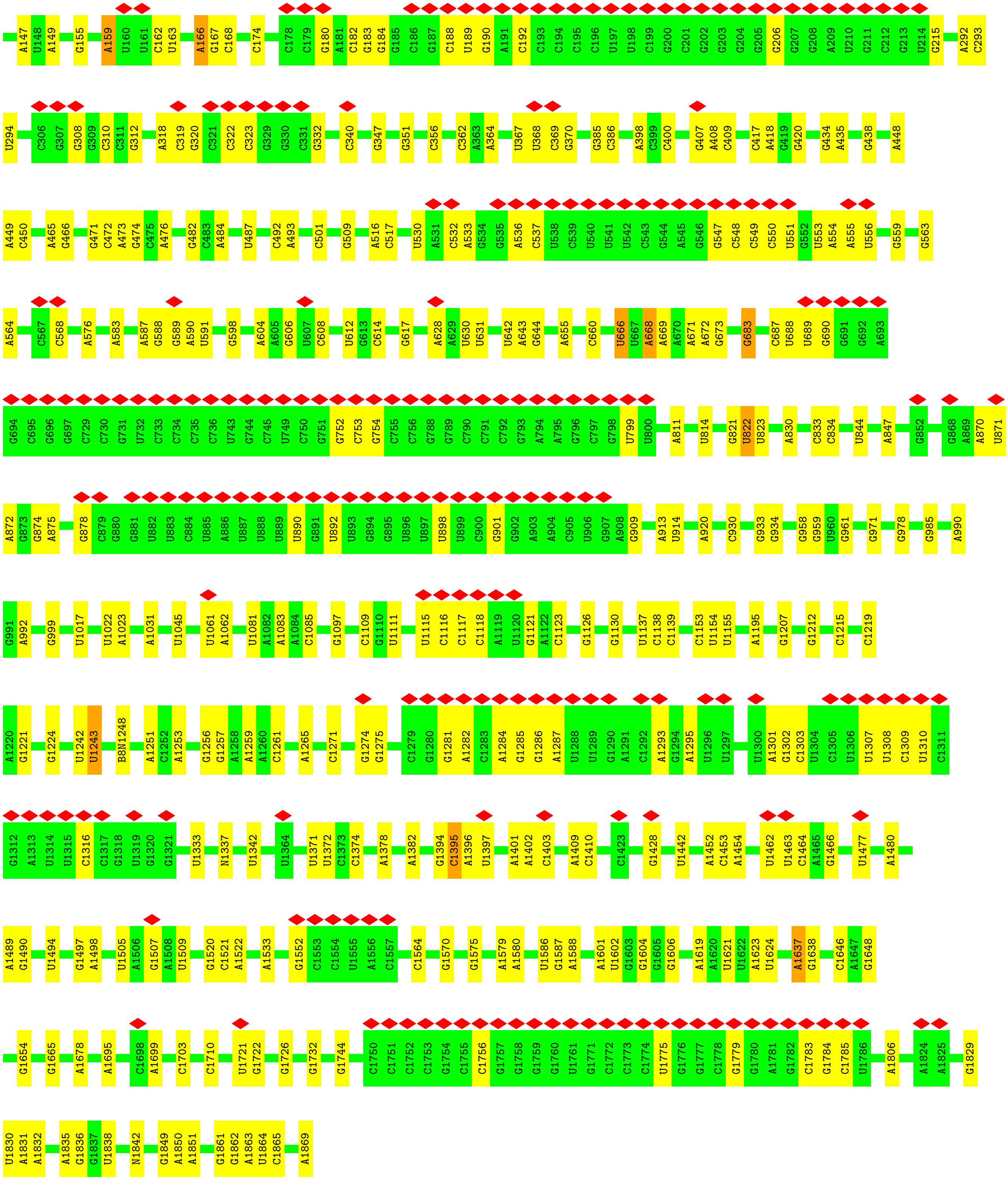
Chain 8:



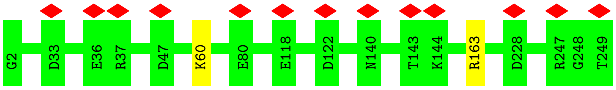
- Molecule 6: 18S rRNA

Chain 9:



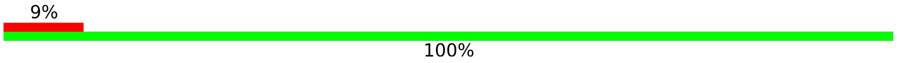


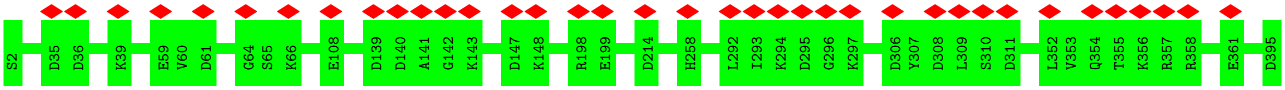
- Molecule 7: 60S ribosomal protein L8



- Molecule 8: 60S ribosomal protein L3

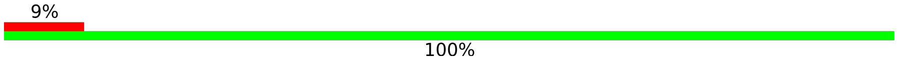
Chain B:

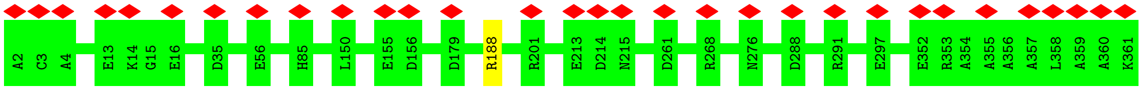




- Molecule 9: 60S ribosomal protein L4

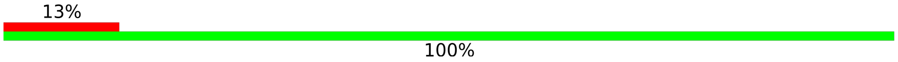
Chain C:

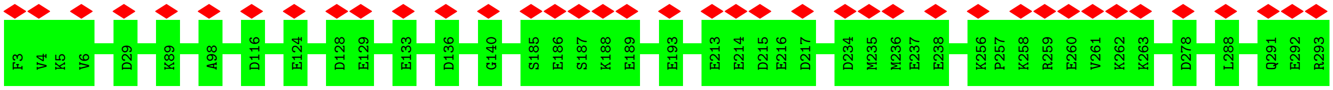




- Molecule 10: Ribosomal_L18_c domain-containing protein

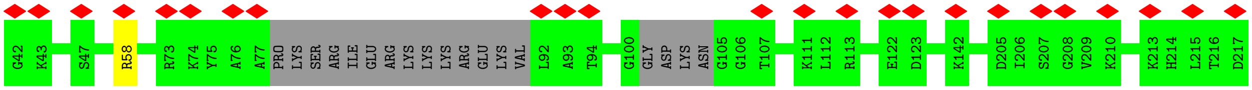
Chain D:

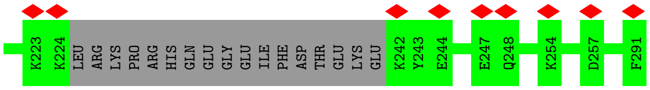




- Molecule 11: 60S ribosomal protein L6

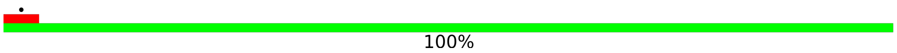
Chain E:

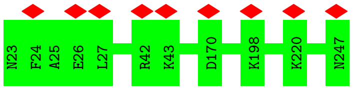




- Molecule 12: 60S ribosomal protein L7

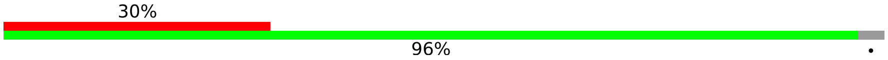
Chain F:

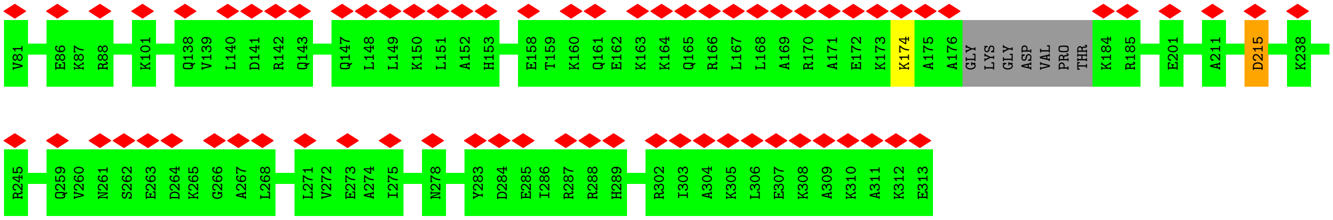




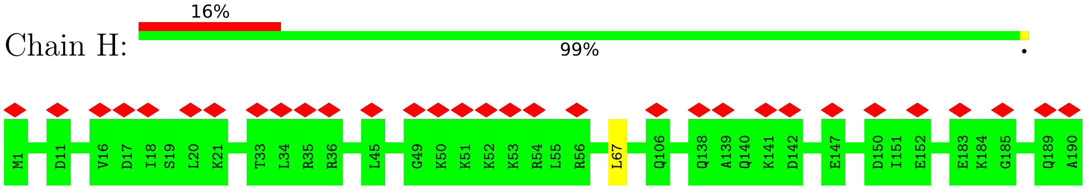
- Molecule 13: 60S ribosomal protein L7a

Chain G:

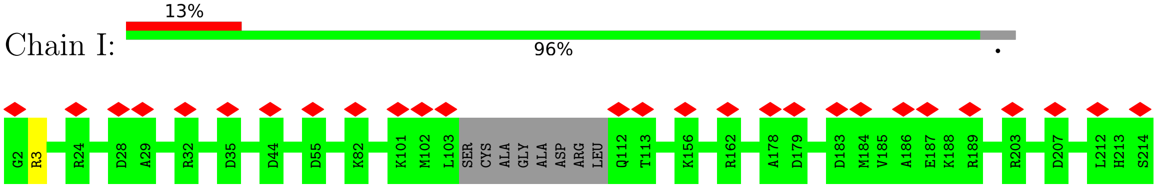




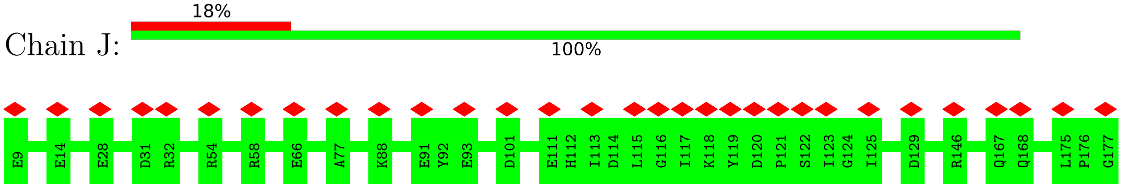
- Molecule 14: 60S ribosomal protein L9



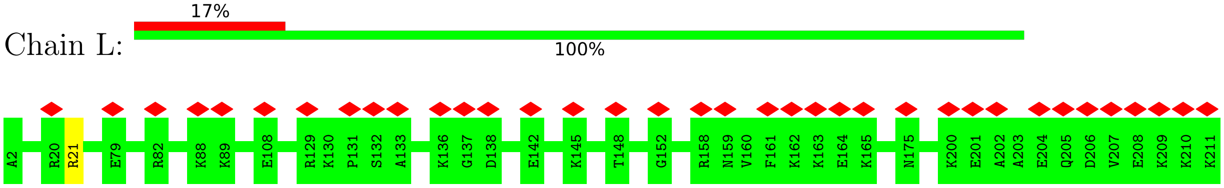
- Molecule 15: Ribosomal protein L10



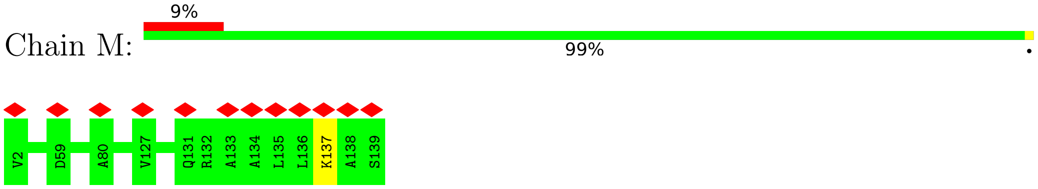
- Molecule 16: 60S ribosomal protein L11



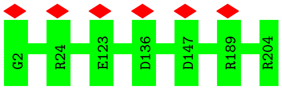
- Molecule 17: 60S ribosomal protein L13



- Molecule 18: 60S ribosomal protein L14

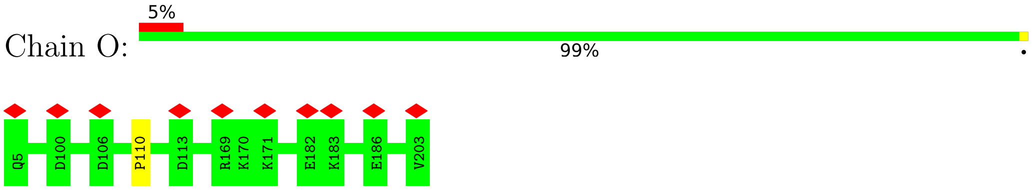


- Molecule 19: 60S ribosomal protein L15



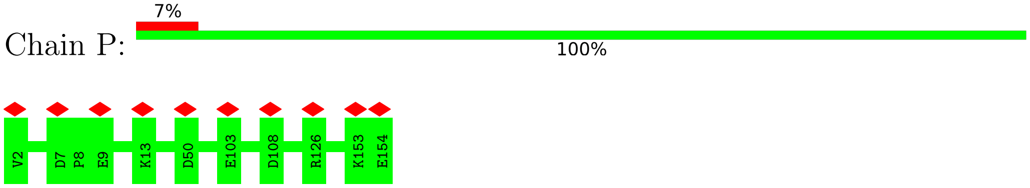
- Molecule 20: 60S ribosomal protein L13a

Chain O:



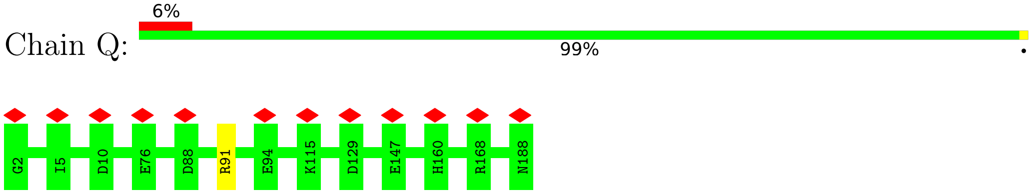
- Molecule 21: 60S ribosomal protein L17

Chain P:



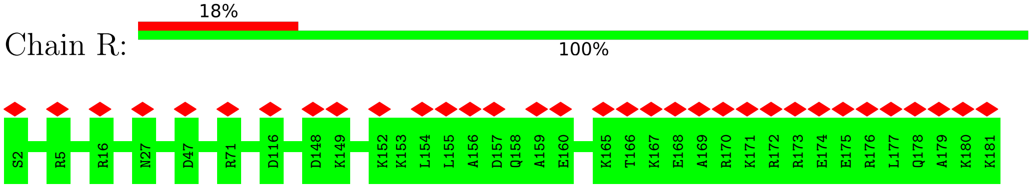
- Molecule 22: 60S ribosomal protein L18

Chain Q:



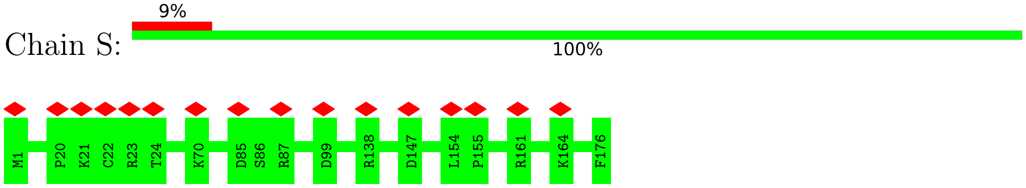
- Molecule 23: 60S ribosomal protein L19

Chain R:



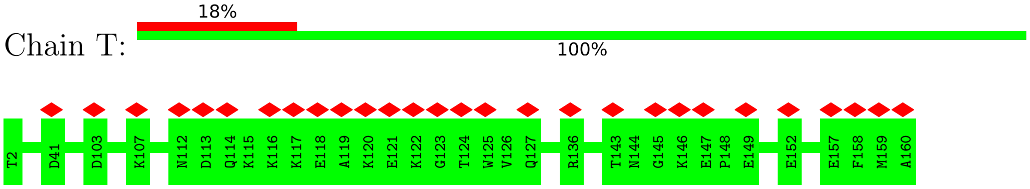
- Molecule 24: 60S ribosomal protein L18a

Chain S:



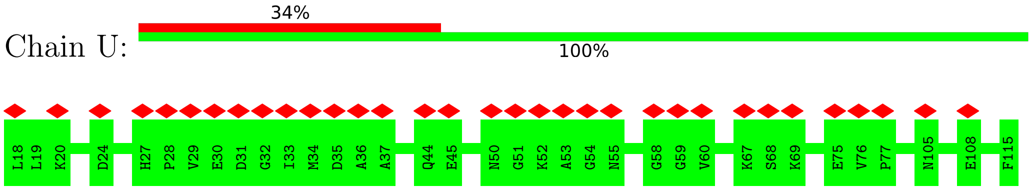
- Molecule 25: 60S ribosomal protein L21

Chain T:



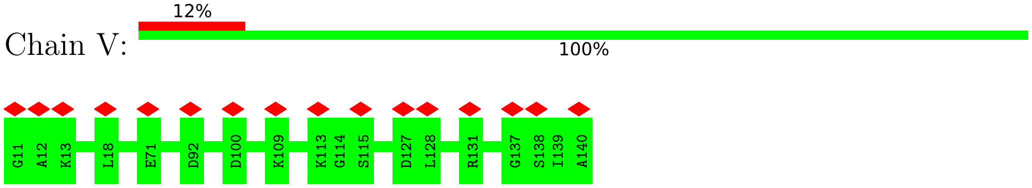
- Molecule 26: 60S ribosomal protein L22

Chain U:



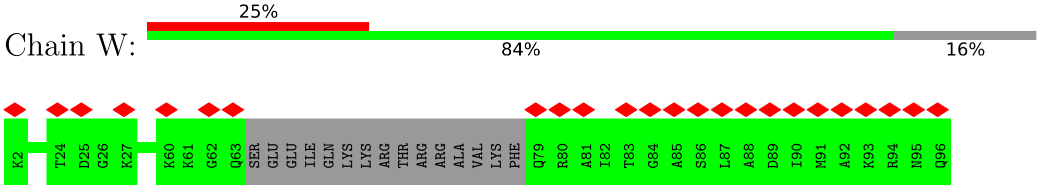
- Molecule 27: 60S ribosomal protein L23

Chain V:



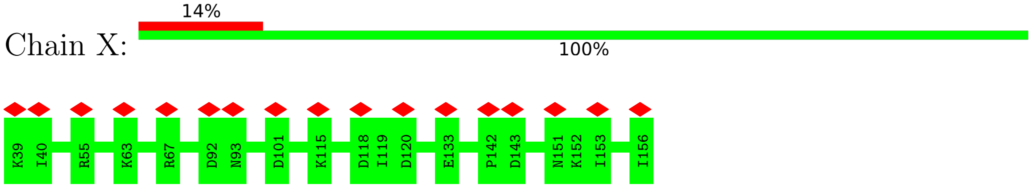
- Molecule 28: Ribosomal protein L24

Chain W:



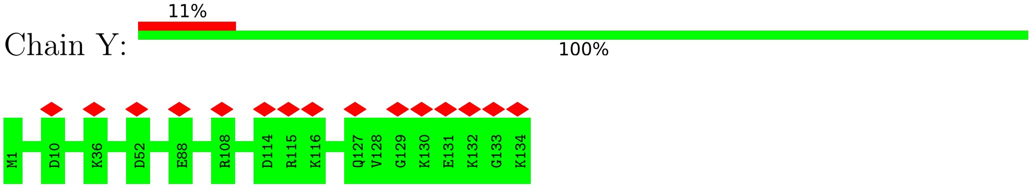
- Molecule 29: 60S ribosomal protein L23a

Chain X:



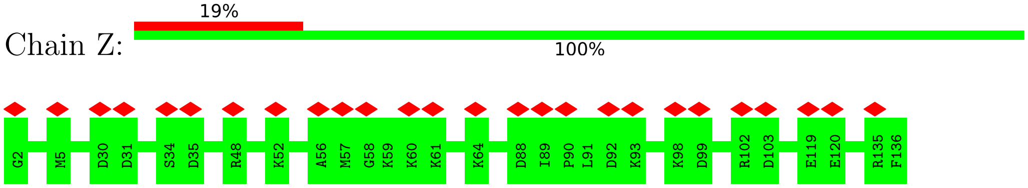
- Molecule 30: 60S ribosomal protein L26

Chain Y:



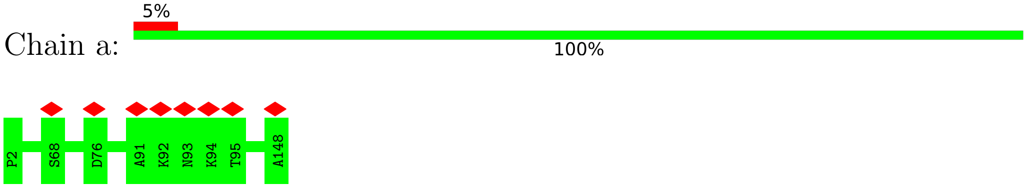
- Molecule 31: 60S ribosomal protein L27

Chain Z:

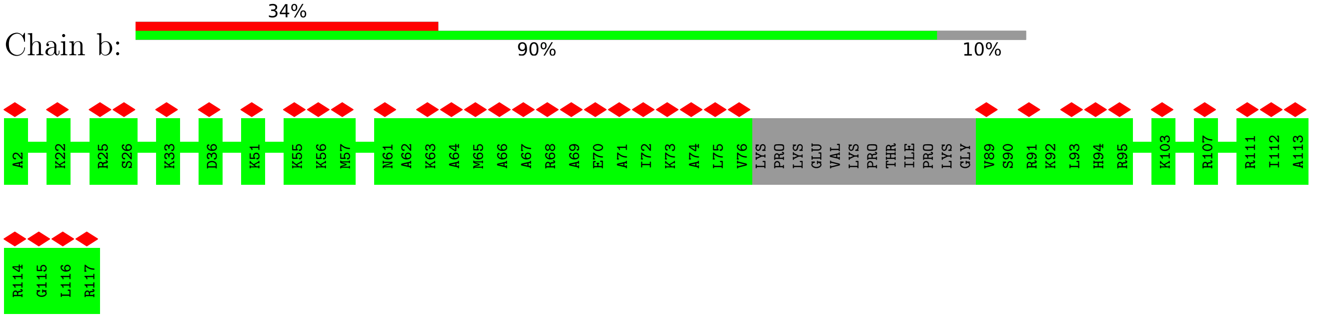


- Molecule 32: 60S ribosomal protein L27a

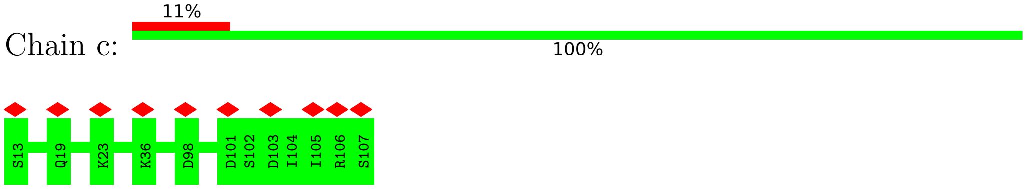
Chain a:



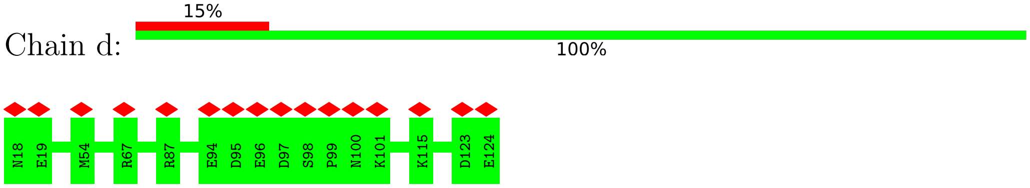
- Molecule 33: 60S ribosomal protein L29



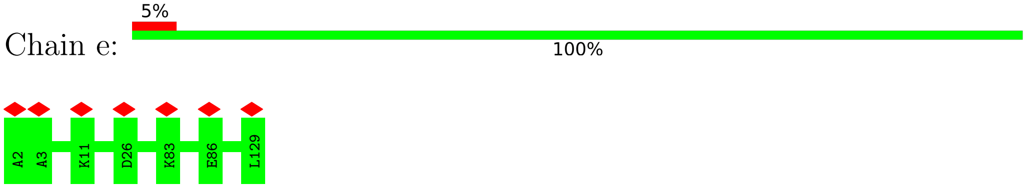
- Molecule 34: 60S ribosomal protein L30



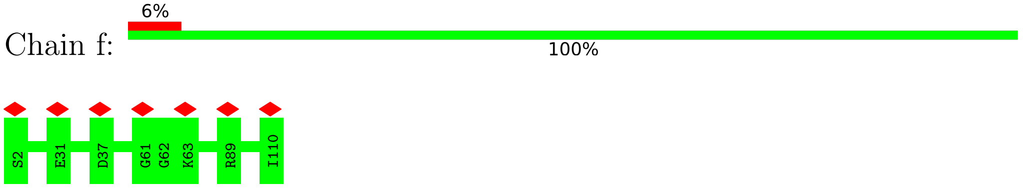
- Molecule 35: 60S ribosomal protein L31



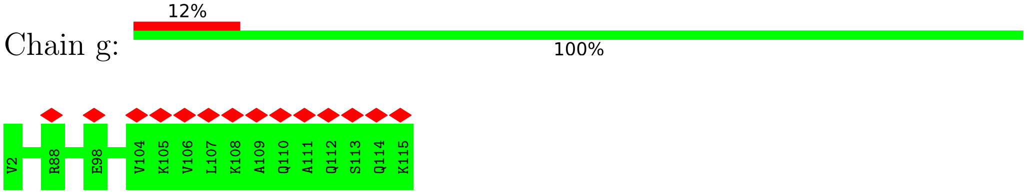
- Molecule 36: 60S ribosomal protein L32



- Molecule 37: 60S ribosomal protein L35a

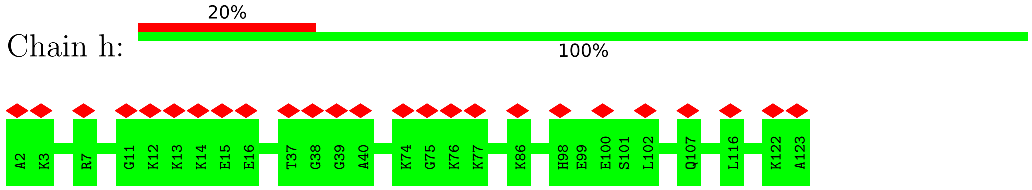


- Molecule 38: 60S ribosomal protein L34



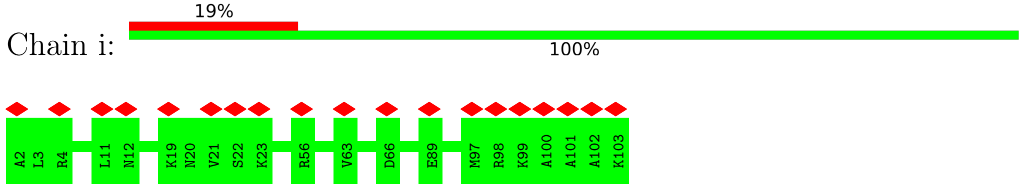
- Molecule 39: 60S ribosomal protein L35

Chain h:



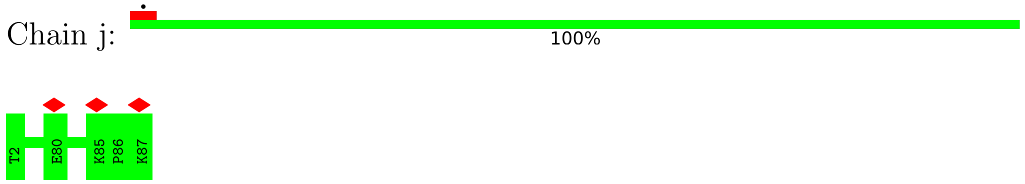
- Molecule 40: 60S ribosomal protein L36

Chain i:



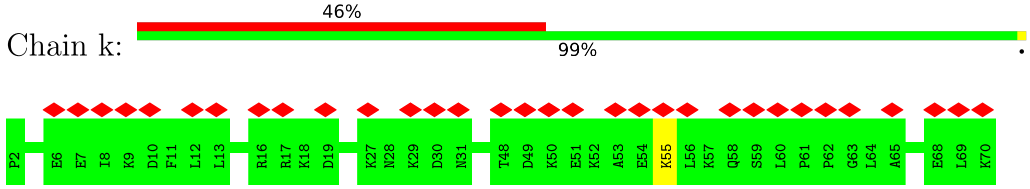
- Molecule 41: 60S ribosomal protein L37

Chain j:



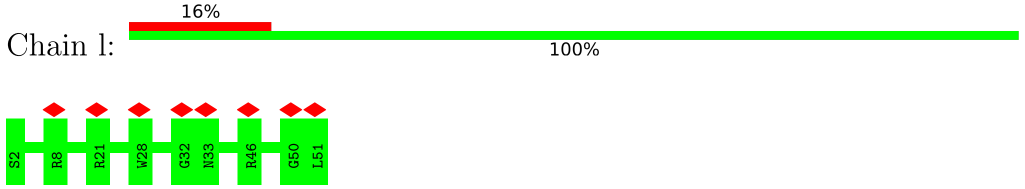
- Molecule 42: 60S ribosomal protein L38

Chain k:



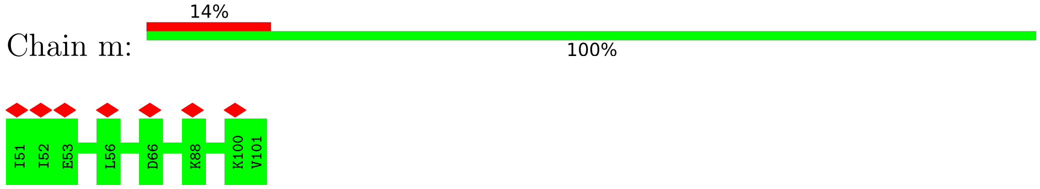
- Molecule 43: 60S ribosomal protein L39

Chain l:



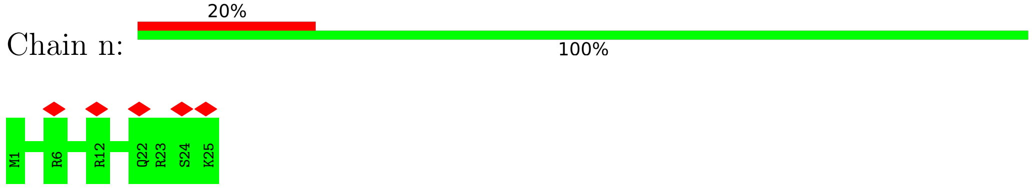
- Molecule 44: 60S ribosomal protein L40

Chain m:

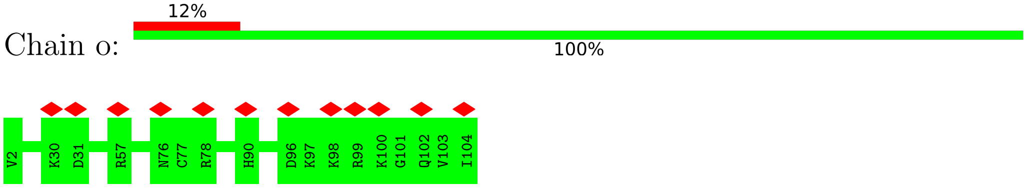


- Molecule 45: eL41

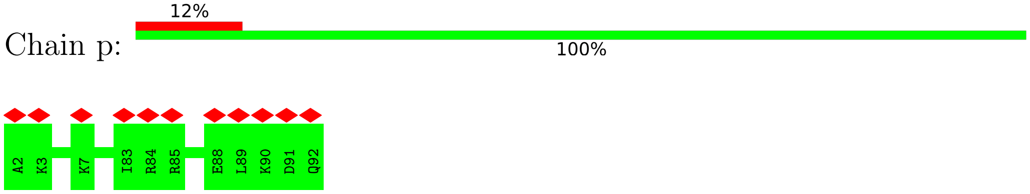
Chain n:



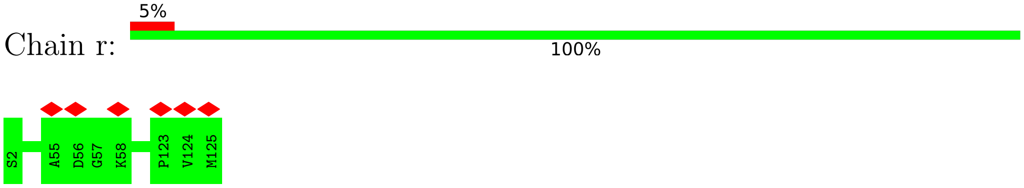
- Molecule 46: 60S ribosomal protein L36a



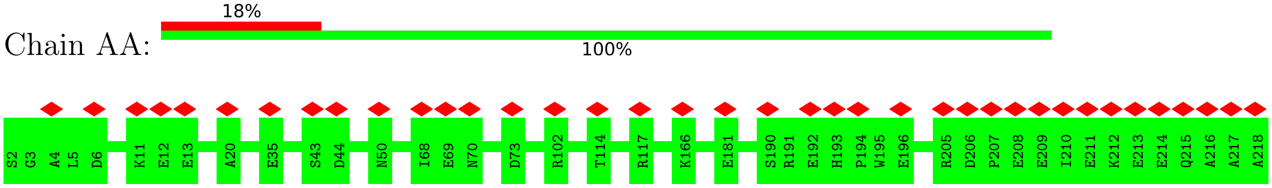
- Molecule 47: 60S ribosomal protein L37a



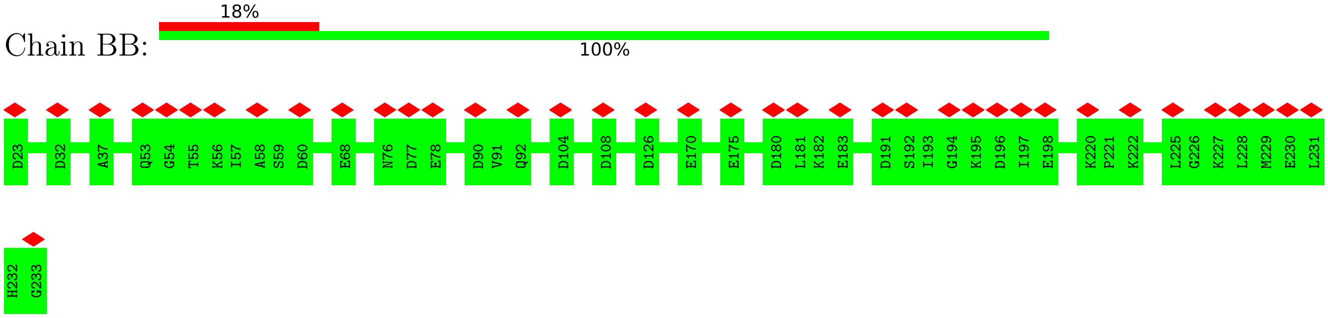
- Molecule 48: 60S ribosomal protein L28



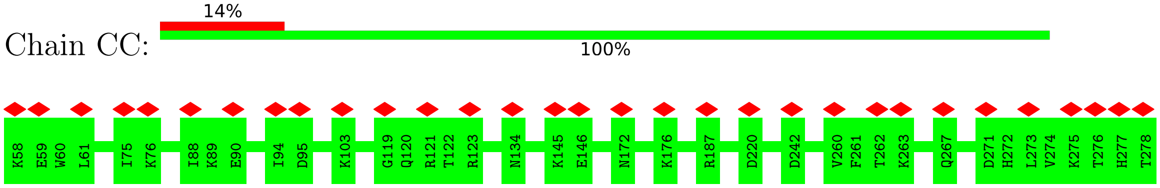
- Molecule 49: 40S_SA_C domain-containing protein



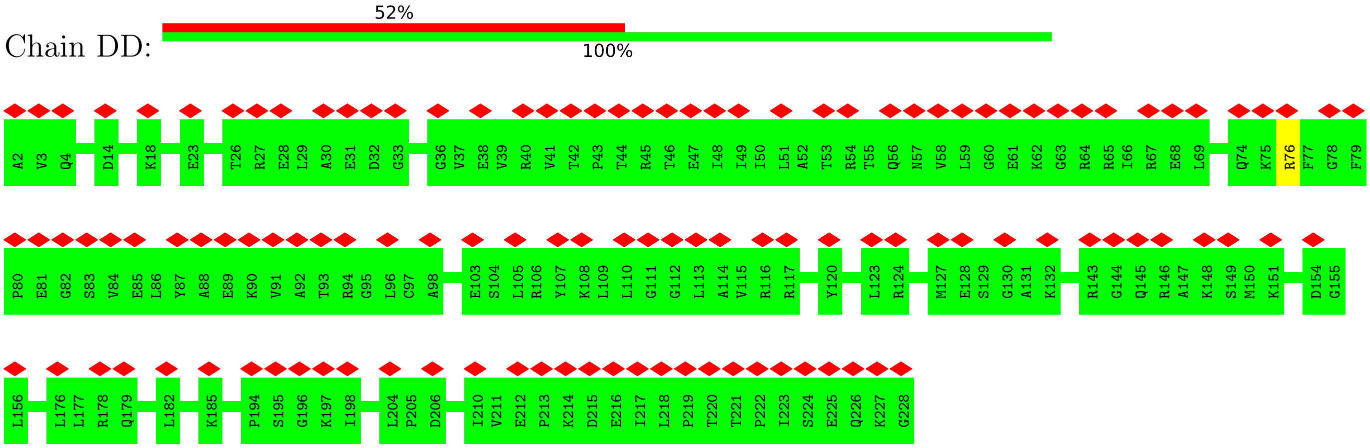
- Molecule 50: 40S ribosomal protein S3a



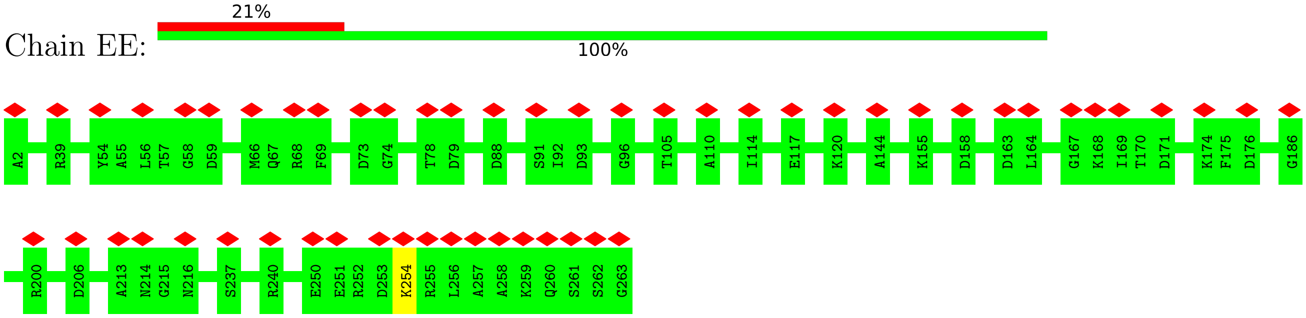
- Molecule 51: 40S ribosomal protein S2



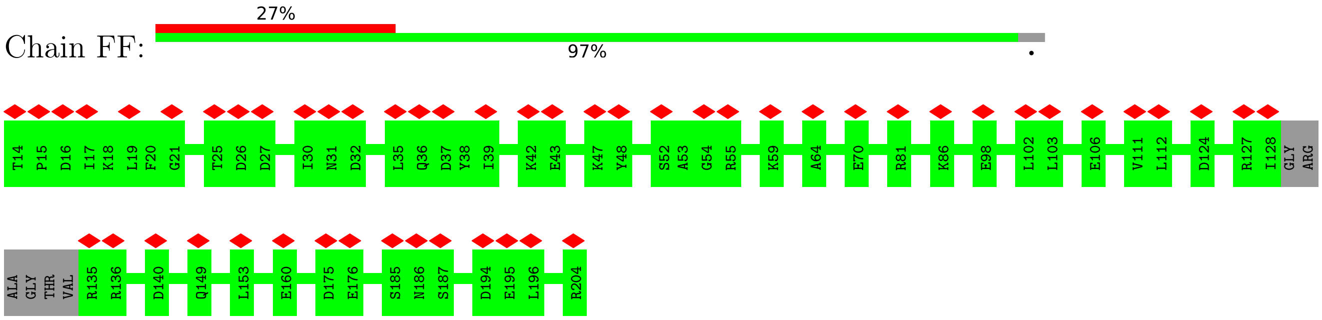
- Molecule 52: 40S ribosomal protein S3



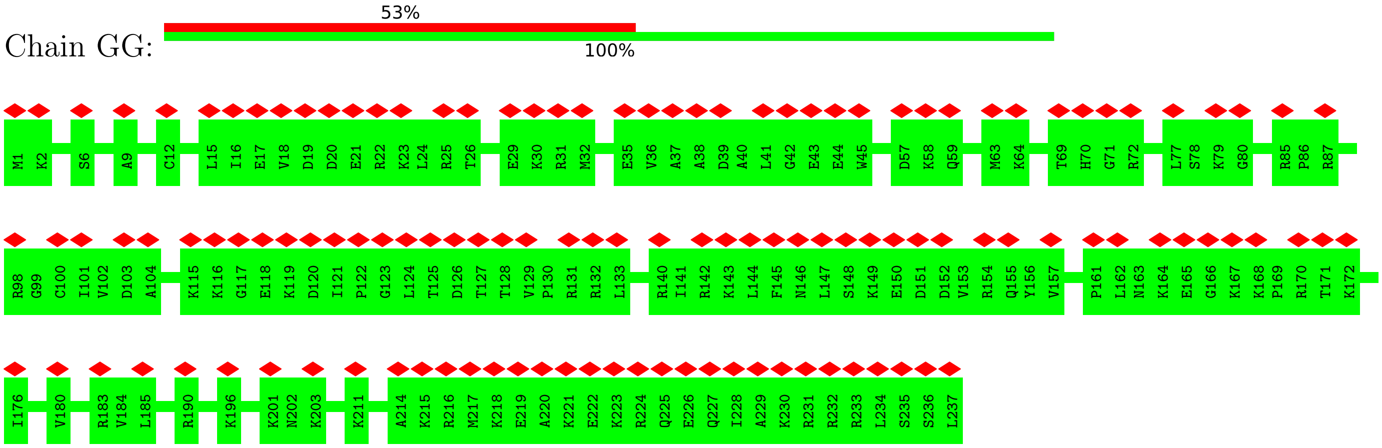
- Molecule 53: 40S ribosomal protein S4



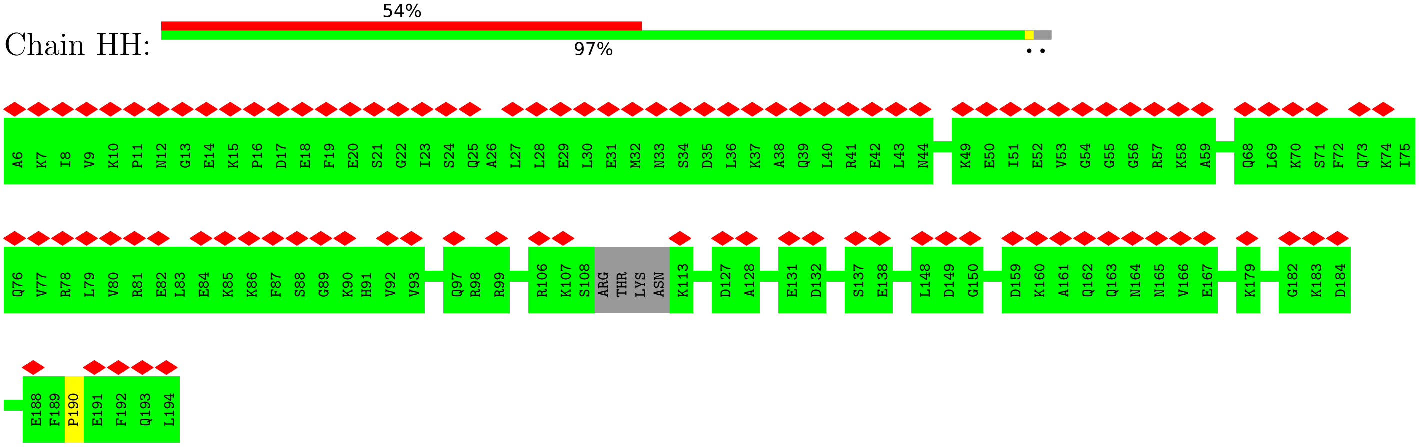
- Molecule 54: Ribosomal protein S5



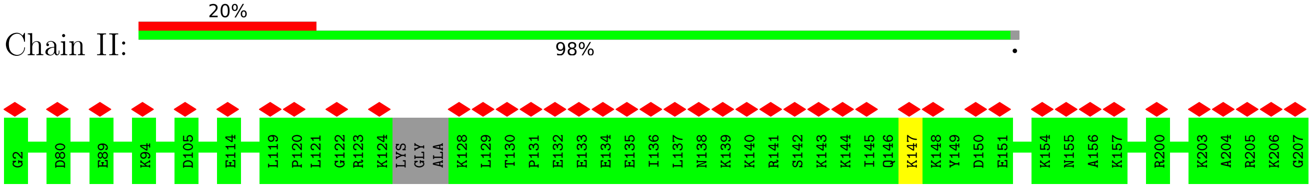
- Molecule 55: 40S ribosomal protein S6



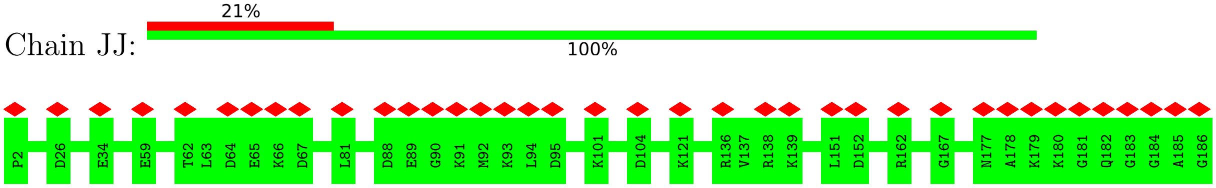
- Molecule 56: 40S ribosomal protein S7



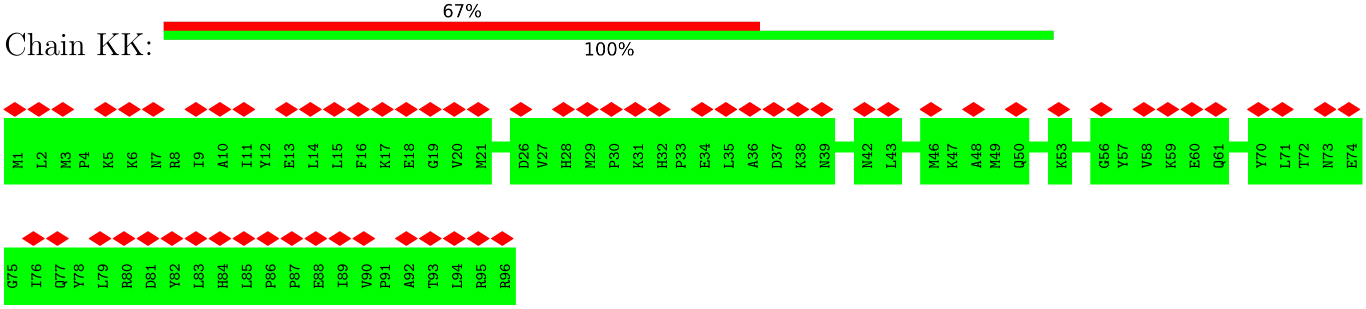
- Molecule 57: 40S ribosomal protein S8



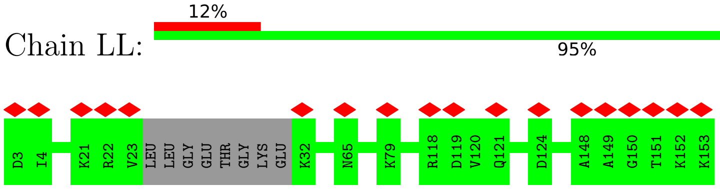
- Molecule 58: 40S ribosomal protein S9



- Molecule 59: 40S ribosomal protein S10

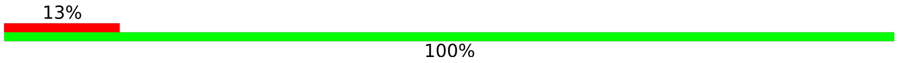


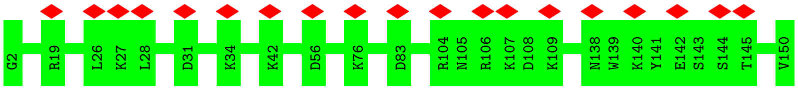
- Molecule 60: 40S ribosomal protein S11



- Molecule 61: 40S ribosomal protein S13

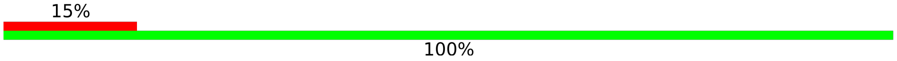
Chain NN:

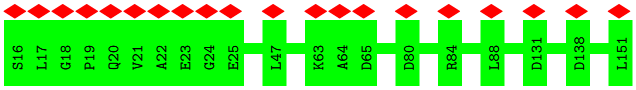




- Molecule 62: 40S ribosomal protein S14

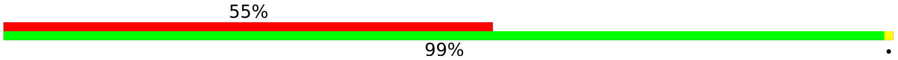
Chain OO:

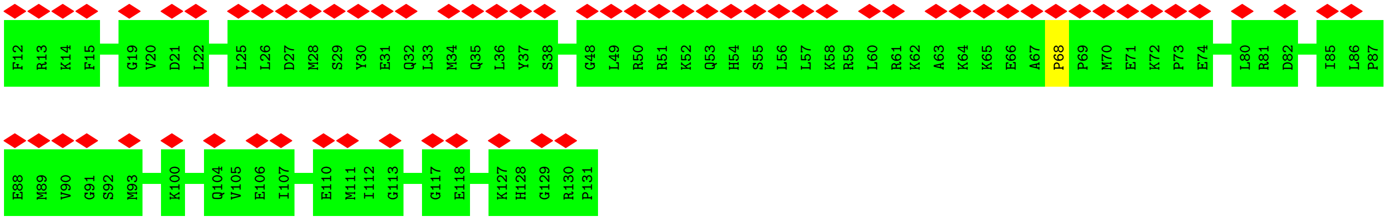




- Molecule 63: 40S ribosomal protein S15

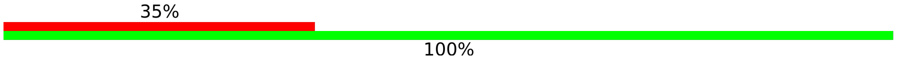
Chain PP:

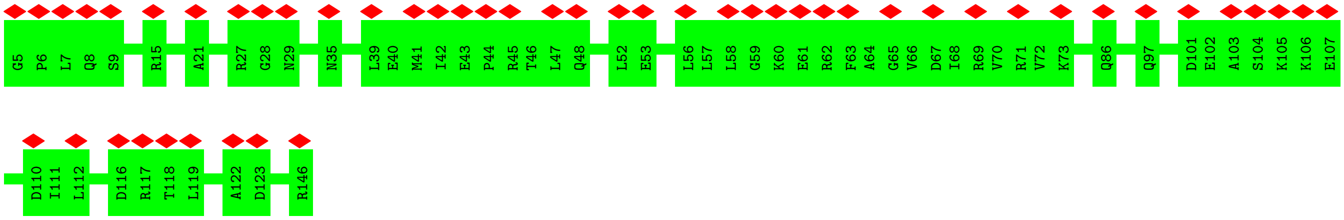




- Molecule 64: 40S ribosomal protein S16

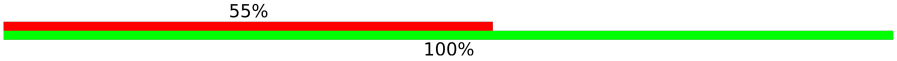
Chain QQ:

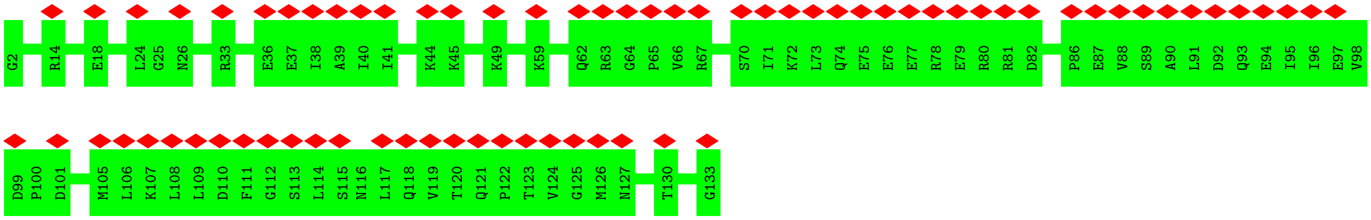




- Molecule 65: 40S ribosomal protein S17

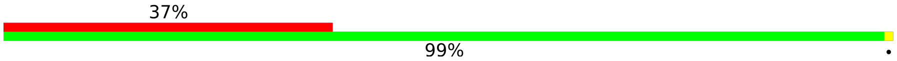
Chain RR:

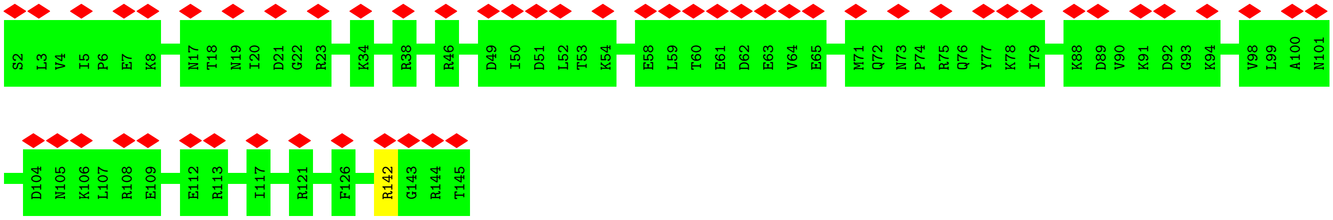




- Molecule 66: 40S ribosomal protein S18

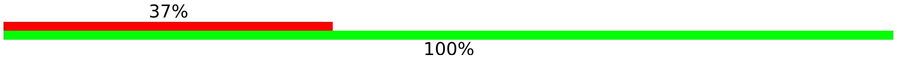
Chain SS:

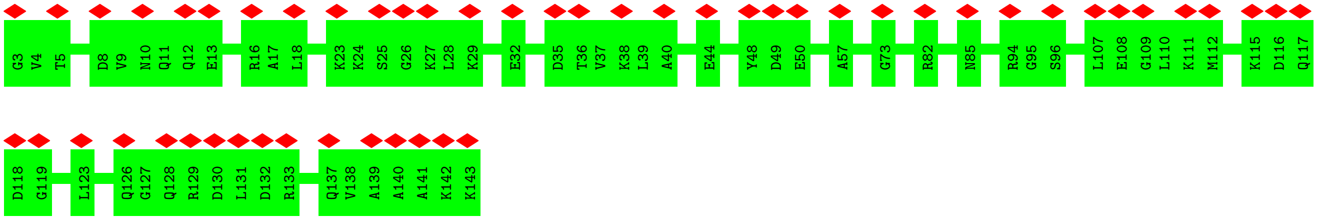




- Molecule 67: 40S ribosomal protein S19

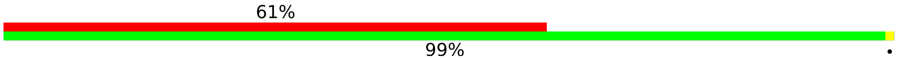
Chain TT:

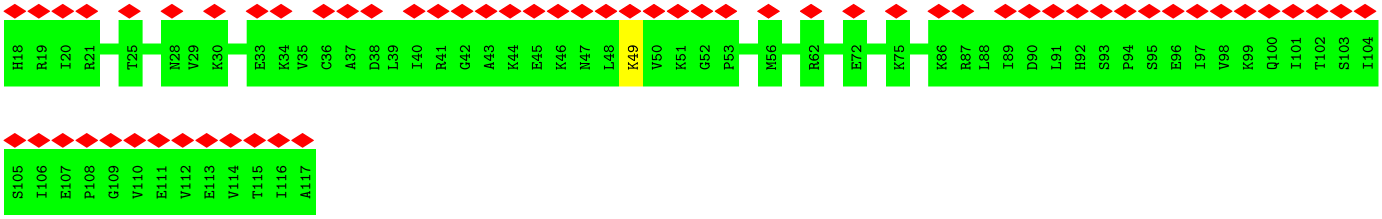




- Molecule 68: 40S ribosomal protein S20

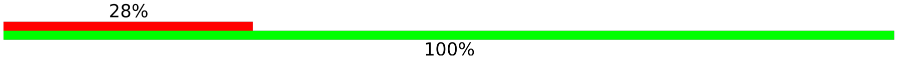
Chain UU:

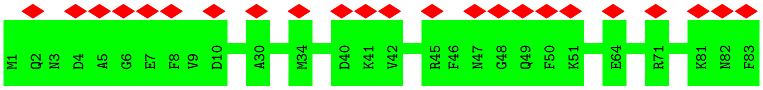




- Molecule 69: eS21

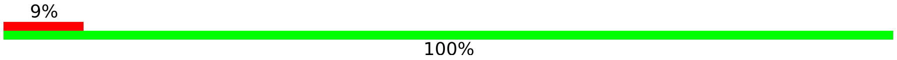
Chain VV:

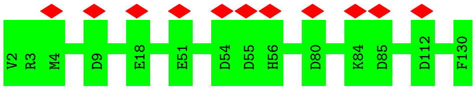




- Molecule 70: 40S ribosomal protein S15a

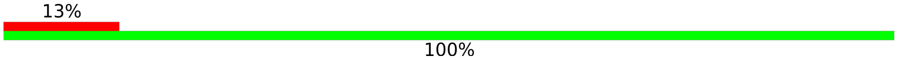
Chain WW:

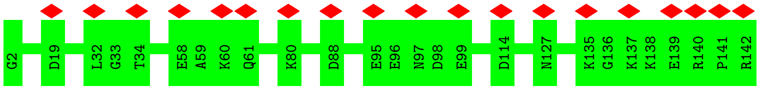




- Molecule 71: 40S ribosomal protein S23

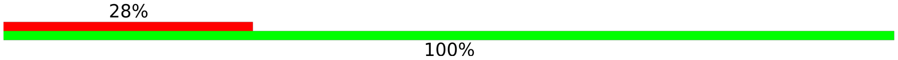
Chain XX:

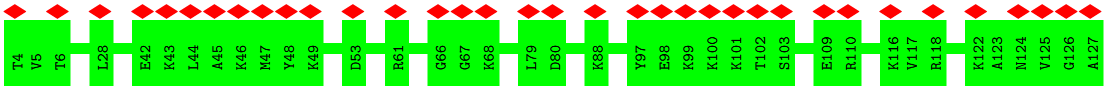




- Molecule 72: 40S ribosomal protein S24

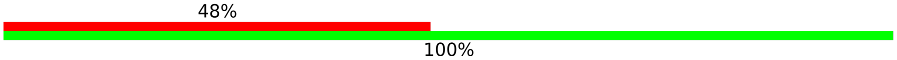
Chain YY:

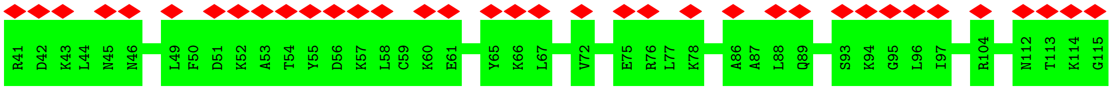




- Molecule 73: 40S ribosomal protein S25

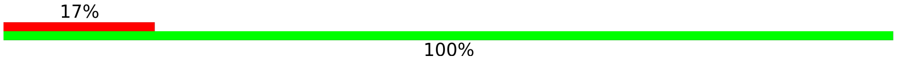
Chain ZZ:

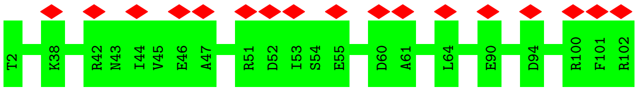




- Molecule 74: eS26

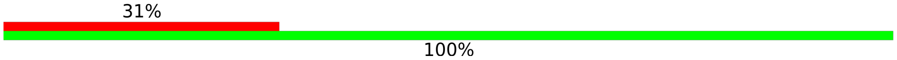
Chain Aa:

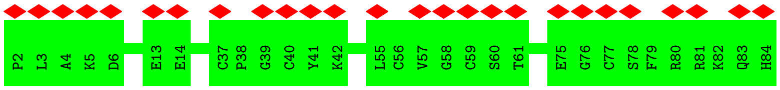




- Molecule 75: 40S ribosomal protein S27

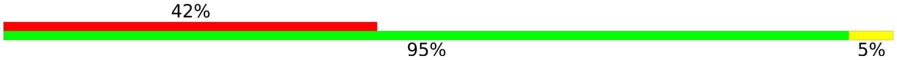
Chain Bb:

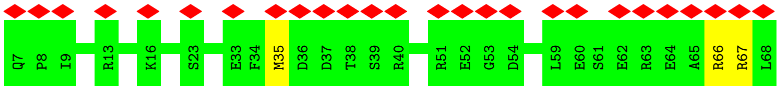




- Molecule 76: 40S ribosomal protein S28

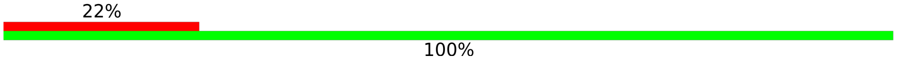
Chain Cc:

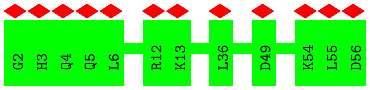




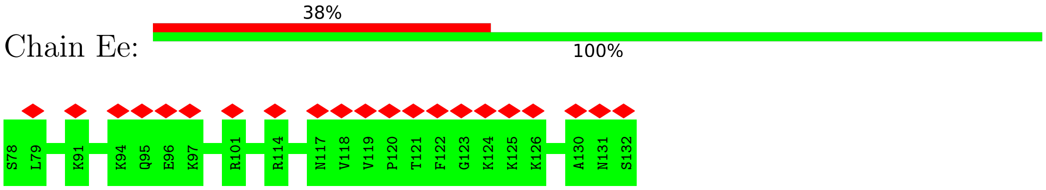
- Molecule 77: 40S ribosomal protein S29

Chain Dd:

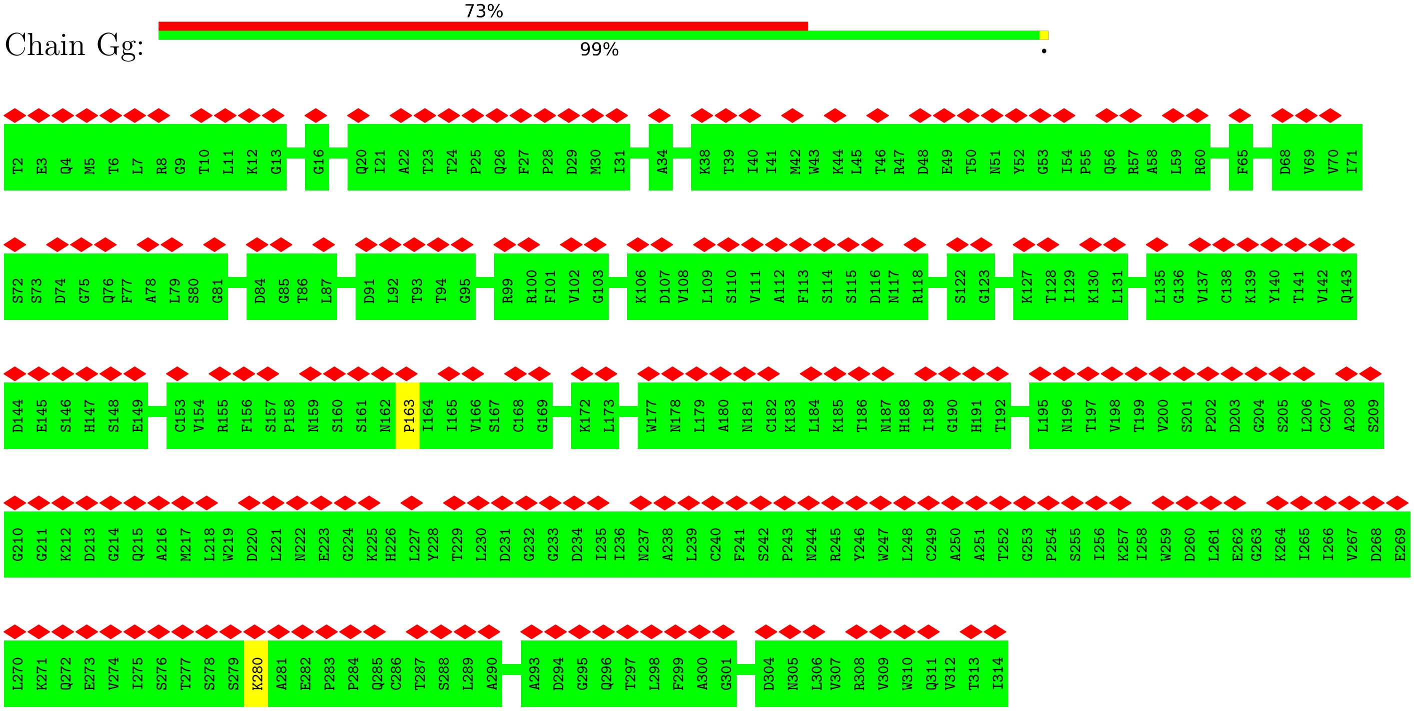




- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Receptor of activated protein C kinase 1



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52555	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.224	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	651.84, 651.84, 651.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.358, 1.358, 1.358	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B9H, B8H, ZN, T6A, OMU, BGH, 6MZ, B8W, UR3, B8N, I4U, M7A, MHG, 7MG, 5MC, 4AC, A2M, PSU, OMG, MA6, B8K, E6G, E7G, B9B, 2MG, B8Q, P7G, 5MU, MQ6, OMC, MLZ, 1MA, B8T, MG, P4U, MMX

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	2	0.28	0/1698	0.83	2/2640 (0.1%)
2	1	0.25	0/145	0.77	0/224
3	5	0.36	0/81475	0.80	34/126990 (0.0%)
4	7	0.34	0/2858	0.73	0/4455
5	8	0.33	0/3540	0.75	0/5513
6	9	0.32	0/39730	0.80	27/61898 (0.0%)
7	A	0.29	0/1936	0.58	0/2596
8	B	0.28	0/3240	0.53	0/4339
9	C	0.28	0/2913	0.56	0/3913
10	D	0.29	0/2427	0.52	0/3250
11	E	0.27	0/1753	0.55	0/2351
12	F	0.29	0/1911	0.53	0/2549
13	G	0.28	0/1861	0.55	1/2504 (0.0%)
14	H	0.27	0/1535	0.57	1/2063 (0.0%)
15	I	0.28	0/1702	0.55	0/2272
16	J	0.28	0/1376	0.59	0/1841
17	L	0.27	0/1733	0.59	0/2316
18	M	0.28	0/1158	0.55	0/1547
19	N	0.29	0/1746	0.58	0/2338
20	O	0.30	0/1662	0.56	0/2222
21	P	0.27	0/1268	0.52	0/1700
22	Q	0.28	0/1539	0.60	0/2054
23	R	0.26	0/1524	0.59	0/2013
24	S	0.29	0/1501	0.55	0/2012
25	T	0.30	0/1326	0.54	0/1770
26	U	0.28	0/814	0.54	0/1092
27	V	0.29	0/987	0.54	0/1324
28	W	0.28	0/666	0.56	0/886
29	X	0.27	0/984	0.55	0/1323
30	Y	0.28	0/1132	0.56	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Z	0.29	0/1130	0.51	0/1507
32	a	0.30	0/1191	0.54	0/1590
33	b	0.26	0/861	0.55	0/1138
34	c	0.30	0/748	0.52	0/1003
35	d	0.27	0/903	0.55	0/1216
36	e	0.28	0/1071	0.53	0/1429
37	f	0.29	0/895	0.58	0/1198
38	g	0.28	0/916	0.58	0/1220
39	h	0.26	0/1021	0.57	0/1348
40	i	0.27	0/841	0.58	0/1112
41	j	0.29	0/720	0.61	0/952
42	k	0.27	0/575	0.53	0/761
43	l	0.25	0/459	0.57	0/608
44	m	0.27	0/415	0.56	0/550
45	n	0.26	0/240	0.69	0/305
46	o	0.27	0/855	0.53	0/1128
47	p	0.29	0/718	0.52	0/953
48	r	0.27	0/1010	0.57	0/1354
49	AA	0.26	0/1747	0.51	0/2374
50	BB	0.27	0/1742	0.51	0/2330
51	CC	0.28	0/1753	0.51	0/2369
52	DD	0.27	0/1788	0.52	0/2407
53	EE	0.27	0/2118	0.54	0/2849
54	FF	0.25	0/1492	0.50	0/2005
55	GG	0.25	0/1946	0.56	0/2590
56	HH	0.37	1/1510 (0.1%)	0.63	3/2022 (0.1%)
57	II	0.26	0/1696	0.54	0/2261
58	JJ	0.26	0/1550	0.57	0/2069
59	KK	0.26	0/834	0.55	0/1125
60	LL	0.29	0/1195	0.54	0/1597
61	NN	0.26	0/1226	0.55	0/1649
62	OO	0.27	0/1029	0.58	0/1380
63	PP	0.32	0/1017	0.63	2/1358 (0.1%)
64	QQ	0.27	0/1146	0.55	0/1534
65	RR	0.26	0/1082	0.52	0/1452
66	SS	0.26	0/1208	0.57	0/1618
67	TT	0.25	0/1115	0.50	0/1493
68	UU	0.25	0/805	0.58	0/1081
69	VV	0.27	0/643	0.54	0/860
70	WW	0.27	0/1051	0.53	0/1406
71	XX	0.27	0/1116	0.52	0/1490
72	YY	0.27	0/1028	0.54	0/1366
73	ZZ	0.27	0/604	0.57	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	Aa	0.28	0/828	0.57	0/1109
75	Bb	0.26	0/665	0.51	0/891
76	Cc	0.25	0/490	0.61	0/656
77	Dd	0.27	0/470	0.57	0/623
78	Ee	0.26	0/447	0.57	0/587
79	Gg	0.40	2/2493 (0.1%)	0.63	3/3394 (0.1%)
All	All	0.32	3/220543 (0.0%)	0.71	73/323626 (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
13	G	0	1
20	O	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	Gg	163	PRO	CG-CD	-14.27	1.03	1.50
56	HH	190	PRO	CG-CD	-9.09	1.20	1.50
79	Gg	163	PRO	N-CD	6.23	1.56	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	Gg	163	PRO	N-CD-CG	-15.55	79.87	103.20
56	HH	190	PRO	N-CD-CG	-11.94	85.29	103.20
79	Gg	163	PRO	CA-N-CD	-10.33	97.03	111.50
56	HH	190	PRO	CA-N-CD	-8.84	99.13	111.50
3	5	133	C	N1-C2-O2	8.52	124.01	118.90
79	Gg	163	PRO	CA-CB-CG	-8.47	87.90	104.00
63	PP	68	PRO	N-CD-CG	-8.11	91.04	103.20
3	5	133	C	C2-N1-C1’	8.03	127.64	118.80
6	9	630	U	C2-N1-C1’	7.78	127.03	117.70
3	5	2019	C	N3-C2-O2	-7.34	116.76	121.90
3	5	1210	C	C2-N1-C1’	7.25	126.78	118.80
3	5	2022	C	N3-C2-O2	-7.16	116.89	121.90
6	9	501	C	C2-N1-C1’	7.15	126.66	118.80
6	9	356	C	C2-N1-C1’	7.00	126.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	133	C	N3-C2-O2	-6.95	117.03	121.90
3	5	1236	C	C2-N1-C1'	6.94	126.43	118.80
6	9	293	C	N1-C2-O2	6.87	123.02	118.90
6	9	293	C	C2-N1-C1'	6.82	126.31	118.80
6	9	630	U	N1-C2-O2	6.77	127.54	122.80
3	5	1210	C	N1-C2-O2	6.66	122.90	118.90
56	HH	190	PRO	CA-CB-CG	-6.50	91.65	104.00
3	5	1639	U	C2-N1-C1'	6.44	125.43	117.70
63	PP	68	PRO	CA-CB-CG	-6.33	91.97	104.00
6	9	630	U	N3-C2-O2	-6.22	117.85	122.20
3	5	100	C	C2-N1-C1'	6.20	125.62	118.80
6	9	356	C	N1-C2-O2	6.17	122.60	118.90
3	5	217	C	N1-C2-O2	6.08	122.55	118.90
6	9	501	C	N1-C2-O2	6.05	122.53	118.90
3	5	4110	C	N3-C2-O2	-5.99	117.71	121.90
3	5	1483	C	N1-C2-O2	5.94	122.47	118.90
6	9	833	C	N1-C2-O2	5.87	122.42	118.90
3	5	2018	C	N1-C2-O2	5.81	122.39	118.90
6	9	1453	C	C2-N1-C1'	5.77	125.15	118.80
3	5	4197	G	N1-C6-O6	-5.70	116.48	119.90
1	2	75	C	C6-N1-C2	-5.68	118.03	120.30
14	H	67	LEU	CA-CB-CG	5.61	128.21	115.30
3	5	133	C	C6-N1-C2	-5.59	118.06	120.30
3	5	1438	U	P-O3'-C3'	5.55	126.36	119.70
6	9	1453	C	N1-C2-O2	5.47	122.18	118.90
3	5	4110	C	N1-C2-O2	5.44	122.17	118.90
3	5	133	C	C6-N1-C1'	-5.43	114.28	120.80
6	9	1637	A	OP2-P-O3'	5.41	117.10	105.20
1	2	75	C	N3-C2-O2	-5.39	118.12	121.90
6	9	293	C	N3-C2-O2	-5.39	118.13	121.90
6	9	1624	U	C2-N1-C1'	5.31	124.07	117.70
3	5	217	C	C2-N1-C1'	5.30	124.63	118.80
3	5	1210	C	N3-C2-O2	-5.30	118.19	121.90
6	9	1261	C	C2-N1-C1'	5.29	124.62	118.80
3	5	115	C	C2-N1-C1'	5.28	124.61	118.80
3	5	1236	C	C6-N1-C1'	-5.27	114.48	120.80
13	G	215	ASP	CB-CG-OD1	5.24	123.02	118.30
3	5	521	C	N3-C2-O2	-5.23	118.24	121.90
3	5	2410	C	C2-N1-C1'	5.22	124.54	118.80
3	5	1639	U	N1-C2-O2	5.21	126.45	122.80
3	5	2022	C	N1-C2-O2	5.19	122.02	118.90
6	9	1123	C	N1-C2-O2	5.19	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	1483	C	C2-N1-C1'	5.17	124.49	118.80
6	9	501	C	C6-N1-C1'	-5.17	114.60	120.80
6	9	1022	U	C2-N1-C1'	5.17	123.90	117.70
6	9	356	C	N3-C2-O2	-5.13	118.31	121.90
6	9	1139	C	C2-N1-C1'	5.12	124.43	118.80
3	5	1236	C	N1-C2-O2	5.11	121.97	118.90
6	9	630	U	C6-N1-C1'	-5.10	114.06	121.20
6	9	666	U	C2-N1-C1'	5.09	123.81	117.70
6	9	1395	C	OP1-P-O3'	5.09	116.39	105.20
3	5	4303	C	C2-N1-C1'	5.08	124.39	118.80
3	5	1210	C	C6-N1-C1'	-5.07	114.72	120.80
3	5	417	G	O4'-C1'-N9	5.04	112.23	108.20
3	5	4197	G	C5-C6-O6	5.04	131.62	128.60
6	9	1637	A	P-O3'-C3'	5.04	125.74	119.70
6	9	1261	C	N1-C2-O2	5.03	121.92	118.90
3	5	4925	U	P-O3'-C3'	5.01	125.72	119.70
6	9	833	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	215	ASP	Peptide
20	O	110	PRO	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	235 (96%)	11 (4%)	0	100	100
8	B	392/394 (100%)	383 (98%)	9 (2%)	0	100	100
9	C	357/360 (99%)	342 (96%)	15 (4%)	0	100	100
10	D	289/291 (99%)	277 (96%)	12 (4%)	0	100	100
11	E	207/250 (83%)	200 (97%)	7 (3%)	0	100	100
12	F	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
13	G	222/233 (95%)	214 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
15	I	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
16	J	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
17	L	208/210 (99%)	204 (98%)	4 (2%)	0	100	100
18	M	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
19	N	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
20	O	197/199 (99%)	192 (98%)	5 (2%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
23	R	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
24	S	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
25	T	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
26	U	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
27	V	128/130 (98%)	126 (98%)	2 (2%)	0	100	100
28	W	76/95 (80%)	74 (97%)	2 (3%)	0	100	100
29	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
30	Y	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
31	Z	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
32	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
33	b	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
34	c	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
35	d	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
36	e	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
41	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	k	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
43	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
44	m	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
47	p	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
48	r	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
49	AA	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
50	BB	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
51	CC	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
52	DD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
53	EE	260/262 (99%)	256 (98%)	4 (2%)	0	100	100
54	FF	181/191 (95%)	169 (93%)	12 (7%)	0	100	100
55	GG	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
56	HH	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
57	II	199/206 (97%)	193 (97%)	6 (3%)	0	100	100
58	JJ	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
59	KK	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
60	LL	139/151 (92%)	136 (98%)	3 (2%)	0	100	100
61	NN	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
62	OO	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
63	PP	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
64	QQ	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
65	RR	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
66	SS	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
67	TT	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
68	UU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
69	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	WW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
71	XX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
72	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
73	ZZ	73/75 (97%)	73 (100%)	0	0	100	100
74	Aa	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
75	Bb	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
76	Cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
77	Dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
78	Ee	53/55 (96%)	53 (100%)	0	0	100	100
79	Gg	311/313 (99%)	289 (93%)	22 (7%)	0	100	100
All	All	10937/11205 (98%)	10582 (97%)	355 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
7	A	190/190 (100%)	188 (99%)	2 (1%)	73	89
8	B	342/342 (100%)	342 (100%)	0	100	100
9	C	299/299 (100%)	298 (100%)	1 (0%)	92	96
10	D	247/247 (100%)	247 (100%)	0	100	100
11	E	189/222 (85%)	188 (100%)	1 (0%)	88	94
12	F	196/196 (100%)	196 (100%)	0	100	100
13	G	195/200 (98%)	194 (100%)	1 (0%)	88	94
14	H	169/169 (100%)	169 (100%)	0	100	100
15	I	175/180 (97%)	174 (99%)	1 (1%)	86	94
16	J	142/142 (100%)	142 (100%)	0	100	100
17	L	175/175 (100%)	174 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	M	117/117 (100%)	116 (99%)	1 (1%)	78	91
19	N	171/171 (100%)	171 (100%)	0	100	100
20	O	171/171 (100%)	171 (100%)	0	100	100
21	P	134/134 (100%)	134 (100%)	0	100	100
22	Q	164/164 (100%)	163 (99%)	1 (1%)	86	94
23	R	159/159 (100%)	159 (100%)	0	100	100
24	S	157/157 (100%)	157 (100%)	0	100	100
25	T	139/139 (100%)	139 (100%)	0	100	100
26	U	88/88 (100%)	88 (100%)	0	100	100
27	V	100/100 (100%)	100 (100%)	0	100	100
28	W	67/81 (83%)	67 (100%)	0	100	100
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	124 (100%)	0	100	100
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	119 (100%)	0	100	100
33	b	84/95 (88%)	84 (100%)	0	100	100
34	c	81/81 (100%)	81 (100%)	0	100	100
35	d	98/98 (100%)	98 (100%)	0	100	100
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	88 (100%)	0	100	100
38	g	98/98 (100%)	98 (100%)	0	100	100
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	73 (100%)	0	100	100
42	k	64/64 (100%)	63 (98%)	1 (2%)	62	84
43	l	47/47 (100%)	47 (100%)	0	100	100
44	m	46/46 (100%)	46 (100%)	0	100	100
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	91 (100%)	0	100	100
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	AA	180/181 (99%)	180 (100%)	0	100	100
50	BB	192/192 (100%)	192 (100%)	0	100	100
51	CC	187/187 (100%)	187 (100%)	0	100	100
52	DD	189/189 (100%)	188 (100%)	1 (0%)	88	94
53	EE	224/224 (100%)	223 (100%)	1 (0%)	91	96
54	FF	158/161 (98%)	158 (100%)	0	100	100
55	GG	207/207 (100%)	207 (100%)	0	100	100
56	HH	165/169 (98%)	165 (100%)	0	100	100
57	II	177/178 (99%)	176 (99%)	1 (1%)	86	94
58	JJ	161/161 (100%)	161 (100%)	0	100	100
59	KK	87/87 (100%)	87 (100%)	0	100	100
60	LL	130/136 (96%)	130 (100%)	0	100	100
61	NN	130/130 (100%)	130 (100%)	0	100	100
62	OO	106/106 (100%)	106 (100%)	0	100	100
63	PP	109/109 (100%)	109 (100%)	0	100	100
64	QQ	117/117 (100%)	117 (100%)	0	100	100
65	RR	119/119 (100%)	119 (100%)	0	100	100
66	SS	125/125 (100%)	124 (99%)	1 (1%)	81	92
67	TT	111/111 (100%)	111 (100%)	0	100	100
68	UU	92/92 (100%)	91 (99%)	1 (1%)	73	89
69	VV	67/67 (100%)	67 (100%)	0	100	100
70	WW	112/112 (100%)	112 (100%)	0	100	100
71	XX	113/113 (100%)	113 (100%)	0	100	100
72	YY	107/107 (100%)	107 (100%)	0	100	100
73	ZZ	66/66 (100%)	66 (100%)	0	100	100
74	Aa	88/88 (100%)	88 (100%)	0	100	100
75	Bb	75/75 (100%)	75 (100%)	0	100	100
76	Cc	55/55 (100%)	52 (94%)	3 (6%)	21	53
77	Dd	48/48 (100%)	48 (100%)	0	100	100
78	Ee	46/46 (100%)	46 (100%)	0	100	100
79	Gg	272/272 (100%)	271 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9552/9635 (99%)	9533 (100%)	19 (0%)	93	97

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	60	LYS
7	A	163	ARG
9	C	188	ARG
11	E	58	ARG
13	G	174	LYS
15	I	3	ARG
17	L	21	ARG
18	M	137	LYS
22	Q	91	ARG
42	k	55	LYS
52	DD	76	ARG
53	EE	254	LYS
57	II	147	LYS
66	SS	142	ARG
68	UU	49	LYS
76	Cc	35	MET
76	Cc	66	ARG
76	Cc	67	ARG
79	Gg	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	100	ASN
7	A	162	ASN
8	B	302	ASN
8	B	315	ASN
9	C	38	ASN
9	C	50	GLN
9	C	60	HIS
9	C	61	GLN
9	C	112	HIS
9	C	215	ASN
9	C	338	ASN
10	D	45	ASN
10	D	175	HIS

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Mol	Chain	Res	Type
10	D	202	GLN
10	D	244	HIS
10	D	282	GLN
11	E	131	HIS
11	E	138	GLN
11	E	194	GLN
11	E	259	GLN
12	F	55	HIS
13	G	91	ASN
13	G	147	GLN
14	H	106	GLN
14	H	188	GLN
15	I	14	ASN
15	I	59	GLN
15	I	73	ASN
15	I	95	HIS
16	J	65	ASN
17	L	19	GLN
17	L	104	ASN
17	L	159	ASN
18	M	20	HIS
18	M	56	GLN
19	N	196	ASN
20	O	72	HIS
22	Q	21	GLN
22	Q	44	ASN
23	R	39	GLN
24	S	77	ASN
24	S	108	GLN
24	S	117	HIS
24	S	125	GLN
24	S	146	HIS
24	S	162	GLN
25	T	3	ASN
25	T	54	HIS
26	U	94	ASN
27	V	36	ASN
28	W	48	GLN
29	X	111	GLN
30	Y	18	HIS
31	Z	79	HIS
31	Z	127	ASN

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Mol	Chain	Res	Type
32	a	34	ASN
32	a	89	ASN
33	b	10	HIS
33	b	12	GLN
33	b	50	ASN
33	b	60	ASN
33	b	94	HIS
34	c	15	ASN
35	d	93	ASN
36	e	23	HIS
36	e	101	HIS
39	h	107	GLN
40	i	12	ASN
40	i	15	HIS
40	i	80	HIS
42	k	31	ASN
42	k	58	GLN
44	m	58	GLN
44	m	61	GLN
44	m	93	ASN
46	o	19	GLN
46	o	36	GLN
46	o	45	GLN
48	r	41	ASN
48	r	83	ASN
49	AA	29	ASN
49	AA	33	GLN
49	AA	50	ASN
49	AA	132	GLN
50	BB	76	ASN
50	BB	149	GLN
50	BB	157	GLN
51	CC	113	GLN
51	CC	115	GLN
52	DD	174	HIS
53	EE	36	HIS
53	EE	50	ASN
53	EE	67	GLN
53	EE	98	ASN
53	EE	188	ASN
54	FF	51	HIS
54	FF	137	GLN

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Mol	Chain	Res	Type
55	GG	227	GLN
56	HH	73	GLN
56	HH	114	GLN
56	HH	186	ASN
57	II	7	ASN
58	JJ	143	ASN
59	KK	7	ASN
59	KK	39	ASN
59	KK	50	GLN
59	KK	61	GLN
59	KK	66	HIS
60	LL	100	ASN
60	LL	121	GLN
61	NN	5	HIS
61	NN	58	HIS
61	NN	105	ASN
62	OO	38	ASN
64	QQ	11	GLN
64	QQ	35	ASN
64	QQ	77	HIS
64	QQ	86	GLN
64	QQ	142	GLN
65	RR	48	ASN
65	RR	83	ASN
65	RR	121	GLN
65	RR	127	ASN
69	VV	33	GLN
70	WW	16	ASN
70	WW	64	ASN
70	WW	70	ASN
70	WW	91	ASN
70	WW	92	ASN
70	WW	113	HIS
71	XX	73	GLN
72	YY	29	HIS
73	ZZ	46	ASN
73	ZZ	106	GLN
74	Aa	43	ASN
75	Bb	29	ASN
77	Dd	28	HIS
77	Dd	45	GLN
78	Ee	95	GLN

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Mol	Chain	Res	Type
79	Gg	143	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	68/76 (89%)	13 (19%)	0
2	1	5/6 (83%)	2 (40%)	0
3	5	3445/3499 (98%)	627 (18%)	46 (1%)
4	7	119/120 (99%)	9 (7%)	0
5	8	148/156 (94%)	25 (16%)	1 (0%)
6	9	1678/1698 (98%)	315 (18%)	17 (1%)
All	All	5463/5555 (98%)	991 (18%)	64 (1%)

All (991) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	11	G
1	2	13	G
1	2	14	C
1	2	19	G
1	2	37	T6A
1	2	42	A
1	2	46	G
1	2	58	A
1	2	70	G
1	2	72	U
1	2	74	C
1	2	75	C
1	2	76	A
2	1	45	C
2	1	46	A
3	5	8	U
3	5	12	A
3	5	13	U
3	5	17	A
3	5	25	A
3	5	39	A
3	5	42	A
3	5	48	G
3	5	49	U
3	5	56	A

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Mol	Chain	Res	Type
3	5	58	G
3	5	59	A
3	5	64	A
3	5	65	A
3	5	66	A
3	5	71	C
3	5	72	C
3	5	73	A
3	5	76	A
3	5	91	G
3	5	104	G
3	5	108	A
3	5	109	G
3	5	110	C
3	5	119	G
3	5	120	A
3	5	126	C
3	5	134	G
3	5	135	G
3	5	136	C
3	5	144	G
3	5	146	G
3	5	159	C
3	5	171	U
3	5	172	C
3	5	173	C
3	5	182	G
3	5	200	U
3	5	201	C
3	5	209	U
3	5	216	C
3	5	219	G
3	5	220	C
3	5	224	U
3	5	233	U
3	5	234	G
3	5	246	G
3	5	265	C
3	5	266	C
3	5	280	G
3	5	297	U
3	5	306	A

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Mol	Chain	Res	Type
3	5	315	G
3	5	316	U
3	5	334	A
3	5	340	C
3	5	344	A
3	5	345	C
3	5	350	C
3	5	362	A
3	5	363	A
3	5	386	A
3	5	387	G
3	5	406	C
3	5	407	A
3	5	409	G
3	5	410	A
3	5	412	G
3	5	413	G
3	5	414	C
3	5	431	G
3	5	432	U
3	5	449	C
3	5	450	G
3	5	452	A
3	5	453	G
3	5	454	U
3	5	455	C
3	5	463	A
3	5	464	G
3	5	467	U
3	5	468	U
3	5	480	C
3	5	483	G
3	5	484	U
3	5	485	C
3	5	486	C
3	5	492	U
3	5	493	G
3	5	496	G
3	5	497	G
3	5	498	C
3	5	499	G
3	5	505	G

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Mol	Chain	Res	Type
3	5	510	U
3	5	666	G
3	5	669	C
3	5	670	G
3	5	685	C
3	5	686	A
3	5	691	C
3	5	696	C
3	5	697	G
3	5	704	C
3	5	705	G
3	5	719	C
3	5	731	G
3	5	738	C
3	5	738(A)	C
3	5	742	G
3	5	749	G
3	5	758	G
3	5	914	U
3	5	915	A
3	5	916	C
3	5	917	A
3	5	918	G
3	5	922	C
3	5	925	C
3	5	926	G
3	5	929	A
3	5	931	C
3	5	932	A
3	5	933	G
3	5	934	C
3	5	935	A
3	5	935(A)	G
3	5	936	C
3	5	938	C
3	5	939	G
3	5	941	C
3	5	943	A
3	5	944	A
3	5	945	U
3	5	959	G
3	5	960	A

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Mol	Chain	Res	Type
3	5	961	G
3	5	964	A
3	5	966	A
3	5	967	C
3	5	983	U
3	5	1072	C
3	5	1078	A
3	5	1079	C
3	5	1081	C
3	5	1084	C
3	5	1098	G
3	5	1175	A
3	5	1179	U
3	5	1180	C
3	5	1187	G
3	5	1193	C
3	5	1211	G
3	5	1212	G
3	5	1215	C
3	5	1234	G
3	5	1235	C
3	5	1236	C
3	5	1237	A
3	5	1239	G
3	5	1272	C
3	5	1273	G
3	5	1274	A
3	5	1275	G
3	5	1276	C
3	5	1280	C
3	5	1284	G
3	5	1287	G
3	5	1292	C
3	5	1293	G
3	5	1295	U
3	5	1296	G
3	5	1301	C
3	5	1303	A
3	5	1304	C
3	5	1313	C
3	5	1314	C
3	5	1326	A2M

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Mol	Chain	Res	Type
3	5	1330	A
3	5	1337	A
3	5	1354	A
3	5	1358	G
3	5	1359	G
3	5	1371	A
3	5	1377	G
3	5	1378	C
3	5	1379	C
3	5	1387	A
3	5	1394	G
3	5	1397	A
3	5	1398	A
3	5	1405	C
3	5	1414	C
3	5	1415	G
3	5	1419	G
3	5	1421	G
3	5	1429	C
3	5	1433	A
3	5	1436	C
3	5	1437	C
3	5	1438	U
3	5	1440	U
3	5	1441	C
3	5	1457	G
3	5	1475	G
3	5	1482	G
3	5	1483	C
3	5	1498	G
3	5	1502	G
3	5	1514	U
3	5	1516	G
3	5	1523	A
3	5	1534	A2M
3	5	1547	A
3	5	1566	C
3	5	1568	C
3	5	1578	U
3	5	1591	U
3	5	1596	U
3	5	1602	U

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Mol	Chain	Res	Type
3	5	1624	G
3	5	1625	OMG
3	5	1631	A
3	5	1633	G
3	5	1634	A
3	5	1641	G
3	5	1654	G
3	5	1661	C
3	5	1676	C
3	5	1677	PSU
3	5	1678	C
3	5	1721	G
3	5	1731	C
3	5	1734	G
3	5	1741	G
3	5	1742	A
3	5	1750	G
3	5	1754	U
3	5	1756	U
3	5	1761	G
3	5	1764	G
3	5	1766	A
3	5	1768	C
3	5	1772	C
3	5	1773	U
3	5	1775	A
3	5	1776	A
3	5	1781	U
3	5	1787	A
3	5	1804	A
3	5	1805	A
3	5	1812	C
3	5	1815	G
3	5	1819	G
3	5	1820	U
3	5	1821	G
3	5	1828	C
3	5	1832	C
3	5	1835	G
3	5	1836	G
3	5	1837	A
3	5	1842	G

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Mol	Chain	Res	Type
3	5	1847	C
3	5	1855	G
3	5	1869	G
3	5	1881	C
3	5	1893	C
3	5	1897	A
3	5	1917	A
3	5	1918	U
3	5	1920	C
3	5	1921	C
3	5	1922	G
3	5	1931	C
3	5	1940	G
3	5	1945	G
3	5	1948	G
3	5	1957	U
3	5	1958	A
3	5	1960	A
3	5	1961	G
3	5	1962	A
3	5	1964	A
3	5	2020	U
3	5	2026	A
3	5	2044	U
3	5	2046	G
3	5	2047	A
3	5	2048	U
3	5	2052	G
3	5	2055	G
3	5	2056	G
3	5	2069	A
3	5	2084	U
3	5	2089	G
3	5	2090	U
3	5	2093	G
3	5	2094	C
3	5	2095	A
3	5	2097	A
3	5	2098	G
3	5	2100	G
3	5	2102	G
3	5	2105	A

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Mol	Chain	Res	Type
3	5	2106	G
3	5	2107	A
3	5	2108	G
3	5	2109	A
3	5	2110	G
3	5	2259	G
3	5	2260	C
3	5	2268	A
3	5	2275	G
3	5	2289	C
3	5	2300	A
3	5	2301	G
3	5	2306	G
3	5	2313	A
3	5	2314	G
3	5	2331	G
3	5	2332	A
3	5	2333	G
3	5	2348	G
3	5	2350	U
3	5	2351	C
3	5	2360	A
3	5	2364	OMG
3	5	2369	U
3	5	2382	A
3	5	2395	A
3	5	2396	A
3	5	2410	C
3	5	2422	OMC
3	5	2424	OMG
3	5	2425	U
3	5	2433	G
3	5	2441	C
3	5	2453	A
3	5	2469	C
3	5	2470	C
3	5	2471	G
3	5	2475	G
3	5	2488	C
3	5	2489	C
3	5	2490	U
3	5	2491	C

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Mol	Chain	Res	Type
3	5	2495	U
3	5	2503	G
3	5	2504	C
3	5	2505	C
3	5	2506	G
3	5	2511	A
3	5	2513	A
3	5	2514	G
3	5	2520	C
3	5	2526	C
3	5	2529	A
3	5	2530	U
3	5	2537	A
3	5	2544	G
3	5	2546	G
3	5	2547	G
3	5	2554	U
3	5	2571	C
3	5	2575	U
3	5	2583	C
3	5	2586	G
3	5	2587	A
3	5	2601	A
3	5	2640	G
3	5	2653	C
3	5	2662	G
3	5	2677	G
3	5	2687	U
3	5	2694	G
3	5	2695	A
3	5	2696	A
3	5	2705	G
3	5	2708	U
3	5	2709	C
3	5	2710	C
3	5	2711	G
3	5	2714	G
3	5	2715	G
3	5	2716	C
3	5	2721	G
3	5	2725	A
3	5	2726	G

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Mol	Chain	Res	Type
3	5	2735	G
3	5	2740	U
3	5	2743	A
3	5	2744	A
3	5	2753	G
3	5	2769	U
3	5	2787	A
3	5	2788	U
3	5	2790	U
3	5	2798	A
3	5	2803	U
3	5	2826	U
3	5	2827	G
3	5	2829	U
3	5	2842	G
3	5	2855	G
3	5	2875	C
3	5	2897	G
3	5	2898	G
3	5	3603	G
3	5	3604	A
3	5	3615	G
3	5	3618	C
3	5	3625	G
3	5	3626	G
3	5	3635	A
3	5	3644	U
3	5	3648	A
3	5	3649	A
3	5	3662	A
3	5	3664	G
3	5	3673	C
3	5	3680	U
3	5	3696	C
3	5	3698	G
3	5	3709	U
3	5	3711	A
3	5	3712	A
3	5	3714	G
3	5	3753	G
3	5	3759	A
3	5	3766	A

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Mol	Chain	Res	Type
3	5	3773	U
3	5	3774	A
3	5	3776	G
3	5	3777	G
3	5	3784	A
3	5	3786	U
3	5	3788	C
3	5	3792	OMG
3	5	3811	G
3	5	3812	C
3	5	3814	U
3	5	3817	A
3	5	3819	G
3	5	3822	U
3	5	3824	A
3	5	3838	U
3	5	3840	U
3	5	3867	A2M
3	5	3876	A
3	5	3877	A
3	5	3878	C
3	5	3879	G
3	5	3889	G
3	5	3898	G
3	5	3901	A
3	5	3905	A
3	5	3906	A
3	5	3907	G
3	5	3908	A
3	5	3915	U
3	5	3916	G
3	5	3917	A
3	5	3938	G
3	5	3939	G
3	5	3946	G
3	5	3947	A
3	5	3948	C
3	5	4061	G
3	5	4066	U
3	5	4076	G
3	5	4085	A
3	5	4086	G

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Mol	Chain	Res	Type
3	5	4116	C
3	5	4118	U
3	5	4119	C
3	5	4120	U
3	5	4122	G
3	5	4125	C
3	5	4127	A
3	5	4158	C
3	5	4162	C
3	5	4163	U
3	5	4166	G
3	5	4170	A
3	5	4180	G
3	5	4183	G
3	5	4191	G
3	5	4195	G
3	5	4203	A
3	5	4212	A
3	5	4221	C
3	5	4229	U
3	5	4233	A
3	5	4251	A
3	5	4254	G
3	5	4255	A
3	5	4258	C
3	5	4266	G
3	5	4268	A
3	5	4271	A
3	5	4273	A
3	5	4281	A
3	5	4291	G
3	5	4305	G
3	5	4306	OMU
3	5	4314	C
3	5	4330	G
3	5	4332	C
3	5	4339	A
3	5	4349	C
3	5	4350	C
3	5	4354	U
3	5	4372	U
3	5	4373	G

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Mol	Chain	Res	Type
3	5	4377	G
3	5	4378	A
3	5	4379	A
3	5	4387	C
3	5	4393	G
3	5	4394	A
3	5	4395	U
3	5	4396	A
3	5	4398	C
3	5	4419	U
3	5	4421	C
3	5	4422	A
3	5	4437	U
3	5	4447	5MC
3	5	4448	G
3	5	4449	A
3	5	4452	U
3	5	4464	A
3	5	4475	G
3	5	4500	PSU
3	5	4510	A
3	5	4511	A
3	5	4512	U
3	5	4513	A
3	5	4519	C
3	5	4520	G
3	5	4523	A2M
3	5	4524	G
3	5	4528	G
3	5	4530	UR3
3	5	4531	PSU
3	5	4535	A
3	5	4548	A
3	5	4549	G
3	5	4560	C
3	5	4567	G
3	5	4573	G
3	5	4575	G
3	5	4584	A
3	5	4586	G
3	5	4589	A
3	5	4590	A

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Mol	Chain	Res	Type
3	5	4627	U
3	5	4636	PSU
3	5	4637	OMG
3	5	4639	G
3	5	4656	A
3	5	4667	C
3	5	4670	C
3	5	4677	U
3	5	4709	U
3	5	4720	C
3	5	4736	C
3	5	4738	C
3	5	4745	G
3	5	4751	G
3	5	4754	G
3	5	4755	G
3	5	4756	C
3	5	4757	C
3	5	4759	C
3	5	4761	G
3	5	4765	G
3	5	4771	C
3	5	4772	C
3	5	4868	G
3	5	4870	OMG
3	5	4871	C
3	5	4875	G
3	5	4882	U
3	5	4883	C
3	5	4885	U
3	5	4895	C
3	5	4903	G
3	5	4904	G
3	5	4906	C
3	5	4910	A
3	5	4911	A
3	5	4912	G
3	5	4914	G
3	5	4915	G
3	5	4921	C
3	5	4924	C
3	5	4926	C

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Mol	Chain	Res	Type
3	5	4931	G
3	5	4934	A
3	5	4937	C
3	5	4943	A
3	5	4944	C
3	5	4948	C
3	5	4950	U
3	5	4951	G
3	5	4956	A
3	5	4958	C
3	5	4960	G
3	5	4963	G
3	5	4966	A
3	5	4976	U
3	5	4988	U
3	5	4990	C
3	5	4993	G
3	5	5013	C
3	5	5014	A
3	5	5017	G
3	5	5041	G
3	5	5047	C
3	5	5050	C
3	5	5053	U
3	5	5054	C
3	5	5055	G
3	5	5061	A
3	5	5062	G
3	5	5069	U
4	7	7	G
4	7	33	U
4	7	53	U
4	7	54	A
4	7	64	G
4	7	100	A
4	7	110	G
4	7	111	C
4	7	120	U
5	8	3	A
5	8	34	U
5	8	35	C
5	8	38	U

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Mol	Chain	Res	Type
5	8	46	G
5	8	59	A
5	8	62	A
5	8	63	U
5	8	75	G
5	8	78	G
5	8	87	G
5	8	90	C
5	8	103	A
5	8	105	C
5	8	110	U
5	8	111	U
5	8	114	G
5	8	124	U
5	8	125	C
5	8	126	C
5	8	127	U
5	8	137	A
5	8	150	C
5	8	151	G
5	8	153	C
6	9	2	A
6	9	3	C
6	9	25	A
6	9	26	U
6	9	33	G
6	9	42	A
6	9	44	U
6	9	45	A
6	9	46	A
6	9	56	G
6	9	58	C
6	9	64	A
6	9	67	C
6	9	68	A
6	9	71	G
6	9	73	C
6	9	74	G
6	9	75	G
6	9	77	A
6	9	79	A
6	9	103	A

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Mol	Chain	Res	Type
6	9	111	A
6	9	113	G
6	9	115	U
6	9	116	OMU
6	9	124	U
6	9	126	G
6	9	129	C
6	9	130	G
6	9	141	A
6	9	143	U
6	9	147	A
6	9	149	A
6	9	155	G
6	9	159	A2M
6	9	162	C
6	9	163	U
6	9	166	A2M
6	9	167	G
6	9	168	C
6	9	180	G
6	9	182	C
6	9	183	G
6	9	184	G
6	9	188	C
6	9	189	U
6	9	190	G
6	9	192	C
6	9	206	G
6	9	215	G
6	9	292	A
6	9	294	U
6	9	308	G
6	9	310	C
6	9	312	G
6	9	318	A
6	9	319	C
6	9	320	G
6	9	322	C
6	9	323	C
6	9	332	G
6	9	340	C
6	9	347	G

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Mol	Chain	Res	Type
6	9	351	G
6	9	362	C
6	9	364	A
6	9	367	U
6	9	368	U
6	9	369	C
6	9	370	G
6	9	385	G
6	9	386	C
6	9	398	A
6	9	400	C
6	9	407	G
6	9	408	A
6	9	409	C
6	9	417	C
6	9	418	A
6	9	420	G
6	9	435	A
6	9	438	G
6	9	448	A
6	9	449	A
6	9	450	C
6	9	465	A
6	9	466	G
6	9	471	G
6	9	472	C
6	9	473	A
6	9	474	G
6	9	476	A
6	9	482	G
6	9	487	U
6	9	492	C
6	9	493	A
6	9	516	A
6	9	530	U
6	9	532	C
6	9	533	A
6	9	536	A
6	9	537	C
6	9	547	G
6	9	548	C
6	9	549	C

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Mol	Chain	Res	Type
6	9	550	C
6	9	551	U
6	9	554	A
6	9	555	A
6	9	556	U
6	9	559	G
6	9	563	G
6	9	564	A
6	9	576	A
6	9	583	A
6	9	587	A
6	9	588	G
6	9	589	G
6	9	590	A
6	9	591	U
6	9	598	G
6	9	604	A
6	9	606	G
6	9	608	C
6	9	614	C
6	9	617	G
6	9	628	A
6	9	631	U
6	9	643	A
6	9	655	A
6	9	660	C
6	9	666	U
6	9	668	A2M
6	9	669	A
6	9	671	A
6	9	672	A
6	9	673	G
6	9	683	OMG
6	9	687	C
6	9	688	U
6	9	689	U
6	9	690	G
6	9	752	G
6	9	753	C
6	9	754	G
6	9	799	U
6	9	811	A

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Mol	Chain	Res	Type
6	9	821	G
6	9	822	PSU
6	9	830	A
6	9	834	C
6	9	844	U
6	9	847	A
6	9	870	A
6	9	871	U
6	9	872	A
6	9	874	G
6	9	875	A
6	9	878	G
6	9	890	U
6	9	892	U
6	9	898	U
6	9	901	G
6	9	909	G
6	9	913	A
6	9	914	U
6	9	920	A
6	9	930	C
6	9	933	G
6	9	934	G
6	9	958	G
6	9	959	G
6	9	961	G
6	9	971	G
6	9	978	G
6	9	985	G
6	9	990	A
6	9	992	A
6	9	999	G
6	9	1017	U
6	9	1023	A
6	9	1045	U
6	9	1061	U
6	9	1062	A
6	9	1083	A
6	9	1085	C
6	9	1097	G
6	9	1109	C
6	9	1111	U

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Mol	Chain	Res	Type
6	9	1115	U
6	9	1116	C
6	9	1117	C
6	9	1118	C
6	9	1121	G
6	9	1126	G
6	9	1130	G
6	9	1138	C
6	9	1153	C
6	9	1154	U
6	9	1155	U
6	9	1195	A
6	9	1207	G
6	9	1212	G
6	9	1215	C
6	9	1221	G
6	9	1224	G
6	9	1242	U
6	9	1243	PSU
6	9	1251	A
6	9	1253	A
6	9	1256	G
6	9	1257	G
6	9	1259	A
6	9	1265	A
6	9	1271	C
6	9	1274	G
6	9	1275	G
6	9	1281	G
6	9	1282	A
6	9	1284	A
6	9	1285	G
6	9	1286	G
6	9	1287	A
6	9	1293	A
6	9	1295	A
6	9	1301	A
6	9	1302	G
6	9	1303	C
6	9	1307	U
6	9	1308	U
6	9	1309	C

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Mol	Chain	Res	Type
6	9	1310	U
6	9	1316	C
6	9	1333	U
6	9	1342	U
6	9	1371	U
6	9	1372	U
6	9	1378	A
6	9	1382	A
6	9	1395	C
6	9	1396	A
6	9	1397	U
6	9	1401	A
6	9	1402	A
6	9	1403	C
6	9	1409	A
6	9	1410	C
6	9	1428	G
6	9	1442	U
6	9	1452	A
6	9	1454	A
6	9	1462	U
6	9	1463	U
6	9	1464	C
6	9	1466	G
6	9	1477	U
6	9	1480	A
6	9	1489	A
6	9	1490	G
6	9	1494	U
6	9	1497	G
6	9	1498	A
6	9	1505	U
6	9	1507	G
6	9	1509	U
6	9	1521	C
6	9	1522	A
6	9	1533	A
6	9	1552	G
6	9	1564	C
6	9	1570	G
6	9	1575	G
6	9	1579	A

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Mol	Chain	Res	Type
6	9	1580	A
6	9	1586	U
6	9	1587	G
6	9	1588	A
6	9	1601	A
6	9	1602	U
6	9	1604	G
6	9	1606	G
6	9	1619	A
6	9	1621	U
6	9	1623	A
6	9	1637	A
6	9	1638	G
6	9	1646	C
6	9	1648	G
6	9	1654	G
6	9	1665	G
6	9	1695	A
6	9	1699	A
6	9	1721	U
6	9	1722	G
6	9	1726	G
6	9	1732	G
6	9	1744	G
6	9	1756	C
6	9	1775	U
6	9	1779	G
6	9	1783	C
6	9	1784	G
6	9	1785	C
6	9	1829	G
6	9	1831	A
6	9	1835	A
6	9	1836	G
6	9	1838	U
6	9	1849	G
6	9	1861	G
6	9	1862	G
6	9	1863	A
6	9	1864	U
6	9	1865	C
6	9	1869	A

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	12	A
3	5	47	A
3	5	48	G
3	5	125	C
3	5	134	G
3	5	171	U
3	5	245	C
3	5	385	A
3	5	406	C
3	5	449	C
3	5	485	C
3	5	491	G
3	5	504	G
3	5	685	C
3	5	696	C
3	5	930	G
3	5	1174	G
3	5	1211	G
3	5	1236	C
3	5	1238	C
3	5	1291	G
3	5	1329	G
3	5	1370	G
3	5	1438	U
3	5	1440	U
3	5	1633	G
3	5	1804	A
3	5	1818	G
3	5	2046	G
3	5	2089	G
3	5	2440	U
3	5	2502	A
3	5	2546	G
3	5	2639	U
3	5	2695	A
3	5	3625	G
3	5	3697	U
3	5	3876	A
3	5	3888	G
3	5	4065	G
3	5	4232	U
3	5	4254	G

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Mol	Chain	Res	Type
3	5	4448	G
3	5	4884	G
3	5	4925	U
3	5	4947	U
5	8	124	U
6	9	110	U
6	9	140	U
6	9	434	G
6	9	465	A
6	9	532	C
6	9	553	U
6	9	642	U
6	9	688	U
6	9	752	G
6	9	870	A
6	9	874	G
6	9	1137	U
6	9	1394	G
6	9	1395	C
6	9	1489	A
6	9	1520	G
6	9	1637	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	I4U	5	1659	3	21,24,25	3.47	9 (42%)	27,34,37	0.94	1 (3%)
3	OMC	5	3909	3	19,22,23	2.95	8 (42%)	26,31,34	0.92	1 (3%)
3	B9B	5	237	3	21,28,29	1.98	3 (14%)	23,40,43	6.24	5 (21%)
6	4AC	9	1842	6	21,24,25	3.17	10 (47%)	29,34,37	1.12	4 (13%)
3	7MG	5	4550	3	22,26,27	3.70	10 (45%)	29,39,42	2.04	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	M7A	9	1806	6	20,25,26	2.01	3 (15%)	28,37,40	3.98	8 (28%)
3	B8Q	5	1456	3	17,22,23	2.86	5 (29%)	22,32,35	2.08	4 (18%)
3	A2M	5	2401	3,80	18,25,26	3.61	8 (44%)	18,36,39	3.36	4 (22%)
3	B8W	5	4129	3	18,26,27	2.10	2 (11%)	21,38,41	2.44	7 (33%)
3	OMC	5	2804	3	19,22,23	2.96	8 (42%)	26,31,34	0.65	0
3	PSU	5	3729	3	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
3	1MA	5	4415	3	16,25,26	4.32	5 (31%)	18,37,40	1.78	3 (16%)
3	B8H	5	3762	3	19,22,23	6.80	6 (31%)	22,32,35	2.34	5 (22%)
6	A2M	9	27	6,80	18,25,26	3.60	8 (44%)	18,36,39	3.27	3 (16%)
3	OMG	5	2424	3	18,26,27	2.48	8 (44%)	19,38,41	1.51	4 (21%)
3	OMG	5	1625	3	18,26,27	2.47	8 (44%)	19,38,41	1.53	4 (21%)
3	5MC	5	4447	3	18,22,23	3.50	7 (38%)	26,32,35	1.06	1 (3%)
3	B8T	5	4483	3	19,22,23	3.55	8 (42%)	26,31,34	0.90	1 (3%)
3	5MC	5	4335	3	18,22,23	3.58	7 (38%)	26,32,35	1.08	1 (3%)
3	OMG	5	373	3	18,26,27	2.47	8 (44%)	19,38,41	1.55	4 (21%)
3	I4U	5	4194	3	21,24,25	3.43	9 (42%)	27,34,37	1.02	1 (3%)
3	A2M	5	398	3	18,25,26	3.60	8 (44%)	18,36,39	3.36	3 (16%)
3	B8K	5	4690	14,3	24,28,29	3.40	11 (45%)	30,42,45	2.35	11 (36%)
6	PSU	9	119	6	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
3	2MG	5	4872	18,3	18,26,27	2.53	7 (38%)	16,38,41	1.58	4 (25%)
3	2MG	5	729	3	18,26,27	2.45	7 (38%)	16,38,41	1.37	3 (18%)
3	A2M	5	2363	3,80	18,25,26	3.62	8 (44%)	18,36,39	3.37	4 (22%)
6	B8Q	9	1219	6,80	17,22,23	2.95	4 (23%)	22,32,35	2.35	7 (31%)
3	E7G	5	1797	3	24,27,28	3.98	11 (45%)	30,40,43	2.28	10 (33%)
3	2MG	5	1517	3	18,26,27	2.43	7 (38%)	16,38,41	1.45	4 (25%)
6	5MC	9	1374	6	18,22,23	3.55	7 (38%)	26,32,35	1.07	2 (7%)
3	PSU	5	4531	3	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
3	OMG	5	3792	3	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
6	OMG	9	644	6	18,26,27	2.44	8 (44%)	19,38,41	1.49	4 (21%)
3	P7G	5	1909	3	24,28,29	4.06	11 (45%)	27,41,44	1.56	2 (7%)
3	OMC	5	3869	3	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
3	PSU	5	4500	3	18,21,22	1.06	1 (5%)	22,30,33	1.86	5 (22%)
6	PSU	9	823	6	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
3	B8K	5	3897	3	24,28,29	3.34	11 (45%)	30,42,45	2.33	10 (33%)
3	B9H	5	2786	3	20,25,26	3.09	3 (15%)	22,35,38	1.46	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMC	5	3701	3,80	19,22,23	2.96	8 (42%)	26,31,34	0.69	0
6	OMU	9	116	6	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
3	OMG	5	2364	3	18,26,27	2.43	8 (44%)	19,38,41	1.50	4 (21%)
6	PSU	9	822	6	18,21,22	1.07	1 (5%)	22,30,33	1.84	6 (27%)
1	T6A	2	37	1	27,34,35	0.98	1 (3%)	29,49,52	2.48	7 (24%)
3	A2M	5	1326	3	18,25,26	3.61	8 (44%)	18,36,39	3.37	4 (22%)
3	OMG	5	4637	3	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
6	MA6	9	1851	6	19,26,27	1.37	3 (15%)	18,38,41	4.33	3 (16%)
6	PSU	9	1081	6	18,21,22	0.99	1 (5%)	22,30,33	1.76	4 (18%)
3	B8T	5	4671	3	19,22,23	3.58	8 (42%)	26,31,34	0.89	1 (3%)
3	OMG	5	4196	3	18,26,27	2.45	8 (44%)	19,38,41	1.53	4 (21%)
3	OMG	5	1883	3	18,26,27	2.50	8 (44%)	19,38,41	1.59	4 (21%)
3	P7G	5	3880	3	24,28,29	3.93	11 (45%)	27,41,44	1.69	3 (11%)
3	A2M	5	4571	3	18,25,26	3.63	8 (44%)	18,36,39	3.38	3 (16%)
3	B8W	5	4529	3,80	18,26,27	2.10	2 (11%)	21,38,41	2.43	9 (42%)
3	OMC	5	4536	3	19,22,23	2.95	8 (42%)	26,31,34	0.69	0
3	PSU	5	4293	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	A2M	5	4523	3,80	18,25,26	3.60	7 (38%)	18,36,39	3.28	3 (16%)
3	A2M	5	3785	3	18,25,26	3.65	8 (44%)	18,36,39	3.41	5 (27%)
3	OMG	5	4623	3	18,26,27	2.47	8 (44%)	19,38,41	1.53	4 (21%)
6	5MU	9	814	6	19,22,23	4.91	7 (36%)	28,32,35	3.60	9 (32%)
3	PSU	5	1582	3	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	5	3825	3	18,25,26	3.60	7 (38%)	18,36,39	3.30	3 (16%)
3	PSU	5	4628	3	18,21,22	1.06	1 (5%)	22,30,33	1.86	4 (18%)
3	OMC	5	2861	3	19,22,23	3.01	8 (42%)	26,31,34	0.78	0
3	UR3	5	4597	3	19,22,23	2.82	6 (31%)	26,32,35	1.19	2 (7%)
6	MMX	9	568	6	19,23,24	3.94	5 (26%)	22,33,36	2.84	5 (22%)
3	PSU	5	1677	3	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)
6	6MZ	9	1832	6,80	18,25,26	1.83	3 (16%)	16,36,39	3.52	4 (25%)
6	OMC	9	1710	6	19,22,23	3.00	8 (42%)	26,31,34	0.73	0
6	A2M	9	159	6	18,25,26	3.60	8 (44%)	18,36,39	3.45	4 (22%)
9	MLZ	C	333	9	8,9,10	0.81	0	4,9,11	0.63	0
3	MHG	5	4371	3	29,32,33	3.81	11 (37%)	34,46,49	2.38	11 (32%)
6	OMC	9	174	6	19,22,23	3.04	8 (42%)	26,31,34	0.72	0
3	M7A	5	4564	3	20,25,26	1.98	3 (15%)	28,37,40	3.89	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	6MZ	5	4220	3	18,25,26	1.90	3 (16%)	16,36,39	3.59	3 (18%)
3	B8W	5	2380	3	18,26,27	2.10	2 (11%)	21,38,41	2.42	7 (33%)
3	A2M	5	3723	3	18,25,26	3.59	8 (44%)	18,36,39	3.26	4 (22%)
3	P4U	5	1348	3	21,24,25	3.55	8 (38%)	27,33,36	1.00	1 (3%)
6	UR3	9	1830	6	19,22,23	2.83	6 (31%)	26,32,35	1.39	3 (11%)
3	OMG	5	1316	3	18,26,27	2.46	8 (44%)	19,38,41	1.54	4 (21%)
3	5MU	5	4083	3	19,22,23	4.90	7 (36%)	28,32,35	3.55	9 (32%)
3	B8H	5	4296	3	19,22,23	6.81	6 (31%)	22,32,35	2.38	5 (22%)
6	A2M	9	484	6	18,25,26	3.62	8 (44%)	18,36,39	3.37	4 (22%)
3	OMG	5	4370	3	18,26,27	2.48	8 (44%)	19,38,41	1.52	4 (21%)
3	B8W	5	4185	3	18,26,27	2.10	2 (11%)	21,38,41	2.42	7 (33%)
44	MLZ	m	72	44	8,9,10	0.77	0	4,9,11	0.58	0
6	A2M	9	166	6	18,25,26	3.62	8 (44%)	18,36,39	3.42	5 (27%)
6	OMU	9	121	6	19,22,23	3.00	8 (42%)	26,31,34	1.73	5 (19%)
3	E7G	5	2297	3	24,27,28	3.99	11 (45%)	30,40,43	2.22	10 (33%)
3	OMU	5	4620	3	19,22,23	2.98	8 (42%)	26,31,34	1.76	5 (19%)
3	A2M	5	3718	3	18,25,26	3.61	8 (44%)	18,36,39	3.29	4 (22%)
3	PSU	5	4442	3	18,21,22	1.08	2 (11%)	22,30,33	1.87	6 (27%)
3	PSU	5	2508	3	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
3	UR3	5	1866	3	19,22,23	2.84	7 (36%)	26,32,35	1.29	2 (7%)
6	OMC	9	1703	6	19,22,23	2.95	8 (42%)	26,31,34	0.70	0
3	A2M	5	3867	3	18,25,26	3.62	8 (44%)	18,36,39	3.35	4 (22%)
6	OMC	9	517	6	19,22,23	3.01	8 (42%)	26,31,34	0.75	0
3	7MG	5	2522	3	22,26,27	3.68	10 (45%)	29,39,42	2.03	9 (31%)
3	A2M	5	1871	3,80	18,25,26	3.60	7 (38%)	18,36,39	3.36	3 (16%)
3	PSU	5	4450	3,80	18,21,22	1.05	1 (5%)	22,30,33	1.79	5 (22%)
3	OMC	5	2422	3,80	19,22,23	2.99	8 (42%)	26,31,34	0.75	0
3	OMG	5	2773	3	18,26,27	2.51	8 (44%)	19,38,41	1.53	4 (21%)
3	A2M	5	1524	3	18,25,26	3.60	7 (38%)	18,36,39	3.36	4 (22%)
3	OMG	5	4494	3	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
3	B9B	5	2754	3	21,28,29	1.99	3 (14%)	23,40,43	6.49	5 (21%)
6	OMG	9	509	6,80	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
3	1MA	5	1322	3,80	16,25,26	4.22	5 (31%)	18,37,40	1.88	3 (16%)
6	A2M	9	668	6,80	18,25,26	3.64	9 (50%)	18,36,39	3.41	3 (16%)
3	PSU	5	4636	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PSU	5	4403	3	18,21,22	1.07	1 (5%)	22,30,33	1.69	5 (22%)
6	OMG	9	683	6	18,26,27	2.49	8 (44%)	19,38,41	1.55	4 (21%)
3	OMC	5	2365	3	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
6	PSU	9	1243	6	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
6	A2M	9	1031	6	18,25,26	3.60	8 (44%)	18,36,39	3.40	3 (16%)
3	OMG	5	1522	3	18,26,27	2.45	8 (44%)	19,38,41	1.51	4 (21%)
6	PSU	9	612	6	18,21,22	1.03	1 (5%)	22,30,33	1.75	5 (22%)
6	A2M	9	1678	6	18,25,26	3.56	8 (44%)	18,36,39	3.36	3 (16%)
3	UR3	5	4530	3	19,22,23	2.79	7 (36%)	26,32,35	1.26	2 (7%)
6	MA6	9	1850	6	19,26,27	1.42	3 (15%)	18,38,41	4.20	3 (16%)
3	A2M	5	1534	3,80	18,25,26	3.61	8 (44%)	18,36,39	3.36	3 (16%)
3	E6G	5	4355	3	20,27,28	2.81	3 (15%)	22,39,42	3.07	7 (31%)
6	4AC	9	1337	6	21,24,25	3.23	9 (42%)	29,34,37	1.06	3 (10%)
3	PSU	5	1683	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	B9B	5	1574	3	21,28,29	2.00	3 (14%)	23,40,43	6.43	5 (21%)
3	OMG	5	2050	3	18,26,27	2.44	8 (44%)	19,38,41	1.51	4 (21%)
3	BGH	5	3899	3,80	25,29,30	4.49	19 (76%)	31,43,46	2.31	12 (38%)
3	PSU	5	3764	3	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
5	OMU	8	14	5,3	19,22,23	2.98	8 (42%)	26,31,34	1.70	5 (19%)
3	5MC	5	3782	3	18,22,23	3.51	7 (38%)	26,32,35	1.06	2 (7%)
3	B8H	5	1860	3	19,22,23	6.81	6 (31%)	22,32,35	2.34	5 (22%)
3	7MG	5	1605	3	22,26,27	3.73	10 (45%)	29,39,42	2.06	9 (31%)
3	OMU	5	4306	3	19,22,23	2.98	8 (42%)	26,31,34	1.73	5 (19%)
3	OMC	5	3887	3	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
3	B8W	5	4472	3	18,26,27	2.10	2 (11%)	21,38,41	2.39	7 (33%)
6	B8N	9	1248	6	24,29,30	3.06	7 (29%)	29,42,45	1.72	5 (17%)
3	PSU	5	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
3	OMG	5	4870	3	18,26,27	2.51	8 (44%)	19,38,41	1.54	4 (21%)

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
3	I4U	5	1659	3	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	5	3909	3	-	2/9/27/28	0/2/2/2
3	B9B	5	237	3	-	5/7/29/30	0/3/3/3
6	4AC	9	1842	6	-	0/11/29/30	0/2/2/2
3	7MG	5	4550	3	-	0/7/37/38	0/3/3/3
6	M7A	9	1806	6	-	2/7/37/38	0/3/3/3
3	B8Q	5	1456	3	-	0/7/42/43	0/2/2/2
3	A2M	5	2401	3,80	-	0/5/27/28	0/3/3/3
3	B8W	5	4129	3	-	2/5/27/28	0/3/3/3
3	OMC	5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	5	3729	3	-	2/7/25/26	0/2/2/2
3	1MA	5	4415	3	-	1/3/25/26	0/3/3/3
3	B8H	5	3762	3	-	2/7/25/26	0/2/2/2
6	A2M	9	27	6,80	-	1/5/27/28	0/3/3/3
3	OMG	5	2424	3	-	2/5/27/28	0/3/3/3
3	OMG	5	1625	3	-	2/5/27/28	0/3/3/3
3	5MC	5	4447	3	-	0/7/25/26	0/2/2/2
3	B8T	5	4483	3	-	0/7/27/28	0/2/2/2
3	5MC	5	4335	3	-	0/7/25/26	0/2/2/2
3	OMG	5	373	3	-	0/5/27/28	0/3/3/3
3	I4U	5	4194	3	-	2/9/29/30	0/2/2/2
3	A2M	5	398	3	-	2/5/27/28	0/3/3/3
3	B8K	5	4690	14,3	-	0/11/41/42	0/3/3/3
6	PSU	9	119	6	-	0/7/25/26	0/2/2/2
3	2MG	5	4872	18,3	-	0/5/27/28	0/3/3/3
3	2MG	5	729	3	-	1/5/27/28	0/3/3/3
3	A2M	5	2363	3,80	-	0/5/27/28	0/3/3/3
6	B8Q	9	1219	6,80	-	2/7/42/43	0/2/2/2
3	E7G	5	1797	3	-	2/9/39/40	0/3/3/3
3	2MG	5	1517	3	-	0/5/27/28	0/3/3/3
6	5MC	9	1374	6	-	0/7/25/26	0/2/2/2
3	PSU	5	4531	3	-	1/7/25/26	0/2/2/2
3	OMG	5	3792	3	-	2/5/27/28	0/3/3/3
6	OMG	9	644	6	-	3/5/27/28	0/3/3/3
3	P7G	5	1909	3	-	1/10/40/41	0/3/3/3
3	OMC	5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4500	3	-	3/7/25/26	0/2/2/2
6	PSU	9	823	6	-	0/7/25/26	0/2/2/2
3	B8K	5	3897	3	-	3/11/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B9H	5	2786	3	-	1/12/47/48	0/2/2/2
3	OMC	5	3701	3,80	-	4/9/27/28	0/2/2/2
6	OMU	9	116	6	-	2/9/27/28	0/2/2/2
3	OMG	5	2364	3	-	3/5/27/28	0/3/3/3
6	PSU	9	822	6	-	0/7/25/26	0/2/2/2
1	T6A	2	37	1	-	4/19/41/42	0/3/3/3
3	A2M	5	1326	3	-	1/5/27/28	0/3/3/3
3	OMG	5	4637	3	-	2/5/27/28	0/3/3/3
6	MA6	9	1851	6	-	2/7/29/30	0/3/3/3
6	PSU	9	1081	6	-	0/7/25/26	0/2/2/2
3	B8T	5	4671	3	-	1/7/27/28	0/2/2/2
3	OMG	5	4196	3	-	0/5/27/28	0/3/3/3
3	OMG	5	1883	3	-	2/5/27/28	0/3/3/3
3	P7G	5	3880	3	-	2/10/40/41	0/3/3/3
3	A2M	5	4571	3	-	1/5/27/28	0/3/3/3
3	B8W	5	4529	3,80	-	2/5/27/28	0/3/3/3
3	OMC	5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	5	4523	3,80	-	2/5/27/28	0/3/3/3
3	A2M	5	3785	3	-	3/5/27/28	0/3/3/3
3	OMG	5	4623	3	-	0/5/27/28	0/3/3/3
6	5MU	9	814	6	-	0/7/25/26	0/2/2/2
3	PSU	5	1582	3	-	0/7/25/26	0/2/2/2
3	A2M	5	3825	3	-	1/5/27/28	0/3/3/3
3	PSU	5	4628	3	-	0/7/25/26	0/2/2/2
3	OMC	5	2861	3	-	1/9/27/28	0/2/2/2
3	UR3	5	4597	3	-	0/7/25/26	0/2/2/2
6	MMX	9	568	6	-	4/9/44/45	0/2/2/2
3	PSU	5	1677	3	-	5/7/25/26	0/2/2/2
6	6MZ	9	1832	6,80	-	0/5/27/28	0/3/3/3
6	OMC	9	1710	6	-	0/9/27/28	0/2/2/2
6	A2M	9	159	6	-	3/5/27/28	0/3/3/3
9	MLZ	C	333	9	-	3/7/8/10	-
3	MHG	5	4371	3	-	6/16/46/47	0/3/3/3
6	OMC	9	174	6	-	1/9/27/28	0/2/2/2
3	M7A	5	4564	3	-	0/7/37/38	0/3/3/3
3	6MZ	5	4220	3	-	1/5/27/28	0/3/3/3
3	B8W	5	2380	3	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	5	3723	3	-	0/5/27/28	0/3/3/3
3	P4U	5	1348	3	-	3/10/29/30	0/2/2/2
6	UR3	9	1830	6	-	2/7/25/26	0/2/2/2
3	OMG	5	1316	3	-	1/5/27/28	0/3/3/3
3	5MU	5	4083	3	-	0/7/25/26	0/2/2/2
3	B8H	5	4296	3	-	3/7/25/26	0/2/2/2
6	A2M	9	484	6	-	0/5/27/28	0/3/3/3
3	OMG	5	4370	3	-	0/5/27/28	0/3/3/3
3	B8W	5	4185	3	-	2/5/27/28	0/3/3/3
44	MLZ	m	72	44	-	1/7/8/10	-
6	A2M	9	166	6	-	2/5/27/28	0/3/3/3
6	OMU	9	121	6	-	0/9/27/28	0/2/2/2
3	E7G	5	2297	3	-	3/9/39/40	0/3/3/3
3	OMU	5	4620	3	-	1/9/27/28	0/2/2/2
3	A2M	5	3718	3	-	1/5/27/28	0/3/3/3
3	PSU	5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	5	2508	3	-	0/7/25/26	0/2/2/2
3	UR3	5	1866	3	-	0/7/25/26	0/2/2/2
6	OMC	9	1703	6	-	2/9/27/28	0/2/2/2
3	A2M	5	3867	3	-	3/5/27/28	0/3/3/3
6	OMC	9	517	6	-	0/9/27/28	0/2/2/2
3	7MG	5	2522	3	-	0/7/37/38	0/3/3/3
3	A2M	5	1871	3,80	-	0/5/27/28	0/3/3/3
3	PSU	5	4450	3,80	-	2/7/25/26	0/2/2/2
3	OMC	5	2422	3,80	-	1/9/27/28	0/2/2/2
3	OMG	5	2773	3	-	1/5/27/28	0/3/3/3
3	A2M	5	1524	3	-	0/5/27/28	0/3/3/3
3	OMG	5	4494	3	-	0/5/27/28	0/3/3/3
3	B9B	5	2754	3	-	3/7/29/30	0/3/3/3
6	OMG	9	509	6,80	-	0/5/27/28	0/3/3/3
3	1MA	5	1322	3,80	-	0/3/25/26	0/3/3/3
6	A2M	9	668	6,80	-	3/5/27/28	0/3/3/3
3	PSU	5	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	5	4403	3	-	2/7/25/26	0/2/2/2
6	OMG	9	683	6	-	2/5/27/28	0/3/3/3
3	OMC	5	2365	3	-	0/9/27/28	0/2/2/2
6	PSU	9	1243	6	-	2/7/25/26	0/2/2/2
6	A2M	9	1031	6	-	0/5/27/28	0/3/3/3
3	OMG	5	1522	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	9	612	6	-	0/7/25/26	0/2/2/2
6	A2M	9	1678	6	-	1/5/27/28	0/3/3/3
3	UR3	5	4530	3	-	2/7/25/26	0/2/2/2
6	MA6	9	1850	6	-	0/7/29/30	0/3/3/3
3	A2M	5	1534	3,80	-	2/5/27/28	0/3/3/3
3	E6G	5	4355	3	-	4/6/28/29	0/3/3/3
6	4AC	9	1337	6	-	0/11/29/30	0/2/2/2
3	PSU	5	1683	3	-	0/7/25/26	0/2/2/2
3	B9B	5	1574	3	-	3/7/29/30	0/3/3/3
3	OMG	5	2050	3	-	0/5/27/28	0/3/3/3
3	BGH	5	3899	3,80	-	1/13/43/44	0/3/3/3
3	PSU	5	3764	3	-	2/7/25/26	0/2/2/2
5	OMU	8	14	5,3	-	1/9/27/28	0/2/2/2
3	5MC	5	3782	3	-	2/7/25/26	0/2/2/2
3	B8H	5	1860	3	-	0/7/25/26	0/2/2/2
3	7MG	5	1605	3	-	0/7/37/38	0/3/3/3
3	OMU	5	4306	3	-	0/9/27/28	0/2/2/2
3	OMC	5	3887	3	-	1/9/27/28	0/2/2/2
3	B8W	5	4472	3	-	2/5/27/28	0/3/3/3
6	B8N	9	1248	6	-	1/16/34/35	0/2/2/2
3	PSU	5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	5	4870	3	-	4/5/27/28	0/3/3/3

All (852) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1860	B8H	C6-C5	-16.61	1.11	1.34
3	5	4296	B8H	C6-C5	-16.58	1.11	1.34
3	5	3762	B8H	C6-C5	-16.51	1.11	1.34
3	5	1860	B8H	C4-N3	-15.74	1.09	1.38
3	5	4296	B8H	C4-N3	-15.74	1.09	1.38
3	5	3762	B8H	C4-N3	-15.62	1.09	1.38
3	5	4415	1MA	C2-N3	15.53	1.47	1.29
3	5	1322	1MA	C2-N3	15.10	1.47	1.29
3	5	4296	B8H	C4-C5	13.31	1.82	1.44
3	5	3762	B8H	C4-C5	13.29	1.82	1.44
3	5	1860	B8H	C4-C5	13.22	1.81	1.44
3	5	3762	B8H	C6-N1	12.35	1.66	1.36
3	5	1860	B8H	C6-N1	12.29	1.66	1.36
3	5	4296	B8H	C6-N1	12.29	1.66	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3899	BGH	C3'-C2'	-12.23	1.25	1.52
6	9	814	5MU	C2-N1	11.39	1.56	1.38
3	5	4083	5MU	C2-N1	11.14	1.56	1.38
3	5	4083	5MU	C6-N1	10.92	1.56	1.38
6	9	814	5MU	C6-N1	10.70	1.56	1.38
3	5	1348	P4U	C4-N3	10.50	1.44	1.31
3	5	1659	I4U	C4-N3	10.36	1.44	1.31
3	5	4355	E6G	O6-C6	10.32	1.44	1.35
6	9	568	MMX	C4-N3	10.21	1.54	1.45
3	5	4194	I4U	C4-N3	10.18	1.44	1.31
6	9	814	5MU	C4-C5	9.83	1.61	1.44
3	5	4083	5MU	C4-C5	9.82	1.61	1.44
3	5	4690	B8K	C8-N9	9.71	1.51	1.46
3	5	2297	E7G	C8-N9	9.64	1.51	1.46
3	5	1797	E7G	C8-N9	9.57	1.51	1.46
6	9	568	MMX	C2-N1	9.36	1.49	1.37
3	5	4371	MHG	C8-N9	9.35	1.51	1.46
3	5	1909	P7G	C8-N9	9.35	1.51	1.46
3	5	4335	5MC	C6-C5	9.28	1.49	1.34
3	5	2786	B9H	C2-N3	9.20	1.48	1.37
3	5	4447	5MC	C6-C5	9.18	1.49	1.34
6	9	1374	5MC	C6-C5	9.13	1.49	1.34
3	5	3897	B8K	C8-N9	9.10	1.51	1.46
3	5	3782	5MC	C6-C5	9.01	1.49	1.34
3	5	2522	7MG	C8-N9	9.00	1.51	1.46
6	9	159	A2M	C3'-C4'	-8.95	1.30	1.53
3	5	4523	A2M	C3'-C4'	-8.89	1.30	1.53
3	5	4571	A2M	C3'-C4'	-8.89	1.30	1.53
3	5	1524	A2M	C3'-C4'	-8.89	1.30	1.53
3	5	4550	7MG	C8-N9	8.89	1.50	1.46
3	5	398	A2M	C3'-C4'	-8.88	1.30	1.53
3	5	1909	P7G	C5-N7	8.85	1.45	1.35
6	9	27	A2M	C3'-C4'	-8.84	1.30	1.53
6	9	166	A2M	C3'-C4'	-8.84	1.30	1.53
3	5	1534	A2M	C3'-C4'	-8.83	1.30	1.53
3	5	1605	7MG	C8-N9	8.83	1.50	1.46
6	9	668	A2M	C3'-C4'	-8.83	1.30	1.53
3	5	3718	A2M	C3'-C4'	-8.81	1.30	1.53
3	5	3880	P7G	C8-N9	8.80	1.50	1.46
3	5	1871	A2M	C3'-C4'	-8.79	1.30	1.53
3	5	3867	A2M	C3'-C4'	-8.78	1.30	1.53
3	5	3825	A2M	C3'-C4'	-8.76	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	484	A2M	C3'-C4'	-8.73	1.30	1.53
3	5	2401	A2M	C3'-C4'	-8.72	1.30	1.53
6	9	1031	A2M	C3'-C4'	-8.71	1.30	1.53
6	9	1678	A2M	C3'-C4'	-8.70	1.30	1.53
3	5	2363	A2M	C3'-C4'	-8.70	1.30	1.53
6	9	568	MMX	C2-N3	8.66	1.48	1.37
3	5	3723	A2M	C3'-C4'	-8.66	1.30	1.53
3	5	1326	A2M	C3'-C4'	-8.65	1.30	1.53
3	5	1797	E7G	C5-N7	8.54	1.45	1.35
3	5	2297	E7G	C5-N7	8.50	1.45	1.35
3	5	3880	P7G	C5-N7	8.48	1.45	1.35
3	5	1456	B8Q	C6-C5	8.45	1.52	1.33
3	5	3785	A2M	C3'-C4'	-8.31	1.31	1.53
6	9	1219	B8Q	C6-C5	8.31	1.52	1.33
3	5	4371	MHG	C2-N3	8.12	1.47	1.31
3	5	3899	BGH	C8-N9	8.09	1.50	1.46
3	5	4129	B8W	C2-N2	8.02	1.49	1.33
3	5	4529	B8W	C2-N2	7.98	1.49	1.33
3	5	4472	B8W	C2-N2	7.94	1.49	1.33
3	5	2380	B8W	C2-N2	7.93	1.49	1.33
3	5	4371	MHG	C5-N7	7.93	1.44	1.35
3	5	4185	B8W	C2-N2	7.87	1.49	1.33
3	5	3785	A2M	O4'-C4'	7.85	1.62	1.45
6	9	1248	B8N	C4-N3	-7.83	1.25	1.40
3	5	2401	A2M	O4'-C4'	7.79	1.62	1.45
6	9	1248	B8N	C6-N1	7.78	1.55	1.36
6	9	668	A2M	O4'-C1'	-7.76	1.30	1.41
3	5	3718	A2M	O4'-C4'	7.74	1.62	1.45
3	5	3785	A2M	O4'-C1'	-7.73	1.30	1.41
6	9	166	A2M	O4'-C4'	7.71	1.62	1.45
3	5	1605	7MG	C5-N7	7.71	1.44	1.35
3	5	3723	A2M	O4'-C4'	7.68	1.62	1.45
3	5	398	A2M	O4'-C4'	7.67	1.62	1.45
3	5	1871	A2M	O4'-C4'	7.61	1.62	1.45
6	9	1031	A2M	O4'-C4'	7.61	1.62	1.45
3	5	3825	A2M	O4'-C4'	7.61	1.62	1.45
3	5	1534	A2M	O4'-C4'	7.59	1.61	1.45
6	9	484	A2M	O4'-C4'	7.56	1.61	1.45
6	9	27	A2M	O4'-C4'	7.56	1.61	1.45
3	5	4550	7MG	C5-N7	7.56	1.44	1.35
3	5	2363	A2M	O4'-C1'	-7.53	1.30	1.41
3	5	4523	A2M	O4'-C4'	7.52	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1326	A2M	O4'-C4'	7.52	1.61	1.45
6	9	814	5MU	C4-N3	-7.51	1.24	1.38
3	5	1326	A2M	O4'-C1'	-7.50	1.30	1.41
3	5	3867	A2M	O4'-C1'	-7.48	1.30	1.41
6	9	159	A2M	O4'-C4'	7.46	1.61	1.45
3	5	3867	A2M	O4'-C4'	7.45	1.61	1.45
3	5	2363	A2M	O4'-C4'	7.44	1.61	1.45
3	5	4083	5MU	C4-N3	-7.42	1.25	1.38
3	5	4571	A2M	O4'-C4'	7.42	1.61	1.45
3	5	4571	A2M	O4'-C1'	-7.40	1.30	1.41
6	9	1678	A2M	O4'-C4'	7.39	1.61	1.45
3	5	1524	A2M	O4'-C4'	7.35	1.61	1.45
3	5	2522	7MG	C5-N7	7.35	1.44	1.35
3	5	4671	B8T	C2-N3	7.28	1.51	1.36
6	9	484	A2M	O4'-C1'	-7.27	1.30	1.41
3	5	1524	A2M	O4'-C1'	-7.27	1.30	1.41
3	5	4483	B8T	C2-N3	7.26	1.51	1.36
6	9	166	A2M	O4'-C1'	-7.21	1.31	1.41
3	5	3825	A2M	O4'-C1'	-7.21	1.31	1.41
6	9	668	A2M	O4'-C4'	7.20	1.61	1.45
6	9	159	A2M	O4'-C1'	-7.18	1.31	1.41
6	9	27	A2M	O4'-C1'	-7.15	1.31	1.41
6	9	1031	A2M	O4'-C1'	-7.15	1.31	1.41
6	9	1678	A2M	O4'-C1'	-7.11	1.31	1.41
3	5	1871	A2M	O4'-C1'	-7.10	1.31	1.41
3	5	1534	A2M	O4'-C1'	-7.07	1.31	1.41
3	5	3723	A2M	O4'-C1'	-7.05	1.31	1.41
3	5	4671	B8T	C4-N3	7.05	1.45	1.32
3	5	2786	B9H	C6-C5	7.03	1.49	1.33
3	5	3718	A2M	O4'-C1'	-7.03	1.31	1.41
3	5	4523	A2M	O4'-C1'	-7.02	1.31	1.41
3	5	2401	A2M	O4'-C1'	-7.00	1.31	1.41
3	5	398	A2M	O4'-C1'	-6.99	1.31	1.41
6	9	1337	4AC	C4-N3	6.97	1.44	1.32
6	9	121	OMU	C2-N1	6.96	1.49	1.38
3	5	4483	B8T	C4-N3	6.91	1.44	1.32
6	9	116	OMU	C2-N1	6.88	1.49	1.38
3	5	1866	UR3	C2-N1	6.87	1.48	1.38
6	9	1830	UR3	C2-N1	6.87	1.48	1.38
3	5	4620	OMU	C2-N1	6.85	1.49	1.38
3	5	4306	OMU	C2-N1	6.84	1.49	1.38
3	5	4671	B8T	C6-C5	6.84	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	8	14	OMU	C2-N1	6.83	1.49	1.38
6	9	1219	B8Q	C2-N3	6.83	1.46	1.35
3	5	4483	B8T	C6-C5	6.82	1.50	1.35
6	9	1842	4AC	C4-N3	6.76	1.44	1.32
3	5	4530	UR3	C6-C5	6.74	1.50	1.35
3	5	3897	B8K	C2-N3	6.73	1.49	1.33
6	9	116	OMU	C2-N3	6.73	1.50	1.38
5	8	14	OMU	C2-N3	6.70	1.49	1.38
3	5	4306	OMU	C2-N3	6.70	1.49	1.38
6	9	121	OMU	C2-N3	6.69	1.49	1.38
3	5	4597	UR3	C6-C5	6.68	1.50	1.35
3	5	4690	B8K	C2-N3	6.67	1.49	1.33
3	5	4597	UR3	C2-N1	6.65	1.48	1.38
6	9	1830	UR3	C6-C5	6.64	1.50	1.35
3	5	2786	B9H	C2-N1	6.64	1.48	1.38
3	5	4620	OMU	C2-N3	6.62	1.49	1.38
6	9	814	5MU	C6-C5	6.60	1.45	1.34
3	5	1866	UR3	C6-C5	6.60	1.50	1.35
3	5	3880	P7G	C4-N9	6.55	1.45	1.35
3	5	4220	6MZ	C6-N6	6.54	1.45	1.35
3	5	4083	5MU	C6-C5	6.50	1.45	1.34
6	9	174	OMC	C2-N3	6.42	1.49	1.36
3	5	3869	OMC	C2-N3	6.40	1.49	1.36
6	9	1374	5MC	C4-N3	6.39	1.44	1.34
3	5	2861	OMC	C2-N3	6.39	1.49	1.36
3	5	1456	B8Q	C2-N3	6.37	1.46	1.35
6	9	1710	OMC	C2-N3	6.36	1.49	1.36
3	5	4335	5MC	C4-N3	6.35	1.44	1.34
3	5	4371	MHG	C8-N7	6.34	1.51	1.45
3	5	1909	P7G	C4-N9	6.33	1.44	1.35
6	9	1832	6MZ	C6-N6	6.32	1.45	1.35
6	9	517	OMC	C2-N3	6.32	1.49	1.36
3	5	3782	5MC	C4-N3	6.32	1.44	1.34
3	5	2422	OMC	C2-N3	6.30	1.49	1.36
3	5	2365	OMC	C2-N3	6.30	1.49	1.36
3	5	4194	I4U	C6-C5	6.29	1.49	1.35
3	5	3887	OMC	C2-N3	6.29	1.49	1.36
3	5	3880	P7G	C4-N3	6.28	1.48	1.37
6	9	1703	OMC	C2-N3	6.28	1.49	1.36
3	5	2804	OMC	C2-N3	6.27	1.49	1.36
3	5	4371	MHG	C2-N1	6.27	1.46	1.36
3	5	4671	B8T	C4-N4	6.26	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	1337	4AC	C6-C5	6.24	1.49	1.35
3	5	3909	OMC	C2-N3	6.23	1.49	1.36
3	5	1909	P7G	C4-N3	6.23	1.48	1.37
3	5	4483	B8T	C4-N4	6.21	1.48	1.35
3	5	3701	OMC	C2-N3	6.21	1.49	1.36
3	5	4530	UR3	C2-N1	6.21	1.47	1.38
3	5	4536	OMC	C2-N3	6.20	1.48	1.36
3	5	2297	E7G	C4-N9	6.18	1.44	1.37
3	5	1574	B9B	O6-C6	6.18	1.40	1.35
3	5	1659	I4U	C6-C5	6.17	1.49	1.35
3	5	1797	E7G	C8-N7	6.16	1.51	1.45
3	5	1348	P4U	C6-C5	6.15	1.49	1.35
3	5	2297	E7G	C8-N7	6.15	1.51	1.45
3	5	1909	P7G	C8-N7	6.12	1.51	1.45
6	9	1842	4AC	C6-C5	6.10	1.49	1.35
3	5	1348	P4U	C2-N3	6.10	1.48	1.36
3	5	1797	E7G	C4-N9	6.06	1.44	1.37
6	9	174	OMC	C6-C5	6.04	1.49	1.35
3	5	4335	5MC	C2-N3	6.04	1.48	1.36
3	5	3782	5MC	C2-N3	6.02	1.48	1.36
6	9	517	OMC	C6-C5	6.02	1.49	1.35
3	5	2861	OMC	C6-C5	6.02	1.49	1.35
3	5	4447	5MC	C4-N3	6.02	1.44	1.34
3	5	2754	B9B	O6-C6	6.01	1.40	1.35
3	5	2365	OMC	C6-C5	6.00	1.49	1.35
3	5	3701	OMC	C6-C5	6.00	1.49	1.35
3	5	4355	E6G	C2-N2	5.99	1.45	1.33
3	5	237	B9B	O6-C6	5.99	1.40	1.35
6	9	1710	OMC	C6-C5	5.96	1.48	1.35
3	5	3869	OMC	C6-C5	5.95	1.48	1.35
3	5	4536	OMC	C6-C5	5.95	1.48	1.35
6	9	1337	4AC	C2-N3	5.95	1.48	1.36
6	9	1703	OMC	C6-C5	5.94	1.48	1.35
6	9	1374	5MC	C2-N3	5.94	1.48	1.36
3	5	2804	OMC	C6-C5	5.94	1.48	1.35
3	5	2422	OMC	C6-C5	5.93	1.48	1.35
3	5	3887	OMC	C6-C5	5.93	1.48	1.35
3	5	2522	7MG	C2-N3	5.89	1.47	1.33
6	9	1842	4AC	C2-N3	5.89	1.48	1.36
3	5	3909	OMC	C6-C5	5.88	1.48	1.35
3	5	1659	I4U	C2-N3	5.88	1.48	1.36
3	5	1909	P7G	C2-N2	5.88	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4550	7MG	C2-N3	5.86	1.47	1.33
3	5	1605	7MG	C2-N3	5.85	1.47	1.33
3	5	1797	E7G	C2-N3	5.83	1.47	1.33
3	5	3880	P7G	C2-N2	5.83	1.48	1.34
3	5	1797	E7G	C4-N3	5.82	1.48	1.34
3	5	2297	E7G	C2-N3	5.82	1.47	1.33
3	5	2297	E7G	C4-N3	5.77	1.48	1.34
3	5	4447	5MC	C2-N3	5.76	1.48	1.36
3	5	3897	B8K	C4-N9	5.74	1.44	1.37
6	9	1248	B8N	C2-N1	5.74	1.56	1.39
3	5	1866	UR3	C2-N3	5.72	1.50	1.39
3	5	4194	I4U	C2-N3	5.72	1.48	1.36
6	9	1806	M7A	C4-N9	5.72	1.48	1.38
3	5	2754	B9B	C2-N2	5.72	1.45	1.33
3	5	4597	UR3	C2-N3	5.70	1.50	1.39
3	5	1605	7MG	C4-N9	5.70	1.44	1.37
3	5	237	B9B	C2-N2	5.65	1.45	1.33
3	5	4620	OMU	C6-C5	5.62	1.48	1.35
6	9	121	OMU	C6-C5	5.61	1.48	1.35
3	5	4530	UR3	C2-N3	5.61	1.49	1.39
6	9	116	OMU	C6-C5	5.61	1.48	1.35
6	9	509	OMG	C2-N3	5.59	1.46	1.33
3	5	4564	M7A	C4-N9	5.59	1.48	1.38
3	5	1574	B9B	C2-N2	5.58	1.45	1.33
3	5	4550	7MG	C4-N3	5.58	1.47	1.34
3	5	4371	MHG	C2-N2	5.58	1.45	1.33
3	5	4306	OMU	C6-C5	5.57	1.48	1.35
3	5	4371	MHG	C4-N9	5.55	1.44	1.37
5	8	14	OMU	C6-C5	5.55	1.47	1.35
3	5	4870	OMG	C2-N3	5.55	1.46	1.33
3	5	1605	7MG	C4-N3	5.54	1.47	1.34
6	9	1830	UR3	C2-N3	5.54	1.49	1.39
3	5	4550	7MG	C4-N9	5.54	1.44	1.37
3	5	4637	OMG	C2-N3	5.53	1.46	1.33
3	5	2424	OMG	C2-N3	5.52	1.46	1.33
3	5	2773	OMG	C2-N3	5.51	1.46	1.33
3	5	2522	7MG	C4-N3	5.50	1.47	1.34
3	5	1883	OMG	C2-N3	5.49	1.46	1.33
3	5	4370	OMG	C2-N3	5.48	1.46	1.33
6	9	1248	B8N	C6-C5	5.47	1.42	1.34
3	5	3792	OMG	C2-N3	5.47	1.46	1.33
3	5	4494	OMG	C2-N3	5.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	683	OMG	C2-N3	5.46	1.46	1.33
3	5	3899	BGH	C2-N3	5.45	1.46	1.33
3	5	1316	OMG	C2-N3	5.45	1.46	1.33
3	5	1625	OMG	C2-N3	5.45	1.46	1.33
3	5	4196	OMG	C2-N3	5.42	1.46	1.33
6	9	644	OMG	C2-N3	5.42	1.46	1.33
3	5	4623	OMG	C2-N3	5.40	1.46	1.33
3	5	3899	BGH	C4-N3	5.39	1.47	1.34
3	5	1522	OMG	C2-N3	5.38	1.46	1.33
3	5	4371	MHG	C4-N3	5.37	1.47	1.34
3	5	373	OMG	C2-N3	5.36	1.46	1.33
3	5	2522	7MG	C4-N9	5.35	1.43	1.37
3	5	2364	OMG	C2-N3	5.34	1.46	1.33
3	5	4690	B8K	C4-N9	5.31	1.43	1.37
3	5	4415	1MA	C2-N1	5.31	1.45	1.35
3	5	729	2MG	C2-N2	5.31	1.45	1.33
3	5	4872	2MG	C2-N2	5.30	1.45	1.33
3	5	1909	P7G	C2-N1	5.30	1.46	1.33
3	5	3899	BGH	C2'-C1'	5.29	1.66	1.53
3	5	2050	OMG	C2-N3	5.28	1.46	1.33
3	5	3880	P7G	C2-N1	5.26	1.45	1.33
3	5	1517	2MG	C2-N2	5.25	1.45	1.33
3	5	3880	P7G	C8-N7	5.22	1.50	1.45
3	5	2422	OMC	C4-N3	5.18	1.44	1.34
6	9	174	OMC	C4-N3	5.16	1.44	1.34
3	5	1797	E7G	C2-N2	5.15	1.46	1.34
3	5	3869	OMC	C4-N3	5.14	1.44	1.34
6	9	1710	OMC	C4-N3	5.13	1.44	1.34
3	5	2297	E7G	C2-N2	5.12	1.46	1.34
3	5	1322	1MA	C2-N1	5.11	1.45	1.35
6	9	517	OMC	C4-N3	5.11	1.44	1.34
3	5	729	2MG	C4-N3	5.11	1.49	1.37
3	5	3899	BGH	O4'-C1'	-5.10	1.29	1.42
3	5	3887	OMC	C4-N3	5.07	1.44	1.34
3	5	2365	OMC	C4-N3	5.05	1.44	1.34
3	5	2861	OMC	C4-N3	5.05	1.44	1.34
3	5	4536	OMC	C4-N3	5.04	1.44	1.34
6	9	1703	OMC	C4-N3	5.04	1.44	1.34
3	5	4872	2MG	C2-N1	5.03	1.44	1.36
3	5	3701	OMC	C4-N3	5.02	1.44	1.34
3	5	2804	OMC	C4-N3	5.00	1.44	1.34
6	9	174	OMC	C4-N4	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1517	2MG	C4-N3	4.96	1.49	1.37
6	9	1710	OMC	C4-N4	4.91	1.45	1.33
3	5	2804	OMC	C4-N4	4.91	1.45	1.33
3	5	2861	OMC	C4-N4	4.90	1.45	1.33
3	5	1605	7MG	C2-N2	4.89	1.45	1.34
3	5	3869	OMC	C4-N4	4.88	1.45	1.33
3	5	3909	OMC	C4-N3	4.87	1.44	1.34
6	9	517	OMC	C4-N4	4.87	1.45	1.33
6	9	1703	OMC	C4-N4	4.86	1.45	1.33
3	5	2522	7MG	C2-N2	4.86	1.45	1.34
3	5	2422	OMC	C4-N4	4.86	1.45	1.33
3	5	3887	OMC	C4-N4	4.85	1.45	1.33
3	5	4536	OMC	C4-N4	4.85	1.45	1.33
3	5	3701	OMC	C4-N4	4.84	1.45	1.33
3	5	3909	OMC	C4-N4	4.82	1.45	1.33
3	5	2365	OMC	C4-N4	4.82	1.45	1.33
3	5	3792	OMG	C4-N3	4.79	1.49	1.37
6	9	509	OMG	C4-N3	4.79	1.49	1.37
3	5	4550	7MG	C2-N2	4.78	1.45	1.34
3	5	1883	OMG	C4-N3	4.77	1.48	1.37
3	5	4494	OMG	C4-N3	4.76	1.48	1.37
3	5	4870	OMG	C4-N3	4.76	1.48	1.37
3	5	2773	OMG	C4-N3	4.75	1.48	1.37
3	5	2424	OMG	C4-N3	4.75	1.48	1.37
3	5	4370	OMG	C4-N3	4.74	1.48	1.37
3	5	1316	OMG	C4-N3	4.73	1.48	1.37
3	5	1522	OMG	C4-N3	4.73	1.48	1.37
6	9	683	OMG	C4-N3	4.72	1.48	1.37
3	5	3899	BGH	C4-N9	4.72	1.43	1.37
3	5	373	OMG	C4-N3	4.71	1.48	1.37
3	5	4637	OMG	C4-N3	4.71	1.48	1.37
3	5	4623	OMG	C4-N3	4.71	1.48	1.37
3	5	2050	OMG	C4-N3	4.68	1.48	1.37
3	5	4196	OMG	C4-N3	4.66	1.48	1.37
3	5	1625	OMG	C4-N3	4.65	1.48	1.37
6	9	1219	B8Q	C2-N1	4.65	1.45	1.38
6	9	1842	4AC	C7-N4	4.65	1.45	1.37
6	9	644	OMG	C4-N3	4.65	1.48	1.37
3	5	1348	P4U	O4-C4	4.62	1.40	1.35
6	9	1337	4AC	C7-N4	4.59	1.45	1.37
3	5	1517	2MG	C2-N1	4.58	1.44	1.36
3	5	4671	B8T	C2-N1	4.58	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	1659	I4U	C5-C4	4.57	1.49	1.43
3	5	2364	OMG	C4-N3	4.56	1.48	1.37
3	5	3899	BGH	C2-N2	4.56	1.45	1.34
6	9	174	OMC	C2-N1	4.55	1.49	1.40
3	5	4872	2MG	C4-N3	4.54	1.48	1.37
6	9	517	OMC	C2-N1	4.53	1.49	1.40
3	5	4194	I4U	C5-C4	4.52	1.49	1.43
3	5	4447	5MC	C6-N1	4.50	1.45	1.38
3	5	729	2MG	C2-N1	4.50	1.43	1.36
6	9	1374	5MC	C6-N1	4.49	1.45	1.38
3	5	4483	B8T	C2-N1	4.49	1.49	1.40
3	5	4335	5MC	C6-N1	4.47	1.45	1.38
3	5	3897	B8K	C4-N3	4.47	1.44	1.34
3	5	3909	OMC	C2-N1	4.46	1.49	1.40
3	5	3762	B8H	C2-N3	4.44	1.45	1.38
3	5	4690	B8K	C4-N3	4.43	1.44	1.34
3	5	3869	OMC	C2-N1	4.43	1.49	1.40
3	5	3899	BGH	C5'-C4'	-4.42	1.37	1.51
3	5	2422	OMC	C2-N1	4.41	1.49	1.40
6	9	1710	OMC	C2-N1	4.40	1.49	1.40
3	5	2861	OMC	C2-N1	4.39	1.49	1.40
3	5	3782	5MC	C6-N1	4.38	1.45	1.38
6	9	1374	5MC	C4-N4	4.35	1.45	1.34
3	5	4296	B8H	C2-N3	4.35	1.45	1.38
3	5	4335	5MC	C4-N4	4.34	1.45	1.34
3	5	4564	M7A	C6-N6	4.31	1.44	1.34
3	5	1348	P4U	C5-C4	4.30	1.48	1.43
3	5	3887	OMC	C2-N1	4.30	1.49	1.40
6	9	1806	M7A	C6-N6	4.30	1.44	1.34
3	5	2804	OMC	C2-N1	4.28	1.49	1.40
3	5	3782	5MC	C4-N4	4.27	1.45	1.34
3	5	3701	OMC	C2-N1	4.26	1.49	1.40
3	5	3782	5MC	C2-N1	4.26	1.49	1.40
3	5	1860	B8H	C2-N3	4.25	1.45	1.38
3	5	3899	BGH	O4'-C4'	4.25	1.54	1.45
3	5	2365	OMC	C2-N1	4.25	1.49	1.40
6	9	1337	4AC	C4-N4	4.24	1.45	1.39
3	5	4447	5MC	C4-N4	4.23	1.45	1.34
6	9	568	MMX	C5-C4	-4.23	1.48	1.52
6	9	1703	OMC	C2-N1	4.23	1.49	1.40
6	9	116	OMU	C4-N3	4.19	1.46	1.38
5	8	14	OMU	C4-N3	4.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	121	OMU	C4-N3	4.17	1.46	1.38
6	9	1374	5MC	C2-N1	4.15	1.49	1.40
6	9	1842	4AC	C4-N4	4.15	1.45	1.39
3	5	4536	OMC	C2-N1	4.11	1.48	1.40
3	5	4335	5MC	C2-N1	4.10	1.48	1.40
6	9	1337	4AC	C5-C4	4.09	1.49	1.40
3	5	1348	P4U	C2-N1	4.08	1.48	1.40
3	5	4306	OMU	C4-N3	4.07	1.45	1.38
6	9	1842	4AC	C2-N1	4.07	1.48	1.40
3	5	4620	OMU	C4-N3	4.06	1.45	1.38
6	9	1337	4AC	C2-N1	4.04	1.48	1.40
6	9	683	OMG	C2-N2	4.03	1.43	1.34
3	5	4447	5MC	C2-N1	4.03	1.48	1.40
3	5	4415	1MA	C4-N3	4.03	1.50	1.37
3	5	4870	OMG	C2-N2	4.02	1.43	1.34
3	5	4637	OMG	C2-N2	4.01	1.43	1.34
3	5	2773	OMG	C2-N2	4.01	1.43	1.34
6	9	1806	M7A	C5-N7	4.00	1.49	1.39
3	5	1883	OMG	C2-N2	3.99	1.43	1.34
3	5	4623	OMG	C2-N2	3.98	1.43	1.34
3	5	2424	OMG	C2-N2	3.98	1.43	1.34
3	5	4370	OMG	C2-N2	3.97	1.43	1.34
3	5	4872	2MG	C6-N1	3.97	1.43	1.37
3	5	4690	B8K	C5-C6	3.97	1.53	1.43
3	5	1316	OMG	C2-N2	3.96	1.43	1.34
3	5	2364	OMG	C2-N2	3.96	1.43	1.34
3	5	3792	OMG	C2-N2	3.96	1.43	1.34
3	5	1659	I4U	C2-N1	3.95	1.48	1.40
3	5	2050	OMG	C2-N2	3.95	1.43	1.34
3	5	4564	M7A	C5-N7	3.95	1.48	1.39
3	5	373	OMG	C2-N2	3.95	1.43	1.34
3	5	1456	B8Q	C2-N1	3.94	1.44	1.38
3	5	1522	OMG	C2-N2	3.94	1.43	1.34
3	5	4196	OMG	C2-N2	3.93	1.43	1.34
6	9	1842	4AC	C5-C4	3.93	1.49	1.40
3	5	4494	OMG	C2-N2	3.92	1.43	1.34
3	5	1625	OMG	C2-N2	3.92	1.43	1.34
3	5	3880	P7G	C2-N3	3.91	1.47	1.37
6	9	644	OMG	C2-N2	3.89	1.43	1.34
3	5	1322	1MA	C4-N3	3.89	1.49	1.37
3	5	3897	B8K	C5-C6	3.89	1.53	1.43
3	5	4671	B8T	C5-C4	3.84	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2773	OMG	C6-N1	3.83	1.43	1.37
3	5	3899	BGH	C5-N7	3.83	1.46	1.39
3	5	4194	I4U	C2-N1	3.82	1.48	1.40
6	9	509	OMG	C2-N2	3.82	1.43	1.34
3	5	3899	BGH	C5-C6	3.79	1.53	1.43
3	5	4870	OMG	C6-N1	3.77	1.43	1.37
3	5	4483	B8T	C5-C4	3.74	1.48	1.40
3	5	1605	7MG	C2-N1	3.73	1.46	1.37
6	9	683	OMG	C6-N1	3.72	1.43	1.37
3	5	2522	7MG	C2-N1	3.72	1.46	1.37
3	5	1909	P7G	C2-N3	3.71	1.46	1.37
3	5	3792	OMG	C6-N1	3.70	1.43	1.37
3	5	1883	OMG	C6-N1	3.69	1.43	1.37
3	5	4370	OMG	C6-N1	3.68	1.43	1.37
3	5	1625	OMG	C6-N1	3.67	1.43	1.37
3	5	2424	OMG	C6-N1	3.67	1.43	1.37
3	5	4494	OMG	C6-N1	3.67	1.43	1.37
3	5	373	OMG	C6-N1	3.67	1.43	1.37
6	9	1248	B8N	C1'-C5	3.67	1.58	1.50
3	5	4690	B8K	C5-N7	3.66	1.45	1.39
3	5	4690	B8K	C6-N1	3.64	1.45	1.38
3	5	4550	7MG	C2-N1	3.64	1.46	1.37
3	5	1797	E7G	C2-N1	3.64	1.46	1.37
3	5	2050	OMG	C6-N1	3.63	1.43	1.37
3	5	2364	OMG	C6-N1	3.62	1.43	1.37
3	5	4196	OMG	C6-N1	3.62	1.43	1.37
6	9	644	OMG	C6-N1	3.61	1.43	1.37
3	5	4623	OMG	C6-N1	3.61	1.43	1.37
3	5	2297	E7G	C2-N1	3.61	1.46	1.37
3	5	1909	P7G	C6-N1	3.56	1.44	1.38
3	5	4637	OMG	C6-N1	3.56	1.43	1.37
3	5	3897	B8K	C5-N7	3.55	1.45	1.39
3	5	1522	OMG	C6-N1	3.54	1.43	1.37
3	5	3897	B8K	C6-N1	3.49	1.45	1.38
3	5	4690	B8K	C2-N2	3.46	1.42	1.34
6	9	509	OMG	C6-N1	3.46	1.43	1.37
3	5	4550	7MG	C5-C6	3.45	1.52	1.43
3	5	4371	MHG	C5-C6	3.45	1.52	1.43
3	5	2297	E7G	C5-C6	3.44	1.52	1.43
3	5	1316	OMG	C6-N1	3.44	1.43	1.37
3	5	1605	7MG	C5-C6	3.44	1.52	1.43
3	5	3897	B8K	C2-N2	3.43	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4531	PSU	C6-C5	3.41	1.39	1.35
6	9	823	PSU	C6-C5	3.40	1.39	1.35
3	5	3899	BGH	C2-N1	3.40	1.46	1.37
3	5	4690	B8K	C2-N1	3.40	1.46	1.37
3	5	3880	P7G	C6-N1	3.37	1.44	1.38
3	5	1517	2MG	C6-N1	3.37	1.42	1.37
3	5	4636	PSU	C6-C5	3.36	1.39	1.35
3	5	1797	E7G	C6-N1	3.36	1.45	1.38
3	5	4403	PSU	C6-C5	3.36	1.39	1.35
3	5	1797	E7G	C5-C6	3.35	1.52	1.43
3	5	4293	PSU	C6-C5	3.35	1.39	1.35
6	9	1243	PSU	C6-C5	3.34	1.39	1.35
3	5	4597	UR3	C6-N1	3.34	1.46	1.38
3	5	2508	PSU	C6-C5	3.33	1.39	1.35
3	5	3897	B8K	C2-N1	3.32	1.45	1.37
3	5	729	2MG	C6-N1	3.32	1.42	1.37
3	5	3764	PSU	C6-C5	3.31	1.39	1.35
6	9	822	PSU	C6-C5	3.31	1.39	1.35
3	5	1866	UR3	C6-N1	3.30	1.46	1.38
6	9	1830	UR3	C6-N1	3.29	1.45	1.38
3	5	2522	7MG	C5-C6	3.28	1.52	1.43
3	5	4530	UR3	C6-N1	3.27	1.45	1.38
6	9	174	OMC	C6-N1	3.27	1.45	1.38
3	5	3729	PSU	C6-C5	3.26	1.39	1.35
3	5	1909	P7G	O6-C6	-3.26	1.18	1.23
3	5	4628	PSU	C6-C5	3.25	1.39	1.35
6	9	119	PSU	C6-C5	3.25	1.39	1.35
3	5	2297	E7G	C6-N1	3.24	1.44	1.38
3	5	4500	PSU	C6-C5	3.24	1.39	1.35
3	5	4194	I4U	C6-N1	3.24	1.45	1.38
3	5	3715	PSU	C6-C5	3.22	1.39	1.35
3	5	3880	P7G	O6-C6	-3.21	1.18	1.23
3	5	3887	OMC	C6-N1	3.21	1.45	1.38
6	9	517	OMC	C6-N1	3.21	1.45	1.38
3	5	4872	2MG	C5-C6	3.20	1.53	1.47
3	5	2861	OMC	C6-N1	3.19	1.45	1.38
3	5	4690	B8K	C71-N7	3.19	1.46	1.39
6	9	1710	OMC	C6-N1	3.18	1.45	1.38
3	5	1605	7MG	C6-N1	3.18	1.44	1.38
3	5	2365	OMC	C6-N1	3.18	1.45	1.38
3	5	1683	PSU	C6-C5	3.18	1.39	1.35
3	5	1582	PSU	C6-C5	3.17	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	612	PSU	C6-C5	3.17	1.39	1.35
3	5	2804	OMC	C6-N1	3.16	1.45	1.38
3	5	3785	A2M	O3'-C3'	3.16	1.50	1.43
3	5	3899	BGH	C6-N1	3.15	1.44	1.38
3	5	4442	PSU	C6-C5	3.15	1.39	1.35
3	5	4371	MHG	C6-N1	3.15	1.44	1.38
6	9	1678	A2M	C6-N6	3.15	1.45	1.34
3	5	4194	I4U	O4-C41	-3.15	1.39	1.47
3	5	2422	OMC	C6-N1	3.14	1.45	1.38
3	5	4450	PSU	C6-C5	3.14	1.39	1.35
3	5	3718	A2M	C6-N6	3.14	1.45	1.34
6	9	159	A2M	C6-N6	3.14	1.45	1.34
3	5	4536	OMC	C6-N1	3.13	1.45	1.38
3	5	1659	I4U	C6-N1	3.13	1.45	1.38
6	9	484	A2M	C6-N6	3.12	1.45	1.34
3	5	4671	B8T	C6-N1	3.12	1.45	1.38
3	5	3869	OMC	C6-N1	3.12	1.45	1.38
3	5	398	A2M	C6-N6	3.12	1.45	1.34
6	9	668	A2M	C6-N6	3.12	1.45	1.34
3	5	3723	A2M	C6-N6	3.12	1.45	1.34
3	5	3701	OMC	C6-N1	3.12	1.45	1.38
3	5	4523	A2M	C6-N6	3.12	1.45	1.34
3	5	4483	B8T	C6-N1	3.12	1.45	1.38
3	5	2401	A2M	C6-N6	3.11	1.45	1.34
3	5	3825	A2M	C6-N6	3.11	1.45	1.34
6	9	27	A2M	C6-N6	3.10	1.45	1.34
3	5	2522	7MG	C6-N1	3.10	1.44	1.38
3	5	1871	A2M	C6-N6	3.10	1.45	1.34
3	5	4355	E6G	C5-C4	-3.10	1.32	1.40
6	9	1031	A2M	C6-N6	3.09	1.45	1.34
3	5	3867	A2M	C6-N6	3.09	1.45	1.34
3	5	1534	A2M	C6-N6	3.08	1.45	1.34
3	5	4571	A2M	C6-N6	3.08	1.45	1.34
3	5	3880	P7G	C5-C4	3.08	1.43	1.37
3	5	1524	A2M	C6-N6	3.08	1.45	1.34
6	9	1337	4AC	C6-N1	3.07	1.45	1.38
3	5	1677	PSU	C6-C5	3.07	1.38	1.35
3	5	3909	OMC	O2-C2	-3.07	1.18	1.23
6	9	1703	OMC	C6-N1	3.07	1.45	1.38
3	5	1326	A2M	C6-N6	3.07	1.45	1.34
6	9	484	A2M	O3'-C3'	3.06	1.50	1.43
3	5	2363	A2M	C6-N6	3.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3785	A2M	C6-N6	3.04	1.45	1.34
6	9	1081	PSU	C6-C5	3.04	1.38	1.35
3	5	1348	P4U	C6-N1	3.03	1.45	1.38
3	5	3897	B8K	C71-N7	3.02	1.46	1.39
3	5	4447	5MC	O2-C2	-3.02	1.18	1.23
3	5	1909	P7G	C5-C4	3.02	1.43	1.37
3	5	729	2MG	C5-C6	3.01	1.53	1.47
3	5	1659	I4U	O4-C41	-3.01	1.40	1.47
3	5	4550	7MG	C6-N1	3.01	1.44	1.38
6	9	166	A2M	C6-N6	3.00	1.45	1.34
3	5	4306	OMU	O4-C4	-3.00	1.18	1.24
3	5	4620	OMU	O4-C4	-2.99	1.18	1.24
6	9	121	OMU	O4-C4	-2.98	1.18	1.24
5	8	14	OMU	O4-C4	-2.97	1.18	1.24
6	9	1851	MA6	C9-N6	2.97	1.52	1.45
3	5	4870	OMG	C5-C6	2.96	1.53	1.47
6	9	668	A2M	O3'-C3'	2.95	1.49	1.43
3	5	3899	BGH	C71-N7	2.95	1.46	1.39
3	5	2773	OMG	C5-C6	2.95	1.53	1.47
3	5	3909	OMC	C6-N1	2.94	1.45	1.38
3	5	2401	A2M	O3'-C3'	2.94	1.49	1.43
6	9	1850	MA6	C9-N6	2.94	1.52	1.45
6	9	1842	4AC	C6-N1	2.94	1.45	1.38
6	9	1850	MA6	C2-N3	2.94	1.36	1.32
3	5	4335	5MC	O2-C2	-2.93	1.18	1.23
6	9	814	5MU	O4-C4	-2.92	1.18	1.23
3	5	1517	2MG	C5-C6	2.92	1.53	1.47
3	5	2363	A2M	O3'-C3'	2.92	1.49	1.43
3	5	4623	OMG	C5-C6	2.91	1.53	1.47
6	9	1031	A2M	O3'-C3'	2.91	1.49	1.43
6	9	116	OMU	O4-C4	-2.91	1.18	1.24
3	5	4671	B8T	O2-C2	-2.90	1.18	1.23
3	5	3792	OMG	C5-C6	2.90	1.53	1.47
3	5	3723	A2M	O3'-C3'	2.90	1.49	1.43
3	5	4083	5MU	O4-C4	-2.90	1.18	1.23
6	9	1374	5MC	O2-C2	-2.89	1.18	1.23
3	5	2364	OMG	C5-C6	2.89	1.53	1.47
3	5	1659	I4U	O2-C2	-2.88	1.18	1.23
6	9	644	OMG	C5-C6	2.88	1.53	1.47
3	5	1574	B9B	C5-C4	-2.88	1.33	1.40
3	5	1522	OMG	C5-C6	2.87	1.53	1.47
6	9	683	OMG	C5-C6	2.87	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4370	OMG	C5-C6	2.86	1.53	1.47
3	5	1326	A2M	O3'-C3'	2.86	1.49	1.43
3	5	4523	A2M	O3'-C3'	2.85	1.49	1.43
3	5	3825	A2M	C5-C4	-2.85	1.33	1.40
3	5	3718	A2M	O3'-C3'	2.85	1.49	1.43
3	5	373	OMG	C5-C6	2.84	1.53	1.47
6	9	509	OMG	C5-C6	2.84	1.53	1.47
3	5	1534	A2M	C5-C4	-2.84	1.33	1.40
6	9	1678	A2M	O3'-C3'	2.83	1.49	1.43
3	5	4571	A2M	O3'-C3'	2.83	1.49	1.43
3	5	4483	B8T	O2-C2	-2.83	1.18	1.23
3	5	3899	BGH	O6-C6	-2.83	1.18	1.23
3	5	1524	A2M	O3'-C3'	2.82	1.49	1.43
6	9	1031	A2M	C5-C4	-2.82	1.33	1.40
3	5	2861	OMC	O2-C2	-2.82	1.18	1.23
6	9	27	A2M	O3'-C3'	2.82	1.49	1.43
3	5	1625	OMG	C5-C6	2.81	1.53	1.47
3	5	3899	BGH	O3'-C3'	2.81	1.49	1.43
3	5	1348	P4U	O2-C2	-2.81	1.18	1.23
3	5	4194	I4U	O2-C2	-2.81	1.18	1.23
3	5	4523	A2M	C5-C4	-2.81	1.33	1.40
3	5	3867	A2M	C5-C4	-2.81	1.33	1.40
3	5	1534	A2M	O2'-C2'	-2.81	1.35	1.42
3	5	4637	OMG	C5-C6	2.80	1.53	1.47
3	5	373	OMG	C5-C4	-2.80	1.35	1.43
3	5	2365	OMC	O2-C2	-2.80	1.18	1.23
3	5	237	B9B	C5-C4	-2.80	1.33	1.40
3	5	398	A2M	O3'-C3'	2.80	1.49	1.43
6	9	668	A2M	C5-C4	-2.80	1.33	1.40
3	5	4185	B8W	C5-C4	-2.80	1.33	1.40
3	5	3887	OMC	O2-C2	-2.79	1.18	1.23
6	9	121	OMU	C6-N1	2.79	1.44	1.38
3	5	1534	A2M	O3'-C3'	2.79	1.49	1.43
3	5	2363	A2M	C5-C4	-2.78	1.33	1.40
3	5	3867	A2M	O3'-C3'	2.78	1.49	1.43
3	5	1871	A2M	C5-C4	-2.78	1.33	1.40
6	9	166	A2M	C5-C4	-2.78	1.33	1.40
3	5	2424	OMG	C5-C6	2.78	1.53	1.47
3	5	1524	A2M	C5-C4	-2.78	1.33	1.40
3	5	4536	OMC	O2-C2	-2.78	1.18	1.23
3	5	1871	A2M	O3'-C3'	2.77	1.49	1.43
3	5	1316	OMG	C5-C6	2.77	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3785	A2M	C5-C4	-2.76	1.33	1.40
3	5	2754	B9B	C5-C4	-2.76	1.33	1.40
3	5	4196	OMG	C5-C6	2.76	1.53	1.47
3	5	398	A2M	C5-C4	-2.76	1.33	1.40
3	5	3701	OMC	O2-C2	-2.76	1.18	1.23
3	5	1326	A2M	C5-C4	-2.76	1.33	1.40
6	9	1850	MA6	C5-C4	-2.76	1.33	1.40
6	9	116	OMU	C6-N1	2.76	1.44	1.38
6	9	1851	MA6	C2-N3	2.75	1.36	1.32
3	5	1883	OMG	C5-C4	-2.75	1.36	1.43
3	5	4306	OMU	C6-N1	2.74	1.44	1.38
6	9	1703	OMC	O2-C2	-2.74	1.18	1.23
3	5	4872	2MG	C5-C4	-2.74	1.36	1.43
3	5	1316	OMG	C5-C4	-2.74	1.36	1.43
6	9	517	OMC	O2-C2	-2.74	1.18	1.23
3	5	1883	OMG	O6-C6	-2.74	1.17	1.23
3	5	3825	A2M	O3'-C3'	2.74	1.49	1.43
6	9	484	A2M	C5-C4	-2.73	1.33	1.40
3	5	2401	A2M	C5-C4	-2.73	1.33	1.40
6	9	27	A2M	C5-C4	-2.73	1.33	1.40
6	9	159	A2M	O3'-C3'	2.73	1.49	1.43
3	5	2364	OMG	C5-C4	-2.73	1.36	1.43
3	5	2380	B8W	C5-C4	-2.72	1.33	1.40
6	9	1337	4AC	O2-C2	-2.72	1.18	1.23
5	8	14	OMU	C6-N1	2.72	1.44	1.38
6	9	1678	A2M	C5-C4	-2.72	1.33	1.40
3	5	4571	A2M	C5-C4	-2.72	1.33	1.40
3	5	3785	A2M	O2'-C2'	-2.72	1.35	1.42
3	5	3869	OMC	O2-C2	-2.71	1.18	1.23
3	5	4571	A2M	O2'-C2'	-2.71	1.35	1.42
6	9	1851	MA6	C5-C4	-2.71	1.33	1.40
3	5	2804	OMC	O2-C2	-2.71	1.18	1.23
3	5	2401	A2M	O2'-C2'	-2.71	1.35	1.42
3	5	2422	OMC	O2-C2	-2.71	1.18	1.23
3	5	398	A2M	O2'-C2'	-2.70	1.35	1.42
3	5	3897	B8K	C5-C4	2.70	1.46	1.38
3	5	1522	OMG	C5-C4	-2.70	1.36	1.43
6	9	1678	A2M	O2'-C2'	-2.70	1.35	1.42
3	5	3782	5MC	O2-C2	-2.70	1.18	1.23
3	5	4472	B8W	C5-C4	-2.70	1.33	1.40
3	5	4494	OMG	C5-C4	-2.69	1.36	1.43
3	5	4620	OMU	C6-N1	2.69	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	1710	OMC	O2-C2	-2.69	1.18	1.23
6	9	1842	4AC	O2-C2	-2.69	1.18	1.23
3	5	2050	OMG	C5-C4	-2.69	1.36	1.43
3	5	1625	OMG	C5-C4	-2.68	1.36	1.43
6	9	1031	A2M	O2'-C2'	-2.68	1.35	1.42
3	5	4196	OMG	C5-C4	-2.68	1.36	1.43
3	5	4494	OMG	C5-C6	2.68	1.52	1.47
3	5	4550	7MG	O6-C6	-2.68	1.18	1.23
6	9	166	A2M	O3'-C3'	2.68	1.49	1.43
3	5	4370	OMG	C5-C4	-2.67	1.36	1.43
3	5	3723	A2M	C5-C4	-2.67	1.33	1.40
6	9	683	OMG	C5-C4	-2.67	1.36	1.43
3	5	3718	A2M	C5-C4	-2.67	1.33	1.40
3	5	1871	A2M	O2'-C2'	-2.67	1.35	1.42
3	5	4523	A2M	O2'-C2'	-2.66	1.35	1.42
3	5	2050	OMG	C5-C6	2.66	1.52	1.47
6	9	159	A2M	C5-C4	-2.66	1.33	1.40
3	5	3792	OMG	C5-C4	-2.66	1.36	1.43
3	5	2522	7MG	O6-C6	-2.66	1.18	1.23
3	5	2424	OMG	C5-C4	-2.65	1.36	1.43
3	5	4623	OMG	C5-C4	-2.65	1.36	1.43
3	5	4220	6MZ	C5-C4	-2.65	1.33	1.40
3	5	4870	OMG	C5-C4	-2.65	1.36	1.43
6	9	166	A2M	O2'-C2'	-2.64	1.35	1.42
6	9	1832	6MZ	C5-C4	-2.64	1.33	1.40
6	9	484	A2M	O2'-C2'	-2.64	1.35	1.42
3	5	1524	A2M	O2'-C2'	-2.64	1.35	1.42
3	5	4690	B8K	C5-C4	2.63	1.46	1.38
3	5	1605	7MG	O6-C6	-2.63	1.18	1.23
6	9	644	OMG	C5-C4	-2.63	1.36	1.43
6	9	174	OMC	O2-C2	-2.63	1.18	1.23
6	9	27	A2M	O2'-C2'	-2.63	1.35	1.42
3	5	2363	A2M	O2'-C2'	-2.62	1.35	1.42
3	5	3718	A2M	O2'-C2'	-2.62	1.35	1.42
3	5	2050	OMG	O6-C6	-2.61	1.18	1.23
3	5	3867	A2M	O2'-C2'	-2.61	1.35	1.42
3	5	1883	OMG	C5-C6	2.61	1.52	1.47
3	5	3723	A2M	O2'-C2'	-2.61	1.35	1.42
3	5	3825	A2M	O2'-C2'	-2.61	1.35	1.42
3	5	373	OMG	O6-C6	-2.61	1.18	1.23
3	5	4637	OMG	C5-C4	-2.60	1.36	1.43
6	9	509	OMG	O6-C6	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	3899	BGH	C1'-N9	-2.60	1.41	1.46
3	5	2773	OMG	C5-C4	-2.60	1.36	1.43
3	5	4494	OMG	O6-C6	-2.58	1.18	1.23
3	5	4623	OMG	O6-C6	-2.57	1.18	1.23
3	5	2297	E7G	O6-C6	-2.57	1.18	1.23
3	5	1326	A2M	O2'-C2'	-2.57	1.36	1.42
3	5	1625	OMG	O6-C6	-2.56	1.18	1.23
3	5	1316	OMG	O6-C6	-2.56	1.18	1.23
3	5	4370	OMG	O6-C6	-2.55	1.18	1.23
3	5	1797	E7G	O6-C6	-2.55	1.18	1.23
3	5	4129	B8W	C5-C4	-2.55	1.34	1.40
6	9	509	OMG	C5-C4	-2.55	1.36	1.43
3	5	4637	OMG	O6-C6	-2.54	1.18	1.23
3	5	4083	5MU	O2-C2	-2.54	1.18	1.23
6	9	174	OMC	C5-C4	2.53	1.48	1.42
6	9	683	OMG	O6-C6	-2.52	1.18	1.23
6	9	1710	OMC	C5-C4	2.52	1.48	1.42
3	5	1517	2MG	C5-C4	-2.52	1.36	1.43
6	9	668	A2M	O2'-C2'	-2.52	1.36	1.42
3	5	1522	OMG	O6-C6	-2.52	1.18	1.23
3	5	4196	OMG	O6-C6	-2.51	1.18	1.23
3	5	4529	B8W	C5-C4	-2.51	1.34	1.40
3	5	1322	1MA	CM1-N1	-2.50	1.41	1.46
3	5	2424	OMG	O6-C6	-2.50	1.18	1.23
6	9	517	OMC	C5-C4	2.49	1.48	1.42
3	5	4870	OMG	O6-C6	-2.49	1.18	1.23
3	5	4870	OMG	C2-N1	2.48	1.43	1.37
3	5	3792	OMG	O6-C6	-2.48	1.18	1.23
6	9	159	A2M	O2'-C2'	-2.48	1.36	1.42
3	5	2773	OMG	C2-N1	2.48	1.43	1.37
5	8	14	OMU	O2-C2	-2.48	1.18	1.23
3	5	2364	OMG	O6-C6	-2.47	1.18	1.23
3	5	4620	OMU	O2-C2	-2.46	1.18	1.23
6	9	814	5MU	O2-C2	-2.46	1.18	1.23
3	5	4194	I4U	O4-C4	2.46	1.40	1.35
3	5	3701	OMC	C5-C4	2.46	1.48	1.42
6	9	644	OMG	O6-C6	-2.46	1.18	1.23
3	5	2773	OMG	O6-C6	-2.46	1.18	1.23
6	9	683	OMG	C2-N1	2.45	1.43	1.37
3	5	4306	OMU	O2-C2	-2.45	1.18	1.23
3	5	4623	OMG	C2-N1	2.44	1.43	1.37
3	5	729	2MG	C5-C4	-2.44	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	2861	OMC	C5-C4	2.43	1.48	1.42
3	5	4371	MHG	O6-C6	-2.42	1.19	1.23
3	5	1659	I4U	O4-C4	2.41	1.40	1.35
3	5	2050	OMG	C2-N1	2.41	1.43	1.37
6	9	116	OMU	O2-C2	-2.41	1.18	1.23
3	5	1883	OMG	C2-N1	2.40	1.43	1.37
3	5	3887	OMC	C5-C4	2.40	1.48	1.42
3	5	2365	OMC	C5-C4	2.40	1.48	1.42
3	5	373	OMG	C2-N1	2.39	1.43	1.37
3	5	4370	OMG	C2-N1	2.38	1.43	1.37
3	5	4220	6MZ	C2-N3	2.38	1.35	1.32
3	5	4196	OMG	C2-N1	2.38	1.43	1.37
3	5	4637	OMG	C2-N1	2.38	1.43	1.37
6	9	644	OMG	C2-N1	2.38	1.43	1.37
3	5	1625	OMG	C2-N1	2.37	1.43	1.37
3	5	4494	OMG	C2-N1	2.37	1.43	1.37
3	5	3869	OMC	C5-C4	2.37	1.48	1.42
3	5	3792	OMG	C2-N1	2.36	1.43	1.37
6	9	509	OMG	C2-N1	2.36	1.43	1.37
6	9	121	OMU	O2-C2	-2.36	1.18	1.23
3	5	2424	OMG	C2-N1	2.35	1.43	1.37
3	5	1316	OMG	C2-N1	2.35	1.43	1.37
3	5	4536	OMC	C5-C4	2.35	1.48	1.42
3	5	2422	OMC	C5-C4	2.35	1.48	1.42
3	5	1517	2MG	O6-C6	-2.34	1.18	1.23
3	5	2364	OMG	C2-N1	2.34	1.43	1.37
1	2	37	T6A	C5-C4	2.34	1.47	1.40
6	9	116	OMU	C5-C4	2.33	1.48	1.43
3	5	4620	OMU	C5-C4	2.31	1.48	1.43
3	5	2804	OMC	C5-C4	2.31	1.48	1.42
3	5	3909	OMC	C5-C4	2.31	1.48	1.42
6	9	121	OMU	C5-C4	2.31	1.48	1.43
3	5	4306	OMU	C5-C4	2.30	1.48	1.43
6	9	1703	OMC	C5-C4	2.30	1.48	1.42
3	5	4872	2MG	O6-C6	-2.29	1.18	1.23
3	5	1522	OMG	C2-N1	2.29	1.43	1.37
6	9	1832	6MZ	C2-N3	2.28	1.35	1.32
3	5	4530	UR3	O2-C2	-2.27	1.18	1.22
3	5	4415	1MA	CM1-N1	-2.25	1.42	1.46
3	5	1322	1MA	C5-C4	-2.25	1.37	1.43
3	5	729	2MG	O6-C6	-2.22	1.18	1.23
3	5	4530	UR3	C5-C4	2.20	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	8	14	OMU	C5-C4	2.19	1.48	1.43
3	5	3723	A2M	C2-N3	2.18	1.35	1.32
3	5	1456	B8Q	O2-C2	-2.18	1.18	1.22
6	9	1830	UR3	O2-C2	-2.18	1.18	1.22
3	5	3899	BGH	C3'-C4'	2.17	1.58	1.53
6	9	1830	UR3	C5-C4	2.17	1.49	1.43
3	5	4571	A2M	C2-N3	2.16	1.35	1.32
3	5	1866	UR3	C4-N3	2.15	1.45	1.40
3	5	1860	B8H	O4-C4	-2.15	1.19	1.23
3	5	4530	UR3	C4-N3	2.14	1.45	1.40
3	5	1534	A2M	C2-N3	2.14	1.35	1.32
6	9	166	A2M	C2-N3	2.14	1.35	1.32
3	5	1866	UR3	C5-C4	2.14	1.49	1.43
6	9	159	A2M	C2-N3	2.13	1.35	1.32
3	5	2401	A2M	C2-N3	2.13	1.35	1.32
3	5	4597	UR3	C4-N3	2.12	1.45	1.40
3	5	4597	UR3	C5-C4	2.12	1.49	1.43
6	9	668	A2M	O5'-C5'	-2.12	1.39	1.44
6	9	1248	B8N	O4-C4	-2.11	1.18	1.23
3	5	3718	A2M	C2-N3	2.11	1.35	1.32
3	5	3785	A2M	C2-N3	2.10	1.35	1.32
6	9	484	A2M	C2-N3	2.10	1.35	1.32
6	9	1678	A2M	C2-N3	2.10	1.35	1.32
6	9	1842	4AC	O7-C7	-2.09	1.18	1.23
6	9	1248	B8N	O2-C2	-2.08	1.18	1.22
6	9	1031	A2M	C2-N3	2.08	1.35	1.32
6	9	1219	B8Q	O2-C2	-2.08	1.18	1.22
3	5	4415	1MA	C5-C4	-2.08	1.37	1.43
6	9	568	MMX	O2-C2	-2.08	1.18	1.22
3	5	3762	B8H	O4-C4	-2.07	1.19	1.23
3	5	1456	B8Q	C6-N1	2.07	1.43	1.38
6	9	27	A2M	C2-N3	2.06	1.35	1.32
3	5	4296	B8H	O4-C4	-2.06	1.19	1.23
3	5	398	A2M	C2-N3	2.06	1.35	1.32
3	5	2363	A2M	C2-N3	2.05	1.35	1.32
3	5	3867	A2M	C2-N3	2.05	1.35	1.32
3	5	1326	A2M	C2-N3	2.05	1.35	1.32
6	9	668	A2M	C2-N3	2.02	1.35	1.32
3	5	1866	UR3	O2-C2	-2.01	1.18	1.22
3	5	4442	PSU	O4'-C1'	-2.01	1.41	1.43

All (564) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	2754	B9B	O6-C6-N1	-29.76	94.43	120.12
3	5	1574	B9B	O6-C6-N1	-29.59	94.58	120.12
3	5	237	B9B	O6-C6-N1	-28.62	95.42	120.12
6	9	1851	MA6	N1-C6-N6	-16.50	99.69	117.06
6	9	1850	MA6	N1-C6-N6	-15.83	100.40	117.06
6	9	1806	M7A	C5-C6-N6	13.89	147.46	123.74
3	5	4564	M7A	C5-C6-N6	13.81	147.33	123.74
3	5	4220	6MZ	C1'-N9-C4	-12.86	104.04	126.64
6	9	1832	6MZ	C1'-N9-C4	-12.36	104.92	126.64
6	9	814	5MU	C5-C4-N3	11.98	125.53	115.31
6	9	1806	M7A	N6-C6-N1	-11.86	92.38	118.35
3	5	4083	5MU	C5-C4-N3	11.83	125.41	115.31
3	5	4564	M7A	N6-C6-N1	-11.64	92.86	118.35
6	9	1031	A2M	C5-C6-N6	10.76	136.70	120.35
6	9	159	A2M	C5-C6-N6	10.67	136.57	120.35
6	9	668	A2M	C5-C6-N6	10.63	136.50	120.35
3	5	4571	A2M	C5-C6-N6	10.57	136.41	120.35
3	5	2401	A2M	C5-C6-N6	10.56	136.40	120.35
3	5	2363	A2M	C5-C6-N6	10.56	136.39	120.35
3	5	1524	A2M	C5-C6-N6	10.54	136.36	120.35
3	5	398	A2M	C5-C6-N6	10.53	136.35	120.35
6	9	484	A2M	C5-C6-N6	10.50	136.30	120.35
6	9	1678	A2M	C5-C6-N6	10.49	136.30	120.35
3	5	3825	A2M	C5-C6-N6	10.47	136.27	120.35
3	5	1326	A2M	C5-C6-N6	10.46	136.25	120.35
3	5	3867	A2M	C5-C6-N6	10.46	136.25	120.35
3	5	1534	A2M	C5-C6-N6	10.46	136.24	120.35
3	5	1871	A2M	C5-C6-N6	10.45	136.24	120.35
3	5	3785	A2M	C5-C6-N6	10.41	136.17	120.35
3	5	3718	A2M	C5-C6-N6	10.40	136.15	120.35
6	9	166	A2M	C5-C6-N6	10.38	136.13	120.35
6	9	27	A2M	C5-C6-N6	10.30	136.00	120.35
3	5	3723	A2M	C5-C6-N6	10.25	135.93	120.35
3	5	4523	A2M	C5-C6-N6	10.20	135.85	120.35
6	9	814	5MU	C5-C6-N1	-10.19	112.85	123.34
3	5	4083	5MU	C5-C6-N1	-9.75	113.31	123.34
3	5	4355	E6G	O6-C6-N1	9.39	128.23	120.12
6	9	568	MMX	N3-C2-N1	8.66	122.52	116.83
1	2	37	T6A	C2-N1-C6	7.64	123.14	116.59
6	9	568	MMX	C4-N3-C2	-7.55	114.56	121.62
6	9	1031	A2M	N6-C6-N1	-7.40	103.21	118.57
6	9	159	A2M	N6-C6-N1	-7.33	103.36	118.57
6	9	166	A2M	N6-C6-N1	-7.32	103.38	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2401	A2M	N6-C6-N1	-7.26	103.49	118.57
6	9	668	A2M	N6-C6-N1	-7.25	103.52	118.57
3	5	4571	A2M	N6-C6-N1	-7.24	103.54	118.57
3	5	1871	A2M	N6-C6-N1	-7.24	103.55	118.57
3	5	2363	A2M	N6-C6-N1	-7.24	103.56	118.57
3	5	3825	A2M	N6-C6-N1	-7.23	103.57	118.57
6	9	484	A2M	N6-C6-N1	-7.22	103.59	118.57
3	5	1326	A2M	N6-C6-N1	-7.22	103.59	118.57
3	5	398	A2M	N6-C6-N1	-7.21	103.61	118.57
3	5	1524	A2M	N6-C6-N1	-7.20	103.63	118.57
3	5	1534	A2M	N6-C6-N1	-7.19	103.65	118.57
3	5	3785	A2M	N6-C6-N1	-7.19	103.66	118.57
3	5	3867	A2M	N6-C6-N1	-7.18	103.67	118.57
6	9	1678	A2M	N6-C6-N1	-7.15	103.73	118.57
3	5	4523	A2M	N6-C6-N1	-7.04	103.97	118.57
3	5	3718	A2M	N6-C6-N1	-7.00	104.04	118.57
6	9	27	A2M	N6-C6-N1	-6.99	104.07	118.57
3	5	3723	A2M	N6-C6-N1	-6.93	104.19	118.57
3	5	4296	B8H	C4-N3-C2	-6.86	118.47	127.35
3	5	3762	B8H	C4-N3-C2	-6.74	118.63	127.35
3	5	1860	B8H	C4-N3-C2	-6.72	118.64	127.35
3	5	3880	P7G	C4-C5-N7	6.72	110.22	106.67
3	5	4371	MHG	C2-N3-C4	6.59	120.21	112.04
3	5	4355	E6G	N2-C2-N3	6.25	127.98	117.79
1	2	37	T6A	N6-C10-N11	6.19	122.41	113.76
3	5	1909	P7G	C4-C5-N7	6.11	109.90	106.67
3	5	1456	B8Q	N3-C2-N1	6.02	124.21	117.13
3	5	2380	B8W	N2-C2-N3	5.87	127.36	117.79
6	9	1850	MA6	C1'-N9-C4	-5.85	116.36	126.64
3	5	4129	B8W	N2-C2-N3	5.84	127.31	117.79
3	5	3762	B8H	N3-C2-N1	5.80	121.41	115.14
3	5	4296	B8H	N3-C2-N1	5.79	121.40	115.14
3	5	1860	B8H	N3-C2-N1	5.71	121.31	115.14
3	5	1322	1MA	N1-C2-N3	-5.71	119.37	126.02
3	5	4564	M7A	N3-C2-N1	-5.70	119.69	128.60
3	5	4529	B8W	N2-C2-N3	5.68	127.05	117.79
6	9	166	A2M	N3-C2-N1	-5.68	119.80	128.68
3	5	1871	A2M	N3-C2-N1	-5.67	119.81	128.68
6	9	668	A2M	N3-C2-N1	-5.65	119.84	128.68
3	5	1797	E7G	C4-C5-N7	5.65	109.94	104.91
6	9	1678	A2M	N3-C2-N1	-5.65	119.85	128.68
3	5	4185	B8W	N2-C2-N3	5.64	126.98	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	1851	MA6	C1'-N9-C4	-5.63	116.76	126.64
3	5	398	A2M	N3-C2-N1	-5.62	119.89	128.68
3	5	1326	A2M	N3-C2-N1	-5.62	119.90	128.68
6	9	159	A2M	N3-C2-N1	-5.61	119.91	128.68
3	5	4472	B8W	N2-C2-N3	5.60	126.92	117.79
3	5	4371	MHG	C4-C5-N7	5.60	109.89	104.91
3	5	4523	A2M	N3-C2-N1	-5.57	119.98	128.68
6	9	1031	A2M	N3-C2-N1	-5.54	120.02	128.68
6	9	27	A2M	N3-C2-N1	-5.53	120.04	128.68
3	5	4571	A2M	N3-C2-N1	-5.52	120.05	128.68
3	5	2786	B9H	C31-N3-C2	5.52	124.10	117.21
6	9	1806	M7A	N3-C2-N1	-5.51	119.98	128.60
3	5	1524	A2M	N3-C2-N1	-5.50	120.08	128.68
3	5	1534	A2M	N3-C2-N1	-5.50	120.09	128.68
3	5	3867	A2M	N3-C2-N1	-5.50	120.09	128.68
3	5	3897	B8K	C5-C6-N1	5.48	120.65	110.99
3	5	3785	A2M	N3-C2-N1	-5.47	120.13	128.68
3	5	4690	B8K	C5-C6-N1	5.46	120.62	110.99
3	5	2401	A2M	N3-C2-N1	-5.46	120.15	128.68
3	5	2363	A2M	N3-C2-N1	-5.46	120.15	128.68
3	5	4472	B8W	N3-C2-N1	-5.45	119.96	127.22
3	5	2297	E7G	C4-C5-N7	5.42	109.73	104.91
6	9	1851	MA6	N3-C2-N1	-5.42	120.21	128.68
3	5	4415	1MA	N1-C2-N3	-5.41	119.71	126.02
3	5	1456	B8Q	C31-N3-C4	5.41	122.40	114.25
3	5	4529	B8W	N3-C2-N1	-5.41	120.01	127.22
6	9	1850	MA6	N3-C2-N1	-5.40	120.24	128.68
3	5	4129	B8W	N3-C2-N1	-5.37	120.05	127.22
6	9	1832	6MZ	N3-C2-N1	-5.37	120.28	128.68
3	5	3899	BGH	C5-C6-N1	5.37	120.44	110.99
3	5	4306	OMU	C4-N3-C2	-5.36	119.51	126.58
6	9	484	A2M	N3-C2-N1	-5.36	120.31	128.68
3	5	4355	E6G	N3-C2-N1	-5.36	120.08	127.22
3	5	4620	OMU	C4-N3-C2	-5.33	119.55	126.58
3	5	3723	A2M	N3-C2-N1	-5.33	120.34	128.68
3	5	4185	B8W	N3-C2-N1	-5.31	120.14	127.22
6	9	121	OMU	C4-N3-C2	-5.30	119.59	126.58
3	5	3825	A2M	N3-C2-N1	-5.29	120.41	128.68
3	5	3718	A2M	N3-C2-N1	-5.28	120.43	128.68
3	5	4220	6MZ	N3-C2-N1	-5.27	120.44	128.68
3	5	1797	E7G	C5-C6-N1	5.23	120.21	110.99
6	9	1219	B8Q	N3-C2-N1	5.17	123.20	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2380	B8W	N3-C2-N1	-5.14	120.36	127.22
6	9	116	OMU	C4-N3-C2	-5.13	119.81	126.58
3	5	2754	B9B	N3-C2-N1	-5.09	120.43	127.22
5	8	14	OMU	C4-N3-C2	-5.08	119.88	126.58
3	5	2297	E7G	C5-C6-N1	5.07	119.93	110.99
3	5	4371	MHG	C5-C6-N1	5.04	119.87	110.99
3	5	1605	7MG	C5-C6-N1	5.03	119.86	110.99
6	9	1248	B8N	C5-C4-N3	5.03	125.48	116.17
3	5	237	B9B	N3-C2-N1	-5.02	120.53	127.22
3	5	4550	7MG	C5-C6-N1	5.02	119.83	110.99
3	5	3897	B8K	C4-C5-N7	5.00	109.36	104.91
3	5	1574	B9B	N3-C2-N1	-5.00	120.56	127.22
6	9	1219	B8Q	C31-N3-C4	4.97	121.74	114.25
3	5	2522	7MG	C5-C6-N1	4.95	119.71	110.99
6	9	1219	B8Q	C1'-N1-C2	4.92	125.30	116.99
3	5	1677	PSU	C4-N3-C2	-4.92	119.25	126.34
3	5	4564	M7A	N3-C4-N9	4.87	133.03	126.87
6	9	1806	M7A	N3-C4-N9	4.87	133.02	126.87
6	9	814	5MU	C4-N3-C2	-4.84	121.09	127.35
3	5	4083	5MU	O4-C4-C5	-4.78	119.36	124.90
6	9	814	5MU	O4-C4-C5	-4.78	119.36	124.90
3	5	4636	PSU	C4-N3-C2	-4.78	119.46	126.34
3	5	4450	PSU	C4-N3-C2	-4.77	119.47	126.34
3	5	2508	PSU	C4-N3-C2	-4.75	119.49	126.34
3	5	4531	PSU	C4-N3-C2	-4.75	119.50	126.34
6	9	823	PSU	C4-N3-C2	-4.74	119.51	126.34
3	5	4083	5MU	C4-N3-C2	-4.72	121.24	127.35
3	5	4628	PSU	N1-C2-N3	4.72	120.47	115.13
3	5	4690	B8K	C4-C5-N7	4.71	109.10	104.91
3	5	4500	PSU	C4-N3-C2	-4.70	119.56	126.34
3	5	4442	PSU	C4-N3-C2	-4.69	119.58	126.34
3	5	4628	PSU	C4-N3-C2	-4.69	119.58	126.34
3	5	1677	PSU	N1-C2-N3	4.68	120.43	115.13
3	5	4531	PSU	N1-C2-N3	4.67	120.42	115.13
6	9	1081	PSU	C4-N3-C2	-4.67	119.62	126.34
3	5	4690	B8K	C2-N3-C4	4.66	120.59	112.30
6	9	823	PSU	N1-C2-N3	4.65	120.39	115.13
3	5	2508	PSU	N1-C2-N3	4.64	120.38	115.13
3	5	1797	E7G	C2-N3-C4	4.63	120.56	112.30
3	5	1866	UR3	C4-N3-C2	-4.63	120.20	124.56
3	5	1683	PSU	C4-N3-C2	-4.63	119.67	126.34
3	5	3897	B8K	C2-N3-C4	4.60	120.50	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4083	5MU	N3-C2-N1	4.60	120.99	114.89
6	9	1243	PSU	C4-N3-C2	-4.60	119.72	126.34
3	5	4450	PSU	N1-C2-N3	4.60	120.34	115.13
6	9	822	PSU	C4-N3-C2	-4.59	119.72	126.34
3	5	4293	PSU	C4-N3-C2	-4.59	119.72	126.34
3	5	4293	PSU	N1-C2-N3	4.59	120.33	115.13
6	9	1806	M7A	C4-N9-C1'	-4.58	115.72	126.60
3	5	4442	PSU	N1-C2-N3	4.58	120.32	115.13
3	5	3899	BGH	C2-N3-C4	4.57	120.44	112.30
3	5	1582	PSU	C4-N3-C2	-4.56	119.77	126.34
6	9	822	PSU	N1-C2-N3	4.56	120.30	115.13
3	5	4500	PSU	N1-C2-N3	4.55	120.28	115.13
3	5	4530	UR3	C4-N3-C2	-4.54	120.28	124.56
6	9	1219	B8Q	O2-C2-N3	-4.52	116.31	122.95
3	5	4636	PSU	N1-C2-N3	4.52	120.25	115.13
3	5	3715	PSU	C4-N3-C2	-4.52	119.83	126.34
3	5	2297	E7G	C2-N3-C4	4.50	120.32	112.30
3	5	3729	PSU	C4-N3-C2	-4.50	119.85	126.34
6	9	1830	UR3	C4-N3-C2	-4.49	120.33	124.56
6	9	814	5MU	N3-C2-N1	4.49	120.85	114.89
3	5	4550	7MG	C2-N3-C4	4.49	120.29	112.30
3	5	1605	7MG	C2-N3-C4	4.47	120.27	112.30
6	9	612	PSU	C4-N3-C2	-4.46	119.91	126.34
3	5	1683	PSU	N1-C2-N3	4.46	120.19	115.13
3	5	3729	PSU	N1-C2-N3	4.45	120.18	115.13
3	5	4690	B8K	C72-C71-N7	4.45	125.55	118.86
3	5	2754	B9B	C2-N3-C4	4.45	120.43	115.36
3	5	3715	PSU	N1-C2-N3	4.43	120.15	115.13
3	5	1582	PSU	N1-C2-N3	4.43	120.15	115.13
6	9	1081	PSU	N1-C2-N3	4.43	120.15	115.13
6	9	612	PSU	N1-C2-N3	4.41	120.12	115.13
6	9	1243	PSU	N1-C2-N3	4.40	120.12	115.13
6	9	119	PSU	N1-C2-N3	4.39	120.11	115.13
3	5	3764	PSU	N1-C2-N3	4.36	120.07	115.13
3	5	3899	BGH	C4-C5-N7	4.35	108.78	104.91
6	9	119	PSU	C4-N3-C2	-4.33	120.10	126.34
3	5	1574	B9B	C2-N3-C4	4.32	120.29	115.36
3	5	4185	B8W	C2-N3-C4	4.32	120.29	115.36
1	2	37	T6A	N6-C6-N1	4.31	124.49	118.72
3	5	3764	PSU	C4-N3-C2	-4.30	120.14	126.34
3	5	2522	7MG	C2-N3-C4	4.30	119.96	112.30
3	5	4597	UR3	C4-N3-C2	-4.29	120.53	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2754	B9B	N2-C2-N3	4.28	124.76	117.79
3	5	4403	PSU	C4-N3-C2	-4.26	120.20	126.34
3	5	237	B9B	N2-C2-N3	4.25	124.72	117.79
3	5	4403	PSU	N1-C2-N3	4.25	119.94	115.13
3	5	2297	E7G	C5-C4-N3	-4.25	120.04	128.13
3	5	4415	1MA	C5-C6-N1	4.24	120.22	113.90
3	5	3897	B8K	C72-C71-N7	4.24	125.23	118.86
3	5	1797	E7G	C5-C4-N3	-4.23	120.08	128.13
6	9	1248	B8N	C4-N3-C2	-4.22	120.12	125.46
3	5	4472	B8W	C2-N3-C4	4.21	120.17	115.36
3	5	4550	7MG	C5-C4-N3	-4.21	120.10	128.13
3	5	237	B9B	C2-N3-C4	4.20	120.16	115.36
3	5	1605	7MG	C5-C4-N3	-4.19	120.14	128.13
3	5	4529	B8W	C2-N3-C4	4.16	120.11	115.36
3	5	4129	B8W	C2-N3-C4	4.12	120.07	115.36
3	5	4371	MHG	C5-C4-N3	-4.11	120.30	128.13
3	5	2522	7MG	C5-C4-N3	-4.10	120.33	128.13
3	5	1322	1MA	C5-C6-N1	4.08	119.99	113.90
3	5	2380	B8W	O6-C6-N1	4.07	124.67	119.03
3	5	1574	B9B	N2-C2-N3	4.03	124.36	117.79
3	5	4371	MHG	C2-N1-C6	-4.02	119.85	124.48
3	5	4355	E6G	C2-N3-C4	4.01	119.94	115.36
3	5	2380	B8W	C2-N3-C4	3.95	119.87	115.36
1	2	37	T6A	N3-C2-N1	-3.93	122.54	128.68
3	5	4083	5MU	C5M-C5-C6	-3.91	117.63	122.85
3	5	4620	OMU	N3-C2-N1	3.89	120.05	114.89
3	5	4306	OMU	N3-C2-N1	3.85	120.00	114.89
1	2	37	T6A	C12-N11-C10	3.84	128.34	121.94
3	5	3899	BGH	C5-C4-N9	3.83	111.32	106.35
6	9	121	OMU	N3-C2-N1	3.81	119.95	114.89
6	9	814	5MU	C5M-C5-C6	-3.75	117.84	122.85
6	9	116	OMU	N3-C2-N1	3.74	119.86	114.89
3	5	1456	B8Q	O2-C2-N3	-3.73	117.47	122.95
3	5	4690	B8K	C5-C4-N9	3.72	111.17	106.35
3	5	4083	5MU	C5M-C5-C4	3.70	122.84	118.77
3	5	1883	OMG	C5-C6-N1	3.68	120.44	113.95
3	5	4194	I4U	C5-C4-N3	-3.68	119.32	124.91
3	5	4447	5MC	C5-C6-N1	-3.66	119.57	123.34
5	8	14	OMU	N3-C2-N1	3.59	119.66	114.89
3	5	4196	OMG	C5-C6-N1	3.58	120.28	113.95
6	9	568	MMX	O2-C2-N3	-3.58	117.53	122.07
3	5	3897	B8K	C5-C4-N3	-3.58	121.31	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	1316	OMG	C5-C6-N1	3.57	120.26	113.95
3	5	3899	BGH	C72-C71-N7	3.57	124.23	118.86
3	5	1860	B8H	C5-C4-N3	3.57	124.65	116.58
6	9	509	OMG	C5-C6-N1	3.56	120.25	113.95
3	5	4296	B8H	C5-C4-N3	3.56	124.64	116.58
3	5	4637	OMG	C5-C6-N1	3.55	120.23	113.95
6	9	1374	5MC	C5-C6-N1	-3.55	119.68	123.34
3	5	4494	OMG	C5-C6-N1	3.55	120.22	113.95
3	5	2424	OMG	C5-C6-N1	3.55	120.21	113.95
3	5	4370	OMG	C5-C6-N1	3.55	120.21	113.95
3	5	373	OMG	C5-C6-N1	3.54	120.21	113.95
3	5	4870	OMG	C5-C6-N1	3.54	120.20	113.95
3	5	1522	OMG	C5-C6-N1	3.51	120.14	113.95
3	5	4335	5MC	C5-C6-N1	-3.50	119.73	123.34
3	5	1517	2MG	C5-C6-N1	3.50	120.13	113.95
3	5	2773	OMG	C5-C6-N1	3.50	120.13	113.95
3	5	4623	OMG	C5-C6-N1	3.50	120.13	113.95
3	5	4185	B8W	C1'-N9-C4	-3.49	120.52	126.64
6	9	683	OMG	C5-C6-N1	3.49	120.11	113.95
3	5	2050	OMG	C5-C6-N1	3.48	120.10	113.95
3	5	3792	OMG	C5-C6-N1	3.48	120.10	113.95
3	5	4872	2MG	C5-C6-N1	3.48	120.10	113.95
3	5	1625	OMG	C5-C6-N1	3.48	120.10	113.95
3	5	3782	5MC	C5-C6-N1	-3.47	119.77	123.34
3	5	1659	I4U	C5-C4-N3	-3.47	119.64	124.91
3	5	3762	B8H	C5-C4-N3	3.47	124.42	116.58
3	5	2364	OMG	C5-C6-N1	3.46	120.07	113.95
3	5	4185	B8W	O6-C6-N1	3.44	123.80	119.03
3	5	729	2MG	C5-C6-N1	3.44	120.02	113.95
1	2	37	T6A	O10-C10-N6	-3.42	117.84	123.62
3	5	4355	E6G	N2-C2-N1	-3.41	111.94	117.25
6	9	644	OMG	C5-C6-N1	3.40	119.96	113.95
3	5	1348	P4U	C5-C4-N3	-3.40	119.73	124.91
3	5	4564	M7A	C2-N3-C4	3.40	119.79	111.75
3	5	4564	M7A	C4-N9-C1'	-3.40	118.53	126.60
3	5	4129	B8W	C1'-N9-C4	-3.40	120.67	126.64
6	9	1806	M7A	C2-N3-C4	3.39	119.75	111.75
3	5	4690	B8K	C5-C4-N3	-3.38	121.69	128.13
3	5	1860	B8H	O2-C2-N1	-3.36	119.09	122.87
3	5	4296	B8H	O2-C2-N1	-3.36	119.09	122.87
3	5	2522	7MG	C4-C5-N7	3.35	110.17	105.53
6	9	121	OMU	C5-C4-N3	3.34	119.83	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4306	OMU	C5-C4-N3	3.33	119.83	114.84
3	5	4872	2MG	CM2-N2-C2	-3.33	116.51	123.86
3	5	3899	BGH	C5-C4-N3	-3.31	121.82	128.13
3	5	4472	B8W	C1'-N9-C4	-3.31	120.83	126.64
6	9	814	5MU	C5M-C5-C4	3.30	122.40	118.77
5	8	14	OMU	C5-C4-N3	3.29	119.76	114.84
6	9	568	MMX	C31-N3-C2	3.29	121.67	117.44
3	5	4620	OMU	C5-C4-N3	3.28	119.75	114.84
3	5	3762	B8H	O2-C2-N1	-3.28	119.18	122.87
6	9	116	OMU	C5-C4-N3	3.26	119.72	114.84
3	5	3897	B8K	C5-C4-N9	3.23	110.54	106.35
6	9	509	OMG	C2-N1-C6	-3.21	119.18	125.10
3	5	3897	B8K	N9-C8-N7	3.21	107.64	103.33
3	5	2380	B8W	N2-C2-N1	-3.20	112.27	117.25
3	5	2297	E7G	C5-C4-N9	3.15	110.43	106.35
3	5	1625	OMG	C2-N1-C6	-3.13	119.34	125.10
3	5	4550	7MG	C4-C5-N7	3.13	109.87	105.53
3	5	4494	OMG	C2-N1-C6	-3.12	119.34	125.10
3	5	1883	OMG	C2-N1-C6	-3.12	119.35	125.10
3	5	2380	B8W	C1'-N9-C4	-3.11	121.17	126.64
3	5	2424	OMG	C2-N1-C6	-3.11	119.37	125.10
3	5	4637	OMG	C2-N1-C6	-3.11	119.38	125.10
3	5	4196	OMG	C2-N1-C6	-3.10	119.39	125.10
3	5	4690	B8K	N9-C8-N7	3.10	107.48	103.33
3	5	1797	E7G	C5-C4-N9	3.09	110.36	106.35
6	9	644	OMG	C2-N1-C6	-3.08	119.42	125.10
3	5	4623	OMG	C2-N1-C6	-3.08	119.43	125.10
3	5	1605	7MG	C5-C4-N9	3.07	110.33	106.35
3	5	1605	7MG	C4-C5-N7	3.06	109.78	105.53
3	5	1316	OMG	C2-N1-C6	-3.06	119.46	125.10
3	5	4371	MHG	C5-C4-N9	3.05	110.31	106.35
6	9	1219	B8Q	C6-N1-C2	-3.05	119.06	121.79
5	8	14	OMU	O4-C4-C5	-3.05	119.80	125.16
3	5	3792	OMG	C2-N1-C6	-3.05	119.49	125.10
3	5	4370	OMG	C2-N1-C6	-3.04	119.51	125.10
3	5	2364	OMG	C2-N1-C6	-3.03	119.51	125.10
6	9	1806	M7A	C71-N7-C5	-3.03	112.36	124.01
3	5	2773	OMG	C2-N1-C6	-3.02	119.54	125.10
3	5	4870	OMG	C2-N1-C6	-3.01	119.56	125.10
6	9	1248	B8N	N3-C2-N1	2.97	120.96	116.76
3	5	3899	BGH	N9-C8-N7	2.97	107.31	103.33
3	5	4550	7MG	C5-C4-N9	2.97	110.20	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4129	B8W	N2-C2-N1	-2.97	112.64	117.25
3	5	1797	E7G	O6-C6-C5	-2.95	120.31	127.54
3	5	2050	OMG	C2-N1-C6	-2.94	119.68	125.10
6	9	116	OMU	O4-C4-C5	-2.94	119.99	125.16
6	9	683	OMG	C2-N1-C6	-2.93	119.69	125.10
3	5	4371	MHG	O6-C6-C5	-2.92	120.36	127.54
3	5	4628	PSU	O2-C2-N1	-2.92	119.57	122.79
3	5	4620	OMU	O4-C4-C5	-2.92	120.03	125.16
3	5	2522	7MG	C5-C4-N9	2.92	110.13	106.35
3	5	373	OMG	C2-N1-C6	-2.91	119.74	125.10
3	5	1522	OMG	C2-N1-C6	-2.91	119.74	125.10
6	9	1830	UR3	C1'-N1-C2	2.91	121.90	116.99
6	9	568	MMX	C5-C6-N1	2.87	115.43	110.71
3	5	3764	PSU	O2-C2-N1	-2.87	119.63	122.79
3	5	4306	OMU	O4-C4-C5	-2.87	120.11	125.16
3	5	4220	6MZ	C2-N1-C6	2.87	119.05	116.59
6	9	121	OMU	O4-C4-C5	-2.87	120.12	125.16
3	5	4529	B8W	C2-N1-C6	2.86	120.67	116.08
6	9	822	PSU	O2-C2-N1	-2.85	119.65	122.79
3	5	1605	7MG	C2-N1-C6	-2.85	119.90	125.10
3	5	1797	E7G	C2-N1-C6	-2.85	119.90	125.10
3	5	1322	1MA	C8-N7-C5	2.84	108.40	102.99
3	5	4529	B8W	C1'-N9-C4	-2.84	121.65	126.64
3	5	2297	E7G	C2-N1-C6	-2.84	119.92	125.10
3	5	4550	7MG	N9-C4-N3	2.83	129.70	125.47
3	5	1909	P7G	N9-C8-N7	2.81	107.40	103.38
3	5	373	OMG	C8-N7-C5	2.81	108.34	102.99
3	5	4370	OMG	C8-N7-C5	2.81	108.33	102.99
3	5	4185	B8W	N2-C2-N1	-2.81	112.89	117.25
3	5	2522	7MG	O6-C6-C5	-2.79	120.69	127.54
3	5	2522	7MG	C2-N1-C6	-2.79	120.02	125.10
3	5	4529	B8W	N2-C2-N1	-2.77	112.94	117.25
3	5	1605	7MG	O6-C6-C5	-2.77	120.75	127.54
3	5	3715	PSU	O2-C2-N1	-2.77	119.74	122.79
3	5	4296	B8H	O4-C4-N3	-2.76	114.82	120.12
3	5	4872	2MG	C8-N7-C5	2.76	108.25	102.99
3	5	2297	E7G	O6-C6-C5	-2.76	120.76	127.54
3	5	4623	OMG	C8-N7-C5	2.76	108.25	102.99
3	5	4529	B8W	O6-C6-C5	2.76	119.96	116.01
3	5	1522	OMG	C8-N7-C5	2.76	108.25	102.99
6	9	1337	4AC	C6-C5-C4	2.76	120.34	116.96
6	9	683	OMG	C8-N7-C5	2.75	108.24	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	9	1842	4AC	C6-C5-C4	2.75	120.33	116.96
3	5	4550	7MG	C2-N1-C6	-2.75	120.09	125.10
3	5	2773	OMG	C8-N7-C5	2.74	108.21	102.99
3	5	1797	E7G	N9-C4-N3	2.74	129.57	125.47
3	5	4870	OMG	C8-N7-C5	2.73	108.19	102.99
3	5	3729	PSU	O2-C2-N1	-2.73	119.79	122.79
3	5	2522	7MG	N9-C4-N3	2.72	129.54	125.47
3	5	3792	OMG	C8-N7-C5	2.72	108.18	102.99
3	5	4129	B8W	C2-N1-C6	2.72	120.45	116.08
3	5	1605	7MG	N9-C4-N3	2.72	129.53	125.47
3	5	2297	E7G	N9-C4-N3	2.72	129.53	125.47
3	5	1316	OMG	C8-N7-C5	2.71	108.16	102.99
6	9	644	OMG	C8-N7-C5	2.71	108.16	102.99
3	5	4415	1MA	C8-N7-C5	2.70	108.14	102.99
3	5	4442	PSU	O2-C2-N1	-2.69	119.82	122.79
3	5	2364	OMG	C8-N7-C5	2.69	108.11	102.99
3	5	1677	PSU	O2-C2-N1	-2.69	119.83	122.79
3	5	1860	B8H	O4-C4-N3	-2.68	114.98	120.12
3	5	1883	OMG	O6-C6-C5	-2.68	119.14	124.37
3	5	3897	B8K	C2-N1-C6	-2.68	120.22	125.10
3	5	1625	OMG	C8-N7-C5	2.67	108.08	102.99
3	5	2754	B9B	C61-O6-C6	-2.67	112.53	117.51
3	5	4483	B8T	C6-C5-C4	2.67	120.22	116.96
6	9	509	OMG	C8-N7-C5	2.66	108.06	102.99
3	5	4472	B8W	N2-C2-N1	-2.65	113.13	117.25
3	5	4196	OMG	C8-N7-C5	2.65	108.04	102.99
6	9	1219	B8Q	C31-N3-C2	2.64	121.63	117.79
6	9	1832	6MZ	C2-N1-C6	2.64	118.85	116.59
3	5	4550	7MG	O6-C6-C5	-2.64	121.07	127.54
3	5	4472	B8W	C2-N1-C6	2.64	120.32	116.08
3	5	4690	B8K	C6-C5-C4	-2.63	117.19	122.62
3	5	4293	PSU	O2-C2-N1	-2.63	119.89	122.79
3	5	3899	BGH	C6-C5-C4	-2.63	117.20	122.62
6	9	612	PSU	O2-C2-N1	-2.63	119.90	122.79
3	5	4355	E6G	C61-O6-C6	-2.63	114.96	117.56
6	9	1248	B8N	O4-C4-N3	-2.63	115.52	119.98
3	5	3899	BGH	C2'-C1'-N9	-2.63	108.80	114.14
3	5	4494	OMG	C8-N7-C5	2.63	107.99	102.99
3	5	4371	MHG	N9-C4-N3	2.62	129.39	125.47
3	5	2424	OMG	C8-N7-C5	2.61	107.97	102.99
6	9	814	5MU	O4-C4-N3	-2.61	115.11	120.12
3	5	4636	PSU	O2-C2-N1	-2.61	119.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	3762	B8H	O4-C4-N3	-2.61	115.12	120.12
3	5	4690	B8K	C2-N1-C6	-2.60	120.36	125.10
3	5	4371	MHG	C72-C71-N7	-2.60	109.85	112.41
3	5	4500	PSU	O2-C2-N1	-2.58	119.95	122.79
6	9	1081	PSU	O2-C2-N1	-2.58	119.95	122.79
3	5	1883	OMG	C8-N7-C5	2.58	107.91	102.99
3	5	1605	7MG	N9-C8-N7	2.58	107.07	103.38
3	5	3880	P7G	N9-C8-N7	2.58	107.07	103.38
6	9	1243	PSU	O2-C2-N1	-2.58	119.95	122.79
3	5	3785	A2M	O4'-C1'-C2'	-2.58	102.12	106.59
6	9	1806	M7A	C5-C4-N3	-2.57	120.58	126.62
3	5	4500	PSU	C6-C5-C4	2.57	120.00	118.20
3	5	4530	UR3	C6-N1-C2	-2.57	119.49	121.79
3	5	4671	B8T	C6-C5-C4	2.57	120.10	116.96
3	5	4531	PSU	C6-C5-C4	2.57	119.99	118.20
3	5	2050	OMG	C8-N7-C5	2.56	107.88	102.99
3	5	729	2MG	C8-N7-C5	2.55	107.85	102.99
3	5	4637	OMG	C8-N7-C5	2.55	107.85	102.99
3	5	4083	5MU	O4-C4-N3	-2.55	115.24	120.12
3	5	237	B9B	C61-O6-C6	-2.54	112.76	117.51
6	9	823	PSU	O2-C2-N1	-2.54	119.99	122.79
3	5	4564	M7A	C5-C4-N3	-2.54	120.66	126.62
3	5	4531	PSU	O2-C2-N1	-2.53	120.00	122.79
6	9	1830	UR3	C6-N1-C2	-2.53	119.52	121.79
3	5	3718	A2M	C1'-N9-C4	2.52	131.08	126.64
3	5	4472	B8W	O6-C6-N1	2.52	122.53	119.03
6	9	119	PSU	O2-C2-N1	-2.50	120.04	122.79
3	5	2363	A2M	C1'-N9-C4	2.49	131.02	126.64
3	5	3764	PSU	C6-N1-C2	-2.49	120.14	122.68
3	5	3897	B8K	C6-C5-C4	-2.49	117.49	122.62
3	5	4450	PSU	O2-C2-N1	-2.49	120.05	122.79
3	5	1517	2MG	C8-N7-C5	2.48	107.71	102.99
3	5	4494	OMG	O6-C6-C5	-2.47	119.54	124.37
6	9	1842	4AC	N4-C4-N3	2.47	118.00	113.85
3	5	1625	OMG	O6-C6-C5	-2.47	119.54	124.37
3	5	3723	A2M	C1'-N9-C4	2.46	130.96	126.64
3	5	4355	E6G	C2-N1-C6	2.45	120.01	116.08
3	5	4628	PSU	C6-N1-C2	-2.44	120.19	122.68
3	5	4442	PSU	O4'-C1'-C2'	2.44	108.58	105.14
3	5	4083	5MU	O2-C2-N1	-2.44	119.55	122.79
3	5	4403	PSU	O4'-C1'-C2'	2.43	108.58	105.14
3	5	1683	PSU	O2-C2-N1	-2.43	120.11	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4371	MHG	N1-C2-N3	-2.41	120.23	123.95
3	5	2522	7MG	N9-C8-N7	2.40	106.82	103.38
3	5	1316	OMG	O6-C6-C5	-2.40	119.68	124.37
3	5	2050	OMG	O6-C6-C5	-2.40	119.68	124.37
6	9	1832	6MZ	C9-N6-C6	-2.40	120.80	122.87
3	5	3899	BGH	C2-N1-C6	-2.40	120.73	125.10
3	5	2508	PSU	O2-C2-N1	-2.39	120.16	122.79
3	5	3729	PSU	C6-N1-C2	-2.39	120.24	122.68
6	9	1219	B8Q	C1'-N1-C6	-2.39	115.64	120.84
3	5	4529	B8W	C4-C5-N7	-2.39	106.91	109.40
3	5	1677	PSU	C6-C5-C4	2.38	119.86	118.20
3	5	1797	E7G	N9-C8-N7	2.38	106.78	103.38
3	5	1326	A2M	C1'-N9-C4	2.37	130.81	126.64
6	9	159	A2M	C1'-N9-C4	2.37	130.81	126.64
3	5	2424	OMG	O6-C6-C5	-2.36	119.77	124.37
3	5	1517	2MG	O6-C6-C5	-2.35	119.78	124.37
3	5	4872	2MG	O6-C6-C5	-2.33	119.82	124.37
6	9	1248	B8N	O4'-C1'-C2'	2.32	108.42	105.14
3	5	3909	OMC	O2-C2-N3	-2.32	118.56	122.33
6	9	119	PSU	C6-N1-C2	-2.32	120.31	122.68
6	9	612	PSU	C6-N1-C2	-2.31	120.32	122.68
5	8	14	OMU	C1'-N1-C2	2.31	121.75	117.57
3	5	4403	PSU	C6-N1-C2	-2.31	120.33	122.68
3	5	4196	OMG	O6-C6-C5	-2.30	119.89	124.37
3	5	2297	E7G	N9-C8-N7	2.30	106.66	103.38
3	5	2786	B9H	O2-C2-N1	-2.30	117.34	122.72
6	9	1337	4AC	N4-C4-N3	2.29	117.70	113.85
3	5	2773	OMG	O6-C6-C5	-2.29	119.91	124.37
3	5	1456	B8Q	C31-N3-C2	2.28	121.11	117.79
3	5	4637	OMG	O6-C6-C5	-2.28	119.91	124.37
3	5	4564	M7A	C71-N7-C5	-2.28	115.25	124.01
3	5	2297	E7G	C8-N7-C71	2.28	125.93	120.50
3	5	3792	OMG	O6-C6-C5	-2.27	119.94	124.37
3	5	4185	B8W	C2-N1-C6	2.27	119.72	116.08
3	5	1797	E7G	C8-N7-C71	2.26	125.89	120.50
3	5	1574	B9B	C61-O6-C6	-2.26	113.28	117.51
6	9	822	PSU	O4'-C1'-C2'	2.25	108.32	105.14
3	5	4293	PSU	C6-N1-C2	-2.25	120.38	122.68
3	5	4306	OMU	O2-C2-N1	-2.25	119.80	122.79
3	5	4597	UR3	C6-N1-C2	-2.25	119.78	121.79
3	5	4450	PSU	C6-N1-C2	-2.25	120.39	122.68
6	9	822	PSU	C6-N1-C2	-2.24	120.39	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	4690	B8K	O6-C6-C5	-2.24	122.04	127.54
3	5	4620	OMU	O2-C2-N1	-2.23	119.82	122.79
3	5	2364	OMG	O6-C6-C5	-2.23	120.03	124.37
3	5	4370	OMG	O6-C6-C5	-2.22	120.03	124.37
6	9	683	OMG	O6-C6-C5	-2.22	120.03	124.37
6	9	116	OMU	O2-C2-N1	-2.22	119.83	122.79
3	5	3715	PSU	C6-N1-C2	-2.22	120.42	122.68
3	5	3880	P7G	C5-C4-N3	-2.22	120.09	124.00
3	5	729	2MG	O6-C6-C5	-2.21	120.05	124.37
3	5	4550	7MG	N9-C8-N7	2.21	106.54	103.38
3	5	373	OMG	O6-C6-C5	-2.21	120.06	124.37
3	5	4371	MHG	N9-C8-N7	2.21	106.53	103.38
3	5	1582	PSU	O2-C2-N1	-2.21	120.36	122.79
3	5	4870	OMG	O6-C6-C5	-2.20	120.07	124.37
3	5	2380	B8W	C2-N1-C6	2.20	119.61	116.08
6	9	823	PSU	C6-N1-C2	-2.20	120.43	122.68
6	9	612	PSU	O4'-C1'-C2'	2.20	108.24	105.14
3	5	3867	A2M	C1'-N9-C4	2.19	130.50	126.64
3	5	3897	B8K	O6-C6-C5	-2.19	122.16	127.54
3	5	1866	UR3	C1'-N1-C2	2.19	120.69	116.99
3	5	4442	PSU	C6-N1-C2	-2.19	120.44	122.68
6	9	644	OMG	O6-C6-C5	-2.18	120.11	124.37
6	9	484	A2M	C1'-N9-C4	2.18	130.47	126.64
3	5	3782	5MC	CM5-C5-C6	-2.18	119.94	122.85
3	5	4450	PSU	C6-C5-C4	2.17	119.71	118.20
6	9	1842	4AC	C5-C4-N3	-2.16	119.12	122.59
6	9	121	OMU	O2-C2-N1	-2.16	119.92	122.79
3	5	4531	PSU	C6-N1-C2	-2.15	120.48	122.68
3	5	1582	PSU	C6-N1-C2	-2.15	120.48	122.68
3	5	2401	A2M	C1'-N9-C4	2.15	130.42	126.64
6	9	823	PSU	C6-C5-C4	2.15	119.70	118.20
6	9	822	PSU	C6-C5-C4	2.14	119.70	118.20
3	5	4623	OMG	O6-C6-C5	-2.14	120.19	124.37
6	9	509	OMG	O6-C6-C5	-2.13	120.21	124.37
6	9	1337	4AC	C5-C4-N3	-2.13	119.16	122.59
6	9	166	A2M	C2'-C3'-C4'	2.13	106.62	101.99
3	5	1517	2MG	CM2-N2-C2	-2.12	119.17	123.86
6	9	166	A2M	C5'-C4'-C3'	-2.12	107.22	115.18
3	5	3899	BGH	N1-C2-N3	-2.12	119.37	123.32
3	5	4500	PSU	C6-N1-C2	-2.11	120.53	122.68
3	5	4442	PSU	C6-C5-C4	2.11	119.67	118.20
3	5	2508	PSU	C6-N1-C2	-2.10	120.54	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	37	T6A	C3'-C2'-C1'	2.10	104.13	100.98
3	5	1683	PSU	C6-N1-C2	-2.10	120.54	122.68
3	5	1522	OMG	O6-C6-C5	-2.09	120.28	124.37
6	9	1842	4AC	CM7-C7-N4	2.09	118.92	115.29
3	5	1524	A2M	C1'-N9-C4	2.09	130.32	126.64
6	9	1243	PSU	C6-N1-C2	-2.09	120.54	122.68
3	5	4129	B8W	C4-C5-N7	-2.07	107.24	109.40
6	9	814	5MU	C6-C5-C4	2.07	119.76	118.03
3	5	4636	PSU	C6-N1-C2	-2.06	120.58	122.68
3	5	4529	B8W	C5-C6-N1	-2.05	119.36	123.26
6	9	1081	PSU	O4'-C1'-C2'	2.04	108.03	105.14
3	5	3785	A2M	C1'-N9-C4	2.04	130.23	126.64
3	5	4403	PSU	O2-C2-N1	-2.03	120.56	122.79
3	5	3899	BGH	O6-C6-C5	-2.03	122.57	127.54
3	5	2786	B9H	C6-N1-C2	-2.02	119.98	121.79
3	5	4690	B8K	N1-C2-N3	-2.02	119.55	123.32
6	9	1374	5MC	CM5-C5-C6	-2.01	120.17	122.85

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	37	T6A	N6-C10-N11-C12
1	2	37	T6A	O10-C10-N11-C12
3	5	237	B9B	C5-C6-O6-C61
3	5	237	B9B	N1-C6-O6-C61
3	5	237	B9B	C3'-C4'-C5'-O5'
3	5	237	B9B	O4'-C4'-C5'-O5'
3	5	237	B9B	C62-C61-O6-C6
3	5	1316	OMG	C1'-C2'-O2'-CM2
3	5	1326	A2M	C1'-C2'-O2'-CM'
3	5	1348	P4U	N3-C4-O4-C41
3	5	1348	P4U	C3'-C4'-C5'-O5'
3	5	1348	P4U	O4'-C4'-C5'-O5'
3	5	1574	B9B	C5-C6-O6-C61
3	5	1574	B9B	N1-C6-O6-C61
3	5	1677	PSU	C2'-C1'-C5-C4
3	5	1677	PSU	C2'-C1'-C5-C6
3	5	1677	PSU	O4'-C1'-C5-C6
3	5	1797	E7G	O4'-C4'-C5'-O5'
3	5	2364	OMG	O4'-C4'-C5'-O5'
3	5	2364	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	5	2380	B8W	C5-C6-O6-C61
3	5	2380	B8W	N1-C6-O6-C61
3	5	2380	B8W	C3’-C4’-C5’-O5’
3	5	2380	B8W	O4’-C4’-C5’-O5’
3	5	2424	OMG	O4’-C4’-C5’-O5’
3	5	2424	OMG	C3’-C4’-C5’-O5’
3	5	2754	B9B	C5-C6-O6-C61
3	5	2754	B9B	N1-C6-O6-C61
3	5	2773	OMG	C1’-C2’-O2’-CM2
3	5	2861	OMC	C1’-C2’-O2’-CM2
3	5	3701	OMC	C2’-C1’-N1-C6
3	5	3718	A2M	C1’-C2’-O2’-CM’
3	5	3762	B8H	C3’-C4’-C5’-O5’
3	5	3762	B8H	O4’-C4’-C5’-O5’
3	5	3792	OMG	O4’-C4’-C5’-O5’
3	5	3792	OMG	C3’-C4’-C5’-O5’
3	5	3825	A2M	C1’-C2’-O2’-CM’
3	5	3867	A2M	O4’-C4’-C5’-O5’
3	5	3867	A2M	C3’-C4’-C5’-O5’
3	5	3867	A2M	C1’-C2’-O2’-CM’
3	5	3880	P7G	O4’-C4’-C5’-O5’
3	5	3899	BGH	C1’-C2’-O2’-C6’
3	5	4129	B8W	C5-C6-O6-C61
3	5	4129	B8W	N1-C6-O6-C61
3	5	4185	B8W	C5-C6-O6-C61
3	5	4185	B8W	N1-C6-O6-C61
3	5	4220	6MZ	N1-C6-N6-C9
3	5	4355	E6G	C5-C6-O6-C61
3	5	4355	E6G	N1-C6-O6-C61
3	5	4403	PSU	O4’-C1’-C5-C4
3	5	4403	PSU	O4’-C1’-C5-C6
3	5	4450	PSU	C2’-C1’-C5-C4
3	5	4472	B8W	C5-C6-O6-C61
3	5	4472	B8W	N1-C6-O6-C61
3	5	4500	PSU	C3’-C4’-C5’-O5’
3	5	4523	A2M	O4’-C4’-C5’-O5’
3	5	4523	A2M	C3’-C4’-C5’-O5’
3	5	4529	B8W	C5-C6-O6-C61
3	5	4529	B8W	N1-C6-O6-C61
3	5	4530	UR3	O4’-C4’-C5’-O5’
3	5	4530	UR3	C3’-C4’-C5’-O5’
3	5	4531	PSU	O4’-C4’-C5’-O5’

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Mol	Chain	Res	Type	Atoms
3	5	4620	OMU	C1'-C2'-O2'-CM2
3	5	4636	PSU	C2'-C1'-C5-C6
3	5	4870	OMG	O4'-C4'-C5'-O5'
3	5	4870	OMG	C3'-C4'-C5'-O5'
5	8	14	OMU	C1'-C2'-O2'-CM2
6	9	27	A2M	C1'-C2'-O2'-CM'
6	9	116	OMU	C3'-C4'-C5'-O5'
6	9	116	OMU	O4'-C4'-C5'-O5'
6	9	159	A2M	C3'-C4'-C5'-O5'
6	9	159	A2M	C1'-C2'-O2'-CM'
6	9	166	A2M	C3'-C4'-C5'-O5'
6	9	174	OMC	C1'-C2'-O2'-CM2
6	9	568	MMX	O4'-C1'-N1-C2
6	9	568	MMX	O4'-C1'-N1-C6
6	9	668	A2M	C1'-C2'-O2'-CM'
6	9	683	OMG	O4'-C4'-C5'-O5'
6	9	1248	B8N	C31-C32-C33-C34
6	9	1678	A2M	C1'-C2'-O2'-CM'
6	9	1830	UR3	O4'-C1'-N1-C2
6	9	1851	MA6	O4'-C4'-C5'-O5'
6	9	1830	UR3	O4'-C1'-N1-C6
3	5	3701	OMC	C2'-C1'-N1-C2
1	2	37	T6A	O4'-C4'-C5'-O5'
3	5	398	A2M	O4'-C4'-C5'-O5'
3	5	1797	E7G	C3'-C4'-C5'-O5'
3	5	3764	PSU	C3'-C4'-C5'-O5'
3	5	3785	A2M	O4'-C4'-C5'-O5'
3	5	3785	A2M	C3'-C4'-C5'-O5'
3	5	3880	P7G	C3'-C4'-C5'-O5'
3	5	3897	B8K	C3'-C4'-C5'-O5'
3	5	3897	B8K	O4'-C4'-C5'-O5'
3	5	4194	I4U	O4'-C4'-C5'-O5'
3	5	4355	E6G	O4'-C4'-C5'-O5'
3	5	4371	MHG	O4'-C4'-C5'-O5'
3	5	4500	PSU	O4'-C4'-C5'-O5'
6	9	159	A2M	O4'-C4'-C5'-O5'
6	9	166	A2M	O4'-C4'-C5'-O5'
6	9	668	A2M	O4'-C4'-C5'-O5'
6	9	668	A2M	C3'-C4'-C5'-O5'
6	9	683	OMG	C3'-C4'-C5'-O5'
6	9	1851	MA6	C3'-C4'-C5'-O5'
9	C	333	MLZ	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	2	37	T6A	C3'-C4'-C5'-O5'
3	5	2364	OMG	C3'-C4'-C5'-O5'
3	5	3764	PSU	O4'-C4'-C5'-O5'
3	5	4194	I4U	C3'-C4'-C5'-O5'
3	5	4355	E6G	C3'-C4'-C5'-O5'
6	9	568	MMX	C3'-C4'-C5'-O5'
3	5	4371	MHG	C2'-C1'-N9-C8
3	5	4870	OMG	C3'-C2'-O2'-CM2
3	5	1574	B9B	O6-C61-C62-C63
3	5	4637	OMG	C3'-C4'-C5'-O5'
3	5	398	A2M	C3'-C4'-C5'-O5'
6	9	568	MMX	O4'-C4'-C5'-O5'
3	5	4371	MHG	C75-C73-C74-C76
3	5	2297	E7G	C3'-C4'-C5'-O5'
6	9	644	OMG	C3'-C4'-C5'-O5'
6	9	1243	PSU	O4'-C4'-C5'-O5'
3	5	3729	PSU	O4'-C4'-C5'-O5'
3	5	2786	B9H	C32-C31-N3-C2
3	5	1625	OMG	C3'-C4'-C5'-O5'
3	5	1883	OMG	C3'-C4'-C5'-O5'
3	5	2297	E7G	O4'-C4'-C5'-O5'
3	5	4296	B8H	O4'-C4'-C5'-O5'
3	5	3897	B8K	C4'-C5'-O5'-P
3	5	4870	OMG	C4'-C5'-O5'-P
3	5	3782	5MC	O4'-C4'-C5'-O5'
3	5	1909	P7G	C72-C71-N7-C8
3	5	3701	OMC	O4'-C1'-N1-C2
3	5	3701	OMC	O4'-C1'-N1-C6
9	C	333	MLZ	N-CA-CB-CG
3	5	1677	PSU	O4'-C4'-C5'-O5'
3	5	4296	B8H	C3'-C4'-C5'-O5'
3	5	4371	MHG	C3'-C4'-C5'-O5'
3	5	4637	OMG	O4'-C4'-C5'-O5'
9	C	333	MLZ	C-CA-CB-CG
3	5	1534	A2M	C4'-C5'-O5'-P
6	9	1703	OMC	O4'-C4'-C5'-O5'
6	9	644	OMG	O4'-C4'-C5'-O5'
3	5	3785	A2M	C3'-C2'-O2'-CM'
3	5	4371	MHG	C72-C73-C74-C76
3	5	1625	OMG	C4'-C5'-O5'-P
6	9	1219	B8Q	C2'-C1'-N1-C2
3	5	3909	OMC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
6	9	1219	B8Q	C2'-C1'-N1-C6
3	5	4500	PSU	C4'-C5'-O5'-P
3	5	1677	PSU	O4'-C1'-C5-C4
3	5	4296	B8H	O4'-C1'-C5-C4
3	5	4450	PSU	O4'-C1'-C5-C4
6	9	1243	PSU	C3'-C4'-C5'-O5'
3	5	1883	OMG	O4'-C4'-C5'-O5'
3	5	3729	PSU	C3'-C4'-C5'-O5'
3	5	4571	A2M	C1'-C2'-O2'-CM'
3	5	3909	OMC	C2'-C1'-N1-C2
3	5	1534	A2M	O4'-C4'-C5'-O5'
6	9	1806	M7A	C2'-C1'-N9-C8
3	5	2297	E7G	C72-C71-N7-C8
3	5	4636	PSU	O4'-C1'-C5-C6
44	m	72	MLZ	CG-CD-CE-NZ
3	5	4371	MHG	O4'-C1'-N9-C8
3	5	2754	B9B	C4'-C5'-O5'-P
3	5	2422	OMC	O4'-C4'-C5'-O5'
3	5	4636	PSU	O4'-C4'-C5'-O5'
6	9	1806	M7A	O4'-C4'-C5'-O5'
3	5	1659	I4U	C42-C41-O4-C4
3	5	4671	B8T	C4'-C5'-O5'-P
3	5	729	2MG	O4'-C4'-C5'-O5'
3	5	3782	5MC	C3'-C4'-C5'-O5'
3	5	4415	1MA	C3'-C4'-C5'-O5'
6	9	1703	OMC	C3'-C4'-C5'-O5'
3	5	3887	OMC	C4'-C5'-O5'-P
6	9	644	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 304 ligands modelled in this entry, 303 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
81	MQ6	5	5296	-	39,42,42	1.49	5 (12%)	38,65,65	1.76	6 (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
81	MQ6	5	5296	-	-	10/26/73/73	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5296	MQ6	O37-C06	-4.94	1.33	1.43
81	5	5296	MQ6	C16-C15	3.44	1.59	1.54
81	5	5296	MQ6	C05-C06	3.20	1.59	1.54
81	5	5296	MQ6	C07-C06	-2.70	1.50	1.53
81	5	5296	MQ6	O38-C02	-2.11	1.39	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	5	5296	MQ6	O37-C06-C07	5.83	123.04	109.40
81	5	5296	MQ6	O14-C12-C06	5.39	121.28	111.27
81	5	5296	MQ6	C23-C22-C21	-3.05	112.69	119.42
81	5	5296	MQ6	O14-C12-O13	-2.88	118.78	123.97
81	5	5296	MQ6	C28-C29-N25	2.62	107.74	103.95
81	5	5296	MQ6	C20-C21-C22	-2.25	117.50	121.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	5	5296	MQ6	C04-C05-C06-C07
81	5	5296	MQ6	C04-C05-C06-O37

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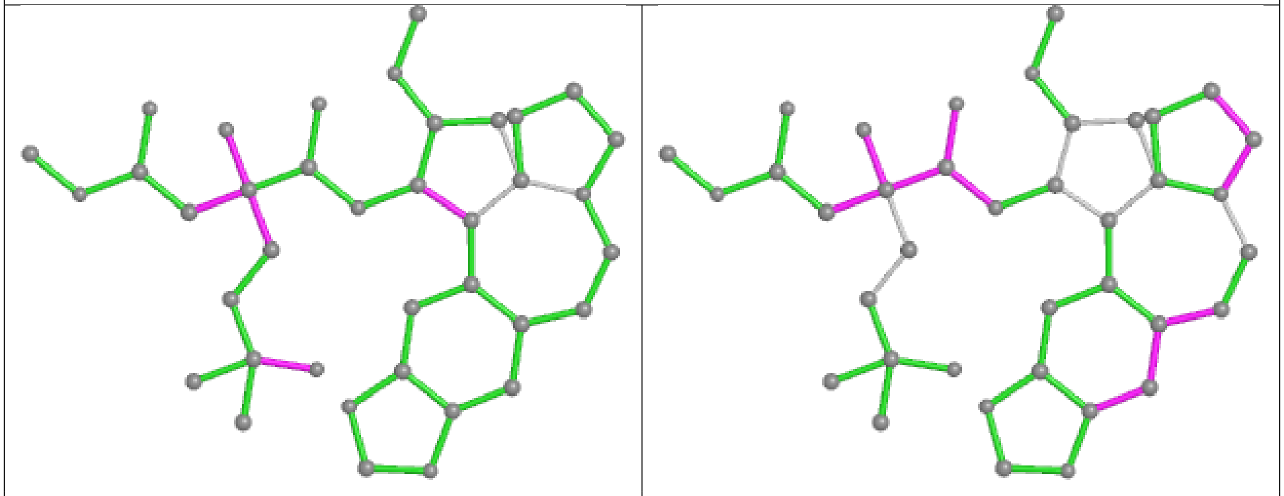
Mol	Chain	Res	Type	Atoms
81	5	5296	MQ6	C15-C31-O32-C33
81	5	5296	MQ6	C30-C31-O32-C33
81	5	5296	MQ6	C12-C06-C07-C08
81	5	5296	MQ6	C04-C05-C06-C12
81	5	5296	MQ6	C01-C02-C04-C05
81	5	5296	MQ6	C03-C02-C04-C05
81	5	5296	MQ6	O38-C02-C04-C05
81	5	5296	MQ6	C02-C04-C05-C06

There are no ring outliers.

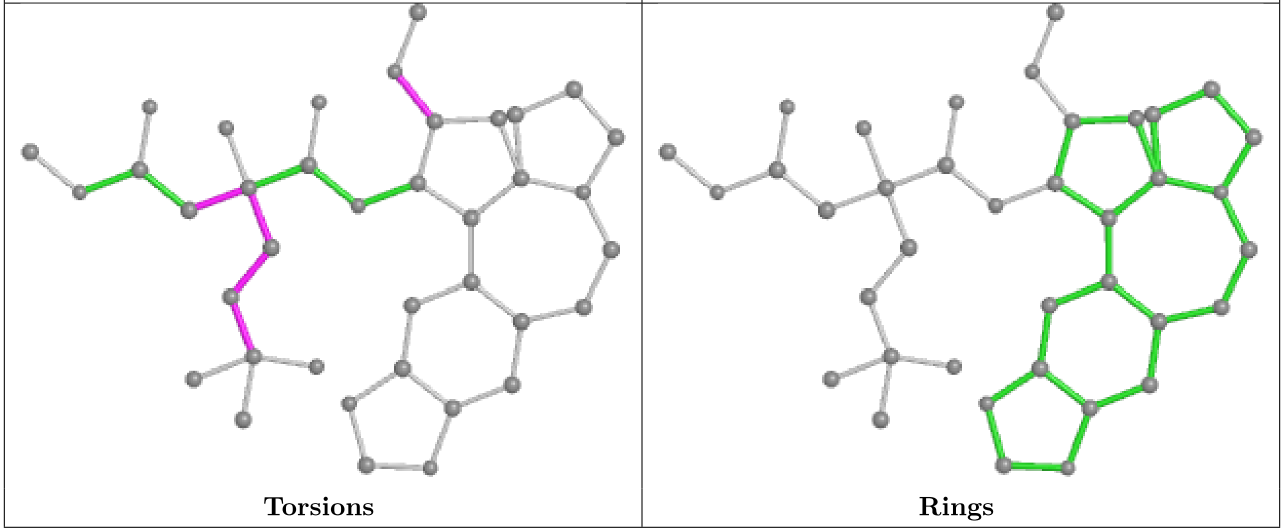
No monomer is involved in short contacts.

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 then 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.

Ligand MQ6 5 5296



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	5	25
6	9	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.42
1	5	1252:C	O3'	1271:G	P	35.84
1	5	1219:G	O3'	1233:G	P	19.81
1	5	4101:C	O3'	4107:G	P	18.15
1	9	1761:U	O3'	1771:G	P	17.60
1	5	523:C	O3'	638:G	P	17.44
1	9	834:C	O3'	841:G	P	17.26
1	9	756:C	O3'	788:G	P	17.08
1	5	1407:G	O3'	1410:C	P	16.49
1	9	323:C	O3'	329:G	P	16.48
1	5	3949:A	O3'	4060:U	P	16.31
1	5	4138:C	O3'	4146:G	P	16.23
1	9	1417:C	O3'	1423:C	P	16.19
1	5	990:U	O3'	1064:G	P	16.14
1	5	1696:C	O3'	1720:C	P	16.01
1	5	4777:C	O3'	4859:C	P	15.94
1	9	697:G	O3'	729:C	P	15.79
1	9	130:G	O3'	140:U	P	15.56
1	5	1969:G	O3'	2017:A	P	15.32
1	5	5022:U	O3'	5028:G	P	14.28
1	5	760:G	O3'	904:C	P	14.21
1	5	2901:G	O3'	3597:G	P	13.99
1	5	1364:U	O3'	1368:A	P	13.57
1	5	182:G	O3'	189:G	P	9.46
1	5	4729:A	O3'	4735:G	P	9.42
1	5	1180:C	O3'	1183:C	P	9.32
1	9	225:G	O3'	287:U	P	8.77
1	5	500:G	O3'	504:G	P	5.54
1	9	745:C	O3'	749:U	P	5.36
1	5	512:U	O3'	515:C	P	5.06
1	9	736:C	O3'	743:U	P	5.06
1	9	1432:U	O3'	1438:A	P	4.44
1	5	1100:U	O3'	1168:G	P	4.09
1	5	4740:G	O3'	4743:G	P	3.98
1	5	4899:G	O3'	4902:C	P	3.55
1	5	1239:G	O3'	1244:G	P	3.53

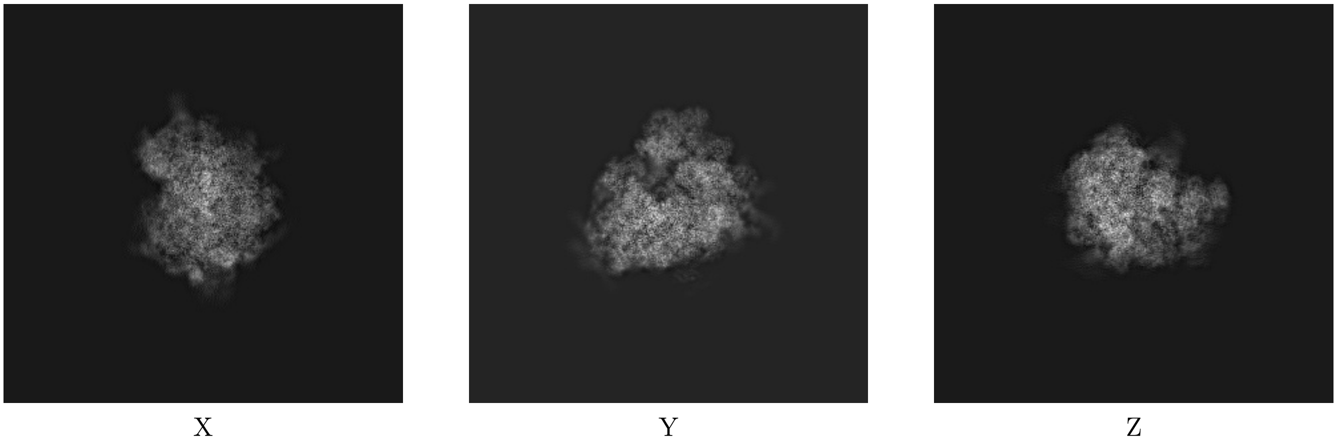
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-26444. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

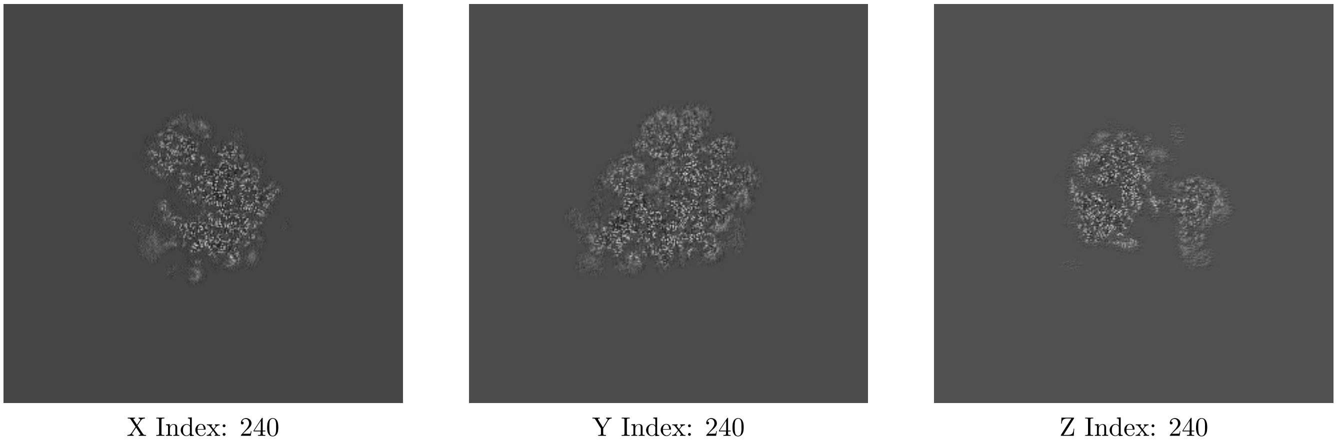
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

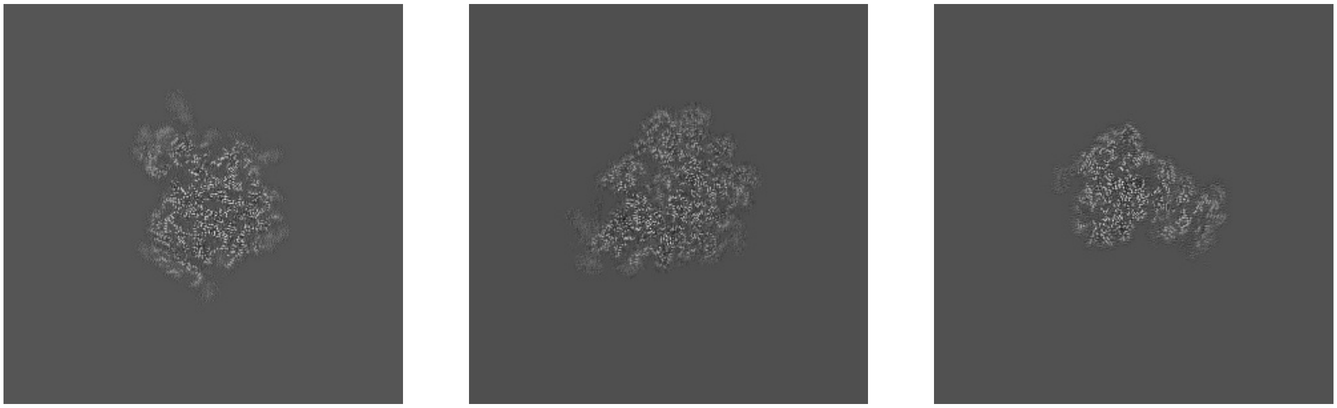
6.2.1 Primary map


X Index: 240 Y Index: 240 Z Index: 240

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

6.3 Largest variance slices

6.3.1 Primary map

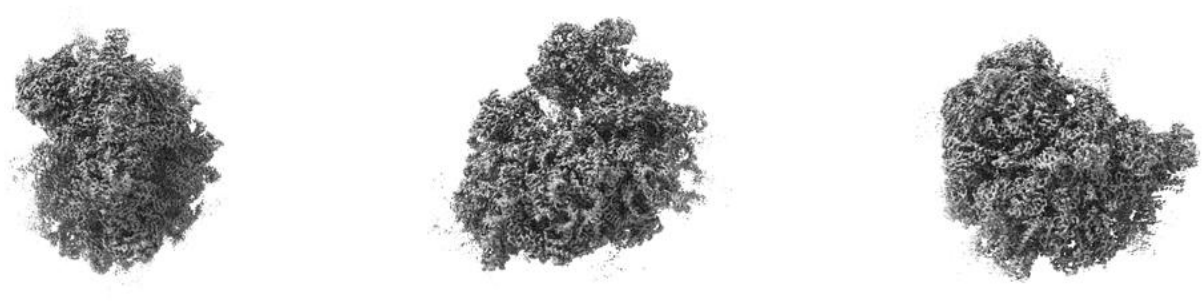


X Index: 218 Y Index: 242 Z Index: 254

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

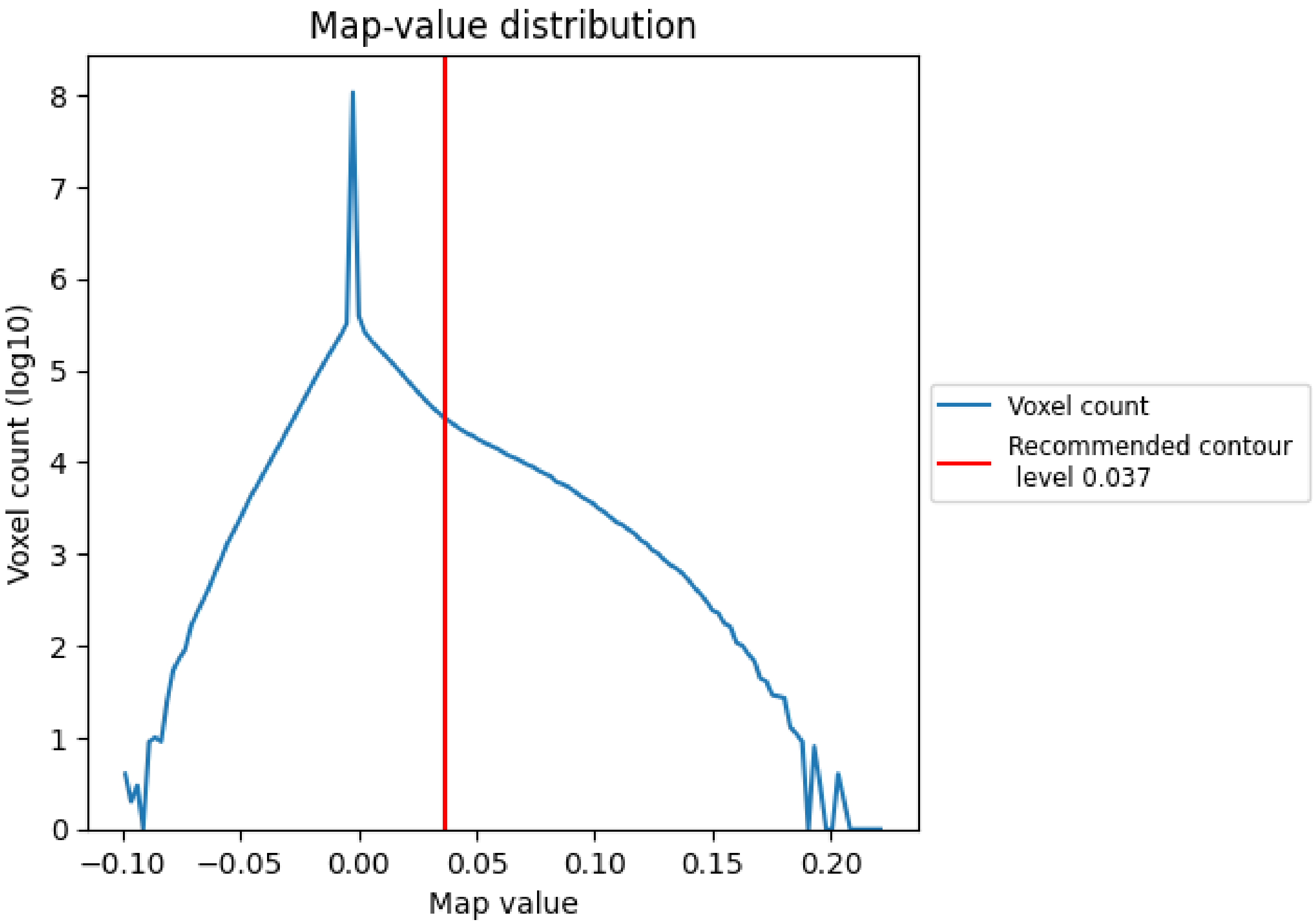
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

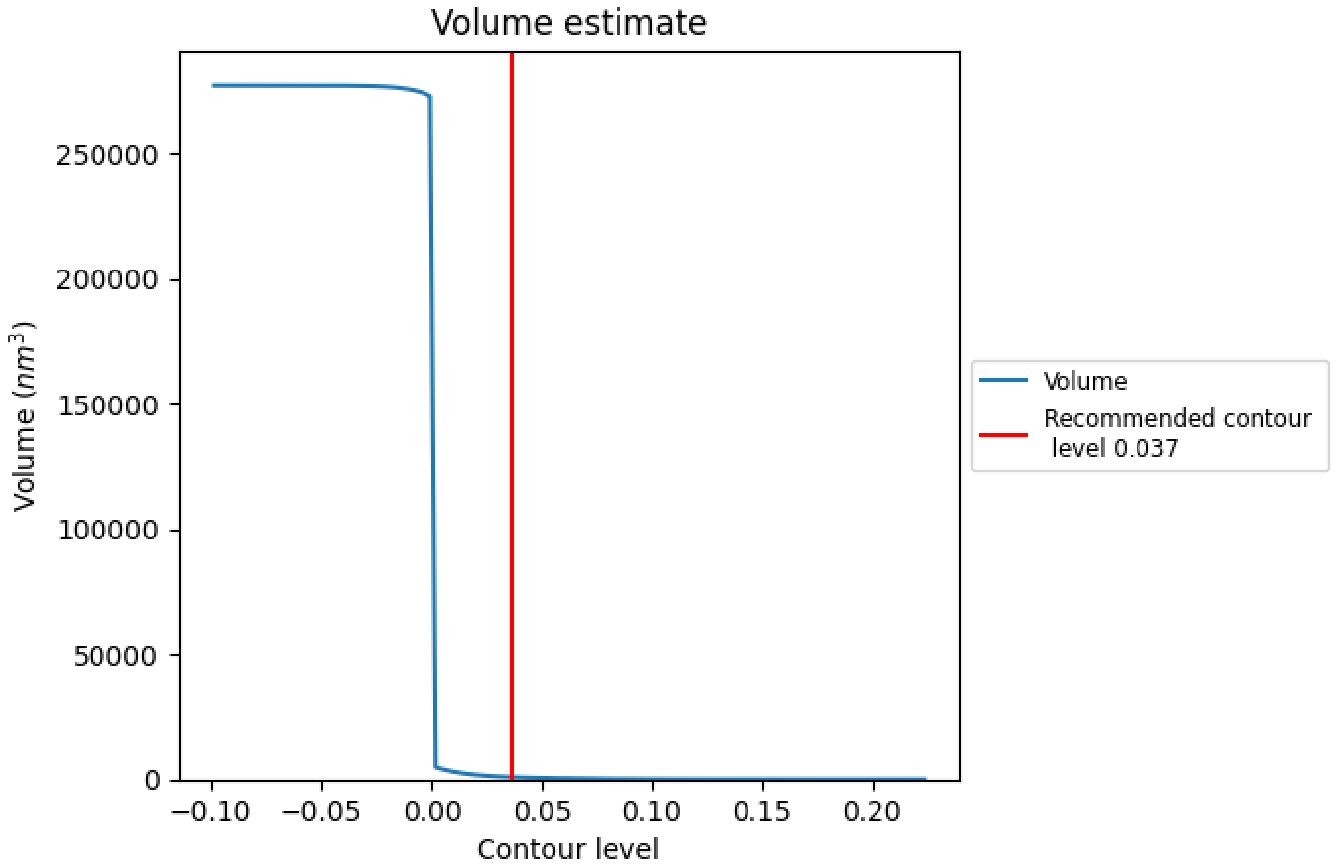
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

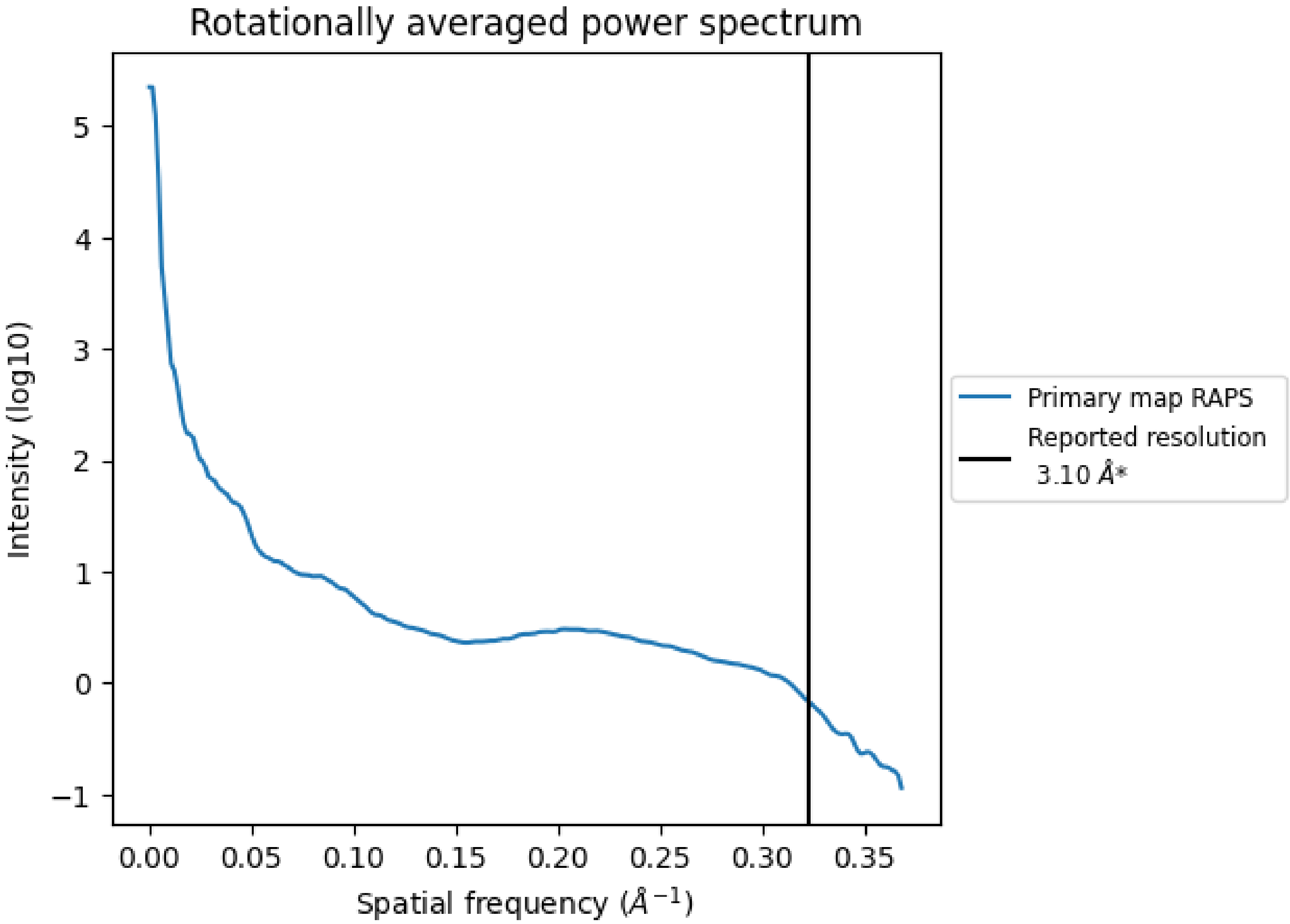
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 860 nm^3; this corresponds to an approximate mass of 777 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 0.323 Å^{-1}

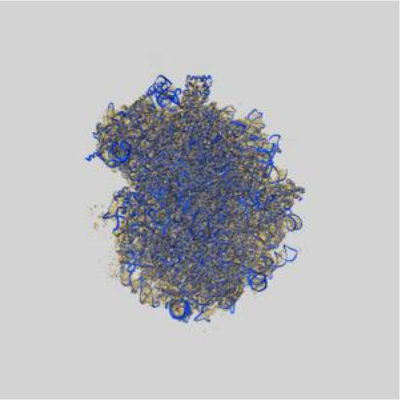
8 Fourier-Shell correlation

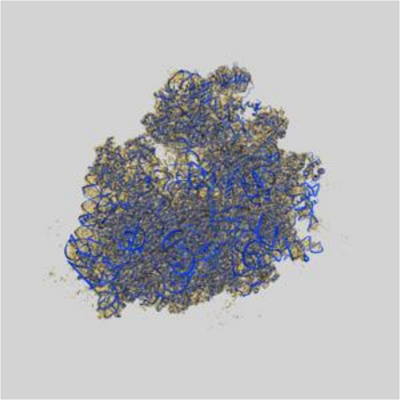
This section was not generated. No FSC curve or half-maps provided.

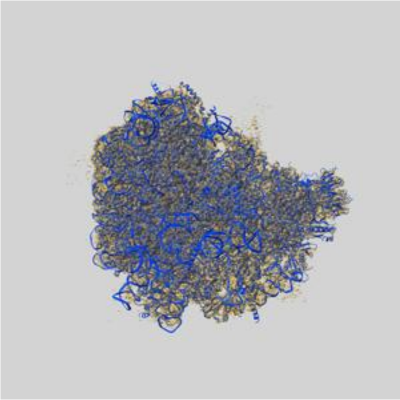
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26444 and PDB model 7UCJ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay

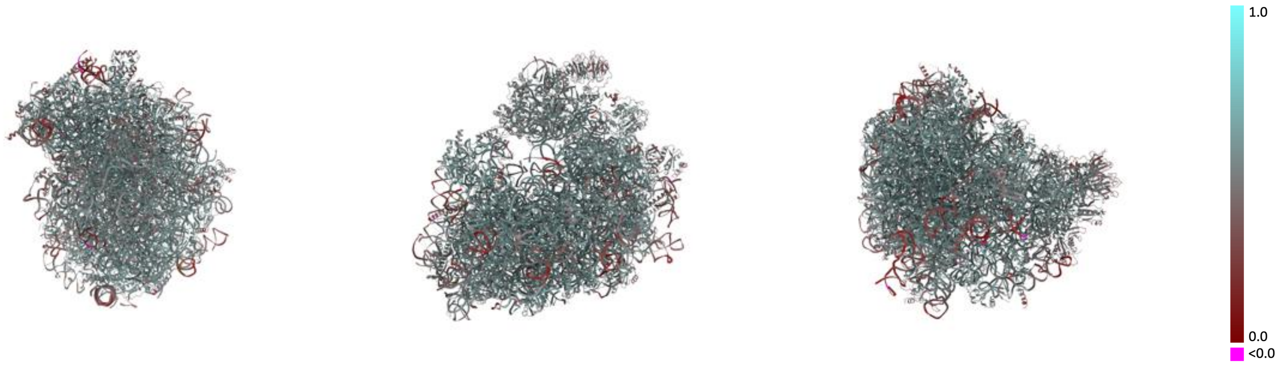

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.037 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.

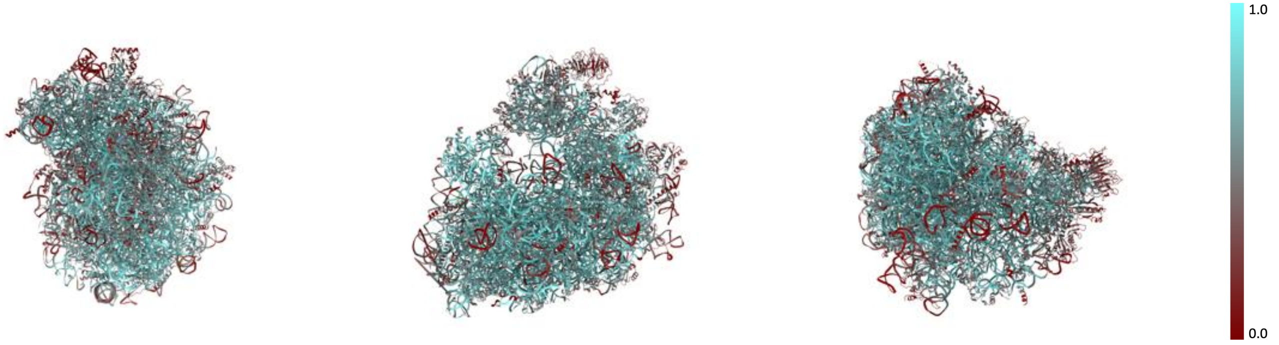
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according 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.

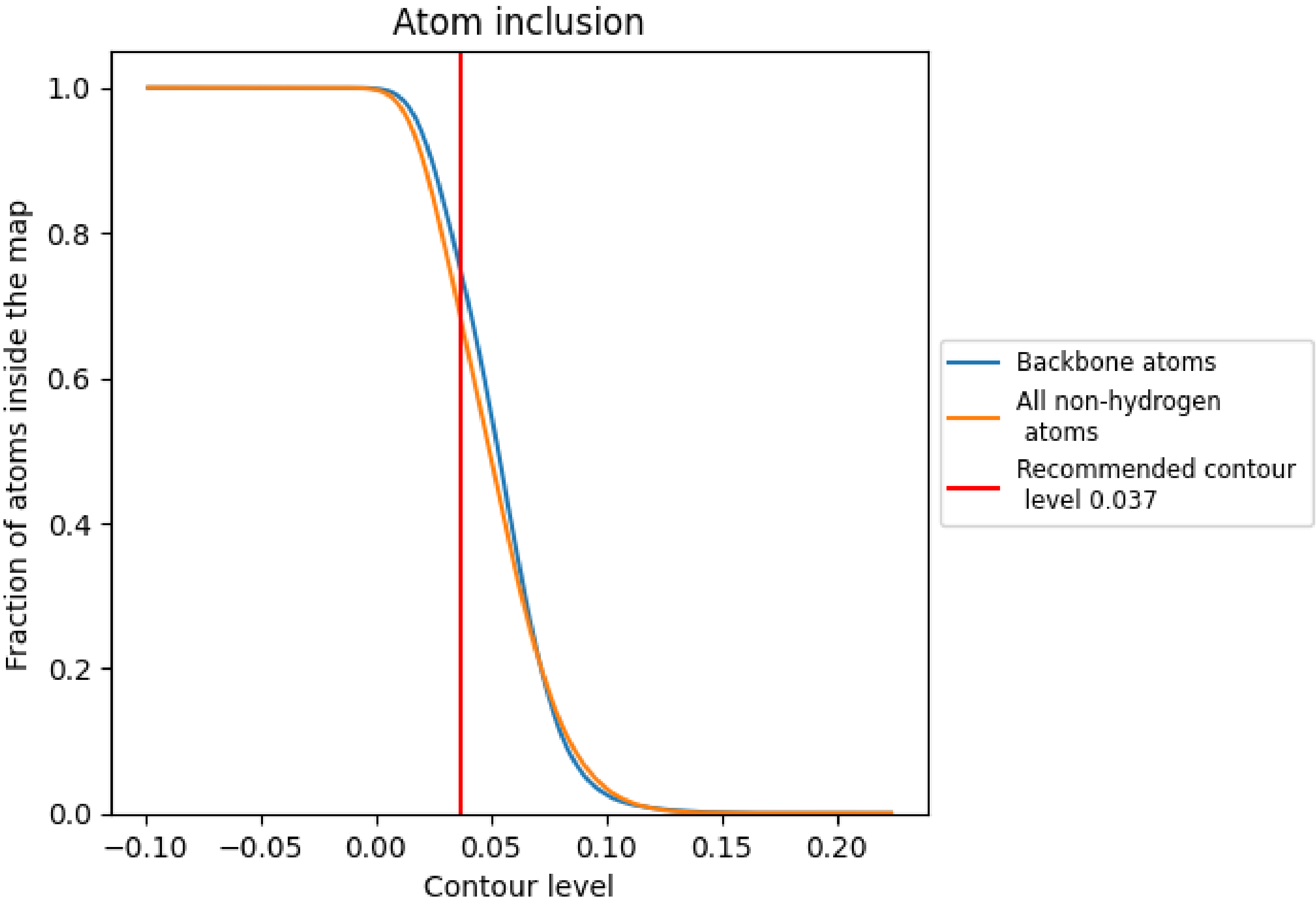
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.037).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6801	0.5390
1	0.5692	0.5540
2	0.3911	0.4900
5	0.7638	0.5420
7	0.8752	0.5830
8	0.7924	0.5570
9	0.7123	0.5210
A	0.7135	0.5930
AA	0.5734	0.5400
Aa	0.6343	0.5590
B	0.6818	0.5770
BB	0.5763	0.5470
Bb	0.5164	0.5230
C	0.7005	0.5780
CC	0.6057	0.5560
Cc	0.4468	0.4960
D	0.6535	0.5540
DD	0.3960	0.4800
Dd	0.5995	0.5400
E	0.6216	0.5500
EE	0.5590	0.5380
Ee	0.4343	0.4930
F	0.7244	0.5820
FF	0.5094	0.5200
G	0.5107	0.5170
GG	0.3876	0.4690
Gg	0.2936	0.4390
H	0.5913	0.5520
HH	0.3785	0.4890
I	0.6601	0.5690
II	0.5817	0.5430
J	0.5854	0.5320
JJ	0.5713	0.5290
KK	0.3380	0.4390
L	0.6132	0.5460

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Chain	Atom inclusion	Q-score
LL	0.6377	0.5690
M	0.6524	0.5510
N	0.7403	0.5920
NN	0.6338	0.5570
O	0.6886	0.5720
OO	0.6079	0.5570
P	0.7042	0.5840
PP	0.4135	0.4740
Q	0.7062	0.5890
QQ	0.5037	0.5210
R	0.6190	0.5560
RR	0.3863	0.4940
S	0.6868	0.5760
SS	0.4795	0.4940
T	0.6405	0.5630
TT	0.4822	0.5130
U	0.4974	0.5010
UU	0.3450	0.4750
V	0.6639	0.5830
VV	0.5113	0.5390
W	0.5689	0.5390
WW	0.6416	0.5680
X	0.6106	0.5530
XX	0.6022	0.5680
Y	0.6364	0.5520
YY	0.5178	0.5120
Z	0.6179	0.5560
ZZ	0.4271	0.4790
a	0.7484	0.5910
b	0.5252	0.5220
c	0.6519	0.5680
d	0.6371	0.5630
e	0.7030	0.5920
f	0.7363	0.5900
g	0.6395	0.5590
h	0.5955	0.5410
i	0.5905	0.5380
j	0.7429	0.5940
k	0.4596	0.4890
l	0.6276	0.5630
m	0.6757	0.5600
n	0.6376	0.5840

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Chain	Atom inclusion	Q-score
o	▬ 0.6548	▬ 0.5840
p	▬ 0.6662	▬ 0.5780
r	▬ 0.7168	▬ 0.5840