Full wwPDB EM Validation Report ⓘ

Dec 21, 2023 – 12:43 PM EST

PDB ID	:	8SCB
EMDB ID	:	EMD-40344
Title	:	Terminating ribosome with SRI-41315
Authors	:	Yip, M.C.J.; Coelho, J.P.L.; Oltion, K.; Tauton, J.; Shao, S.
Deposited on	:	2023-04-05
Resolution	:	2.50 Å(reported)

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

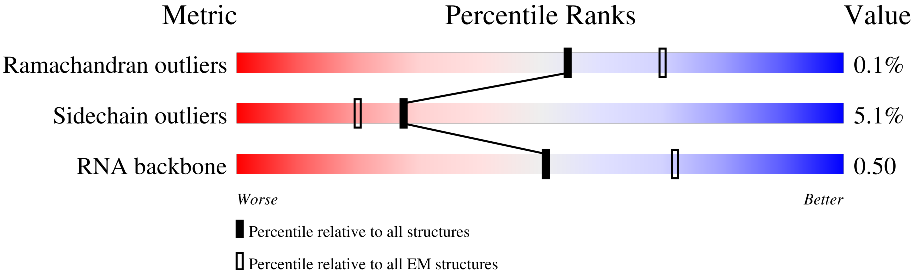
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

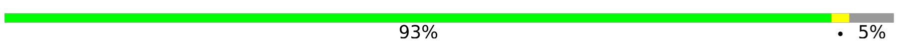
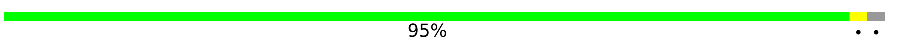
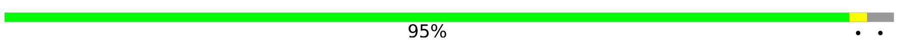
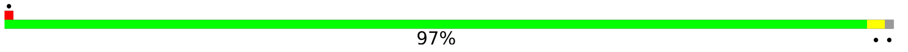
The reported resolution of this entry is 2.50 Å.

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	A	257	
2	B	403	
3	C	413	
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	

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Mol	Chain	Length	Quality of chain
9	I	214	93% • 5%
10	J	178	89% • 6%
11	L	211	• 96% •
12	M	218	• 63% 37%
13	N	204	98% •
14	O	203	93% • •
15	P	184	81% • 17%
16	Q	188	97% • •
17	R	196	5% 88% • 9%
18	S	176	97% •
19	T	160	• 99% •
20	U	128	73% • 23%
21	V	140	92% • 7%
22	W	157	• 39% • 60%
23	X	156	73% • 26%
24	Y	145	• 89% • 8%
25	Z	136	94% 5% •
26	a	148	96% • •
27	b	245	• 30% • 69%
28	c	115	76% 6% 18%
29	d	125	• 79% • 20%
30	e	135	94% • 5%
31	f	110	98% ••
32	g	117	• 94% • •
33	h	123	94% 5% •

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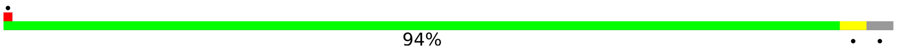
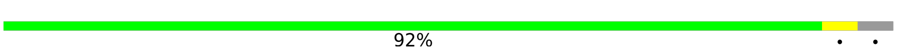
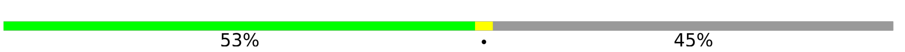
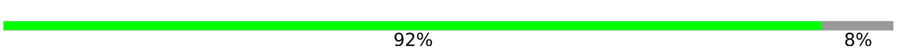
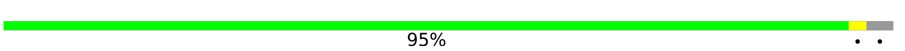
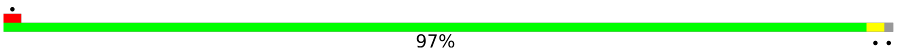
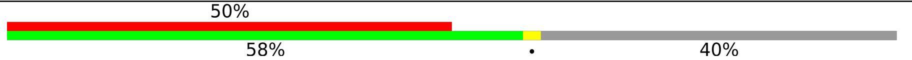
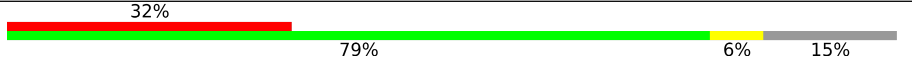
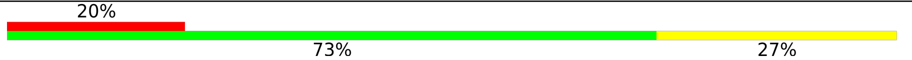
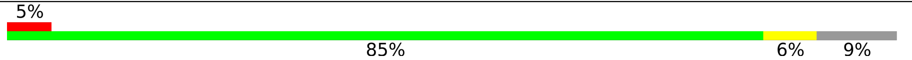
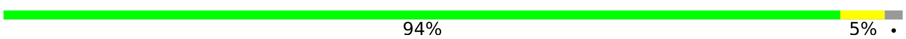
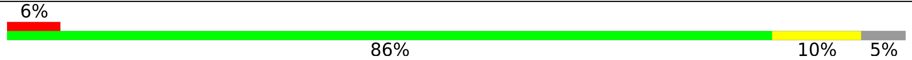
Mol	Chain	Length	Quality of chain
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	93	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	130	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	

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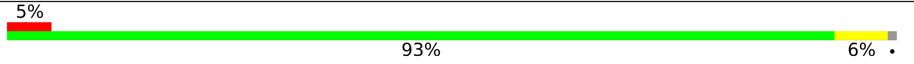
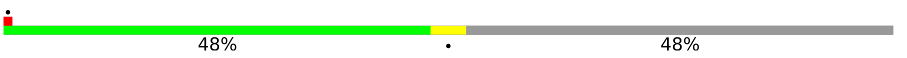
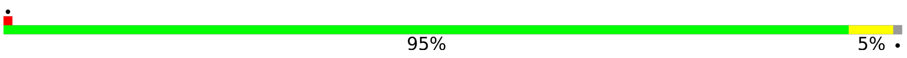
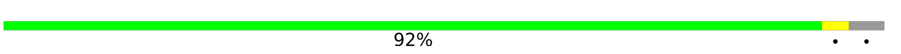
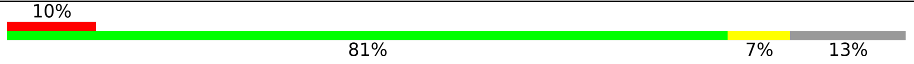
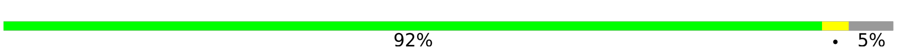
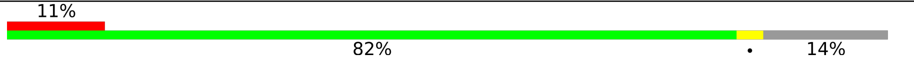
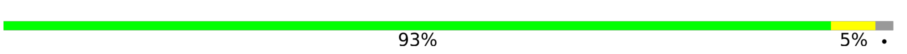
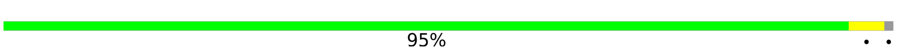
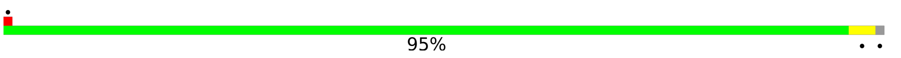
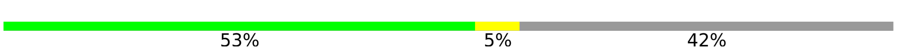
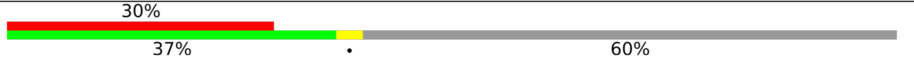
Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	

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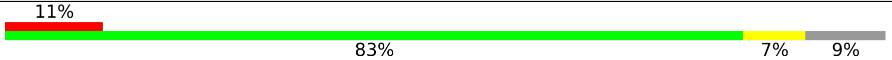
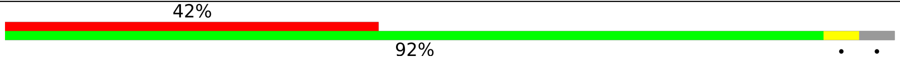
Mol	Chain	Length	Quality of chain
84	gg	317	
85	hh	197	
86	ii	459	
87	jj	599	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
90	ZVM	ii	501	X	-	-	-

2 Entry composition ⓘ

There are 92 unique types of molecules in this entry. The entry contains 222478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	244	1868	1171	382	309	6	0	0

- Molecule 2 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	394	3148	2007	591	537	13	0	0

- Molecule 3 is a protein called 60S ribosomal protein L4.

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

- Molecule 4 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	289	2361	1495	431	421	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1726	1110	327	286	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L7.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	218	1768	1127	341	296	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called 60S ribosomal protein L9.

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

- Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	204	1655	1051	319	272	13	0	0

- Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	167	1336	846	249	235	6	0	0

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called 60S ribosomal protein L14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	198	1621	1046	317	253	5	0	0

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called Ribosomal protein L18.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	4	ASP	ASN	conflict	UNP G1TFE0
Q	14	ARG	TRP	conflict	UNP G1TFE0
Q	53	MET	LEU	conflict	UNP G1TFE0
Q	58	ARG	TRP	conflict	UNP G1TFE0
Q	75	ARG	GLN	conflict	UNP G1TFE0
Q	80	ALA	PRO	conflict	UNP G1TFE0
Q	86	VAL	ILE	conflict	UNP G1TFE0
Q	104	ARG	HIS	conflict	UNP G1TFE0
Q	110	ARG	CYS	conflict	UNP G1TFE0
Q	137	VAL	GLY	conflict	UNP G1TFE0
Q	157	GLY	ARG	conflict	UNP G1TFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 17 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	179	Total 1502	C 930	N 327	O 236	S 9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	CYS	conflict	UNP G1TJR3
R	64	ARG	GLN	conflict	UNP G1TJR3
R	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	LEU	VAL	conflict	UNP G1TSG1
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	60	VAL	ALA	conflict	UNP G1TSG1
U	62	SER	THR	conflict	UNP G1TSG1
U	63	LEU	ILE	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1
U	106	THR	SER	conflict	UNP G1TSG1
U	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 21 is a protein called Ribosomal protein L23.

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

- Molecule 22 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	63	528	337	103	85	3	0	0

- Molecule 23 is a protein called eL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	116	949	606	178	164	1	0	0

- Molecule 24 is a protein called uL24.

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

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

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

- Molecule 26 is a protein called 60S ribosomal protein L27a.

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

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	464	130	132	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	100	Total	C	N	O	S	0	0
			833	530	163	138	2		

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called 60S ribosomal protein L34.

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

- Molecule 33 is a protein called eL35.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	68	559	360	101	97	1	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	49	438	280	95	62	1	0	0

- Molecule 38 is a protein called Ubiquitin A-52 residue ribosomal protein fusion product 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	51	421	260	89	66	6	0	0

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	23	222	134	61	25	2	0	0

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	r	125	1001	621	206	168	6	0	0

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	s	190	1461	931	255	266	9	0	0

- Molecule 44 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	t	141	1059	662	195	199	3	0	0

- Molecule 45 is a protein called NC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	1	15	125	82	20	22	1	0	0

- Molecule 46 is a RNA chain called P_tRNA.

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

- Molecule 47 is a RNA chain called E_tRNA.

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

- Molecule 48 is a RNA chain called 28S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	5	3530	75735	33780	13869	24556	3530	0	0

- Molecule 49 is a RNA chain called 5S_rRNA.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 50 is a RNA chain called 5.8S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	8	156	3315	1481	585	1094	155	0	0

- Molecule 51 is a RNA chain called 18S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1692	Total 36134	C 16163	N 6486	O 11794	P 1691	0	0

- Molecule 52 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	206	Total 1624	C 1035	N 287	O 294	S 8	0	0

- Molecule 53 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	212	Total 1722	C 1093	N 308	O 307	S 14	0	0

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	216	Total 1674	C 1085	N 286	O 294	S 9	0	0

- Molecule 55 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	221	Total 1723	C 1098	N 311	O 307	S 7	0	0

- Molecule 56 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	259	Total 2059	C 1316	N 383	O 352	S 8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17
EE	51	ARG	LYS	conflict	UNP G1TK17
EE	78	THR	ALA	conflict	UNP G1TK17
EE	156	VAL	MET	conflict	UNP G1TK17

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	181	Total 1441	C 902	N 273	O 259	S 7	0	0

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	177	Total 1425	C 912	N 258	O 254	S 1	0	0

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	II	206	Total 1686	C 1058	N 332	O 291	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 61 is a protein called uS4.

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

- Molecule 62 is a protein called S10_plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	86	Total 729	C 479	N 127	O 118	S 5	0	0

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	LL	136	1123	717	210	190	6	0	0

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	MM	122	939	588	166	176	9	0	0

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	NN	150	1208	773	229	205	1	0	0

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	OO	127	957	585	189	177	6	0	0

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	PP	117	968	615	181	165	7	0	0

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	QQ	140	1117	710	211	193	3	0	0

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	RR	118	962	604	179	176	3	0	0

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SS	140	1162	731	234	196	1	0	0

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	TT	138	1075	674	206	192	3	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	UU	102	807	507	153	143	4	0	0

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	VV	81	617	380	114	118	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
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	YY	123	1006	637	197	167	5	0	0

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	ZZ	72	574	368	104	101	1	0	0

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	aa	98	781	486	161	129	5	0	0

There are 3 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
aa	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 79 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	bb	79	628	395	117	110	6	0	0

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	cc	61	479	292	95	90	2	0	0

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	dd	53	445	278	90	72	5	0	0

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	ee	47	380	231	86	62	1	0	0

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	ff	63	527	336	99	86	6	0	0

- Molecule 84 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	gg	304	2371	1496	414	449	12	0	0

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
85	hh	11	236	106	44	75	11	0	0

- Molecule 86 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	ii	416	3280	2087	559	623	11	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	expression tag	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495
ii	183	ALA	GLY	conflict	UNP P62495
ii	184	ALA	GLY	conflict	UNP P62495

- Molecule 87 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	578	Total 4558	C 2914	N 780	O 835	S 29	0	0

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A	2	Total 2	Mg 2	0
88	I	2	Total 2	Mg 2	0
88	N	1	Total 1	Mg 1	0
88	P	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	a	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms	AltConf
88	e	1	Total Mg 1 1	0
88	f	1	Total Mg 1 1	0
88	g	1	Total Mg 1 1	0
88	o	1	Total Mg 1 1	0
88	2	2	Total Mg 2 2	0
88	5	221	Total Mg 221 221	0
88	7	6	Total Mg 6 6	0
88	8	2	Total Mg 2 2	0
88	9	64	Total Mg 64 64	0
88	EE	1	Total Mg 1 1	0
88	LL	1	Total Mg 1 1	0
88	OO	1	Total Mg 1 1	0
88	XX	1	Total Mg 1 1	0
88	hh	1	Total Mg 1 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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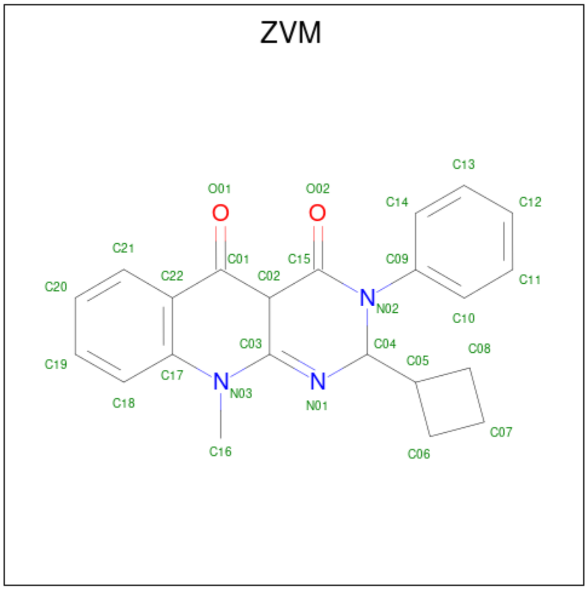
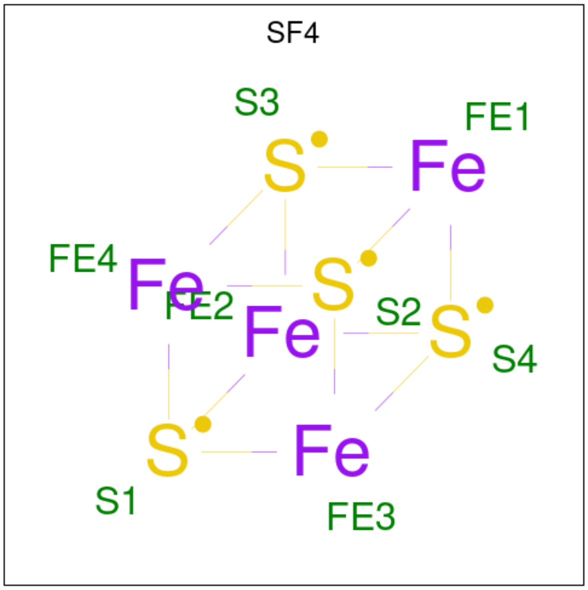
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
89	aa	1	1	1	0
			Total	Zn	
89	dd	1	1	1	0
			Total	Zn	
89	ff	1	1	1	0

- Molecule 90 is (2S,4aS)-2-cyclobutyl-10-methyl-3-phenyl-2,10-dihydropyrimido[4,5-b]quinoline-4,5(3H,4aH)-dione (three-letter code: ZVM) (formula: $C_{22}H_{21}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
90	ii	1	27	22	3	2	0

- Molecule 91 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
91	jj	1	Total Fe S 8 4 4	0
91	jj	1	Total Fe S 8 4 4	0

- Molecule 92 is water.

Mol	Chain	Residues	Atoms	AltConf
92	A	6	Total O 6 6	0
92	B	2	Total O 2 2	0
92	C	1	Total O 1 1	0
92	F	1	Total O 1 1	0
92	I	1	Total O 1 1	0
92	L	1	Total O 1 1	0
92	N	4	Total O 4 4	0
92	Q	1	Total O 1 1	0
92	R	1	Total O 1 1	0
92	V	2	Total O 2 2	0

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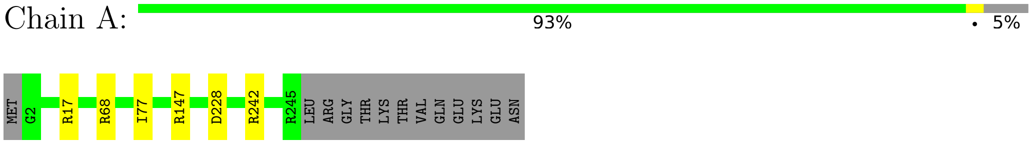
Mol	Chain	Residues	Atoms	AltConf
92	X	2	Total O 2 2	0
92	a	5	Total O 5 5	0
92	e	5	Total O 5 5	0
92	j	1	Total O 1 1	0
92	o	2	Total O 2 2	0
92	5	723	Total O 723 723	0
92	7	13	Total O 13 13	0
92	8	8	Total O 8 8	0
92	9	173	Total O 173 173	0
92	II	1	Total O 1 1	0
92	OO	1	Total O 1 1	0
92	XX	1	Total O 1 1	0
92	aa	1	Total O 1 1	0
92	ii	2	Total O 2 2	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.

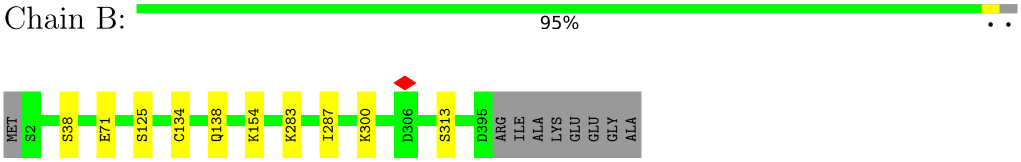
- Molecule 1: Ribosomal protein L8

Chain A:



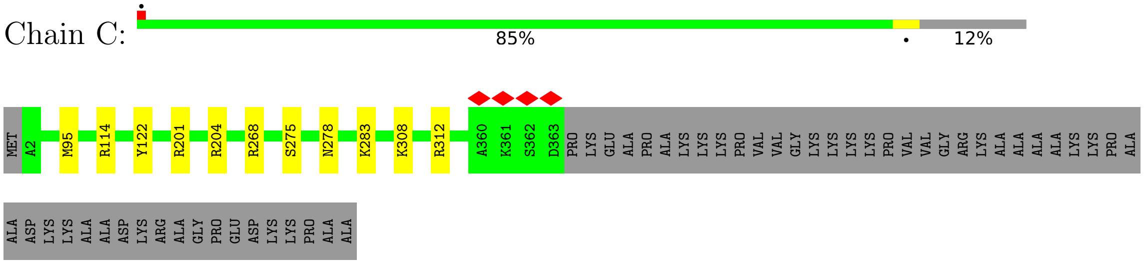
- Molecule 2: Ribosomal protein L3

Chain B:



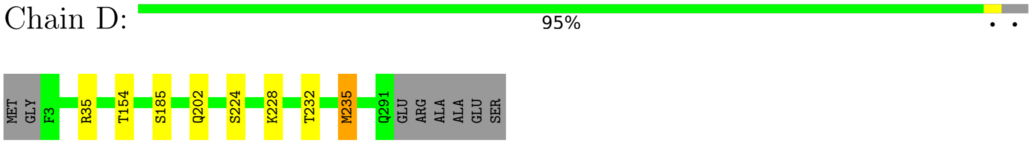
- Molecule 3: 60S ribosomal protein L4

Chain C:



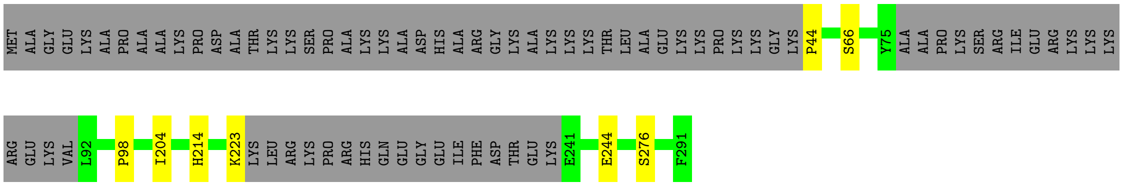
- Molecule 4: Ribosomal_L18_c domain-containing protein

Chain D:



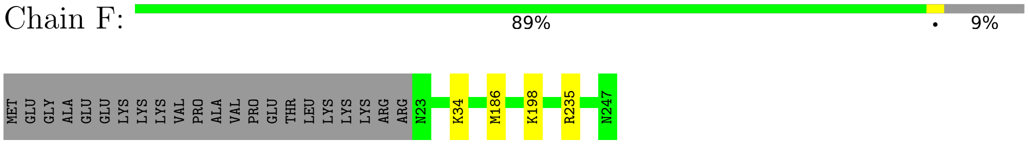
- Molecule 5: 60S ribosomal protein L6

Chain E:



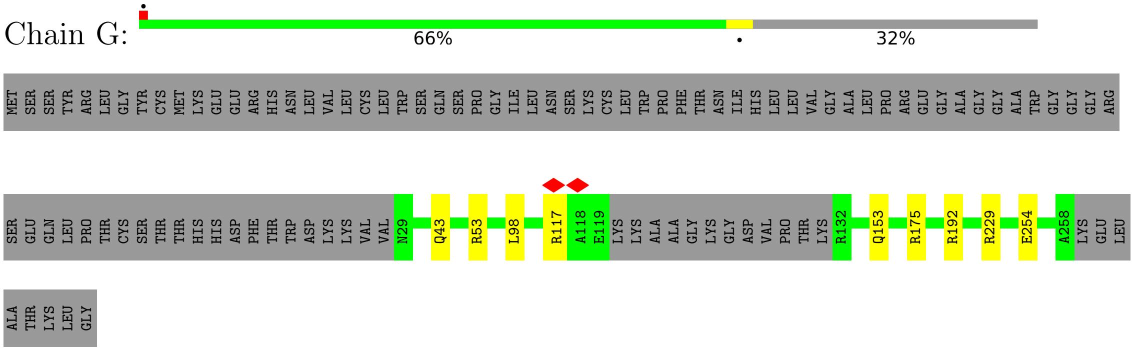
- Molecule 6: 60S ribosomal protein L7

Chain F:



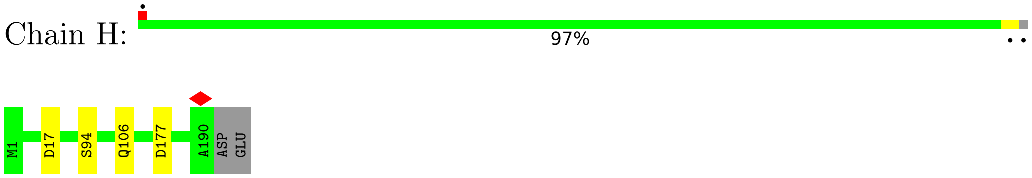
- Molecule 7: 60S ribosomal protein L7a

Chain G:



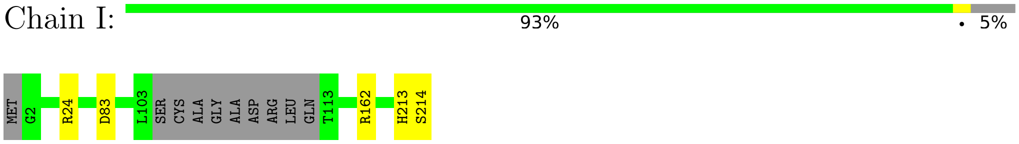
- Molecule 8: 60S ribosomal protein L9

Chain H:



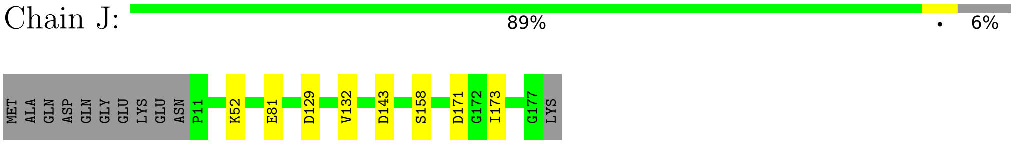
- Molecule 9: 60S ribosomal protein L10

Chain I:



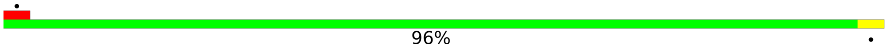
- Molecule 10: 60S ribosomal protein L11

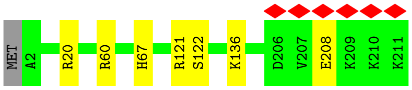
Chain J:



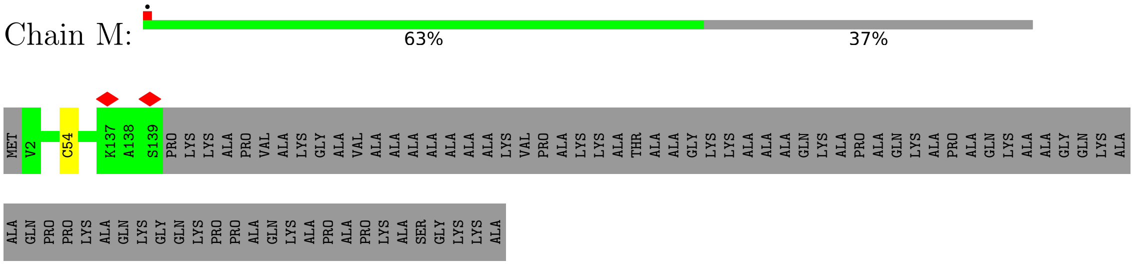
- Molecule 11: eL13

Chain L:

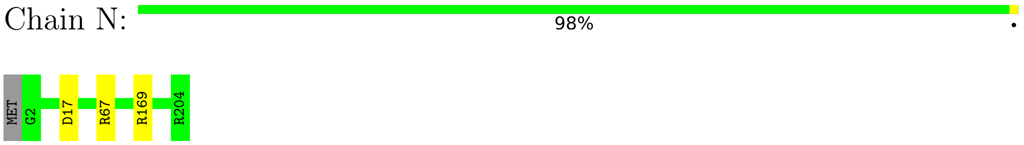




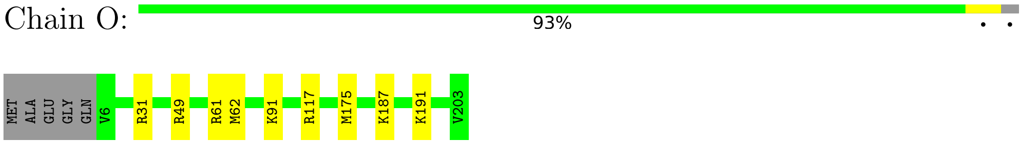
- Molecule 12: 60S ribosomal protein L14



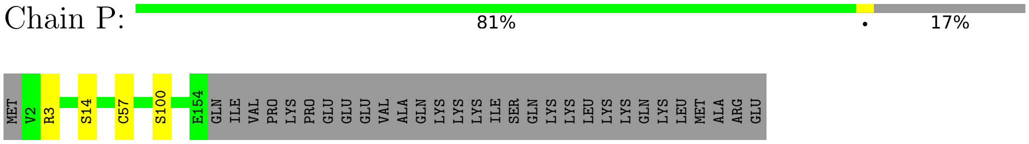
- Molecule 13: Ribosomal protein L15



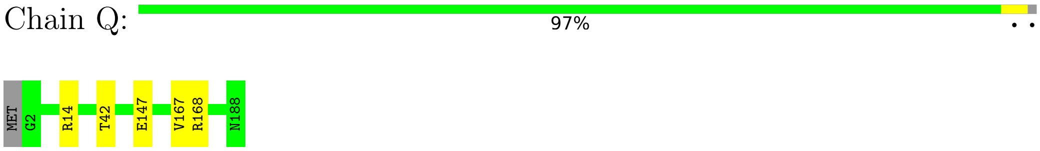
- Molecule 14: uL13



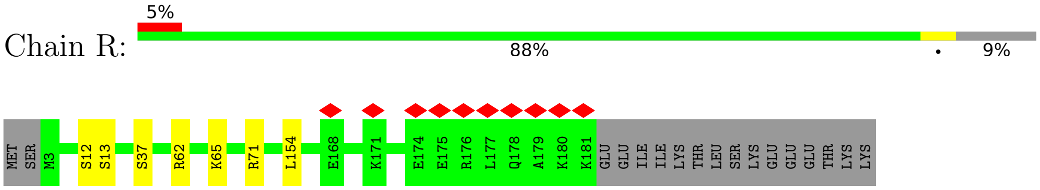
- Molecule 15: uL22



- Molecule 16: Ribosomal protein L18

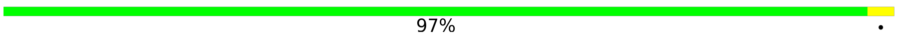


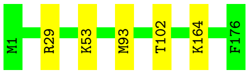
- Molecule 17: Ribosomal protein L19



- Molecule 18: eL20

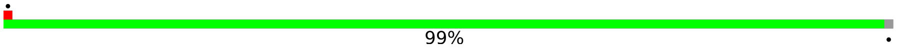
Chain S:

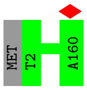




- Molecule 19: eL21

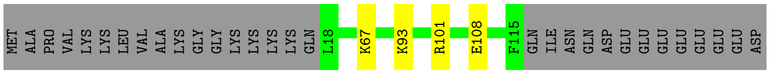
Chain T:





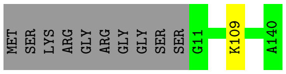
- Molecule 20: eL22

Chain U:



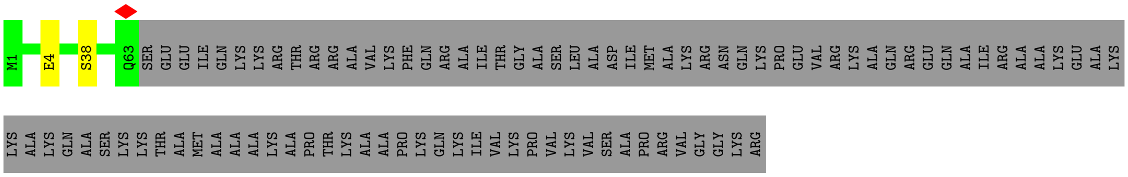
- Molecule 21: Ribosomal protein L23

Chain V:



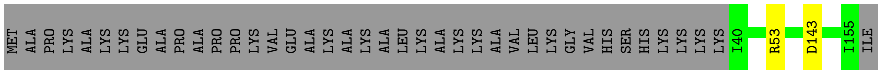
- Molecule 22: 60S ribosomal protein L24

Chain W:



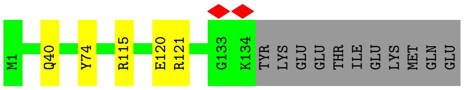
- Molecule 23: eL23

Chain X:

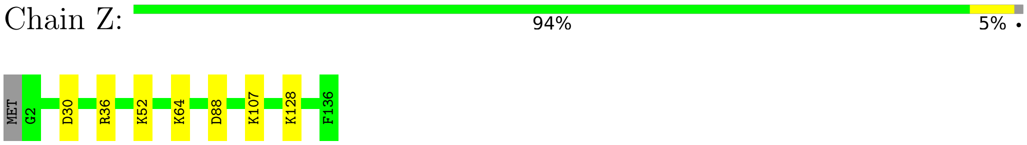


- Molecule 24: uL24

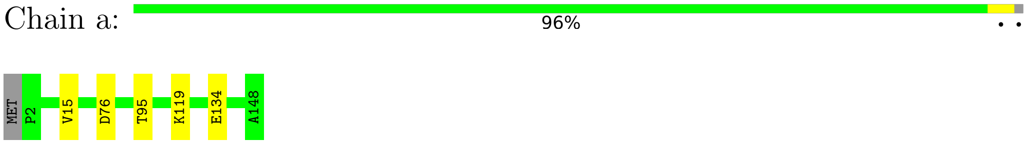
Chain Y:



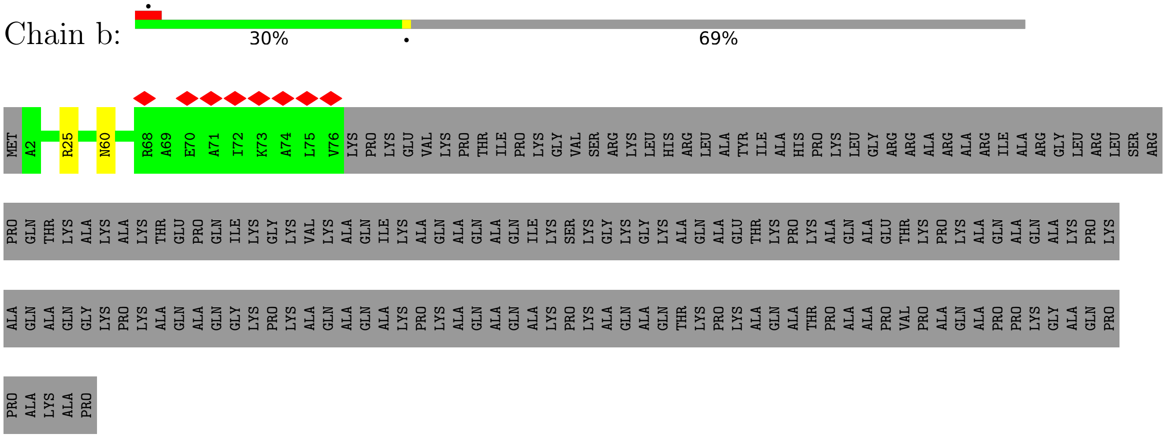
- Molecule 25: 60S ribosomal protein L27



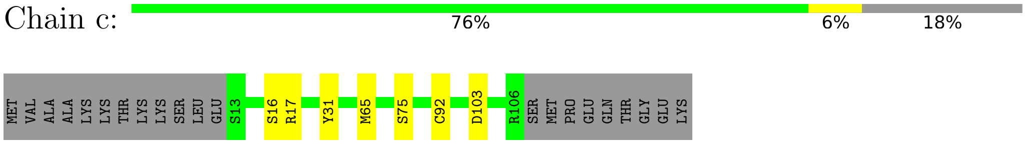
- Molecule 26: 60S ribosomal protein L27a



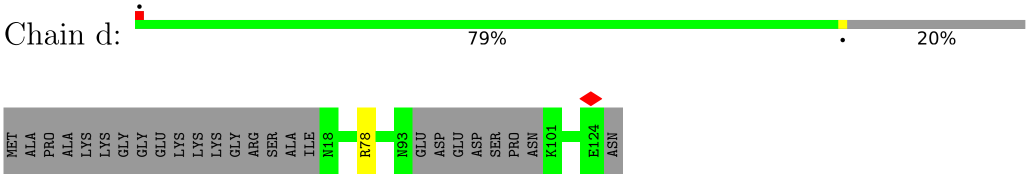
- Molecule 27: 60S ribosomal protein L29



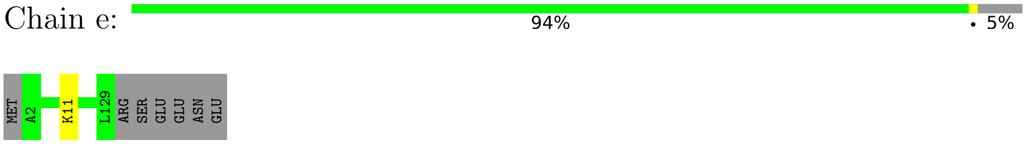
- Molecule 28: eL30



- Molecule 29: eL31

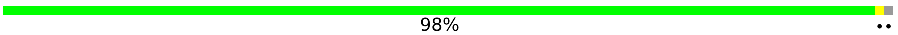


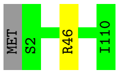
- Molecule 30: eL32



- Molecule 31: eL33

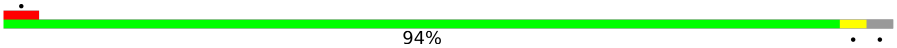
Chain f:

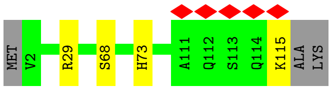




- Molecule 32: 60S ribosomal protein L34

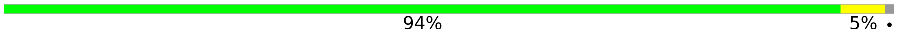
Chain g:

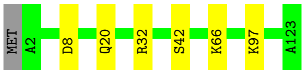




- Molecule 33: eL35

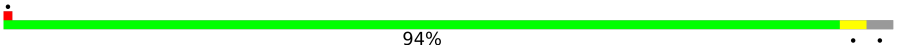
Chain h:

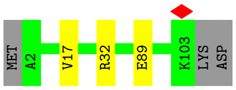




- Molecule 34: 60S ribosomal protein L36

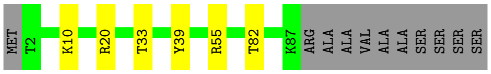
Chain i:





- Molecule 35: Ribosomal protein L37

Chain j:

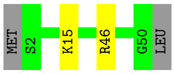


- Molecule 36: 60S ribosomal protein L38

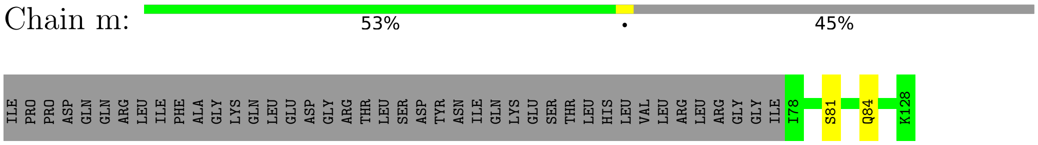
Chain k:

- Molecule 37: eL39

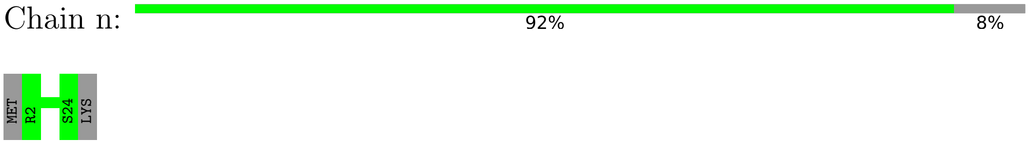
Chain l:



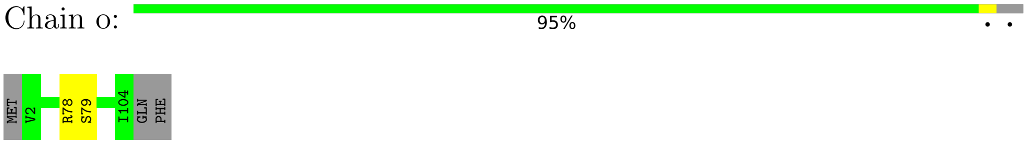
- Molecule 38: Ubiquitin A-52 residue ribosomal protein fusion product 1



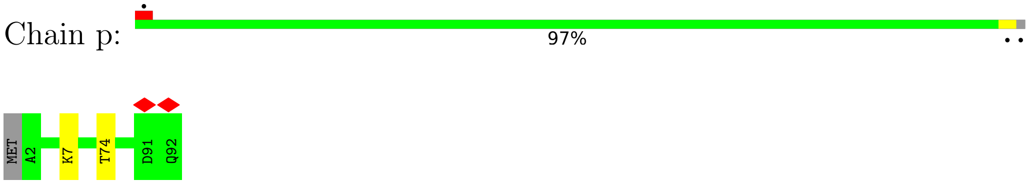
- Molecule 39: eL41



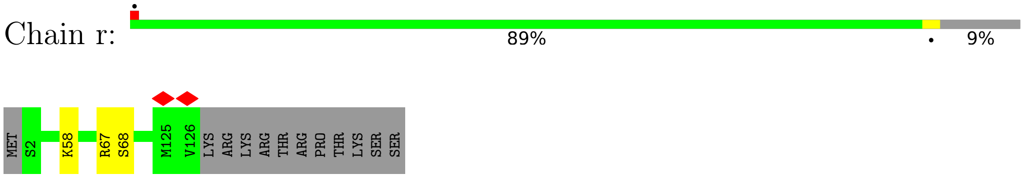
- Molecule 40: eL42



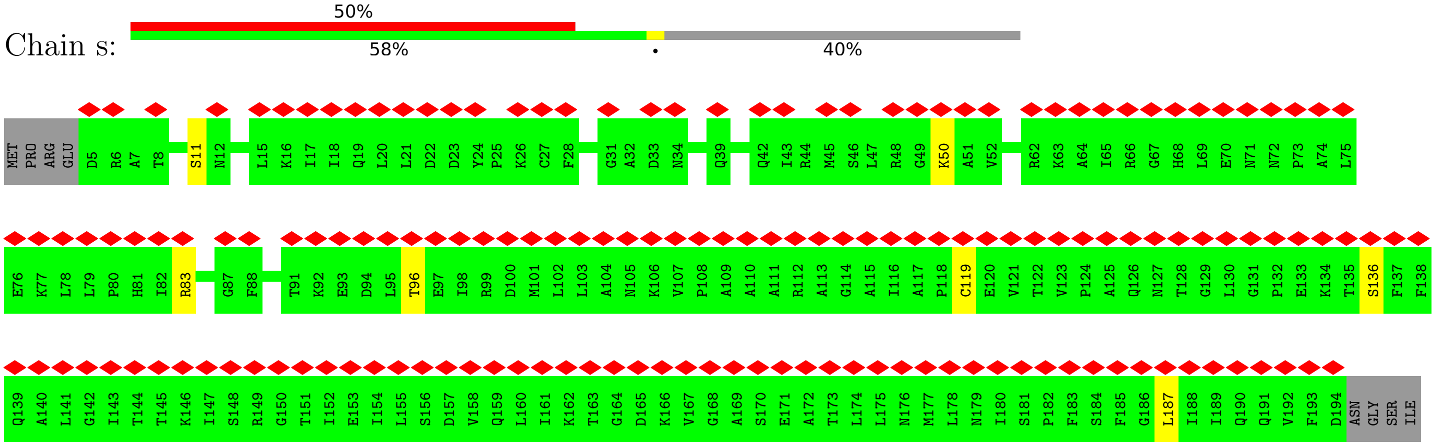
- Molecule 41: eL43

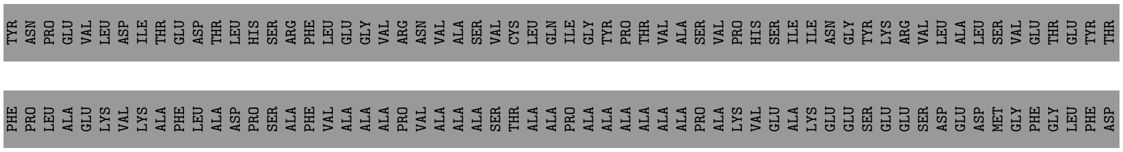


- Molecule 42: eL28



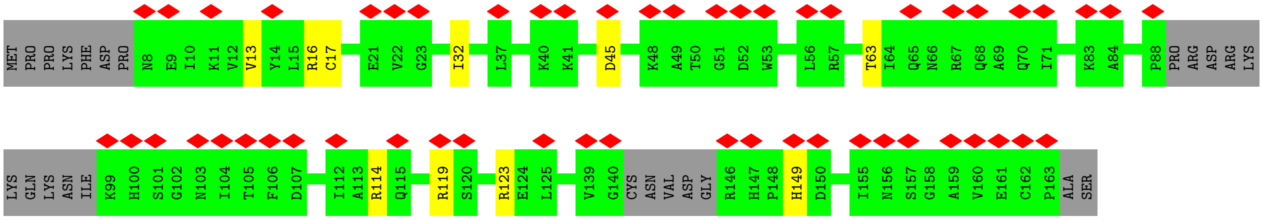
- Molecule 43: 60S acidic ribosomal protein P0





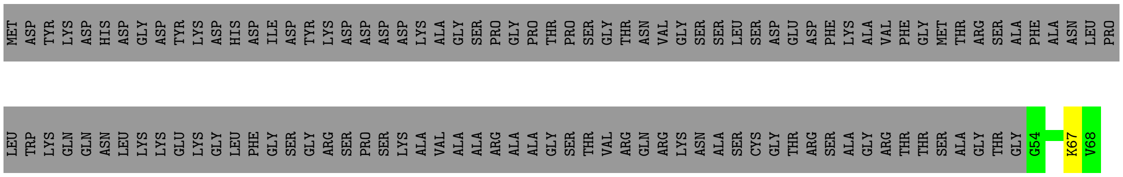
- Molecule 44: 60S ribosomal protein L12

Chain t:



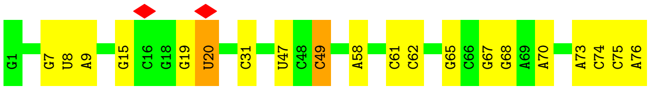
- Molecule 45: NC

Chain 1:



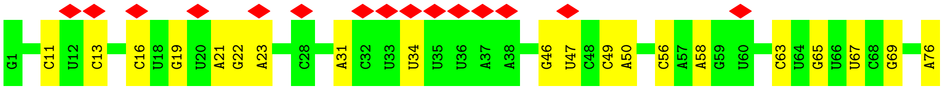
- Molecule 46: P_tRNA

Chain 2:



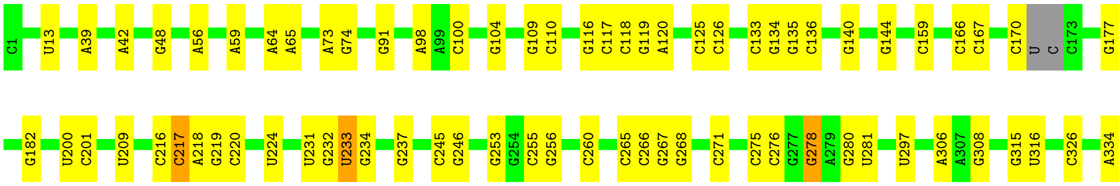
- Molecule 47: E_tRNA

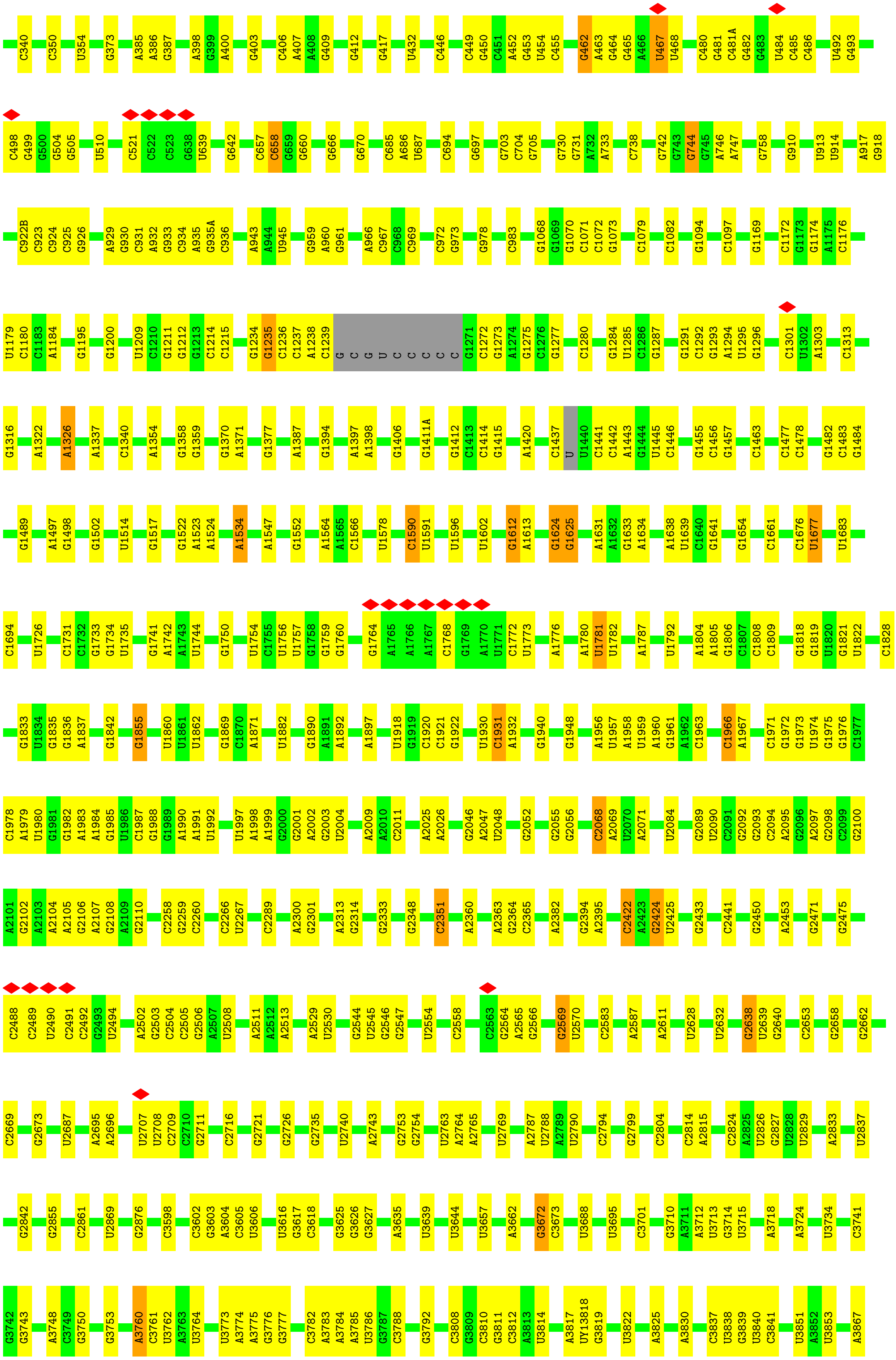
Chain 3:



- Molecule 48: 28S_rRNA

Chain 5:




C340 C350 U354 G373 A385 A386 G387 A398 G399 A400 G403 C406 A407 A408 G409 G412 G417 U432 C446 C449 G450 C451 A452 G453 U454 C455 G462 A463 G464 G465 A466 U467 U468 C480 G481 C481A G482 G483 U484 C485 C486 U492 G493
C498 G499 G500 G504 G505 U510 C521 C522 C523 G638 U639 G642 C657 C658 G659 G660 G666 G670 C685 A686 U687 C694 G697 G703 C704 G705 G730 G731 A732 A733 C738 G742 G743 G744 G745 A746 A747 G758 G910 U913 U914 A917 G918
C922B C923 C924 C925 G926 A929 G930 C931 A932 G933 C934 A935 G935A C936 A943 A944 U945 G959 A960 G961 A966 C967 C968 C969 C972 G973 G978 C983 G1068 G1069 G1070 C1071 C1072 G1073 C1079 C1082 G1094 C1097 G1169 C1172 G1173 G1174 A1175 C1176
U1179 C1180 C1183 A1184 G1195 G1200 U1209 C1210 G1211 G1212 G1213 C1214 C1215 G1234 G1235 C1236 C1237 A1238 C1239 G C G U C C C C C G1271 C1272 G1273 A1274 G1275 C1276 G1277 C1280 G1284 U1285 C1286 G1287 G1291 C1292 G1293 A1294 U1295 G1296 C1301 U1302 A1303 C1313
G1316 A1322 A1326 A1337 C1340 A1354 G1358 G1359 G1370 A1371 G1377 A1387 G1394 A1397 A1398 G1406 G1411A G1412 C1413 C1414 G1415 A1420 C1437 U U1440 C1441 C1442 A1443 G1444 U1445 C1446 G1455 C1456 G1457 C1463 C1477 C1478 G1482 C1483 G1484
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C1694 U1726 C1731 C1732 G1733 G1734 U1735 G1741 A1742 A1743 U1744 G1750 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 A1776 A1780 U1781 U1782 A1787 U1792 A1804 A1805 G1806 C1807 C1808 C1809 G1818 G1819 U1820 G1821 U1822 C1828
G1833 U1834 G1835 G1836 A1837 G1842 G1855 U1860 U1861 U1862 G1869 C1870 A1871 U1882 G1890 A1891 A1892 A1897 U1918 G1919 C1920 C1921 G1922 U1930 C1931 A1932 G1940 G1948 A1956 U1957 A1958 U1959 A1960 G1961 A1962 C1963 C1966 A1967 C1971 G1972 G1973 U1974 G1975 G1976 C1977
C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 U1997 A1998 A1999 G2000 G2001 A2002 G2003 U2004 A2009 A2010 C2011 A2025 A2026 G2046 A2047 U2048 G2052 G2055 G2056 C2068 A2069 U2070 A2071 U2084 G2089 U2090 C2091 G2092 G2093 C2094 A2095 G2096 A2097 G2098 C2099 G2100
A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 A2109 G2110 C2258 G2259 C2260 C2266 U2267 C2289 A2300 G2301 A2313 G2314 G2333 G2348 C2351 A2360 A2363 G2364 C2365 A2382 G2394 A2395 C2422 A2423 G2424 U2425 G2433 C2441 G2450 A2453 G2471 G2475
C2488 C2489 U2490 C2491 C2492 G2493 U2494 A2502 G2503 C2504 C2505 G2506 A2507 U2508 A2511 A2512 A2513 A2529 U2530 G2544 U2545 G2546 G2547 U2554 C2558 C2563 G2564 A2565 G2566 G2569 U2570 C2583 A2587 A2611 U2628 U2632 G2638 U2639 G2640 C2653 G2658 G2662
C2669 G2673 U2687 A2695 A2696 U2707 U2708 C2709 C2710 G2711 C2716 G2721 G2726 G2735 U2740 A2743 G2753 G2754 U2763 A2764 A2765 U2769 A2787 U2788 A2789 U2790 C2794 G2799 C2804 C2814 A2815 C2824 A2825 U2826 G2827 U2828 U2829 A2833 U2837
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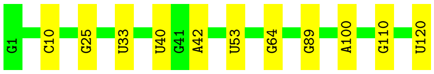
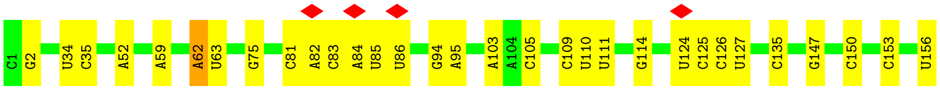
- Molecule 49: 5S_rRNA

Chain 7:



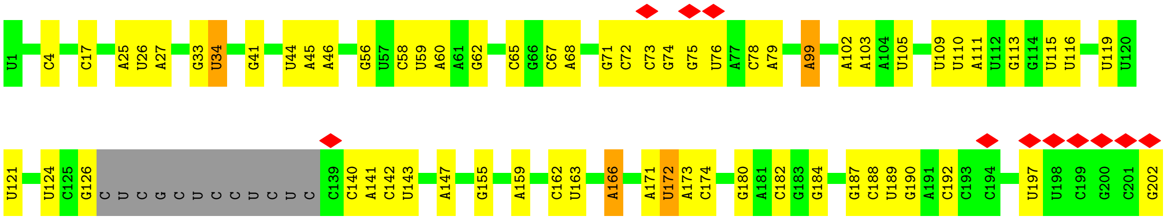
- Molecule 50: 5.8S_rRNA

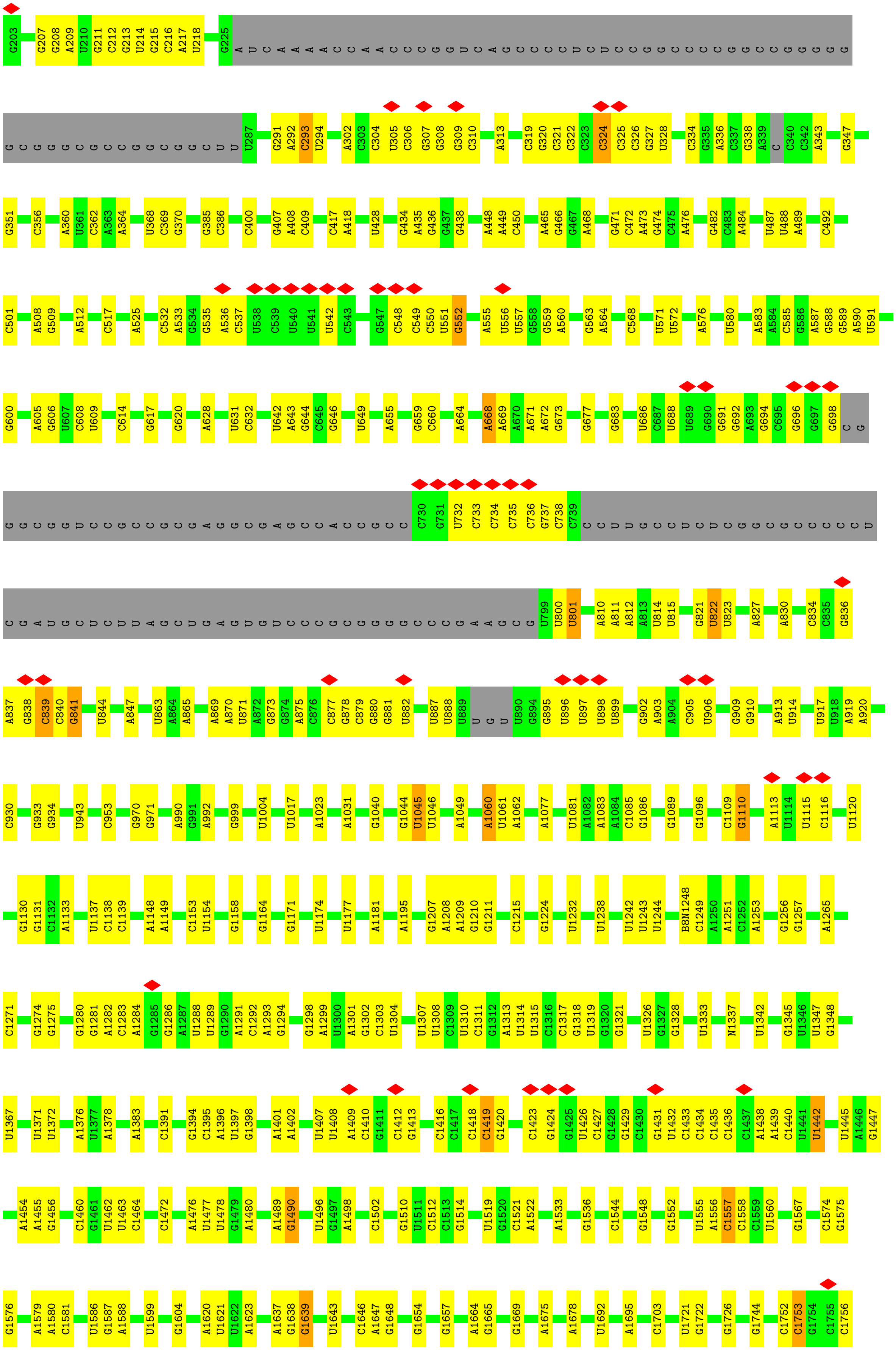
Chain 8:



- Molecule 51: 18S_rRNA

Chain 9:




G203 G207 G208 A209 U210 G211 C212 G213 U214 G215 C216 A217 U218 G225 A U C A A A A C C A A C C C G G U C A G C C C C U C U C C G G C C C C G G C C G G G G G
G C G G G C G C C G G C G G C U U U287 G291 A292 C293 U294 A302 C303 C304 U305 C306 G307 G308 G309 C310 A313 C319 G320 C321 C322 C323 C324 C325 C326 G327 U328 C334 G335 A336 C337 G338 A339 C C340 C342 A343 G347
G351 C356 A360 U361 C362 A363 A364 U368 C369 G370 G385 C386 C400 G407 A408 C409 C417 A418 U428 G434 A435 G436 G437 G438 A448 A449 C450 A465 G466 G467 A468 G471 C472 A473 G474 C475 A476 G482 C483 A484 U487 U488 A489 C492
C501 A508 G509 A512 C517 A525 C532 A533 G534 G535 A536 C537 U538 C539 U540 U541 U542 C543 G547 C548 C549 C550 U551 G552 A555 U556 U557 G558 G559 A560 G563 A564 C568 U571 U572 A576 U580 A583 A584 C585 G586 A587 G588 G589 A590 U591
G600 A605 G606 U607 C608 U609 C614 G617 G620 A628 U631 C632 U642 A643 G644 C645 G646 U649 A655 G659 C660 A664 A668 A669 A670 A671 A672 G673 G677 G683 U686 C687 U688 U689 G690 G691 G692 A693 G694 C695 G696 G697 G698 C G
G G C G G U C C G C C G C G A G G C G A G C C A C C G C C C730 G731 U732 C733 C734 C735 C736 G737 C738 C739 C C U U G C C U C U C G G C G C C C C C U
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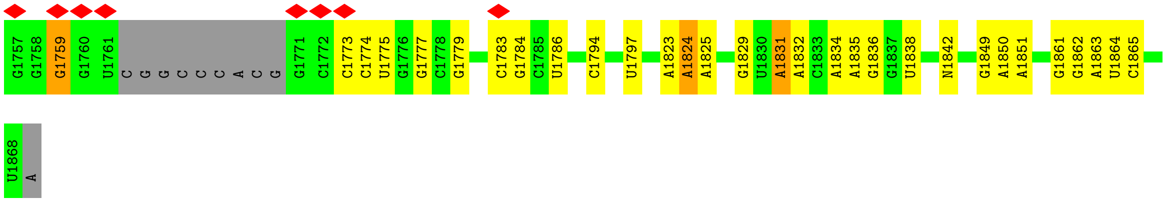
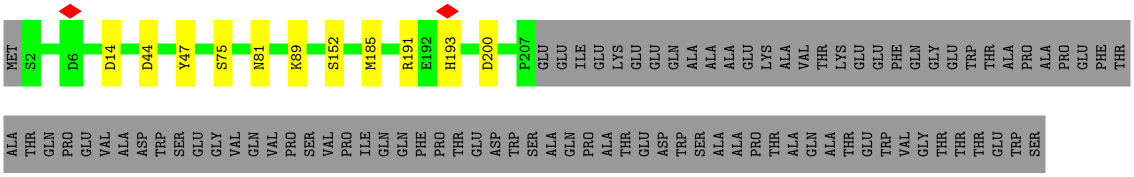
A837 G838 C839 C840 G841 U844 A847 U863 A864 A865 A869 A870 U871 A872 G873 G874 A875 C876 C877 G878 C879 G880 G881 U882 U887 U888 U889 U G U U890 G894 G895 U896 U897 U898 U899 G902 A903 A904 C905 U906 G909 G910 A913 U914 U917 U918 A919 A920
G930 G933 G934 U943 C953 G970 G971 A990 G991 A992 G999 U1004 U1017 A1023 A1031 G1040 G1044 U1045 U1046 A1049 A1060 U1061 A1062 A1077 U1081 A1082 A1083 A1084 C1085 G1086 G1089 G1096 C1109 G1110 A1113 U1114 U1115 C1116 U1120
G1130 G1131 C1132 A1133 U1137 C1138 C1139 A1148 A1149 C1153 U1154 G1158 G1164 G1171 U1174 U1177 A1181 A1195 G1207 A1208 A1209 G1210 G1211 C1215 G1224 U1232 U1238 U1242 U1243 U1244 B8N1248 C1249 A1250 A1251 C1252 A1253 G1256 G1257 A1265
C1271 G1274 G1275 G1280 G1281 A1282 C1283 A1284 G1285 G1286 A1287 U1288 U1289 G1290 A1291 C1292 A1293 G1294 G1298 A1299 U1300 A1301 G1302 C1303 U1304 U1307 U1308 C1309 U1310 C1311 G1312 A1313 U1314 U1315 C1316 C1317 G1318 U1319 G1320 G1321 U1326 G1327 G1328 U1333 N1337 U1342 G1345 U1346 U1347 G1348
U1367 U1371 U1372 A1376 U1377 A1378 A1383 C1391 G1394 C1395 A1396 U1397 G1398 A1401 A1402 U1407 U1408 A1409 C1410 G1411 C1412 G1413 C1416 C1417 C1418 C1419 G1420 C1423 G1424 G1425 U1426 C1427 G1428 G1429 C1430 G1431 U1432 C1433 C1434 C1435 C1436 C1437 A1438 A1439 C1440 U1441 U1442 U1445 A1446 G1447
A1454 A1455 G1456 C1460 G1461 U1462 U1463 C1464 C1472 A1476 U1477 U1478 G1479 A1480 A1489 G1490 U1496 G1497 A1498 C1502 G1510 U1511 C1512 C1513 G1514 U1519 G1520 C1521 A1522 A1533 G1536 C1544 G1548 G1552 U1555 A1556 C1557 C1558 C1559 U1560 G1567 C1574 G1575
G1576 A1579 A1580 C1581 U1586 G1587 A1588 U1599 G1604 A1620 U1621 U1622 A1623 A1637 G1638 G1639 U1643 C1646 A1647 G1648 G1654 G1657 A1664 G1665 G1669 A1675 A1678 U1692 A1695 C1703 U1721 G1722 G1726 G1744 C1752 C1753 G1754 C1755 C1756



- Molecule 52: uS2 (SA)

Chain AA:

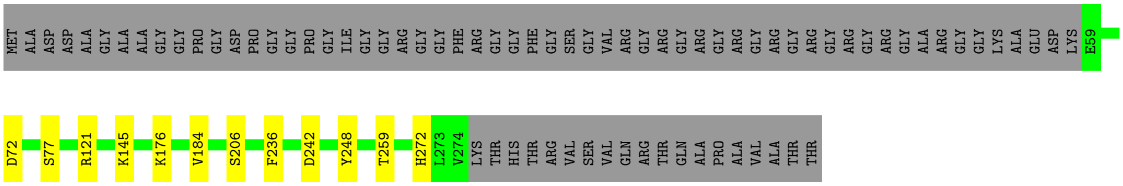


- Molecule 53: eS1

Chain BB:

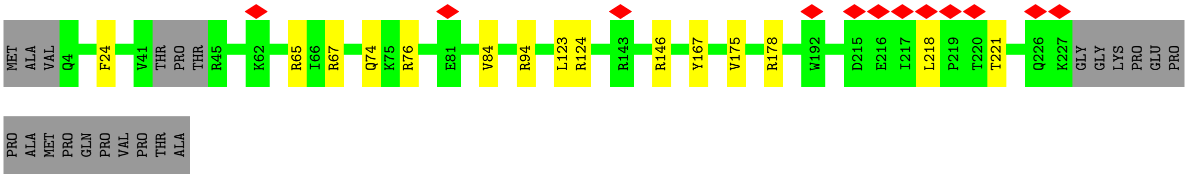
- Molecule 54: uS5

Chain CC:



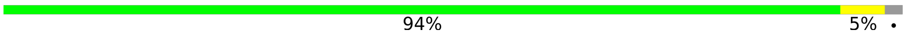
- Molecule 55: Ribosomal protein S3

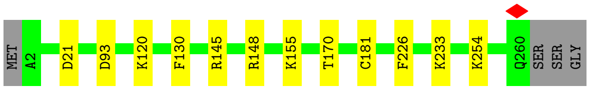
Chain DD:



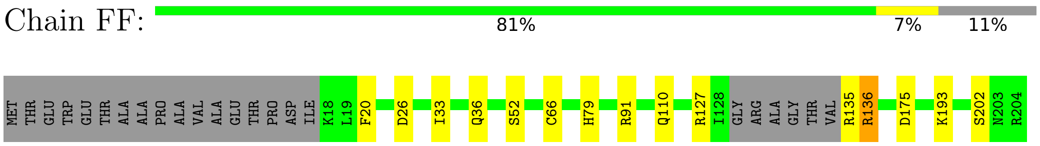
- Molecule 56: eS4 (S4 X isoform)

Chain EE:

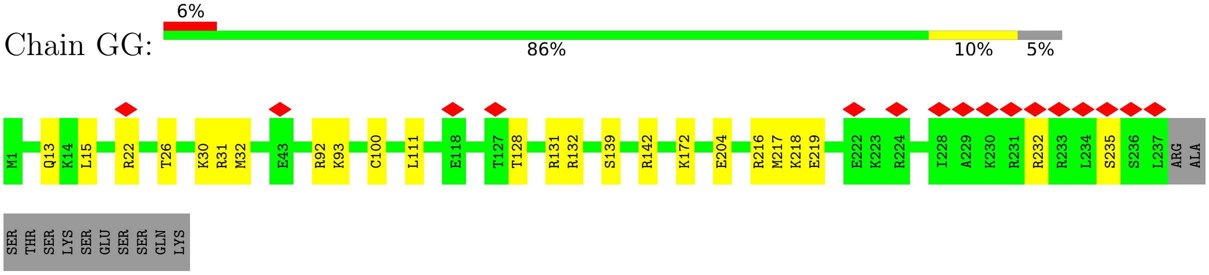




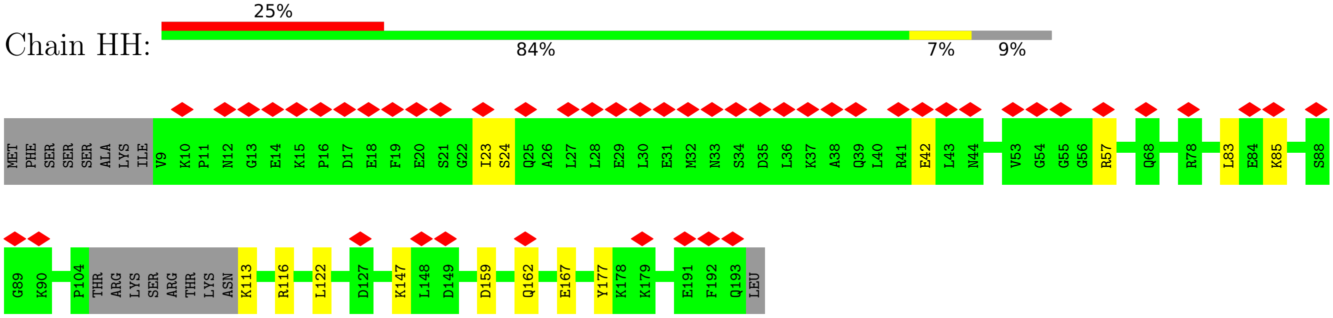
- Molecule 57: uS7



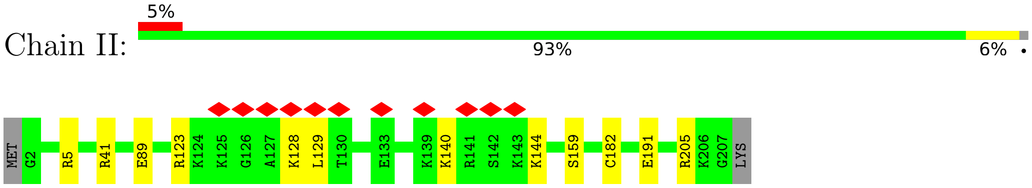
- Molecule 58: eS6



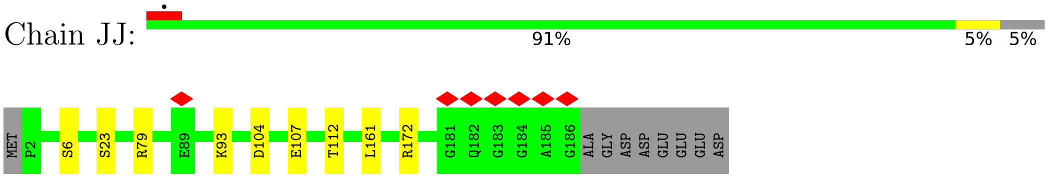
- Molecule 59: eS7



- Molecule 60: eS8



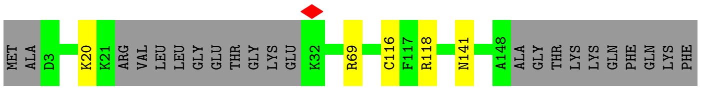
- Molecule 61: uS4



- Molecule 62: S10_plectin domain-containing protein

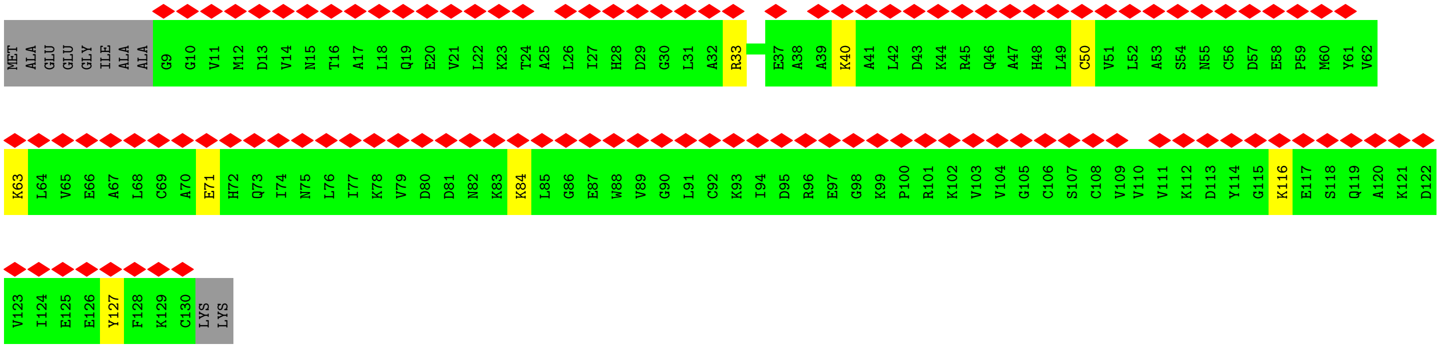
- Molecule 63: uS17

Chain LL:



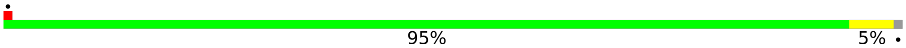
- Molecule 64: eS12

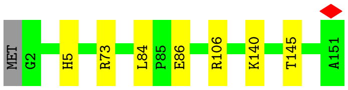
Chain MM:



- Molecule 65: uS15

Chain NN:



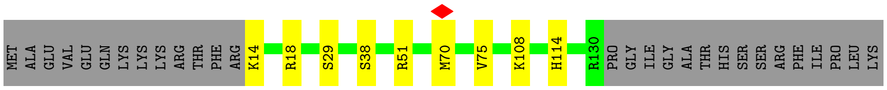


- Molecule 66: uS11

Chain OO:

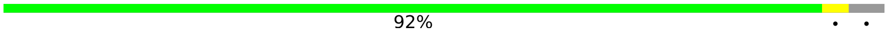
- Molecule 67: uS19

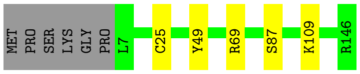
Chain PP:



- Molecule 68: uS9

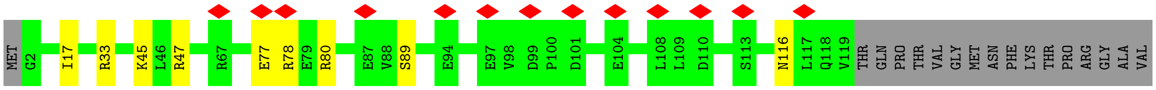
Chain QQ:





- Molecule 69: eS17

Chain RR:

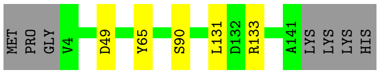


- Molecule 70: uS13

Chain SS:

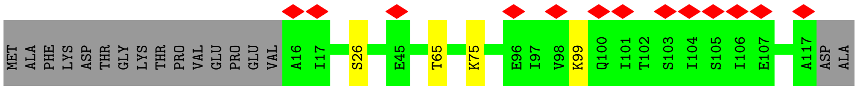
- Molecule 71: eS19

Chain TT:



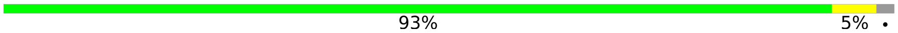
- Molecule 72: uS10

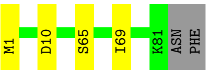
Chain UU:



- Molecule 73: eS21

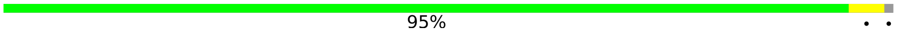
Chain VV:

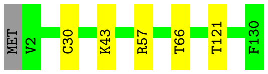




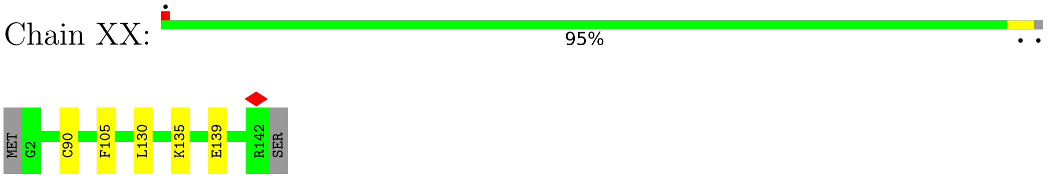
- Molecule 74: uS8

Chain WW:

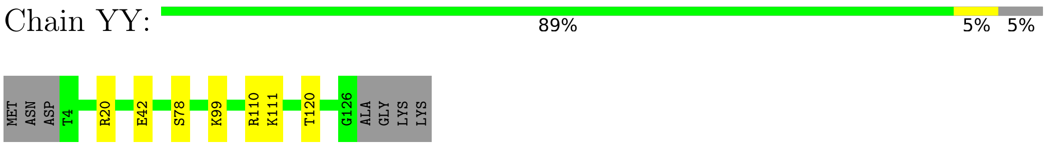




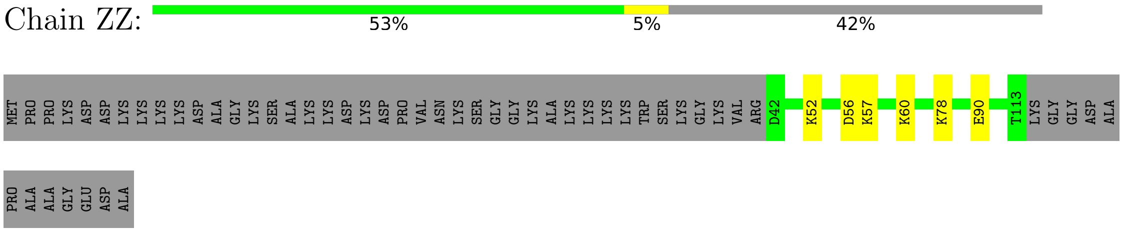
- Molecule 75: uS12



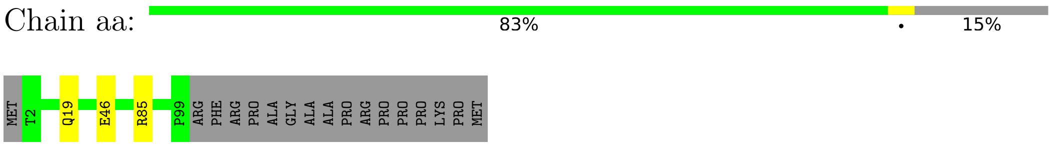
- Molecule 76: 40S ribosomal protein S24



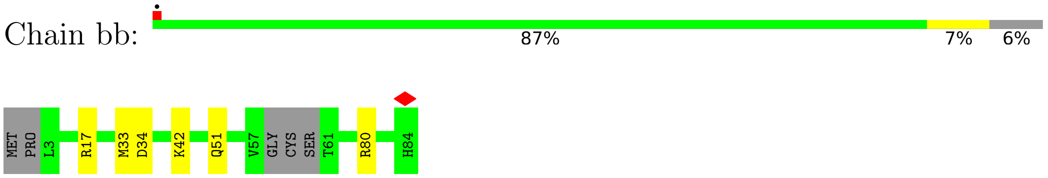
- Molecule 77: eS25



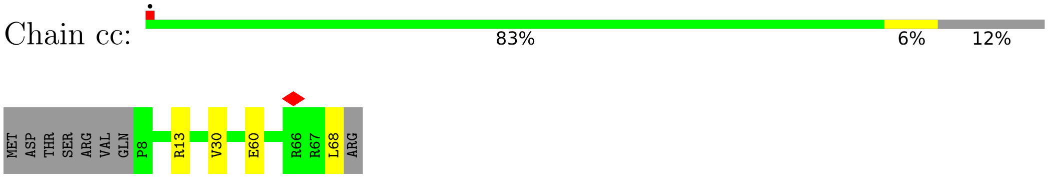
- Molecule 78: 40S ribosomal protein S26



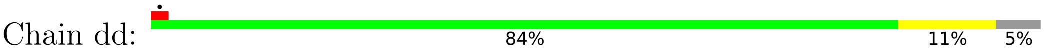
- Molecule 79: eS27

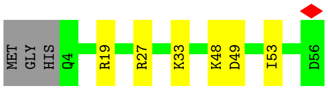


- Molecule 80: eS28



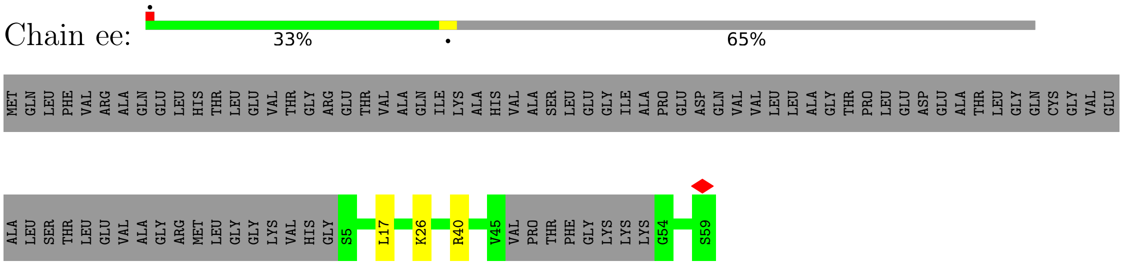
- Molecule 81: uS14





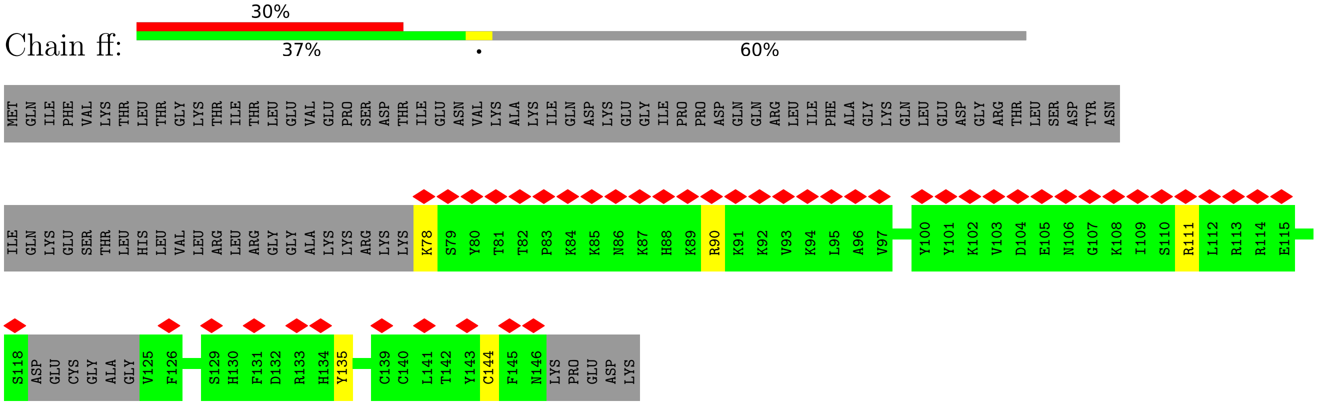
- Molecule 82: eS30

Chain ee:



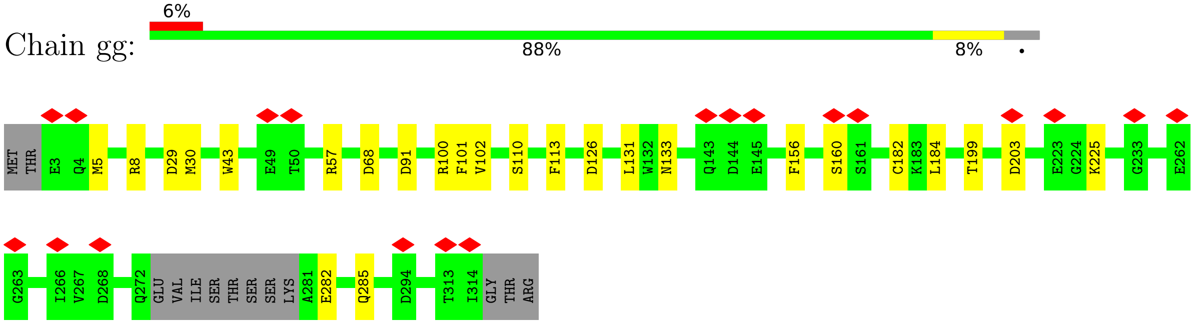
- Molecule 83: eS31

Chain ff:



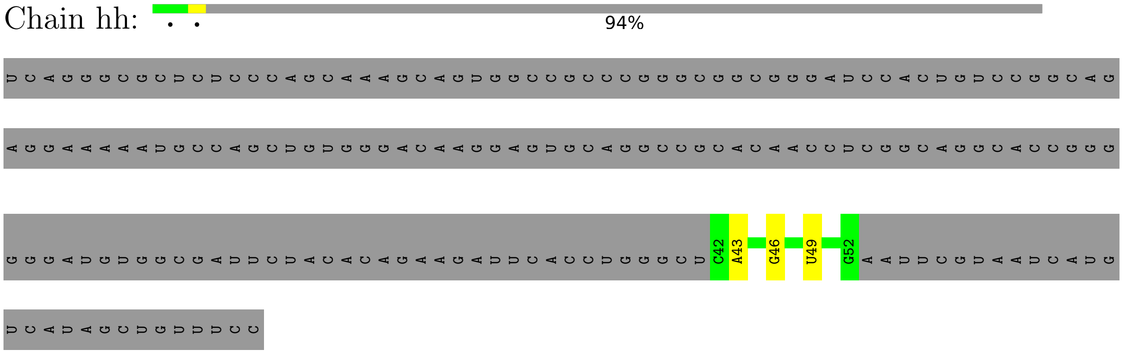
- Molecule 84: Receptor for Activated C Kinase 1 (RACK1)

Chain gg:

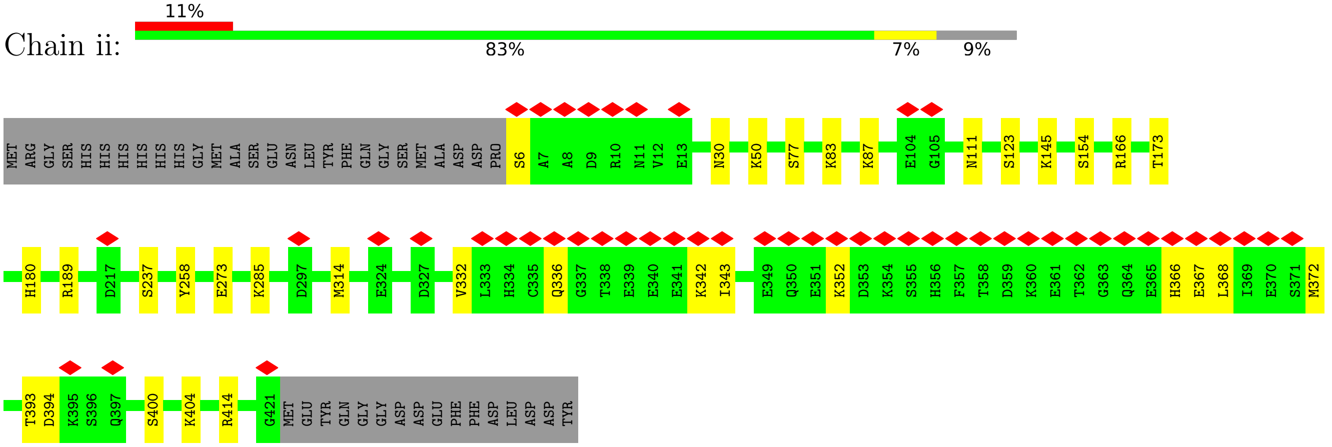


- Molecule 85: mRNA

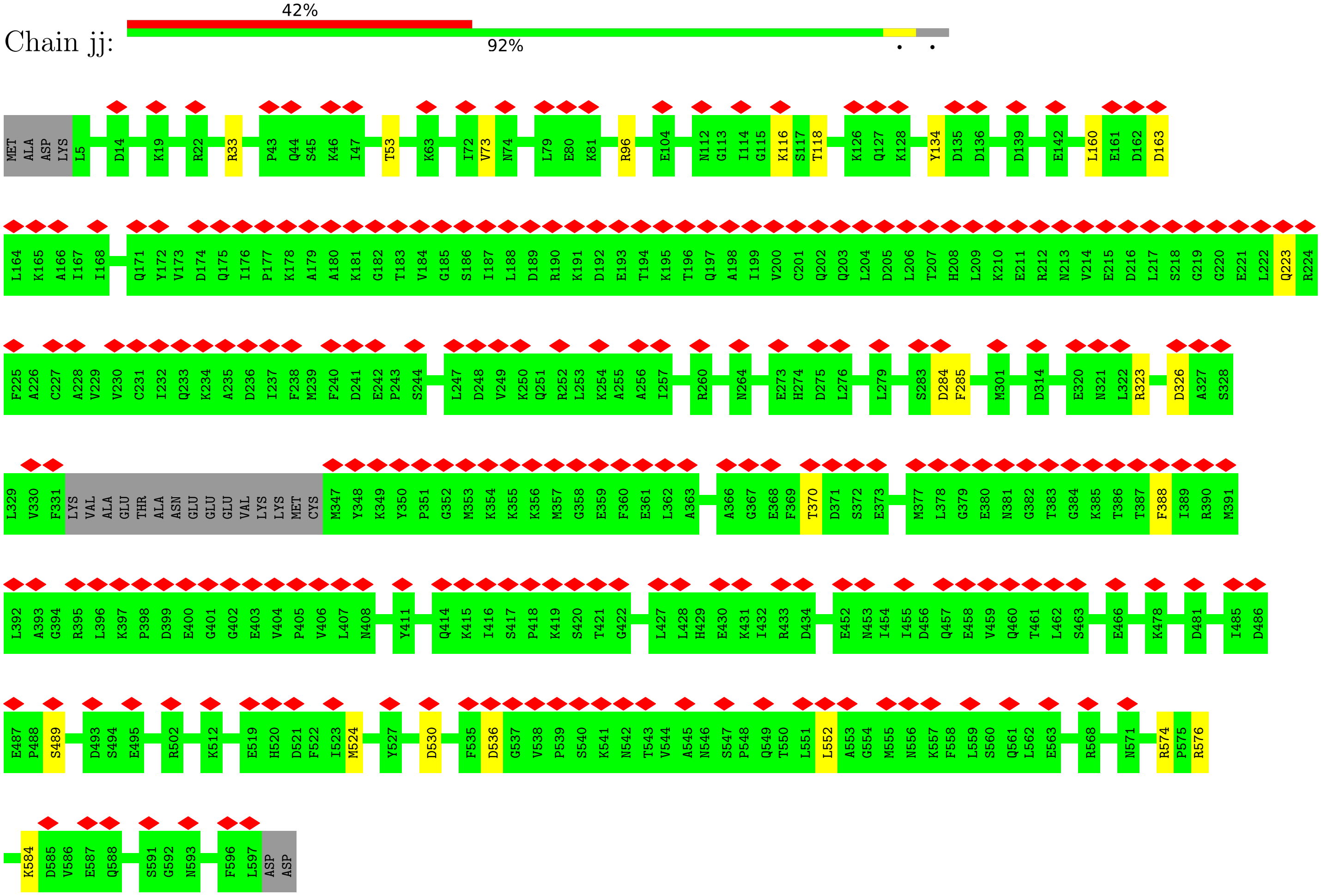
Chain hh:



- Molecule 86: Eukaryotic peptide chain release factor subunit 1



- Molecule 87: ATP binding cassette subfamily E member 1



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90190	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 $(e^-/\text{Å}^2)$	53.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: UR3, ZVM, 1MA, PSU, UY1, OMG, B8N, G7M, B9B, A2M, 6MZ, 2MG, OMU, MG, SF4, MA6, ZN, 5MC, 4AC, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/1906	0.65	0/2556
2	B	0.39	0/3216	0.59	0/4311
3	C	0.38	0/2937	0.63	0/3946
4	D	0.38	0/2407	0.60	0/3224
5	E	0.37	0/1760	0.61	0/2362
6	F	0.40	0/1911	0.61	0/2549
7	G	0.36	0/1799	0.61	0/2424
8	H	0.36	0/1535	0.61	0/2063
9	I	0.37	0/1693	0.60	0/2260
10	J	0.36	0/1359	0.62	0/1817
11	L	0.36	0/1733	0.64	0/2316
12	M	0.36	0/1158	0.58	0/1547
13	N	0.42	0/1746	0.67	0/2338
14	O	0.37	0/1653	0.64	0/2210
15	P	0.39	0/1268	0.59	0/1700
16	Q	0.39	0/1539	0.68	0/2054
17	R	0.33	0/1518	0.65	0/2005
18	S	0.40	0/1501	0.63	0/2012
19	T	0.38	0/1326	0.59	0/1770
20	U	0.39	0/814	0.61	0/1092
21	V	0.38	0/987	0.61	0/1324
22	W	0.40	0/541	0.58	0/720
23	X	0.35	0/966	0.60	0/1301
24	Y	0.37	0/1132	0.62	0/1504
25	Z	0.41	0/1130	0.63	0/1507
26	a	0.41	0/1191	0.61	0/1590
27	b	0.39	0/619	0.57	0/818
28	c	0.39	0/742	0.58	0/995
29	d	0.36	0/846	0.62	0/1136
30	e	0.40	0/1071	0.62	0/1429
31	f	0.43	0/895	0.68	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.37	0/916	0.64	0/1220
33	h	0.35	0/1021	0.61	0/1348
34	i	0.35	0/841	0.64	0/1112
35	j	0.40	0/720	0.66	0/952
36	k	0.38	0/565	0.66	0/750
37	l	0.37	0/450	0.64	0/597
38	m	0.40	0/427	0.60	0/564
39	n	0.39	0/223	0.83	0/284
40	o	0.40	0/855	0.63	0/1128
41	p	0.37	0/718	0.60	0/953
42	r	0.38	0/1017	0.65	0/1364
43	s	0.31	0/1483	0.56	0/2000
44	t	0.29	0/1071	0.58	0/1444
45	1	0.37	0/129	0.58	0/173
46	2	0.55	0/1805	1.00	2/2809 (0.1%)
47	3	0.46	0/1777	0.99	0/2763
48	5	0.83	5/82331 (0.0%)	0.99	95/128398 (0.1%)
49	7	0.77	0/2858	0.88	0/4455
50	8	0.83	1/3675 (0.0%)	0.93	6/5725 (0.1%)
51	9	0.69	7/38943 (0.0%)	0.98	69/60686 (0.1%)
52	AA	0.34	0/1661	0.57	0/2259
53	BB	0.34	0/1749	0.58	0/2340
54	CC	0.35	0/1710	0.56	0/2312
55	DD	0.35	0/1749	0.60	0/2350
56	EE	0.35	0/2101	0.63	0/2828
57	FF	0.33	0/1461	0.57	0/1961
58	GG	0.33	0/1946	0.65	0/2590
59	HH	0.34	0/1447	0.60	0/1939
60	II	0.35	0/1715	0.64	0/2287
61	JJ	0.33	0/1550	0.64	0/2069
62	KK	0.36	0/752	0.59	0/1014
63	LL	0.37	0/1143	0.61	0/1529
64	MM	0.30	0/949	0.53	0/1274
65	NN	0.34	0/1232	0.59	0/1656
66	OO	0.39	0/969	0.71	0/1298
67	PP	0.33	0/986	0.63	0/1316
68	QQ	0.36	0/1134	0.62	0/1517
69	RR	0.34	0/973	0.61	0/1304
70	SS	0.33	0/1180	0.62	0/1581
71	TT	0.34	0/1093	0.60	0/1466
72	UU	0.32	0/817	0.62	0/1097
73	VV	0.34	0/623	0.61	0/833
74	WW	0.35	0/1051	0.59	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	XX	0.34	0/1116	0.61	0/1490
76	YY	0.35	0/1023	0.61	0/1359
77	ZZ	0.32	0/580	0.59	0/780
78	aa	0.36	0/794	0.64	0/1065
79	bb	0.33	0/640	0.58	0/856
80	cc	0.34	0/481	0.71	0/643
81	dd	0.35	0/455	0.65	0/603
82	ee	0.32	0/381	0.64	0/498
83	ff	0.34	0/538	0.64	0/713
84	gg	0.32	0/2427	0.58	0/3303
85	hh	0.63	0/264	0.95	0/409
86	ii	0.35	0/3333	0.59	0/4483
87	jj	0.31	0/4644	0.55	0/6272
All	All	0.63	13/233391 (0.0%)	0.85	172/341503 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
57	FF	0	1
63	LL	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	8	62	A	N9-C4	-7.30	1.33	1.37
48	5	978	G	N9-C4	-6.25	1.32	1.38
51	9	1675	A	N9-C4	-5.92	1.34	1.37
48	5	3775	A	N3-C4	-5.74	1.31	1.34
51	9	1130	G	N9-C4	-5.71	1.33	1.38
48	5	1890	G	N9-C4	-5.43	1.33	1.38
51	9	1834	A	N9-C4	-5.33	1.34	1.37
51	9	1675	A	N3-C4	-5.29	1.31	1.34
51	9	1620	A	N3-C4	-5.23	1.31	1.34
51	9	1834	A	N3-C4	-5.19	1.31	1.34
48	5	1890	G	N3-C4	-5.15	1.31	1.35
48	5	978	G	C2-N3	-5.15	1.28	1.32
51	9	1620	A	N9-C4	-5.04	1.34	1.37

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	978	G	N3-C4-N9	-11.15	119.31	126.00
51	9	1779	G	N3-C4-N9	9.76	131.85	126.00
48	5	1612	G	N9-C4-C5	-9.75	101.50	105.40
48	5	255	C	N1-C2-O2	9.63	124.68	118.90
48	5	978	G	N3-C4-C5	9.42	133.31	128.60
48	5	978	G	N3-C2-N2	-9.31	113.39	119.90
48	5	1890	G	N3-C4-N9	-9.18	120.49	126.00
51	9	356	C	C2-N1-C1'	8.89	128.58	118.80
48	5	255	C	N3-C2-O2	-8.80	115.74	121.90
48	5	417	G	O4'-C1'-N9	8.77	115.21	108.20
48	5	2638	G	N3-C4-N9	-8.61	120.83	126.00
48	5	1890	G	C2-N3-C4	-8.56	107.62	111.90
51	9	1779	G	C4-N9-C1'	8.34	137.34	126.50
48	5	2638	G	N3-C4-C5	7.98	132.59	128.60
48	5	2638	G	C2-N3-C4	-7.85	107.97	111.90
51	9	488	U	N3-C2-O2	-7.83	116.72	122.20
48	5	1612	G	C4-C5-N7	7.82	113.93	110.80
48	5	1612	G	N3-C4-N9	7.81	130.69	126.00
51	9	1130	G	N3-C4-C5	7.77	132.48	128.60
48	5	3775	A	C8-N9-C4	-7.74	102.70	105.80
48	5	462	G	N3-C4-N9	-7.72	121.37	126.00
51	9	1779	G	C8-N9-C1'	-7.63	117.08	127.00
51	9	1318	G	C4-N9-C1'	7.61	136.40	126.50
48	5	1612	G	C6-C5-N7	-7.61	125.84	130.40
50	8	62	A	N3-C4-N9	-7.59	121.32	127.40
51	9	1130	G	C2-N3-C4	-7.57	108.11	111.90
51	9	1130	G	N3-C4-N9	-7.52	121.49	126.00
51	9	501	C	C2-N1-C1'	7.51	127.06	118.80
48	5	3775	A	N1-C2-N3	7.50	133.05	129.30
51	9	1348	G	N3-C4-N9	-7.48	121.52	126.00
51	9	839	C	C2-N1-C1'	7.44	126.99	118.80
48	5	255	C	C5-C4-N4	7.40	125.38	120.20
51	9	1779	G	C6-C5-N7	-7.38	125.97	130.40
51	9	1779	G	N3-C4-C5	-7.24	124.98	128.60
48	5	1890	G	N3-C2-N2	-7.14	114.91	119.90
51	9	1834	A	C8-N9-C4	-7.10	102.96	105.80
48	5	1612	G	C8-N9-C1'	-7.09	117.79	127.00
51	9	1318	G	C8-N9-C1'	-7.08	117.80	127.00
51	9	1109	C	O4'-C1'-N1	6.98	113.79	108.20
48	5	3775	A	C2-N3-C4	-6.98	107.11	110.60
51	9	356	C	C6-N1-C1'	-6.85	112.58	120.80
48	5	2638	G	N3-C2-N2	-6.83	115.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1318	G	N3-C4-N9	6.78	130.07	126.00
48	5	978	G	N1-C2-N2	6.78	122.30	116.20
51	9	356	C	N1-C2-O2	6.67	122.90	118.90
50	8	62	A	N3-C4-C5	6.65	131.45	126.80
48	5	1890	G	N3-C4-C5	6.64	131.92	128.60
48	5	1235	G	N3-C4-N9	-6.62	122.03	126.00
51	9	692	G	C8-N9-C1'	-6.59	118.43	127.00
51	9	488	U	N1-C2-O2	6.56	127.39	122.80
51	9	692	G	N3-C4-N9	6.54	129.93	126.00
48	5	255	C	N3-C4-N4	-6.53	113.43	118.00
48	5	4404	U	O4'-C1'-N1	6.46	113.37	108.20
48	5	3775	A	N7-C8-N9	6.43	117.01	113.80
51	9	501	C	C6-N1-C2	-6.41	117.73	120.30
51	9	839	C	N1-C2-O2	6.40	122.74	118.90
48	5	1890	G	C8-N9-C4	-6.36	103.86	106.40
48	5	2471	G	C4-C5-N7	6.33	113.33	110.80
48	5	233	U	O4'-C1'-N1	6.30	113.24	108.20
51	9	1557	C	C2-N1-C1'	6.29	125.72	118.80
51	9	501	C	N3-C2-O2	-6.29	117.50	121.90
51	9	1318	G	C6-C5-N7	-6.27	126.64	130.40
48	5	1552	G	O4'-C1'-N9	6.26	113.20	108.20
48	5	4864	U	O4'-C1'-N1	6.25	113.20	108.20
51	9	1824	A	O4'-C1'-N9	6.20	113.16	108.20
48	5	4949	G	C4-N9-C1'	6.20	134.55	126.50
48	5	278	G	O4'-C1'-N9	-6.16	103.28	108.20
48	5	4527	G	O4'-C1'-N9	6.15	113.12	108.20
48	5	100	C	N3-C2-O2	-6.13	117.61	121.90
51	9	905	C	N3-C2-O2	-6.13	117.61	121.90
51	9	692	G	C4-N9-C1'	6.11	134.45	126.50
48	5	1890	G	N1-C2-N3	6.09	127.56	123.90
51	9	1348	G	N3-C4-C5	6.06	131.63	128.60
51	9	1675	A	C2-N3-C4	-5.98	107.61	110.60
48	5	3741	C	N3-C2-O2	-5.98	117.72	121.90
51	9	1456	G	C8-N9-C4	-5.96	104.02	106.40
51	9	501	C	N1-C2-O2	5.94	122.46	118.90
48	5	4949	G	C6-C5-N7	-5.80	126.92	130.40
48	5	2814	C	C2-N1-C1'	5.79	125.16	118.80
51	9	1759	G	N3-C4-N9	5.78	129.47	126.00
48	5	1590	C	P-O3'-C3'	5.77	126.63	119.70
51	9	1773	C	N1-C2-O2	5.77	122.36	118.90
51	9	692	G	C6-C5-N7	-5.76	126.94	130.40
48	5	1612	G	C5-C6-O6	-5.76	125.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	4635	A	N7-C8-N9	5.71	116.65	113.80
48	5	48	G	O4'-C1'-N9	5.71	112.77	108.20
51	9	841	G	N3-C4-N9	5.70	129.42	126.00
48	5	2394	G	O4'-C1'-N9	5.68	112.74	108.20
51	9	905	C	N1-C2-O2	5.68	122.31	118.90
48	5	3837	C	N1-C2-O2	-5.66	115.50	118.90
48	5	4233	A	O4'-C1'-N9	5.66	112.73	108.20
48	5	100	C	C6-N1-C2	-5.65	118.04	120.30
48	5	1235	G	N3-C4-C5	5.65	131.42	128.60
51	9	1773	C	C2-N1-C1'	5.64	125.00	118.80
51	9	1779	G	N9-C4-C5	-5.64	103.14	105.40
51	9	692	G	N9-C4-C5	-5.64	103.14	105.40
48	5	4626	A	O4'-C1'-N9	5.63	112.70	108.20
48	5	4719	G	N3-C4-C5	5.62	131.41	128.60
51	9	1110	G	C8-N9-C4	-5.62	104.15	106.40
48	5	3775	A	N9-C4-C5	5.62	108.05	105.80
50	8	62	A	C4-N9-C1'	-5.61	116.21	126.30
48	5	1180	C	C2-N1-C1'	5.59	124.95	118.80
51	9	324	C	C2-N1-C1'	5.56	124.92	118.80
48	5	308	G	O4'-C1'-N9	5.56	112.65	108.20
48	5	3775	A	O4'-C1'-N9	5.56	112.65	108.20
51	9	293	C	C2-N1-C1'	5.55	124.91	118.80
48	5	744	G	N3-C4-N9	5.55	129.33	126.00
48	5	1890	G	N7-C8-N9	5.54	115.87	113.10
46	2	20	U	C2-N1-C1'	5.54	124.34	117.70
48	5	5016	A	O4'-C1'-N9	5.53	112.62	108.20
51	9	659	G	C4-N9-C1'	5.52	133.68	126.50
48	5	4949	G	C8-N9-C1'	-5.51	119.83	127.00
51	9	839	C	C6-N1-C1'	-5.51	114.19	120.80
48	5	1612	G	C4-N9-C1'	5.51	133.66	126.50
51	9	1834	A	N7-C8-N9	5.50	116.55	113.80
48	5	1966	C	C2-N1-C1'	5.49	124.84	118.80
48	5	1855	G	O5'-P-OP1	-5.46	100.79	105.70
48	5	4719	G	OP1-P-O3'	5.46	117.20	105.20
51	9	1557	C	N1-C2-O2	5.46	122.17	118.90
51	9	1753	C	N3-C2-O2	-5.45	118.09	121.90
51	9	1834	A	C2-N3-C4	-5.44	107.88	110.60
48	5	462	G	N3-C4-C5	5.44	131.32	128.60
48	5	3672	G	N3-C2-N2	-5.44	116.09	119.90
50	8	62	A	C8-N9-C1'	5.43	137.48	127.70
48	5	1890	G	N9-C4-C5	5.42	107.57	105.40
48	5	4949	G	O4'-C1'-N9	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2558	C	N1-C2-O2	-5.40	115.66	118.90
51	9	1752	C	N1-C2-O2	5.40	122.14	118.90
51	9	691	G	C8-N9-C4	-5.38	104.25	106.40
50	8	62	A	C2-N3-C4	-5.36	107.92	110.60
48	5	1931	C	O4'-C1'-N1	5.35	112.48	108.20
51	9	919	A	O4'-C1'-N9	5.34	112.47	108.20
51	9	1779	G	C4-C5-N7	5.34	112.93	110.80
48	5	1235	G	N3-C2-N2	-5.31	116.18	119.90
51	9	1536	G	C2-N3-C4	5.30	114.55	111.90
48	5	978	G	C8-N9-C1'	5.30	133.89	127.00
48	5	1808	C	N1-C2-O2	-5.29	115.72	118.90
48	5	4936	G	N9-C4-C5	-5.29	103.29	105.40
48	5	4468	U	C5-C4-O4	5.27	129.06	125.90
51	9	1675	A	N3-C4-N9	-5.27	123.19	127.40
51	9	1831	A	O5'-P-OP2	-5.27	100.96	105.70
48	5	4922	C	C2-N1-C1'	5.25	124.58	118.80
48	5	744	G	C8-N9-C1'	-5.25	120.18	127.00
48	5	1624	G	O4'-C1'-N9	5.25	112.40	108.20
48	5	2068	C	C6-N1-C2	-5.24	118.20	120.30
51	9	1060	A	O4'-C1'-N9	5.22	112.38	108.20
51	9	1834	A	N3-C4-N9	-5.18	123.25	127.40
46	2	49	C	N1-C2-O2	5.17	122.00	118.90
48	5	978	G	C4-N9-C1'	-5.17	119.78	126.50
51	9	677	G	N9-C4-C5	-5.17	103.33	105.40
51	9	1419	C	C2-N1-C1'	5.16	124.48	118.80
48	5	1612	G	N1-C6-O6	5.13	122.98	119.90
51	9	1130	G	C5-N7-C8	-5.13	101.73	104.30
51	9	1110	G	N7-C8-N9	5.11	115.66	113.10
48	5	1882	U	C5-C4-O4	-5.11	122.83	125.90
51	9	488	U	C2-N1-C1'	5.09	123.81	117.70
48	5	3876	A	N1-C6-N6	5.08	121.65	118.60
48	5	5016	A	C5-N7-C8	-5.07	101.36	103.90
48	5	658	C	C2-N1-C1'	5.07	124.37	118.80
48	5	217	C	C2-N1-C1'	5.06	124.37	118.80
48	5	467	U	C2-N1-C1'	-5.05	111.64	117.70
48	5	2471	G	N9-C4-C5	-5.04	103.38	105.40
51	9	1834	A	N9-C4-C5	5.03	107.81	105.80
50	8	62	A	C4-C5-C6	-5.03	114.49	117.00
51	9	1164	G	N3-C4-N9	5.02	129.01	126.00
48	5	744	G	C6-C5-N7	-5.02	127.39	130.40
48	5	1639	U	C2-N1-C1'	5.01	123.72	117.70
48	5	4391	G	N1-C6-O6	-5.01	116.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	552	G	C4-N9-C1'	5.01	133.02	126.50
48	5	1463	C	N1-C2-O2	-5.01	115.89	118.90
48	5	2569	G	N3-C2-N2	-5.00	116.40	119.90
48	5	1973	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	FF	136	ARG	Sidechain
63	LL	118	ARG	Sidechain

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	
1	A	242/257 (94%)	226 (93%)	16 (7%)	0	100	100
2	B	392/403 (97%)	376 (96%)	16 (4%)	0	100	100
3	C	360/413 (87%)	348 (97%)	12 (3%)	0	100	100
4	D	287/297 (97%)	270 (94%)	16 (6%)	1 (0%)	41	61
5	E	209/291 (72%)	189 (90%)	20 (10%)	0	100	100
6	F	223/247 (90%)	218 (98%)	5 (2%)	0	100	100
7	G	214/319 (67%)	202 (94%)	12 (6%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	200/214 (94%)	193 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	165/178 (93%)	151 (92%)	13 (8%)	1 (1%)	25	43
11	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
12	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
13	N	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
14	O	196/203 (97%)	187 (95%)	8 (4%)	1 (0%)	29	48
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
16	Q	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
17	R	177/196 (90%)	172 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	96/128 (75%)	88 (92%)	8 (8%)	0	100	100
21	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
22	W	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
23	X	114/156 (73%)	108 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
25	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
26	a	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	22	39
27	b	73/245 (30%)	70 (96%)	3 (4%)	0	100	100
28	c	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
29	d	96/125 (77%)	94 (98%)	2 (2%)	0	100	100
30	e	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
31	f	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
32	g	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
33	h	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
34	i	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
35	j	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
36	k	66/70 (94%)	60 (91%)	5 (8%)	1 (2%)	10	18
37	l	47/51 (92%)	45 (96%)	2 (4%)	0	100	100
38	m	49/93 (53%)	47 (96%)	2 (4%)	0	100	100
39	n	21/25 (84%)	21 (100%)	0	0	100	100
40	o	101/106 (95%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
42	r	123/137 (90%)	113 (92%)	10 (8%)	0	100	100
43	s	188/318 (59%)	163 (87%)	25 (13%)	0	100	100
44	t	135/165 (82%)	113 (84%)	21 (16%)	1 (1%)	22	39
45	1	13/130 (10%)	11 (85%)	2 (15%)	0	100	100
52	AA	204/295 (69%)	189 (93%)	15 (7%)	0	100	100
53	BB	210/264 (80%)	200 (95%)	10 (5%)	0	100	100
54	CC	214/293 (73%)	202 (94%)	12 (6%)	0	100	100
55	DD	217/243 (89%)	196 (90%)	21 (10%)	0	100	100
56	EE	257/263 (98%)	231 (90%)	26 (10%)	0	100	100
57	FF	177/204 (87%)	163 (92%)	13 (7%)	1 (1%)	25	43
58	GG	235/249 (94%)	205 (87%)	29 (12%)	1 (0%)	34	54
59	HH	173/194 (89%)	146 (84%)	27 (16%)	0	100	100
60	II	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
61	JJ	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
62	KK	84/165 (51%)	76 (90%)	8 (10%)	0	100	100
63	LL	132/158 (84%)	125 (95%)	7 (5%)	0	100	100
64	MM	120/132 (91%)	91 (76%)	29 (24%)	0	100	100
65	NN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
66	OO	125/168 (74%)	121 (97%)	4 (3%)	0	100	100
67	PP	115/145 (79%)	106 (92%)	9 (8%)	0	100	100
68	QQ	138/146 (94%)	128 (93%)	10 (7%)	0	100	100
69	RR	116/135 (86%)	106 (91%)	10 (9%)	0	100	100
70	SS	138/152 (91%)	130 (94%)	8 (6%)	0	100	100
71	TT	136/145 (94%)	124 (91%)	12 (9%)	0	100	100
72	UU	100/119 (84%)	89 (89%)	11 (11%)	0	100	100
73	VV	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
76	YY	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
77	ZZ	70/125 (56%)	64 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	aa	96/115 (84%)	86 (90%)	10 (10%)	0	100	100
79	bb	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
80	cc	59/69 (86%)	54 (92%)	5 (8%)	0	100	100
81	dd	51/56 (91%)	45 (88%)	6 (12%)	0	100	100
82	ee	43/133 (32%)	37 (86%)	6 (14%)	0	100	100
83	ff	59/156 (38%)	49 (83%)	10 (17%)	0	100	100
84	gg	300/317 (95%)	252 (84%)	48 (16%)	0	100	100
86	ii	414/459 (90%)	380 (92%)	33 (8%)	1 (0%)	47	68
87	jj	574/599 (96%)	529 (92%)	44 (8%)	1 (0%)	47	68
All	All	12249/14542 (84%)	11407 (93%)	832 (7%)	10 (0%)	54	73

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	GG	128	THR
57	FF	33	ILE
86	ii	180	HIS
26	a	15	VAL
10	J	173	ILE
14	O	187	LYS
4	D	235	MET
87	jj	96	ARG
36	k	61	PRO
44	t	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/199 (94%)	181 (97%)	6 (3%)	39	65
2	B	336/348 (97%)	326 (97%)	10 (3%)	41	68
3	C	302/337 (90%)	291 (96%)	11 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	245/250 (98%)	237 (97%)	8 (3%)	38	64
5	E	191/251 (76%)	183 (96%)	8 (4%)	30	54
6	F	196/215 (91%)	192 (98%)	4 (2%)	55	79
7	G	189/272 (70%)	180 (95%)	9 (5%)	25	48
8	H	169/171 (99%)	165 (98%)	4 (2%)	49	74
9	I	174/181 (96%)	169 (97%)	5 (3%)	42	69
10	J	140/149 (94%)	133 (95%)	7 (5%)	24	46
11	L	175/176 (99%)	168 (96%)	7 (4%)	31	56
12	M	117/161 (73%)	116 (99%)	1 (1%)	78	92
13	N	171/172 (99%)	168 (98%)	3 (2%)	59	81
14	O	170/173 (98%)	162 (95%)	8 (5%)	26	49
15	P	134/163 (82%)	130 (97%)	4 (3%)	41	68
16	Q	164/165 (99%)	159 (97%)	5 (3%)	41	68
17	R	158/175 (90%)	151 (96%)	7 (4%)	28	52
18	S	157/157 (100%)	152 (97%)	5 (3%)	39	65
19	T	139/140 (99%)	139 (100%)	0	100	100
20	U	88/114 (77%)	84 (96%)	4 (4%)	27	51
21	V	100/107 (94%)	99 (99%)	1 (1%)	76	90
22	W	55/126 (44%)	53 (96%)	2 (4%)	35	61
23	X	104/134 (78%)	102 (98%)	2 (2%)	57	80
24	Y	124/135 (92%)	119 (96%)	5 (4%)	31	56
25	Z	117/118 (99%)	110 (94%)	7 (6%)	19	37
26	a	119/120 (99%)	115 (97%)	4 (3%)	37	63
27	b	62/184 (34%)	60 (97%)	2 (3%)	39	65
28	c	80/98 (82%)	73 (91%)	7 (9%)	10	19
29	d	91/110 (83%)	90 (99%)	1 (1%)	73	89
30	e	114/121 (94%)	113 (99%)	1 (1%)	78	92
31	f	88/89 (99%)	87 (99%)	1 (1%)	73	89
32	g	98/100 (98%)	94 (96%)	4 (4%)	30	55
33	h	109/110 (99%)	103 (94%)	6 (6%)	21	41
34	i	86/89 (97%)	83 (96%)	3 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	j	73/80 (91%)	67 (92%)	6 (8%)	11	22
36	k	63/65 (97%)	57 (90%)	6 (10%)	8	17
37	l	46/48 (96%)	44 (96%)	2 (4%)	29	53
38	m	47/84 (56%)	45 (96%)	2 (4%)	29	53
39	n	22/24 (92%)	22 (100%)	0	100	100
40	o	91/94 (97%)	89 (98%)	2 (2%)	52	77
41	p	74/75 (99%)	72 (97%)	2 (3%)	44	71
42	r	109/121 (90%)	106 (97%)	3 (3%)	43	70
43	s	159/258 (62%)	152 (96%)	7 (4%)	28	52
44	t	115/137 (84%)	106 (92%)	9 (8%)	12	24
45	1	13/102 (13%)	12 (92%)	1 (8%)	13	25
52	AA	172/244 (70%)	161 (94%)	11 (6%)	17	33
53	BB	193/231 (84%)	185 (96%)	8 (4%)	30	55
54	CC	182/225 (81%)	170 (93%)	12 (7%)	16	32
55	DD	185/202 (92%)	170 (92%)	15 (8%)	11	23
56	EE	222/225 (99%)	210 (95%)	12 (5%)	22	42
57	FF	154/170 (91%)	140 (91%)	14 (9%)	9	18
58	GG	207/218 (95%)	184 (89%)	23 (11%)	6	11
59	HH	158/174 (91%)	144 (91%)	14 (9%)	9	19
60	II	178/180 (99%)	166 (93%)	12 (7%)	16	31
61	JJ	161/168 (96%)	152 (94%)	9 (6%)	21	40
62	KK	78/136 (57%)	71 (91%)	7 (9%)	9	19
63	LL	125/142 (88%)	121 (97%)	4 (3%)	39	65
64	MM	102/108 (94%)	94 (92%)	8 (8%)	12	24
65	NN	130/131 (99%)	123 (95%)	7 (5%)	22	42
66	OO	100/130 (77%)	92 (92%)	8 (8%)	12	23
67	PP	106/130 (82%)	97 (92%)	9 (8%)	10	21
68	QQ	116/121 (96%)	111 (96%)	5 (4%)	29	53
69	RR	107/121 (88%)	98 (92%)	9 (8%)	11	21
70	SS	122/132 (92%)	112 (92%)	10 (8%)	11	22
71	TT	109/115 (95%)	104 (95%)	5 (5%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	UU	93/107 (87%)	89 (96%)	4 (4%)	29	53
73	VV	65/67 (97%)	61 (94%)	4 (6%)	18	35
74	WW	112/113 (99%)	107 (96%)	5 (4%)	27	51
75	XX	113/115 (98%)	108 (96%)	5 (4%)	28	52
76	YY	107/112 (96%)	100 (94%)	7 (6%)	17	33
77	ZZ	64/103 (62%)	58 (91%)	6 (9%)	8	17
78	aa	85/98 (87%)	82 (96%)	3 (4%)	36	62
79	bb	72/76 (95%)	66 (92%)	6 (8%)	11	22
80	cc	54/62 (87%)	50 (93%)	4 (7%)	13	27
81	dd	47/49 (96%)	41 (87%)	6 (13%)	4	8
82	ee	39/106 (37%)	36 (92%)	3 (8%)	13	25
83	ff	59/140 (42%)	54 (92%)	5 (8%)	10	21
84	gg	263/275 (96%)	238 (90%)	25 (10%)	8	17
86	ii	358/394 (91%)	326 (91%)	32 (9%)	9	19
87	jj	508/526 (97%)	485 (96%)	23 (4%)	27	51
All	All	10707/12344 (87%)	10165 (95%)	542 (5%)	27	45

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	68	ARG
1	A	77	ILE
1	A	147	ARG
1	A	228	ASP
1	A	242	ARG
2	B	38	SER
2	B	71	GLU
2	B	125	SER
2	B	134	CYS
2	B	138	GLN
2	B	154	LYS
2	B	283	LYS
2	B	287	ILE
2	B	300	LYS
2	B	313	SER
3	C	95	MET

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Mol	Chain	Res	Type
3	C	114	ARG
3	C	122	TYR
3	C	201	ARG
3	C	204	ARG
3	C	268	ARG
3	C	275	SER
3	C	278	ASN
3	C	283	LYS
3	C	308	LYS
3	C	312	ARG
4	D	35	ARG
4	D	154	THR
4	D	185	SER
4	D	202	GLN
4	D	224	SER
4	D	228	LYS
4	D	232	THR
4	D	235	MET
5	E	44	PRO
5	E	66	SER
5	E	98	PRO
5	E	204	ILE
5	E	214	HIS
5	E	223	LYS
5	E	244	GLU
5	E	276	SER
6	F	34	LYS
6	F	186	MET
6	F	198	LYS
6	F	235	ARG
7	G	43	GLN
7	G	53	ARG
7	G	98	LEU
7	G	117	ARG
7	G	153	GLN
7	G	175	ARG
7	G	192	ARG
7	G	229	ARG
7	G	254	GLU
8	H	17	ASP
8	H	94	SER
8	H	106	GLN

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Mol	Chain	Res	Type
8	H	177	ASP
9	I	24	ARG
9	I	83	ASP
9	I	162	ARG
9	I	213	HIS
9	I	214	SER
10	J	52	LYS
10	J	81	GLU
10	J	129	ASP
10	J	132	VAL
10	J	143	ASP
10	J	158	SER
10	J	171	ASP
11	L	20	ARG
11	L	60	ARG
11	L	67	HIS
11	L	121	ARG
11	L	122	SER
11	L	136	LYS
11	L	208	GLU
12	M	54	CYS
13	N	17	ASP
13	N	67	ARG
13	N	169	ARG
14	O	31	ARG
14	O	49	ARG
14	O	61	ARG
14	O	62	MET
14	O	91	LYS
14	O	117	ARG
14	O	175	MET
14	O	191	LYS
15	P	3	ARG
15	P	14	SER
15	P	57	CYS
15	P	100	SER
16	Q	14	ARG
16	Q	42	THR
16	Q	147	GLU
16	Q	167	VAL
16	Q	168	ARG
17	R	12	SER

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Mol	Chain	Res	Type
17	R	13	SER
17	R	37	SER
17	R	62	ARG
17	R	65	LYS
17	R	71	ARG
17	R	154	LEU
18	S	29	ARG
18	S	53	LYS
18	S	93	MET
18	S	102	THR
18	S	164	LYS
20	U	67	LYS
20	U	93	LYS
20	U	101	ARG
20	U	108	GLU
21	V	109	LYS
22	W	4	GLU
22	W	38	SER
23	X	53	ARG
23	X	143	ASP
24	Y	40	GLN
24	Y	74	TYR
24	Y	115	ARG
24	Y	120	GLU
24	Y	121	ARG
25	Z	30	ASP
25	Z	36	ARG
25	Z	52	LYS
25	Z	64	LYS
25	Z	88	ASP
25	Z	107	LYS
25	Z	128	LYS
26	a	76	ASP
26	a	95	THR
26	a	119	LYS
26	a	134	GLU
27	b	25	ARG
27	b	60	ASN
28	c	16	SER
28	c	17	ARG
28	c	31	TYR
28	c	65	MET

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Mol	Chain	Res	Type
28	c	75	SER
28	c	92	CYS
28	c	103	ASP
29	d	78	ARG
30	e	11	LYS
31	f	46	ARG
32	g	29	ARG
32	g	68	SER
32	g	73	HIS
32	g	115	LYS
33	h	8	ASP
33	h	20	GLN
33	h	32	ARG
33	h	42	SER
33	h	66	LYS
33	h	97	LYS
34	i	17	VAL
34	i	32	ARG
34	i	89	GLU
35	j	10	LYS
35	j	20	ARG
35	j	33	THR
35	j	39	TYR
35	j	55	ARG
35	j	82	THR
36	k	9	LYS
36	k	14	THR
36	k	16	ARG
36	k	48	THR
36	k	54	GLU
36	k	61	PRO
37	l	15	LYS
37	l	46	ARG
38	m	81	SER
38	m	84	GLN
40	o	78	ARG
40	o	79	SER
41	p	7	LYS
41	p	74	THR
42	r	58	LYS
42	r	67	ARG
42	r	68	SER

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Mol	Chain	Res	Type
43	s	11	SER
43	s	50	LYS
43	s	83	ARG
43	s	96	THR
43	s	119	CYS
43	s	136	SER
43	s	187	LEU
44	t	13	VAL
44	t	16	ARG
44	t	17	CYS
44	t	45	ASP
44	t	63	THR
44	t	114	ARG
44	t	119	ARG
44	t	123	ARG
44	t	149	HIS
45	1	67	LYS
52	AA	14	ASP
52	AA	44	ASP
52	AA	47	TYR
52	AA	75	SER
52	AA	81	ASN
52	AA	89	LYS
52	AA	152	SER
52	AA	185	MET
52	AA	191	ARG
52	AA	193	HIS
52	AA	200	ASP
53	BB	23	ASP
53	BB	88	THR
53	BB	95	ASN
53	BB	115	LYS
53	BB	131	ASP
53	BB	147	ASN
53	BB	172	MET
53	BB	208	HIS
54	CC	72	ASP
54	CC	77	SER
54	CC	121	ARG
54	CC	145	LYS
54	CC	176	LYS
54	CC	184	VAL

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Mol	Chain	Res	Type
54	CC	206	SER
54	CC	236	PHE
54	CC	242	ASP
54	CC	248	TYR
54	CC	259	THR
54	CC	272	HIS
55	DD	24	PHE
55	DD	65	ARG
55	DD	67	ARG
55	DD	74	GLN
55	DD	76	ARG
55	DD	84	VAL
55	DD	94	ARG
55	DD	123	LEU
55	DD	124	ARG
55	DD	146	ARG
55	DD	167	TYR
55	DD	175	VAL
55	DD	178	ARG
55	DD	218	LEU
55	DD	221	THR
56	EE	21	ASP
56	EE	93	ASP
56	EE	120	LYS
56	EE	130	PHE
56	EE	145	ARG
56	EE	148	ARG
56	EE	155	LYS
56	EE	170	THR
56	EE	181	CYS
56	EE	226	PHE
56	EE	233	LYS
56	EE	254	LYS
57	FF	20	PHE
57	FF	26	ASP
57	FF	36	GLN
57	FF	52	SER
57	FF	66	CYS
57	FF	79	HIS
57	FF	91	ARG
57	FF	110	GLN
57	FF	127	ARG

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Mol	Chain	Res	Type
57	FF	135	ARG
57	FF	136	ARG
57	FF	175	ASP
57	FF	193	LYS
57	FF	202	SER
58	GG	13	GLN
58	GG	15	LEU
58	GG	22	ARG
58	GG	26	THR
58	GG	30	LYS
58	GG	31	ARG
58	GG	32	MET
58	GG	92	ARG
58	GG	93	LYS
58	GG	100	CYS
58	GG	111	LEU
58	GG	131	ARG
58	GG	132	ARG
58	GG	139	SER
58	GG	142	ARG
58	GG	172	LYS
58	GG	204	GLU
58	GG	216	ARG
58	GG	217	MET
58	GG	218	LYS
58	GG	219	GLU
58	GG	232	ARG
58	GG	235	SER
59	HH	23	ILE
59	HH	24	SER
59	HH	42	GLU
59	HH	57	ARG
59	HH	83	LEU
59	HH	85	LYS
59	HH	113	LYS
59	HH	116	ARG
59	HH	122	LEU
59	HH	147	LYS
59	HH	159	ASP
59	HH	162	GLN
59	HH	167	GLU
59	HH	177	TYR

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Mol	Chain	Res	Type
60	II	5	ARG
60	II	41	ARG
60	II	89	GLU
60	II	123	ARG
60	II	128	LYS
60	II	129	LEU
60	II	140	LYS
60	II	144	LYS
60	II	159	SER
60	II	182	CYS
60	II	191	GLU
60	II	205	ARG
61	JJ	6	SER
61	JJ	23	SER
61	JJ	79	ARG
61	JJ	93	LYS
61	JJ	104	ASP
61	JJ	107	GLU
61	JJ	112	THR
61	JJ	161	LEU
61	JJ	172	ARG
62	KK	6	LYS
62	KK	16	PHE
62	KK	24	LYS
62	KK	39	ASN
62	KK	61	GLN
62	KK	81	ASP
62	KK	82	TYR
63	LL	20	LYS
63	LL	69	ARG
63	LL	116	CYS
63	LL	141	ASN
64	MM	33	ARG
64	MM	40	LYS
64	MM	50	CYS
64	MM	63	LYS
64	MM	71	GLU
64	MM	84	LYS
64	MM	116	LYS
64	MM	127	TYR
65	NN	5	HIS
65	NN	73	ARG

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Mol	Chain	Res	Type
65	NN	84	LEU
65	NN	86	GLU
65	NN	106	ARG
65	NN	140	LYS
65	NN	145	THR
66	OO	34	PHE
66	OO	47	LEU
66	OO	48	SER
66	OO	75	MET
66	OO	137	SER
66	OO	138	ASP
66	OO	146	ARG
66	OO	151	LEU
67	PP	14	LYS
67	PP	18	ARG
67	PP	29	SER
67	PP	38	SER
67	PP	51	ARG
67	PP	70	MET
67	PP	75	VAL
67	PP	108	LYS
67	PP	114	HIS
68	QQ	25	CYS
68	QQ	49	TYR
68	QQ	69	ARG
68	QQ	87	SER
68	QQ	109	LYS
69	RR	17	ILE
69	RR	33	ARG
69	RR	45	LYS
69	RR	47	ARG
69	RR	77	GLU
69	RR	78	ARG
69	RR	80	ARG
69	RR	89	SER
69	RR	116	ASN
70	SS	8	LYS
70	SS	23	ARG
70	SS	30	ILE
70	SS	34	LYS
70	SS	55	ARG
70	SS	62	ASP

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Mol	Chain	Res	Type
70	SS	83	PHE
70	SS	86	ARG
70	SS	115	LYS
70	SS	135	HIS
71	TT	49	ASP
71	TT	65	TYR
71	TT	90	SER
71	TT	131	LEU
71	TT	133	ARG
72	UU	26	SER
72	UU	65	THR
72	UU	75	LYS
72	UU	99	LYS
73	VV	1	MET
73	VV	10	ASP
73	VV	65	SER
73	VV	69	ILE
74	WW	30	CYS
74	WW	43	LYS
74	WW	57	ARG
74	WW	66	THR
74	WW	121	THR
75	XX	90	CYS
75	XX	105	PHE
75	XX	130	LEU
75	XX	135	LYS
75	XX	139	GLU
76	YY	20	ARG
76	YY	42	GLU
76	YY	78	SER
76	YY	99	LYS
76	YY	110	ARG
76	YY	111	LYS
76	YY	120	THR
77	ZZ	52	LYS
77	ZZ	56	ASP
77	ZZ	57	LYS
77	ZZ	60	LYS
77	ZZ	78	LYS
77	ZZ	90	GLU
78	aa	19	GLN
78	aa	46	GLU

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Mol	Chain	Res	Type
78	aa	85	ARG
79	bb	17	ARG
79	bb	33	MET
79	bb	34	ASP
79	bb	42	LYS
79	bb	51	GLN
79	bb	80	ARG
80	cc	13	ARG
80	cc	30	VAL
80	cc	60	GLU
80	cc	68	LEU
81	dd	19	ARG
81	dd	27	ARG
81	dd	33	LYS
81	dd	48	LYS
81	dd	49	ASP
81	dd	53	ILE
82	ee	17	LEU
82	ee	26	LYS
82	ee	40	ARG
83	ff	78	LYS
83	ff	90	ARG
83	ff	111	ARG
83	ff	135	TYR
83	ff	144	CYS
84	gg	5	MET
84	gg	8	ARG
84	gg	29	ASP
84	gg	30	MET
84	gg	43	TRP
84	gg	57	ARG
84	gg	68	ASP
84	gg	91	ASP
84	gg	100	ARG
84	gg	101	PHE
84	gg	102	VAL
84	gg	110	SER
84	gg	113	PHE
84	gg	126	ASP
84	gg	131	LEU
84	gg	133	ASN
84	gg	156	PHE

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Mol	Chain	Res	Type
84	gg	160	SER
84	gg	182	CYS
84	gg	184	LEU
84	gg	199	THR
84	gg	203	ASP
84	gg	225	LYS
84	gg	282	GLU
84	gg	285	GLN
86	ii	6	SER
86	ii	30	ASN
86	ii	50	LYS
86	ii	77	SER
86	ii	83	LYS
86	ii	87	LYS
86	ii	111	ASN
86	ii	123	SER
86	ii	145	LYS
86	ii	154	SER
86	ii	166	ARG
86	ii	173	THR
86	ii	189	ARG
86	ii	237	SER
86	ii	258	TYR
86	ii	273	GLU
86	ii	285	LYS
86	ii	314	MET
86	ii	332	VAL
86	ii	336	GLN
86	ii	342	LYS
86	ii	343	ILE
86	ii	352	LYS
86	ii	366	HIS
86	ii	367	GLU
86	ii	368	LEU
86	ii	372	MET
86	ii	393	THR
86	ii	394	ASP
86	ii	400	SER
86	ii	404	LYS
86	ii	414	ARG
87	jj	33	ARG
87	jj	53	THR

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Mol	Chain	Res	Type
87	jj	73	VAL
87	jj	116	LYS
87	jj	118	THR
87	jj	134	TYR
87	jj	160	LEU
87	jj	163	ASP
87	jj	223	GLN
87	jj	284	ASP
87	jj	285	PHE
87	jj	323	ARG
87	jj	326	ASP
87	jj	370	THR
87	jj	388	PHE
87	jj	489	SER
87	jj	524	MET
87	jj	530	ASP
87	jj	536	ASP
87	jj	552	LEU
87	jj	574	ARG
87	jj	576	ARG
87	jj	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	8	GLN
62	KK	61	GLN
70	SS	97	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	0
47	3	72/75 (96%)	20 (27%)	0
48	5	3502/3543 (98%)	648 (18%)	72 (2%)
49	7	119/120 (99%)	11 (9%)	0
50	8	155/156 (99%)	29 (18%)	3 (1%)
51	9	1676/1869 (89%)	439 (26%)	36 (2%)
85	hh	10/197 (5%)	3 (30%)	0
All	All	5608/6036 (92%)	1170 (20%)	111 (1%)

All (1170) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	7	G
46	2	8	U
46	2	9	A
46	2	15	G
46	2	19	G
46	2	20	U
46	2	31	C
46	2	47	U
46	2	49	C
46	2	58	A
46	2	61	C
46	2	62	C
46	2	65	G
46	2	67	G
46	2	68	G
46	2	70	A
46	2	73	A
46	2	74	C
46	2	75	C
46	2	76	A
47	3	11	C
47	3	13	C
47	3	16	C
47	3	19	G
47	3	21	A
47	3	22	G
47	3	23	A
47	3	31	A
47	3	34	U
47	3	46	G
47	3	47	U
47	3	49	C
47	3	50	A
47	3	56	C
47	3	58	A
47	3	63	C
47	3	65	G
47	3	67	U
47	3	69	G
47	3	76	A
48	5	13	U
48	5	39	A

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Mol	Chain	Res	Type
48	5	56	A
48	5	59	A
48	5	64	A
48	5	65	A
48	5	73	A
48	5	74	G
48	5	91	G
48	5	98	A
48	5	104	G
48	5	109	G
48	5	110	C
48	5	116	G
48	5	117	C
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	140	G
48	5	144	G
48	5	159	C
48	5	166	C
48	5	167	C
48	5	170	C
48	5	177	G
48	5	182	G
48	5	200	U
48	5	201	C
48	5	209	U
48	5	216	C
48	5	218	A
48	5	219	G
48	5	220	C
48	5	224	U
48	5	232	G
48	5	233	U
48	5	234	G
48	5	246	G
48	5	253	G
48	5	256	G

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Mol	Chain	Res	Type
48	5	260	C
48	5	265	C
48	5	266	C
48	5	267	G
48	5	268	G
48	5	271	C
48	5	276	C
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	315	G
48	5	316	U
48	5	326	C
48	5	334	A
48	5	340	C
48	5	350	C
48	5	354	U
48	5	386	A
48	5	387	G
48	5	403	G
48	5	407	A
48	5	409	G
48	5	412	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	462	G
48	5	463	A
48	5	464	G
48	5	465	G
48	5	467	U
48	5	468	U
48	5	481	G
48	5	481(A)	C
48	5	482	G
48	5	484	U

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Mol	Chain	Res	Type
48	5	485	C
48	5	486	C
48	5	492	U
48	5	493	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	521	C
48	5	639	U
48	5	642	G
48	5	657	C
48	5	658	C
48	5	660	G
48	5	666	G
48	5	670	G
48	5	685	C
48	5	686	A
48	5	687	U
48	5	694	C
48	5	697	G
48	5	703	G
48	5	704	C
48	5	705	G
48	5	730	G
48	5	731	G
48	5	733	A
48	5	738	C
48	5	742	G
48	5	744	G
48	5	746	A
48	5	747	A
48	5	758	G
48	5	910	G
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	923	C
48	5	925	C
48	5	926	G
48	5	929	A

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Mol	Chain	Res	Type
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C
48	5	943	A
48	5	945	U
48	5	959	G
48	5	960	A
48	5	961	G
48	5	966	A
48	5	967	C
48	5	969	C
48	5	972	C
48	5	973	G
48	5	983	C
48	5	1068	G
48	5	1070	G
48	5	1071	C
48	5	1072	C
48	5	1073	G
48	5	1079	C
48	5	1082	C
48	5	1094	G
48	5	1097	C
48	5	1169	G
48	5	1172	C
48	5	1174	G
48	5	1176	C
48	5	1179	U
48	5	1184	A
48	5	1195	G
48	5	1200	G
48	5	1209	U
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G

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Mol	Chain	Res	Type
48	5	1236	C
48	5	1237	C
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1275	G
48	5	1277	G
48	5	1280	C
48	5	1284	G
48	5	1285	U
48	5	1287	G
48	5	1292	C
48	5	1293	G
48	5	1294	A
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1313	C
48	5	1326	A2M
48	5	1337	A
48	5	1354	A
48	5	1358	G
48	5	1359	G
48	5	1371	A
48	5	1377	G
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1406	G
48	5	1411(A)	G
48	5	1412	G
48	5	1414	C
48	5	1415	G
48	5	1420	A
48	5	1437	C
48	5	1441	C
48	5	1442	C
48	5	1443	A
48	5	1445	U
48	5	1446	C

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Mol	Chain	Res	Type
48	5	1456	C
48	5	1457	G
48	5	1477	C
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1514	U
48	5	1523	A
48	5	1534	A2M
48	5	1547	A
48	5	1564	A
48	5	1566	C
48	5	1578	U
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	OMG
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1638	A
48	5	1641	G
48	5	1654	G
48	5	1661	C
48	5	1676	C
48	5	1677	PSU
48	5	1694	C
48	5	1726	U
48	5	1731	C
48	5	1734	G
48	5	1735	U
48	5	1741	G
48	5	1742	A
48	5	1750	G

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Mol	Chain	Res	Type
48	5	1754	U
48	5	1756	U
48	5	1757	U
48	5	1759	G
48	5	1760	G
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1780	A
48	5	1781	PSU
48	5	1787	A
48	5	1804	A
48	5	1805	A
48	5	1806	G
48	5	1809	C
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1892	A
48	5	1897	A
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1930	U
48	5	1931	C
48	5	1932	A
48	5	1940	G
48	5	1948	G
48	5	1957	U
48	5	1958	A
48	5	1959	U

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Mol	Chain	Res	Type
48	5	1960	A
48	5	1961	G
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1971	C
48	5	1972	G
48	5	1974	U
48	5	1975	G
48	5	1976	G
48	5	1978	C
48	5	1979	A
48	5	1980	U
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1987	C
48	5	1988	G
48	5	1990	A
48	5	1991	A
48	5	1992	U
48	5	1997	U
48	5	1998	A
48	5	1999	A
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2009	A
48	5	2011	C
48	5	2025	A
48	5	2026	A
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2069	A
48	5	2071	A
48	5	2084	U
48	5	2089	G

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Mol	Chain	Res	Type
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2267	U
48	5	2289	C
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2333	G
48	5	2348	G
48	5	2351	OMC
48	5	2360	A
48	5	2382	A
48	5	2395	A
48	5	2422	OMC
48	5	2424	OMG
48	5	2425	U
48	5	2433	G
48	5	2441	C
48	5	2450	G
48	5	2453	A
48	5	2475	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2492	C

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Mol	Chain	Res	Type
48	5	2494	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2511	A
48	5	2513	A
48	5	2529	A
48	5	2530	U
48	5	2544	G
48	5	2545	U
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2564	G
48	5	2565	A
48	5	2566	G
48	5	2569	G
48	5	2570	U
48	5	2583	C
48	5	2587	A
48	5	2611	A
48	5	2628	U
48	5	2638	G
48	5	2640	G
48	5	2653	C
48	5	2658	G
48	5	2662	G
48	5	2669	C
48	5	2673	G
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2711	G
48	5	2716	C
48	5	2721	G
48	5	2726	G
48	5	2735	G
48	5	2740	U

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Mol	Chain	Res	Type
48	5	2743	A
48	5	2753	G
48	5	2754	G
48	5	2763	U
48	5	2764	A
48	5	2765	A
48	5	2769	U
48	5	2788	U
48	5	2790	U
48	5	2799	G
48	5	2826	U
48	5	2827	G
48	5	2829	U
48	5	2833	A
48	5	2842	G
48	5	2855	G
48	5	2869	U
48	5	3598	C
48	5	3602	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3616	U
48	5	3617	G
48	5	3618	C
48	5	3625	G
48	5	3626	G
48	5	3635	A
48	5	3644	U
48	5	3657	U
48	5	3662	A
48	5	3673	C
48	5	3688	U
48	5	3710	G
48	5	3712	A
48	5	3713	U
48	5	3714	G
48	5	3743	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3760	A2M

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Mol	Chain	Res	Type
48	5	3761	C
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3783	A
48	5	3784	A
48	5	3786	U
48	5	3788	C
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3897	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3939	G
48	5	3943	A
48	5	3948	C
48	5	4066	U
48	5	4069	U
48	5	4076	G
48	5	4084	G
48	5	4096	C
48	5	4097	G
48	5	4119	C
48	5	4120	U
48	5	4122	G
48	5	4127	A

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Mol	Chain	Res	Type
48	5	4134	C
48	5	4158	C
48	5	4161	G
48	5	4163	U
48	5	4170	A
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4203	A
48	5	4221	C
48	5	4225	G
48	5	4229	U
48	5	4233	A
48	5	4251	A
48	5	4252	C
48	5	4254	G
48	5	4258	C
48	5	4266	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4304	A
48	5	4305	G
48	5	4314	C
48	5	4329	G
48	5	4330	G
48	5	4339	A
48	5	4349	C
48	5	4364	G
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4394	A
48	5	4395	U
48	5	4419	U

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Mol	Chain	Res	Type
48	5	4421	C
48	5	4422	A
48	5	4430	G
48	5	4439	U
48	5	4440	G
48	5	4448	G
48	5	4449	A
48	5	4464	A
48	5	4475	G
48	5	4500	PSU
48	5	4512	U
48	5	4513	A
48	5	4519	C
48	5	4524	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4590	A
48	5	4606	G
48	5	4636	U
48	5	4637	OMG
48	5	4656	A
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4700	A
48	5	4709	U
48	5	4720	C
48	5	4736	C
48	5	4740	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4769	G

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Mol	Chain	Res	Type
48	5	4771	C
48	5	4772	C
48	5	4776	G
48	5	4860	G
48	5	4867	G
48	5	4870	G
48	5	4871	C
48	5	4873	G
48	5	4875	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4895	C
48	5	4896	G
48	5	4903	G
48	5	4904	G
48	5	4905	C
48	5	4906	C
48	5	4907	G
48	5	4908	G
48	5	4912	G
48	5	4914	G
48	5	4917	C
48	5	4921	C
48	5	4922	C
48	5	4923	U
48	5	4924	C
48	5	4926	C
48	5	4933	C
48	5	4934	A
48	5	4944	C
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4960	G
48	5	4963	G
48	5	4964	C
48	5	4966	A

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Mol	Chain	Res	Type
48	5	4967	A
48	5	4976	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4993	G
48	5	5007	A
48	5	5014	A
48	5	5017	G
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5061	A
48	5	5062	G
49	7	10	C
49	7	25	G
49	7	33	U
49	7	40	U
49	7	42	A
49	7	53	U
49	7	64	G
49	7	89	G
49	7	100	A
49	7	110	G
49	7	120	U
50	8	2	G
50	8	34	U
50	8	35	C
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	81	C
50	8	82	A
50	8	83	C
50	8	84	A
50	8	85	U
50	8	86	U
50	8	94	G
50	8	95	A

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Mol	Chain	Res	Type
50	8	103	A
50	8	105	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	114	G
50	8	125	C
50	8	126	C
50	8	127	U
50	8	135	C
50	8	147	G
50	8	150	C
50	8	153	C
50	8	156	U
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	34	PSU
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	62	G
51	9	65	C
51	9	67	C
51	9	68	A
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	76	U
51	9	78	C
51	9	79	A
51	9	99	A2M
51	9	103	A

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Mol	Chain	Res	Type
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	124	U
51	9	126	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	162	C
51	9	163	U
51	9	166	A2M
51	9	171	A
51	9	172	OMU
51	9	173	A
51	9	180	G
51	9	182	C
51	9	184	G
51	9	187	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	192	C
51	9	197	U
51	9	202	G
51	9	207	G
51	9	209	A
51	9	211	G
51	9	212	C
51	9	214	U
51	9	215	G
51	9	216	C
51	9	217	A
51	9	291	G
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	305	U

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Mol	Chain	Res	Type
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	313	A
51	9	319	C
51	9	320	G
51	9	321	C
51	9	322	C
51	9	324	C
51	9	325	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	334	C
51	9	336	A
51	9	338	G
51	9	343	A
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	369	C
51	9	370	G
51	9	385	G
51	9	386	C
51	9	400	C
51	9	408	A
51	9	409	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	465	A
51	9	466	G
51	9	471	G
51	9	472	C

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Mol	Chain	Res	Type
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	489	A
51	9	492	C
51	9	508	A
51	9	525	A
51	9	532	C
51	9	533	A
51	9	535	G
51	9	536	A
51	9	537	C
51	9	542	U
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	552	G
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	564	A
51	9	568	C
51	9	571	U
51	9	576	A
51	9	580	U
51	9	583	A
51	9	585	C
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	600	G
51	9	605	A
51	9	606	G
51	9	608	C
51	9	614	C

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Mol	Chain	Res	Type
51	9	617	G
51	9	620	G
51	9	628	A
51	9	631	U
51	9	632	C
51	9	643	A
51	9	646	G
51	9	655	A
51	9	660	C
51	9	664	A
51	9	668	A2M
51	9	669	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	688	U
51	9	694	G
51	9	696	G
51	9	698	G
51	9	732	U
51	9	733	C
51	9	734	C
51	9	735	C
51	9	736	C
51	9	737	G
51	9	738	C
51	9	800	U
51	9	801	PSU
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	PSU
51	9	823	U
51	9	827	A
51	9	830	A
51	9	834	C
51	9	836	G
51	9	837	A
51	9	838	G
51	9	839	C
51	9	840	C

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Mol	Chain	Res	Type
51	9	841	G
51	9	844	U
51	9	847	A
51	9	865	A
51	9	870	A
51	9	871	U
51	9	873	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	881	G
51	9	882	U
51	9	887	U
51	9	888	U
51	9	895	G
51	9	896	U
51	9	897	U
51	9	898	U
51	9	899	U
51	9	902	G
51	9	903	A
51	9	906	U
51	9	909	G
51	9	910	G
51	9	913	A
51	9	914	U
51	9	917	U
51	9	920	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	953	C
51	9	970	G
51	9	971	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1017	U
51	9	1023	A

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Mol	Chain	Res	Type
51	9	1040	G
51	9	1044	G
51	9	1045	PSU
51	9	1049	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1077	A
51	9	1083	A
51	9	1085	C
51	9	1086	G
51	9	1089	G
51	9	1096	G
51	9	1110	G
51	9	1113	A
51	9	1115	U
51	9	1116	C
51	9	1120	U
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1158	G
51	9	1171	G
51	9	1181	A
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1209	A
51	9	1210	G
51	9	1211	G
51	9	1215	C
51	9	1224	G
51	9	1242	U
51	9	1243	U
51	9	1249	C
51	9	1251	A
51	9	1253	A

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Mol	Chain	Res	Type
51	9	1256	G
51	9	1257	G
51	9	1265	A
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1280	G
51	9	1281	G
51	9	1282	A
51	9	1283	C
51	9	1284	A
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1291	A
51	9	1292	C
51	9	1293	A
51	9	1294	G
51	9	1298	G
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1310	U
51	9	1311	C
51	9	1313	A
51	9	1314	U
51	9	1315	U
51	9	1317	C
51	9	1319	U
51	9	1321	G
51	9	1333	U
51	9	1342	U
51	9	1345	G
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1394	G

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Mol	Chain	Res	Type
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1401	A
51	9	1402	A
51	9	1407	U
51	9	1408	U
51	9	1409	A
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1416	C
51	9	1418	C
51	9	1419	C
51	9	1420	G
51	9	1423	C
51	9	1424	G
51	9	1426	U
51	9	1427	C
51	9	1429	G
51	9	1431	G
51	9	1432	U
51	9	1433	C
51	9	1434	C
51	9	1435	C
51	9	1436	C
51	9	1438	A
51	9	1439	A
51	9	1440	C
51	9	1442	OMU
51	9	1447	G
51	9	1454	A
51	9	1455	A
51	9	1460	C
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1472	C
51	9	1476	A
51	9	1477	U
51	9	1478	U

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Mol	Chain	Res	Type
51	9	1480	A
51	9	1489	A
51	9	1490	OMG
51	9	1496	U
51	9	1498	A
51	9	1502	C
51	9	1510	G
51	9	1512	C
51	9	1514	G
51	9	1519	U
51	9	1521	C
51	9	1522	A
51	9	1533	A
51	9	1544	C
51	9	1548	G
51	9	1552	G
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1558	C
51	9	1560	U
51	9	1567	G
51	9	1574	C
51	9	1575	G
51	9	1576	G
51	9	1579	A
51	9	1580	A
51	9	1581	C
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1599	U
51	9	1604	G
51	9	1621	U
51	9	1623	A
51	9	1637	A
51	9	1638	G
51	9	1639	G7M
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1657	G

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Mol	Chain	Res	Type
51	9	1664	A
51	9	1665	G
51	9	1669	G
51	9	1695	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1744	G
51	9	1753	C
51	9	1756	C
51	9	1759	G
51	9	1774	C
51	9	1775	U
51	9	1777	G
51	9	1783	C
51	9	1784	G
51	9	1786	U
51	9	1794	C
51	9	1797	U
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1864	U
51	9	1865	C
85	hh	43	A
85	hh	46	G
85	hh	49	U

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	42	A
48	5	125	C

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Mol	Chain	Res	Type
48	5	133	C
48	5	134	G
48	5	217	C
48	5	231	U
48	5	245	C
48	5	265	C
48	5	267	G
48	5	275	C
48	5	278	G
48	5	385	A
48	5	406	C
48	5	449	C
48	5	480	C
48	5	485	C
48	5	504	G
48	5	922(B)	C
48	5	924	C
48	5	930	G
48	5	959	G
48	5	1072	C
48	5	1211	G
48	5	1236	C
48	5	1238	A
48	5	1291	G
48	5	1370	G
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1590	C
48	5	1625	OMG
48	5	1633	G
48	5	1733	G
48	5	1818	G
48	5	1956	A
48	5	1975	G
48	5	1978	C
48	5	1982	G
48	5	1990	A
48	5	1991	A
48	5	2046	G
48	5	2068	C
48	5	2089	G

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Mol	Chain	Res	Type
48	5	2104	A
48	5	2258	C
48	5	2266	C
48	5	2488	C
48	5	2502	A
48	5	2529	A
48	5	2587	A
48	5	2639	U
48	5	2695	A
48	5	2794	C
48	5	3603	G
48	5	3625	G
48	5	3672	G
48	5	3876	A
48	5	3888	G
48	5	4119	C
48	5	4232	U
48	5	4378	A
48	5	4394	A
48	5	4395	U
48	5	4448	G
48	5	4548	A
48	5	4699	U
48	5	4719	G
48	5	4884	G
48	5	4925	U
48	5	4932	U
48	5	4947	U
50	8	81	C
50	8	94	G
50	8	124	U
51	9	72	C
51	9	102	A
51	9	110	U
51	9	140	C
51	9	208	G
51	9	213	G
51	9	215	G
51	9	291	G
51	9	327	G
51	9	369	C
51	9	407	G

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Mol	Chain	Res	Type
51	9	417	C
51	9	434	G
51	9	465	A
51	9	532	C
51	9	563	G
51	9	642	U
51	9	840	C
51	9	869	A
51	9	870	A
51	9	1137	U
51	9	1281	G
51	9	1394	G
51	9	1395	C
51	9	1408	U
51	9	1418	C
51	9	1432	U
51	9	1463	U
51	9	1477	U
51	9	1490	OMG
51	9	1556	A
51	9	1637	A
51	9	1646	C
51	9	1647	A
51	9	1824	A
51	9	1835	A

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

163 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	$\#\|Z\| > 2$
48	OMC	5	2365	48	19,22,23	2.83	8 (42%)	26,31,34	0.66	0
48	A2M	5	3718	48	18,25,26	4.28	7 (38%)	18,36,39	3.45	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
51	A2M	9	512	51	18,25,26	4.21	6 (33%)	18,36,39	3.77	3 (16%)
51	PSU	9	1367	51	18,20,22	1.09	1 (5%)	21,28,33	1.80	4 (19%)
48	A2M	5	400	48	18,25,26	4.17	8 (44%)	18,36,39	3.04	3 (16%)
48	OMC	5	2422	48,88	19,22,23	2.92	8 (42%)	26,31,34	0.70	0
48	OMU	5	2837	48	19,22,23	2.80	6 (31%)	26,31,34	1.90	6 (23%)
48	PSU	5	4299	48	18,20,22	0.96	1 (5%)	21,28,33	1.83	3 (14%)
48	PSU	5	4628	48	18,20,22	1.16	1 (5%)	21,28,33	2.07	5 (23%)
51	A2M	9	166	51	18,25,26	4.13	6 (33%)	18,36,39	3.44	3 (16%)
48	PSU	5	4423	48	18,20,22	0.97	1 (5%)	21,28,33	1.87	3 (14%)
51	OMG	9	644	51	18,26,27	2.40	8 (44%)	19,38,41	1.37	3 (15%)
48	OMG	5	3899	48	18,26,27	2.40	8 (44%)	19,38,41	1.44	4 (21%)
51	OMG	9	436	51	18,26,27	2.49	8 (44%)	19,38,41	1.53	4 (21%)
48	PSU	5	1677	48	18,20,22	1.20	2 (11%)	21,28,33	2.06	3 (14%)
48	OMC	5	2351	48	19,22,23	2.73	8 (42%)	26,31,34	0.81	0
51	OMU	9	1442	51	19,22,23	2.80	6 (31%)	26,31,34	1.72	4 (15%)
48	PSU	5	4552	48	18,20,22	1.11	1 (5%)	21,28,33	1.83	3 (14%)
51	OMG	9	683	51	18,26,27	2.55	8 (44%)	19,38,41	1.72	4 (21%)
48	UY1	5	3818	48,88	19,22,23	4.18	9 (47%)	22,31,34	1.94	5 (22%)
48	PSU	5	4353	48	18,20,22	1.07	1 (5%)	21,28,33	1.99	5 (23%)
51	PSU	9	119	51	18,20,22	1.01	1 (5%)	21,28,33	1.90	5 (23%)
48	PSU	5	4420	48	18,20,22	1.07	1 (5%)	21,28,33	1.95	4 (19%)
51	OMC	9	1703	51	19,22,23	2.95	8 (42%)	26,31,34	0.79	0
51	PSU	9	1081	51	18,20,22	1.09	1 (5%)	21,28,33	1.92	6 (28%)
51	PSU	9	1445	51	18,20,22	0.99	1 (5%)	21,28,33	1.73	4 (19%)
48	OMG	5	3792	48	18,26,27	2.34	7 (38%)	19,38,41	1.44	4 (21%)
48	OMC	5	3841	48	19,22,23	2.81	8 (42%)	26,31,34	0.88	0
48	OMG	5	4392	48	18,26,27	2.33	8 (44%)	19,38,41	1.50	4 (21%)
51	OMU	9	121	51	19,22,23	2.68	6 (31%)	26,31,34	1.79	6 (23%)
48	A2M	5	3760	48,88	18,25,26	4.26	7 (38%)	18,36,39	3.48	3 (16%)
51	A2M	9	27	51	18,25,26	4.12	6 (33%)	18,36,39	3.44	3 (16%)
51	PSU	9	105	51	18,20,22	1.08	1 (5%)	21,28,33	1.88	3 (14%)
48	A2M	5	3830	48	18,25,26	4.11	7 (38%)	18,36,39	3.42	3 (16%)
48	OMG	5	4623	48	18,26,27	2.49	8 (44%)	19,38,41	1.64	4 (21%)
48	5MC	5	4447	48,88	18,22,23	3.35	7 (38%)	26,32,35	1.16	2 (7%)
51	PSU	9	1244	51	18,20,22	1.11	1 (5%)	21,28,33	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	A2M	5	4523	48,88	18,25,26	4.12	7 (38%)	18,36,39	3.52	3 (16%)
48	PSU	5	4442	48	18,20,22	1.04	1 (5%)	21,28,33	1.97	5 (23%)
51	PSU	9	218	51	18,20,22	1.08	1 (5%)	21,28,33	2.16	6 (28%)
51	PSU	9	801	51	18,20,22	1.20	2 (11%)	21,28,33	1.57	4 (19%)
51	PSU	9	815	51	18,20,22	1.00	1 (5%)	21,28,33	2.05	5 (23%)
48	OMC	5	2804	48	19,22,23	2.78	8 (42%)	26,31,34	0.71	0
51	PSU	9	1347	51	18,20,22	1.03	1 (5%)	21,28,33	1.89	5 (23%)
48	PSU	5	1683	48,88	18,20,22	1.17	1 (5%)	21,28,33	1.91	4 (19%)
48	PSU	5	4361	48	18,20,22	1.06	1 (5%)	21,28,33	1.90	3 (14%)
48	A2M	5	3867	48	18,25,26	4.11	6 (33%)	18,36,39	3.39	3 (16%)
51	OMG	9	509	51,88	18,26,27	2.41	7 (38%)	19,38,41	1.45	4 (21%)
51	A2M	9	159	51	18,25,26	4.28	7 (38%)	18,36,39	3.43	3 (16%)
48	A2M	5	1524	48	18,25,26	4.08	7 (38%)	18,36,39	3.44	3 (16%)
48	UR3	5	4530	48	19,22,23	2.60	7 (36%)	26,32,35	1.21	3 (11%)
48	OMU	5	4227	48	19,22,23	2.79	7 (36%)	26,31,34	1.74	5 (19%)
48	A2M	5	3724	48	18,25,26	4.28	7 (38%)	18,36,39	3.23	3 (16%)
51	4AC	9	1842	51	21,24,25	3.03	10 (47%)	29,34,37	1.04	2 (6%)
48	PSU	5	4532	48	18,20,22	1.06	1 (5%)	21,28,33	1.67	2 (9%)
51	A2M	9	99	51,88	18,25,26	4.28	7 (38%)	18,36,39	3.41	3 (16%)
48	A2M	5	1326	48	18,25,26	4.16	7 (38%)	18,36,39	3.39	3 (16%)
48	2MG	5	1517	48	18,26,27	2.22	7 (38%)	16,38,41	1.52	3 (18%)
48	OMG	5	2876	48	18,26,27	2.43	8 (44%)	19,38,41	1.38	3 (15%)
51	A2M	9	1031	51	18,25,26	4.21	7 (38%)	18,36,39	3.30	3 (16%)
51	MA6	9	1850	51	19,26,27	1.19	1 (5%)	18,38,41	4.45	3 (16%)
48	PSU	5	1792	48	18,20,22	1.00	1 (5%)	21,28,33	1.79	3 (14%)
51	PSU	9	1692	51	18,20,22	1.08	1 (5%)	21,28,33	1.68	3 (14%)
51	PSU	9	649	51	18,20,22	1.01	1 (5%)	21,28,33	1.79	3 (14%)
48	OMG	5	4499	48	18,26,27	2.52	8 (44%)	19,38,41	1.56	4 (21%)
48	OMG	5	373	48	18,26,27	2.42	8 (44%)	19,38,41	1.57	3 (15%)
51	PSU	9	1643	51	18,20,22	0.99	1 (5%)	21,28,33	1.97	3 (14%)
51	PSU	9	1004	51	18,20,22	1.07	1 (5%)	21,28,33	1.88	4 (19%)
48	B9B	5	237	48	21,28,29	1.99	3 (14%)	23,40,43	2.04	8 (34%)
48	PSU	5	2508	48	18,20,22	1.03	1 (5%)	21,28,33	1.81	4 (19%)
48	OMG	5	2364	48	18,26,27	2.43	8 (44%)	19,38,41	1.54	3 (15%)
51	PSU	9	572	51	18,20,22	1.02	1 (5%)	21,28,33	1.84	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	OMG	5	1625	48,88	18,26,27	2.56	8 (44%)	19,38,41	1.72	4 (21%)
51	6MZ	9	1832	51,88	18,25,26	1.89	2 (11%)	16,36,39	2.01	2 (12%)
48	OMU	5	3925	48	19,22,23	2.77	7 (36%)	26,31,34	1.77	4 (15%)
48	PSU	5	4457	48	18,20,22	1.10	1 (5%)	21,28,33	1.67	3 (14%)
51	OMC	9	517	51	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
51	PSU	9	863	51	18,20,22	0.94	1 (5%)	21,28,33	1.82	3 (14%)
51	PSU	9	822	51	18,20,22	1.16	3 (16%)	21,28,33	2.11	6 (28%)
51	OMU	9	428	51	19,22,23	2.83	7 (36%)	26,31,34	1.68	5 (19%)
51	G7M	9	1639	51,46	20,26,27	2.64	8 (40%)	17,39,42	1.08	2 (11%)
48	OMG	5	1522	48	18,26,27	2.43	8 (44%)	19,38,41	1.54	4 (21%)
48	OMG	5	4637	48	18,26,27	2.40	8 (44%)	19,38,41	1.55	4 (21%)
48	PSU	5	1744	48,88	18,20,22	0.93	1 (5%)	21,28,33	1.90	3 (14%)
51	MA6	9	1851	51	19,26,27	1.13	2 (10%)	18,38,41	5.21	3 (16%)
48	OMC	5	3701	48,88	19,22,23	2.75	8 (42%)	26,31,34	1.01	1 (3%)
48	OMG	5	4618	48	18,26,27	2.40	8 (44%)	19,38,41	1.66	5 (26%)
51	PSU	9	609	51	18,20,22	1.01	1 (5%)	21,28,33	1.90	4 (19%)
48	OMG	5	4370	48	18,26,27	2.40	8 (44%)	19,38,41	1.55	5 (26%)
48	A2M	5	398	48	18,25,26	4.29	7 (38%)	18,36,39	3.38	3 (16%)
51	4AC	9	1337	51	21,24,25	3.12	10 (47%)	29,34,37	0.99	1 (3%)
51	OMU	9	116	51	19,22,23	2.76	6 (31%)	26,31,34	1.68	5 (19%)
48	OMC	5	4536	48	19,22,23	2.77	8 (42%)	26,31,34	0.85	0
48	PSU	5	3920	48	18,20,22	1.02	1 (5%)	21,28,33	2.06	4 (19%)
48	PSU	5	3695	48	18,20,22	1.01	1 (5%)	21,28,33	1.86	4 (19%)
48	OMU	5	4620	48	19,22,23	2.79	7 (36%)	26,31,34	1.76	4 (15%)
48	OMU	5	4498	48	19,22,23	2.77	8 (42%)	26,31,34	1.81	5 (19%)
48	A2M	5	2787	48	18,25,26	4.14	8 (44%)	18,36,39	3.25	3 (16%)
48	PSU	5	4403	48	18,20,22	1.06	1 (5%)	21,28,33	1.78	3 (14%)
51	PSU	9	1232	51	18,20,22	1.14	1 (5%)	21,28,33	1.82	3 (14%)
48	PSU	5	1781	48	18,20,22	1.09	1 (5%)	21,28,33	1.85	4 (19%)
48	A2M	5	1871	48,88	18,25,26	4.10	7 (38%)	18,36,39	3.33	3 (16%)
51	A2M	9	468	51	18,25,26	4.25	8 (44%)	18,36,39	3.43	4 (22%)
51	A2M	9	484	51	18,25,26	4.28	7 (38%)	18,36,39	3.68	3 (16%)
48	OMU	5	4306	48	19,22,23	2.82	7 (36%)	26,31,34	1.74	4 (15%)
48	OMC	5	3808	48	19,22,23	2.73	8 (42%)	26,31,34	0.64	0
51	A2M	9	1383	51	18,25,26	4.27	7 (38%)	18,36,39	3.63	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	PSU	5	1782	48	18,20,22	1.04	1 (5%)	21,28,33	1.90	4 (19%)
48	PSU	5	2632	48	18,20,22	1.08	1 (5%)	21,28,33	1.86	4 (19%)
48	PSU	5	4293	48	18,20,22	1.16	1 (5%)	21,28,33	1.78	3 (14%)
51	OMU	9	172	51	19,22,23	2.81	7 (36%)	26,31,34	1.71	5 (19%)
48	PSU	5	4500	48	18,20,22	1.06	2 (11%)	21,28,33	1.96	5 (23%)
48	PSU	5	1860	48	18,20,22	0.98	1 (5%)	21,28,33	1.81	4 (19%)
48	OMG	5	1316	48	18,26,27	2.43	8 (44%)	19,38,41	1.64	3 (15%)
48	OMC	5	2861	48	19,22,23	2.93	8 (42%)	26,31,34	0.82	1 (3%)
48	A2M	5	2815	48	18,25,26	4.12	7 (38%)	18,36,39	3.39	3 (16%)
48	5MC	5	3782	48,88	18,22,23	3.27	7 (38%)	26,32,35	1.14	2 (7%)
48	OMC	5	3887	48	19,22,23	2.78	7 (36%)	26,31,34	0.76	0
48	PSU	5	1862	48	18,20,22	1.06	1 (5%)	21,28,33	1.88	4 (19%)
51	PSU	9	814	51	18,20,22	1.03	1 (5%)	21,28,33	1.93	5 (23%)
51	PSU	9	1045	51	18,20,22	1.09	1 (5%)	21,28,33	2.02	5 (23%)
51	PSU	9	1046	51	18,20,22	1.07	1 (5%)	21,28,33	1.81	5 (23%)
48	OMC	5	2824	48	19,22,23	2.83	8 (42%)	26,31,34	0.93	1 (3%)
48	PSU	5	4579	48	18,20,22	1.00	1 (5%)	21,28,33	1.78	3 (14%)
48	PSU	5	3764	48	18,20,22	1.12	1 (5%)	21,28,33	1.93	4 (19%)
50	OMG	8	75	50	18,26,27	2.39	8 (44%)	19,38,41	1.53	5 (26%)
48	OMC	5	3869	48	19,22,23	2.82	7 (36%)	26,31,34	0.74	0
48	A2M	5	4571	48	18,25,26	4.29	8 (44%)	18,36,39	3.52	3 (16%)
51	OMC	9	174	51	19,22,23	2.90	8 (42%)	26,31,34	0.92	0
51	PSU	9	1177	51	18,20,22	1.03	1 (5%)	21,28,33	1.67	4 (19%)
48	PSU	5	3762	48	18,20,22	1.08	1 (5%)	21,28,33	2.01	4 (19%)
48	OMC	5	1340	48	19,22,23	2.96	8 (42%)	26,31,34	1.00	2 (7%)
51	OMC	9	1391	51	19,22,23	2.95	8 (42%)	26,31,34	0.96	1 (3%)
48	OMG	5	2424	48	18,26,27	2.41	8 (44%)	19,38,41	1.53	4 (21%)
51	OMG	9	1490	51,88	18,26,27	2.37	7 (38%)	19,38,41	1.39	4 (21%)
48	A2M	5	3825	48	18,25,26	4.21	8 (44%)	18,36,39	3.11	3 (16%)
48	OMC	5	4456	48	19,22,23	2.79	8 (42%)	26,31,34	0.76	0
48	PSU	5	3639	48	18,20,22	1.10	1 (5%)	21,28,33	1.80	3 (14%)
48	PSU	5	4296	48	18,20,22	1.15	1 (5%)	21,28,33	1.85	3 (14%)
48	OMG	5	3627	48	18,26,27	2.43	8 (44%)	19,38,41	1.50	3 (15%)
48	A2M	5	1534	48,88	18,25,26	4.26	7 (38%)	18,36,39	3.43	3 (16%)
51	PSU	9	1238	51	18,20,22	1.15	2 (11%)	21,28,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	PSU	5	3851	48	18,20,22	1.06	2 (11%)	21,28,33	1.94	4 (19%)
51	PSU	9	1174	51	18,20,22	1.06	1 (5%)	21,28,33	1.96	4 (19%)
48	6MZ	5	4220	48	18,25,26	1.99	2 (11%)	16,36,39	1.99	2 (12%)
48	A2M	5	3785	48	18,25,26	3.97	7 (38%)	18,36,39	3.37	3 (16%)
48	OMG	5	4228	48	18,26,27	2.37	8 (44%)	19,38,41	1.46	3 (15%)
51	A2M	9	668	51,88	18,25,26	4.18	7 (38%)	18,36,39	3.53	4 (22%)
51	A2M	9	1678	51	18,25,26	4.17	6 (33%)	18,36,39	3.61	3 (16%)
48	A2M	5	2363	48,88	18,25,26	4.21	7 (38%)	18,36,39	3.47	3 (16%)
48	PSU	5	3734	48	18,20,22	1.12	1 (5%)	21,28,33	1.82	5 (23%)
48	PSU	5	3853	48	18,20,22	1.15	1 (5%)	21,28,33	2.07	4 (19%)
51	B8N	9	1248	51	24,29,30	3.01	6 (25%)	29,42,45	1.89	5 (17%)
51	OMG	9	1328	51	18,26,27	2.42	8 (44%)	19,38,41	1.46	4 (21%)
51	PSU	9	686	51	18,20,22	0.98	1 (5%)	21,28,33	2.16	4 (19%)
48	PSU	5	3715	48	18,20,22	1.06	3 (16%)	21,28,33	1.99	6 (28%)
48	PSU	5	4521	48,88	18,20,22	1.18	2 (11%)	21,28,33	2.12	6 (28%)
48	OMG	5	4494	48	18,26,27	2.33	8 (44%)	19,38,41	1.48	5 (26%)
51	PSU	9	34	51	18,20,22	1.10	1 (5%)	21,28,33	1.85	4 (19%)
48	1MA	5	1322	48,88	16,25,26	3.53	4 (25%)	18,37,40	1.84	3 (16%)
51	OMU	9	1326	51	19,22,23	2.76	7 (36%)	26,31,34	1.83	5 (19%)
48	OMG	5	4196	48,46	18,26,27	2.47	7 (38%)	19,38,41	1.49	4 (21%)
51	PSU	9	109	51	18,20,22	1.13	1 (5%)	21,28,33	1.91	4 (19%)

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
48	OMC	5	2365	48	-	0/9/27/28	0/2/2/2
48	A2M	5	3718	48	-	0/5/27/28	0/3/3/3
51	A2M	9	512	51	-	1/5/27/28	0/3/3/3
51	PSU	9	1367	51	-	0/6/24/26	0/2/2/2
48	A2M	5	400	48	-	0/5/27/28	0/3/3/3
48	OMC	5	2422	48,88	-	1/9/27/28	0/2/2/2
48	OMU	5	2837	48	-	1/9/27/28	0/2/2/2
48	PSU	5	4299	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4628	48	-	0/6/24/26	0/2/2/2
51	A2M	9	166	51	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	5	4423	48	-	0/6/24/26	0/2/2/2
51	OMG	9	644	51	-	1/5/27/28	0/3/3/3
48	OMG	5	3899	48	-	0/5/27/28	0/3/3/3
51	OMG	9	436	51	-	0/5/27/28	0/3/3/3
48	PSU	5	1677	48	-	0/6/24/26	0/2/2/2
48	OMC	5	2351	48	-	2/9/27/28	0/2/2/2
51	OMU	9	1442	51	-	2/9/27/28	0/2/2/2
48	PSU	5	4552	48	-	0/6/24/26	0/2/2/2
51	OMG	9	683	51	-	2/5/27/28	0/3/3/3
48	UY1	5	3818	48,88	-	3/9/27/28	0/2/2/2
48	PSU	5	4353	48	-	0/6/24/26	0/2/2/2
51	PSU	9	119	51	-	0/6/24/26	0/2/2/2
48	PSU	5	4420	48	-	0/6/24/26	0/2/2/2
51	OMC	9	1703	51	-	2/9/27/28	0/2/2/2
51	PSU	9	1081	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1445	51	-	1/6/24/26	0/2/2/2
48	OMG	5	3792	48	-	2/5/27/28	0/3/3/3
48	OMC	5	3841	48	-	0/9/27/28	0/2/2/2
48	OMG	5	4392	48	-	0/5/27/28	0/3/3/3
51	OMU	9	121	51	-	1/9/27/28	0/2/2/2
48	A2M	5	3760	48,88	-	3/5/27/28	0/3/3/3
51	A2M	9	27	51	-	0/5/27/28	0/3/3/3
51	PSU	9	105	51	-	0/6/24/26	0/2/2/2
48	A2M	5	3830	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4623	48	-	0/5/27/28	0/3/3/3
48	5MC	5	4447	48,88	-	4/7/25/26	0/2/2/2
51	PSU	9	1244	51	-	0/6/24/26	0/2/2/2
48	A2M	5	4523	48,88	-	0/5/27/28	0/3/3/3
48	PSU	5	4442	48	-	0/6/24/26	0/2/2/2
51	PSU	9	218	51	-	0/6/24/26	0/2/2/2
51	PSU	9	801	51	-	2/6/24/26	0/2/2/2
51	PSU	9	815	51	-	0/6/24/26	0/2/2/2
48	OMC	5	2804	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1347	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1683	48,88	-	0/6/24/26	0/2/2/2
48	PSU	5	4361	48	-	0/6/24/26	0/2/2/2
48	A2M	5	3867	48	-	1/5/27/28	0/3/3/3
51	OMG	9	509	51,88	-	0/5/27/28	0/3/3/3
51	A2M	9	159	51	-	0/5/27/28	0/3/3/3
48	A2M	5	1524	48	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	UR3	5	4530	48	-	0/7/25/26	0/2/2/2
48	OMU	5	4227	48	-	0/9/27/28	0/2/2/2
48	A2M	5	3724	48	-	0/5/27/28	0/3/3/3
51	4AC	9	1842	51	-	0/11/29/30	0/2/2/2
48	PSU	5	4532	48	-	0/6/24/26	0/2/2/2
51	A2M	9	99	51,88	-	2/5/27/28	0/3/3/3
48	A2M	5	1326	48	-	1/5/27/28	0/3/3/3
48	2MG	5	1517	48	-	0/5/27/28	0/3/3/3
48	OMG	5	2876	48	-	0/5/27/28	0/3/3/3
51	A2M	9	1031	51	-	1/5/27/28	0/3/3/3
51	MA6	9	1850	51	-	0/7/29/30	0/3/3/3
48	PSU	5	1792	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1692	51	-	0/6/24/26	0/2/2/2
51	PSU	9	649	51	-	0/6/24/26	0/2/2/2
48	OMG	5	4499	48	-	2/5/27/28	0/3/3/3
48	OMG	5	373	48	-	1/5/27/28	0/3/3/3
51	PSU	9	1643	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1004	51	-	0/6/24/26	0/2/2/2
48	B9B	5	237	48	-	2/7/29/30	0/3/3/3
48	PSU	5	2508	48	-	0/6/24/26	0/2/2/2
48	OMG	5	2364	48	-	3/5/27/28	0/3/3/3
51	PSU	9	572	51	-	0/6/24/26	0/2/2/2
48	OMG	5	1625	48,88	-	1/5/27/28	0/3/3/3
51	6MZ	9	1832	51,88	-	0/5/27/28	0/3/3/3
48	OMU	5	3925	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4457	48	-	0/6/24/26	0/2/2/2
51	OMC	9	517	51	-	0/9/27/28	0/2/2/2
51	PSU	9	863	51	-	2/6/24/26	0/2/2/2
51	PSU	9	822	51	-	2/6/24/26	0/2/2/2
51	OMU	9	428	51	-	4/9/27/28	0/2/2/2
51	G7M	9	1639	51,46	-	2/3/25/26	0/3/3/3
48	OMG	5	1522	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4637	48	-	0/5/27/28	0/3/3/3
48	PSU	5	1744	48,88	-	0/6/24/26	0/2/2/2
51	MA6	9	1851	51	-	3/7/29/30	0/3/3/3
48	OMC	5	3701	48,88	-	4/9/27/28	0/2/2/2
48	OMG	5	4618	48	-	0/5/27/28	0/3/3/3
51	PSU	9	609	51	-	0/6/24/26	0/2/2/2
48	OMG	5	4370	48	-	0/5/27/28	0/3/3/3
48	A2M	5	398	48	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
51	OMU	9	116	51	-	0/9/27/28	0/2/2/2
48	OMC	5	4536	48	-	0/9/27/28	0/2/2/2
48	PSU	5	3920	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3695	48	-	0/6/24/26	0/2/2/2
48	OMU	5	4620	48	-	0/9/27/28	0/2/2/2
48	OMU	5	4498	48	-	0/9/27/28	0/2/2/2
48	A2M	5	2787	48	-	0/5/27/28	0/3/3/3
48	PSU	5	4403	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1232	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1781	48	-	2/6/24/26	0/2/2/2
48	A2M	5	1871	48,88	-	0/5/27/28	0/3/3/3
51	A2M	9	468	51	-	1/5/27/28	0/3/3/3
51	A2M	9	484	51	-	0/5/27/28	0/3/3/3
48	OMU	5	4306	48	-	0/9/27/28	0/2/2/2
48	OMC	5	3808	48	-	0/9/27/28	0/2/2/2
51	A2M	9	1383	51	-	0/5/27/28	0/3/3/3
48	PSU	5	1782	48	-	0/6/24/26	0/2/2/2
48	PSU	5	2632	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4293	48	-	0/6/24/26	0/2/2/2
51	OMU	9	172	51	-	2/9/27/28	0/2/2/2
48	PSU	5	4500	48	-	2/6/24/26	0/2/2/2
48	PSU	5	1860	48	-	0/6/24/26	0/2/2/2
48	OMG	5	1316	48	-	0/5/27/28	0/3/3/3
48	OMC	5	2861	48	-	0/9/27/28	0/2/2/2
48	A2M	5	2815	48	-	2/5/27/28	0/3/3/3
48	5MC	5	3782	48,88	-	0/7/25/26	0/2/2/2
48	OMC	5	3887	48	-	0/9/27/28	0/2/2/2
48	PSU	5	1862	48	-	0/6/24/26	0/2/2/2
51	PSU	9	814	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1045	51	-	2/6/24/26	0/2/2/2
51	PSU	9	1046	51	-	0/6/24/26	0/2/2/2
48	OMC	5	2824	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4579	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3764	48	-	0/6/24/26	0/2/2/2
50	OMG	8	75	50	-	0/5/27/28	0/3/3/3
48	OMC	5	3869	48	-	0/9/27/28	0/2/2/2
48	A2M	5	4571	48	-	0/5/27/28	0/3/3/3
51	OMC	9	174	51	-	0/9/27/28	0/2/2/2
51	PSU	9	1177	51	-	0/6/24/26	0/2/2/2
48	PSU	5	3762	48	-	0/6/24/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMC	5	1340	48	-	0/9/27/28	0/2/2/2
51	OMC	9	1391	51	-	0/9/27/28	0/2/2/2
48	OMG	5	2424	48	-	3/5/27/28	0/3/3/3
51	OMG	9	1490	51,88	-	2/5/27/28	0/3/3/3
48	A2M	5	3825	48	-	0/5/27/28	0/3/3/3
48	OMC	5	4456	48	-	0/9/27/28	0/2/2/2
48	PSU	5	3639	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4296	48	-	0/6/24/26	0/2/2/2
48	OMG	5	3627	48	-	0/5/27/28	0/3/3/3
48	A2M	5	1534	48,88	-	2/5/27/28	0/3/3/3
51	PSU	9	1238	51	-	0/6/24/26	0/2/2/2
48	PSU	5	3851	48	-	1/6/24/26	0/2/2/2
51	PSU	9	1174	51	-	0/6/24/26	0/2/2/2
48	6MZ	5	4220	48	-	0/5/27/28	0/3/3/3
48	A2M	5	3785	48	-	2/5/27/28	0/3/3/3
48	OMG	5	4228	48	-	1/5/27/28	0/3/3/3
51	A2M	9	668	51,88	-	2/5/27/28	0/3/3/3
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
48	A2M	5	2363	48,88	-	0/5/27/28	0/3/3/3
48	PSU	5	3734	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3853	48	-	0/6/24/26	0/2/2/2
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
51	OMG	9	1328	51	-	1/5/27/28	0/3/3/3
51	PSU	9	686	51	-	0/6/24/26	0/2/2/2
48	PSU	5	3715	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4521	48,88	-	0/6/24/26	0/2/2/2
48	OMG	5	4494	48	-	2/5/27/28	0/3/3/3
51	PSU	9	34	51	-	4/6/24/26	0/2/2/2
48	1MA	5	1322	48,88	-	0/3/25/26	0/3/3/3
51	OMU	9	1326	51	-	0/9/27/28	0/2/2/2
48	OMG	5	4196	48,46	-	0/5/27/28	0/3/3/3
51	PSU	9	109	51	-	0/6/24/26	0/2/2/2

All (788) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1383	A2M	O4'-C1'	15.51	1.62	1.41
48	5	3724	A2M	O4'-C1'	15.46	1.62	1.41
51	9	99	A2M	O4'-C1'	15.44	1.62	1.41
48	5	398	A2M	O4'-C1'	15.43	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	159	A2M	O4'-C1'	15.36	1.62	1.41
48	5	3718	A2M	O4'-C1'	15.36	1.62	1.41
51	9	484	A2M	O4'-C1'	15.35	1.62	1.41
48	5	3760	A2M	O4'-C1'	15.28	1.62	1.41
48	5	4571	A2M	O4'-C1'	15.14	1.62	1.41
51	9	468	A2M	O4'-C1'	15.12	1.62	1.41
51	9	1031	A2M	O4'-C1'	15.11	1.62	1.41
51	9	512	A2M	O4'-C1'	15.09	1.62	1.41
48	5	1534	A2M	O4'-C1'	15.06	1.62	1.41
48	5	3825	A2M	O4'-C1'	15.05	1.62	1.41
48	5	2363	A2M	O4'-C1'	15.01	1.62	1.41
51	9	1678	A2M	O4'-C1'	14.94	1.61	1.41
51	9	27	A2M	O4'-C1'	14.70	1.61	1.41
51	9	166	A2M	O4'-C1'	14.70	1.61	1.41
48	5	400	A2M	O4'-C1'	14.69	1.61	1.41
48	5	2815	A2M	O4'-C1'	14.63	1.61	1.41
48	5	1326	A2M	O4'-C1'	14.62	1.61	1.41
48	5	2787	A2M	O4'-C1'	14.59	1.61	1.41
48	5	4523	A2M	O4'-C1'	14.57	1.61	1.41
51	9	668	A2M	O4'-C1'	14.57	1.61	1.41
48	5	3830	A2M	O4'-C1'	14.56	1.61	1.41
48	5	3867	A2M	O4'-C1'	14.47	1.61	1.41
48	5	1871	A2M	O4'-C1'	14.46	1.61	1.41
48	5	1524	A2M	O4'-C1'	14.21	1.60	1.41
48	5	3785	A2M	O4'-C1'	14.05	1.60	1.41
48	5	1322	1MA	C2-N3	12.62	1.44	1.29
48	5	3818	UY1	C6-C5	10.75	1.47	1.35
48	5	3818	UY1	C2-N1	9.25	1.49	1.36
48	5	3782	5MC	C6-C5	9.05	1.49	1.34
48	5	4447	5MC	C6-C5	8.66	1.48	1.34
48	5	4220	6MZ	C6-N6	7.39	1.47	1.35
51	9	1248	B8N	C6-N1	7.38	1.54	1.36
51	9	1248	B8N	C4-N3	-7.11	1.27	1.40
51	9	668	A2M	O4'-C4'	-7.08	1.29	1.45
51	9	1442	OMU	C2-N1	6.97	1.49	1.38
48	5	2837	OMU	C2-N1	6.93	1.49	1.38
51	9	1832	6MZ	C6-N6	6.85	1.46	1.35
48	5	1524	A2M	O4'-C4'	-6.83	1.29	1.45
48	5	4571	A2M	O4'-C4'	-6.80	1.29	1.45
48	5	4530	UR3	C2-N1	6.76	1.48	1.38
48	5	1534	A2M	O4'-C4'	-6.75	1.29	1.45
48	5	3818	UY1	C2-N3	6.71	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4620	OMU	C2-N1	6.68	1.49	1.38
48	5	3867	A2M	O4'-C4'	-6.62	1.30	1.45
51	9	428	OMU	C2-N1	6.58	1.49	1.38
51	9	428	OMU	C2-N3	6.50	1.49	1.38
48	5	400	A2M	O4'-C4'	-6.49	1.30	1.45
51	9	116	OMU	C2-N1	6.49	1.48	1.38
48	5	2815	A2M	O4'-C4'	-6.48	1.30	1.45
48	5	3925	OMU	C2-N1	6.48	1.48	1.38
51	9	1248	B8N	C2-N1	6.46	1.58	1.39
48	5	2363	A2M	O4'-C4'	-6.46	1.30	1.45
51	9	1391	OMC	C2-N3	6.45	1.49	1.36
48	5	4306	OMU	C2-N1	6.45	1.48	1.38
48	5	4227	OMU	C2-N1	6.43	1.48	1.38
48	5	1326	A2M	O4'-C4'	-6.41	1.30	1.45
48	5	1871	A2M	O4'-C4'	-6.41	1.30	1.45
48	5	3760	A2M	O4'-C4'	-6.40	1.30	1.45
51	9	1639	G7M	C2-N2	6.40	1.49	1.34
51	9	159	A2M	O4'-C4'	-6.40	1.30	1.45
51	9	1031	A2M	O4'-C4'	-6.40	1.30	1.45
51	9	27	A2M	O4'-C4'	-6.37	1.30	1.45
51	9	484	A2M	O4'-C4'	-6.36	1.30	1.45
51	9	172	OMU	C2-N3	6.36	1.49	1.38
48	5	3718	A2M	O4'-C4'	-6.34	1.30	1.45
51	9	468	A2M	O4'-C4'	-6.31	1.30	1.45
48	5	1340	OMC	C2-N3	6.31	1.49	1.36
51	9	1337	4AC	C6-C5	6.30	1.49	1.35
48	5	398	A2M	O4'-C4'	-6.29	1.30	1.45
48	5	2787	A2M	O4'-C4'	-6.29	1.30	1.45
51	9	517	OMC	C2-N3	6.29	1.49	1.36
48	5	4523	A2M	O4'-C4'	-6.27	1.31	1.45
51	9	517	OMC	C6-C5	6.26	1.49	1.35
51	9	172	OMU	C2-N1	6.24	1.48	1.38
48	5	2422	OMC	C2-N3	6.21	1.49	1.36
48	5	3887	OMC	C2-N3	6.21	1.48	1.36
48	5	3830	A2M	O4'-C4'	-6.20	1.31	1.45
48	5	4498	OMU	C2-N1	6.20	1.48	1.38
48	5	237	B9B	O6-C6	6.19	1.40	1.35
51	9	1326	OMU	C2-N1	6.18	1.48	1.38
51	9	99	A2M	O4'-C4'	-6.17	1.31	1.45
51	9	1703	OMC	C2-N3	6.17	1.48	1.36
51	9	121	OMU	C2-N1	6.15	1.48	1.38
51	9	512	A2M	O4'-C4'	-6.15	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3825	A2M	O4'-C4'	-6.13	1.31	1.45
48	5	1340	OMC	C6-C5	6.13	1.49	1.35
51	9	1678	A2M	O4'-C4'	-6.12	1.31	1.45
51	9	166	A2M	O4'-C4'	-6.11	1.31	1.45
48	5	2861	OMC	C2-N3	6.10	1.48	1.36
51	9	1442	OMU	C2-N3	6.08	1.48	1.38
48	5	3724	A2M	O4'-C4'	-6.08	1.31	1.45
48	5	3785	A2M	O4'-C4'	-6.05	1.31	1.45
51	9	174	OMC	C6-C5	6.03	1.49	1.35
51	9	1391	OMC	C6-C5	6.02	1.49	1.35
51	9	1383	A2M	O4'-C4'	-6.02	1.31	1.45
51	9	116	OMU	C2-N3	6.02	1.48	1.38
48	5	4536	OMC	C6-C5	6.00	1.49	1.35
51	9	1326	OMU	C2-N3	6.00	1.48	1.38
51	9	121	OMU	C2-N3	5.99	1.48	1.38
48	5	2837	OMU	C2-N3	5.99	1.48	1.38
48	5	4498	OMU	C2-N3	5.96	1.48	1.38
48	5	4620	OMU	C2-N3	5.96	1.48	1.38
48	5	3869	OMC	C6-C5	5.93	1.48	1.35
51	9	174	OMC	C2-N3	5.92	1.48	1.36
48	5	3841	OMC	C6-C5	5.91	1.48	1.35
48	5	4306	OMU	C6-C5	5.90	1.48	1.35
48	5	2804	OMC	C2-N3	5.90	1.48	1.36
51	9	1703	OMC	C6-C5	5.89	1.48	1.35
48	5	4227	OMU	C2-N3	5.89	1.48	1.38
48	5	2365	OMC	C6-C5	5.88	1.48	1.35
48	5	2365	OMC	C2-N3	5.87	1.48	1.36
48	5	2861	OMC	C6-C5	5.87	1.48	1.35
51	9	1248	B8N	C6-C5	5.87	1.43	1.34
48	5	3925	OMU	C2-N3	5.87	1.48	1.38
51	9	172	OMU	C6-C5	5.87	1.48	1.35
48	5	3841	OMC	C2-N3	5.86	1.48	1.36
51	9	1842	4AC	C6-C5	5.83	1.48	1.35
48	5	2422	OMC	C6-C5	5.83	1.48	1.35
48	5	4447	5MC	C4-N3	5.82	1.44	1.34
48	5	2351	OMC	C6-C5	5.79	1.48	1.35
48	5	3701	OMC	C6-C5	5.78	1.48	1.35
51	9	116	OMU	C6-C5	5.78	1.48	1.35
51	9	1337	4AC	C4-N3	5.77	1.42	1.32
48	5	2824	OMC	C6-C5	5.76	1.48	1.35
51	9	1842	4AC	C4-N3	5.74	1.42	1.32
48	5	4306	OMU	C2-N3	5.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4456	OMC	C2-N3	5.74	1.48	1.36
51	9	1326	OMU	C6-C5	5.73	1.48	1.35
48	5	2824	OMC	C2-N3	5.72	1.48	1.36
48	5	2804	OMC	C6-C5	5.66	1.48	1.35
51	9	436	OMG	C2-N3	5.65	1.46	1.33
48	5	4456	OMC	C6-C5	5.64	1.48	1.35
48	5	4498	OMU	C6-C5	5.64	1.48	1.35
48	5	4227	OMU	C6-C5	5.64	1.48	1.35
48	5	3925	OMU	C6-C5	5.64	1.48	1.35
48	5	4447	5MC	C2-N3	5.62	1.47	1.36
48	5	4620	OMU	C6-C5	5.61	1.48	1.35
48	5	3869	OMC	C2-N3	5.61	1.47	1.36
48	5	3808	OMC	C6-C5	5.56	1.48	1.35
48	5	3808	OMC	C2-N3	5.56	1.47	1.36
48	5	4536	OMC	C2-N3	5.54	1.47	1.36
51	9	683	OMG	C2-N3	5.53	1.46	1.33
48	5	4530	UR3	C6-C5	5.52	1.47	1.35
51	9	428	OMU	C6-C5	5.51	1.47	1.35
51	9	1442	OMU	C6-C5	5.47	1.47	1.35
48	5	4196	OMG	C2-N3	5.47	1.46	1.33
48	5	3701	OMC	C2-N3	5.42	1.47	1.36
48	5	1625	OMG	C2-N3	5.42	1.46	1.33
48	5	2351	OMC	C2-N3	5.39	1.47	1.36
48	5	237	B9B	C2-N2	5.38	1.44	1.33
48	5	4499	OMG	C2-N3	5.37	1.46	1.33
48	5	3887	OMC	C6-C5	5.35	1.47	1.35
51	9	509	OMG	C2-N3	5.32	1.46	1.33
48	5	2837	OMU	C6-C5	5.30	1.47	1.35
48	5	4623	OMG	C2-N3	5.30	1.46	1.33
51	9	1328	OMG	C2-N3	5.26	1.46	1.33
48	5	3818	UY1	C1'-C5	-5.25	1.38	1.50
51	9	121	OMU	C6-C5	5.24	1.47	1.35
51	9	1639	G7M	C2-N3	5.18	1.45	1.33
51	9	1337	4AC	C2-N3	5.17	1.46	1.36
48	5	373	OMG	C2-N3	5.16	1.45	1.33
48	5	4637	OMG	C2-N3	5.14	1.45	1.33
48	5	2876	OMG	C2-N3	5.13	1.45	1.33
48	5	1340	OMC	C4-N4	5.10	1.45	1.33
48	5	3627	OMG	C2-N3	5.08	1.45	1.33
51	9	1337	4AC	C4-N4	5.08	1.47	1.39
48	5	4370	OMG	C2-N3	5.08	1.45	1.33
48	5	3782	5MC	C4-N3	5.07	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3782	5MC	C2-N3	5.07	1.46	1.36
48	5	2364	OMG	C2-N3	5.07	1.45	1.33
51	9	644	OMG	C2-N3	5.07	1.45	1.33
48	5	2424	OMG	C2-N3	5.05	1.45	1.33
48	5	4499	OMG	C4-N3	5.05	1.49	1.37
48	5	3899	OMG	C2-N3	5.04	1.45	1.33
51	9	1391	OMC	C4-N4	5.02	1.45	1.33
48	5	1316	OMG	C2-N3	5.02	1.45	1.33
48	5	4392	OMG	C2-N3	5.00	1.45	1.33
51	9	509	OMG	C4-N3	5.00	1.49	1.37
51	9	683	OMG	C4-N3	5.00	1.49	1.37
50	8	75	OMG	C2-N3	4.99	1.45	1.33
51	9	436	OMG	C4-N3	4.98	1.49	1.37
48	5	3792	OMG	C2-N3	4.97	1.45	1.33
51	9	1842	4AC	C2-N3	4.96	1.46	1.36
48	5	2876	OMG	C4-N3	4.93	1.49	1.37
48	5	4623	OMG	C4-N3	4.90	1.49	1.37
48	5	4637	OMG	C4-N3	4.89	1.49	1.37
48	5	4618	OMG	C2-N3	4.88	1.45	1.33
48	5	1522	OMG	C2-N3	4.87	1.45	1.33
48	5	4494	OMG	C2-N3	4.87	1.45	1.33
48	5	1625	OMG	C4-N3	4.85	1.49	1.37
48	5	4196	OMG	C4-N3	4.85	1.49	1.37
51	9	1842	4AC	C7-N4	4.80	1.46	1.37
48	5	1517	2MG	C2-N2	4.79	1.44	1.33
48	5	3899	OMG	C4-N3	4.78	1.49	1.37
48	5	373	OMG	C4-N3	4.78	1.49	1.37
51	9	1703	OMC	C2-N1	4.75	1.50	1.40
51	9	1703	OMC	C4-N3	4.73	1.44	1.34
51	9	644	OMG	C4-N3	4.72	1.48	1.37
51	9	1639	G7M	C4-N3	4.70	1.48	1.37
48	5	4370	OMG	C4-N3	4.69	1.48	1.37
51	9	517	OMC	C4-N3	4.69	1.44	1.34
48	5	4228	OMG	C2-N3	4.67	1.44	1.33
51	9	1703	OMC	C4-N4	4.67	1.44	1.33
48	5	1522	OMG	C4-N3	4.67	1.48	1.37
48	5	3887	OMC	C4-N3	4.66	1.43	1.34
48	5	3869	OMC	C4-N4	4.65	1.44	1.33
48	5	3818	UY1	C6-N1	4.65	1.44	1.36
48	5	3627	OMG	C4-N3	4.64	1.48	1.37
51	9	174	OMC	C4-N3	4.64	1.43	1.34
48	5	4228	OMG	C4-N3	4.63	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1490	OMG	C2-N3	4.62	1.44	1.33
51	9	517	OMC	C4-N4	4.61	1.44	1.33
48	5	2422	OMC	C4-N3	4.60	1.43	1.34
51	9	1328	OMG	C4-N3	4.60	1.48	1.37
48	5	4456	OMC	C4-N4	4.58	1.44	1.33
48	5	2824	OMC	C4-N4	4.57	1.44	1.33
51	9	174	OMC	C4-N4	4.57	1.44	1.33
48	5	1625	OMG	C2-N2	4.56	1.45	1.34
48	5	2364	OMG	C4-N3	4.56	1.48	1.37
48	5	2861	OMC	C4-N4	4.56	1.44	1.33
48	5	3792	OMG	C4-N3	4.56	1.48	1.37
48	5	2861	OMC	C4-N3	4.55	1.43	1.34
48	5	2365	OMC	C4-N4	4.54	1.44	1.33
48	5	1316	OMG	C4-N3	4.52	1.48	1.37
48	5	2422	OMC	C4-N4	4.51	1.44	1.33
48	5	4530	UR3	C2-N3	4.49	1.47	1.39
48	5	3887	OMC	C4-N4	4.49	1.44	1.33
51	9	1337	4AC	C7-N4	4.48	1.45	1.37
48	5	2424	OMG	C4-N3	4.48	1.48	1.37
48	5	3841	OMC	C4-N4	4.46	1.44	1.33
48	5	2365	OMC	C4-N3	4.45	1.43	1.34
51	9	1490	OMG	C4-N3	4.45	1.48	1.37
48	5	3869	OMC	C4-N3	4.43	1.43	1.34
51	9	644	OMG	C2-N2	4.43	1.44	1.34
48	5	4196	OMG	C2-N2	4.42	1.44	1.34
48	5	4618	OMG	C4-N3	4.42	1.48	1.37
48	5	4392	OMG	C4-N3	4.42	1.48	1.37
50	8	75	OMG	C4-N3	4.42	1.48	1.37
48	5	4456	OMC	C4-N3	4.42	1.43	1.34
48	5	2804	OMC	C4-N4	4.39	1.44	1.33
48	5	4536	OMC	C4-N4	4.38	1.44	1.33
51	9	1391	OMC	C4-N3	4.37	1.43	1.34
48	5	4499	OMG	C2-N2	4.36	1.44	1.34
51	9	683	OMG	C2-N2	4.36	1.44	1.34
51	9	436	OMG	C2-N2	4.35	1.44	1.34
48	5	2861	OMC	C2-N1	4.35	1.49	1.40
48	5	4623	OMG	C2-N2	4.34	1.44	1.34
48	5	2422	OMC	C2-N1	4.33	1.49	1.40
51	9	1842	4AC	C4-N4	4.33	1.46	1.39
48	5	4494	OMG	C4-N3	4.31	1.47	1.37
48	5	2424	OMG	C2-N2	4.30	1.44	1.34
51	9	517	OMC	C2-N1	4.30	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4447	5MC	C6-N1	4.30	1.45	1.38
51	9	1490	OMG	C2-N2	4.30	1.44	1.34
48	5	3701	OMC	C4-N3	4.29	1.43	1.34
48	5	1340	OMC	C4-N3	4.28	1.43	1.34
48	5	3808	OMC	C4-N4	4.27	1.44	1.33
50	8	75	OMG	C2-N2	4.26	1.44	1.34
48	5	2364	OMG	C2-N2	4.26	1.44	1.34
48	5	373	OMG	C2-N2	4.25	1.44	1.34
51	9	509	OMG	C2-N2	4.25	1.44	1.34
51	9	1328	OMG	C2-N2	4.22	1.44	1.34
48	5	4370	OMG	C2-N2	4.21	1.44	1.34
48	5	3899	OMG	C2-N2	4.20	1.44	1.34
48	5	2351	OMC	C4-N3	4.19	1.43	1.34
51	9	174	OMC	C2-N1	4.18	1.49	1.40
48	5	2824	OMC	C2-N1	4.18	1.49	1.40
48	5	3841	OMC	C4-N3	4.18	1.42	1.34
48	5	2351	OMC	C4-N4	4.17	1.43	1.33
51	9	1391	OMC	C2-N1	4.16	1.49	1.40
48	5	3808	OMC	C2-N1	4.16	1.49	1.40
48	5	3701	OMC	C4-N4	4.16	1.43	1.33
48	5	4228	OMG	C2-N2	4.15	1.44	1.34
48	5	2804	OMC	C4-N3	4.14	1.42	1.34
48	5	3627	OMG	C2-N2	4.14	1.44	1.34
48	5	3782	5MC	C6-N1	4.13	1.45	1.38
48	5	2824	OMC	C4-N3	4.13	1.42	1.34
48	5	4618	OMG	C2-N2	4.13	1.44	1.34
48	5	3701	OMC	C2-N1	4.12	1.48	1.40
48	5	3808	OMC	C4-N3	4.12	1.42	1.34
48	5	3792	OMG	C2-N2	4.11	1.44	1.34
48	5	4494	OMG	C2-N2	4.09	1.43	1.34
51	9	1639	G7M	C6-N1	4.06	1.43	1.37
48	5	1522	OMG	C2-N2	4.01	1.43	1.34
48	5	2876	OMG	C2-N2	4.00	1.43	1.34
48	5	2351	OMC	C2-N1	3.97	1.48	1.40
48	5	4536	OMC	C4-N3	3.96	1.42	1.34
48	5	1316	OMG	C2-N2	3.94	1.43	1.34
48	5	4536	OMC	C2-N1	3.93	1.48	1.40
48	5	4447	5MC	C4-N4	3.93	1.44	1.34
48	5	3782	5MC	C4-N4	3.91	1.44	1.34
48	5	2804	OMC	C2-N1	3.91	1.48	1.40
48	5	4637	OMG	C2-N2	3.89	1.43	1.34
48	5	1340	OMC	C2-N1	3.88	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1322	1MA	C2-N1	3.87	1.43	1.35
48	5	1517	2MG	C6-N1	3.86	1.43	1.37
51	9	1337	4AC	C5-C4	3.85	1.49	1.40
51	9	1842	4AC	C5-C4	3.85	1.49	1.40
48	5	3841	OMC	C2-N1	3.84	1.48	1.40
51	9	1842	4AC	C2-N1	3.83	1.48	1.40
48	5	1517	2MG	C2-N1	3.78	1.42	1.36
48	5	2365	OMC	C2-N1	3.73	1.48	1.40
48	5	3869	OMC	C2-N1	3.71	1.48	1.40
48	5	3887	OMC	C2-N1	3.71	1.48	1.40
48	5	4456	OMC	C2-N1	3.70	1.48	1.40
48	5	4392	OMG	C2-N2	3.69	1.43	1.34
51	9	1248	B8N	O4-C4	-3.66	1.15	1.23
48	5	1625	OMG	C6-N1	3.66	1.43	1.37
48	5	4456	OMC	O2-C2	-3.66	1.16	1.23
48	5	2824	OMC	O2-C2	-3.65	1.16	1.23
48	5	4447	5MC	C2-N1	3.64	1.47	1.40
48	5	4306	OMU	O2-C2	-3.63	1.16	1.23
48	5	4293	PSU	C6-C5	3.63	1.39	1.35
48	5	3734	PSU	C6-C5	3.63	1.39	1.35
48	5	3782	5MC	C2-N1	3.62	1.47	1.40
48	5	2861	OMC	O2-C2	-3.59	1.17	1.23
48	5	4306	OMU	O4-C4	-3.58	1.17	1.24
51	9	468	A2M	O3'-C3'	-3.55	1.34	1.43
48	5	3869	OMC	O2-C2	-3.55	1.17	1.23
48	5	4536	OMC	O2-C2	-3.54	1.17	1.23
51	9	801	PSU	C6-C5	3.52	1.39	1.35
48	5	1683	PSU	C6-C5	3.50	1.39	1.35
48	5	3925	OMU	O4-C4	-3.47	1.17	1.24
48	5	3701	OMC	O2-C2	-3.47	1.17	1.23
48	5	2804	OMC	O2-C2	-3.46	1.17	1.23
48	5	1322	1MA	C4-N3	3.44	1.48	1.37
48	5	4420	PSU	C6-C5	3.43	1.39	1.35
48	5	3853	PSU	C6-C5	3.41	1.39	1.35
48	5	4296	PSU	C6-C5	3.39	1.39	1.35
48	5	1340	OMC	O2-C2	-3.39	1.17	1.23
48	5	3841	OMC	O2-C2	-3.39	1.17	1.23
48	5	2365	OMC	O2-C2	-3.39	1.17	1.23
51	9	1842	4AC	O2-C2	-3.39	1.17	1.23
48	5	1862	PSU	C6-C5	3.37	1.39	1.35
48	5	4457	PSU	C6-C5	3.37	1.39	1.35
51	9	1238	PSU	C6-C5	3.37	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3808	OMC	O2-C2	-3.37	1.17	1.23
51	9	121	OMU	O4-C4	-3.37	1.18	1.24
48	5	3782	5MC	O2-C2	-3.36	1.17	1.23
48	5	4628	PSU	C6-C5	3.36	1.39	1.35
48	5	4620	OMU	O2-C2	-3.35	1.16	1.23
51	9	109	PSU	C6-C5	3.34	1.39	1.35
51	9	1639	G7M	C5-C6	3.34	1.54	1.45
51	9	1337	4AC	O2-C2	-3.34	1.17	1.23
51	9	822	PSU	C6-C5	3.34	1.39	1.35
48	5	2351	OMC	O2-C2	-3.34	1.17	1.23
51	9	34	PSU	C6-C5	3.33	1.39	1.35
51	9	174	OMC	O2-C2	-3.33	1.17	1.23
48	5	1517	2MG	C4-N3	3.33	1.45	1.37
48	5	2632	PSU	C6-C5	3.32	1.39	1.35
51	9	1692	PSU	C6-C5	3.32	1.39	1.35
51	9	1442	OMU	C4-N3	3.32	1.44	1.38
51	9	1244	PSU	C6-C5	3.31	1.39	1.35
51	9	1367	PSU	C6-C5	3.31	1.39	1.35
51	9	428	OMU	C4-N3	3.31	1.44	1.38
48	5	3925	OMU	O2-C2	-3.30	1.17	1.23
48	5	4498	OMU	O4-C4	-3.30	1.18	1.24
51	9	1490	OMG	C5-C4	-3.28	1.34	1.43
51	9	1337	4AC	C6-N1	3.28	1.45	1.38
51	9	1490	OMG	C6-N1	3.28	1.42	1.37
48	5	4227	OMU	O2-C2	-3.27	1.17	1.23
51	9	166	A2M	C6-N6	3.27	1.46	1.34
48	5	2422	OMC	O2-C2	-3.27	1.17	1.23
51	9	1326	OMU	C4-N3	3.27	1.44	1.38
48	5	2837	OMU	O2-C2	-3.26	1.17	1.23
48	5	4521	PSU	C6-C5	3.26	1.39	1.35
51	9	105	PSU	C6-C5	3.25	1.39	1.35
48	5	4620	OMU	O4-C4	-3.25	1.18	1.24
51	9	1232	PSU	C6-C5	3.25	1.39	1.35
48	5	4571	A2M	O3'-C3'	-3.24	1.35	1.43
48	5	4523	A2M	O3'-C3'	-3.24	1.35	1.43
48	5	2364	OMG	C5-C6	3.24	1.54	1.47
48	5	3764	PSU	C6-C5	3.23	1.39	1.35
48	5	1522	OMG	C6-N1	3.22	1.42	1.37
48	5	1782	PSU	C6-C5	3.21	1.39	1.35
51	9	172	OMU	C4-N3	3.21	1.44	1.38
48	5	3869	OMC	C6-N1	3.21	1.45	1.38
51	9	1004	PSU	C6-C5	3.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1328	OMG	C6-N1	3.20	1.42	1.37
51	9	609	PSU	C6-C5	3.20	1.39	1.35
48	5	4499	OMG	C6-N1	3.19	1.42	1.37
51	9	484	A2M	C5-C4	-3.19	1.32	1.40
48	5	4447	5MC	O2-C2	-3.19	1.17	1.23
51	9	1337	4AC	C2-N1	3.19	1.46	1.40
51	9	1174	PSU	C6-C5	3.18	1.39	1.35
51	9	1045	PSU	C6-C5	3.18	1.39	1.35
51	9	1326	OMU	O2-C2	-3.18	1.17	1.23
51	9	1046	PSU	C6-C5	3.18	1.39	1.35
51	9	159	A2M	O3'-C3'	-3.18	1.35	1.43
51	9	683	OMG	C6-N1	3.18	1.42	1.37
48	5	2861	OMC	C6-N1	3.18	1.45	1.38
51	9	218	PSU	C6-C5	3.18	1.39	1.35
51	9	1177	PSU	C6-C5	3.18	1.39	1.35
48	5	2422	OMC	C6-N1	3.17	1.45	1.38
51	9	1391	OMC	C6-N1	3.17	1.45	1.38
51	9	572	PSU	C6-C5	3.17	1.39	1.35
51	9	166	A2M	O3'-C3'	-3.16	1.35	1.43
51	9	99	A2M	C5-C4	-3.16	1.32	1.40
48	5	4532	PSU	C6-C5	3.16	1.39	1.35
48	5	4623	OMG	C5-C4	-3.15	1.35	1.43
48	5	2424	OMG	C6-N1	3.15	1.42	1.37
48	5	4498	OMU	C4-N3	3.15	1.44	1.38
48	5	4618	OMG	C6-N1	3.14	1.42	1.37
48	5	2424	OMG	C5-C4	-3.14	1.35	1.43
48	5	4571	A2M	C6-N6	3.14	1.45	1.34
48	5	4498	OMU	O2-C2	-3.14	1.17	1.23
48	5	3792	OMG	C5-C4	-3.13	1.35	1.43
48	5	2787	A2M	C5-C4	-3.13	1.32	1.40
48	5	3718	A2M	C5-C4	-3.13	1.32	1.40
50	8	75	OMG	C6-N1	3.13	1.42	1.37
48	5	2824	OMC	C6-N1	3.13	1.45	1.38
51	9	1678	A2M	C6-N6	3.13	1.45	1.34
48	5	4552	PSU	C6-C5	3.12	1.39	1.35
51	9	517	OMC	C6-N1	3.12	1.45	1.38
48	5	3841	OMC	C6-N1	3.12	1.45	1.38
48	5	4227	OMU	O4-C4	-3.12	1.18	1.24
48	5	3627	OMG	C5-C6	3.11	1.53	1.47
51	9	1081	PSU	C6-C5	3.11	1.38	1.35
48	5	3825	A2M	C6-N6	3.11	1.45	1.34
48	5	1340	OMC	C6-N1	3.11	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	2837	OMU	O4-C4	-3.11	1.18	1.24
51	9	512	A2M	O2'-C2'	3.10	1.50	1.42
48	5	1871	A2M	C5-C4	-3.10	1.32	1.40
51	9	1850	MA6	C5-C4	-3.09	1.32	1.40
51	9	1678	A2M	O2'-C2'	3.09	1.50	1.42
48	5	1326	A2M	O3'-C3'	-3.09	1.35	1.43
48	5	2365	OMC	C6-N1	3.08	1.45	1.38
48	5	1677	PSU	C6-C5	3.08	1.38	1.35
48	5	2351	OMC	C6-N1	3.08	1.45	1.38
48	5	1534	A2M	C5-C4	-3.07	1.32	1.40
48	5	1316	OMG	C6-N1	3.07	1.42	1.37
48	5	4623	OMG	C6-N1	3.07	1.42	1.37
48	5	4571	A2M	C5-C4	-3.07	1.32	1.40
48	5	398	A2M	O3'-C3'	-3.06	1.35	1.43
48	5	373	OMG	O6-C6	-3.06	1.17	1.23
48	5	4392	OMG	C5-C4	-3.06	1.35	1.43
48	5	1677	PSU	O4'-C1'	-3.06	1.39	1.43
48	5	1316	OMG	C5-C6	3.06	1.53	1.47
51	9	512	A2M	O3'-C3'	-3.06	1.35	1.43
48	5	1326	A2M	O2'-C2'	3.05	1.50	1.42
51	9	1391	OMC	O2-C2	-3.05	1.18	1.23
48	5	3887	OMC	O2-C2	-3.05	1.18	1.23
48	5	4618	OMG	C5-C4	-3.05	1.35	1.43
48	5	3762	PSU	C6-C5	3.05	1.38	1.35
48	5	3760	A2M	O3'-C3'	-3.04	1.35	1.43
51	9	649	PSU	C6-C5	3.04	1.38	1.35
48	5	398	A2M	C6-N6	3.04	1.45	1.34
48	5	373	OMG	C5-C4	-3.04	1.35	1.43
51	9	468	A2M	C6-N6	3.03	1.45	1.34
48	5	3818	UY1	C4-N3	3.03	1.44	1.38
51	9	1703	OMC	C6-N1	3.03	1.45	1.38
48	5	3830	A2M	O3'-C3'	-3.03	1.35	1.43
48	5	3639	PSU	C6-C5	3.03	1.38	1.35
48	5	1522	OMG	O6-C6	-3.03	1.17	1.23
48	5	3627	OMG	C6-N1	3.03	1.42	1.37
51	9	668	A2M	O3'-C3'	-3.03	1.35	1.43
48	5	4228	OMG	C5-C6	3.02	1.53	1.47
48	5	4442	PSU	C6-C5	3.02	1.38	1.35
51	9	1031	A2M	C5-C4	-3.02	1.32	1.40
48	5	1322	1MA	C5-C4	-3.02	1.35	1.43
48	5	1860	PSU	C6-C5	3.02	1.38	1.35
48	5	3701	OMC	C6-N1	3.02	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3724	A2M	O3'-C3'	-3.02	1.35	1.43
48	5	4227	OMU	C4-N3	3.01	1.43	1.38
48	5	2363	A2M	O3'-C3'	-3.01	1.35	1.43
51	9	1851	MA6	C5-C4	-3.01	1.33	1.40
51	9	1328	OMG	C5-C4	-3.01	1.35	1.43
51	9	174	OMC	C6-N1	3.01	1.45	1.38
48	5	4361	PSU	C6-C5	3.00	1.38	1.35
48	5	3867	A2M	O3'-C3'	-3.00	1.35	1.43
48	5	1534	A2M	O3'-C3'	-3.00	1.35	1.43
51	9	815	PSU	C6-C5	3.00	1.38	1.35
51	9	517	OMC	O2-C2	-2.99	1.18	1.23
48	5	1522	OMG	C5-C4	-2.99	1.35	1.43
51	9	116	OMU	C4-N3	2.99	1.43	1.38
48	5	3724	A2M	C6-N6	2.98	1.44	1.34
48	5	1781	PSU	C6-C5	2.98	1.38	1.35
51	9	512	A2M	C6-N6	2.98	1.44	1.34
48	5	4637	OMG	C5-C4	-2.98	1.35	1.43
48	5	1522	OMG	C5-C6	2.97	1.53	1.47
48	5	4392	OMG	C5-C6	2.97	1.53	1.47
48	5	2508	PSU	C6-C5	2.97	1.38	1.35
48	5	4618	OMG	O6-C6	-2.97	1.17	1.23
51	9	484	A2M	C6-N6	2.96	1.44	1.34
51	9	119	PSU	C6-C5	2.96	1.38	1.35
51	9	668	A2M	C6-N6	2.96	1.44	1.34
51	9	159	A2M	C6-N6	2.96	1.44	1.34
48	5	3760	A2M	C6-N6	2.96	1.44	1.34
48	5	1316	OMG	O6-C6	-2.96	1.17	1.23
48	5	1316	OMG	C5-C4	-2.96	1.35	1.43
48	5	1524	A2M	C5-C4	-2.95	1.33	1.40
48	5	2815	A2M	C5-C4	-2.95	1.33	1.40
48	5	2804	OMC	C6-N1	2.95	1.45	1.38
51	9	27	A2M	C6-N6	2.95	1.44	1.34
51	9	1383	A2M	O3'-C3'	-2.94	1.36	1.43
51	9	1643	PSU	C6-C5	2.94	1.38	1.35
51	9	172	OMU	O4-C4	-2.94	1.18	1.24
51	9	428	OMU	O4-C4	-2.94	1.18	1.24
48	5	3808	OMC	C6-N1	2.94	1.45	1.38
48	5	2364	OMG	C5-C4	-2.94	1.35	1.43
48	5	237	B9B	C5-C4	-2.94	1.33	1.40
48	5	3718	A2M	O2'-C2'	2.93	1.50	1.42
48	5	3830	A2M	C5-C4	-2.93	1.33	1.40
51	9	1445	PSU	C6-C5	2.93	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3867	A2M	C5-C4	-2.93	1.33	1.40
51	9	121	OMU	O2-C2	-2.93	1.17	1.23
48	5	4370	OMG	C5-C4	-2.93	1.35	1.43
48	5	2787	A2M	O3'-C3'	-2.92	1.36	1.43
51	9	1347	PSU	C6-C5	2.92	1.38	1.35
48	5	4536	OMC	C6-N1	2.92	1.45	1.38
48	5	1524	A2M	C6-N6	2.92	1.44	1.34
48	5	1517	2MG	C5-C4	-2.92	1.35	1.43
48	5	4571	A2M	O2'-C2'	2.92	1.50	1.42
48	5	4494	OMG	C5-C4	-2.92	1.35	1.43
48	5	3785	A2M	C5-C4	-2.91	1.33	1.40
48	5	4353	PSU	C6-C5	2.91	1.38	1.35
51	9	1442	OMU	O4-C4	-2.90	1.18	1.24
48	5	4196	OMG	O6-C6	-2.90	1.17	1.23
48	5	4392	OMG	O6-C6	-2.90	1.17	1.23
48	5	2363	A2M	C5-C4	-2.89	1.33	1.40
48	5	3818	UY1	O2-C2	-2.89	1.17	1.23
48	5	3867	A2M	C6-N6	2.88	1.44	1.34
48	5	4499	OMG	C5-C4	-2.88	1.35	1.43
48	5	3887	OMC	C6-N1	2.88	1.44	1.38
51	9	509	OMG	O6-C6	-2.88	1.17	1.23
51	9	1383	A2M	O2'-C2'	2.88	1.50	1.42
51	9	1383	A2M	C6-N6	2.88	1.44	1.34
51	9	1678	A2M	C5-C4	-2.88	1.33	1.40
48	5	1625	OMG	O6-C6	-2.88	1.17	1.23
51	9	668	A2M	C5-C4	-2.87	1.33	1.40
48	5	3792	OMG	C6-N1	2.87	1.42	1.37
48	5	400	A2M	O3'-C3'	-2.86	1.36	1.43
48	5	2787	A2M	C6-N6	2.86	1.44	1.34
48	5	2876	OMG	C5-C6	2.86	1.53	1.47
51	9	644	OMG	C5-C6	2.86	1.53	1.47
48	5	4494	OMG	O6-C6	-2.86	1.17	1.23
51	9	683	OMG	C5-C6	2.86	1.53	1.47
48	5	1625	OMG	C5-C4	-2.86	1.35	1.43
48	5	400	A2M	C5-C4	-2.86	1.33	1.40
48	5	398	A2M	C5-C4	-2.85	1.33	1.40
51	9	814	PSU	C6-C5	2.85	1.38	1.35
48	5	2363	A2M	O2'-C2'	2.85	1.49	1.42
51	9	172	OMU	O2-C2	-2.85	1.17	1.23
48	5	1871	A2M	C6-N6	2.85	1.44	1.34
48	5	1534	A2M	C6-N6	2.85	1.44	1.34
48	5	4403	PSU	C6-C5	2.85	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1842	4AC	C6-N1	2.84	1.44	1.38
48	5	2815	A2M	O3'-C3'	-2.84	1.36	1.43
51	9	99	A2M	O3'-C3'	-2.84	1.36	1.43
48	5	3825	A2M	O3'-C3'	-2.84	1.36	1.43
51	9	484	A2M	O2'-C2'	2.84	1.49	1.42
51	9	1703	OMC	O2-C2	-2.83	1.18	1.23
51	9	1031	A2M	C6-N6	2.83	1.44	1.34
48	5	3724	A2M	C5-C4	-2.83	1.33	1.40
48	5	4523	A2M	C6-N6	2.83	1.44	1.34
48	5	4623	OMG	O6-C6	-2.83	1.17	1.23
48	5	1534	A2M	O2'-C2'	2.83	1.49	1.42
48	5	400	A2M	C6-N6	2.83	1.44	1.34
48	5	2837	OMU	C4-N3	2.82	1.43	1.38
51	9	683	OMG	C5-C4	-2.82	1.35	1.43
48	5	3760	A2M	O2'-C2'	2.82	1.49	1.42
48	5	3627	OMG	C5-C4	-2.82	1.35	1.43
48	5	4228	OMG	C6-N1	2.82	1.42	1.37
48	5	1871	A2M	O3'-C3'	-2.81	1.36	1.43
51	9	159	A2M	O2'-C2'	2.81	1.49	1.42
48	5	1326	A2M	C5-C4	-2.81	1.33	1.40
51	9	1031	A2M	O3'-C3'	-2.81	1.36	1.43
51	9	116	OMU	O2-C2	-2.81	1.17	1.23
48	5	2363	A2M	C6-N6	2.80	1.44	1.34
48	5	1524	A2M	O3'-C3'	-2.80	1.36	1.43
48	5	3899	OMG	C5-C4	-2.80	1.35	1.43
51	9	1326	OMU	O4-C4	-2.80	1.19	1.24
48	5	3718	A2M	O3'-C3'	-2.80	1.36	1.43
51	9	436	OMG	C5-C4	-2.80	1.35	1.43
51	9	99	A2M	C6-N6	2.80	1.44	1.34
48	5	3899	OMG	C6-N1	2.80	1.42	1.37
48	5	1326	A2M	C6-N6	2.80	1.44	1.34
48	5	1524	A2M	O2'-C2'	2.80	1.49	1.42
51	9	644	OMG	C6-N1	2.80	1.42	1.37
48	5	2815	A2M	C6-N6	2.80	1.44	1.34
48	5	4196	OMG	C5-C4	-2.79	1.35	1.43
48	5	4500	PSU	C6-C5	2.79	1.38	1.35
48	5	4370	OMG	O6-C6	-2.79	1.17	1.23
51	9	1383	A2M	C5-C4	-2.79	1.33	1.40
51	9	27	A2M	O3'-C3'	-2.79	1.36	1.43
48	5	4196	OMG	C6-N1	2.79	1.42	1.37
48	5	3760	A2M	C5-C4	-2.79	1.33	1.40
51	9	116	OMU	O4-C4	-2.79	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4618	OMG	C5-C6	2.79	1.53	1.47
48	5	3718	A2M	C6-N6	2.78	1.44	1.34
48	5	4370	OMG	C6-N1	2.78	1.42	1.37
48	5	4530	UR3	C6-N1	2.77	1.44	1.38
50	8	75	OMG	C5-C6	2.76	1.53	1.47
48	5	3785	A2M	C6-N6	2.76	1.44	1.34
51	9	159	A2M	C5-C4	-2.76	1.33	1.40
48	5	2364	OMG	O6-C6	-2.76	1.17	1.23
51	9	484	A2M	O3'-C3'	-2.75	1.36	1.43
51	9	166	A2M	O2'-C2'	2.75	1.49	1.42
48	5	4456	OMC	C6-N1	2.75	1.44	1.38
51	9	468	A2M	C5-C4	-2.75	1.33	1.40
48	5	4228	OMG	C5-C4	-2.75	1.36	1.43
51	9	668	A2M	O2'-C2'	2.75	1.49	1.42
48	5	4637	OMG	C5-C6	2.75	1.53	1.47
48	5	2815	A2M	O2'-C2'	2.74	1.49	1.42
48	5	3818	UY1	O4-C4	-2.74	1.18	1.23
50	8	75	OMG	C5-C4	-2.74	1.36	1.43
48	5	4579	PSU	C6-C5	2.74	1.38	1.35
48	5	4523	A2M	C5-C4	-2.74	1.33	1.40
48	5	3825	A2M	O2'-C2'	2.74	1.49	1.42
48	5	4228	OMG	O6-C6	-2.74	1.17	1.23
51	9	121	OMU	C4-N3	2.73	1.43	1.38
48	5	4530	UR3	O2-C2	-2.73	1.17	1.22
51	9	863	PSU	C6-C5	2.73	1.38	1.35
51	9	166	A2M	C5-C4	-2.72	1.33	1.40
48	5	1792	PSU	C6-C5	2.72	1.38	1.35
48	5	2787	A2M	O2'-C2'	2.72	1.49	1.42
51	9	512	A2M	C5-C4	-2.72	1.33	1.40
48	5	398	A2M	O2'-C2'	2.71	1.49	1.42
48	5	4637	OMG	O6-C6	-2.71	1.17	1.23
48	5	2876	OMG	C6-N1	2.71	1.41	1.37
48	5	3851	PSU	C6-C5	2.71	1.38	1.35
51	9	436	OMG	C6-N1	2.70	1.41	1.37
48	5	3899	OMG	C5-C6	2.70	1.52	1.47
51	9	686	PSU	C6-C5	2.70	1.38	1.35
48	5	3830	A2M	O2'-C2'	2.69	1.49	1.42
48	5	4370	OMG	C5-C6	2.69	1.52	1.47
48	5	3627	OMG	O6-C6	-2.69	1.17	1.23
48	5	2364	OMG	C6-N1	2.69	1.41	1.37
48	5	2424	OMG	O6-C6	-2.69	1.17	1.23
48	5	4523	A2M	O2'-C2'	2.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1490	OMG	C5-C6	2.68	1.52	1.47
51	9	436	OMG	O6-C6	-2.68	1.17	1.23
48	5	3830	A2M	C6-N6	2.68	1.43	1.34
48	5	3792	OMG	O6-C6	-2.67	1.17	1.23
51	9	1639	G7M	C2-N1	2.67	1.44	1.37
48	5	3825	A2M	C5-C4	-2.67	1.33	1.40
51	9	27	A2M	O2'-C2'	2.66	1.49	1.42
51	9	99	A2M	O2'-C2'	2.66	1.49	1.42
48	5	3920	PSU	C6-C5	2.66	1.38	1.35
48	5	2876	OMG	C5-C4	-2.65	1.36	1.43
51	9	468	A2M	O2'-C2'	2.65	1.49	1.42
48	5	4494	OMG	C6-N1	2.65	1.41	1.37
48	5	2876	OMG	O6-C6	-2.64	1.17	1.23
48	5	4423	PSU	C6-C5	2.63	1.38	1.35
51	9	428	OMU	O2-C2	-2.63	1.18	1.23
51	9	1678	A2M	O3'-C3'	-2.63	1.36	1.43
48	5	1871	A2M	O2'-C2'	2.63	1.49	1.42
51	9	1832	6MZ	C5-C4	-2.63	1.34	1.40
48	5	3724	A2M	O2'-C2'	2.61	1.49	1.42
48	5	1744	PSU	C6-C5	2.60	1.38	1.35
48	5	2424	OMG	C5-C6	2.60	1.52	1.47
48	5	3715	PSU	C6-C5	2.60	1.38	1.35
48	5	4499	OMG	O6-C6	-2.58	1.18	1.23
48	5	4637	OMG	C6-N1	2.58	1.41	1.37
48	5	3899	OMG	O6-C6	-2.58	1.18	1.23
48	5	400	A2M	O2'-C2'	2.58	1.49	1.42
48	5	3867	A2M	O2'-C2'	2.57	1.49	1.42
48	5	1517	2MG	O6-C6	-2.57	1.18	1.23
48	5	4220	6MZ	C5-C4	-2.57	1.34	1.40
48	5	3695	PSU	C6-C5	2.57	1.38	1.35
48	5	3818	UY1	O4'-C1'	-2.57	1.40	1.43
48	5	4299	PSU	C6-C5	2.57	1.38	1.35
48	5	4623	OMG	C5-C6	2.57	1.52	1.47
51	9	1248	B8N	C32-C33	2.56	1.58	1.53
51	9	644	OMG	C2-N1	2.56	1.44	1.37
51	9	509	OMG	C5-C4	-2.56	1.36	1.43
51	9	1842	4AC	O7-C7	-2.56	1.17	1.23
51	9	509	OMG	C6-N1	2.54	1.41	1.37
48	5	4494	OMG	C5-C6	2.54	1.52	1.47
51	9	1703	OMC	C5-C4	2.54	1.48	1.42
48	5	373	OMG	C5-C6	2.54	1.52	1.47
48	5	4499	OMG	C2-N1	2.53	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1442	OMU	O2-C2	-2.53	1.18	1.23
51	9	1490	OMG	O6-C6	-2.53	1.18	1.23
51	9	644	OMG	C5-C4	-2.52	1.36	1.43
48	5	4530	UR3	O4-C4	-2.52	1.18	1.23
51	9	1031	A2M	O2'-C2'	2.52	1.49	1.42
50	8	75	OMG	O6-C6	-2.52	1.18	1.23
51	9	1328	OMG	O6-C6	-2.52	1.18	1.23
48	5	3785	A2M	O2'-C2'	2.51	1.49	1.42
51	9	27	A2M	C5-C4	-2.50	1.34	1.40
51	9	517	OMC	C5-C4	2.48	1.48	1.42
48	5	4196	OMG	C5-C6	2.47	1.52	1.47
51	9	683	OMG	O6-C6	-2.47	1.18	1.23
48	5	2365	OMC	C5-C4	2.47	1.48	1.42
48	5	1871	A2M	O5'-C5'	-2.40	1.38	1.44
51	9	1337	4AC	O7-C7	-2.40	1.17	1.23
50	8	75	OMG	C2-N1	2.38	1.43	1.37
48	5	1534	A2M	O5'-C5'	-2.38	1.38	1.44
48	5	4306	OMU	C4-N3	2.37	1.42	1.38
48	5	4499	OMG	C5-C6	2.37	1.52	1.47
51	9	1328	OMG	C5-C6	2.37	1.52	1.47
48	5	4456	OMC	C5-C4	2.36	1.48	1.42
48	5	3825	A2M	O5'-C5'	-2.36	1.39	1.44
51	9	174	OMC	C5-C4	2.35	1.48	1.42
48	5	2824	OMC	C5-C4	2.35	1.48	1.42
48	5	2364	OMG	C2-N1	2.34	1.43	1.37
48	5	2876	OMG	C2-N1	2.34	1.43	1.37
48	5	3925	OMU	C4-N3	2.34	1.42	1.38
48	5	4620	OMU	C4-N3	2.34	1.42	1.38
51	9	468	A2M	O5'-C5'	-2.33	1.39	1.44
48	5	1522	OMG	C2-N1	2.33	1.43	1.37
51	9	1639	G7M	O6-C6	-2.33	1.18	1.23
48	5	398	A2M	C2-N3	2.32	1.35	1.32
48	5	1340	OMC	C5-C4	2.31	1.48	1.42
48	5	3724	A2M	O5'-C5'	-2.31	1.39	1.44
48	5	3830	A2M	O5'-C5'	-2.31	1.39	1.44
48	5	4392	OMG	C6-N1	2.30	1.41	1.37
48	5	1326	A2M	O5'-C5'	-2.29	1.39	1.44
48	5	1524	A2M	O5'-C5'	-2.28	1.39	1.44
48	5	3785	A2M	O5'-C5'	-2.28	1.39	1.44
51	9	801	PSU	O4'-C1'	-2.28	1.40	1.43
48	5	4571	A2M	O5'-C5'	-2.28	1.39	1.44
51	9	1328	OMG	C2-N1	2.27	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	2422	OMC	C5-C4	2.27	1.48	1.42
51	9	683	OMG	C2-N1	2.27	1.43	1.37
48	5	4228	OMG	C2-N1	2.27	1.43	1.37
51	9	436	OMG	C2-N1	2.26	1.43	1.37
48	5	2861	OMC	C5-C4	2.25	1.48	1.42
48	5	400	A2M	O5'-C5'	-2.25	1.39	1.44
51	9	99	A2M	O5'-C5'	-2.24	1.39	1.44
48	5	1625	OMG	C2-N1	2.24	1.43	1.37
48	5	3785	A2M	O3'-C3'	-2.23	1.37	1.43
51	9	484	A2M	O5'-C5'	-2.23	1.39	1.44
48	5	2804	OMC	C5-C4	2.22	1.48	1.42
48	5	4523	A2M	O5'-C5'	-2.22	1.39	1.44
48	5	3841	OMC	C5-C4	2.22	1.48	1.42
51	9	436	OMG	C5-C6	2.21	1.51	1.47
48	5	4500	PSU	O4'-C1'	-2.20	1.40	1.43
48	5	4618	OMG	C2-N1	2.20	1.43	1.37
51	9	644	OMG	O6-C6	-2.20	1.18	1.23
48	5	2351	OMC	C5-C4	2.20	1.48	1.42
48	5	2815	A2M	O5'-C5'	-2.20	1.39	1.44
48	5	4370	OMG	C2-N1	2.20	1.43	1.37
48	5	3715	PSU	O4'-C1'	-2.20	1.40	1.43
48	5	3715	PSU	C4-C5	-2.19	1.37	1.44
48	5	1517	2MG	CM2-N2	2.19	1.49	1.45
48	5	1316	OMG	C2-N1	2.19	1.43	1.37
48	5	3627	OMG	C2-N1	2.19	1.43	1.37
48	5	3701	OMC	C5-C4	2.18	1.47	1.42
51	9	1031	A2M	O5'-C5'	-2.18	1.39	1.44
48	5	1625	OMG	C5-C6	2.18	1.51	1.47
48	5	4494	OMG	C2-N1	2.17	1.43	1.37
48	5	2363	A2M	O5'-C5'	-2.16	1.39	1.44
51	9	428	OMU	C6-N1	2.16	1.43	1.38
51	9	1383	A2M	O5'-C5'	-2.16	1.39	1.44
48	5	373	OMG	C6-N1	2.16	1.41	1.37
48	5	373	OMG	C2-N1	2.15	1.43	1.37
48	5	3792	OMG	C5-C6	2.14	1.51	1.47
48	5	400	A2M	C2-N3	2.14	1.35	1.32
48	5	2787	A2M	C2-N3	2.14	1.35	1.32
48	5	3808	OMC	C5-C4	2.13	1.47	1.42
51	9	822	PSU	O4'-C1'	-2.13	1.40	1.43
51	9	668	A2M	O5'-C5'	-2.12	1.39	1.44
48	5	4637	OMG	C2-N1	2.12	1.42	1.37
51	9	159	A2M	C2-N3	2.11	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3925	OMU	C5-C4	2.11	1.48	1.43
48	5	4536	OMC	C5-C4	2.10	1.47	1.42
48	5	3851	PSU	O4'-C1'	-2.09	1.40	1.43
48	5	3760	A2M	C2-N3	2.09	1.35	1.32
51	9	1326	OMU	C5-C4	2.09	1.48	1.43
51	9	172	OMU	C5-C4	2.09	1.48	1.43
48	5	3718	A2M	O5'-C5'	-2.07	1.39	1.44
48	5	2424	OMG	C2-N1	2.07	1.42	1.37
51	9	1391	OMC	C5-C4	2.07	1.47	1.42
48	5	3825	A2M	C2-N3	2.07	1.35	1.32
48	5	2787	A2M	O5'-C5'	-2.07	1.39	1.44
48	5	4306	OMU	C6-N1	2.07	1.43	1.38
51	9	1639	G7M	C8-N7	2.06	1.36	1.33
51	9	1851	MA6	C2-N3	2.06	1.35	1.32
51	9	509	OMG	C2-N1	2.06	1.42	1.37
51	9	1238	PSU	C4-C5	-2.05	1.38	1.44
48	5	4227	OMU	C5-C4	2.05	1.48	1.43
48	5	4620	OMU	C6-N1	2.04	1.42	1.38
48	5	4392	OMG	C2-N1	2.03	1.42	1.37
48	5	4530	UR3	C5-C4	2.03	1.49	1.43
48	5	4498	OMU	C6-N1	2.02	1.42	1.38
51	9	468	A2M	C2-N3	2.02	1.35	1.32
48	5	4498	OMU	C5-C4	2.01	1.48	1.43
48	5	4521	PSU	O4'-C1'	-2.01	1.41	1.43
51	9	822	PSU	C4-C5	-2.01	1.38	1.44
48	5	3899	OMG	C2-N1	2.01	1.42	1.37
48	5	4623	OMG	C2-N1	2.01	1.42	1.37
48	5	4571	A2M	C2-N3	2.00	1.35	1.32

All (554) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1851	MA6	N1-C6-N6	-18.65	97.42	117.06
51	9	1850	MA6	N1-C6-N6	-15.52	100.72	117.06
51	9	512	A2M	C5-C6-N6	11.97	138.54	120.35
51	9	484	A2M	C5-C6-N6	11.70	138.13	120.35
51	9	1678	A2M	C5-C6-N6	11.45	137.75	120.35
48	5	4523	A2M	C5-C6-N6	11.26	137.47	120.35
51	9	1383	A2M	C5-C6-N6	11.15	137.29	120.35
48	5	2363	A2M	C5-C6-N6	11.14	137.28	120.35
48	5	3760	A2M	C5-C6-N6	11.10	137.22	120.35
48	5	4571	A2M	C5-C6-N6	11.09	137.20	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	27	A2M	C5-C6-N6	11.06	137.16	120.35
51	9	159	A2M	C5-C6-N6	10.98	137.04	120.35
51	9	668	A2M	C5-C6-N6	10.98	137.04	120.35
51	9	99	A2M	C5-C6-N6	10.90	136.92	120.35
48	5	3718	A2M	C5-C6-N6	10.89	136.90	120.35
48	5	1524	A2M	C5-C6-N6	10.85	136.85	120.35
48	5	1534	A2M	C5-C6-N6	10.80	136.76	120.35
51	9	166	A2M	C5-C6-N6	10.74	136.67	120.35
48	5	3830	A2M	C5-C6-N6	10.71	136.63	120.35
51	9	468	A2M	C5-C6-N6	10.70	136.62	120.35
48	5	2815	A2M	C5-C6-N6	10.70	136.61	120.35
48	5	1326	A2M	C5-C6-N6	10.68	136.58	120.35
48	5	398	A2M	C5-C6-N6	10.62	136.50	120.35
48	5	3867	A2M	C5-C6-N6	10.60	136.46	120.35
48	5	1871	A2M	C5-C6-N6	10.47	136.26	120.35
48	5	3785	A2M	C5-C6-N6	10.47	136.26	120.35
51	9	1031	A2M	C5-C6-N6	10.35	136.09	120.35
48	5	3724	A2M	C5-C6-N6	10.18	135.82	120.35
48	5	3825	A2M	C5-C6-N6	10.08	135.68	120.35
48	5	2787	A2M	C5-C6-N6	10.05	135.63	120.35
51	9	1851	MA6	C1'-N9-C4	-9.96	109.14	126.64
48	5	400	A2M	C5-C6-N6	9.44	134.70	120.35
51	9	1850	MA6	C1'-N9-C4	-9.00	110.83	126.64
51	9	512	A2M	N6-C6-N1	-8.01	101.95	118.57
51	9	484	A2M	N6-C6-N1	-7.96	102.06	118.57
51	9	1678	A2M	N6-C6-N1	-7.88	102.23	118.57
48	5	3760	A2M	N6-C6-N1	-7.70	102.59	118.57
48	5	4571	A2M	N6-C6-N1	-7.70	102.59	118.57
48	5	2363	A2M	N6-C6-N1	-7.67	102.65	118.57
51	9	1383	A2M	N6-C6-N1	-7.63	102.74	118.57
48	5	4523	A2M	N6-C6-N1	-7.56	102.89	118.57
51	9	99	A2M	N6-C6-N1	-7.55	102.89	118.57
51	9	668	A2M	N6-C6-N1	-7.54	102.93	118.57
48	5	398	A2M	N6-C6-N1	-7.51	102.98	118.57
51	9	159	A2M	N6-C6-N1	-7.50	103.00	118.57
48	5	3718	A2M	N6-C6-N1	-7.38	103.26	118.57
48	5	2815	A2M	N6-C6-N1	-7.33	103.36	118.57
51	9	468	A2M	N6-C6-N1	-7.31	103.41	118.57
51	9	27	A2M	N6-C6-N1	-7.29	103.44	118.57
48	5	3785	A2M	N6-C6-N1	-7.29	103.45	118.57
48	5	3867	A2M	N6-C6-N1	-7.24	103.54	118.57
48	5	3830	A2M	N6-C6-N1	-7.21	103.61	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	1524	A2M	N6-C6-N1	-7.15	103.74	118.57
48	5	1534	A2M	N6-C6-N1	-7.14	103.75	118.57
48	5	3724	A2M	N6-C6-N1	-7.08	103.88	118.57
51	9	1031	A2M	N6-C6-N1	-7.00	104.04	118.57
48	5	2787	A2M	N6-C6-N1	-6.99	104.06	118.57
48	5	1326	A2M	N6-C6-N1	-6.98	104.08	118.57
51	9	166	A2M	N6-C6-N1	-6.95	104.16	118.57
48	5	1871	A2M	N6-C6-N1	-6.67	104.72	118.57
48	5	3825	A2M	N6-C6-N1	-6.56	104.97	118.57
48	5	400	A2M	N6-C6-N1	-6.16	105.79	118.57
51	9	166	A2M	N3-C2-N1	-6.12	119.11	128.68
51	9	484	A2M	N3-C2-N1	-6.03	119.26	128.68
51	9	512	A2M	N3-C2-N1	-5.95	119.38	128.68
48	5	3830	A2M	N3-C2-N1	-5.93	119.41	128.68
51	9	1832	6MZ	N3-C2-N1	-5.90	119.46	128.68
48	5	1871	A2M	N3-C2-N1	-5.88	119.48	128.68
51	9	1031	A2M	N3-C2-N1	-5.82	119.58	128.68
48	5	3867	A2M	N3-C2-N1	-5.77	119.67	128.68
48	5	4498	OMU	C4-N3-C2	-5.73	119.03	126.58
48	5	237	B9B	N3-C2-N1	-5.72	119.59	127.22
51	9	1851	MA6	N3-C2-N1	-5.72	119.73	128.68
48	5	1326	A2M	N3-C2-N1	-5.71	119.75	128.68
51	9	1383	A2M	N3-C2-N1	-5.70	119.76	128.68
48	5	4571	A2M	N3-C2-N1	-5.69	119.78	128.68
48	5	2815	A2M	N3-C2-N1	-5.68	119.80	128.68
51	9	1326	OMU	C4-N3-C2	-5.66	119.11	126.58
51	9	468	A2M	N3-C2-N1	-5.65	119.85	128.68
48	5	4523	A2M	N3-C2-N1	-5.63	119.87	128.68
51	9	668	A2M	N3-C2-N1	-5.63	119.88	128.68
48	5	2837	OMU	C4-N3-C2	-5.61	119.18	126.58
48	5	1524	A2M	N3-C2-N1	-5.59	119.94	128.68
48	5	3718	A2M	N3-C2-N1	-5.56	119.99	128.68
48	5	1534	A2M	N3-C2-N1	-5.53	120.03	128.68
51	9	686	PSU	C4-N3-C2	-5.51	118.40	126.34
48	5	4220	6MZ	N3-C2-N1	-5.49	120.09	128.68
51	9	27	A2M	N3-C2-N1	-5.49	120.10	128.68
48	5	4521	PSU	N1-C2-N3	5.45	121.31	115.13
48	5	3925	OMU	C4-N3-C2	-5.45	119.39	126.58
51	9	1678	A2M	N3-C2-N1	-5.44	120.17	128.68
51	9	218	PSU	N1-C2-N3	5.44	121.29	115.13
48	5	2787	A2M	N3-C2-N1	-5.43	120.19	128.68
48	5	4227	OMU	C4-N3-C2	-5.42	119.43	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3760	A2M	N3-C2-N1	-5.38	120.26	128.68
48	5	398	A2M	N3-C2-N1	-5.37	120.28	128.68
48	5	2363	A2M	N3-C2-N1	-5.35	120.32	128.68
48	5	3785	A2M	N3-C2-N1	-5.34	120.33	128.68
48	5	3724	A2M	N3-C2-N1	-5.33	120.35	128.68
48	5	3762	PSU	C4-N3-C2	-5.32	118.67	126.34
51	9	99	A2M	N3-C2-N1	-5.31	120.37	128.68
51	9	218	PSU	C4-N3-C2	-5.31	118.69	126.34
51	9	1248	B8N	C5-C4-N3	5.31	126.00	116.17
48	5	4620	OMU	C4-N3-C2	-5.28	119.62	126.58
48	5	4306	OMU	C4-N3-C2	-5.26	119.64	126.58
51	9	159	A2M	N3-C2-N1	-5.25	120.47	128.68
51	9	1850	MA6	N3-C2-N1	-5.25	120.48	128.68
48	5	3853	PSU	N1-C2-N3	5.23	121.05	115.13
48	5	4628	PSU	N1-C2-N3	5.21	121.03	115.13
51	9	172	OMU	C4-N3-C2	-5.21	119.71	126.58
48	5	1677	PSU	C4-N3-C2	-5.20	118.85	126.34
51	9	1442	OMU	C4-N3-C2	-5.19	119.73	126.58
51	9	121	OMU	C4-N3-C2	-5.19	119.73	126.58
51	9	1643	PSU	C4-N3-C2	-5.17	118.89	126.34
48	5	4628	PSU	C4-N3-C2	-5.17	118.89	126.34
48	5	1322	1MA	N1-C2-N3	-5.16	120.00	126.02
48	5	1677	PSU	N1-C2-N3	5.14	120.96	115.13
48	5	400	A2M	N3-C2-N1	-5.13	120.66	128.68
48	5	3920	PSU	C4-N3-C2	-5.12	118.97	126.34
48	5	1683	PSU	N1-C2-N3	5.11	120.92	115.13
51	9	1174	PSU	N1-C2-N3	5.11	120.92	115.13
51	9	822	PSU	N1-C2-N3	5.11	120.91	115.13
48	5	4442	PSU	N1-C2-N3	5.10	120.91	115.13
51	9	1045	PSU	N1-C2-N3	5.10	120.90	115.13
48	5	4353	PSU	N1-C2-N3	5.09	120.90	115.13
51	9	428	OMU	C4-N3-C2	-5.08	119.88	126.58
51	9	686	PSU	N1-C2-N3	5.07	120.87	115.13
48	5	3851	PSU	N1-C2-N3	5.06	120.86	115.13
51	9	1045	PSU	C4-N3-C2	-5.05	119.06	126.34
48	5	3920	PSU	N1-C2-N3	5.03	120.83	115.13
51	9	109	PSU	N1-C2-N3	5.02	120.82	115.13
48	5	4220	6MZ	C2-N1-C6	5.01	120.89	116.59
51	9	1244	PSU	C4-N3-C2	-5.01	119.12	126.34
51	9	1248	B8N	C4-N3-C2	-5.01	119.12	125.46
48	5	3825	A2M	N3-C2-N1	-5.00	120.86	128.68
48	5	3853	PSU	C4-N3-C2	-4.99	119.15	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3762	PSU	N1-C2-N3	4.98	120.78	115.13
51	9	105	PSU	N1-C2-N3	4.98	120.78	115.13
48	5	3764	PSU	C4-N3-C2	-4.97	119.17	126.34
51	9	1643	PSU	N1-C2-N3	4.97	120.76	115.13
51	9	814	PSU	C4-N3-C2	-4.96	119.19	126.34
48	5	4361	PSU	N1-C2-N3	4.96	120.75	115.13
51	9	116	OMU	C4-N3-C2	-4.96	120.04	126.58
48	5	4423	PSU	C4-N3-C2	-4.95	119.20	126.34
51	9	815	PSU	N1-C2-N3	4.94	120.73	115.13
48	5	3764	PSU	N1-C2-N3	4.94	120.72	115.13
48	5	4361	PSU	C4-N3-C2	-4.94	119.23	126.34
51	9	822	PSU	C4-N3-C2	-4.93	119.23	126.34
51	9	109	PSU	C4-N3-C2	-4.93	119.23	126.34
51	9	815	PSU	C4-N3-C2	-4.93	119.23	126.34
51	9	1081	PSU	N1-C2-N3	4.93	120.71	115.13
48	5	4299	PSU	C4-N3-C2	-4.92	119.25	126.34
51	9	1347	PSU	C4-N3-C2	-4.92	119.25	126.34
48	5	4552	PSU	C4-N3-C2	-4.90	119.28	126.34
51	9	1174	PSU	C4-N3-C2	-4.90	119.28	126.34
48	5	1683	PSU	C4-N3-C2	-4.90	119.28	126.34
51	9	1832	6MZ	C2-N1-C6	4.88	120.78	116.59
51	9	34	PSU	N1-C2-N3	4.87	120.65	115.13
48	5	4296	PSU	N1-C2-N3	4.83	120.61	115.13
48	5	3695	PSU	C4-N3-C2	-4.83	119.38	126.34
51	9	1004	PSU	N1-C2-N3	4.83	120.60	115.13
48	5	3851	PSU	C4-N3-C2	-4.83	119.38	126.34
51	9	814	PSU	N1-C2-N3	4.82	120.59	115.13
51	9	119	PSU	C4-N3-C2	-4.81	119.41	126.34
48	5	4420	PSU	N1-C2-N3	4.81	120.58	115.13
48	5	1744	PSU	C4-N3-C2	-4.80	119.43	126.34
48	5	2632	PSU	N1-C2-N3	4.80	120.56	115.13
51	9	1244	PSU	N1-C2-N3	4.80	120.56	115.13
48	5	1782	PSU	N1-C2-N3	4.80	120.56	115.13
48	5	3695	PSU	N1-C2-N3	4.79	120.56	115.13
48	5	4442	PSU	C4-N3-C2	-4.79	119.44	126.34
51	9	609	PSU	N1-C2-N3	4.78	120.55	115.13
48	5	1781	PSU	C4-N3-C2	-4.78	119.45	126.34
48	5	4521	PSU	C4-N3-C2	-4.78	119.45	126.34
48	5	4353	PSU	C4-N3-C2	-4.77	119.46	126.34
48	5	4579	PSU	C4-N3-C2	-4.77	119.46	126.34
51	9	649	PSU	C4-N3-C2	-4.76	119.47	126.34
48	5	4420	PSU	C4-N3-C2	-4.76	119.48	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1238	PSU	C4-N3-C2	-4.75	119.49	126.34
48	5	1860	PSU	N1-C2-N3	4.74	120.51	115.13
51	9	1232	PSU	N1-C2-N3	4.74	120.50	115.13
48	5	4293	PSU	C4-N3-C2	-4.74	119.52	126.34
48	5	1792	PSU	C4-N3-C2	-4.73	119.52	126.34
51	9	105	PSU	C4-N3-C2	-4.73	119.52	126.34
48	5	1782	PSU	C4-N3-C2	-4.73	119.52	126.34
51	9	1081	PSU	C4-N3-C2	-4.73	119.52	126.34
48	5	2632	PSU	C4-N3-C2	-4.72	119.53	126.34
48	5	4403	PSU	C4-N3-C2	-4.72	119.54	126.34
48	5	4423	PSU	N1-C2-N3	4.72	120.47	115.13
51	9	609	PSU	C4-N3-C2	-4.72	119.55	126.34
51	9	1004	PSU	C4-N3-C2	-4.71	119.55	126.34
48	5	4500	PSU	N1-C2-N3	4.70	120.46	115.13
51	9	119	PSU	N1-C2-N3	4.70	120.46	115.13
48	5	4457	PSU	C4-N3-C2	-4.70	119.56	126.34
51	9	863	PSU	C4-N3-C2	-4.70	119.57	126.34
48	5	1862	PSU	N1-C2-N3	4.69	120.44	115.13
48	5	1744	PSU	N1-C2-N3	4.68	120.44	115.13
48	5	4296	PSU	C4-N3-C2	-4.68	119.60	126.34
48	5	1862	PSU	C4-N3-C2	-4.67	119.61	126.34
48	5	2508	PSU	C4-N3-C2	-4.65	119.63	126.34
51	9	1046	PSU	N1-C2-N3	4.65	120.40	115.13
48	5	4500	PSU	C4-N3-C2	-4.65	119.64	126.34
48	5	3639	PSU	C4-N3-C2	-4.64	119.65	126.34
51	9	1232	PSU	C4-N3-C2	-4.62	119.68	126.34
48	5	3639	PSU	N1-C2-N3	4.62	120.36	115.13
48	5	4532	PSU	C4-N3-C2	-4.62	119.69	126.34
48	5	3734	PSU	N1-C2-N3	4.61	120.35	115.13
51	9	1367	PSU	C4-N3-C2	-4.61	119.70	126.34
48	5	4403	PSU	N1-C2-N3	4.60	120.34	115.13
51	9	572	PSU	N1-C2-N3	4.60	120.34	115.13
51	9	1238	PSU	N1-C2-N3	4.60	120.34	115.13
51	9	1347	PSU	N1-C2-N3	4.60	120.34	115.13
48	5	4552	PSU	N1-C2-N3	4.59	120.33	115.13
48	5	2508	PSU	N1-C2-N3	4.57	120.30	115.13
48	5	1860	PSU	C4-N3-C2	-4.52	119.83	126.34
51	9	1692	PSU	C4-N3-C2	-4.51	119.84	126.34
48	5	4299	PSU	N1-C2-N3	4.50	120.23	115.13
48	5	3818	UY1	N1-C2-N3	4.50	120.23	115.13
48	5	3734	PSU	C4-N3-C2	-4.50	119.85	126.34
48	5	3818	UY1	C4-N3-C2	-4.50	119.86	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	572	PSU	C4-N3-C2	-4.50	119.86	126.34
48	5	1781	PSU	N1-C2-N3	4.49	120.22	115.13
51	9	1046	PSU	C4-N3-C2	-4.49	119.87	126.34
51	9	649	PSU	N1-C2-N3	4.48	120.21	115.13
51	9	1367	PSU	N1-C2-N3	4.48	120.21	115.13
48	5	4579	PSU	N1-C2-N3	4.46	120.19	115.13
48	5	1792	PSU	N1-C2-N3	4.45	120.17	115.13
48	5	4293	PSU	N1-C2-N3	4.45	120.17	115.13
48	5	4306	OMU	N3-C2-N1	4.42	120.75	114.89
51	9	34	PSU	C4-N3-C2	-4.42	119.98	126.34
48	5	3715	PSU	N1-C2-N3	4.38	120.09	115.13
51	9	1177	PSU	N1-C2-N3	4.36	120.07	115.13
51	9	1177	PSU	C4-N3-C2	-4.34	120.08	126.34
51	9	1445	PSU	N1-C2-N3	4.32	120.03	115.13
51	9	863	PSU	N1-C2-N3	4.31	120.02	115.13
48	5	3715	PSU	C4-N3-C2	-4.28	120.17	126.34
51	9	1692	PSU	N1-C2-N3	4.27	119.97	115.13
51	9	1326	OMU	N3-C2-N1	4.25	120.54	114.89
51	9	1445	PSU	C4-N3-C2	-4.21	120.27	126.34
48	5	237	B9B	C2-N3-C4	4.21	120.16	115.36
48	5	4623	OMG	C5-C6-N1	4.12	121.22	113.95
48	5	4530	UR3	C4-N3-C2	-4.08	120.72	124.56
48	5	4532	PSU	N1-C2-N3	4.07	119.74	115.13
51	9	116	OMU	N3-C2-N1	4.05	120.27	114.89
51	9	801	PSU	N1-C2-N3	4.03	119.70	115.13
48	5	4457	PSU	N1-C2-N3	4.02	119.69	115.13
51	9	801	PSU	C4-N3-C2	-4.00	120.57	126.34
48	5	4420	PSU	O2-C2-N1	-3.99	118.40	122.79
51	9	815	PSU	O2-C2-N1	-3.96	118.43	122.79
51	9	1442	OMU	N3-C2-N1	3.92	120.09	114.89
48	5	3925	OMU	C5-C4-N3	3.91	120.68	114.84
51	9	863	PSU	O2-C2-N1	-3.88	118.52	122.79
48	5	4498	OMU	C5-C4-N3	3.88	120.64	114.84
48	5	4498	OMU	N3-C2-N1	3.88	120.04	114.89
48	5	1322	1MA	C5-C6-N1	3.87	119.67	113.90
48	5	3818	UY1	C6-C5-C4	3.84	120.88	118.20
48	5	3853	PSU	O2-C2-N1	-3.82	118.58	122.79
48	5	2837	OMU	N3-C2-N1	3.82	119.95	114.89
48	5	4620	OMU	C5-C4-N3	3.79	120.51	114.84
48	5	3715	PSU	O2-C2-N1	-3.77	118.64	122.79
48	5	4227	OMU	C5-C4-N3	3.76	120.46	114.84
48	5	3782	5MC	C5-C6-N1	-3.76	119.47	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	4620	OMU	N3-C2-N1	3.75	119.87	114.89
51	9	686	PSU	O2-C2-N1	-3.75	118.66	122.79
48	5	1625	OMG	C5-C6-N1	3.75	120.57	113.95
48	5	3925	OMU	N3-C2-N1	3.74	119.85	114.89
48	5	4227	OMU	N3-C2-N1	3.73	119.84	114.89
48	5	4499	OMG	C5-C6-N1	3.72	120.52	113.95
48	5	4447	5MC	C5-C6-N1	-3.66	119.57	123.34
51	9	436	OMG	C5-C6-N1	3.66	120.41	113.95
51	9	572	PSU	O2-C2-N1	-3.66	118.76	122.79
51	9	428	OMU	C5-C4-N3	3.65	120.30	114.84
48	5	2837	OMU	C5-C4-N3	3.65	120.30	114.84
48	5	4196	OMG	C5-C6-N1	3.64	120.37	113.95
51	9	683	OMG	C5-C6-N1	3.63	120.36	113.95
48	5	1316	OMG	C5-C6-N1	3.63	120.36	113.95
51	9	172	OMU	N3-C2-N1	3.61	119.68	114.89
51	9	1643	PSU	O2-C2-N1	-3.61	118.82	122.79
48	5	4392	OMG	C5-C6-N1	3.59	120.29	113.95
51	9	121	OMU	C5-C4-N3	3.59	120.21	114.84
51	9	509	OMG	C5-C6-N1	3.55	120.22	113.95
48	5	1625	OMG	O6-C6-C5	-3.55	117.45	124.37
48	5	3715	PSU	C6-C5-C4	3.53	120.67	118.20
48	5	4370	OMG	C5-C6-N1	3.53	120.19	113.95
51	9	609	PSU	O2-C2-N1	-3.50	118.93	122.79
48	5	4500	PSU	O2-C2-N1	-3.50	118.94	122.79
48	5	4306	OMU	C5-C4-N3	3.50	120.07	114.84
48	5	4618	OMG	C5-C6-N1	3.49	120.11	113.95
50	8	75	OMG	C5-C6-N1	3.49	120.11	113.95
48	5	1522	OMG	C5-C6-N1	3.46	120.07	113.95
48	5	4521	PSU	C6-C5-C4	3.46	120.61	118.20
51	9	121	OMU	N3-C2-N1	3.45	119.48	114.89
51	9	172	OMU	C5-C4-N3	3.45	120.00	114.84
48	5	1517	2MG	C5-C6-N1	3.45	120.04	113.95
51	9	428	OMU	O4-C4-C5	-3.44	119.11	125.16
48	5	2424	OMG	C5-C6-N1	3.44	120.03	113.95
48	5	4637	OMG	C5-C6-N1	3.44	120.02	113.95
48	5	4623	OMG	C2-N1-C6	-3.42	118.79	125.10
48	5	373	OMG	C5-C6-N1	3.42	119.98	113.95
48	5	4392	OMG	C2-N1-C6	-3.40	118.83	125.10
48	5	2364	OMG	C5-C6-N1	3.40	119.96	113.95
48	5	1625	OMG	C2-N1-C6	-3.39	118.85	125.10
51	9	1326	OMU	C5-C4-N3	3.38	119.90	114.84
51	9	1248	B8N	N3-C2-N1	3.37	121.52	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3627	OMG	C5-C6-N1	3.36	119.88	113.95
51	9	1328	OMG	C5-C6-N1	3.35	119.87	113.95
48	5	2424	OMG	C2-N1-C6	-3.32	118.99	125.10
48	5	1862	PSU	O2-C2-N1	-3.31	119.14	122.79
51	9	218	PSU	C6-C5-C4	3.31	120.51	118.20
48	5	2876	OMG	C2-N1-C6	-3.31	119.01	125.10
48	5	4628	PSU	O2-C2-N1	-3.31	119.15	122.79
51	9	683	OMG	C2-N1-C6	-3.28	119.06	125.10
48	5	2364	OMG	C2-N1-C6	-3.27	119.08	125.10
51	9	822	PSU	C6-C5-C4	3.26	120.48	118.20
51	9	436	OMG	C2-N1-C6	-3.25	119.11	125.10
48	5	1677	PSU	O2-C2-N1	-3.23	119.23	122.79
48	5	3762	PSU	O2-C2-N1	-3.21	119.26	122.79
48	5	3920	PSU	O2-C2-N1	-3.20	119.27	122.79
48	5	4521	PSU	O2-C2-N1	-3.19	119.27	122.79
48	5	4494	OMG	C5-C6-N1	3.19	119.58	113.95
51	9	116	OMU	C5-C4-N3	3.18	119.61	114.84
48	5	4499	OMG	C2-N1-C6	-3.18	119.24	125.10
51	9	1174	PSU	O2-C2-N1	-3.17	119.30	122.79
48	5	3818	UY1	C6-N1-C2	-3.17	119.44	122.68
50	8	75	OMG	C2-N1-C6	-3.16	119.28	125.10
48	5	3899	OMG	C5-C6-N1	3.15	119.51	113.95
51	9	1442	OMU	O4-C4-C5	-3.14	119.63	125.16
51	9	428	OMU	N3-C2-N1	3.14	119.06	114.89
48	5	3792	OMG	C5-C6-N1	3.14	119.50	113.95
48	5	4618	OMG	C2-N1-C6	-3.14	119.32	125.10
48	5	237	B9B	C2-N1-C6	3.14	121.12	116.08
48	5	4228	OMG	C5-C6-N1	3.12	119.46	113.95
48	5	4637	OMG	C2-N1-C6	-3.12	119.35	125.10
48	5	4370	OMG	C2-N1-C6	-3.10	119.38	125.10
51	9	683	OMG	CM2-O2'-C2'	3.10	122.65	114.52
48	5	1744	PSU	O2-C2-N1	-3.08	119.41	122.79
48	5	4353	PSU	C6-C5-C4	3.07	120.34	118.20
48	5	1517	2MG	C8-N7-C5	3.06	108.81	102.99
48	5	4196	OMG	C2-N1-C6	-3.05	119.47	125.10
48	5	373	OMG	C2-N1-C6	-3.05	119.47	125.10
51	9	644	OMG	C5-C6-N1	3.05	119.34	113.95
51	9	822	PSU	O2-C2-N1	-3.05	119.43	122.79
48	5	1782	PSU	O2-C2-N1	-3.05	119.43	122.79
48	5	237	B9B	N2-C2-N3	3.04	122.75	117.79
48	5	1792	PSU	O2-C2-N1	-3.04	119.45	122.79
51	9	119	PSU	O2-C2-N1	-3.04	119.45	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1328	OMG	C2-N1-C6	-3.02	119.53	125.10
51	9	1442	OMU	C5-C4-N3	3.02	119.35	114.84
51	9	509	OMG	C2-N1-C6	-3.01	119.55	125.10
48	5	1522	OMG	C2-N1-C6	-3.00	119.58	125.10
48	5	2364	OMG	C8-N7-C5	2.99	108.69	102.99
48	5	373	OMG	C8-N7-C5	2.98	108.67	102.99
48	5	4370	OMG	C8-N7-C5	2.98	108.66	102.99
48	5	4494	OMG	C2-N1-C6	-2.97	119.63	125.10
48	5	2876	OMG	C5-C6-N1	2.96	119.19	113.95
51	9	683	OMG	C8-N7-C5	2.95	108.62	102.99
48	5	4423	PSU	O2-C2-N1	-2.95	119.54	122.79
48	5	4499	OMG	O6-C6-C5	-2.95	118.61	124.37
48	5	3627	OMG	C8-N7-C5	2.94	108.58	102.99
48	5	3899	OMG	C8-N7-C5	2.93	108.57	102.99
48	5	1316	OMG	C2-N1-C6	-2.92	119.72	125.10
51	9	686	PSU	C6-C5-C4	2.92	120.24	118.20
51	9	644	OMG	C2-N1-C6	-2.91	119.75	125.10
51	9	34	PSU	C6-N1-C2	-2.90	119.72	122.68
51	9	1326	OMU	O2-C2-N1	-2.89	118.95	122.79
48	5	3627	OMG	C2-N1-C6	-2.89	119.78	125.10
48	5	4637	OMG	C8-N7-C5	2.88	108.48	102.99
48	5	4500	PSU	C6-C5-C4	2.87	120.21	118.20
48	5	1316	OMG	C8-N7-C5	2.86	108.43	102.99
48	5	4442	PSU	O2-C2-N1	-2.86	119.65	122.79
48	5	2837	OMU	O2-C2-N1	-2.85	118.99	122.79
48	5	4498	OMU	O4-C4-C5	-2.84	120.16	125.16
51	9	436	OMG	O6-C6-C5	-2.84	118.82	124.37
48	5	3851	PSU	O2-C2-N1	-2.84	119.66	122.79
48	5	4618	OMG	C8-N7-C5	2.83	108.39	102.99
51	9	218	PSU	O2-C2-N1	-2.83	119.67	122.79
51	9	1490	OMG	C5-C6-N1	2.83	118.95	113.95
51	9	1248	B8N	O4-C4-N3	-2.82	115.18	119.98
51	9	116	OMU	O2-C2-N1	-2.81	119.05	122.79
48	5	3920	PSU	C6-C5-C4	2.80	120.16	118.20
48	5	2876	OMG	C8-N7-C5	2.79	108.31	102.99
48	5	4228	OMG	C2-N1-C6	-2.77	119.99	125.10
51	9	1639	G7M	C2-N1-C6	-2.75	120.03	125.10
48	5	1860	PSU	O2-C2-N1	-2.75	119.77	122.79
51	9	1842	4AC	O2-C2-N3	-2.75	117.86	122.33
48	5	4498	OMU	O2-C2-N1	-2.75	119.14	122.79
48	5	3792	OMG	O6-C6-C5	-2.75	119.01	124.37
48	5	4637	OMG	O6-C6-C5	-2.74	119.03	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1238	PSU	C6-C5-C4	2.73	120.11	118.20
51	9	814	PSU	O2-C2-N1	-2.73	119.78	122.79
51	9	1326	OMU	O4-C4-C5	-2.72	120.37	125.16
48	5	2837	OMU	C2'-C1'-N1	-2.72	108.94	114.22
51	9	1045	PSU	O2-C2-N1	-2.72	119.80	122.79
51	9	121	OMU	O4-C4-C5	-2.71	120.39	125.16
48	5	4228	OMG	C8-N7-C5	2.71	108.15	102.99
48	5	2837	OMU	O4-C4-C5	-2.70	120.40	125.16
48	5	3851	PSU	C6-N1-C2	-2.69	119.93	122.68
50	8	75	OMG	C8-N7-C5	2.69	108.11	102.99
48	5	1522	OMG	C8-N7-C5	2.68	108.09	102.99
51	9	1445	PSU	C6-N1-C2	-2.67	119.95	122.68
51	9	1045	PSU	C6-C5-C4	2.67	120.06	118.20
48	5	4623	OMG	O6-C6-C5	-2.67	119.17	124.37
48	5	2424	OMG	O6-C6-C5	-2.66	119.17	124.37
48	5	1625	OMG	C8-N7-C5	2.65	108.05	102.99
51	9	1004	PSU	O2-C2-N1	-2.65	119.87	122.79
48	5	3899	OMG	C2-N1-C6	-2.65	120.22	125.10
51	9	1244	PSU	O2-C2-N1	-2.64	119.89	122.79
48	5	4579	PSU	O2-C2-N1	-2.62	119.91	122.79
51	9	649	PSU	O2-C2-N1	-2.61	119.91	122.79
51	9	644	OMG	C8-N7-C5	2.59	107.92	102.99
48	5	4196	OMG	C8-N7-C5	2.59	107.92	102.99
48	5	3639	PSU	O2-C2-N1	-2.58	119.95	122.79
51	9	105	PSU	C6-N1-C2	-2.58	120.05	122.68
48	5	3792	OMG	C2-N1-C6	-2.58	120.35	125.10
51	9	34	PSU	O2-C2-N1	-2.56	119.97	122.79
51	9	121	OMU	CM2-O2'-C2'	2.56	121.24	114.52
48	5	1683	PSU	O2-C2-N1	-2.55	119.98	122.79
48	5	3925	OMU	O4-C4-C5	-2.54	120.70	125.16
48	5	4392	OMG	C8-N7-C5	2.53	107.81	102.99
51	9	1244	PSU	C6-C5-C4	2.53	119.97	118.20
51	9	436	OMG	C8-N7-C5	2.52	107.79	102.99
51	9	509	OMG	O6-C6-C5	-2.52	119.45	124.37
48	5	2424	OMG	C8-N7-C5	2.52	107.79	102.99
48	5	3853	PSU	C6-N1-C2	-2.52	120.11	122.68
51	9	822	PSU	C6-N1-C2	-2.52	120.11	122.68
48	5	4628	PSU	C6-C5-C4	2.52	119.96	118.20
48	5	1781	PSU	O2-C2-N1	-2.51	120.03	122.79
48	5	4499	OMG	C8-N7-C5	2.51	107.77	102.99
48	5	2632	PSU	O2-C2-N1	-2.50	120.03	122.79
51	9	1046	PSU	O2-C2-N1	-2.50	120.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4442	PSU	C6-C5-C4	2.50	119.95	118.20
51	9	815	PSU	C6-N1-C2	-2.50	120.13	122.68
48	5	4494	OMG	C8-N7-C5	2.50	107.75	102.99
48	5	1683	PSU	C6-N1-C2	-2.49	120.14	122.68
48	5	4620	OMU	O4-C4-C5	-2.48	120.79	125.16
48	5	4623	OMG	C8-N7-C5	2.48	107.71	102.99
51	9	1328	OMG	O6-C6-C5	-2.47	119.55	124.37
48	5	4447	5MC	CM5-C5-C6	-2.47	119.55	122.85
48	5	1517	2MG	O6-C6-C5	-2.47	119.55	124.37
51	9	1328	OMG	C8-N7-C5	2.47	107.69	102.99
48	5	4353	PSU	C6-N1-C2	-2.46	120.17	122.68
51	9	1490	OMG	C8-N7-C5	2.46	107.68	102.99
48	5	4227	OMU	O4-C4-C5	-2.46	120.84	125.16
51	9	172	OMU	O4-C4-C5	-2.46	120.84	125.16
48	5	1322	1MA	C8-N7-C5	2.45	107.65	102.99
51	9	428	OMU	O2-C2-N1	-2.44	119.54	122.79
48	5	3764	PSU	O2-C2-N1	-2.44	120.11	122.79
48	5	1782	PSU	C6-C5-C4	2.43	119.90	118.20
51	9	1232	PSU	C6-N1-C2	-2.42	120.20	122.68
51	9	172	OMU	O2-C2-N1	-2.42	119.57	122.79
48	5	2632	PSU	C6-N1-C2	-2.42	120.21	122.68
51	9	1490	OMG	O6-C6-C5	-2.42	119.65	124.37
51	9	116	OMU	O4-C4-C5	-2.41	120.92	125.16
48	5	237	B9B	C1'-N9-C4	-2.41	122.41	126.64
48	5	2824	OMC	O2-C2-N3	-2.40	118.42	122.33
51	9	109	PSU	C6-N1-C2	-2.40	120.22	122.68
48	5	4227	OMU	O2-C2-N1	-2.40	119.60	122.79
48	5	4361	PSU	O2-C2-N1	-2.40	120.15	122.79
51	9	1174	PSU	C6-N1-C2	-2.39	120.23	122.68
48	5	4521	PSU	C6-N1-C2	-2.39	120.24	122.68
51	9	815	PSU	C6-C5-C4	2.38	119.86	118.20
51	9	468	A2M	C5'-C4'-C3'	-2.37	106.31	115.18
51	9	1347	PSU	O2-C2-N1	-2.37	120.19	122.79
48	5	4299	PSU	O2-C2-N1	-2.36	120.19	122.79
48	5	3718	A2M	C1'-N9-C4	-2.34	122.53	126.64
51	9	1046	PSU	C6-N1-C2	-2.34	120.29	122.68
48	5	4530	UR3	C6-N1-C2	-2.34	119.69	121.79
48	5	1860	PSU	C6-N1-C2	-2.33	120.30	122.68
51	9	1445	PSU	O2-C2-N1	-2.33	120.23	122.79
48	5	4392	OMG	O6-C6-C5	-2.32	119.84	124.37
48	5	4618	OMG	O6-C6-C5	-2.32	119.85	124.37
48	5	3695	PSU	C6-N1-C2	-2.32	120.31	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4353	PSU	O2-C2-N1	-2.32	120.24	122.79
48	5	1340	OMC	C5-C4-N3	-2.31	117.39	121.33
51	9	1692	PSU	O2-C2-N1	-2.31	120.25	122.79
48	5	4552	PSU	O2-C2-N1	-2.31	120.25	122.79
51	9	1081	PSU	C6-C5-C4	2.30	119.81	118.20
48	5	4442	PSU	C6-N1-C2	-2.30	120.33	122.68
51	9	572	PSU	C6-N1-C2	-2.30	120.33	122.68
48	5	3792	OMG	C8-N7-C5	2.30	107.37	102.99
51	9	801	PSU	O2-C2-N1	-2.30	120.26	122.79
51	9	822	PSU	O4'-C1'-C2'	2.28	108.36	105.14
48	5	4500	PSU	C6-N1-C2	-2.28	120.36	122.68
51	9	1367	PSU	C6-N1-C2	-2.27	120.36	122.68
48	5	3734	PSU	C6-C5-C4	2.27	119.78	118.20
51	9	1248	B8N	C31-N3-C4	2.26	120.64	117.31
51	9	1490	OMG	C2-N1-C6	-2.25	120.95	125.10
51	9	801	PSU	C6-N1-C2	-2.25	120.38	122.68
51	9	1177	PSU	C6-N1-C2	-2.24	120.39	122.68
51	9	1383	A2M	C2'-C3'-C4'	-2.23	97.14	101.99
51	9	1081	PSU	O4'-C1'-C2'	2.23	108.29	105.14
51	9	1367	PSU	O2-C2-N1	-2.22	120.34	122.79
48	5	3701	OMC	O2-C2-N3	-2.22	118.72	122.33
48	5	4618	OMG	N2-C2-N1	2.22	121.44	116.71
48	5	3715	PSU	O4'-C1'-C2'	2.21	108.26	105.14
48	5	1781	PSU	C6-C5-C4	2.21	119.74	118.20
48	5	3715	PSU	C6-N1-C2	-2.20	120.43	122.68
48	5	4457	PSU	O2-C2-N1	-2.19	120.38	122.79
48	5	4420	PSU	C6-N1-C2	-2.19	120.44	122.68
48	5	3782	5MC	CM5-C5-C6	-2.19	119.92	122.85
51	9	1639	G7M	N2-C2-N1	2.19	121.38	116.71
48	5	237	B9B	O6-C6-N1	-2.19	118.24	120.12
48	5	4494	OMG	N2-C2-N1	2.18	121.35	116.71
51	9	609	PSU	C6-N1-C2	-2.18	120.46	122.68
51	9	1004	PSU	C6-N1-C2	-2.17	120.46	122.68
48	5	4296	PSU	C6-N1-C2	-2.17	120.47	122.68
48	5	3695	PSU	O2-C2-N1	-2.17	120.40	122.79
50	8	75	OMG	O6-C6-C5	-2.16	120.16	124.37
51	9	119	PSU	C6-N1-C2	-2.15	120.49	122.68
48	5	3734	PSU	O2-C2-N1	-2.15	120.43	122.79
48	5	1862	PSU	C6-C5-C4	2.14	119.70	118.20
51	9	1045	PSU	C6-N1-C2	-2.14	120.49	122.68
51	9	814	PSU	C6-C5-C4	2.14	119.69	118.20
48	5	4293	PSU	C6-N1-C2	-2.13	120.50	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	237	B9B	C5-C6-N1	-2.12	119.22	123.26
48	5	4306	OMU	O2-C2-N1	-2.12	119.96	122.79
51	9	1081	PSU	O2-C2-N1	-2.12	120.45	122.79
50	8	75	OMG	N2-C2-N1	2.12	121.23	116.71
51	9	668	A2M	C3'-C2'-C1'	2.12	106.88	102.89
51	9	1177	PSU	O2-C2-N1	-2.12	120.46	122.79
48	5	3764	PSU	C6-N1-C2	-2.12	120.52	122.68
51	9	1347	PSU	C6-N1-C2	-2.12	120.52	122.68
48	5	2508	PSU	O2-C2-N1	-2.12	120.46	122.79
48	5	3818	UY1	O4'-C1'-C2'	2.12	108.41	104.48
48	5	4196	OMG	O6-C6-C5	-2.12	120.24	124.37
48	5	3734	PSU	C6-N1-C2	-2.11	120.53	122.68
48	5	1522	OMG	N2-C2-N1	2.10	121.19	116.71
48	5	237	B9B	C61-O6-C6	2.09	121.41	117.51
48	5	1340	OMC	C6-C5-C4	2.09	120.87	117.50
51	9	814	PSU	C6-N1-C2	-2.08	120.55	122.68
48	5	4494	OMG	O6-C6-C5	-2.08	120.31	124.37
48	5	3762	PSU	C6-N1-C2	-2.08	120.56	122.68
51	9	121	OMU	C1'-N1-C2	2.07	121.32	117.57
51	9	119	PSU	C6-C5-C4	2.07	119.64	118.20
51	9	1046	PSU	O4'-C1'-C2'	2.06	108.05	105.14
51	9	218	PSU	C5-C6-N1	-2.05	119.03	122.11
51	9	509	OMG	C8-N7-C5	2.04	106.89	102.99
48	5	2861	OMC	O2-C2-N3	-2.04	119.01	122.33
48	5	4530	UR3	C1'-N1-C2	2.04	120.44	116.99
48	5	4403	PSU	O4'-C1'-C2'	2.04	108.02	105.14
51	9	1391	OMC	O2-C2-N3	-2.04	119.02	122.33
51	9	1842	4AC	C6-C5-C4	2.04	119.45	116.96
48	5	4521	PSU	O4'-C1'-C2'	2.03	108.01	105.14
48	5	4628	PSU	O4'-C1'-C2'	2.03	108.00	105.14
51	9	109	PSU	O2-C2-N1	-2.03	120.56	122.79
51	9	1081	PSU	C6-N1-C2	-2.03	120.61	122.68
48	5	4370	OMG	N2-C2-N1	2.02	121.02	116.71
51	9	218	PSU	C6-N1-C2	-2.02	120.61	122.68
51	9	1238	PSU	C5-C6-N1	-2.01	119.09	122.11
51	9	1337	4AC	C5-C4-N4	2.01	126.41	122.92
48	5	4370	OMG	O6-C6-C5	-2.01	120.44	124.37
51	9	1347	PSU	O4-C4-C5	-2.01	118.80	124.05
48	5	2508	PSU	C6-N1-C2	-2.01	120.63	122.68
48	5	3899	OMG	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	5	237	B9B	C5-C6-O6-C61
48	5	237	B9B	N1-C6-O6-C61
48	5	1781	PSU	C3'-C4'-C5'-O5'
48	5	2424	OMG	O4'-C4'-C5'-O5'
48	5	2424	OMG	C1'-C2'-O2'-CM2
48	5	3701	OMC	C2'-C1'-N1-C2
48	5	3701	OMC	C2'-C1'-N1-C6
48	5	3785	A2M	O4'-C4'-C5'-O5'
48	5	3818	UY1	O4'-C4'-C5'-O5'
48	5	4228	OMG	C3'-C2'-O2'-CM2
48	5	4500	PSU	C3'-C4'-C5'-O5'
48	5	4500	PSU	O4'-C4'-C5'-O5'
51	9	34	PSU	O4'-C4'-C5'-O5'
51	9	121	OMU	C1'-C2'-O2'-CM2
51	9	166	A2M	C3'-C4'-C5'-O5'
51	9	668	A2M	O4'-C4'-C5'-O5'
51	9	683	OMG	C1'-C2'-O2'-CM2
51	9	801	PSU	C3'-C4'-C5'-O5'
51	9	1248	B8N	N3-C31-C32-C33
51	9	1248	B8N	C31-C32-C33-N34
51	9	1328	OMG	C1'-C2'-O2'-CM2
51	9	1851	MA6	O4'-C4'-C5'-O5'
48	5	2364	OMG	O4'-C4'-C5'-O5'
48	5	2424	OMG	C3'-C4'-C5'-O5'
51	9	99	A2M	O4'-C4'-C5'-O5'
51	9	166	A2M	O4'-C4'-C5'-O5'
51	9	822	PSU	C3'-C4'-C5'-O5'
51	9	1442	OMU	O4'-C4'-C5'-O5'
51	9	1490	OMG	O4'-C4'-C5'-O5'
48	5	1781	PSU	O4'-C4'-C5'-O5'
48	5	2364	OMG	C3'-C4'-C5'-O5'
48	5	2815	A2M	O4'-C4'-C5'-O5'
48	5	3760	A2M	C3'-C4'-C5'-O5'
48	5	3785	A2M	C3'-C4'-C5'-O5'
48	5	3818	UY1	C3'-C4'-C5'-O5'
51	9	34	PSU	C3'-C4'-C5'-O5'
51	9	99	A2M	C3'-C4'-C5'-O5'
51	9	668	A2M	C3'-C4'-C5'-O5'
51	9	822	PSU	O4'-C4'-C5'-O5'
51	9	1045	PSU	C3'-C4'-C5'-O5'
51	9	1639	G7M	O4'-C4'-C5'-O5'
51	9	1639	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
51	9	1851	MA6	C3'-C4'-C5'-O5'
51	9	1703	OMC	O4'-C4'-C5'-O5'
51	9	1045	PSU	O4'-C4'-C5'-O5'
48	5	2815	A2M	C3'-C4'-C5'-O5'
48	5	3760	A2M	O4'-C4'-C5'-O5'
51	9	172	OMU	O4'-C4'-C5'-O5'
51	9	801	PSU	O4'-C4'-C5'-O5'
48	5	4447	5MC	C2'-C1'-N1-C6
51	9	428	OMU	C2'-C1'-N1-C6
51	9	172	OMU	C3'-C4'-C5'-O5'
51	9	1442	OMU	C3'-C4'-C5'-O5'
48	5	3818	UY1	C4'-C5'-O5'-P
48	5	1625	OMG	C3'-C2'-O2'-CM2
51	9	1248	B8N	C32-C33-C34-O36
51	9	512	A2M	O4'-C4'-C5'-O5'
51	9	1248	B8N	C32-C33-C34-O35
48	5	1534	A2M	C4'-C5'-O5'-P
51	9	1490	OMG	C4'-C5'-O5'-P
48	5	1524	A2M	C3'-C2'-O2'-CM'
51	9	1031	A2M	C3'-C2'-O2'-CM'
48	5	4447	5MC	O4'-C1'-N1-C6
48	5	1326	A2M	C4'-C5'-O5'-P
48	5	4447	5MC	O4'-C1'-N1-C2
48	5	3792	OMG	O4'-C4'-C5'-O5'
48	5	3792	OMG	C3'-C4'-C5'-O5'
51	9	683	OMG	C3'-C4'-C5'-O5'
48	5	3701	OMC	O4'-C1'-N1-C6
51	9	428	OMU	O4'-C1'-N1-C6
48	5	4447	5MC	C2'-C1'-N1-C2
51	9	1851	MA6	C4'-C5'-O5'-P
48	5	3701	OMC	O4'-C1'-N1-C2
51	9	644	OMG	C4'-C5'-O5'-P
51	9	468	A2M	C3'-C4'-C5'-O5'
51	9	428	OMU	C2'-C1'-N1-C2
51	9	34	PSU	O4'-C1'-C5-C4
51	9	1445	PSU	O4'-C1'-C5-C4
48	5	4499	OMG	C3'-C2'-O2'-CM2
48	5	3851	PSU	C3'-C4'-C5'-O5'
51	9	1703	OMC	C3'-C4'-C5'-O5'
51	9	428	OMU	O4'-C1'-N1-C2
48	5	1534	A2M	O4'-C4'-C5'-O5'
48	5	2364	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
48	5	4494	OMG	C1'-C2'-O2'-CM2
48	5	4499	OMG	C1'-C2'-O2'-CM2
48	5	2837	OMU	C3'-C4'-C5'-O5'
51	9	863	PSU	C3'-C4'-C5'-O5'
51	9	863	PSU	O4'-C4'-C5'-O5'
51	9	34	PSU	O4'-C1'-C5-C6
48	5	2351	OMC	O4'-C4'-C5'-O5'
48	5	2422	OMC	O4'-C4'-C5'-O5'
48	5	3867	A2M	C3'-C4'-C5'-O5'
48	5	2351	OMC	C2'-C1'-N1-C2
48	5	3760	A2M	C3'-C2'-O2'-CM'
48	5	4494	OMG	C3'-C2'-O2'-CM2
48	5	373	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 323 ligands modelled in this entry, 320 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	ZVM	ii	501	88	29,31,31	4.74	20 (68%)	31,46,46	2.79	8 (25%)
91	SF4	jj	602	87	0,12,12	-	-	-		
91	SF4	jj	601	87	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	ZVM	ii	501	88	2/2/8/8	2/4/50/50	0/3/5/5
91	SF4	jj	602	87	-	-	0/6/5/5
91	SF4	jj	601	87	-	-	0/6/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	ii	501	ZVM	O01-C01	12.06	1.39	1.22
90	ii	501	ZVM	O02-C15	9.72	1.39	1.22
90	ii	501	ZVM	C03-N01	7.44	1.38	1.27
90	ii	501	ZVM	C10-C09	7.21	1.53	1.39
90	ii	501	ZVM	C13-C14	6.59	1.52	1.38
90	ii	501	ZVM	C04-N02	-5.99	1.42	1.47
90	ii	501	ZVM	C12-C11	5.47	1.52	1.38
90	ii	501	ZVM	C02-C03	-5.46	1.40	1.52
90	ii	501	ZVM	C03-N03	5.35	1.47	1.37
90	ii	501	ZVM	C05-C04	4.95	1.59	1.54
90	ii	501	ZVM	C14-C09	-3.97	1.31	1.39
90	ii	501	ZVM	C17-N03	3.83	1.49	1.40
90	ii	501	ZVM	C21-C22	-3.83	1.33	1.39
90	ii	501	ZVM	C08-C05	-3.62	1.45	1.54
90	ii	501	ZVM	C11-C10	-3.42	1.31	1.38
90	ii	501	ZVM	C06-C05	-3.32	1.45	1.54
90	ii	501	ZVM	C15-N02	2.96	1.40	1.36
90	ii	501	ZVM	C07-C06	2.65	1.65	1.54
90	ii	501	ZVM	C07-C08	2.58	1.65	1.54
90	ii	501	ZVM	C12-C13	-2.38	1.31	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	ii	501	ZVM	C05-C04-N01	12.11	121.33	109.90
90	ii	501	ZVM	C02-C03-N03	4.39	121.20	114.49
90	ii	501	ZVM	N02-C04-N01	4.29	119.25	113.37
90	ii	501	ZVM	C07-C06-C05	-3.70	85.41	88.34
90	ii	501	ZVM	C07-C08-C05	-3.25	85.77	88.34
90	ii	501	ZVM	C22-C01-C02	2.80	120.36	116.63
90	ii	501	ZVM	C21-C22-C17	2.74	121.99	118.82
90	ii	501	ZVM	C02-C15-N02	2.26	119.16	116.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
90	ii	501	ZVM	C02
90	ii	501	ZVM	C04

All (2) torsion outliers are listed below:

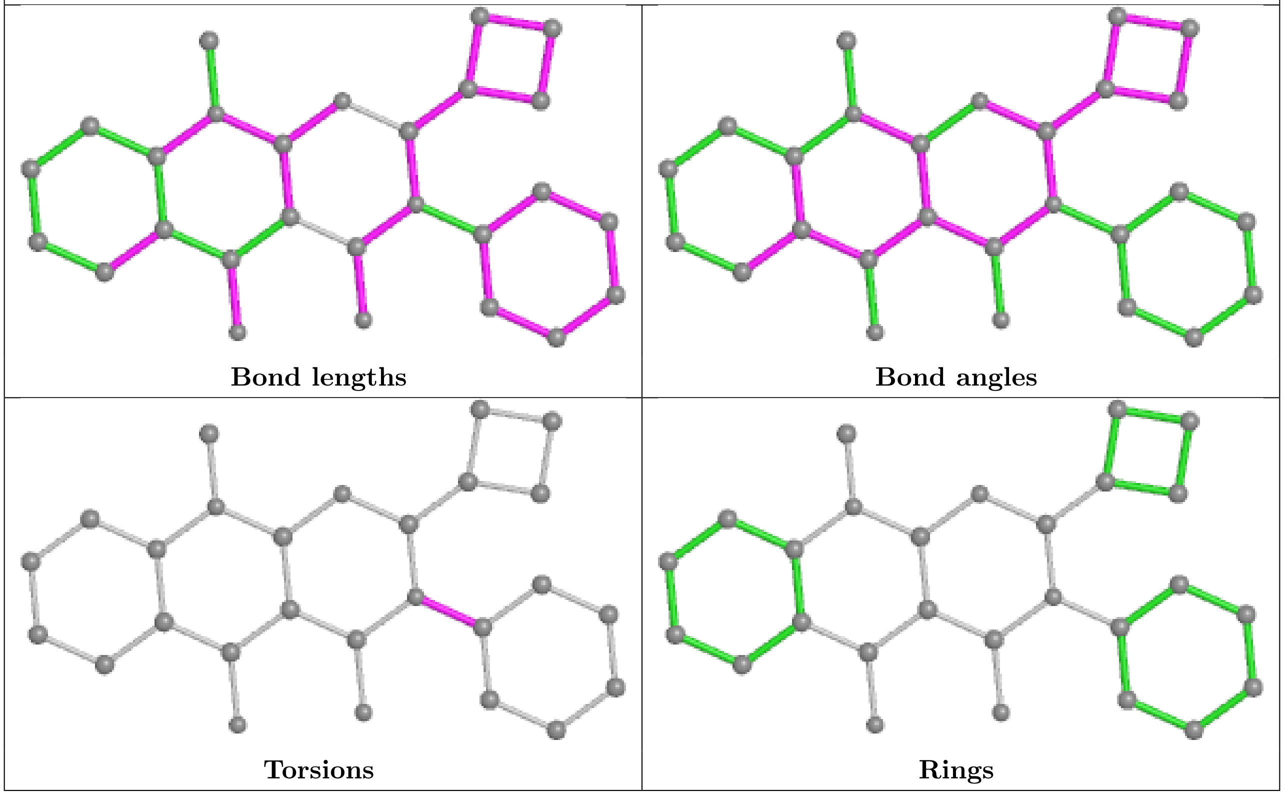
Mol	Chain	Res	Type	Atoms
90	ii	501	ZVM	C10-C09-N02-C04
90	ii	501	ZVM	C14-C09-N02-C04

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 ZVM ii 501



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
48	5	23
51	9	3
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.98
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	16.99
1	5	1696:C	O3'	1720:C	P	16.41
1	5	990:C	O3'	1064:G	P	15.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	523:C	O3’	638:G	P	15.09
1	5	4138:C	O3’	4146:G	P	15.05
1	5	1364:U	O3’	1368:A	P	14.32
1	5	4777:C	O3’	4859:C	P	14.25
1	5	4101:C	O3’	4107:G	P	13.97
1	5	5022:U	O3’	5028:G	P	13.74
1	5	182:G	O3’	189:G	P	13.69
1	5	760:G	O3’	904:C	P	13.62
1	5	2901:G	O3’	3597:G	P	12.67
1	5	3948:C	O3’	4065:G	P	12.45
1	9	890:U	O3’	894:G	P	12.31
1	5	1180:C	O3’	1183:C	P	9.35
1	5	4729:A	O3’	4735:G	P	8.97
1	5	1980:U	O3’	1981:G	P	7.17
1	5	1981:G	O3’	1982:G	P	6.96
1	5	512:U	O3’	515:C	P	6.64
1	5	4740:G	O3’	4743:G	P	6.62
1	5	500:G	O3’	504:G	P	6.28
1	3	19:G	O3’	20:U	P	5.95
1	3	16:C	O3’	18:U	P	5.54
1	2	16:C	O3’	18:G	P	5.42
1	5	1100:U	O3’	1168:G	P	4.14
1	9	873:G	O3’	874:G	P	3.50
1	9	900:C	O3’	901:G	P	3.23

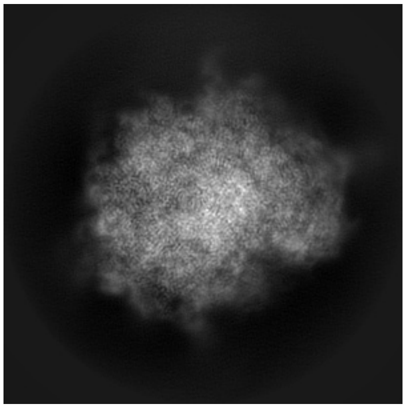
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40344. These allow visual inspection of the internal detail of the map and identification of artifacts.

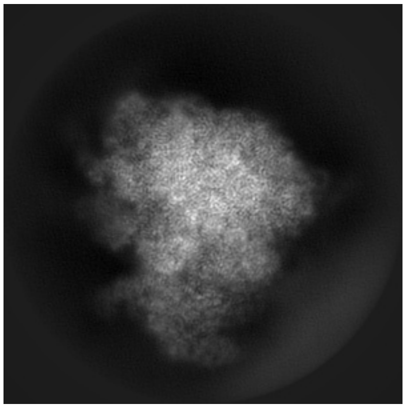
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

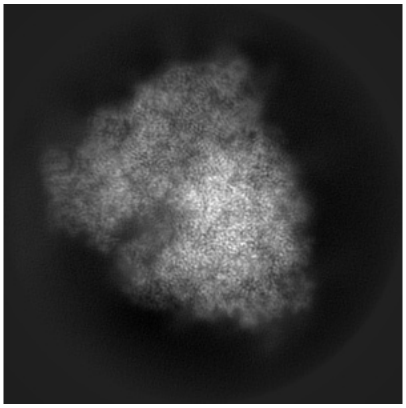
6.1.1 Primary map



X

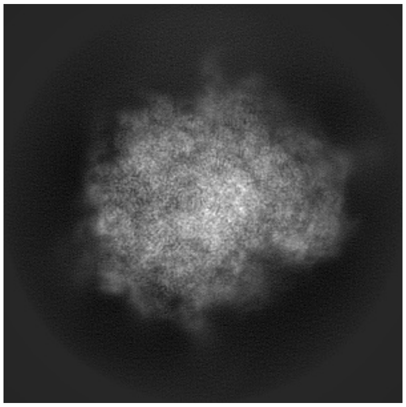


Y

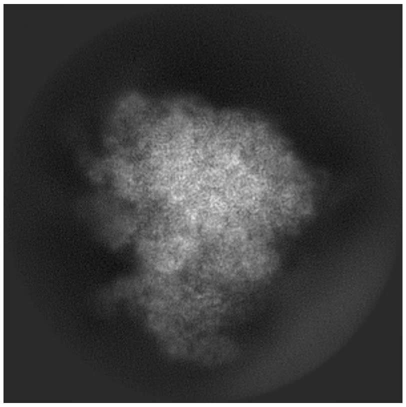


Z

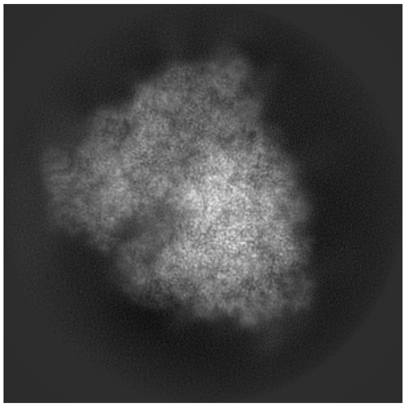
6.1.2 Raw map



X



Y

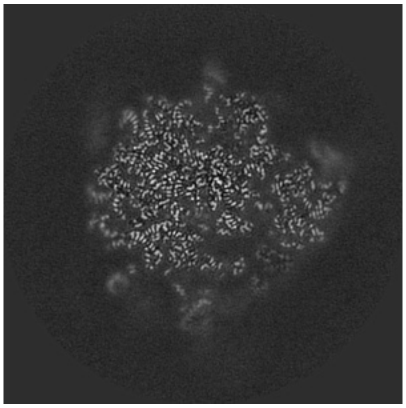


Z

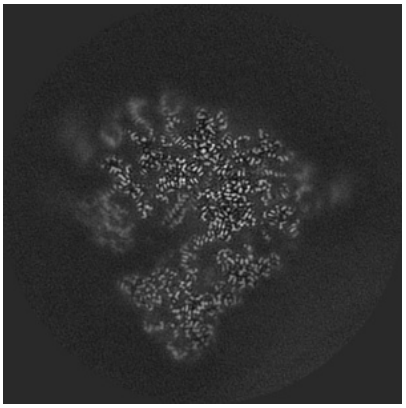
The images above show the map projected in three orthogonal directions.

6.2 Central slices

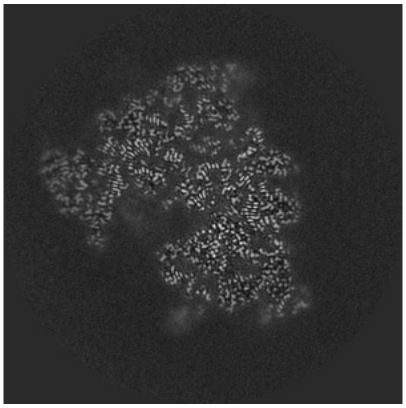
6.2.1 Primary map



X Index: 240

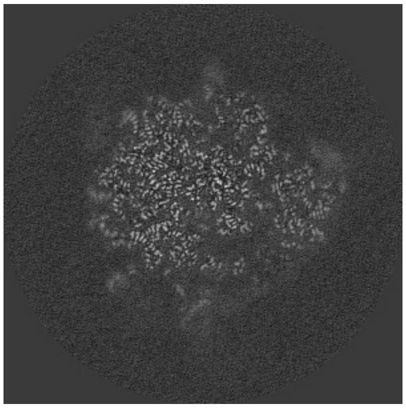


Y Index: 240

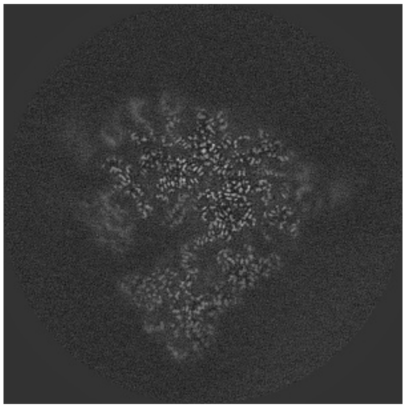


Z Index: 240

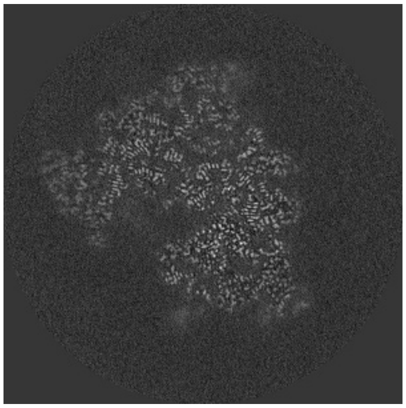
6.2.2 Raw map



X Index: 240



Y Index: 240

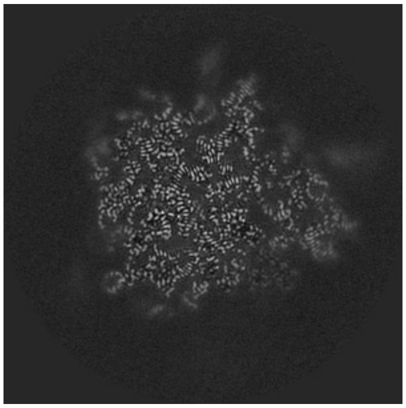


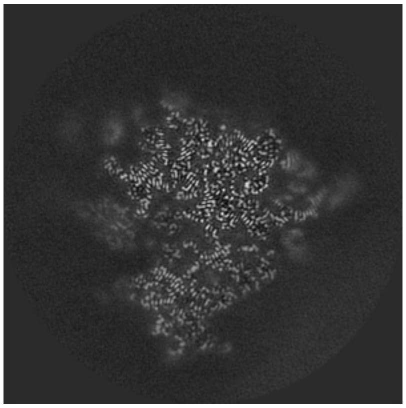
Z Index: 240

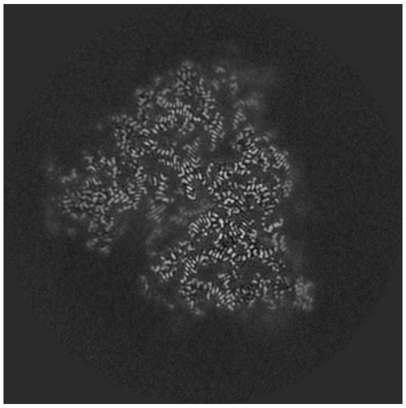
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

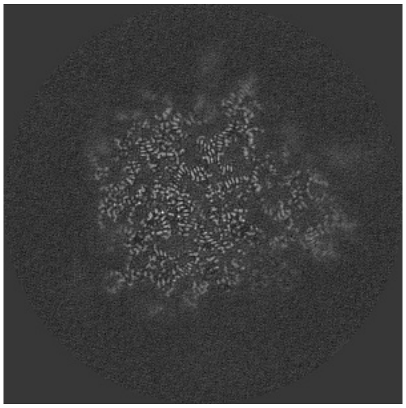
6.3.1 Primary map

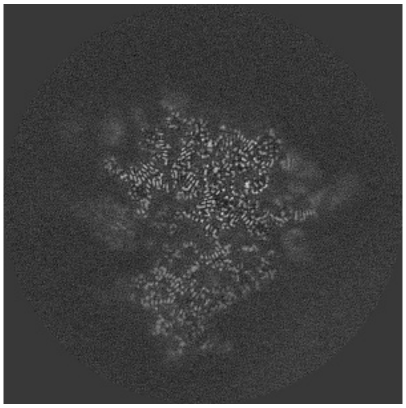

X Index: 261

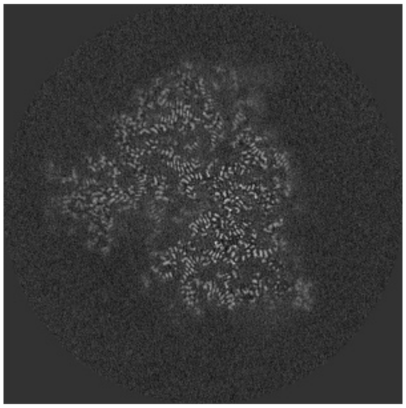

Y Index: 250


Z Index: 227

6.3.2 Raw map


X Index: 261

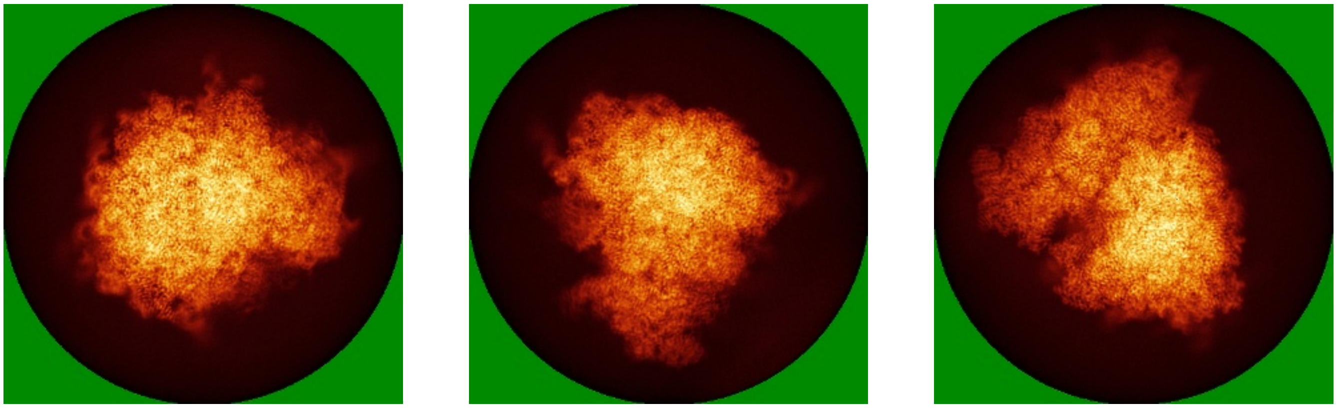

Y Index: 250


Z Index: 228

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

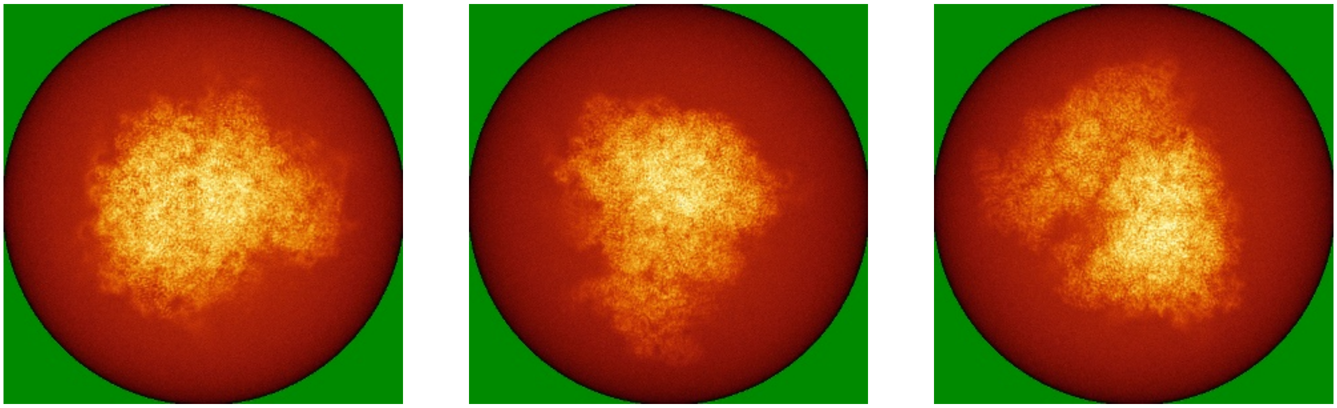
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

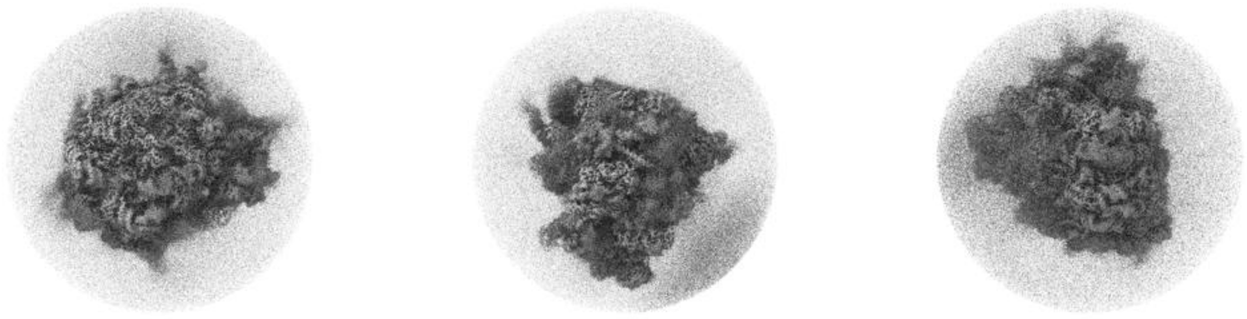
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

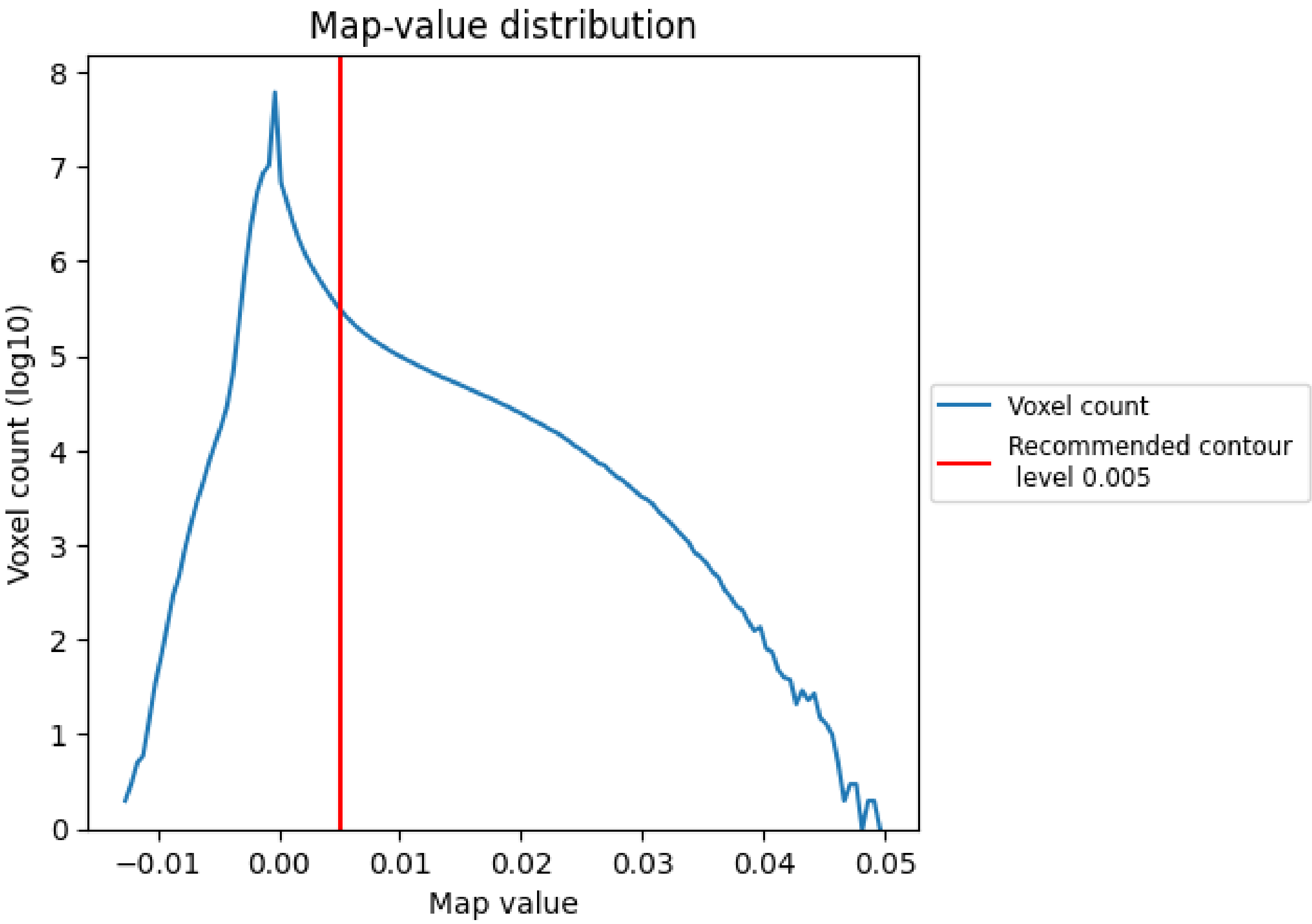
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

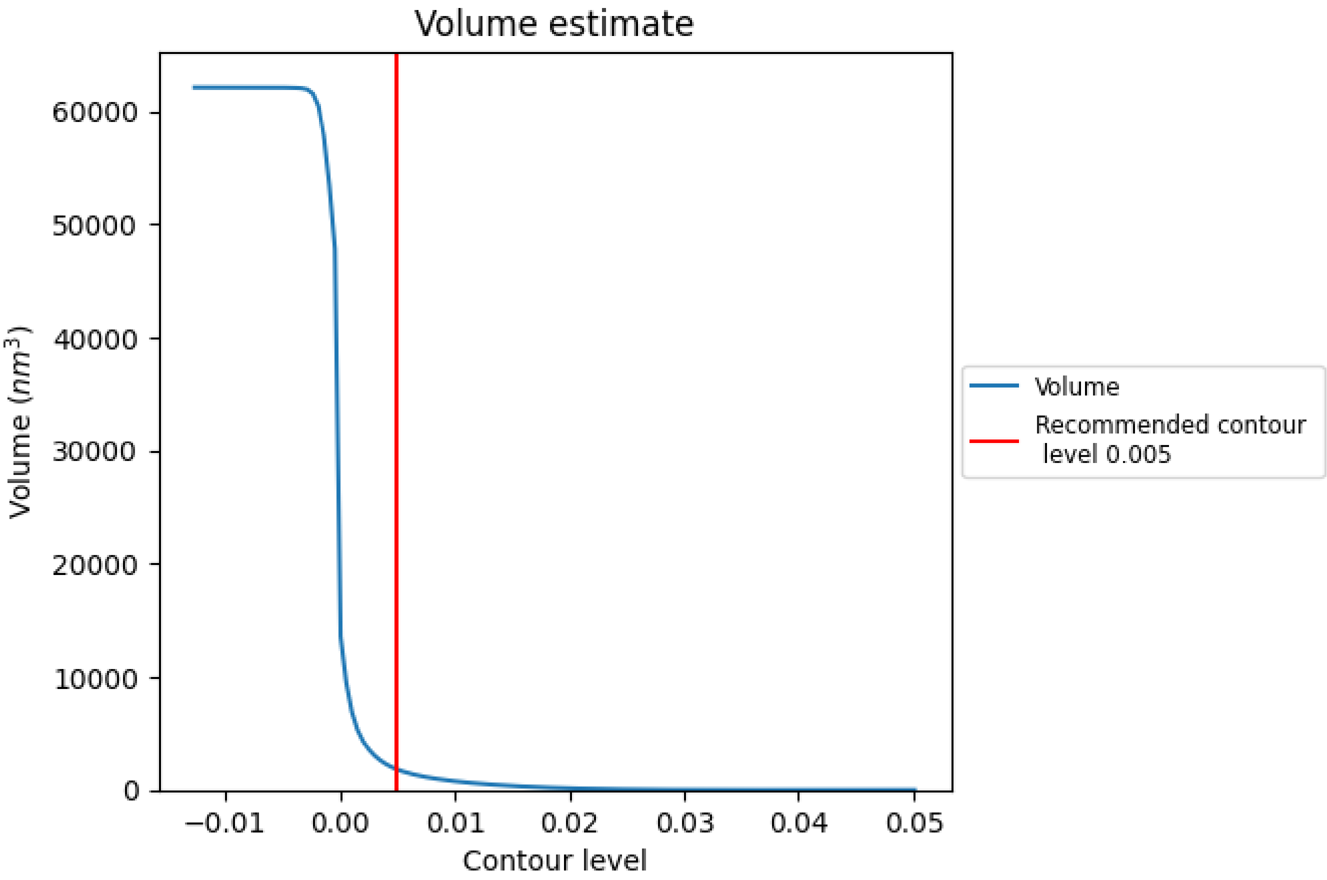
This section contains the results of statistical analysis of the map.

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.

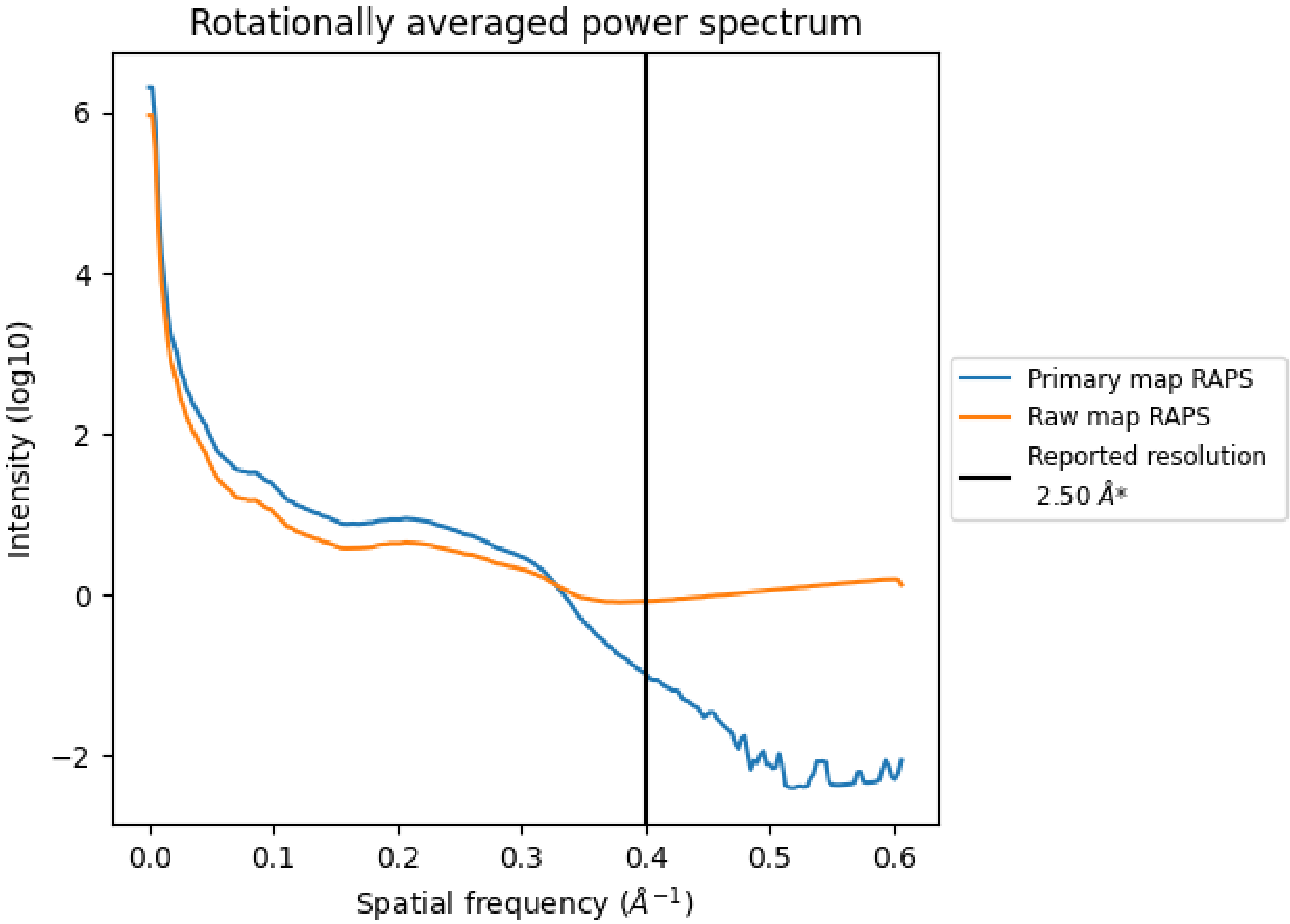
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1812 nm^3; this corresponds to an approximate mass of 1637 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 ⓘ

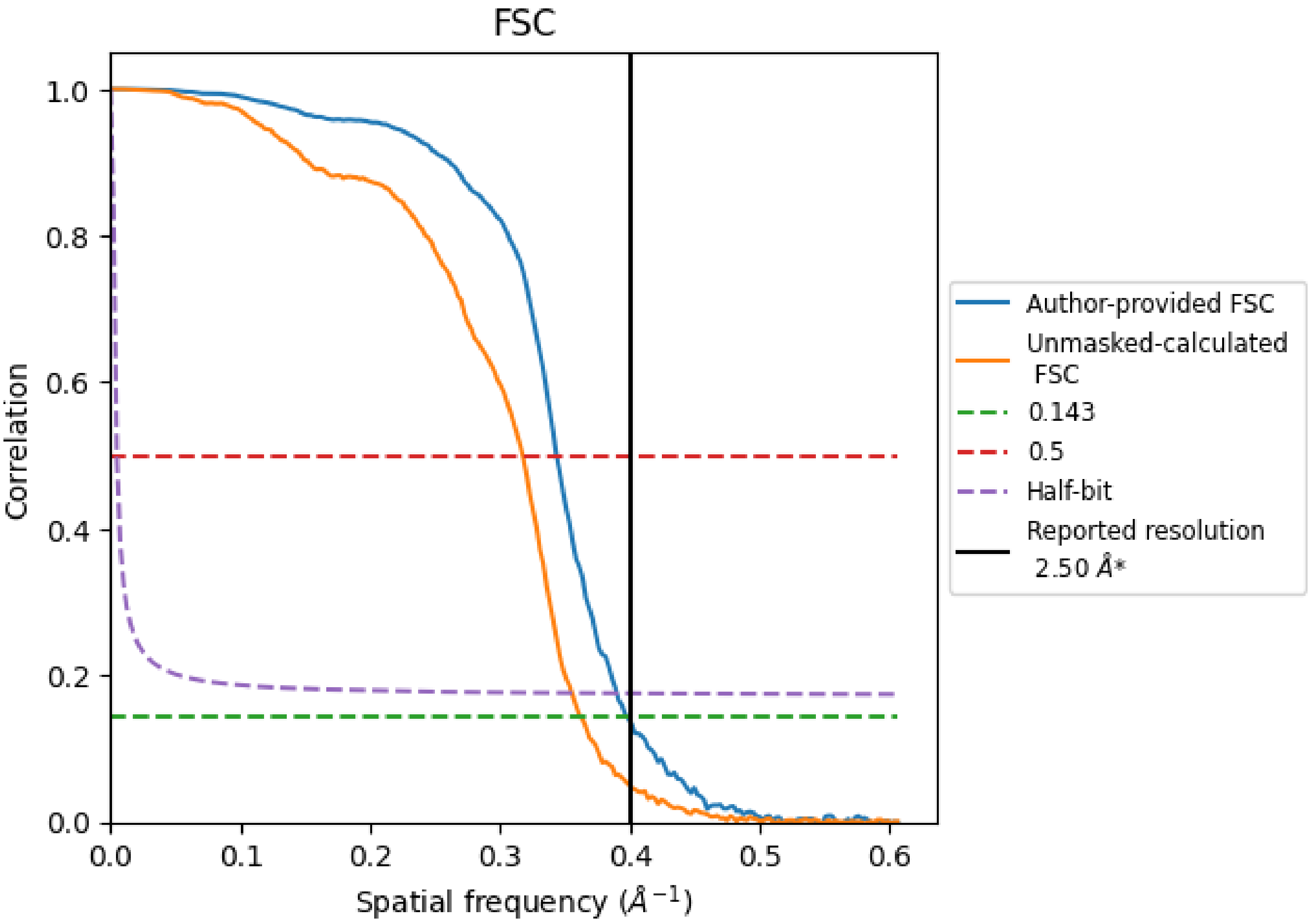


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates ⓘ

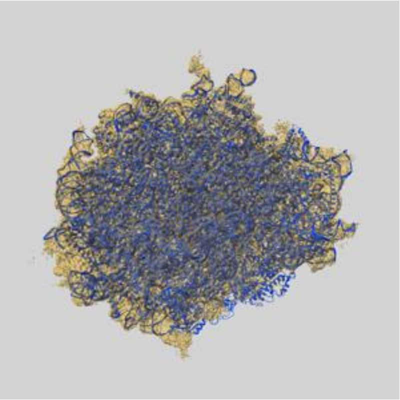
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.91	2.56
Unmasked-calculated*	2.76	3.15	2.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.5 by more than 10 %

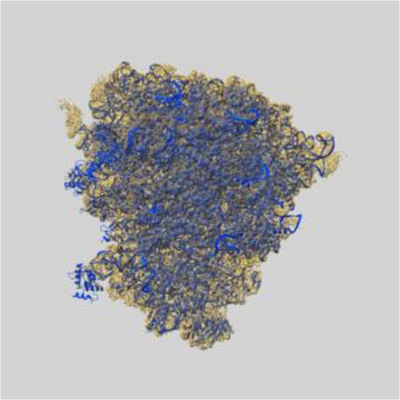
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-40344 and PDB model 8SCB. Per-residue inclusion information can be found in section 3 on page 27.

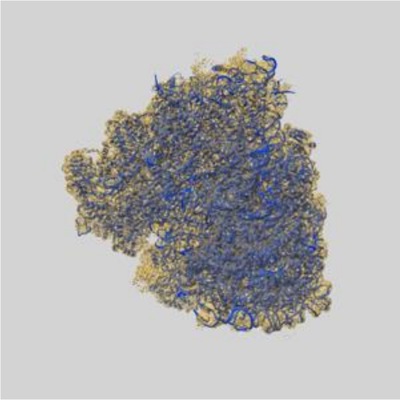
9.1 Map-model overlay ⓘ



X



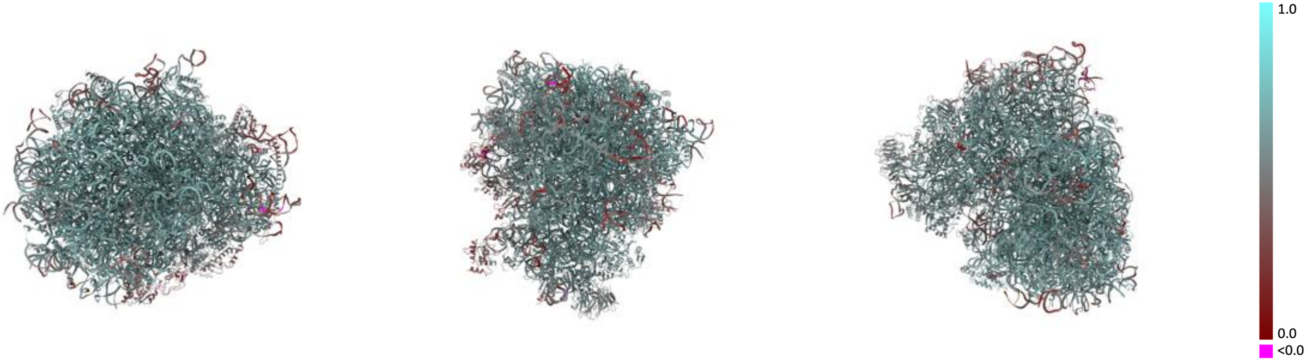
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

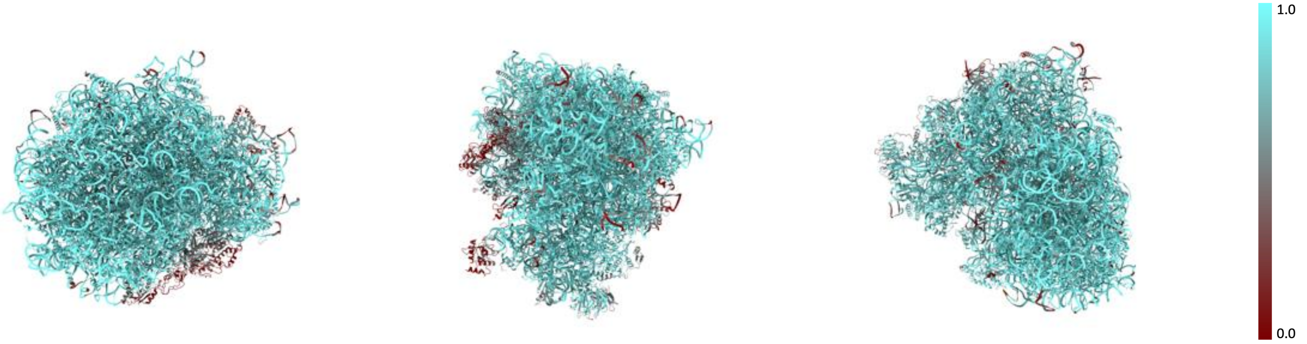
9.2 Q-score mapped to coordinate model ⓘ



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.

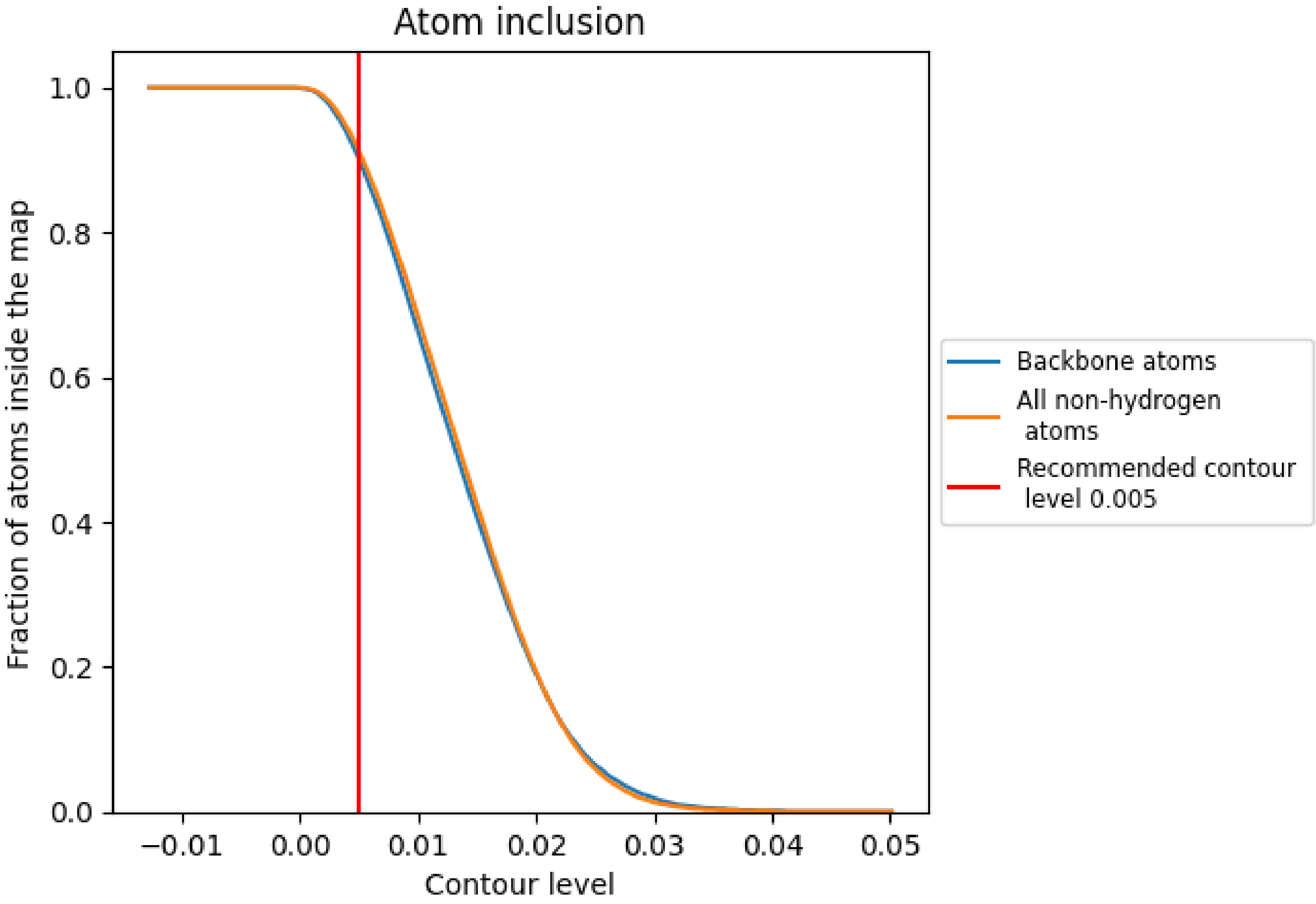
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.5890
1	0.9590	0.6230
2	0.9490	0.5410
3	0.5710	0.3940
5	0.9750	0.6070
7	0.9950	0.6350
8	0.9630	0.6010
9	0.9380	0.5680
A	0.9860	0.6570
AA	0.8810	0.5860
B	0.9700	0.6410
BB	0.9000	0.5920
C	0.9670	0.6410
CC	0.9270	0.6040
D	0.9380	0.6090
DD	0.8180	0.5420
E	0.9520	0.6100
EE	0.9280	0.5870
F	0.9690	0.6450
FF	0.9060	0.5780
G	0.9140	0.5970
GG	0.7990	0.5030
H	0.9330	0.6160
HH	0.5830	0.4750
I	0.9590	0.6300
II	0.8730	0.5680
J	0.9180	0.5910
JJ	0.9020	0.5760
KK	0.8390	0.5400
L	0.9210	0.6130
LL	0.9440	0.6250
M	0.9470	0.6130
MM	0.1120	0.3190
N	0.9900	0.6560
NN	0.9280	0.6010

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Chain	Atom inclusion	Q-score
O	0.9690	0.6370
OO	0.9570	0.6170
P	0.9640	0.6460
PP	0.8780	0.5590
Q	0.9730	0.6490
QQ	0.9080	0.5780
R	0.9000	0.6030
RR	0.7450	0.5450
S	0.9760	0.6450
SS	0.8830	0.5660
T	0.9440	0.6210
TT	0.9120	0.5790
U	0.8820	0.5490
UU	0.7490	0.5170
V	0.9730	0.6440
VV	0.8760	0.5780
W	0.9490	0.6300
WW	0.9550	0.6150
X	0.9530	0.6240
XX	0.9590	0.6230
Y	0.9390	0.6220
YY	0.8960	0.5620
Z	0.9460	0.6140
ZZ	0.8430	0.5540
a	0.9660	0.6480
aa	0.9420	0.6160
b	0.8450	0.5830
bb	0.8470	0.5730
c	0.9440	0.6220
cc	0.8400	0.5680
d	0.9650	0.6330
dd	0.9490	0.5990
e	0.9830	0.6530
ee	0.9060	0.5680
f	0.9790	0.6560
ff	0.2530	0.3490
g	0.9350	0.6170
gg	0.7550	0.5030
h	0.9380	0.6160
hh	0.9920	0.6100
i	0.9210	0.6070
ii	0.7390	0.5290

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Chain	Atom inclusion	Q-score
j	0.9940	0.6520
jj	0.4420	0.5120
k	0.8460	0.5750
l	0.9860	0.6370
m	0.9490	0.6270
n	0.9750	0.6320
o	0.9610	0.6380
p	0.9580	0.6370
r	0.9660	0.6340
s	0.1770	0.2900
t	0.4670	0.3450