Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 11:12 am BST

PDB ID	:	8CMJ
EMDB ID	:	EMD-16729
Title	:	Translocation intermediate 4 (TI-4*) of 80S S. cerevisiae ribosome with eEF2 in the absence of sordarin
Authors	:	Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2023-02-20
Resolution	:	3.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

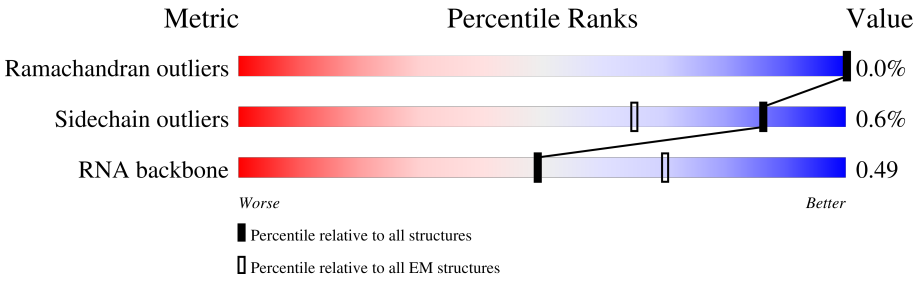
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.79 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%

Mol	Chain	Length	Quality of chain
1	0	135	99%
2	1	108	64% 35%
3	2	119	82% 18%
4	3	82	99%
5	4	67	93% 6%
6	5	56	86% 12%
7	6	63	75% 10% 16%
8	7	319	99%
9	8	152	24% 76%

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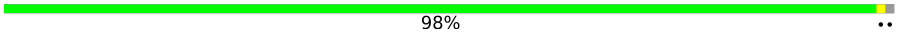
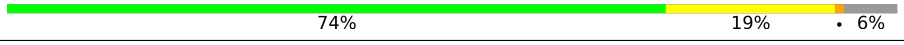
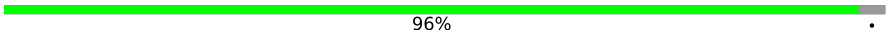
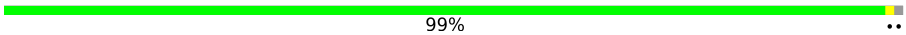
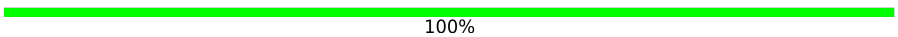
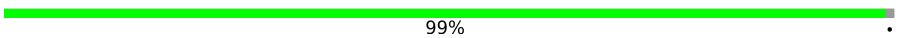
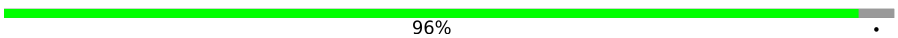
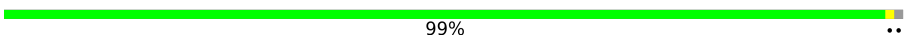
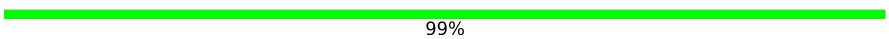
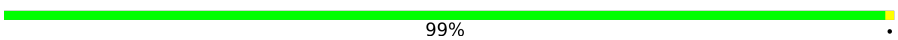
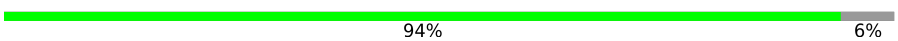
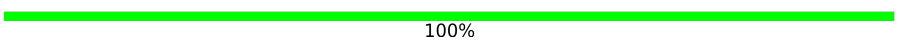
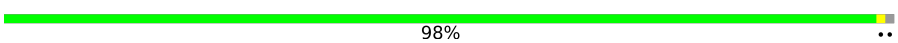
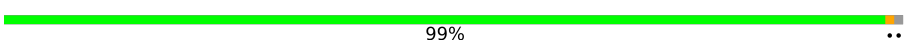
Mol	Chain	Length	Quality of chain
10	A	199	
11	AA	3396	
12	Aa	842	
13	B	184	
14	BB	121	
15	C	186	
16	CC	158	
17	D	189	
18	DD	312	
19	E	172	
20	EE	254	
21	Ee	165	
22	F	160	
23	FF	387	
24	G	121	
25	GG	362	
26	H	137	
27	HH	297	
28	I	155	
29	II	176	
30	J	142	
31	JJ	244	
32	K	127	
33	KK	256	
34	L	136	

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Mol	Chain	Length	Quality of chain
35	LL	191	
36	M	149	
37	MM	221	
38	N	59	
39	NN	174	
40	O	105	
41	OO	199	
42	P	113	
43	PP	138	
44	Q	130	
45	QQ	204	
46	R	107	
47	S	121	
48	T	120	
49	U	100	
50	V	88	
51	W	78	
52	X	51	
53	Y	128	
54	Z	25	
55	a	106	
56	b	92	
57	c	1800	
58	d	252	
59	e	255	

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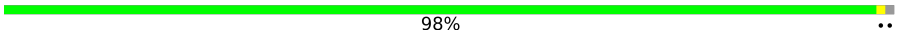
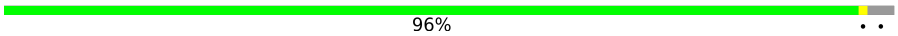
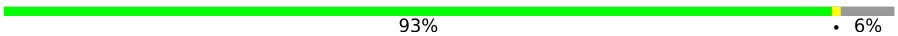
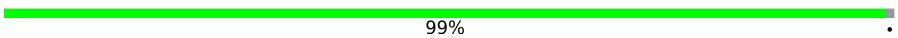
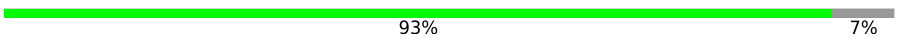
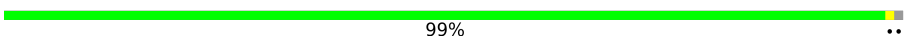
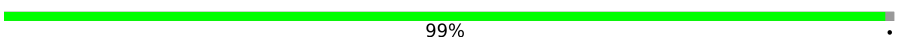
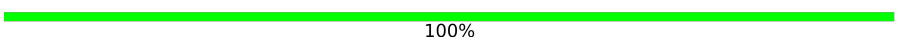
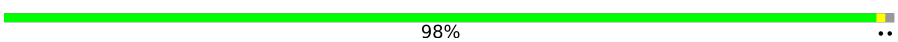
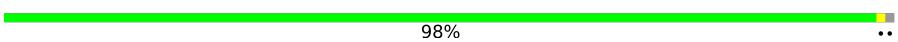
Mol	Chain	Length	Quality of chain
60	f	254	
61	g	240	
62	h	261	
63	i	225	
64	j	236	
65	k	190	
66	l	200	
67	m	197	
68	n	105	
69	o	156	
70	p	151	
71	q	137	
72	r	142	
73	s	143	
74	t	136	
75	u	146	
76	v	144	
77	w	121	
78	x	87	
79	y	130	
80	z	145	

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 202630 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 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	49	404	249	86	65	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	53	Total	C	N	O	S	0	0
			427	269	88	69	1		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	36	Total	C	N	O	S	0	0
			276	173	54	45	4		

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	3197	Total	C	N	O	P	0	0
			68429	30589	12334	22309	3197		

- Molecule 12 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Aa	816	Total	C	N	O	S	0	0
			6368	4051	1088	1198	31		

- Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 14 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 16 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	D	176	Total	C	N	O	0	0
			1423	875	308	240		

- Molecule 18 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DD	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 20 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	EE	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 21 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 24 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	G	97	Total	C	N	O	0	0
			770	499	126	145		

- Molecule 25 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	GG	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 27 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	HH	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 28 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 29 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	II	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 30 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 31 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	K	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	KK	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 34 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	L	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 35 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LL	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 36 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 37 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	MM	215	Total	C	N	O	S	0	0
			1743	1102	331	303	7		

- Molecule 38 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 39 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NN	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 40 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 41 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	OO	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 42 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	P	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	PP	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 44 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Q	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 45 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	QQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 46 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 47 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 48 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 49 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 50 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	V	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 51 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	W	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 52 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 53 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Y	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 54 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 55 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 56 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	b	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 57 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	c	1608	Total	C	N	O	P	0	0
			34321	15360	6093	11260	1608		

- Molecule 58 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 59 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 60 is a protein called 40S ribosomal protein S2.

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

- Molecule 61 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	g	183	Total	C	N	O	S	0	0
			1412	893	260	253	6		

- Molecule 62 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 63 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 64 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 65 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	k	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 66 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	l	184	Total	C	N	O	S	0	0
			1457	906	291	258	2		

- Molecule 67 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	m	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 68 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	n	33	Total	C	N	O	0	0
			300	199	46	55		

- Molecule 69 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	o	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	q	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	r	91	Total	C	N	O	S	0	0
			732	469	138	120	5		

- Molecule 73 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	s	136	Total	C	N	O	0	0
			1069	686	195	188		

- Molecule 74 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	t	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 75 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	u	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 76 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 77 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	w	100	Total	C	N	O	S	0	0
			800	509	144	146	1		

- Molecule 78 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 79 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 80 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	z	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	2	1	Total	Zn	0
			1	1	
81	5	1	Total	Zn	0
			1	1	
81	8	1	Total	Zn	0
			1	1	
81	S	1	Total	Zn	0
			1	1	
81	V	1	Total	Zn	0
			1	1	
81	Y	1	Total	Zn	0
			1	1	
81	a	1	Total	Zn	0
			1	1	
81	b	1	Total	Zn	0
			1	1	

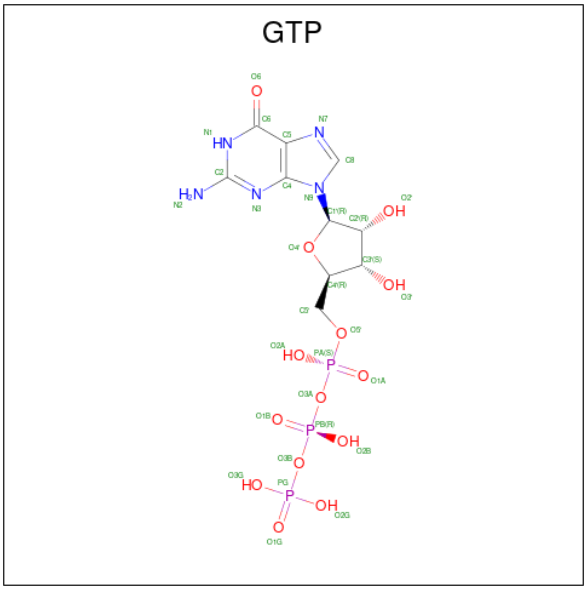
- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
82	AA	119	Total Mg 119 119	0
82	Aa	1	Total Mg 1 1	0
82	BB	3	Total Mg 3 3	0
82	CC	3	Total Mg 3 3	0
82	H	1	Total Mg 1 1	0
82	JJ	1	Total Mg 1 1	0
82	c	25	Total Mg 25 25	0

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
83	AA	9	Total K 9 9	0
83	EE	1	Total K 1 1	0

- Molecule 84 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
84	Aa	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 85 is water.

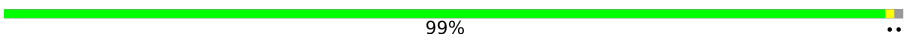
Mol	Chain	Residues	Atoms		AltConf
85	AA	71	Total	O	0
			71	71	
85	B	1	Total	O	0
			1	1	
85	CC	8	Total	O	0
			8	8	
85	F	1	Total	O	0
			1	1	
85	JJ	1	Total	O	0
			1	1	
85	R	1	Total	O	0
			1	1	
85	V	1	Total	O	0
			1	1	
85	c	18	Total	O	0
			18	18	

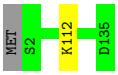
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 40S ribosomal protein S24-A

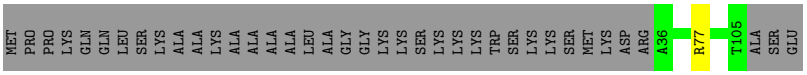
Chain 0:





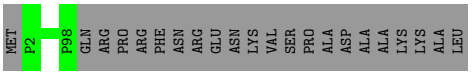
- Molecule 2: 40S ribosomal protein S25-A

Chain 1:



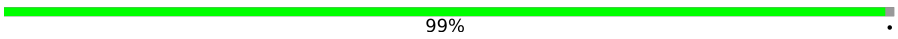
- Molecule 3: 40S ribosomal protein S26

Chain 2:



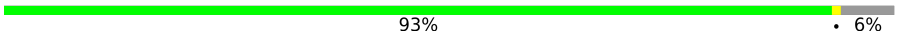
- Molecule 4: 40S ribosomal protein S27-A

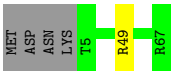
Chain 3:



- Molecule 5: 40S ribosomal protein S28-A

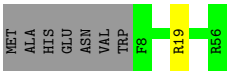
Chain 4:





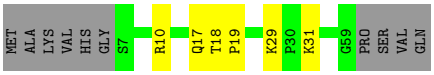
- Molecule 6: HLJ1_G0030400.mRNA.1.CDS.1

Chain 5:



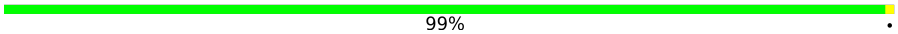
• Molecule 7: 40S ribosomal protein S30-A

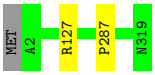
Chain 6:



• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

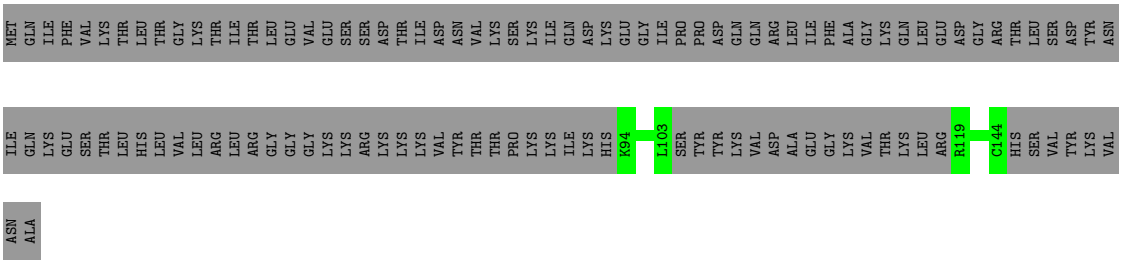
Chain 7:





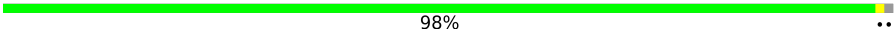
• Molecule 9: Ubiquitin-40S ribosomal protein S31

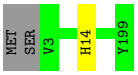
Chain 8:



• Molecule 10: 60S ribosomal protein L16-A

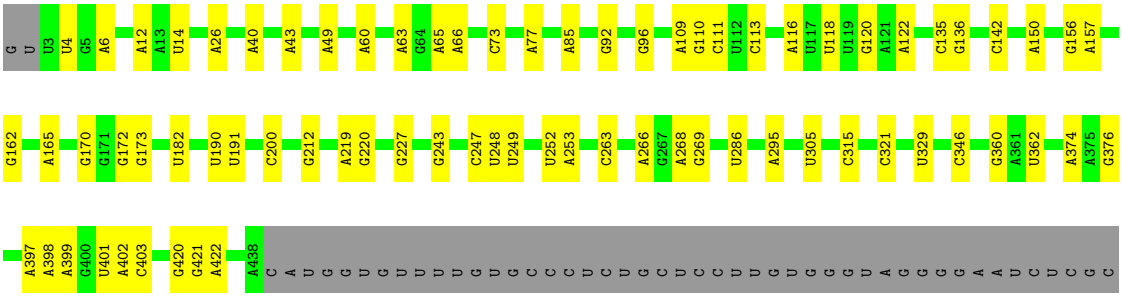
Chain A:

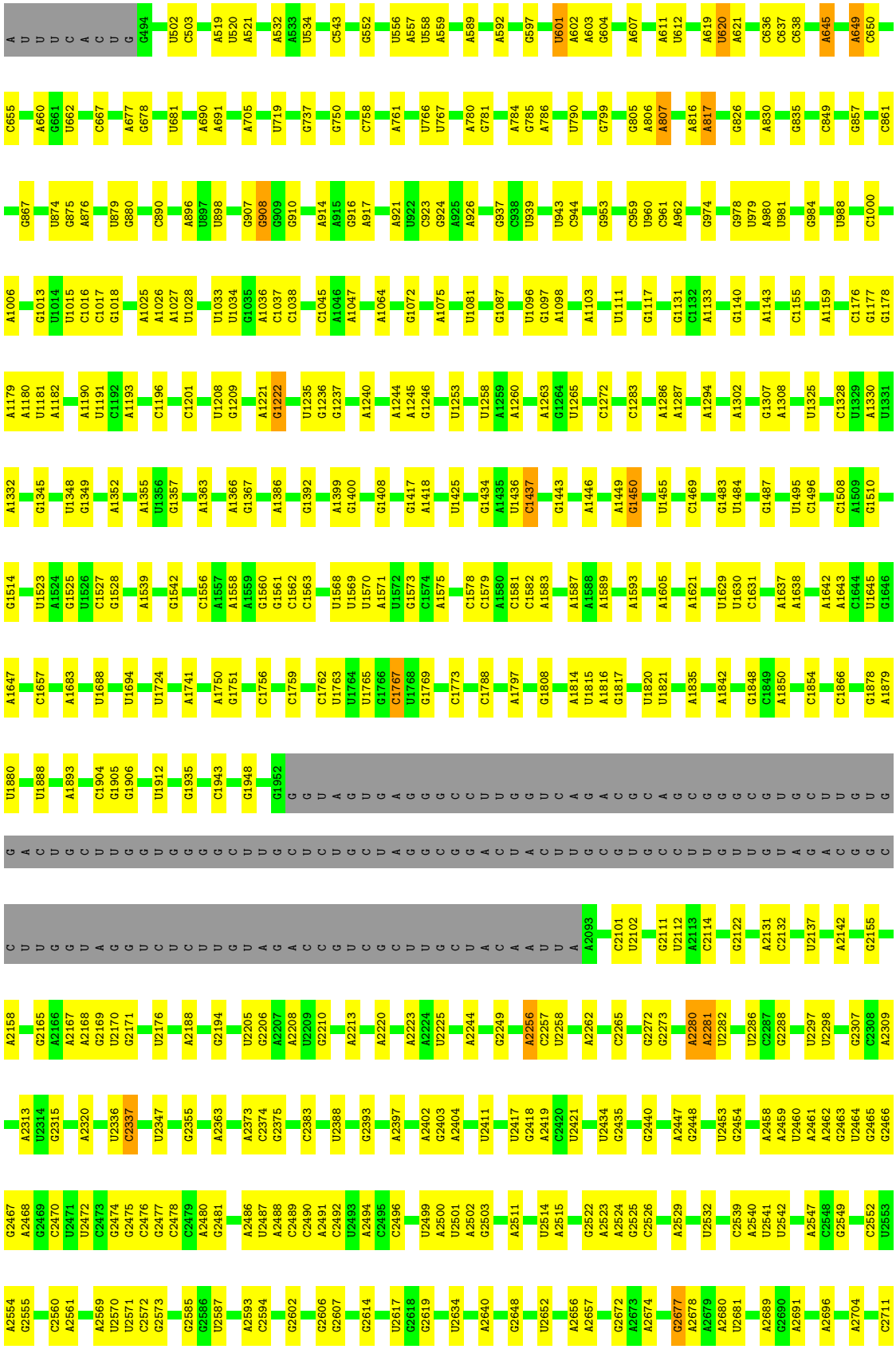


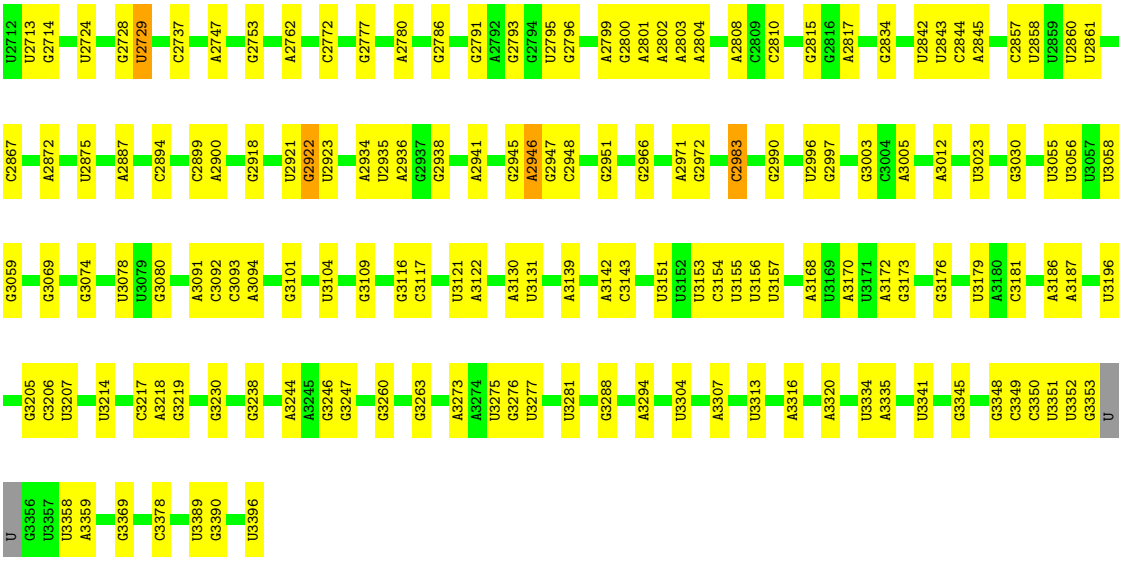


• Molecule 11: 25S ribosomal RNA

Chain AA:

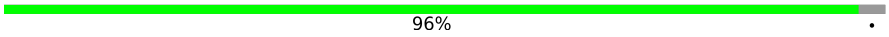






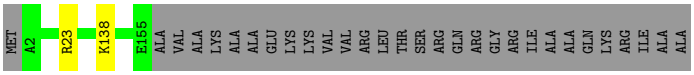
• Molecule 12: Elongation factor 2

Chain Aa:



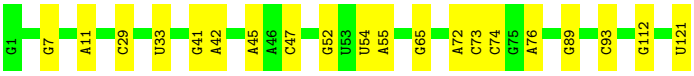
• Molecule 13: 60S ribosomal protein L17-A

Chain B:



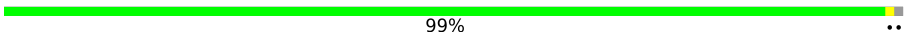
• Molecule 14: 5S ribosomal RNA

Chain BB:



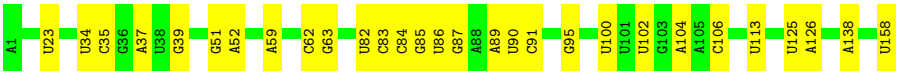
• Molecule 15: 60S ribosomal protein L18-A

Chain C:



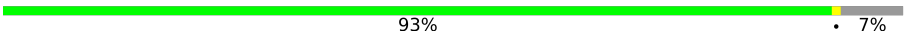
• Molecule 16: 5.8S ribosomal RNA

Chain CC:



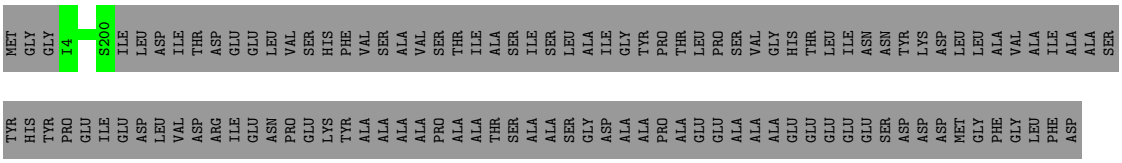
• Molecule 17: 60S ribosomal protein L19-A

Chain D:



• Molecule 18: 60S acidic ribosomal protein P0

Chain DD:



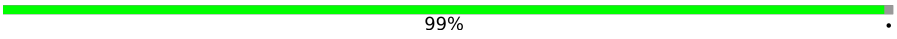
• Molecule 19: 60S ribosomal protein L20-A

Chain E:

There are no outlier residues recorded for this chain.

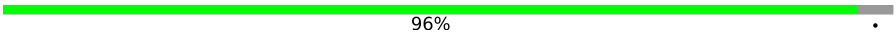
• Molecule 20: 60S ribosomal protein L2-A

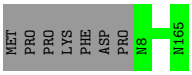
Chain EE:



• Molecule 21: 60S ribosomal protein L12-A

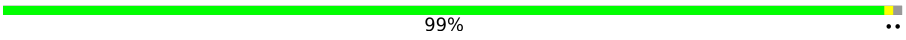
Chain Ee:





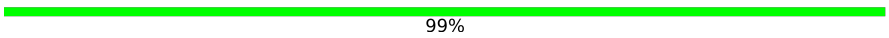
• Molecule 22: 60S ribosomal protein L21-A

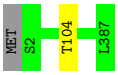
Chain F:



• Molecule 23: 60S ribosomal protein L3

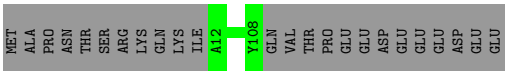
Chain FF:





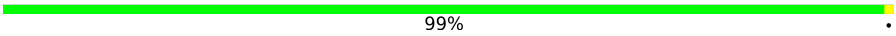
• Molecule 24: 60S ribosomal protein L22-A

Chain G:



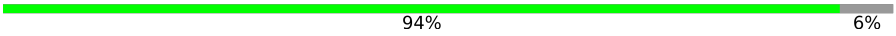
• Molecule 25: 60S ribosomal protein L4-A

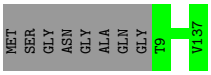
Chain GG:



• Molecule 26: 60S ribosomal protein L23-A

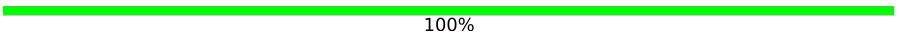
Chain H:





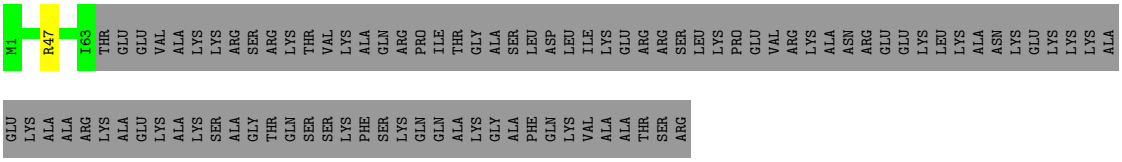
• Molecule 27: 60S ribosomal protein L5

Chain HH:



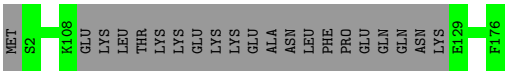
• Molecule 28: 60S ribosomal protein L24-A

Chain I:



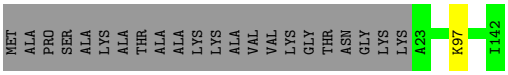
• Molecule 29: 60S ribosomal protein L6-A

Chain II:



• Molecule 30: 60S ribosomal protein L25

Chain J:

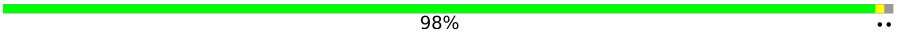


• Molecule 31: 60S ribosomal protein L7-A

Chain JJ:

• Molecule 32: 60S ribosomal protein L26-A

Chain K:

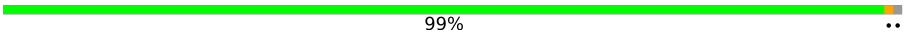


• Molecule 33: 60S ribosomal protein L8-A

Chain KK:

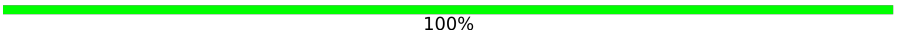
• Molecule 34: 60S ribosomal protein L27-A

Chain L:



• Molecule 35: RPL9A isoform 1

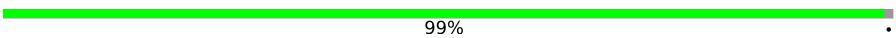
Chain LL:



There are no outlier residues recorded for this chain.

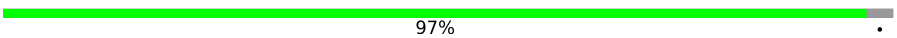
• Molecule 36: 60S ribosomal protein L28

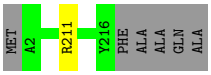
Chain M:



• Molecule 37: 60S ribosomal protein L10

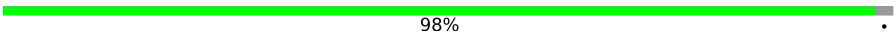
Chain MM:





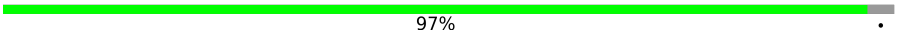
• Molecule 38: 60S ribosomal protein L29

Chain N:



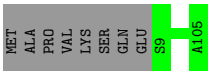
• Molecule 39: 60S ribosomal protein L11-A

Chain NN:



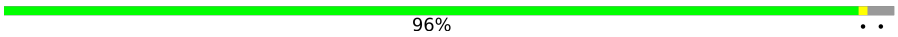
• Molecule 40: 60S ribosomal protein L30

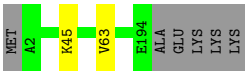
Chain O:



• Molecule 41: 60S ribosomal protein L13-A

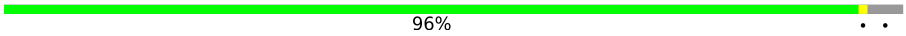
Chain OO:

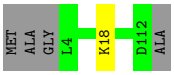




• Molecule 42: 60S ribosomal protein L31-A

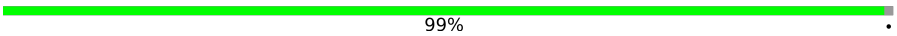
Chain P:





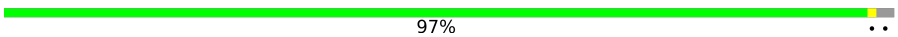
• Molecule 43: 60S ribosomal protein L14-A

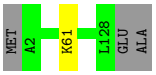
Chain PP:



• Molecule 44: 60S ribosomal protein L32

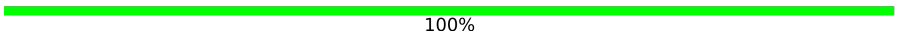
Chain Q:





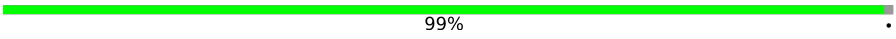
• Molecule 45: 60S ribosomal protein L15-A

Chain QQ:



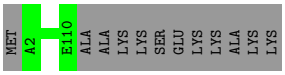
• Molecule 46: 60S ribosomal protein L33-A

Chain R:



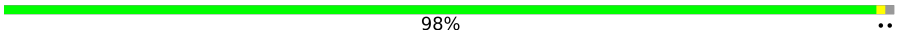
• Molecule 47: 60S ribosomal protein L34-A

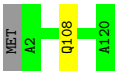
Chain S:



• Molecule 48: 60S ribosomal protein L35-A

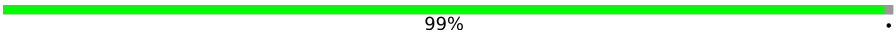
Chain T:





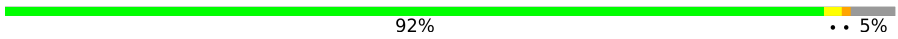
• Molecule 49: 60S ribosomal protein L36-A

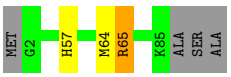
Chain U:



• Molecule 50: 60S ribosomal protein L37-A

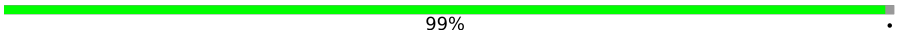
Chain V:





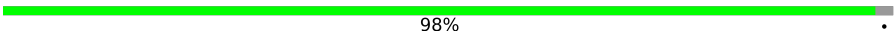
• Molecule 51: 60S ribosomal protein L38

Chain W:



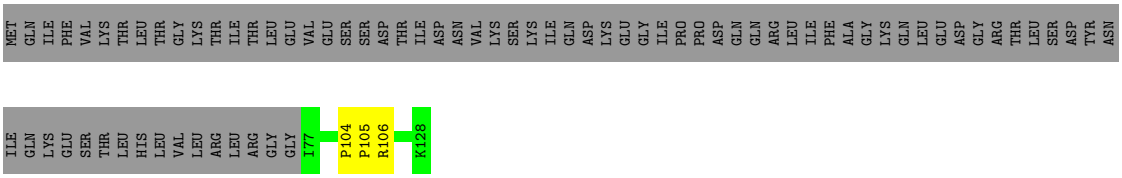
• Molecule 52: 60S ribosomal protein L39

Chain X:



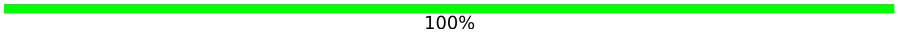
• Molecule 53: Ubiquitin-60S ribosomal protein L40

Chain Y:



• Molecule 54: 60S ribosomal protein L41

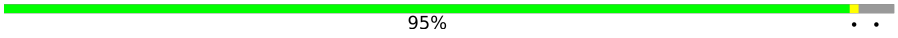
Chain Z:

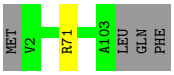


There are no outlier residues recorded for this chain.

• Molecule 55: 60S ribosomal protein L42-A

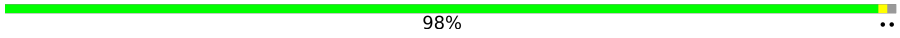
Chain a:

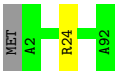




• Molecule 56: 60S ribosomal protein L43-A

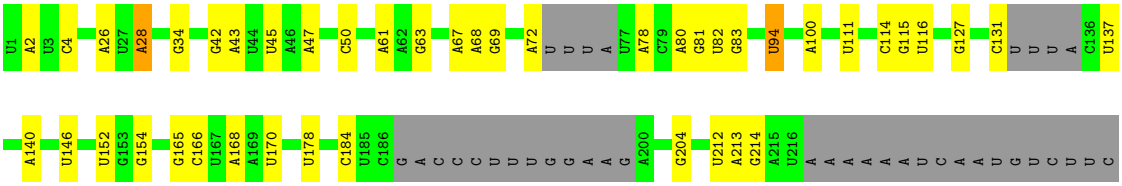
Chain b:

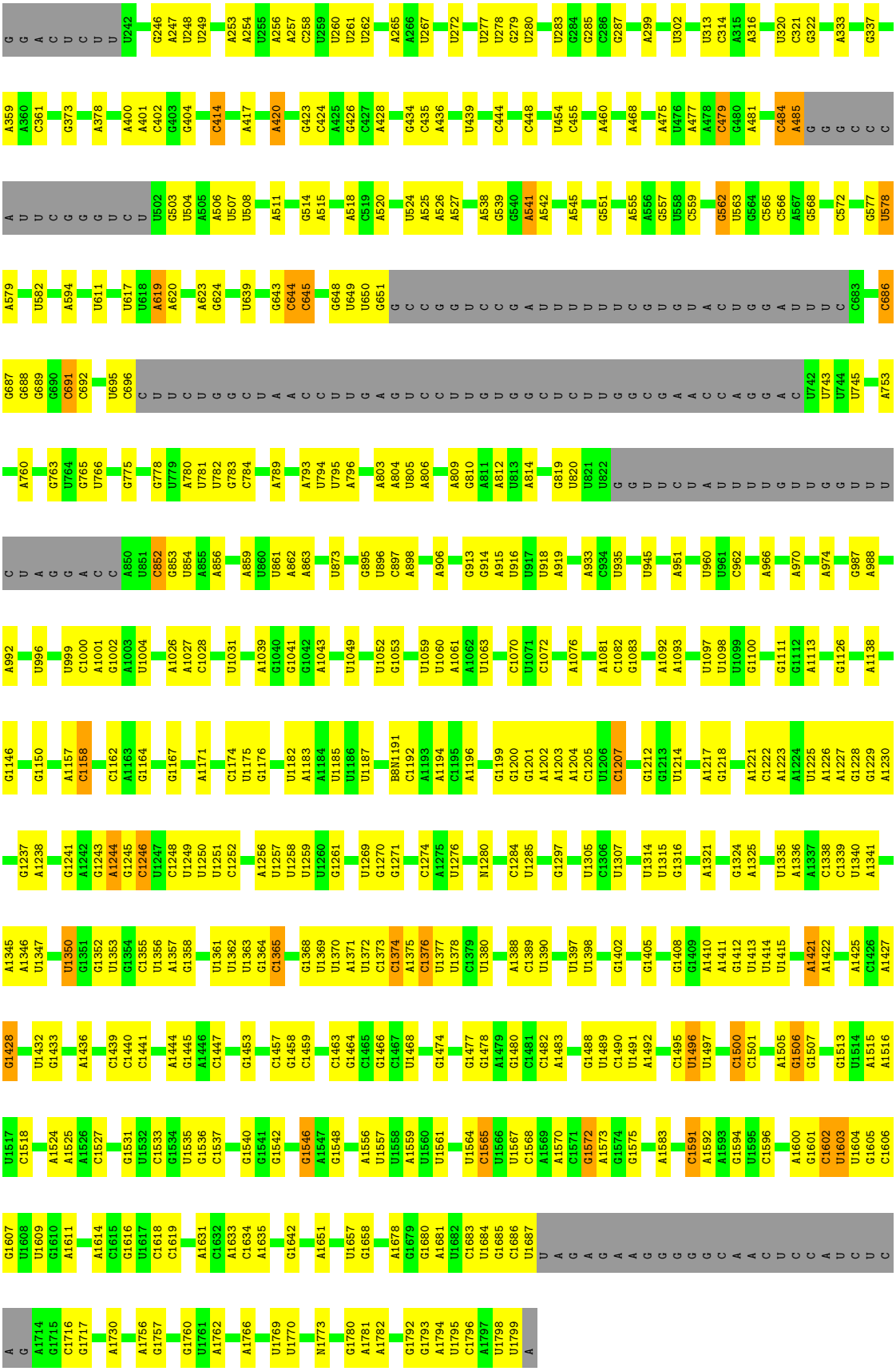




• Molecule 57: 18S ribosomal RNA

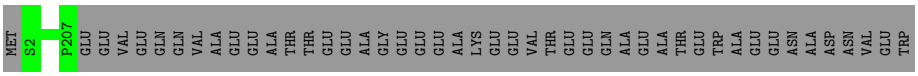
Chain c:





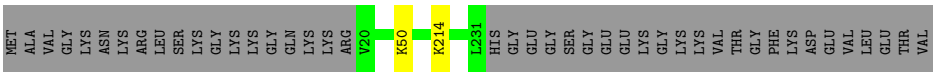
• Molecule 58: 40S ribosomal protein S0-A

Chain d:



• Molecule 59: 40S ribosomal protein S1-A

Chain e:

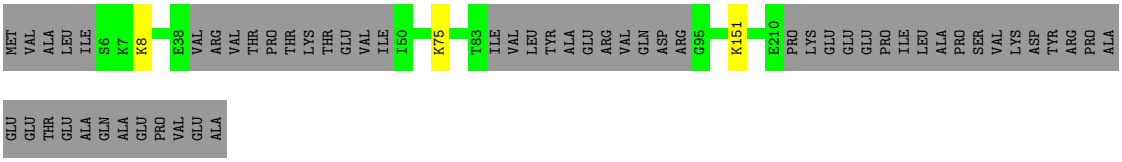


• Molecule 60: 40S ribosomal protein S2

Chain f:

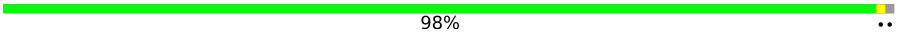
• Molecule 61: RPS3 isoform 1

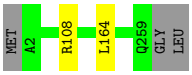
Chain g:



• Molecule 62: 40S ribosomal protein S4-A

Chain h:



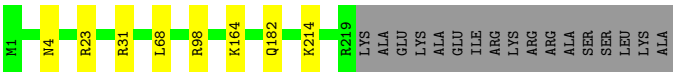


• Molecule 63: 40S ribosomal protein S5

Chain i:

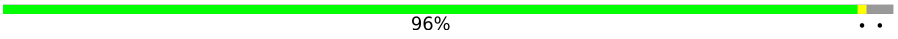
• Molecule 64: 40S ribosomal protein S6-A

Chain j:



• Molecule 65: 40S ribosomal protein S7-A

Chain k:

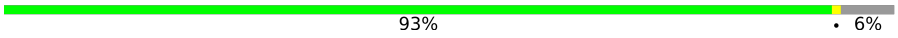


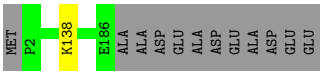
• Molecule 66: 40S ribosomal protein S8-B

Chain l:

• Molecule 67: 40S ribosomal protein S9-A

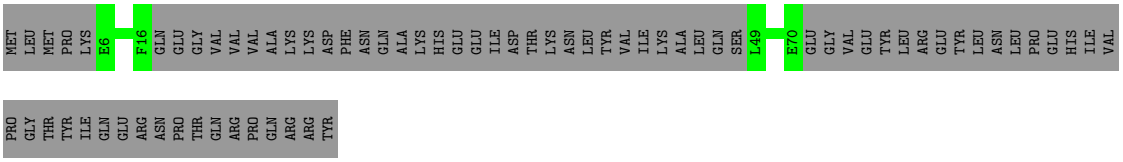
Chain m:





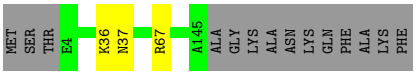
• Molecule 68: 40S ribosomal protein S10-A

Chain n:



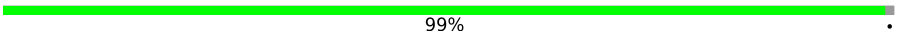
• Molecule 69: 40S ribosomal protein S11-A

Chain o:



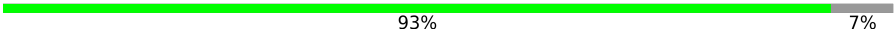
• Molecule 70: 40S ribosomal protein S13

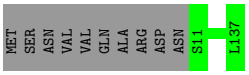
Chain p:



• Molecule 71: 40S ribosomal protein S14-A

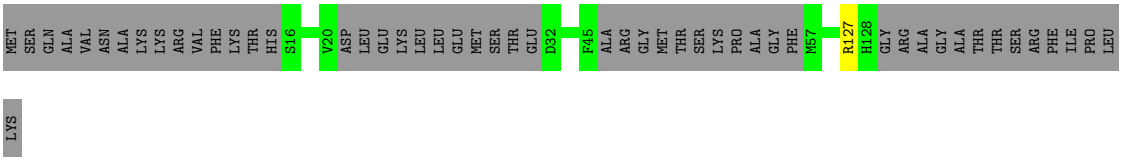
Chain q:





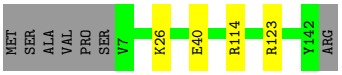
• Molecule 72: 40S ribosomal protein S15

Chain r:



• Molecule 73: 40S ribosomal protein S16-A

Chain s:

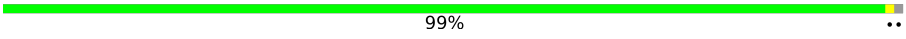


• Molecule 74: 40S ribosomal protein S17-A

Chain t:

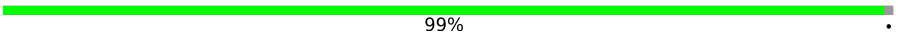
• Molecule 75: 40S ribosomal protein S18-A

Chain u:



• Molecule 76: 40S ribosomal protein S19-A

Chain v:



• Molecule 77: 40S ribosomal protein S20

Chain w:

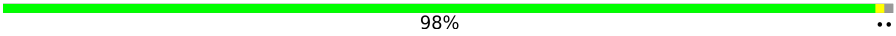
• Molecule 78: 40S ribosomal protein S21-A

Chain x:

There are no outlier residues recorded for this chain.

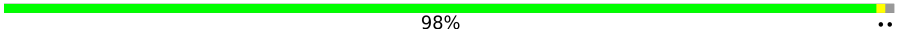
• Molecule 79: 40S ribosomal protein S22-A

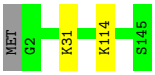
Chain y:



• Molecule 80: 40S ribosomal protein S23-A

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38558	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	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: OMG, A2M, ZN, 4AC, UR3, MG, GTP, G7M, 5MC, K, B8N, MA6, OMU, DDE, 1MA, 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	0	0.28	0/1087	0.60	0/1449
2	1	0.26	0/571	0.66	0/768
3	2	0.31	0/782	0.64	0/1047
4	3	0.29	0/620	0.61	0/838
5	4	0.28	0/499	0.62	0/670
6	5	0.29	0/412	0.60	0/544
7	6	0.57	1/433 (0.2%)	1.05	5/575 (0.9%)
8	7	0.40	1/2489 (0.0%)	0.73	4/3389 (0.1%)
9	8	0.26	0/279	0.60	0/369
10	A	0.33	0/1585	0.54	0/2128
11	AA	0.40	0/75545	0.83	29/117782 (0.0%)
12	Aa	0.28	0/6470	0.55	0/8759
13	B	0.33	0/1245	0.59	0/1676
14	BB	0.38	0/2883	0.80	1/4491 (0.0%)
15	C	0.29	0/1465	0.58	1/1965 (0.1%)
16	CC	0.41	0/3746	0.81	0/5832
17	D	0.29	0/1440	0.58	0/1921
18	DD	0.27	0/1558	0.53	0/2107
19	E	0.34	0/1481	0.61	0/1990
20	EE	0.31	0/1948	0.60	0/2617
21	Ee	0.28	0/1210	0.55	0/1627
22	F	0.30	0/1300	0.55	0/1743
23	FF	0.30	0/3146	0.55	0/4228
24	G	0.30	0/786	0.53	0/1065
25	GG	0.30	0/2800	0.53	0/3790
26	H	0.31	0/978	0.58	0/1316
27	HH	0.30	0/2425	0.53	0/3271
28	I	0.34	0/533	0.57	0/707
29	II	0.30	0/1251	0.56	0/1682
30	J	0.29	0/974	0.55	0/1314
31	JJ	0.35	0/1821	0.54	0/2451
32	K	0.29	0/1004	0.56	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	KK	0.27	0/1836	0.48	0/2481
34	L	0.31	0/1118	0.52	0/1497
35	LL	0.32	0/1539	0.56	0/2073
36	M	0.27	0/1204	0.56	0/1612
37	MM	0.30	0/1779	0.55	0/2386
38	N	0.26	0/473	0.54	0/629
39	NN	0.28	0/1374	0.60	0/1842
40	O	0.32	0/750	0.57	0/1008
41	OO	0.29	0/1568	0.59	0/2106
42	P	0.30	0/897	0.59	0/1205
43	PP	0.28	0/1068	0.55	0/1438
44	Q	0.29	0/1041	0.54	0/1394
45	QQ	0.29	0/1757	0.59	0/2354
46	R	0.35	0/868	0.60	0/1168
47	S	0.30	0/871	0.58	0/1164
48	T	0.28	0/978	0.55	0/1301
49	U	0.27	0/778	0.59	0/1034
50	V	0.31	0/680	0.64	0/901
51	W	0.29	0/618	0.59	0/826
52	X	0.30	0/443	0.67	0/588
53	Y	0.29	0/423	0.62	0/562
54	Z	0.29	0/234	0.88	0/300
55	a	0.29	0/831	0.61	0/1097
56	b	0.30	0/701	0.63	0/934
57	c	0.37	0/37760	0.94	120/58811 (0.2%)
58	d	0.28	0/1623	0.54	0/2222
59	e	0.29	0/1714	0.58	0/2308
60	f	0.29	0/1665	0.56	0/2263
61	g	0.29	0/1429	0.59	0/1913
62	h	0.31	0/2097	0.61	1/2823 (0.0%)
63	i	0.28	0/1591	0.61	0/2151
64	j	0.28	0/1790	0.62	1/2393 (0.0%)
65	k	0.28	0/1506	0.57	0/2028
66	l	0.31	0/1482	0.63	0/1980
67	m	0.28	0/1519	0.59	0/2035
68	n	0.29	0/309	0.49	0/416
69	o	0.30	0/1172	0.61	0/1580
70	p	0.31	0/1215	0.57	0/1638
71	q	0.29	0/901	0.62	0/1217
72	r	0.31	0/747	0.64	0/1002
73	s	0.27	0/1088	0.59	0/1459
74	t	0.27	0/971	0.59	0/1303
75	u	0.27	0/1211	0.60	0/1628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	v	0.26	0/1130	0.56	0/1517
77	w	0.26	0/810	0.57	0/1095
78	x	0.31	0/693	0.60	0/935
79	y	0.31	0/1038	0.57	0/1395
80	z	0.29	0/1139	0.60	0/1518
All	All	0.35	2/215195 (0.0%)	0.76	162/314982 (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
7	6	0	1
31	JJ	0	2
34	L	0	1
50	V	0	1
53	Y	0	1
64	j	0	1
65	k	0	1
69	o	0	1
73	s	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	287	PRO	CG-CD	-13.52	1.06	1.50
7	6	19	PRO	CG-CD	-8.23	1.23	1.50

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	287	PRO	N-CD-CG	-18.44	75.55	103.20
57	c	94	U	C2-N3-C4	14.86	135.92	127.00
57	c	1501	C	N1-C2-O2	14.09	127.35	118.90
8	7	287	PRO	CA-CB-CG	-12.15	80.92	104.00
57	c	1602	C	OP1-P-O3'	-11.57	79.74	105.20
57	c	1175	U	OP1-P-O3'	-11.23	80.50	105.20
57	c	1439	C	OP1-P-O3'	-11.09	80.79	105.20
57	c	1496	U	OP1-P-O3'	-11.08	80.82	105.20
57	c	1440	C	OP1-P-O3'	-11.04	80.91	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	c	804	A	OP1-P-O3'	-11.02	80.95	105.20
57	c	1157	A	OP1-P-O3'	-11.01	80.98	105.20
57	c	82	U	OP1-P-O3'	-10.79	81.46	105.20
57	c	1421	A	OP1-P-O3'	-10.72	81.62	105.20
7	6	19	PRO	N-CD-CG	-10.68	87.18	103.20
57	c	81	G	OP1-P-O3'	-10.67	81.72	105.20
57	c	82	U	OP2-P-O3'	-10.61	81.86	105.20
57	c	804	A	OP2-P-O3'	-10.28	82.58	105.20
57	c	1175	U	OP2-P-O3'	-10.24	82.67	105.20
57	c	81	G	OP2-P-O3'	-9.68	83.90	105.20
57	c	94	U	N1-C2-N3	9.66	120.70	114.90
57	c	1421	A	OP2-P-O3'	-9.53	84.23	105.20
57	c	1507	G	C5-C6-O6	9.51	134.31	128.60
57	c	1374	C	N1-C2-O2	9.51	124.60	118.90
57	c	1440	C	OP2-P-O3'	-9.45	84.41	105.20
57	c	1439	C	OP2-P-O3'	-9.44	84.42	105.20
57	c	1350	U	N3-C2-O2	-9.44	115.59	122.20
57	c	689	G	N3-C4-N9	9.35	131.61	126.00
7	6	18	THR	N-CA-CB	-9.34	92.55	110.30
57	c	1374	C	N3-C2-O2	-9.24	115.44	121.90
57	c	1501	C	N3-C2-O2	-9.11	115.52	121.90
57	c	686	C	N3-C2-O2	-8.98	115.61	121.90
57	c	1496	U	OP2-P-O3'	-8.93	85.57	105.20
57	c	1507	G	N1-C6-O6	-8.66	114.70	119.90
57	c	1602	C	OP2-P-O3'	-8.60	86.29	105.20
57	c	1533	C	N3-C2-O2	-8.50	115.95	121.90
57	c	1506	G	N3-C2-N2	8.42	125.79	119.90
57	c	1157	A	OP2-P-O3'	-8.26	87.02	105.20
57	c	479	C	O4'-C1'-N1	8.14	114.71	108.20
11	AA	1788	C	N3-C2-O2	-8.07	116.25	121.90
57	c	1365	C	N1-C2-O2	8.04	123.73	118.90
7	6	19	PRO	CA-N-CD	-7.99	100.32	111.50
57	c	689	G	C8-N9-C1'	-7.97	116.64	127.00
8	7	287	PRO	CA-N-CD	-7.90	100.44	111.50
57	c	1422	A	OP1-P-OP2	7.82	131.32	119.60
57	c	645	C	N3-C2-O2	-7.57	116.60	121.90
57	c	689	G	N9-C4-C5	-7.56	102.38	105.40
57	c	1603	U	OP1-P-OP2	7.55	130.93	119.60
57	c	1176	G	OP1-P-OP2	7.53	130.89	119.60
8	7	287	PRO	CB-CG-CD	7.47	135.64	106.50
57	c	689	G	C4-N9-C1'	7.42	136.14	126.50
57	c	484	C	N3-C2-O2	-7.40	116.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	c	1500	C	C6-N1-C2	-7.37	117.35	120.30
57	c	1506	G	N9-C4-C5	-7.34	102.46	105.40
57	c	1374	C	C2-N1-C1'	7.33	126.86	118.80
57	c	1716	C	C2-N1-C1'	-7.29	110.78	118.80
57	c	1158	C	OP1-P-OP2	7.29	130.53	119.60
11	AA	1283	C	N3-C2-O2	-7.29	116.80	121.90
57	c	1376	C	C2-N1-C1'	-7.29	110.79	118.80
57	c	691	C	N3-C2-O2	-7.25	116.83	121.90
57	c	686	C	C6-N1-C2	-7.21	117.42	120.30
57	c	83	G	OP1-P-OP2	7.21	130.41	119.60
57	c	805	U	OP1-P-OP2	7.16	130.35	119.60
57	c	1533	C	N1-C2-O2	7.16	123.20	118.90
57	c	1497	U	OP1-P-OP2	7.14	130.31	119.60
57	c	1565	C	N3-C2-O2	-7.09	116.94	121.90
57	c	1440	C	OP1-P-OP2	7.08	130.22	119.60
11	AA	2711	C	N3-C2-O2	-7.06	116.96	121.90
57	c	689	G	C6-C5-N7	-7.06	126.17	130.40
57	c	1441	C	OP1-P-OP2	7.03	130.15	119.60
11	AA	1328	C	N3-C2-O2	-7.03	116.98	121.90
57	c	1591	C	C4'-C3'-O3'	-7.01	94.68	109.40
57	c	686	C	C5-C4-N4	7.01	125.10	120.20
57	c	645	C	N1-C2-O2	7.00	123.10	118.90
57	c	1495	C	N3-C2-O2	-7.00	117.00	121.90
57	c	1350	U	N1-C2-O2	6.95	127.67	122.80
57	c	479	C	C2-N1-C1'	6.90	126.39	118.80
57	c	479	C	N1-C2-O2	6.89	123.03	118.90
11	AA	2137	U	C2-N1-C1'	6.84	125.91	117.70
57	c	82	U	OP1-P-OP2	6.82	129.83	119.60
57	c	691	C	N1-C2-O2	6.80	122.98	118.90
57	c	1376	C	C6-N1-C1'	6.78	128.93	120.80
57	c	1591	C	N1-C1'-C2'	6.75	122.78	114.00
11	AA	2843	U	N1-C2-O2	6.74	127.51	122.80
57	c	648	G	C5-C6-O6	6.72	132.63	128.60
57	c	1500	C	C5-C4-N4	6.72	124.90	120.20
57	c	644	C	N1-C2-O2	6.68	122.91	118.90
11	AA	620	U	C2-N1-C1'	6.64	125.67	117.70
11	AA	2137	U	N1-C2-O2	6.63	127.44	122.80
11	AA	1788	C	N1-C2-O2	6.61	122.86	118.90
11	AA	1328	C	N1-C2-O2	6.57	122.84	118.90
57	c	1500	C	N3-C2-O2	-6.57	117.30	121.90
57	c	1716	C	C6-N1-C1'	6.53	128.63	120.80
57	c	1506	G	N3-C4-N9	6.51	129.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	c	1501	C	N3-C4-C5	6.50	124.50	121.90
57	c	1507	G	N9-C4-C5	6.49	108.00	105.40
57	c	1506	G	C4-C5-N7	6.48	113.39	110.80
11	AA	2843	U	C2-N1-C1'	6.47	125.46	117.70
57	c	1389	C	C2-N1-C1'	6.44	125.89	118.80
11	AA	620	U	N1-C2-O2	6.44	127.31	122.80
57	c	94	U	N3-C2-O2	-6.42	117.70	122.20
57	c	1389	C	C6-N1-C2	-6.39	117.74	120.30
57	c	1246	C	C2-N1-C1'	6.30	125.73	118.80
57	c	1565	C	N1-C2-O2	6.20	122.62	118.90
57	c	479	C	N3-C2-O2	-6.05	117.66	121.90
57	c	689	G	C4-C5-N7	6.04	113.22	110.80
11	AA	620	U	N3-C2-O2	-5.97	118.02	122.20
57	c	1513	G	C5-C6-O6	5.97	132.18	128.60
11	AA	1496	C	C2-N1-C1'	5.94	125.34	118.80
57	c	1565	C	C6-N1-C2	-5.94	117.92	120.30
11	AA	2137	U	N3-C2-O2	-5.93	118.05	122.20
57	c	479	C	C6-N1-C2	-5.93	117.93	120.30
57	c	484	C	N1-C2-O2	5.92	122.45	118.90
57	c	485	A	O4'-C1'-N9	5.91	112.92	108.20
11	AA	1222	G	O4'-C1'-N9	5.90	112.92	108.20
57	c	648	G	N1-C6-O6	-5.86	116.38	119.90
7	6	18	THR	C-N-CD	5.84	140.66	128.40
57	c	572	C	N3-C2-O2	-5.83	117.82	121.90
57	c	1374	C	C6-N1-C2	-5.81	117.98	120.30
11	AA	1176	C	N3-C2-O2	-5.79	117.85	121.90
11	AA	2843	U	N3-C2-O2	-5.75	118.18	122.20
57	c	1507	G	C4-C5-N7	-5.74	108.51	110.80
57	c	962	C	N3-C2-O2	-5.71	117.91	121.90
11	AA	2677	G	O4'-C1'-N9	5.66	112.73	108.20
57	c	644	C	C2-N1-C1'	5.63	125.00	118.80
62	h	164	LEU	CA-CB-CG	5.63	128.25	115.30
57	c	1501	C	C4-C5-C6	-5.62	114.59	117.40
57	c	1716	C	N1-C2-O2	-5.61	115.53	118.90
57	c	962	C	N1-C2-O2	5.61	122.27	118.90
64	j	68	LEU	CA-CB-CG	5.58	128.13	115.30
57	c	1207	C	N1-C2-O2	5.57	122.24	118.90
57	c	686	C	N3-C4-N4	-5.57	114.10	118.00
57	c	1591	C	O4'-C1'-C2'	-5.51	100.29	105.80
57	c	94	U	N3-C4-C5	5.46	117.87	114.60
57	c	1506	G	N1-C2-N2	-5.44	111.31	116.20
7	6	19	PRO	CA-CB-CG	-5.43	93.67	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2711	C	N1-C2-O2	5.42	122.15	118.90
11	AA	3214	U	N3-C2-O2	-5.42	118.41	122.20
57	c	1501	C	N3-C4-N4	-5.42	114.21	118.00
14	BB	89	G	N1-C6-O6	-5.39	116.67	119.90
57	c	1546	G	N3-C4-N9	-5.38	122.78	126.00
57	c	1546	G	N1-C6-O6	-5.32	116.71	119.90
57	c	689	G	N3-C2-N2	5.31	123.62	119.90
11	AA	1283	C	N1-C2-O2	5.30	122.08	118.90
57	c	1389	C	N3-C2-O2	-5.26	118.22	121.90
11	AA	2499	U	N1-C2-O2	5.25	126.47	122.80
11	AA	2983	C	C2-N1-C1'	5.24	124.56	118.80
57	c	689	G	N3-C4-C5	-5.24	125.98	128.60
15	C	95	GLU	C-N-CA	-5.23	108.62	121.70
57	c	852	C	N1-C2-O2	5.18	122.01	118.90
57	c	1244	A	P-O3'-C3'	5.18	125.91	119.70
57	c	1389	C	N1-C2-O2	5.17	122.00	118.90
57	c	1501	C	C2-N1-C1'	5.17	124.48	118.80
57	c	1500	C	C6-N1-C1'	5.14	126.97	120.80
57	c	1565	C	C2-N1-C1'	5.13	124.44	118.80
11	AA	601	U	C2-N1-C1'	5.08	123.79	117.70
57	c	1507	G	N3-C4-N9	-5.07	122.96	126.00
57	c	1513	G	N1-C6-O6	-5.06	116.86	119.90
57	c	686	C	N1-C2-N3	5.05	122.73	119.20
11	AA	1190	A	N1-C2-N3	5.04	131.82	129.30
11	AA	1767	C	C2-N1-C1'	5.04	124.35	118.80
11	AA	3058	U	C2-N1-C1'	5.03	123.74	117.70
11	AA	2857	C	N3-C2-O2	-5.01	118.39	121.90

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	6	17	GLN	Mainchain
31	JJ	158	LYS	Peptide
31	JJ	232	ARG	Peptide
34	L	102	GLU	Peptide
50	V	64	MET	Peptide
53	Y	104	PRO	Peptide
64	j	23	ARG	Sidechain
65	k	64	VAL	Peptide
69	o	37	ASN	Peptide
73	s	40	GLU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
2	1	68/108 (63%)	61 (90%)	7 (10%)	0	100	100
3	2	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
4	3	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
5	4	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
6	5	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
7	6	51/63 (81%)	48 (94%)	3 (6%)	0	100	100
8	7	316/319 (99%)	298 (94%)	18 (6%)	0	100	100
9	8	32/152 (21%)	19 (59%)	13 (41%)	0	100	100
10	A	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
12	Aa	811/842 (96%)	794 (98%)	17 (2%)	0	100	100
13	B	152/184 (83%)	152 (100%)	0	0	100	100
15	C	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
17	D	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
18	DD	195/312 (62%)	192 (98%)	3 (2%)	0	100	100
19	E	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
20	EE	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
21	Ee	156/165 (94%)	148 (95%)	8 (5%)	0	100	100
22	F	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	FF	384/387 (99%)	373 (97%)	11 (3%)	0	100	100
24	G	95/121 (78%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	GG	359/362 (99%)	350 (98%)	9 (2%)	0	100	100
26	H	127/137 (93%)	127 (100%)	0	0	100	100
27	HH	294/297 (99%)	285 (97%)	9 (3%)	0	100	100
28	I	61/155 (39%)	61 (100%)	0	0	100	100
29	II	151/176 (86%)	150 (99%)	1 (1%)	0	100	100
30	J	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
31	JJ	220/244 (90%)	212 (96%)	7 (3%)	1 (0%)	29	66
32	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
33	KK	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
34	L	133/136 (98%)	129 (97%)	3 (2%)	1 (1%)	19	57
35	LL	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
36	M	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
37	MM	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
38	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
39	NN	167/174 (96%)	159 (95%)	8 (5%)	0	100	100
40	O	95/105 (90%)	95 (100%)	0	0	100	100
41	OO	191/199 (96%)	180 (94%)	10 (5%)	1 (0%)	29	66
42	P	107/113 (95%)	105 (98%)	2 (2%)	0	100	100
43	PP	134/138 (97%)	131 (98%)	3 (2%)	0	100	100
44	Q	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
45	QQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
46	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
47	S	107/121 (88%)	107 (100%)	0	0	100	100
48	T	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
49	U	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
50	V	82/88 (93%)	79 (96%)	2 (2%)	1 (1%)	13	50
51	W	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
52	X	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
53	Y	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	7	41
54	Z	23/25 (92%)	23 (100%)	0	0	100	100
55	a	100/106 (94%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	b	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
58	d	204/252 (81%)	193 (95%)	11 (5%)	0	100	100
59	e	210/255 (82%)	196 (93%)	14 (7%)	0	100	100
60	f	215/254 (85%)	201 (94%)	14 (6%)	0	100	100
61	g	177/240 (74%)	170 (96%)	7 (4%)	0	100	100
62	h	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
63	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
64	j	217/236 (92%)	217 (100%)	0	0	100	100
65	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
66	l	180/200 (90%)	169 (94%)	11 (6%)	0	100	100
67	m	183/197 (93%)	175 (96%)	8 (4%)	0	100	100
68	n	29/105 (28%)	29 (100%)	0	0	100	100
69	o	140/156 (90%)	133 (95%)	7 (5%)	0	100	100
70	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	q	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
72	r	85/142 (60%)	80 (94%)	5 (6%)	0	100	100
73	s	134/143 (94%)	126 (94%)	8 (6%)	0	100	100
74	t	119/136 (88%)	114 (96%)	5 (4%)	0	100	100
75	u	143/146 (98%)	134 (94%)	9 (6%)	0	100	100
76	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
77	w	98/121 (81%)	98 (100%)	0	0	100	100
78	x	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
79	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
80	z	142/145 (98%)	132 (93%)	10 (7%)	0	100	100
All	All	11672/13056 (89%)	11284 (97%)	383 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	JJ	159	GLN
50	V	65	ARG
34	L	102	GLU
53	Y	105	PRO
41	OO	63	VAL

5.3.2 Protein sidechains (i)

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	0	112/113 (99%)	111 (99%)	1 (1%)	78 88
2	1	61/89 (68%)	60 (98%)	1 (2%)	62 79
3	2	83/101 (82%)	83 (100%)	0	100 100
4	3	70/71 (99%)	70 (100%)	0	100 100
5	4	56/60 (93%)	55 (98%)	1 (2%)	59 77
6	5	43/49 (88%)	42 (98%)	1 (2%)	50 72
7	6	46/54 (85%)	43 (94%)	3 (6%)	17 48
8	7	259/262 (99%)	258 (100%)	1 (0%)	91 95
9	8	30/135 (22%)	30 (100%)	0	100 100
10	A	160/162 (99%)	159 (99%)	1 (1%)	86 92
12	Aa	694/714 (97%)	691 (100%)	3 (0%)	91 95
13	B	125/146 (86%)	123 (98%)	2 (2%)	62 79
15	C	150/151 (99%)	150 (100%)	0	100 100
17	D	143/154 (93%)	142 (99%)	1 (1%)	84 91
18	DD	167/254 (66%)	167 (100%)	0	100 100
19	E	156/156 (100%)	156 (100%)	0	100 100
20	EE	193/196 (98%)	193 (100%)	0	100 100
21	Ee	129/136 (95%)	129 (100%)	0	100 100
22	F	136/137 (99%)	135 (99%)	1 (1%)	84 91
23	FF	320/323 (99%)	319 (100%)	1 (0%)	92 96
24	G	84/107 (78%)	84 (100%)	0	100 100
25	GG	288/289 (100%)	285 (99%)	3 (1%)	76 86
26	H	101/105 (96%)	101 (100%)	0	100 100
27	HH	244/245 (100%)	244 (100%)	0	100 100
28	I	55/129 (43%)	54 (98%)	1 (2%)	59 77
29	II	133/153 (87%)	133 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	J	104/118 (88%)	103 (99%)	1 (1%)	76 86
31	JJ	186/205 (91%)	186 (100%)	0	100 100
32	K	109/110 (99%)	108 (99%)	1 (1%)	78 88
33	KK	187/208 (90%)	187 (100%)	0	100 100
34	L	115/116 (99%)	115 (100%)	0	100 100
35	LL	171/171 (100%)	171 (100%)	0	100 100
36	M	118/119 (99%)	118 (100%)	0	100 100
37	MM	184/187 (98%)	183 (100%)	1 (0%)	88 94
38	N	46/47 (98%)	46 (100%)	0	100 100
39	NN	147/150 (98%)	147 (100%)	0	100 100
40	O	81/88 (92%)	81 (100%)	0	100 100
41	OO	154/159 (97%)	153 (99%)	1 (1%)	86 92
42	P	94/97 (97%)	93 (99%)	1 (1%)	73 85
43	PP	107/109 (98%)	107 (100%)	0	100 100
44	Q	109/111 (98%)	108 (99%)	1 (1%)	78 88
45	QQ	175/176 (99%)	175 (100%)	0	100 100
46	R	90/91 (99%)	90 (100%)	0	100 100
47	S	94/103 (91%)	94 (100%)	0	100 100
48	T	104/105 (99%)	103 (99%)	1 (1%)	76 86
49	U	81/82 (99%)	81 (100%)	0	100 100
50	V	69/71 (97%)	67 (97%)	2 (3%)	42 67
51	W	68/69 (99%)	68 (100%)	0	100 100
52	X	45/46 (98%)	45 (100%)	0	100 100
53	Y	47/116 (40%)	46 (98%)	1 (2%)	53 74
54	Z	23/23 (100%)	23 (100%)	0	100 100
55	a	87/91 (96%)	86 (99%)	1 (1%)	73 85
56	b	71/72 (99%)	70 (99%)	1 (1%)	67 81
58	d	165/210 (79%)	165 (100%)	0	100 100
59	e	189/224 (84%)	187 (99%)	2 (1%)	73 85
60	f	176/205 (86%)	175 (99%)	1 (1%)	86 92
61	g	145/195 (74%)	142 (98%)	3 (2%)	53 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	h	220/222 (99%)	219 (100%)	1 (0%)	88 94
63	i	172/191 (90%)	171 (99%)	1 (1%)	86 92
64	j	188/201 (94%)	182 (97%)	6 (3%)	39 65
65	k	165/170 (97%)	164 (99%)	1 (1%)	86 92
66	l	146/161 (91%)	146 (100%)	0	100 100
67	m	158/166 (95%)	157 (99%)	1 (1%)	86 92
68	n	32/98 (33%)	32 (100%)	0	100 100
69	o	127/137 (93%)	125 (98%)	2 (2%)	62 79
70	p	127/128 (99%)	127 (100%)	0	100 100
71	q	81/105 (77%)	81 (100%)	0	100 100
72	r	77/118 (65%)	76 (99%)	1 (1%)	69 82
73	s	113/119 (95%)	110 (97%)	3 (3%)	44 69
74	t	105/124 (85%)	104 (99%)	1 (1%)	76 86
75	u	128/129 (99%)	127 (99%)	1 (1%)	81 89
76	v	115/116 (99%)	115 (100%)	0	100 100
77	w	94/114 (82%)	92 (98%)	2 (2%)	53 74
78	x	74/74 (100%)	74 (100%)	0	100 100
79	y	110/111 (99%)	109 (99%)	1 (1%)	78 88
80	z	119/120 (99%)	117 (98%)	2 (2%)	60 78
All	All	9930/10969 (90%)	9868 (99%)	62 (1%)	86 92

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	112	LYS
2	1	77	ARG
5	4	49	ARG
6	5	19	ARG
7	6	10	ARG
7	6	29	LYS
7	6	31	LYS
8	7	127	ARG
10	A	14	HIS
12	Aa	271	ARG
12	Aa	437	MET

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Mol	Chain	Res	Type
12	Aa	555	LYS
13	B	23	ARG
13	B	138	LYS
17	D	166	ASN
22	F	83	ARG
23	FF	104	THR
25	GG	3	ARG
25	GG	43	ASN
25	GG	138	ARG
28	I	47	ARG
30	J	97	LYS
32	K	3	LYS
37	MM	211	ARG
41	OO	45	LYS
42	P	18	LYS
44	Q	61	LYS
48	T	108	GLN
50	V	57	HIS
50	V	65	ARG
53	Y	106	ARG
55	a	71	ARG
56	b	24	ARG
59	e	50	LYS
59	e	214	LYS
60	f	141	ARG
61	g	8	LYS
61	g	75	LYS
61	g	151	LYS
62	h	108	ARG
63	i	222	LYS
64	j	4	ASN
64	j	31	ARG
64	j	98	ARG
64	j	164	LYS
64	j	182	GLN
64	j	214	LYS
65	k	107	ARG
67	m	138	LYS
69	o	36	LYS
69	o	67	ARG
72	r	127	ARG
73	s	26	LYS

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Mol	Chain	Res	Type
73	s	114	ARG
73	s	123	ARG
74	t	59	LYS
75	u	41	ARG
77	w	21	LYS
77	w	52	LYS
79	y	3	ARG
80	z	31	LYS
80	z	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	43	ASN
5	4	27	GLN
8	7	64	HIS
8	7	147	HIS
8	7	224	ASN
12	Aa	644	ASN
13	B	137	ASN
15	C	45	ASN
17	D	75	HIS
17	D	150	GLN
20	EE	211	HIS
22	F	54	HIS
23	FF	165	GLN
23	FF	212	ASN
25	GG	307	GLN
25	GG	311	HIS
25	GG	316	ASN
26	H	98	ASN
29	II	172	HIS
31	JJ	194	HIS
31	JJ	197	GLN
33	KK	138	HIS
34	L	78	ASN
37	MM	59	GLN
37	MM	208	ASN
39	NN	47	GLN
44	Q	49	ASN
46	R	26	ASN
47	S	108	GLN

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Mol	Chain	Res	Type
49	U	12	ASN
52	X	19	GLN
56	b	33	GLN
61	g	74	GLN
61	g	111	ASN
62	h	259	GLN
63	i	128	ASN
63	i	170	GLN
64	j	199	GLN
68	n	58	GLN
70	p	78	ASN
72	r	82	ASN
73	s	139	GLN
74	t	48	ASN
75	u	6	GLN
76	v	16	ASN
76	v	101	ASN
79	y	16	ASN
80	z	18	HIS
80	z	99	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	636 (19%)	21 (0%)
14	BB	120/121 (99%)	18 (15%)	1 (0%)
16	CC	157/158 (99%)	28 (17%)	1 (0%)
57	c	1593/1800 (88%)	468 (29%)	0
All	All	5063/5475 (92%)	1150 (22%)	23 (0%)

All (1150) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	4	U
11	AA	6	A
11	AA	12	A
11	AA	14	U
11	AA	26	A
11	AA	40	A
11	AA	43	A
11	AA	49	A

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Mol	Chain	Res	Type
11	AA	60	A
11	AA	63	A
11	AA	65	A
11	AA	66	A
11	AA	73	C
11	AA	77	A
11	AA	85	A
11	AA	92	G
11	AA	96	G
11	AA	109	A
11	AA	110	G
11	AA	111	C
11	AA	113	C
11	AA	116	A
11	AA	118	U
11	AA	120	G
11	AA	122	A
11	AA	135	C
11	AA	136	G
11	AA	142	C
11	AA	150	A
11	AA	156	G
11	AA	157	A
11	AA	162	G
11	AA	165	A
11	AA	170	G
11	AA	172	G
11	AA	173	G
11	AA	182	U
11	AA	190	U
11	AA	191	U
11	AA	200	C
11	AA	212	G
11	AA	219	A
11	AA	220	G
11	AA	227	G
11	AA	243	G
11	AA	247	C
11	AA	248	U
11	AA	249	U
11	AA	252	U
11	AA	253	A

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Mol	Chain	Res	Type
11	AA	263	C
11	AA	266	A
11	AA	268	A
11	AA	269	G
11	AA	286	U
11	AA	295	A
11	AA	305	U
11	AA	315	C
11	AA	321	C
11	AA	329	U
11	AA	346	C
11	AA	360	G
11	AA	362	U
11	AA	374	A
11	AA	376	G
11	AA	397	A
11	AA	398	A
11	AA	399	A
11	AA	401	U
11	AA	402	A
11	AA	403	C
11	AA	420	G
11	AA	421	G
11	AA	422	A
11	AA	502	U
11	AA	503	C
11	AA	519	A
11	AA	520	U
11	AA	521	A
11	AA	532	A
11	AA	534	U
11	AA	543	C
11	AA	552	G
11	AA	556	U
11	AA	557	A
11	AA	558	U
11	AA	559	A
11	AA	589	A
11	AA	592	A
11	AA	597	G
11	AA	601	U
11	AA	602	A

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Mol	Chain	Res	Type
11	AA	603	A
11	AA	604	G
11	AA	607	A
11	AA	611	A
11	AA	612	U
11	AA	620	U
11	AA	621	A
11	AA	636	C
11	AA	637	C
11	AA	638	C
11	AA	645	1MA
11	AA	649	A2M
11	AA	655	C
11	AA	660	A
11	AA	662	U
11	AA	667	C
11	AA	677	A
11	AA	678	G
11	AA	681	U
11	AA	690	A
11	AA	691	A
11	AA	705	A
11	AA	719	U
11	AA	737	G
11	AA	750	G
11	AA	758	C
11	AA	761	A
11	AA	766	U
11	AA	767	U
11	AA	780	A
11	AA	781	G
11	AA	784	A
11	AA	785	G
11	AA	786	A
11	AA	790	U
11	AA	799	G
11	AA	806	A
11	AA	807	A2M
11	AA	816	A
11	AA	817	A2M
11	AA	826	G
11	AA	830	A

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Mol	Chain	Res	Type
11	AA	835	G
11	AA	849	C
11	AA	857	G
11	AA	861	C
11	AA	874	U
11	AA	875	G
11	AA	879	U
11	AA	880	G
11	AA	890	C
11	AA	896	A
11	AA	907	G
11	AA	908	OMG
11	AA	910	G
11	AA	914	A
11	AA	916	G
11	AA	917	A
11	AA	921	A
11	AA	923	C
11	AA	924	G
11	AA	926	A
11	AA	937	G
11	AA	939	U
11	AA	943	U
11	AA	944	C
11	AA	953	G
11	AA	959	C
11	AA	960	U
11	AA	961	C
11	AA	962	A
11	AA	974	G
11	AA	979	U
11	AA	980	A
11	AA	981	U
11	AA	984	G
11	AA	988	U
11	AA	1000	C
11	AA	1006	A
11	AA	1013	G
11	AA	1015	U
11	AA	1017	C
11	AA	1018	G
11	AA	1025	A

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Mol	Chain	Res	Type
11	AA	1026	A
11	AA	1027	A
11	AA	1028	U
11	AA	1034	U
11	AA	1036	A
11	AA	1037	C
11	AA	1038	C
11	AA	1045	C
11	AA	1047	A
11	AA	1064	A
11	AA	1072	G
11	AA	1075	A
11	AA	1081	U
11	AA	1087	G
11	AA	1096	U
11	AA	1097	G
11	AA	1098	A
11	AA	1103	A
11	AA	1111	U
11	AA	1117	G
11	AA	1131	G
11	AA	1140	G
11	AA	1143	A
11	AA	1155	C
11	AA	1159	A
11	AA	1177	G
11	AA	1178	G
11	AA	1179	A
11	AA	1180	A
11	AA	1181	U
11	AA	1182	A
11	AA	1191	U
11	AA	1193	A
11	AA	1196	C
11	AA	1201	C
11	AA	1208	U
11	AA	1209	G
11	AA	1221	A
11	AA	1222	G
11	AA	1235	U
11	AA	1236	G
11	AA	1237	G

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Mol	Chain	Res	Type
11	AA	1240	A
11	AA	1244	A
11	AA	1245	A
11	AA	1246	G
11	AA	1253	U
11	AA	1258	U
11	AA	1260	A
11	AA	1263	A
11	AA	1265	U
11	AA	1272	C
11	AA	1286	A
11	AA	1287	A
11	AA	1294	A
11	AA	1302	A
11	AA	1307	G
11	AA	1308	A
11	AA	1325	U
11	AA	1330	A
11	AA	1332	A
11	AA	1345	G
11	AA	1348	U
11	AA	1349	G
11	AA	1352	A
11	AA	1355	A
11	AA	1357	G
11	AA	1363	A
11	AA	1366	A
11	AA	1367	G
11	AA	1386	A
11	AA	1392	G
11	AA	1399	A
11	AA	1400	G
11	AA	1408	G
11	AA	1417	G
11	AA	1418	A
11	AA	1425	U
11	AA	1434	G
11	AA	1436	U
11	AA	1437	OMC
11	AA	1443	G
11	AA	1446	A
11	AA	1450	OMG

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Mol	Chain	Res	Type
11	AA	1455	U
11	AA	1469	C
11	AA	1483	G
11	AA	1484	U
11	AA	1487	G
11	AA	1495	U
11	AA	1508	C
11	AA	1510	G
11	AA	1514	G
11	AA	1523	U
11	AA	1525	G
11	AA	1527	C
11	AA	1528	G
11	AA	1539	A
11	AA	1542	G
11	AA	1556	C
11	AA	1558	A
11	AA	1560	G
11	AA	1561	G
11	AA	1562	C
11	AA	1563	C
11	AA	1568	U
11	AA	1569	U
11	AA	1570	U
11	AA	1571	A
11	AA	1573	G
11	AA	1575	A
11	AA	1578	C
11	AA	1579	C
11	AA	1581	C
11	AA	1582	C
11	AA	1583	A
11	AA	1587	A
11	AA	1589	A
11	AA	1593	A
11	AA	1605	A
11	AA	1621	A
11	AA	1629	U
11	AA	1630	U
11	AA	1631	C
11	AA	1637	A
11	AA	1638	A

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Mol	Chain	Res	Type
11	AA	1642	A
11	AA	1643	A
11	AA	1645	U
11	AA	1647	A
11	AA	1657	C
11	AA	1683	A
11	AA	1688	U
11	AA	1694	U
11	AA	1724	U
11	AA	1741	A
11	AA	1750	A
11	AA	1751	G
11	AA	1756	C
11	AA	1759	C
11	AA	1762	C
11	AA	1763	U
11	AA	1765	U
11	AA	1767	C
11	AA	1769	G
11	AA	1773	C
11	AA	1797	A
11	AA	1808	G
11	AA	1814	A
11	AA	1815	U
11	AA	1816	A
11	AA	1817	G
11	AA	1820	U
11	AA	1821	U
11	AA	1835	A
11	AA	1842	A
11	AA	1848	G
11	AA	1850	A
11	AA	1854	C
11	AA	1866	C
11	AA	1878	G
11	AA	1879	A
11	AA	1880	U
11	AA	1893	A
11	AA	1905	G
11	AA	1906	G
11	AA	1912	U
11	AA	1935	G

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Mol	Chain	Res	Type
11	AA	1943	C
11	AA	1948	G
11	AA	2101	C
11	AA	2102	U
11	AA	2111	G
11	AA	2112	U
11	AA	2114	C
11	AA	2122	G
11	AA	2131	A
11	AA	2132	C
11	AA	2155	G
11	AA	2158	A
11	AA	2165	G
11	AA	2167	A
11	AA	2168	A
11	AA	2169	G
11	AA	2170	U
11	AA	2171	G
11	AA	2176	U
11	AA	2188	A
11	AA	2194	G
11	AA	2205	U
11	AA	2206	G
11	AA	2208	A
11	AA	2210	G
11	AA	2213	A
11	AA	2223	A
11	AA	2225	U
11	AA	2244	A
11	AA	2249	G
11	AA	2256	A2M
11	AA	2257	C
11	AA	2258	U
11	AA	2262	A
11	AA	2265	C
11	AA	2272	G
11	AA	2273	G
11	AA	2280	A2M
11	AA	2281	A2M
11	AA	2282	U
11	AA	2286	U
11	AA	2297	U

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Mol	Chain	Res	Type
11	AA	2298	U
11	AA	2307	G
11	AA	2309	A
11	AA	2313	A
11	AA	2315	G
11	AA	2320	A
11	AA	2336	U
11	AA	2337	OMC
11	AA	2355	G
11	AA	2363	A
11	AA	2373	A
11	AA	2374	C
11	AA	2375	G
11	AA	2383	C
11	AA	2388	U
11	AA	2393	G
11	AA	2397	A
11	AA	2402	A
11	AA	2403	G
11	AA	2404	A
11	AA	2411	U
11	AA	2418	G
11	AA	2419	A
11	AA	2434	U
11	AA	2435	G
11	AA	2440	G
11	AA	2447	A
11	AA	2448	G
11	AA	2453	U
11	AA	2454	G
11	AA	2458	A
11	AA	2459	A
11	AA	2460	U
11	AA	2461	A
11	AA	2462	A
11	AA	2463	G
11	AA	2464	U
11	AA	2465	G
11	AA	2466	G
11	AA	2468	A
11	AA	2470	C
11	AA	2472	U

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Mol	Chain	Res	Type
11	AA	2474	G
11	AA	2475	G
11	AA	2476	C
11	AA	2477	G
11	AA	2478	C
11	AA	2480	A
11	AA	2481	G
11	AA	2486	A
11	AA	2487	U
11	AA	2488	A
11	AA	2489	C
11	AA	2490	C
11	AA	2491	A
11	AA	2492	C
11	AA	2494	A
11	AA	2496	C
11	AA	2501	U
11	AA	2502	A
11	AA	2503	G
11	AA	2511	A
11	AA	2514	U
11	AA	2515	A
11	AA	2522	G
11	AA	2523	A
11	AA	2524	A
11	AA	2525	G
11	AA	2526	C
11	AA	2529	A
11	AA	2532	U
11	AA	2539	C
11	AA	2540	A
11	AA	2541	U
11	AA	2542	U
11	AA	2547	A
11	AA	2549	G
11	AA	2552	C
11	AA	2554	A
11	AA	2555	G
11	AA	2560	C
11	AA	2561	A
11	AA	2569	A
11	AA	2570	U

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Mol	Chain	Res	Type
11	AA	2571	U
11	AA	2572	C
11	AA	2573	G
11	AA	2585	G
11	AA	2587	U
11	AA	2593	A
11	AA	2594	C
11	AA	2602	G
11	AA	2606	G
11	AA	2607	G
11	AA	2614	G
11	AA	2617	U
11	AA	2648	G
11	AA	2652	U
11	AA	2656	A
11	AA	2657	A
11	AA	2672	G
11	AA	2674	A
11	AA	2677	G
11	AA	2678	A
11	AA	2680	A
11	AA	2681	U
11	AA	2689	A
11	AA	2691	A
11	AA	2696	A
11	AA	2704	A
11	AA	2713	U
11	AA	2714	G
11	AA	2728	G
11	AA	2729	OMU
11	AA	2737	C
11	AA	2747	A
11	AA	2753	G
11	AA	2762	A
11	AA	2772	C
11	AA	2777	G
11	AA	2780	A
11	AA	2786	G
11	AA	2795	U
11	AA	2796	G
11	AA	2799	A
11	AA	2800	G

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Mol	Chain	Res	Type
11	AA	2801	A
11	AA	2802	A
11	AA	2803	A
11	AA	2804	A
11	AA	2808	A
11	AA	2810	C
11	AA	2817	A
11	AA	2834	G
11	AA	2842	U
11	AA	2844	C
11	AA	2845	A
11	AA	2858	U
11	AA	2860	U
11	AA	2861	U
11	AA	2867	C
11	AA	2872	A
11	AA	2875	U
11	AA	2887	A
11	AA	2894	C
11	AA	2899	C
11	AA	2900	A
11	AA	2918	G
11	AA	2922	OMG
11	AA	2923	U
11	AA	2934	A
11	AA	2935	U
11	AA	2936	A
11	AA	2938	G
11	AA	2941	A
11	AA	2945	G
11	AA	2946	A2M
11	AA	2947	G
11	AA	2951	G
11	AA	2966	G
11	AA	2971	A
11	AA	2972	G
11	AA	2983	C
11	AA	2990	G
11	AA	2996	U
11	AA	2997	G
11	AA	3003	G
11	AA	3005	A

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Mol	Chain	Res	Type
11	AA	3012	A
11	AA	3023	U
11	AA	3030	G
11	AA	3055	U
11	AA	3056	U
11	AA	3059	G
11	AA	3069	G
11	AA	3074	G
11	AA	3078	U
11	AA	3080	G
11	AA	3091	A
11	AA	3092	C
11	AA	3093	C
11	AA	3094	A
11	AA	3101	G
11	AA	3104	U
11	AA	3109	G
11	AA	3116	G
11	AA	3117	C
11	AA	3122	A
11	AA	3130	A
11	AA	3131	U
11	AA	3139	A
11	AA	3142	A
11	AA	3143	C
11	AA	3151	U
11	AA	3153	U
11	AA	3154	C
11	AA	3155	U
11	AA	3156	U
11	AA	3157	U
11	AA	3168	A
11	AA	3170	A
11	AA	3172	A
11	AA	3173	G
11	AA	3176	G
11	AA	3179	U
11	AA	3181	C
11	AA	3186	A
11	AA	3187	A
11	AA	3196	U
11	AA	3205	G

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Mol	Chain	Res	Type
11	AA	3207	U
11	AA	3217	C
11	AA	3218	A
11	AA	3219	G
11	AA	3230	G
11	AA	3238	G
11	AA	3244	A
11	AA	3246	G
11	AA	3247	G
11	AA	3260	G
11	AA	3263	G
11	AA	3273	A
11	AA	3275	U
11	AA	3276	G
11	AA	3277	U
11	AA	3281	U
11	AA	3288	G
11	AA	3294	A
11	AA	3304	U
11	AA	3307	A
11	AA	3313	U
11	AA	3316	A
11	AA	3320	A
11	AA	3334	U
11	AA	3335	A
11	AA	3341	U
11	AA	3345	G
11	AA	3348	G
11	AA	3349	C
11	AA	3350	C
11	AA	3351	U
11	AA	3352	U
11	AA	3353	G
11	AA	3358	U
11	AA	3359	A
11	AA	3369	G
11	AA	3378	C
11	AA	3389	U
11	AA	3390	G
11	AA	3396	U
14	BB	7	G
14	BB	11	A

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Mol	Chain	Res	Type
14	BB	29	C
14	BB	33	U
14	BB	41	G
14	BB	42	A
14	BB	45	A
14	BB	47	C
14	BB	52	G
14	BB	54	U
14	BB	55	A
14	BB	65	G
14	BB	73	C
14	BB	74	C
14	BB	76	A
14	BB	93	C
14	BB	112	G
14	BB	121	U
16	CC	23	U
16	CC	34	U
16	CC	35	C
16	CC	37	A
16	CC	39	G
16	CC	51	G
16	CC	52	A
16	CC	59	A
16	CC	62	C
16	CC	63	G
16	CC	82	U
16	CC	83	C
16	CC	84	C
16	CC	85	G
16	CC	86	U
16	CC	87	G
16	CC	90	U
16	CC	91	C
16	CC	95	G
16	CC	100	U
16	CC	102	U
16	CC	104	A
16	CC	106	C
16	CC	113	U
16	CC	125	U
16	CC	126	A

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Mol	Chain	Res	Type
16	CC	138	A
16	CC	158	U
57	c	2	A
57	c	4	C
57	c	26	A
57	c	28	A2M
57	c	34	G
57	c	42	G
57	c	43	A
57	c	45	U
57	c	47	A
57	c	50	C
57	c	61	A
57	c	63	G
57	c	67	A
57	c	68	A
57	c	69	G
57	c	72	A
57	c	78	A
57	c	80	A
57	c	94	U
57	c	111	U
57	c	114	C
57	c	115	G
57	c	116	U
57	c	127	G
57	c	131	C
57	c	137	U
57	c	140	A
57	c	146	U
57	c	152	U
57	c	154	G
57	c	165	G
57	c	166	C
57	c	168	A
57	c	170	U
57	c	178	U
57	c	184	C
57	c	204	G
57	c	212	U
57	c	213	A
57	c	214	G

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Mol	Chain	Res	Type
57	c	246	G
57	c	247	A
57	c	248	U
57	c	249	U
57	c	253	A
57	c	254	A
57	c	256	A
57	c	257	A
57	c	258	C
57	c	260	U
57	c	261	U
57	c	262	U
57	c	265	A
57	c	267	U
57	c	272	U
57	c	277	U
57	c	278	U
57	c	279	G
57	c	280	U
57	c	283	U
57	c	285	G
57	c	287	G
57	c	299	A
57	c	302	U
57	c	313	U
57	c	314	C
57	c	316	A
57	c	320	U
57	c	321	C
57	c	322	G
57	c	333	A
57	c	337	G
57	c	359	A
57	c	361	C
57	c	373	G
57	c	378	A
57	c	400	A
57	c	401	A
57	c	402	C
57	c	404	G
57	c	414	OMC
57	c	417	A

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Mol	Chain	Res	Type
57	c	420	A2M
57	c	423	G
57	c	424	C
57	c	426	G
57	c	428	A
57	c	434	G
57	c	435	C
57	c	439	U
57	c	444	C
57	c	448	C
57	c	454	U
57	c	455	C
57	c	460	A
57	c	468	A
57	c	475	A
57	c	477	A
57	c	479	C
57	c	481	A
57	c	484	C
57	c	485	A
57	c	503	G
57	c	504	U
57	c	506	A
57	c	507	U
57	c	508	U
57	c	511	A
57	c	514	G
57	c	515	A
57	c	518	A
57	c	520	A
57	c	524	U
57	c	525	A
57	c	526	A
57	c	527	A
57	c	538	A
57	c	539	G
57	c	541	A2M
57	c	542	A
57	c	545	A
57	c	551	G
57	c	555	A
57	c	557	G

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Mol	Chain	Res	Type
57	c	559	C
57	c	562	OMG
57	c	563	U
57	c	565	C
57	c	566	C
57	c	568	G
57	c	577	G
57	c	578	OMU
57	c	579	A
57	c	582	U
57	c	594	A
57	c	611	U
57	c	617	U
57	c	619	A2M
57	c	620	A
57	c	623	A
57	c	624	G
57	c	639	U
57	c	643	G
57	c	644	C
57	c	645	C
57	c	649	U
57	c	650	U
57	c	651	G
57	c	686	C
57	c	687	G
57	c	688	G
57	c	691	C
57	c	692	C
57	c	695	U
57	c	696	C
57	c	743	U
57	c	745	U
57	c	753	A
57	c	760	A
57	c	763	G
57	c	765	G
57	c	766	U
57	c	775	G
57	c	778	G
57	c	780	A
57	c	781	U

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Mol	Chain	Res	Type
57	c	782	U
57	c	783	G
57	c	784	C
57	c	789	A
57	c	793	A
57	c	794	U
57	c	795	U
57	c	803	A
57	c	806	A
57	c	809	A
57	c	810	G
57	c	812	A
57	c	814	A
57	c	819	G
57	c	820	U
57	c	852	C
57	c	853	G
57	c	854	U
57	c	856	A
57	c	859	A
57	c	861	U
57	c	862	A
57	c	863	A
57	c	873	U
57	c	895	G
57	c	896	U
57	c	897	C
57	c	898	A
57	c	906	A
57	c	913	G
57	c	914	G
57	c	915	A
57	c	916	U
57	c	918	U
57	c	919	A
57	c	933	A
57	c	935	U
57	c	945	U
57	c	951	A
57	c	960	U
57	c	966	A
57	c	970	A

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Mol	Chain	Res	Type
57	c	987	G
57	c	988	A
57	c	992	A
57	c	996	U
57	c	999	U
57	c	1000	C
57	c	1001	A
57	c	1002	G
57	c	1004	U
57	c	1026	A
57	c	1027	A
57	c	1028	C
57	c	1031	U
57	c	1039	A
57	c	1041	G
57	c	1043	A
57	c	1049	U
57	c	1052	U
57	c	1053	G
57	c	1059	U
57	c	1060	U
57	c	1061	A
57	c	1063	U
57	c	1070	C
57	c	1072	C
57	c	1076	A
57	c	1081	A
57	c	1082	C
57	c	1083	G
57	c	1092	A
57	c	1093	A
57	c	1097	U
57	c	1098	U
57	c	1100	G
57	c	1111	G
57	c	1113	A
57	c	1138	A
57	c	1146	G
57	c	1150	G
57	c	1158	C
57	c	1162	C
57	c	1164	G

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Mol	Chain	Res	Type
57	c	1167	G
57	c	1171	A
57	c	1174	C
57	c	1182	U
57	c	1183	A
57	c	1185	U
57	c	1187	U
57	c	1192	C
57	c	1194	A
57	c	1196	A
57	c	1199	G
57	c	1200	G
57	c	1201	G
57	c	1202	A
57	c	1203	A
57	c	1204	A
57	c	1205	C
57	c	1207	C
57	c	1212	G
57	c	1214	U
57	c	1217	A
57	c	1218	G
57	c	1221	A
57	c	1222	C
57	c	1223	A
57	c	1225	U
57	c	1226	A
57	c	1227	A
57	c	1228	G
57	c	1229	G
57	c	1230	A
57	c	1237	G
57	c	1238	A
57	c	1241	G
57	c	1243	G
57	c	1244	A
57	c	1245	G
57	c	1246	C
57	c	1248	C
57	c	1249	U
57	c	1250	U
57	c	1251	U

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Mol	Chain	Res	Type
57	c	1252	C
57	c	1256	A
57	c	1257	U
57	c	1258	U
57	c	1259	U
57	c	1261	G
57	c	1270	G
57	c	1274	C
57	c	1276	U
57	c	1284	C
57	c	1285	U
57	c	1297	G
57	c	1305	U
57	c	1307	U
57	c	1314	U
57	c	1315	U
57	c	1316	G
57	c	1321	A
57	c	1324	G
57	c	1325	A
57	c	1335	U
57	c	1336	A
57	c	1338	C
57	c	1339	C
57	c	1340	U
57	c	1341	A
57	c	1345	A
57	c	1346	A
57	c	1347	U
57	c	1350	U
57	c	1352	G
57	c	1353	U
57	c	1355	C
57	c	1356	U
57	c	1357	A
57	c	1358	G
57	c	1361	U
57	c	1362	U
57	c	1363	U
57	c	1364	G
57	c	1365	C
57	c	1368	G

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Mol	Chain	Res	Type
57	c	1369	U
57	c	1370	U
57	c	1371	A
57	c	1372	U
57	c	1373	C
57	c	1374	C
57	c	1375	A
57	c	1376	C
57	c	1377	U
57	c	1378	U
57	c	1380	U
57	c	1388	A
57	c	1390	U
57	c	1397	U
57	c	1398	U
57	c	1402	G
57	c	1405	G
57	c	1408	G
57	c	1410	A
57	c	1411	A
57	c	1412	G
57	c	1413	U
57	c	1414	U
57	c	1415	U
57	c	1421	A
57	c	1425	A
57	c	1427	A
57	c	1428	OMG
57	c	1432	U
57	c	1433	G
57	c	1436	A
57	c	1444	A
57	c	1445	G
57	c	1447	C
57	c	1453	G
57	c	1457	C
57	c	1458	G
57	c	1459	C
57	c	1463	C
57	c	1464	G
57	c	1466	G
57	c	1468	U

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Mol	Chain	Res	Type
57	c	1474	G
57	c	1477	G
57	c	1478	G
57	c	1480	G
57	c	1482	C
57	c	1483	A
57	c	1488	G
57	c	1489	U
57	c	1490	C
57	c	1491	U
57	c	1492	A
57	c	1496	U
57	c	1500	C
57	c	1505	A
57	c	1506	G
57	c	1515	A
57	c	1516	A
57	c	1518	C
57	c	1524	A
57	c	1525	A
57	c	1527	C
57	c	1531	G
57	c	1535	U
57	c	1536	G
57	c	1537	C
57	c	1540	G
57	c	1542	G
57	c	1546	G
57	c	1548	G
57	c	1556	A
57	c	1557	U
57	c	1559	A
57	c	1561	U
57	c	1564	U
57	c	1565	C
57	c	1567	U
57	c	1568	C
57	c	1570	A
57	c	1572	OMG
57	c	1573	A
57	c	1583	A
57	c	1591	C

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Mol	Chain	Res	Type
57	c	1592	A
57	c	1594	G
57	c	1596	C
57	c	1600	A
57	c	1601	G
57	c	1602	C
57	c	1603	U
57	c	1604	U
57	c	1605	G
57	c	1606	C
57	c	1607	G
57	c	1609	U
57	c	1611	A
57	c	1614	A
57	c	1616	G
57	c	1618	C
57	c	1619	C
57	c	1631	A
57	c	1633	A
57	c	1634	C
57	c	1635	A
57	c	1642	G
57	c	1651	A
57	c	1657	U
57	c	1658	G
57	c	1678	A
57	c	1680	G
57	c	1681	A
57	c	1683	C
57	c	1684	U
57	c	1685	G
57	c	1686	C
57	c	1687	U
57	c	1717	G
57	c	1730	A
57	c	1756	A
57	c	1757	G
57	c	1760	G
57	c	1762	A
57	c	1766	A
57	c	1769	U
57	c	1770	U

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Mol	Chain	Res	Type
57	c	1780	G
57	c	1792	G
57	c	1793	G
57	c	1794	A
57	c	1795	U
57	c	1796	C
57	c	1798	U
57	c	1799	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	601	U
11	AA	619	A
11	AA	916	G
11	AA	978	G
11	AA	1016	C
11	AA	1033	U
11	AA	1348	U
11	AA	1562	C
11	AA	1904	C
11	AA	2101	C
11	AA	2167	A
11	AA	2418	G
11	AA	2458	A
11	AA	2467	G
11	AA	2490	C
11	AA	2500	A
11	AA	2501	U
11	AA	2570	U
11	AA	2971	A
11	AA	3121	U
11	AA	3206	C
14	BB	72	A
16	CC	89	A

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

67 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	$\#\|Z\| > 2$
11	OMG	AA	2791	11	18,26,27	1.19	2 (11%)	19,38,41	0.83	1 (5%)
57	OMG	c	1428	57	18,26,27	1.14	2 (11%)	19,38,41	0.82	1 (5%)
11	A2M	AA	1449	82,11	18,25,26	3.63	8 (44%)	18,36,39	3.42	4 (22%)
57	A2M	c	100	82,57	18,25,26	3.63	8 (44%)	18,36,39	3.31	3 (16%)
11	A2M	AA	2256	11	18,25,26	3.58	8 (44%)	18,36,39	3.57	5 (27%)
11	OMG	AA	2288	11	18,26,27	1.18	2 (11%)	19,38,41	0.79	1 (5%)
57	OMG	c	1572	57	18,26,27	1.17	2 (11%)	19,38,41	0.87	1 (5%)
57	4AC	c	1773	57	21,24,25	3.47	10 (47%)	29,34,37	1.61	5 (17%)
11	OMG	AA	1450	11	18,26,27	1.14	2 (11%)	19,38,41	0.80	1 (5%)
11	OMU	AA	1888	11	19,22,23	3.03	8 (42%)	26,31,34	1.72	5 (19%)
11	A2M	AA	2220	11	18,25,26	3.59	8 (44%)	18,36,39	3.45	4 (22%)
57	OMG	c	562	57	18,26,27	1.24	2 (11%)	19,38,41	0.80	0
11	UR3	AA	2634	11	19,22,23	2.76	7 (36%)	26,32,35	1.25	1 (3%)
57	OMC	c	414	57	19,22,23	0.62	0	26,31,34	1.08	2 (7%)
11	5MC	AA	2278	82,11	18,22,23	0.59	0	26,32,35	0.67	0
11	OMC	AA	1437	82,11	19,22,23	0.62	0	26,31,34	1.34	2 (7%)
11	OMU	AA	2347	11	19,22,23	3.00	8 (42%)	26,31,34	1.75	4 (15%)
11	OMC	AA	2948	11	19,22,23	0.61	0	26,31,34	1.03	2 (7%)
12	DDE	Aa	699	12	14,20,21	1.02	1 (7%)	14,28,30	1.17	2 (14%)
11	OMU	AA	898	11	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
11	OMG	AA	2922	11	18,26,27	1.15	2 (11%)	19,38,41	0.87	1 (5%)
11	OMC	AA	2337	11	19,22,23	0.60	0	26,31,34	0.80	1 (3%)
11	OMC	AA	2197	11,83	19,22,23	0.54	0	26,31,34	0.66	0
11	OMU	AA	2421	11	19,22,23	3.02	8 (42%)	26,31,34	1.70	5 (19%)
11	A2M	AA	2280	11	18,25,26	3.63	8 (44%)	18,36,39	3.34	4 (22%)
57	A2M	c	28	80,57	18,25,26	3.62	9 (50%)	18,36,39	3.36	4 (22%)
11	A2M	AA	1133	82,11	18,25,26	3.64	8 (44%)	18,36,39	3.32	3 (16%)
57	4AC	c	1280	57	21,24,25	3.54	10 (47%)	29,34,37	1.77	7 (24%)
57	G7M	c	1575	57	20,26,27	2.46	7 (35%)	17,39,42	1.15	1 (5%)
11	A2M	AA	2640	11	18,25,26	3.58	8 (44%)	18,36,39	3.42	4 (22%)
11	OMU	AA	2724	11	19,22,23	3.02	8 (42%)	26,31,34	1.75	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OMC	AA	2959	11	19,22,23	0.55	0	26,31,34	0.68	0
11	1MA	AA	2142	82,11	16,25,26	0.95	2 (12%)	18,37,40	1.10	2 (11%)
11	OMG	AA	805	11	18,26,27	1.16	2 (11%)	19,38,41	0.83	1 (5%)
11	OMC	AA	650	11	19,22,23	0.55	0	26,31,34	0.80	1 (3%)
11	A2M	AA	2281	11	18,25,26	3.69	9 (50%)	18,36,39	3.41	4 (22%)
11	OMG	AA	2793	11	18,26,27	1.21	2 (11%)	19,38,41	0.76	1 (5%)
11	A2M	AA	876	11	18,25,26	3.62	9 (50%)	18,36,39	3.40	4 (22%)
11	OMC	AA	663	11	19,22,23	0.57	0	26,31,34	0.70	0
57	A2M	c	420	57	18,25,26	3.60	8 (44%)	18,36,39	3.41	3 (16%)
57	OMG	c	1271	57	18,26,27	1.14	2 (11%)	19,38,41	0.79	0
57	MA6	c	1782	57	18,26,27	1.03	2 (11%)	19,38,41	3.50	2 (10%)
57	OMG	c	1126	57	18,26,27	1.20	2 (11%)	19,38,41	0.77	1 (5%)
57	A2M	c	541	57	18,25,26	3.62	8 (44%)	18,36,39	3.29	4 (22%)
11	A2M	AA	807	11	18,25,26	3.61	8 (44%)	18,36,39	3.36	4 (22%)
57	MA6	c	1781	57	18,26,27	1.05	2 (11%)	19,38,41	3.46	2 (10%)
11	5MC	AA	2870	11,83	18,22,23	0.65	0	26,32,35	0.59	0
11	A2M	AA	649	11	18,25,26	3.62	8 (44%)	18,36,39	3.33	4 (22%)
11	A2M	AA	817	82,11	18,25,26	3.63	8 (44%)	18,36,39	3.55	4 (22%)
57	A2M	c	974	57	18,25,26	3.62	8 (44%)	18,36,39	3.43	4 (22%)
57	OMU	c	1269	57	19,22,23	3.12	8 (42%)	26,31,34	1.67	5 (19%)
57	OMC	c	1639	82,57	19,22,23	0.56	0	26,31,34	0.67	0
11	1MA	AA	645	82,11	16,25,26	0.92	2 (12%)	18,37,40	1.03	1 (5%)
57	A2M	c	619	82,57	18,25,26	3.69	9 (50%)	18,36,39	3.39	4 (22%)
11	OMG	AA	908	11	18,26,27	1.20	2 (11%)	19,38,41	0.83	1 (5%)
57	OMC	c	1007	57	19,22,23	0.55	0	26,31,34	0.70	0
57	B8N	c	1191	57	24,29,30	3.07	8 (33%)	29,42,45	1.72	5 (17%)
57	OMU	c	578	57	19,22,23	3.06	8 (42%)	26,31,34	1.69	5 (19%)
11	OMG	AA	867	11,83	18,26,27	1.16	2 (11%)	19,38,41	0.90	2 (10%)
11	OMU	AA	2729	11	19,22,23	3.01	8 (42%)	26,31,34	1.74	4 (15%)
57	A2M	c	436	57	18,25,26	3.61	8 (44%)	18,36,39	3.37	4 (22%)
11	OMU	AA	2417	11	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)
57	A2M	c	796	57	18,25,26	3.64	8 (44%)	18,36,39	3.39	3 (16%)
11	A2M	AA	2946	82,11	18,25,26	3.62	8 (44%)	18,36,39	3.31	4 (22%)
11	OMG	AA	2815	11	18,26,27	1.15	2 (11%)	19,38,41	0.88	1 (5%)
11	OMU	AA	2921	11	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
11	OMG	AA	2619	11	18,26,27	1.16	2 (11%)	19,38,41	0.82	1 (5%)

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
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
57	OMG	c	1428	57	-	3/5/27/28	0/3/3/3
11	A2M	AA	1449	82,11	-	0/5/27/28	0/3/3/3
57	A2M	c	100	82,57	-	0/5/27/28	0/3/3/3
11	A2M	AA	2256	11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
57	OMG	c	1572	57	-	3/5/27/28	0/3/3/3
57	4AC	c	1773	57	-	3/11/29/30	0/2/2/2
11	OMG	AA	1450	11	-	3/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2220	11	-	1/5/27/28	0/3/3/3
57	OMG	c	562	57	-	2/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
57	OMC	c	414	57	-	3/9/27/28	0/2/2/2
11	5MC	AA	2278	82,11	-	2/7/25/26	0/2/2/2
11	OMC	AA	1437	82,11	-	5/9/27/28	0/2/2/2
11	OMU	AA	2347	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2948	11	-	4/9/27/28	0/2/2/2
12	DDE	Aa	699	12	-	12/20/21/23	0/1/1/1
11	OMU	AA	898	11	-	2/9/27/28	0/2/2/2
11	OMG	AA	2922	11	-	2/5/27/28	0/3/3/3
11	OMC	AA	2337	11	-	3/9/27/28	0/2/2/2
11	OMC	AA	2197	11,83	-	2/9/27/28	0/2/2/2
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
57	A2M	c	28	80,57	-	3/5/27/28	0/3/3/3
11	A2M	AA	1133	82,11	-	0/5/27/28	0/3/3/3
57	4AC	c	1280	57	-	6/11/29/30	0/2/2/2
57	G7M	c	1575	57	-	2/3/25/26	0/3/3/3
11	A2M	AA	2640	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2959	11	-	1/9/27/28	0/2/2/2
11	1MA	AA	2142	82,11	-	0/3/25/26	0/3/3/3
11	OMG	AA	805	11	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMC	AA	650	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	2281	11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2793	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
57	A2M	c	420	57	-	3/5/27/28	0/3/3/3
57	OMG	c	1271	57	-	1/5/27/28	0/3/3/3
57	MA6	c	1782	57	-	1/7/29/30	0/3/3/3
57	OMG	c	1126	57	-	1/5/27/28	0/3/3/3
57	A2M	c	541	57	-	3/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	4/5/27/28	0/3/3/3
57	MA6	c	1781	57	-	0/7/29/30	0/3/3/3
11	5MC	AA	2870	11,83	-	5/7/25/26	0/2/2/2
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	817	82,11	-	2/5/27/28	0/3/3/3
57	A2M	c	974	57	-	0/5/27/28	0/3/3/3
57	OMU	c	1269	57	-	5/9/27/28	0/2/2/2
57	OMC	c	1639	82,57	-	0/9/27/28	0/2/2/2
11	1MA	AA	645	82,11	-	2/3/25/26	0/3/3/3
57	A2M	c	619	82,57	-	2/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	3/5/27/28	0/3/3/3
57	OMC	c	1007	57	-	0/9/27/28	0/2/2/2
57	B8N	c	1191	57	-	7/16/34/35	0/2/2/2
57	OMU	c	578	57	-	0/9/27/28	0/2/2/2
11	OMG	AA	867	11,83	-	0/5/27/28	0/3/3/3
11	OMU	AA	2729	11	-	1/9/27/28	0/2/2/2
57	A2M	c	436	57	-	0/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	0/9/27/28	0/2/2/2
57	A2M	c	796	57	-	1/5/27/28	0/3/3/3
11	A2M	AA	2946	82,11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2921	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2619	11	-	0/5/27/28	0/3/3/3

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	28	A2M	C3'-C4'	-9.16	1.29	1.53
11	AA	1133	A2M	C3'-C4'	-8.99	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.99	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	619	A2M	C3'-C4'	-8.95	1.30	1.53
57	c	974	A2M	C3'-C4'	-8.94	1.30	1.53
57	c	796	A2M	C3'-C4'	-8.92	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.89	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.89	1.30	1.53
11	AA	876	A2M	C3'-C4'	-8.88	1.30	1.53
57	c	541	A2M	C3'-C4'	-8.86	1.30	1.53
11	AA	2220	A2M	C3'-C4'	-8.81	1.30	1.53
57	c	420	A2M	C3'-C4'	-8.80	1.30	1.53
57	c	100	A2M	C3'-C4'	-8.79	1.30	1.53
57	c	436	A2M	C3'-C4'	-8.79	1.30	1.53
11	AA	2640	A2M	C3'-C4'	-8.76	1.30	1.53
11	AA	649	A2M	C3'-C4'	-8.75	1.30	1.53
11	AA	807	A2M	C3'-C4'	-8.75	1.30	1.53
11	AA	817	A2M	C3'-C4'	-8.66	1.30	1.53
11	AA	2281	A2M	C3'-C4'	-8.58	1.31	1.53
11	AA	2256	A2M	C3'-C4'	-8.40	1.31	1.53
11	AA	2281	A2M	O4'-C1'	-8.00	1.29	1.41
57	c	1191	B8N	C6-N1	7.87	1.56	1.36
57	c	1191	B8N	C4-N3	-7.85	1.25	1.40
11	AA	817	A2M	O4'-C4'	7.71	1.62	1.45
57	c	619	A2M	O4'-C1'	-7.69	1.30	1.41
57	c	100	A2M	O4'-C4'	7.69	1.62	1.45
11	AA	2946	A2M	O4'-C4'	7.69	1.62	1.45
57	c	420	A2M	O4'-C4'	7.66	1.62	1.45
57	c	796	A2M	O4'-C4'	7.64	1.62	1.45
57	c	436	A2M	O4'-C4'	7.63	1.62	1.45
11	AA	2280	A2M	O4'-C4'	7.62	1.62	1.45
11	AA	2220	A2M	O4'-C4'	7.61	1.62	1.45
11	AA	649	A2M	O4'-C1'	-7.57	1.30	1.41
57	c	974	A2M	O4'-C4'	7.56	1.61	1.45
11	AA	2281	A2M	O4'-C4'	7.56	1.61	1.45
11	AA	807	A2M	O4'-C4'	7.55	1.61	1.45
11	AA	2256	A2M	O4'-C4'	7.54	1.61	1.45
11	AA	2256	A2M	O4'-C1'	-7.52	1.30	1.41
11	AA	1133	A2M	O4'-C4'	7.51	1.61	1.45
11	AA	2640	A2M	O4'-C4'	7.50	1.61	1.45
11	AA	876	A2M	O4'-C4'	7.48	1.61	1.45
57	c	541	A2M	O4'-C4'	7.45	1.61	1.45
57	c	28	A2M	O4'-C4'	7.44	1.61	1.45
11	AA	1449	A2M	O4'-C4'	7.43	1.61	1.45
57	c	1269	OMU	C2-N1	7.41	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	649	A2M	O4'-C4'	7.40	1.61	1.45
11	AA	817	A2M	O4'-C1'	-7.38	1.30	1.41
57	c	619	A2M	O4'-C4'	7.37	1.61	1.45
57	c	1280	4AC	C4-N3	7.33	1.45	1.32
57	c	541	A2M	O4'-C1'	-7.29	1.30	1.41
11	AA	1449	A2M	O4'-C1'	-7.27	1.30	1.41
11	AA	1133	A2M	O4'-C1'	-7.27	1.30	1.41
11	AA	807	A2M	O4'-C1'	-7.26	1.30	1.41
11	AA	2280	A2M	O4'-C1'	-7.25	1.31	1.41
57	c	796	A2M	O4'-C1'	-7.23	1.31	1.41
11	AA	876	A2M	O4'-C1'	-7.21	1.31	1.41
57	c	100	A2M	O4'-C1'	-7.20	1.31	1.41
11	AA	2347	OMU	C2-N1	7.17	1.50	1.38
57	c	1773	4AC	C4-N3	7.17	1.45	1.32
57	c	974	A2M	O4'-C1'	-7.14	1.31	1.41
57	c	436	A2M	O4'-C1'	-7.10	1.31	1.41
11	AA	2640	A2M	O4'-C1'	-7.10	1.31	1.41
57	c	578	OMU	C2-N1	7.09	1.49	1.38
11	AA	2724	OMU	C2-N1	7.09	1.49	1.38
11	AA	1888	OMU	C2-N1	7.07	1.49	1.38
11	AA	2220	A2M	O4'-C1'	-7.06	1.31	1.41
57	c	420	A2M	O4'-C1'	-7.05	1.31	1.41
11	AA	2421	OMU	C2-N1	7.03	1.49	1.38
11	AA	898	OMU	C2-N1	7.02	1.49	1.38
11	AA	2729	OMU	C2-N1	7.02	1.49	1.38
57	c	1269	OMU	C2-N3	7.00	1.50	1.38
57	c	28	A2M	O4'-C1'	-6.99	1.31	1.41
11	AA	2946	A2M	O4'-C1'	-6.98	1.31	1.41
11	AA	2417	OMU	C2-N1	6.89	1.49	1.38
57	c	1773	4AC	C6-C5	6.87	1.51	1.35
57	c	578	OMU	C2-N3	6.86	1.50	1.38
11	AA	898	OMU	C2-N3	6.84	1.50	1.38
11	AA	2921	OMU	C2-N1	6.82	1.49	1.38
11	AA	2724	OMU	C2-N3	6.78	1.50	1.38
11	AA	2921	OMU	C2-N3	6.77	1.50	1.38
11	AA	2421	OMU	C2-N3	6.70	1.49	1.38
11	AA	1888	OMU	C2-N3	6.67	1.49	1.38
11	AA	2417	OMU	C2-N3	6.65	1.49	1.38
57	c	1280	4AC	C6-C5	6.62	1.50	1.35
11	AA	2729	OMU	C2-N3	6.61	1.49	1.38
11	AA	2634	UR3	C6-C5	6.56	1.50	1.35
11	AA	2347	OMU	C2-N3	6.54	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2634	UR3	C2-N1	6.48	1.47	1.38
57	c	1191	B8N	C2-N1	5.86	1.56	1.39
57	c	1280	4AC	C7-N4	5.78	1.47	1.37
57	c	578	OMU	C6-C5	5.74	1.48	1.35
57	c	1269	OMU	C6-C5	5.73	1.48	1.35
11	AA	898	OMU	C6-C5	5.72	1.48	1.35
11	AA	2921	OMU	C6-C5	5.67	1.48	1.35
11	AA	1888	OMU	C6-C5	5.65	1.48	1.35
11	AA	2729	OMU	C6-C5	5.64	1.48	1.35
11	AA	2421	OMU	C6-C5	5.59	1.48	1.35
11	AA	2417	OMU	C6-C5	5.58	1.48	1.35
11	AA	2347	OMU	C6-C5	5.55	1.48	1.35
11	AA	2724	OMU	C6-C5	5.54	1.47	1.35
57	c	1280	4AC	C2-N1	5.51	1.51	1.40
57	c	1575	G7M	C2-N3	5.49	1.46	1.33
11	AA	2634	UR3	C2-N3	5.49	1.49	1.39
57	c	1773	4AC	C7-N4	5.47	1.47	1.37
57	c	1191	B8N	C6-C5	5.32	1.42	1.34
57	c	1280	4AC	C2-N3	5.18	1.46	1.36
57	c	1280	4AC	C4-N4	5.09	1.47	1.39
57	c	1773	4AC	C4-N4	5.07	1.47	1.39
57	c	1773	4AC	C2-N3	5.01	1.46	1.36
57	c	1773	4AC	C2-N1	4.99	1.50	1.40
57	c	1575	G7M	C4-N3	4.97	1.49	1.37
57	c	1575	G7M	C2-N2	4.77	1.45	1.34
57	c	1269	OMU	C4-N3	4.38	1.46	1.38
57	c	578	OMU	C4-N3	4.32	1.46	1.38
11	AA	1888	OMU	C4-N3	4.25	1.46	1.38
57	c	1280	4AC	CM7-C7	4.24	1.59	1.50
11	AA	2417	OMU	C4-N3	4.22	1.46	1.38
11	AA	2729	OMU	C4-N3	4.20	1.46	1.38
11	AA	2421	OMU	C4-N3	4.16	1.46	1.38
11	AA	898	OMU	C4-N3	4.12	1.45	1.38
11	AA	2921	OMU	C4-N3	4.08	1.45	1.38
11	AA	2724	OMU	C4-N3	4.08	1.45	1.38
57	c	1773	4AC	CM7-C7	4.08	1.59	1.50
57	c	1773	4AC	C5-C4	4.05	1.49	1.40
11	AA	2347	OMU	C4-N3	3.99	1.45	1.38
57	c	1280	4AC	C5-C4	3.97	1.49	1.40
57	c	1575	G7M	C6-N1	3.62	1.43	1.37
57	c	1191	B8N	C1'-C5	3.58	1.58	1.50
57	c	1575	G7M	C5-C6	3.29	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	562	OMG	C8-N7	-3.23	1.29	1.35
11	AA	2634	UR3	C6-N1	3.18	1.45	1.38
11	AA	2220	A2M	C6-N6	3.16	1.45	1.34
57	c	420	A2M	C6-N6	3.15	1.45	1.34
11	AA	2281	A2M	C6-N6	3.15	1.45	1.34
11	AA	876	A2M	C6-N6	3.14	1.45	1.34
57	c	541	A2M	C6-N6	3.14	1.45	1.34
57	c	28	A2M	C6-N6	3.13	1.45	1.34
11	AA	807	A2M	C6-N6	3.13	1.45	1.34
11	AA	2640	A2M	C6-N6	3.13	1.45	1.34
11	AA	649	A2M	C6-N6	3.13	1.45	1.34
57	c	619	A2M	C6-N6	3.12	1.45	1.34
11	AA	2256	A2M	O3'-C3'	3.12	1.50	1.43
57	c	619	A2M	O3'-C3'	3.12	1.50	1.43
11	AA	1449	A2M	C6-N6	3.12	1.45	1.34
11	AA	2256	A2M	C6-N6	3.11	1.45	1.34
57	c	100	A2M	C6-N6	3.10	1.45	1.34
11	AA	2280	A2M	C6-N6	3.10	1.45	1.34
11	AA	1133	A2M	C6-N6	3.10	1.45	1.34
57	c	796	A2M	C6-N6	3.10	1.45	1.34
57	c	436	A2M	C6-N6	3.09	1.45	1.34
57	c	541	A2M	O3'-C3'	3.09	1.50	1.43
11	AA	2946	A2M	C6-N6	3.08	1.45	1.34
11	AA	2724	OMU	O4-C4	-3.06	1.18	1.24
11	AA	817	A2M	C6-N6	3.04	1.45	1.34
57	c	1269	OMU	C6-N1	3.03	1.45	1.38
11	AA	2417	OMU	O4-C4	-3.01	1.18	1.24
11	AA	2347	OMU	O4-C4	-3.00	1.18	1.24
11	AA	1888	OMU	O4-C4	-2.99	1.18	1.24
57	c	974	A2M	C6-N6	2.99	1.45	1.34
11	AA	2421	OMU	O4-C4	-2.99	1.18	1.24
11	AA	898	OMU	O4-C4	-2.98	1.18	1.24
57	c	436	A2M	O3'-C3'	2.98	1.50	1.43
11	AA	908	OMG	C8-N7	-2.97	1.30	1.35
11	AA	807	A2M	O3'-C3'	2.97	1.50	1.43
11	AA	2921	OMU	O4-C4	-2.97	1.18	1.24
57	c	1428	OMG	C8-N7	-2.96	1.30	1.35
57	c	1572	OMG	C8-N7	-2.96	1.30	1.35
11	AA	2288	OMG	C8-N7	-2.93	1.30	1.35
11	AA	2729	OMU	O4-C4	-2.93	1.18	1.24
11	AA	817	A2M	O2'-C2'	-2.90	1.35	1.42
57	c	420	A2M	O3'-C3'	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	578	OMU	O4-C4	-2.88	1.18	1.24
11	AA	649	A2M	O3'-C3'	2.88	1.49	1.43
11	AA	2793	OMG	C8-N7	-2.87	1.30	1.35
57	c	974	A2M	C5-C4	-2.87	1.33	1.40
57	c	1126	OMG	C8-N7	-2.86	1.30	1.35
11	AA	2281	A2M	C5-C4	-2.86	1.33	1.40
11	AA	2791	OMG	C8-N7	-2.85	1.30	1.35
11	AA	876	A2M	C5-C4	-2.85	1.33	1.40
11	AA	1133	A2M	C5-C4	-2.84	1.33	1.40
57	c	100	A2M	O3'-C3'	2.83	1.49	1.43
57	c	1269	OMU	O4-C4	-2.83	1.19	1.24
11	AA	2421	OMU	C6-N1	2.82	1.44	1.38
11	AA	2619	OMG	C8-N7	-2.82	1.30	1.35
11	AA	2946	A2M	C5-C4	-2.82	1.33	1.40
57	c	796	A2M	C5-C4	-2.82	1.33	1.40
57	c	578	OMU	C6-N1	2.81	1.44	1.38
11	AA	2220	A2M	O3'-C3'	2.81	1.49	1.43
57	c	420	A2M	C5-C4	-2.81	1.33	1.40
57	c	1575	G7M	C2-N1	2.81	1.44	1.37
57	c	619	A2M	C5-C4	-2.81	1.33	1.40
11	AA	2347	OMU	C6-N1	2.80	1.44	1.38
11	AA	1888	OMU	C6-N1	2.80	1.44	1.38
11	AA	2640	A2M	O3'-C3'	2.79	1.49	1.43
57	c	974	A2M	O3'-C3'	2.79	1.49	1.43
11	AA	1450	OMG	C8-N7	-2.79	1.30	1.35
57	c	796	A2M	O3'-C3'	2.79	1.49	1.43
11	AA	2921	OMU	C6-N1	2.78	1.44	1.38
11	AA	2815	OMG	C8-N7	-2.78	1.30	1.35
57	c	100	A2M	C5-C4	-2.78	1.33	1.40
11	AA	2280	A2M	O3'-C3'	2.77	1.49	1.43
11	AA	2281	A2M	O3'-C3'	2.77	1.49	1.43
11	AA	807	A2M	C5-C4	-2.77	1.33	1.40
57	c	562	OMG	C5-C6	-2.77	1.41	1.47
57	c	974	A2M	O2'-C2'	-2.77	1.35	1.42
11	AA	817	A2M	C5-C4	-2.76	1.33	1.40
11	AA	2946	A2M	O3'-C3'	2.76	1.49	1.43
11	AA	2281	A2M	O2'-C2'	-2.75	1.35	1.42
11	AA	867	OMG	C8-N7	-2.75	1.30	1.35
11	AA	1133	A2M	O2'-C2'	-2.75	1.35	1.42
11	AA	898	OMU	C6-N1	2.74	1.44	1.38
11	AA	2417	OMU	C6-N1	2.74	1.44	1.38
11	AA	2729	OMU	C6-N1	2.74	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1449	A2M	O3'-C3'	2.74	1.49	1.43
57	c	796	A2M	O2'-C2'	-2.74	1.35	1.42
11	AA	2640	A2M	C5-C4	-2.74	1.33	1.40
11	AA	2922	OMG	C8-N7	-2.73	1.30	1.35
11	AA	817	A2M	O3'-C3'	2.73	1.49	1.43
11	AA	876	A2M	O3'-C3'	2.72	1.49	1.43
11	AA	2256	A2M	C5-C4	-2.72	1.33	1.40
11	AA	805	OMG	C8-N7	-2.72	1.30	1.35
11	AA	649	A2M	C5-C4	-2.71	1.33	1.40
57	c	28	A2M	O3'-C3'	2.71	1.49	1.43
11	AA	2946	A2M	O2'-C2'	-2.70	1.35	1.42
11	AA	1449	A2M	O2'-C2'	-2.70	1.35	1.42
57	c	1271	OMG	C8-N7	-2.70	1.30	1.35
57	c	28	A2M	C5-C4	-2.70	1.33	1.40
57	c	619	A2M	O2'-C2'	-2.70	1.35	1.42
11	AA	2724	OMU	C6-N1	2.69	1.44	1.38
11	AA	2793	OMG	C5-C6	-2.69	1.41	1.47
57	c	100	A2M	O2'-C2'	-2.69	1.35	1.42
57	c	541	A2M	C5-C4	-2.68	1.33	1.40
11	AA	2280	A2M	C5-C4	-2.68	1.33	1.40
11	AA	2288	OMG	C5-C6	-2.67	1.42	1.47
11	AA	1449	A2M	C5-C4	-2.67	1.33	1.40
11	AA	876	A2M	O2'-C2'	-2.67	1.35	1.42
57	c	1782	MA6	C5-C4	-2.66	1.33	1.40
57	c	1781	MA6	C5-C4	-2.66	1.33	1.40
57	c	436	A2M	O2'-C2'	-2.65	1.35	1.42
11	AA	2791	OMG	C5-C6	-2.64	1.42	1.47
11	AA	2220	A2M	C5-C4	-2.64	1.33	1.40
11	AA	2280	A2M	O2'-C2'	-2.63	1.35	1.42
11	AA	908	OMG	C5-C6	-2.61	1.42	1.47
11	AA	807	A2M	O2'-C2'	-2.61	1.35	1.42
57	c	436	A2M	C5-C4	-2.60	1.34	1.40
57	c	28	A2M	O2'-C2'	-2.59	1.36	1.42
11	AA	649	A2M	O2'-C2'	-2.59	1.36	1.42
11	AA	1133	A2M	O3'-C3'	2.59	1.49	1.43
57	c	541	A2M	O2'-C2'	-2.58	1.36	1.42
57	c	1126	OMG	C5-C6	-2.58	1.42	1.47
11	AA	2142	1MA	C8-N7	-2.58	1.30	1.35
57	c	1572	OMG	C5-C6	-2.57	1.42	1.47
57	c	420	A2M	O2'-C2'	-2.56	1.36	1.42
57	c	1773	4AC	C6-N1	2.53	1.44	1.38
57	c	1428	OMG	C5-C6	-2.53	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	805	OMG	C5-C6	-2.52	1.42	1.47
11	AA	2640	A2M	O2'-C2'	-2.52	1.36	1.42
57	c	1271	OMG	C5-C6	-2.51	1.42	1.47
11	AA	867	OMG	C5-C6	-2.51	1.42	1.47
11	AA	2619	OMG	C5-C6	-2.50	1.42	1.47
57	c	1782	MA6	C2-N3	2.49	1.36	1.32
11	AA	2347	OMU	O2-C2	-2.48	1.18	1.23
57	c	578	OMU	C5-C4	2.48	1.49	1.43
11	AA	898	OMU	O2-C2	-2.47	1.18	1.23
11	AA	2220	A2M	O2'-C2'	-2.47	1.36	1.42
11	AA	2729	OMU	O2-C2	-2.46	1.18	1.23
11	AA	2724	OMU	O2-C2	-2.45	1.18	1.23
11	AA	1450	OMG	C5-C6	-2.45	1.42	1.47
11	AA	2729	OMU	C5-C4	2.44	1.49	1.43
57	c	1781	MA6	C2-N3	2.42	1.36	1.32
57	c	1280	4AC	C6-N1	2.42	1.43	1.38
11	AA	2815	OMG	C5-C6	-2.41	1.42	1.47
11	AA	2922	OMG	C5-C6	-2.40	1.42	1.47
57	c	1269	OMU	C5-C4	2.40	1.48	1.43
11	AA	2417	OMU	O2-C2	-2.39	1.18	1.23
11	AA	2421	OMU	O2-C2	-2.39	1.18	1.23
11	AA	2921	OMU	O2-C2	-2.38	1.18	1.23
11	AA	645	1MA	C5-C4	-2.36	1.37	1.43
11	AA	2921	OMU	C5-C4	2.36	1.48	1.43
11	AA	1888	OMU	C5-C4	2.34	1.48	1.43
11	AA	2421	OMU	C5-C4	2.33	1.48	1.43
11	AA	1888	OMU	O2-C2	-2.33	1.18	1.23
11	AA	898	OMU	C5-C4	2.31	1.48	1.43
57	c	1773	4AC	O7-C7	-2.31	1.18	1.23
11	AA	2347	OMU	C5-C4	2.30	1.48	1.43
57	c	1280	4AC	O7-C7	-2.30	1.18	1.23
11	AA	2142	1MA	C5-C4	-2.28	1.37	1.43
57	c	578	OMU	O2-C2	-2.25	1.18	1.23
11	AA	2417	OMU	C5-C4	2.25	1.48	1.43
12	Aa	699	DDE	CD2-NE2	2.24	1.39	1.36
57	c	1269	OMU	O2-C2	-2.23	1.19	1.23
57	c	436	A2M	C2-N3	2.22	1.35	1.32
11	AA	645	1MA	C8-N7	-2.19	1.31	1.35
11	AA	2724	OMU	C5-C4	2.18	1.48	1.43
57	c	796	A2M	C2-N3	2.18	1.35	1.32
11	AA	2640	A2M	C2-N3	2.17	1.35	1.32
57	c	541	A2M	C2-N3	2.16	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	28	A2M	O5'-C5'	-2.16	1.39	1.44
57	c	420	A2M	C2-N3	2.16	1.35	1.32
11	AA	2256	A2M	O2'-C2'	-2.16	1.37	1.42
57	c	619	A2M	O5'-C5'	-2.15	1.39	1.44
11	AA	2220	A2M	C2-N3	2.14	1.35	1.32
11	AA	2256	A2M	C2-N3	2.14	1.35	1.32
11	AA	2280	A2M	C2-N3	2.13	1.35	1.32
11	AA	2281	A2M	C2-N3	2.13	1.35	1.32
11	AA	2946	A2M	C2-N3	2.13	1.35	1.32
57	c	28	A2M	C2-N3	2.12	1.35	1.32
57	c	100	A2M	C2-N3	2.12	1.35	1.32
11	AA	1449	A2M	C2-N3	2.12	1.35	1.32
11	AA	649	A2M	C2-N3	2.11	1.35	1.32
57	c	1575	G7M	O6-C6	-2.11	1.19	1.23
11	AA	2634	UR3	C5-C4	2.10	1.49	1.43
57	c	619	A2M	C2-N3	2.10	1.35	1.32
11	AA	876	A2M	C2-N3	2.09	1.35	1.32
11	AA	2281	A2M	O5'-C5'	-2.09	1.39	1.44
11	AA	817	A2M	C2-N3	2.08	1.35	1.32
57	c	1191	B8N	O4-C4	-2.07	1.18	1.23
11	AA	1133	A2M	O5'-C5'	-2.05	1.39	1.44
57	c	974	A2M	C2-N3	2.05	1.35	1.32
11	AA	2634	UR3	O2-C2	-2.04	1.18	1.22
11	AA	2634	UR3	C4-N3	2.03	1.45	1.40
11	AA	876	A2M	O5'-C5'	-2.03	1.39	1.44
11	AA	807	A2M	C2-N3	2.03	1.35	1.32
57	c	1191	B8N	O2-C2	-2.00	1.18	1.22
57	c	1191	B8N	C32-C31	2.00	1.56	1.52

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	c	1782	MA6	N1-C6-N6	-14.09	102.23	117.06
57	c	1781	MA6	N1-C6-N6	-13.88	102.45	117.06
11	AA	817	A2M	C5-C6-N6	11.00	137.07	120.35
11	AA	2256	A2M	C5-C6-N6	10.75	136.68	120.35
11	AA	1449	A2M	C5-C6-N6	10.72	136.64	120.35
57	c	420	A2M	C5-C6-N6	10.71	136.62	120.35
57	c	974	A2M	C5-C6-N6	10.70	136.62	120.35
11	AA	2220	A2M	C5-C6-N6	10.63	136.51	120.35
11	AA	807	A2M	C5-C6-N6	10.58	136.43	120.35
11	AA	2640	A2M	C5-C6-N6	10.56	136.40	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	c	796	A2M	C5-C6-N6	10.55	136.38	120.35
57	c	436	A2M	C5-C6-N6	10.53	136.36	120.35
57	c	619	A2M	C5-C6-N6	10.53	136.36	120.35
11	AA	1133	A2M	C5-C6-N6	10.44	136.22	120.35
57	c	28	A2M	C5-C6-N6	10.43	136.21	120.35
11	AA	876	A2M	C5-C6-N6	10.43	136.21	120.35
11	AA	649	A2M	C5-C6-N6	10.41	136.18	120.35
57	c	100	A2M	C5-C6-N6	10.34	136.07	120.35
11	AA	2281	A2M	C5-C6-N6	10.32	136.04	120.35
57	c	541	A2M	C5-C6-N6	10.29	135.99	120.35
11	AA	2946	A2M	C5-C6-N6	10.29	135.99	120.35
11	AA	2280	A2M	C5-C6-N6	10.22	135.88	120.35
11	AA	817	A2M	N6-C6-N1	-7.59	102.83	118.57
11	AA	2256	A2M	N6-C6-N1	-7.50	103.01	118.57
57	c	974	A2M	N6-C6-N1	-7.45	103.12	118.57
11	AA	2220	A2M	N6-C6-N1	-7.34	103.34	118.57
57	c	420	A2M	N6-C6-N1	-7.32	103.38	118.57
57	c	796	A2M	N6-C6-N1	-7.31	103.40	118.57
11	AA	1449	A2M	N6-C6-N1	-7.29	103.45	118.57
11	AA	876	A2M	N6-C6-N1	-7.21	103.61	118.57
11	AA	807	A2M	N6-C6-N1	-7.20	103.62	118.57
11	AA	2640	A2M	N6-C6-N1	-7.20	103.64	118.57
57	c	619	A2M	N6-C6-N1	-7.19	103.65	118.57
57	c	436	A2M	N6-C6-N1	-7.17	103.69	118.57
57	c	100	A2M	N6-C6-N1	-7.12	103.79	118.57
11	AA	2946	A2M	N6-C6-N1	-7.11	103.81	118.57
57	c	28	A2M	N6-C6-N1	-7.06	103.91	118.57
11	AA	2281	A2M	N6-C6-N1	-7.06	103.91	118.57
11	AA	649	A2M	N6-C6-N1	-7.06	103.92	118.57
11	AA	1133	A2M	N6-C6-N1	-7.05	103.95	118.57
11	AA	2280	A2M	N6-C6-N1	-7.00	104.04	118.57
57	c	541	A2M	N6-C6-N1	-6.97	104.10	118.57
57	c	1280	4AC	CM7-C7-N4	5.87	125.45	115.29
11	AA	2256	A2M	N3-C2-N1	-5.77	119.66	128.68
57	c	796	A2M	N3-C2-N1	-5.75	119.69	128.68
57	c	1773	4AC	CM7-C7-N4	5.72	125.19	115.29
11	AA	2220	A2M	N3-C2-N1	-5.62	119.89	128.68
11	AA	1133	A2M	N3-C2-N1	-5.62	119.90	128.68
57	c	974	A2M	N3-C2-N1	-5.61	119.90	128.68
57	c	28	A2M	N3-C2-N1	-5.61	119.90	128.68
57	c	100	A2M	N3-C2-N1	-5.60	119.93	128.68
57	c	420	A2M	N3-C2-N1	-5.57	119.97	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	876	A2M	N3-C2-N1	-5.56	119.99	128.68
11	AA	2946	A2M	N3-C2-N1	-5.54	120.01	128.68
11	AA	2281	A2M	N3-C2-N1	-5.53	120.04	128.68
57	c	541	A2M	N3-C2-N1	-5.51	120.06	128.68
11	AA	649	A2M	N3-C2-N1	-5.49	120.11	128.68
57	c	1781	MA6	N3-C2-N1	-5.47	120.13	128.68
11	AA	2640	A2M	N3-C2-N1	-5.46	120.14	128.68
11	AA	2280	A2M	N3-C2-N1	-5.46	120.14	128.68
57	c	619	A2M	N3-C2-N1	-5.45	120.15	128.68
11	AA	817	A2M	N3-C2-N1	-5.41	120.22	128.68
11	AA	2729	OMU	C4-N3-C2	-5.40	119.46	126.58
57	c	1782	MA6	N3-C2-N1	-5.38	120.28	128.68
11	AA	2347	OMU	C4-N3-C2	-5.34	119.53	126.58
57	c	436	A2M	N3-C2-N1	-5.34	120.33	128.68
11	AA	1449	A2M	N3-C2-N1	-5.33	120.35	128.68
11	AA	1888	OMU	C4-N3-C2	-5.28	119.62	126.58
11	AA	2417	OMU	C4-N3-C2	-5.28	119.62	126.58
11	AA	2921	OMU	C4-N3-C2	-5.26	119.64	126.58
11	AA	807	A2M	N3-C2-N1	-5.26	120.46	128.68
57	c	578	OMU	C4-N3-C2	-5.25	119.66	126.58
11	AA	2724	OMU	C4-N3-C2	-5.21	119.71	126.58
11	AA	2421	OMU	C4-N3-C2	-5.20	119.72	126.58
57	c	1191	B8N	C5-C4-N3	5.18	125.77	116.17
11	AA	898	OMU	C4-N3-C2	-5.16	119.77	126.58
11	AA	2634	UR3	C4-N3-C2	-4.82	120.02	124.56
57	c	1269	OMU	C4-N3-C2	-4.79	120.26	126.58
57	c	1191	B8N	C4-N3-C2	-4.58	119.67	125.46
11	AA	1437	OMC	C1'-N1-C2	4.33	128.08	118.42
11	AA	898	OMU	N3-C2-N1	4.18	120.44	114.89
11	AA	2921	OMU	N3-C2-N1	3.97	120.16	114.89
11	AA	2347	OMU	N3-C2-N1	3.95	120.13	114.89
11	AA	2724	OMU	N3-C2-N1	3.85	120.00	114.89
11	AA	2729	OMU	N3-C2-N1	3.78	119.91	114.89
57	c	578	OMU	N3-C2-N1	3.69	119.79	114.89
11	AA	2421	OMU	N3-C2-N1	3.67	119.77	114.89
11	AA	1888	OMU	N3-C2-N1	3.58	119.64	114.89
11	AA	2417	OMU	N3-C2-N1	3.54	119.58	114.89
57	c	1269	OMU	N3-C2-N1	3.52	119.56	114.89
11	AA	2417	OMU	C5-C4-N3	3.47	120.03	114.84
11	AA	2421	OMU	C5-C4-N3	3.45	120.00	114.84
11	AA	2729	OMU	C5-C4-N3	3.44	119.98	114.84
11	AA	2347	OMU	C5-C4-N3	3.42	119.96	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	1888	OMU	C5-C4-N3	3.42	119.95	114.84
11	AA	2724	OMU	C5-C4-N3	3.39	119.91	114.84
11	AA	1437	OMC	C1'-N1-C6	-3.25	113.74	120.84
57	c	578	OMU	C5-C4-N3	3.24	119.69	114.84
11	AA	2921	OMU	C5-C4-N3	3.18	119.59	114.84
11	AA	2417	OMU	O4-C4-C5	-3.17	119.58	125.16
57	c	1269	OMU	C5-C4-N3	3.17	119.58	114.84
57	c	414	OMC	C1'-N1-C2	3.17	125.49	118.42
11	AA	2948	OMC	C1'-N1-C2	3.15	125.45	118.42
11	AA	898	OMU	C5-C4-N3	3.05	119.40	114.84
11	AA	2729	OMU	O4-C4-C5	-3.03	119.82	125.16
11	AA	2724	OMU	O4-C4-C5	-3.03	119.83	125.16
11	AA	2421	OMU	O4-C4-C5	-3.01	119.86	125.16
57	c	1575	G7M	C2-N1-C6	-2.95	119.67	125.10
57	c	1191	B8N	N3-C2-N1	2.93	120.90	116.76
11	AA	2347	OMU	O4-C4-C5	-2.92	120.02	125.16
11	AA	2281	A2M	O4'-C1'-C2'	-2.90	101.55	106.59
11	AA	1888	OMU	O4-C4-C5	-2.89	120.08	125.16
57	c	1269	OMU	O4-C4-C5	-2.87	120.12	125.16
57	c	1191	B8N	O4-C4-N3	-2.86	115.12	119.98
57	c	1773	4AC	O7-C7-N4	-2.86	117.19	121.82
57	c	1280	4AC	O7-C7-N4	-2.83	117.23	121.82
57	c	1280	4AC	C6-C5-C4	2.82	120.42	116.96
57	c	578	OMU	O4-C4-C5	-2.82	120.20	125.16
11	AA	2921	OMU	O4-C4-C5	-2.79	120.26	125.16
11	AA	898	OMU	O4-C4-C5	-2.71	120.39	125.16
57	c	414	OMC	C1'-N1-C6	-2.66	115.04	120.84
11	AA	876	A2M	C1'-N9-C4	2.63	131.26	126.64
11	AA	2256	A2M	O4'-C1'-C2'	-2.63	102.03	106.59
11	AA	1449	A2M	C1'-N9-C4	2.57	131.15	126.64
57	c	1773	4AC	C5-C4-N3	-2.56	118.47	122.59
57	c	1280	4AC	O7-C7-CM7	-2.55	117.32	122.06
11	AA	867	OMG	O6-C6-C5	2.55	129.35	124.37
57	c	1280	4AC	C5-C4-N3	-2.55	118.50	122.59
11	AA	2921	OMU	O2-C2-N1	-2.51	119.45	122.79
11	AA	2948	OMC	C1'-N1-C6	-2.51	115.38	120.84
57	c	1280	4AC	O2-C2-N3	-2.47	118.32	122.33
11	AA	898	OMU	O2-C2-N1	-2.45	119.53	122.79
11	AA	2337	OMC	C1'-N1-C2	2.45	123.88	118.42
57	c	541	A2M	C1'-N9-C4	2.42	130.90	126.64
11	AA	2922	OMG	O6-C6-C5	2.42	129.10	124.37
11	AA	2724	OMU	C1'-N1-C2	2.42	121.95	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Aa	699	DDE	CAU-CBW-CBI	-2.41	106.43	111.20
11	AA	2256	A2M	O2'-C2'-C1'	2.40	113.84	109.09
57	c	1773	4AC	O7-C7-CM7	-2.39	117.62	122.06
57	c	1773	4AC	C6-C5-C4	2.38	119.87	116.96
57	c	1280	4AC	C1'-N1-C2	2.35	123.67	118.42
11	AA	2280	A2M	C1'-N9-C4	2.33	130.74	126.64
57	c	436	A2M	C1'-N9-C4	2.31	130.71	126.64
11	AA	2288	OMG	O6-C6-C5	2.31	128.89	124.37
57	c	1269	OMU	C1'-N1-C2	2.30	121.73	117.57
57	c	28	A2M	C1'-N9-C4	2.29	130.66	126.64
11	AA	805	OMG	O6-C6-C5	2.28	128.82	124.37
57	c	1428	OMG	O6-C6-C5	2.27	128.80	124.37
11	AA	2619	OMG	O6-C6-C5	2.26	128.79	124.37
11	AA	2220	A2M	C1'-N9-C4	2.26	130.61	126.64
11	AA	2815	OMG	O6-C6-C5	2.26	128.78	124.37
11	AA	908	OMG	O6-C6-C5	2.25	128.77	124.37
11	AA	2142	1MA	N1-C6-N6	2.22	125.42	119.77
57	c	1572	OMG	O6-C6-C5	2.21	128.69	124.37
11	AA	817	A2M	O4'-C1'-C2'	-2.19	102.78	106.59
11	AA	645	1MA	N1-C6-N6	2.18	125.31	119.77
11	AA	2142	1MA	C5-C6-N1	-2.18	110.65	113.90
11	AA	807	A2M	C1'-N9-C4	2.17	130.46	126.64
11	AA	2417	OMU	O2-C2-N1	-2.16	119.92	122.79
11	AA	2421	OMU	O2-C2-N1	-2.14	119.94	122.79
12	Aa	699	DDE	CBW-CBI-NAD	2.13	118.00	115.28
11	AA	2640	A2M	C1'-N9-C4	2.13	130.39	126.64
11	AA	1450	OMG	O6-C6-C5	2.13	128.53	124.37
11	AA	649	A2M	C1'-N9-C4	2.11	130.35	126.64
11	AA	2946	A2M	C1'-N9-C4	2.11	130.34	126.64
57	c	974	A2M	C1'-N9-C4	2.10	130.34	126.64
11	AA	2791	OMG	O6-C6-C5	2.09	128.45	124.37
57	c	578	OMU	O2-C2-N1	-2.07	120.03	122.79
57	c	1191	B8N	C31-N3-C2	2.07	120.77	117.67
11	AA	2793	OMG	O6-C6-C5	2.04	128.36	124.37
11	AA	650	OMC	C1'-N1-C2	2.03	122.94	118.42
57	c	619	A2M	C1'-N9-C4	2.02	130.20	126.64
11	AA	1888	OMU	O2-C2-N1	-2.01	120.11	122.79
57	c	1126	OMG	O6-C6-C5	2.01	128.30	124.37
11	AA	867	OMG	C5-C6-N1	-2.00	110.42	113.95

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	805	OMG	C1'-C2'-O2'-CM2
11	AA	807	A2M	C1'-C2'-O2'-CM'
11	AA	898	OMU	C1'-C2'-O2'-CM2
11	AA	908	OMG	C3'-C4'-C5'-O5'
11	AA	1437	OMC	C3'-C4'-C5'-O5'
11	AA	1450	OMG	C3'-C4'-C5'-O5'
11	AA	2220	A2M	C1'-C2'-O2'-CM'
11	AA	2256	A2M	C1'-C2'-O2'-CM'
11	AA	2280	A2M	O4'-C4'-C5'-O5'
11	AA	2337	OMC	C1'-C2'-O2'-CM2
11	AA	2337	OMC	C3'-C4'-C5'-O5'
11	AA	2421	OMU	C1'-C2'-O2'-CM2
11	AA	2640	A2M	C1'-C2'-O2'-CM'
11	AA	2724	OMU	C1'-C2'-O2'-CM2
11	AA	2729	OMU	C1'-C2'-O2'-CM2
11	AA	2793	OMG	C1'-C2'-O2'-CM2
11	AA	2870	5MC	C2'-C1'-N1-C2
11	AA	2870	5MC	C2'-C1'-N1-C6
11	AA	2921	OMU	C1'-C2'-O2'-CM2
11	AA	2922	OMG	C3'-C4'-C5'-O5'
11	AA	2946	A2M	C1'-C2'-O2'-CM'
11	AA	2948	OMC	C1'-C2'-O2'-CM2
11	AA	2959	OMC	C1'-C2'-O2'-CM2
12	Aa	699	DDE	CA-CB-CG-ND1
12	Aa	699	DDE	CA-CB-CG-CD2
12	Aa	699	DDE	CAU-CAT-CE1-NE2
12	Aa	699	DDE	CBI-CBW-NCB-CAB
12	Aa	699	DDE	CBI-CBW-NCB-CAC
12	Aa	699	DDE	CBI-CBW-NCB-CAA
12	Aa	699	DDE	CAU-CBW-NCB-CAB
12	Aa	699	DDE	CAU-CBW-NCB-CAC
12	Aa	699	DDE	CAU-CBW-NCB-CAA
12	Aa	699	DDE	CAT-CAU-CBW-NCB
12	Aa	699	DDE	CE1-CAT-CAU-CBW
57	c	28	A2M	C3'-C4'-C5'-O5'
57	c	414	OMC	C1'-C2'-O2'-CM2
57	c	414	OMC	O4'-C4'-C5'-O5'
57	c	420	A2M	O4'-C4'-C5'-O5'
57	c	420	A2M	C1'-C2'-O2'-CM'
57	c	541	A2M	C4'-C5'-O5'-P
57	c	541	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
57	c	541	A2M	C3'-C4'-C5'-O5'
57	c	562	OMG	O4'-C4'-C5'-O5'
57	c	562	OMG	C3'-C4'-C5'-O5'
57	c	619	A2M	O4'-C4'-C5'-O5'
57	c	1191	B8N	O4'-C4'-C5'-O5'
57	c	1191	B8N	C3'-C4'-C5'-O5'
57	c	1191	B8N	C2'-C1'-C5-C6
57	c	1191	B8N	C31-C32-C33-C34
57	c	1191	B8N	C31-C32-C33-N34
57	c	1271	OMG	C1'-C2'-O2'-CM2
57	c	1428	OMG	C1'-C2'-O2'-CM2
57	c	1572	OMG	O4'-C4'-C5'-O5'
11	AA	807	A2M	C3'-C4'-C5'-O5'
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2280	A2M	C3'-C4'-C5'-O5'
11	AA	2337	OMC	O4'-C4'-C5'-O5'
11	AA	2946	A2M	O4'-C4'-C5'-O5'
57	c	28	A2M	O4'-C4'-C5'-O5'
57	c	414	OMC	C3'-C4'-C5'-O5'
57	c	619	A2M	C3'-C4'-C5'-O5'
57	c	1572	OMG	C3'-C4'-C5'-O5'
12	Aa	699	DDE	CAT-CAU-CBW-CBI
11	AA	645	1MA	O4'-C4'-C5'-O5'
11	AA	645	1MA	C3'-C4'-C5'-O5'
11	AA	807	A2M	O4'-C4'-C5'-O5'
11	AA	908	OMG	O4'-C4'-C5'-O5'
11	AA	2278	5MC	O4'-C4'-C5'-O5'
11	AA	2922	OMG	O4'-C4'-C5'-O5'
11	AA	2946	A2M	C3'-C4'-C5'-O5'
57	c	420	A2M	C3'-C4'-C5'-O5'
57	c	1428	OMG	O4'-C4'-C5'-O5'
57	c	1269	OMU	C3'-C2'-O2'-CM2
11	AA	1437	OMC	C2'-C1'-N1-C2
57	c	1428	OMG	C3'-C4'-C5'-O5'
11	AA	1437	OMC	O4'-C4'-C5'-O5'
11	AA	1437	OMC	C2'-C1'-N1-C6
11	AA	2278	5MC	C3'-C4'-C5'-O5'
57	c	1280	4AC	O7-C7-N4-C4
57	c	1280	4AC	CM7-C7-N4-C4
57	c	1773	4AC	O7-C7-N4-C4
57	c	1773	4AC	CM7-C7-N4-C4
11	AA	908	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
11	AA	2256	A2M	C4'-C5'-O5'-P
57	c	1280	4AC	C4'-C5'-O5'-P
57	c	1575	G7M	O4'-C4'-C5'-O5'
57	c	1191	B8N	N3-C31-C32-C33
57	c	1782	MA6	C4'-C5'-O5'-P
11	AA	2281	A2M	O4'-C4'-C5'-O5'
11	AA	807	A2M	C4'-C5'-O5'-P
11	AA	1450	OMG	C4'-C5'-O5'-P
57	c	1572	OMG	C4'-C5'-O5'-P
11	AA	2870	5MC	O4'-C1'-N1-C6
57	c	1269	OMU	O4'-C1'-N1-C6
11	AA	2870	5MC	O4'-C1'-N1-C2
57	c	1280	4AC	C2'-C1'-N1-C6
11	AA	2281	A2M	C3'-C2'-O2'-CM'
11	AA	817	A2M	C4'-C5'-O5'-P
57	c	1280	4AC	C2'-C1'-N1-C2
57	c	1269	OMU	C2'-C1'-N1-C6
11	AA	2870	5MC	C4'-C5'-O5'-P
11	AA	2197	OMC	C2'-C1'-N1-C6
57	c	796	A2M	O4'-C4'-C5'-O5'
11	AA	2948	OMC	C2'-C1'-N1-C6
11	AA	2197	OMC	O4'-C1'-N1-C6
57	c	1269	OMU	C2'-C1'-N1-C2
11	AA	650	OMC	O4'-C4'-C5'-O5'
57	c	1280	4AC	C3'-C4'-C5'-O5'
57	c	1191	B8N	O4'-C1'-C5-C6
11	AA	1437	OMC	C4'-C5'-O5'-P
57	c	1269	OMU	O4'-C1'-N1-C2
11	AA	817	A2M	O4'-C4'-C5'-O5'
11	AA	2256	A2M	O4'-C4'-C5'-O5'
11	AA	2948	OMC	O4'-C4'-C5'-O5'
57	c	1126	OMG	C3'-C4'-C5'-O5'
11	AA	2347	OMU	C2'-C1'-N1-C2
11	AA	2948	OMC	C2'-C1'-N1-C2
11	AA	2815	OMG	C3'-C2'-O2'-CM2
11	AA	2281	A2M	C3'-C4'-C5'-O5'
57	c	1575	G7M	C3'-C4'-C5'-O5'
57	c	1773	4AC	C2'-C1'-N1-C2
57	c	28	A2M	C4'-C5'-O5'-P
11	AA	898	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 172 ligands modelled in this entry, 171 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	GTP	Aa	901	82	26,34,34	0.99	1 (3%)	32,54,54	1.59	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	GTP	Aa	901	82	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Aa	901	GTP	C6-N1	-2.97	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	Aa	901	GTP	PB-O3B-PG	-4.43	117.61	132.83
84	Aa	901	GTP	PA-O3A-PB	-4.25	118.25	132.83
84	Aa	901	GTP	C3'-C2'-C1'	3.25	105.86	100.98
84	Aa	901	GTP	C5-C6-N1	2.17	117.79	113.95
84	Aa	901	GTP	C8-N7-C5	2.09	106.97	102.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

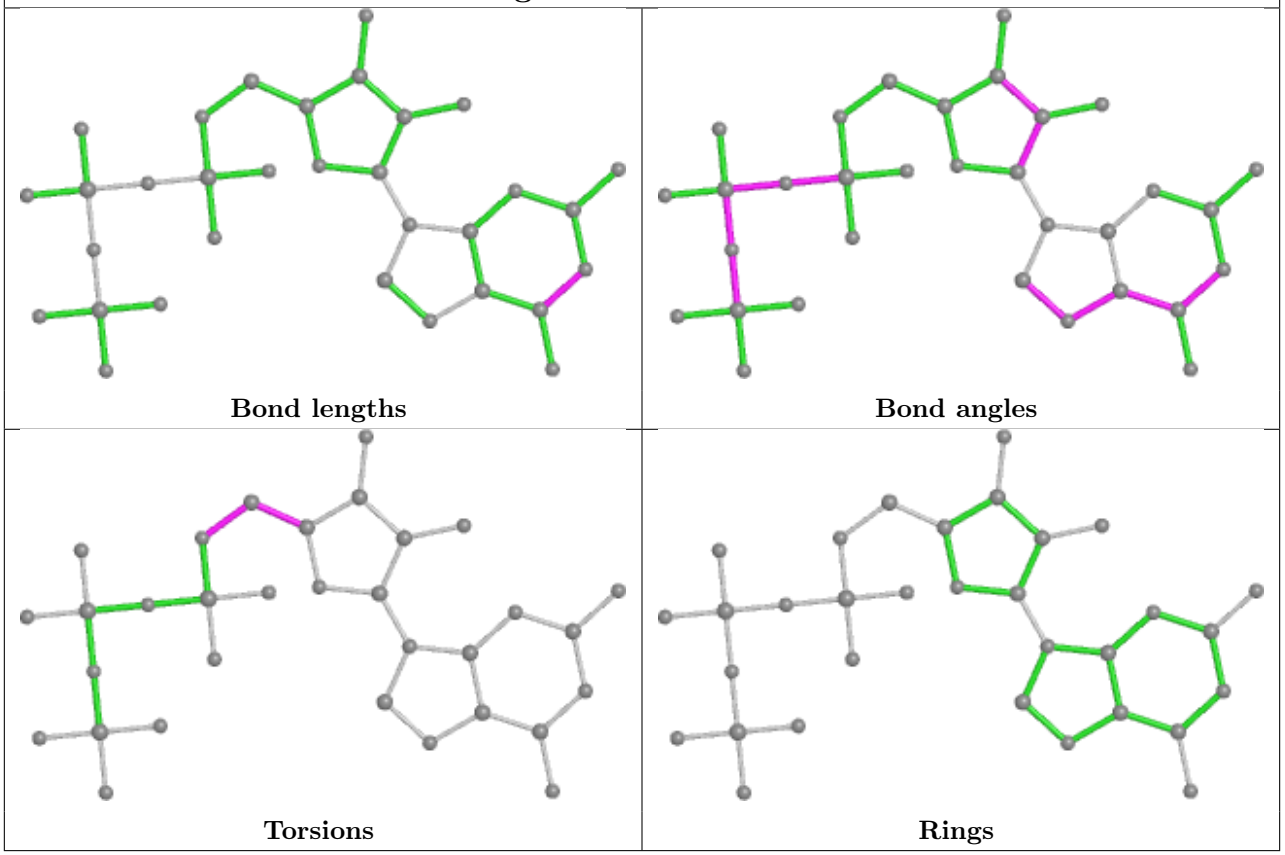
Mol	Chain	Res	Type	Atoms
84	Aa	901	GTP	O4'-C4'-C5'-O5'
84	Aa	901	GTP	C3'-C4'-C5'-O5'
84	Aa	901	GTP	C4'-C5'-O5'-PA

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 GTP Aa 901



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16729. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.