Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 02:17 pm BST

PDB ID	:	8CCS
EMDB ID	:	EMD-16563
Title	:	80S S. cerevisiae ribosome with ligands in hybrid-1 pre-translocation (PRE-H1) complex
Authors	:	Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2023-01-27
Resolution	:	1.97 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:

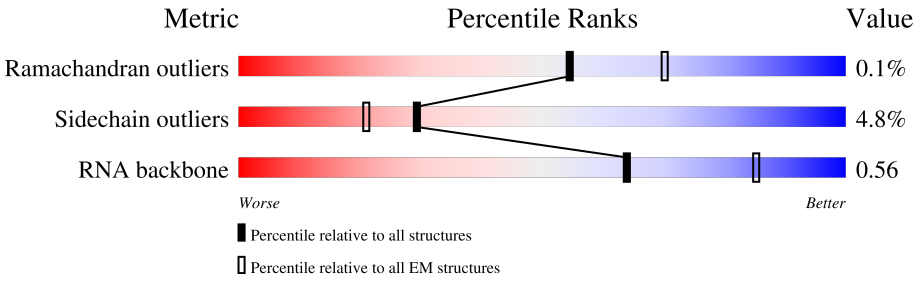
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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	91% 8% ·
2	1	108	62% · 35%
3	2	119	76% 5% 18%
4	3	82	98% ··
5	4	67	85% 9% 6%
6	5	56	80% 14% 5%
7	6	63	76% 8% 16%
8	7	319	87% 12%
9	8	152	22% · 76%

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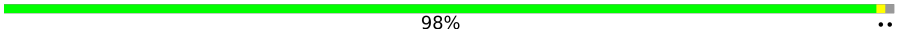
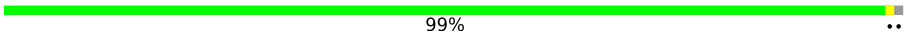
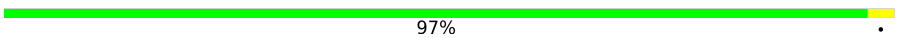
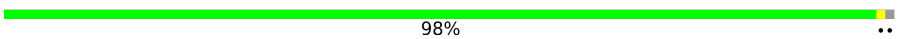
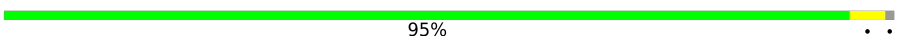
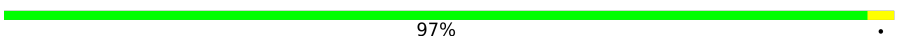
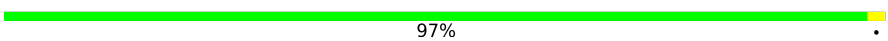
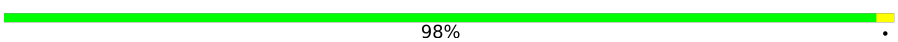
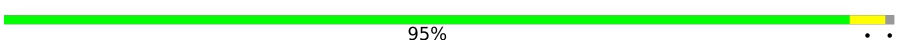
Mol	Chain	Length	Quality of chain
10	A	199	
11	AA	3396	
12	B	184	
13	BB	121	
14	Bb	76	
15	C	186	
16	CC	158	
17	Cc	77	
18	D	189	
19	DD	312	
20	Dd	39	
21	E	172	
22	EE	254	
23	Ee	165	
24	F	160	
25	FF	387	
26	G	121	
27	GG	362	
28	H	137	
29	HH	297	
30	I	155	
31	II	176	
32	J	142	
33	JJ	244	
34	K	127	

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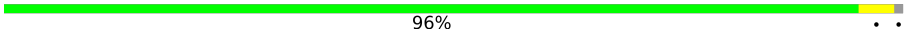
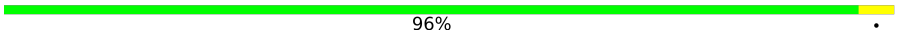
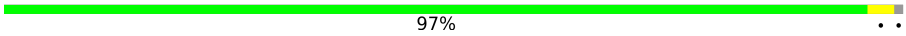
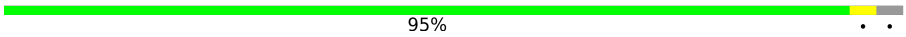
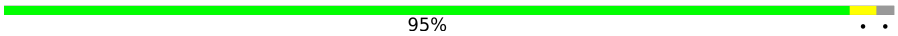
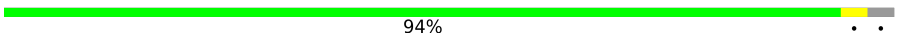
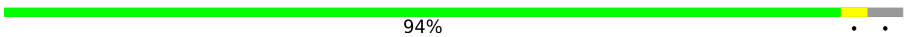
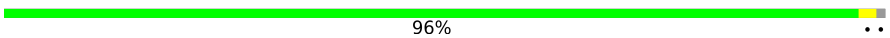
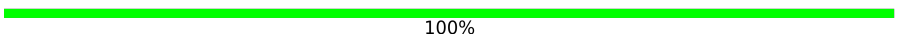
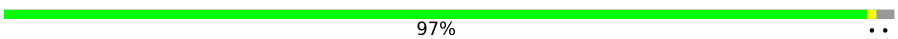
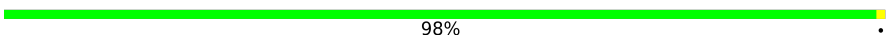
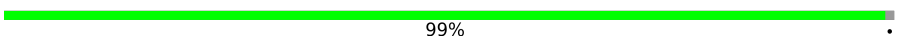
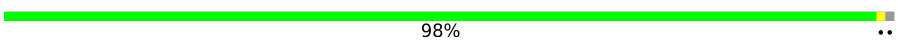
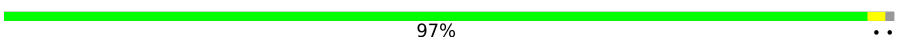
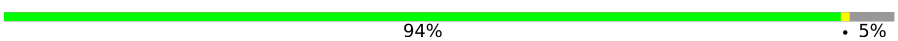
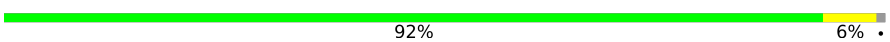
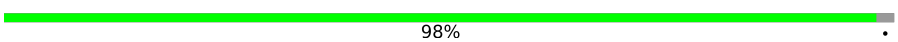
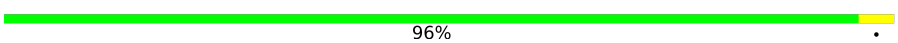
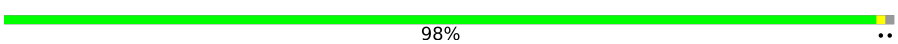
Mol	Chain	Length	Quality of chain
35	KK	256	
36	L	136	
37	LL	191	
38	M	149	
39	MM	221	
40	N	59	
41	NN	174	
42	O	105	
43	OO	199	
44	P	113	
45	PP	138	
46	Pp	2	
47	Q	130	
48	QQ	204	
49	R	107	
50	S	121	
51	T	120	
52	U	100	
53	V	88	
54	W	78	
55	X	51	
56	Y	128	
57	Z	25	
58	a	106	
59	b	92	

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Mol	Chain	Length	Quality of chain
60	c	1800	72% 17% 11%
61	d	252	80% 18%
62	e	255	78% 5% 17%
63	f	254	82% 15%
64	g	240	80% 6% 14%
65	h	261	93% 6%
66	i	225	82% 6% 12%
67	j	236	89% 7%
68	k	190	89% 8%
69	l	200	88% 8%
70	m	197	87% 7% 6%
71	n	105	83% 13%
72	o	156	87% 9%
73	p	151	95%
74	q	137	91% 7%
75	r	142	70% 27%
76	s	143	89% 7%
77	t	136	74% 14% 11%
78	u	146	95% 5%
79	v	144	94% 5%
80	w	121	74% 8% 17%
81	x	87	95% 5%
82	y	130	98%
83	z	145	94% 5%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 201697 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	53	442	274	92	72	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	3190	Total	C	N	O	P	0	0
			68285	30524	12313	22258	3190		

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 13 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 14 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Bb	76	Total	C	N	O	P	0	0
			1638	736	294	533	75		

- 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 RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cc	77	Total	C	N	O	P	0	0
			1644	732	298	537	77		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cc	18	C	U	conflict	GB 170517292

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 19 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 20 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Dd	13	Total	C	N	O	P	0	0
			278	125	50	90	13		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L12-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L3.

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

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

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

- Molecule 27 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L5.

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

- Molecule 30 is a protein called 60S ribosomal protein L24-A.

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

- Molecule 31 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L25.

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

- Molecule 33 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L28.

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

- Molecule 39 is a protein called 60S ribosomal protein L10.

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

- Molecule 40 is a protein called 60S ribosomal protein L29.

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

- Molecule 41 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 42 is a protein called 60S ribosomal protein L30.

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

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 46 is a protein called di-peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Pp	2	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 47 is a protein called 60S ribosomal protein L32.

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

- Molecule 48 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 49 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L38.

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

- Molecule 55 is a protein called 60S ribosomal protein L39.

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

- Molecule 56 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 57 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 58 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 59 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 60 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	c	1604	Total	C	N	O	P	0	0
			34236	15322	6079	11231	1604		

- Molecule 61 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 63 is a protein called 40S ribosomal protein S2.

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

- Molecule 64 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	g	206	Total	C	N	O	S	0	0
			1601	1014	294	287	6		

- Molecule 65 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 66 is a protein called 40S ribosomal protein S5.

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

- Molecule 67 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S8-B.

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

- Molecule 70 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	n	91	Total	C	N	O	S	0	0
			772	503	123	144	2		

- Molecule 72 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S13.

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

- Molecule 74 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	r	104	Total	C	N	O	S	0	0
			837	533	155	143	6		

- Molecule 76 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	s	137	Total	C	N	O	0	0
			1080	692	199	189		

- Molecule 77 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 78 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 79 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 80 is a protein called 40S ribosomal protein S20.

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

- Molecule 81 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 82 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 83 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	2	1	Total	Zn	0
			1	1	
84	5	1	Total	Zn	0
			1	1	
84	8	1	Total	Zn	0
			1	1	
84	S	1	Total	Zn	0
			1	1	
84	V	1	Total	Zn	0
			1	1	
84	Y	1	Total	Zn	0
			1	1	
84	a	1	Total	Zn	0
			1	1	
84	b	1	Total	Zn	0
			1	1	

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	AA	205	Total	Mg	0
			205	205	
85	B	1	Total	Mg	0
			1	1	
85	BB	5	Total	Mg	0
			5	5	
85	Bb	1	Total	Mg	0
			1	1	
85	CC	3	Total	Mg	0
			3	3	
85	Cc	1	Total	Mg	0
			1	1	
85	Dd	1	Total	Mg	0
			1	1	
85	FF	1	Total	Mg	0
			1	1	
85	H	1	Total	Mg	0
			1	1	

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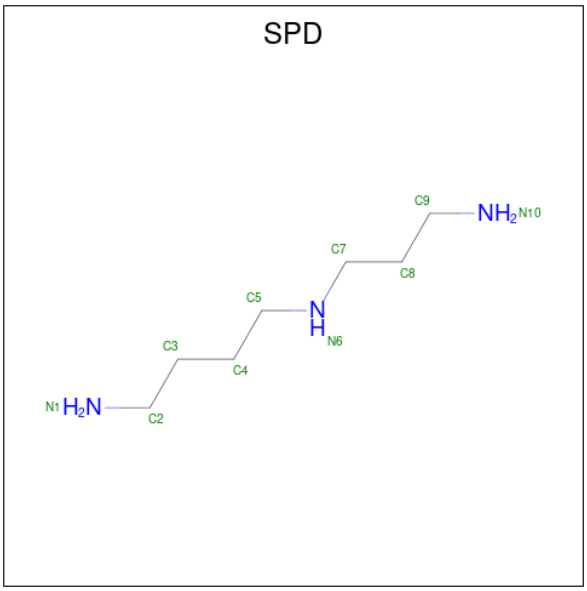
Mol	Chain	Residues	Atoms	AltConf
85	QQ	1	Total Mg 1 1	0
85	V	1	Total Mg 1 1	0
85	c	60	Total Mg 60 60	0

- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
86	AA	12	Total K 12 12	0
86	EE	1	Total K 1 1	0
86	MM	1	Total K 1 1	0
86	Q	1	Total K 1 1	0
86	S	1	Total K 1 1	0
86	a	1	Total K 1 1	0
86	c	4	Total K 4 4	0
86	q	1	Total K 1 1	0

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
87	AA	1	Total C N 10 7 3	0
87	AA	1	Total C N 10 7 3	0
87	AA	1	Total C N 10 7 3	0
87	c	1	Total C N 10 7 3	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms	AltConf
88	2	1	Total O 1 1	0
88	A	2	Total O 2 2	0
88	AA	877	Total O 877 877	0
88	B	3	Total O 3 3	0
88	BB	12	Total O 12 12	0
88	Bb	5	Total O 5 5	0
88	CC	18	Total O 18 18	0
88	Cc	6	Total O 6 6	0

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Mol	Chain	Residues	Atoms	AltConf
88	D	4	Total O 4 4	0
88	Dd	4	Total O 4 4	0
88	EE	9	Total O 9 9	0
88	F	4	Total O 4 4	0
88	FF	4	Total O 4 4	0
88	GG	3	Total O 3 3	0
88	H	3	Total O 3 3	0
88	HH	1	Total O 1 1	0
88	J	1	Total O 1 1	0
88	JJ	2	Total O 2 2	0
88	LL	1	Total O 1 1	0
88	M	3	Total O 3 3	0
88	MM	2	Total O 2 2	0
88	N	1	Total O 1 1	0
88	Q	4	Total O 4 4	0
88	QQ	9	Total O 9 9	0
88	S	2	Total O 2 2	0
88	V	3	Total O 3 3	0
88	a	2	Total O 2 2	0
88	c	226	Total O 226 226	0
88	h	2	Total O 2 2	0

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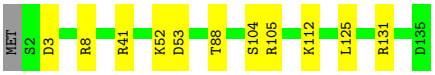
Mol	Chain	Residues	Atoms	AltConf
88	o	2	Total O 2 2	0
88	p	2	Total O 2 2	0
88	q	2	Total O 2 2	0
88	v	3	Total O 3 3	0
88	z	1	Total O 1 1	0

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.

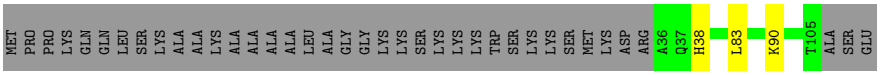
• Molecule 1: 40S ribosomal protein S24-A

Chain 0:



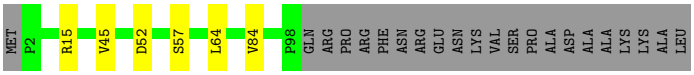
• Molecule 2: 40S ribosomal protein S25-A

Chain 1:



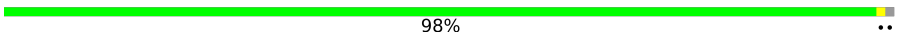
• Molecule 3: 40S ribosomal protein S26

Chain 2:



• Molecule 4: 40S ribosomal protein S27-A

Chain 3:



• Molecule 5: 40S ribosomal protein S28-A

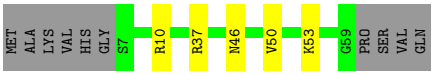
Chain 4:

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

Chain 5:

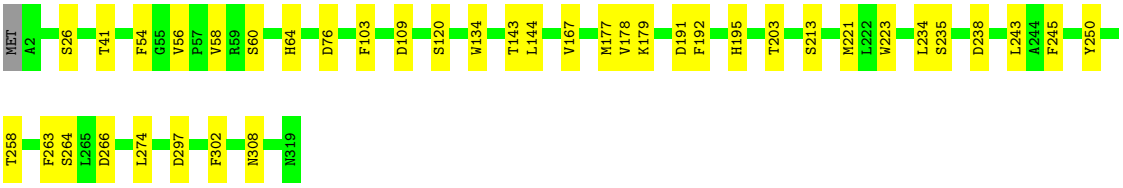
• Molecule 7: 40S ribosomal protein S30-A

Chain 6:



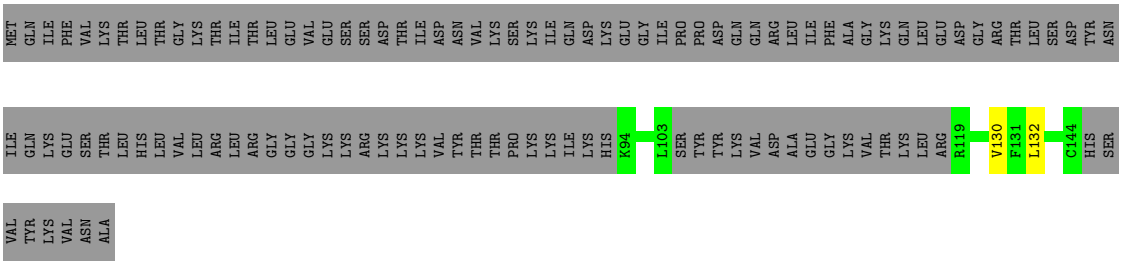
• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

Chain 7:



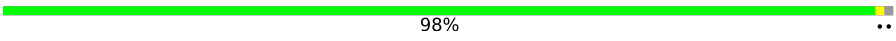
• Molecule 9: Ubiquitin-40S ribosomal protein S31

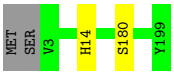
Chain 8:



• Molecule 10: 60S ribosomal protein L16-A

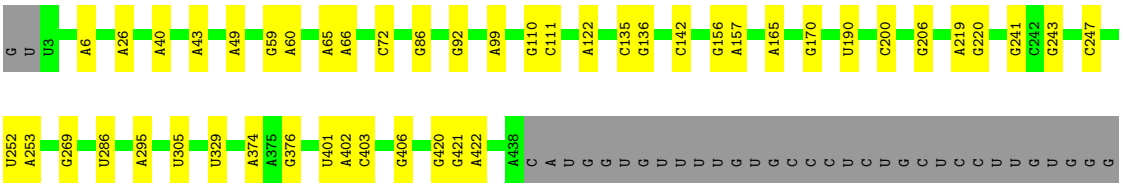
Chain A:

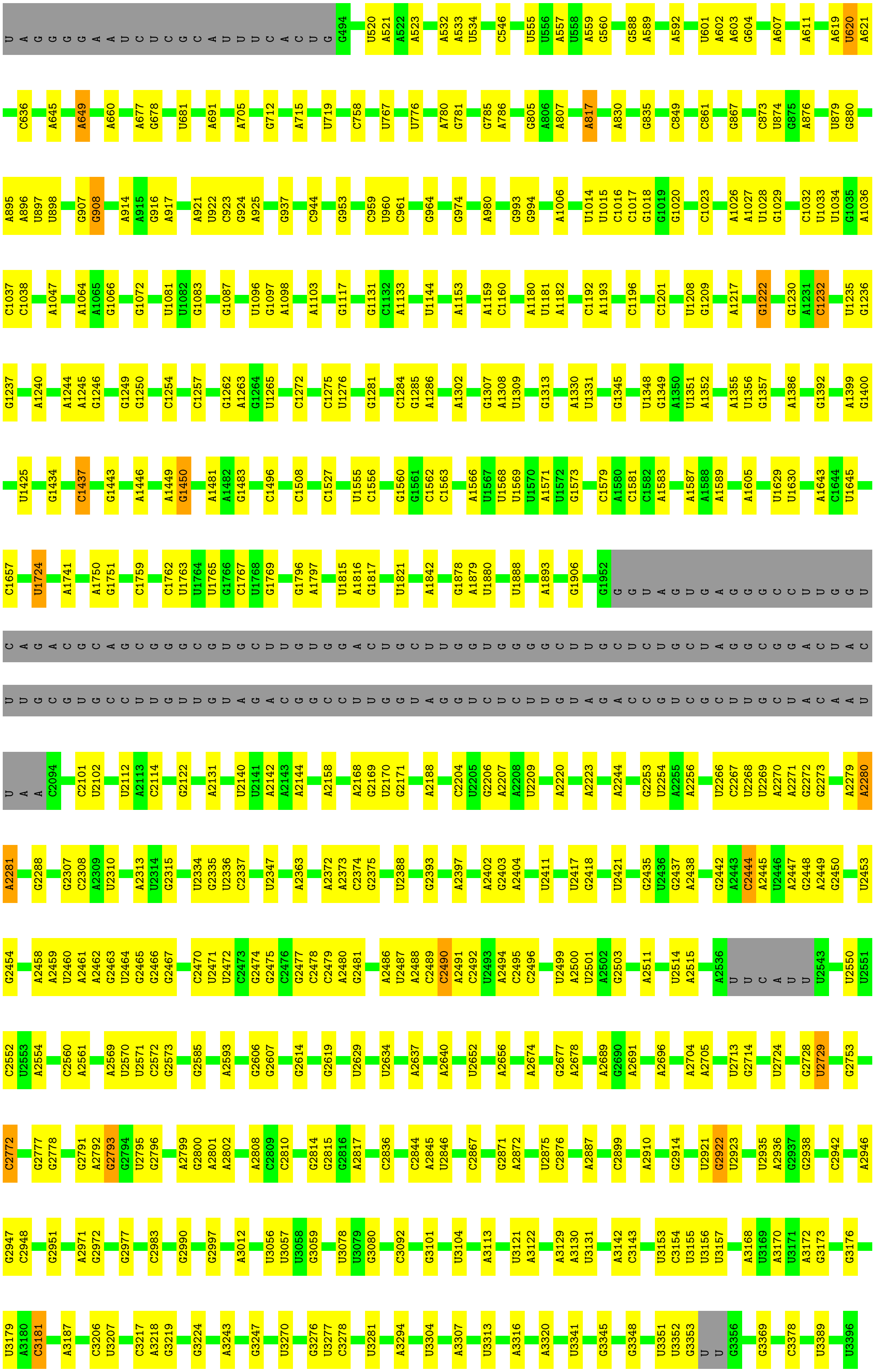




• Molecule 11: 25S ribosomal RNA

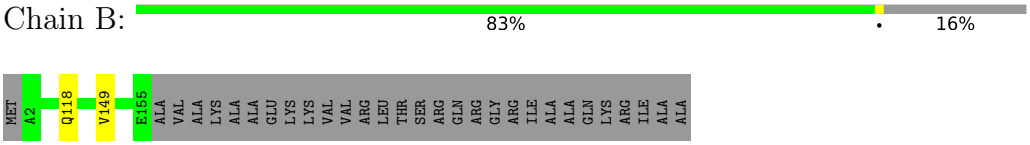
Chain AA:





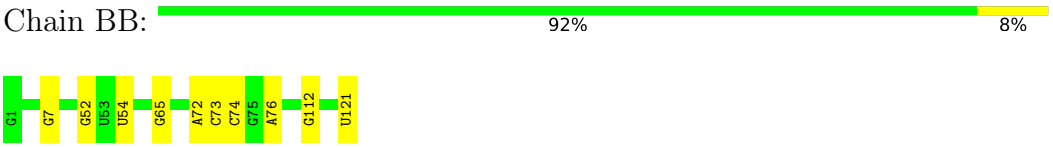
• Molecule 12: 60S ribosomal protein L17-A

Chain B:



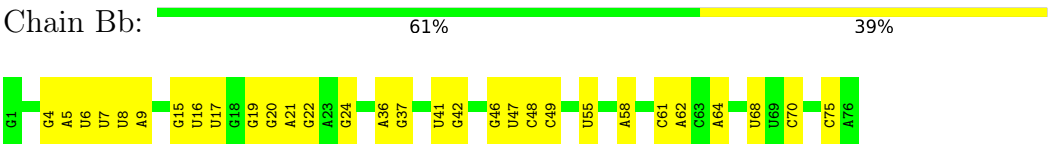
• Molecule 13: 5S ribosomal RNA

Chain BB:



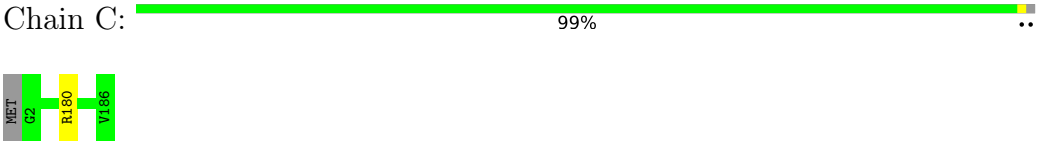
• Molecule 14: Transfer RNA Phe

Chain Bb:



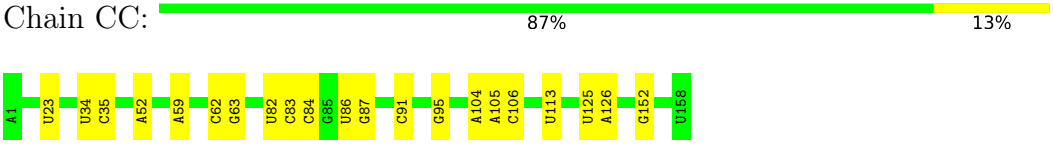
• Molecule 15: 60S ribosomal protein L18-A

Chain C:



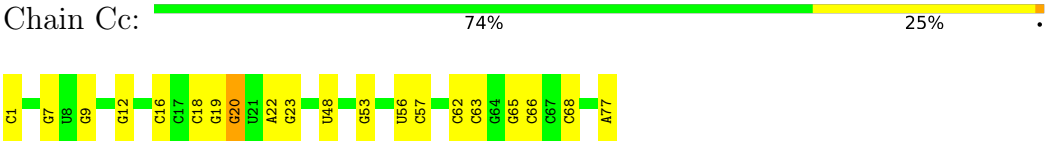
• Molecule 16: 5.8S ribosomal RNA

Chain CC:



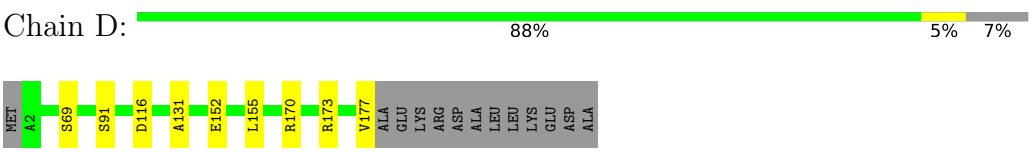
• Molecule 17: Transfer RNA fMet

Chain Cc:



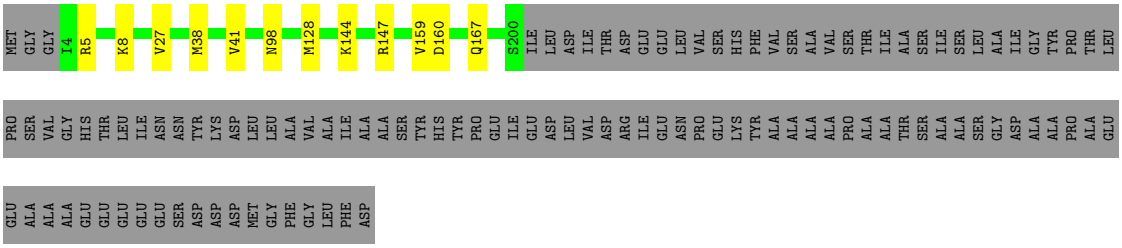
• Molecule 18: 60S ribosomal protein L19-A

Chain D:



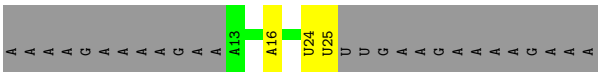
• Molecule 19: 60S acidic ribosomal protein P0

Chain DD:



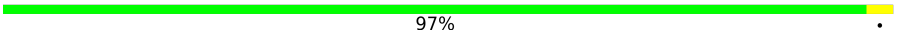
• Molecule 20: Messenger RNA

Chain Dd:



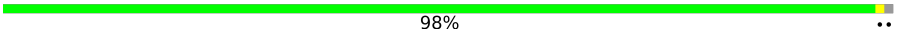
• Molecule 21: 60S ribosomal protein L20-A

Chain E:



• Molecule 22: 60S ribosomal protein L2-A

Chain EE:

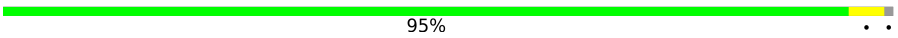


• Molecule 23: 60S ribosomal protein L12-A

Chain Ee:

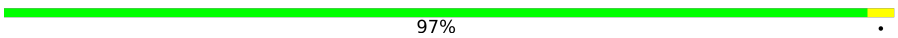
• Molecule 24: 60S ribosomal protein L21-A

Chain F:



• Molecule 25: 60S ribosomal protein L3

Chain FF:

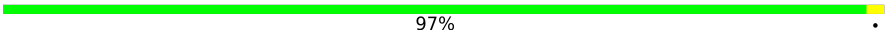


• Molecule 26: 60S ribosomal protein L22-A

Chain G:

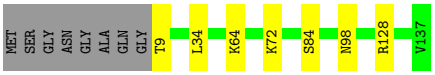
• Molecule 27: 60S ribosomal protein L4-A

Chain GG:



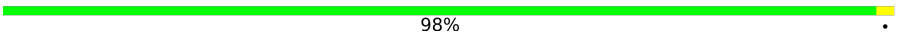
• Molecule 28: 60S ribosomal protein L23-A

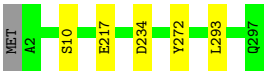
Chain H:



• Molecule 29: 60S ribosomal protein L5

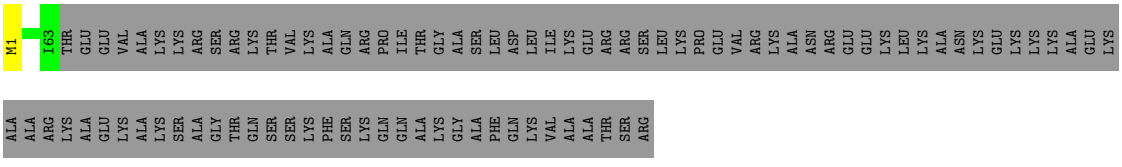
Chain HH:





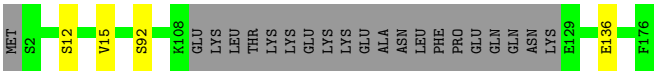
• Molecule 30: 60S ribosomal protein L24-A

Chain I:



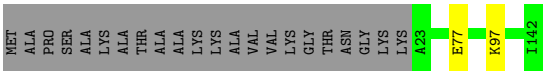
• Molecule 31: 60S ribosomal protein L6-A

Chain II:



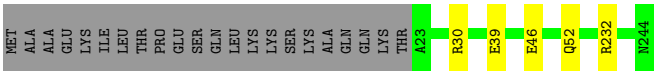
• Molecule 32: 60S ribosomal protein L25

Chain J:



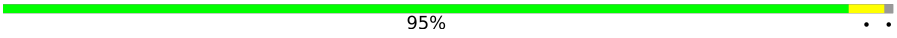
• Molecule 33: 60S ribosomal protein L7-A

Chain JJ:



• Molecule 34: 60S ribosomal protein L26-A

Chain K:

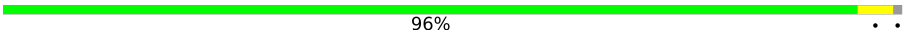


• Molecule 35: 60S ribosomal protein L8-A

Chain KK:

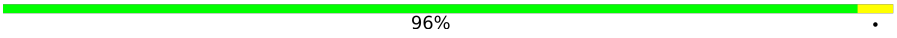
• Molecule 36: 60S ribosomal protein L27-A

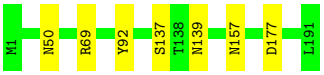
Chain L:



• Molecule 37: 60S ribosomal protein L9-A

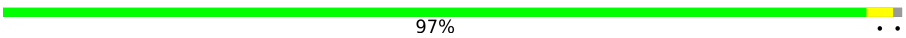
Chain LL:





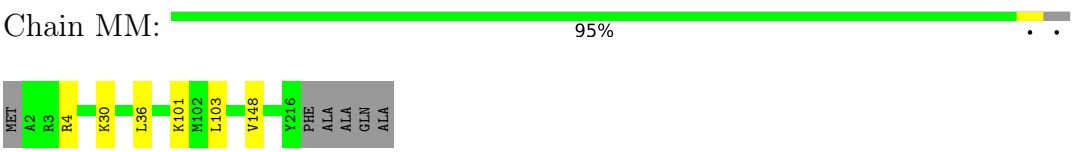
• Molecule 38: 60S ribosomal protein L28

Chain M:



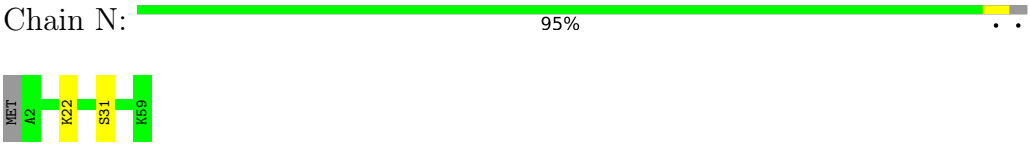
• Molecule 39: 60S ribosomal protein L10

Chain MM:



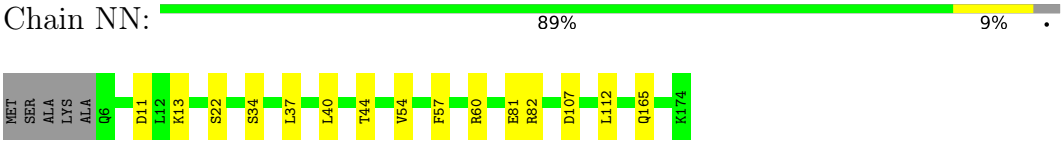
• Molecule 40: 60S ribosomal protein L29

Chain N:



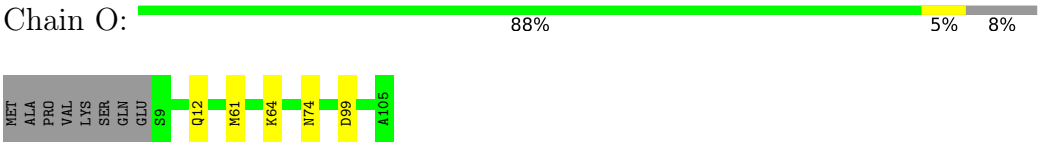
• Molecule 41: 60S ribosomal protein L11-A

Chain NN:



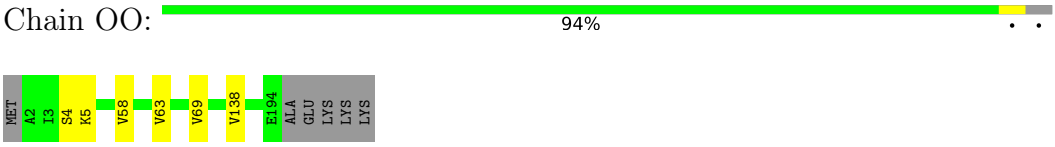
• Molecule 42: 60S ribosomal protein L30

Chain O:



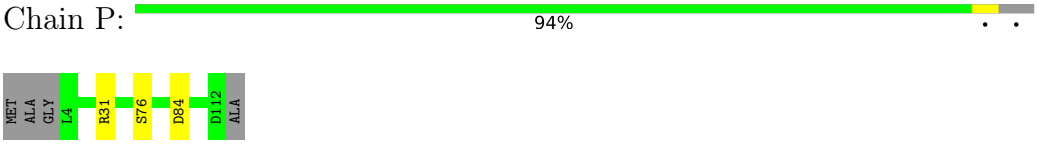
• Molecule 43: 60S ribosomal protein L13-A

Chain OO:



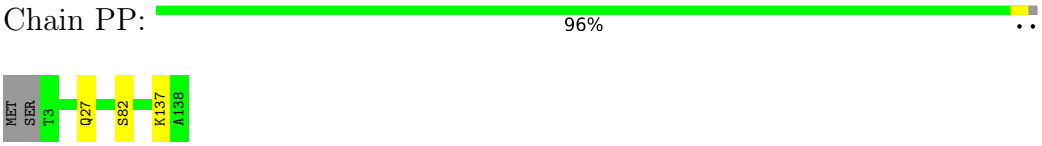
• Molecule 44: 60S ribosomal protein L31-A

Chain P:



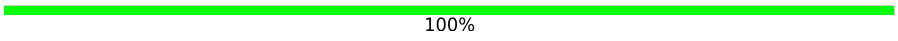
• Molecule 45: 60S ribosomal protein L14-A

Chain PP:



• Molecule 46: di-peptide

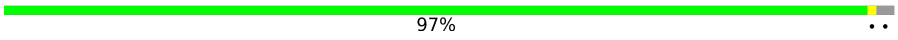
Chain Pp:

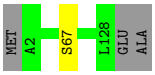


There are no outlier residues recorded for this chain.

• Molecule 47: 60S ribosomal protein L32

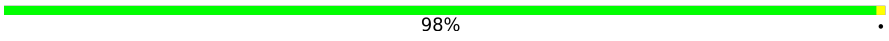
Chain Q:





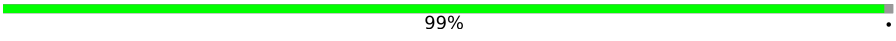
• Molecule 48: 60S ribosomal protein L15-A

Chain QQ:



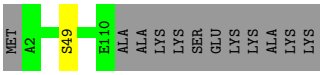
• Molecule 49: 60S ribosomal protein L33-A

Chain R:



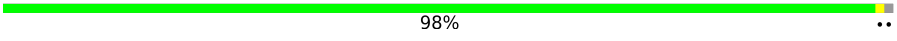
• Molecule 50: 60S ribosomal protein L34-A

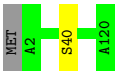
Chain S:



• Molecule 51: 60S ribosomal protein L35-A

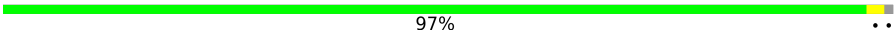
Chain T:





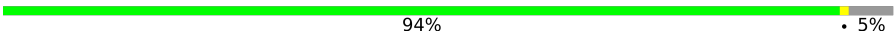
• Molecule 52: 60S ribosomal protein L36-A

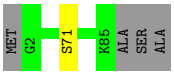
Chain U:



• Molecule 53: 60S ribosomal protein L37-A

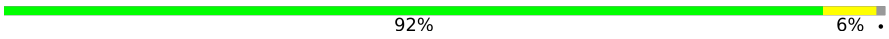
Chain V:





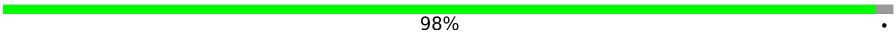
• Molecule 54: 60S ribosomal protein L38

Chain W:



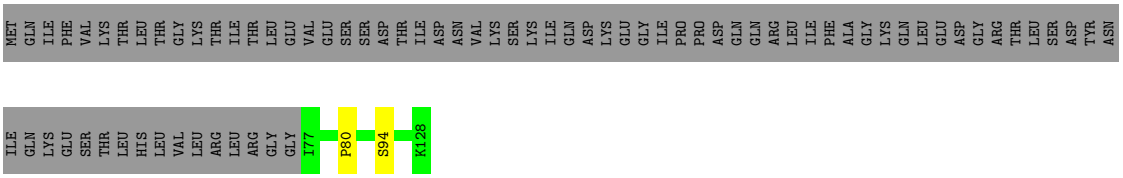
• Molecule 55: 60S ribosomal protein L39

Chain X:



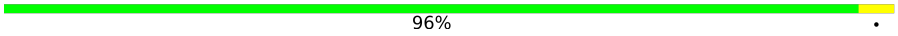
• Molecule 56: Ubiquitin-60S ribosomal protein L40

Chain Y:



• Molecule 57: 60S ribosomal protein L41-A

Chain Z:

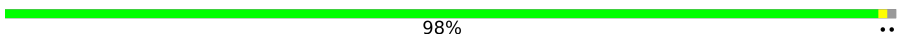


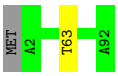
• Molecule 58: 60S ribosomal protein L42-A

Chain a:

• Molecule 59: 60S ribosomal protein L43-A

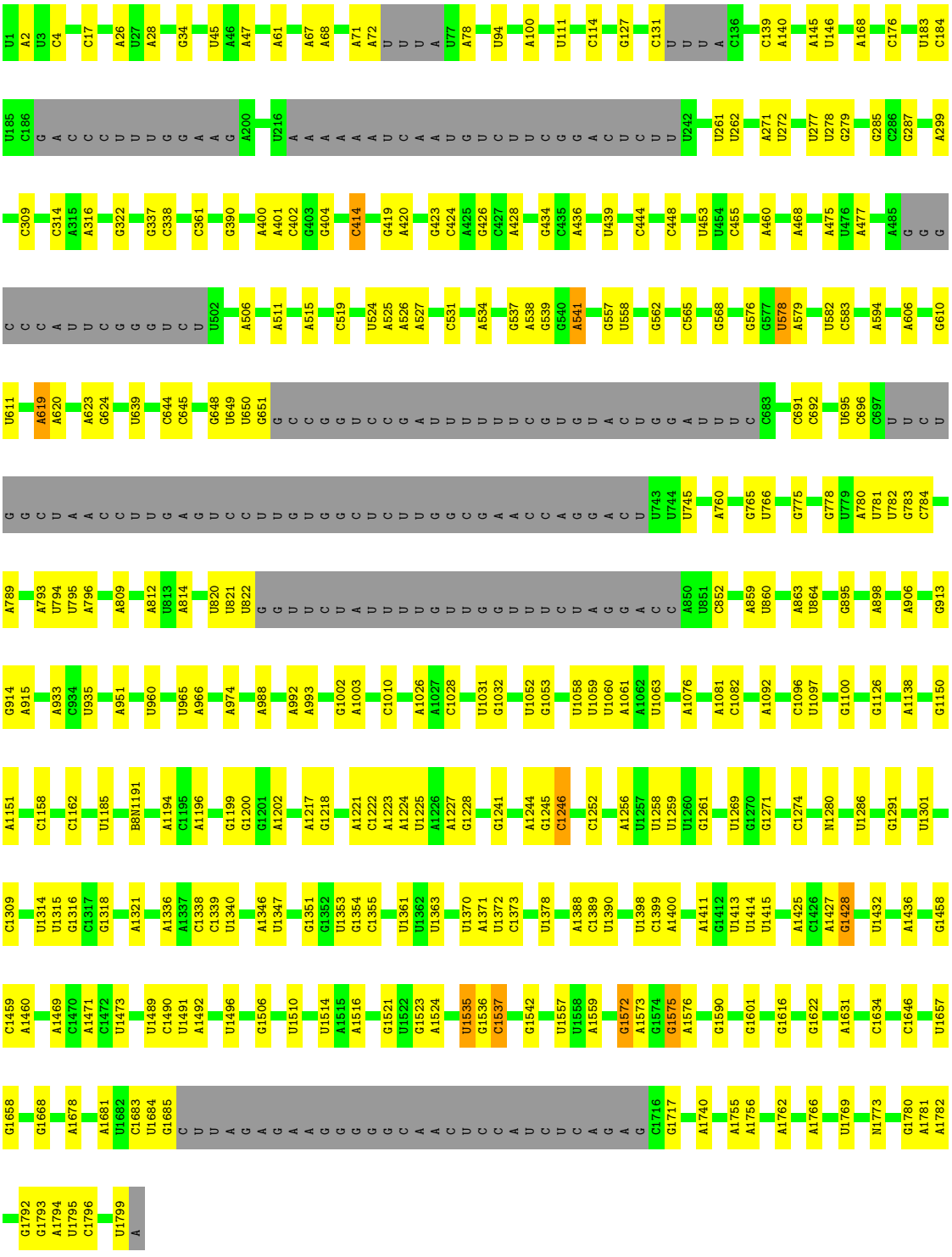
Chain b:





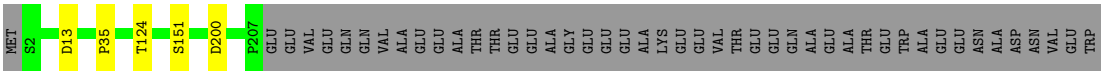
• Molecule 60: 18S ribosomal RNA

Chain c:



• Molecule 61: 40S ribosomal protein S0-A

Chain d:



• Molecule 62: 40S ribosomal protein S1-A

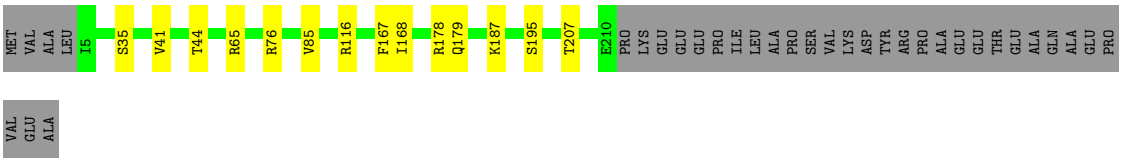
Chain e:

• Molecule 63: 40S ribosomal protein S2

Chain f:

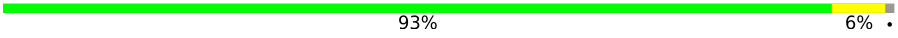
• Molecule 64: RPS3 isoform 1

Chain g:



• Molecule 65: 40S ribosomal protein S4-A

Chain h:

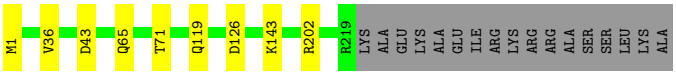


• Molecule 66: 40S ribosomal protein S5

Chain i:

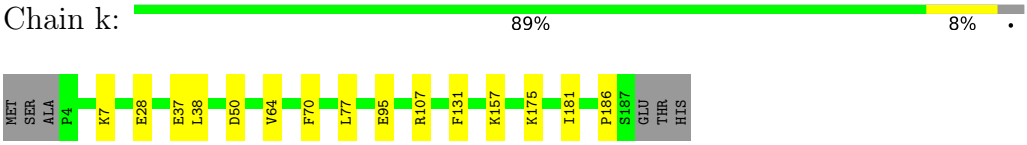
• Molecule 67: 40S ribosomal protein S6-A

Chain j:



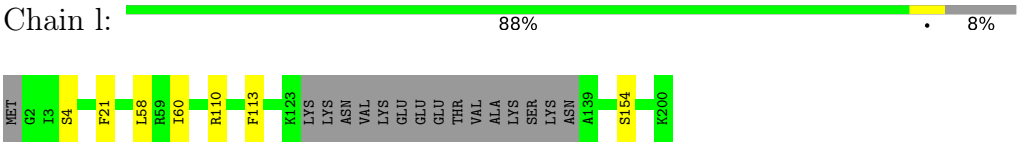
• Molecule 68: 40S ribosomal protein S7-A

Chain k:



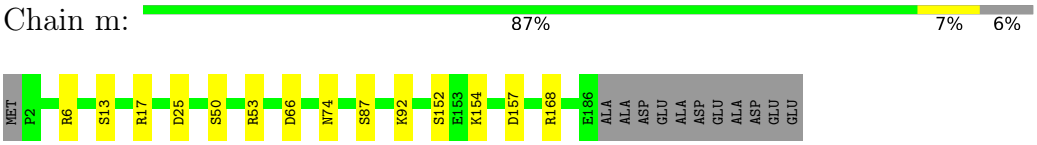
• Molecule 69: 40S ribosomal protein S8-B

Chain l:



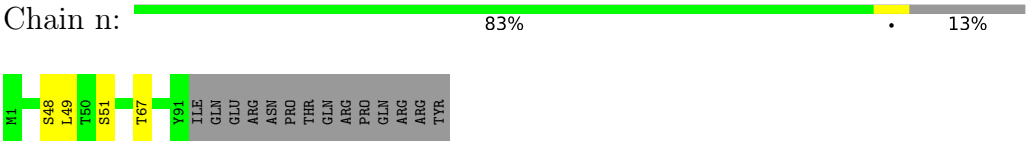
• Molecule 70: 40S ribosomal protein S9-A

Chain m:



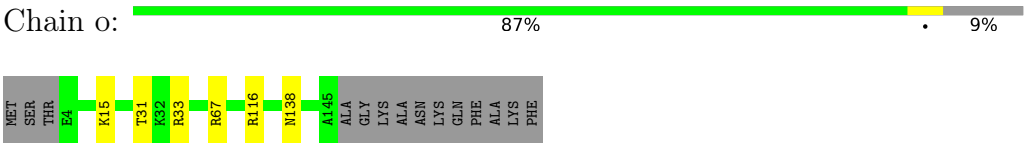
• Molecule 71: 40S ribosomal protein S10-A

Chain n:



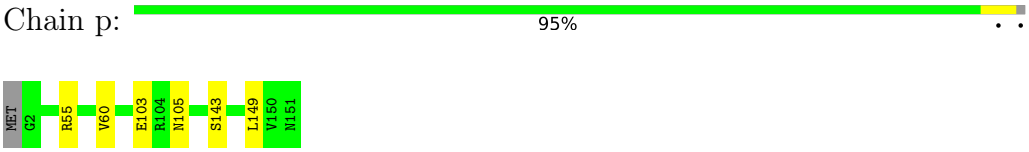
• Molecule 72: 40S ribosomal protein S11-A

Chain o:



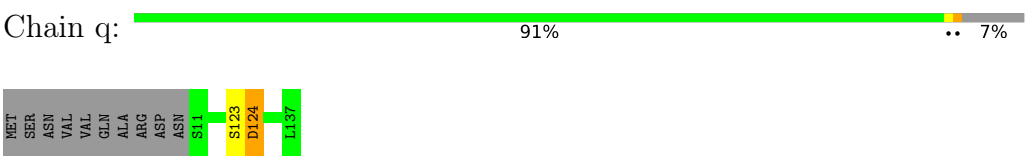
• Molecule 73: 40S ribosomal protein S13

Chain p:



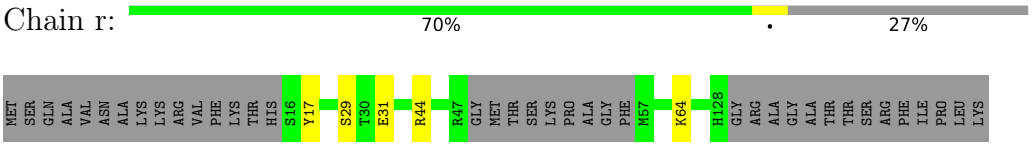
• Molecule 74: 40S ribosomal protein S14-A

Chain q:



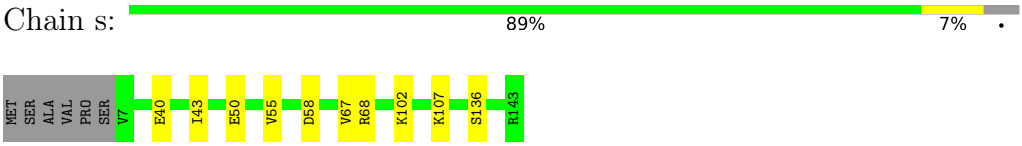
• Molecule 75: 40S ribosomal protein S15

Chain r:



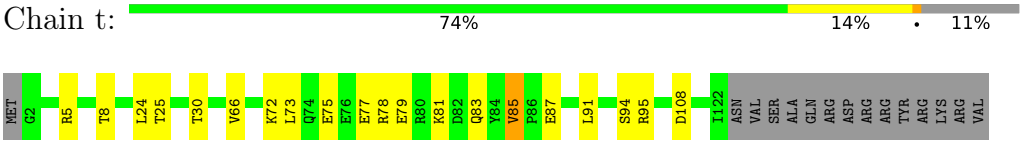
• Molecule 76: 40S ribosomal protein S16-A

Chain s:



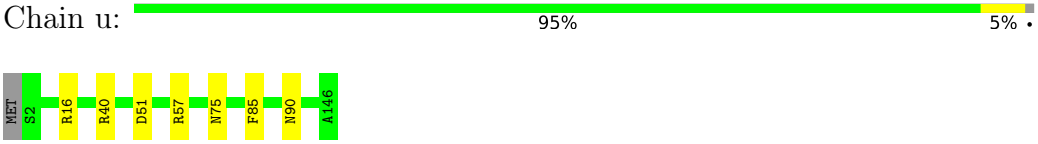
• Molecule 77: 40S ribosomal protein S17-A

Chain t:



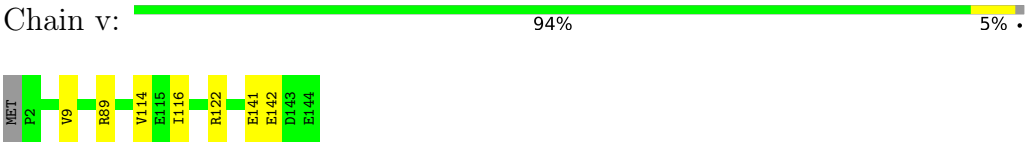
• Molecule 78: 40S ribosomal protein S18-A

Chain u:



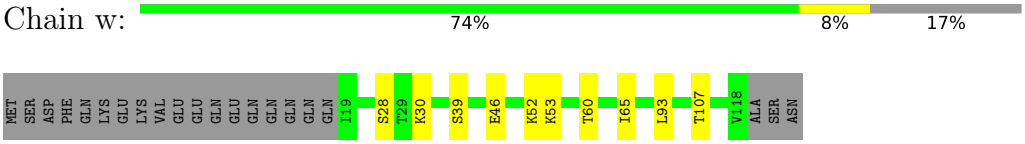
• Molecule 79: 40S ribosomal protein S19-A

Chain v:



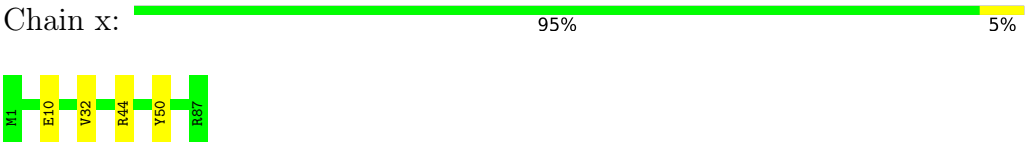
• Molecule 80: 40S ribosomal protein S20

Chain w:



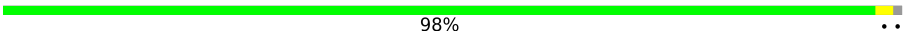
• Molecule 81: 40S ribosomal protein S21-A

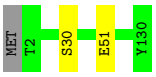
Chain x:



• Molecule 82: 40S ribosomal protein S22-A

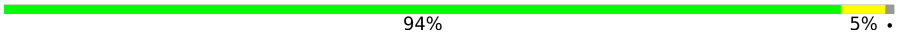
Chain y:





• Molecule 83: 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	55455	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	270000	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: 1MA, ZN, 4AC, A2M, SPD, K, UR3, MG, 5MC, OMG, YYG, OMU, B8N, MA6, OMC, G7M

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	0.55	0/1449
2	1	0.29	0/571	0.68	1/768 (0.1%)
3	2	0.29	0/782	0.62	0/1047
4	3	0.28	0/620	0.54	0/838
5	4	0.29	0/499	0.65	0/670
6	5	0.29	0/452	0.58	0/600
7	6	0.28	0/433	0.59	0/575
8	7	0.27	0/2489	0.58	0/3389
9	8	0.24	0/279	0.51	0/369
10	A	0.33	0/1585	0.54	0/2128
11	AA	0.53	0/75384	0.81	38/117530 (0.0%)
12	B	0.32	0/1245	0.54	0/1676
13	BB	0.48	0/2883	0.76	0/4491
14	Bb	0.30	0/1788	0.84	0/2786
15	C	0.30	0/1465	0.56	0/1965
16	CC	0.53	0/3746	0.78	0/5832
17	Cc	0.41	1/1836 (0.1%)	0.77	1/2859 (0.0%)
18	D	0.28	0/1440	0.58	0/1921
19	DD	0.27	0/1558	0.54	0/2107
20	Dd	0.41	0/311	0.72	0/482
21	E	0.32	0/1481	0.55	0/1990
22	EE	0.32	0/1948	0.58	0/2617
23	Ee	0.25	0/1210	0.52	0/1627
24	F	0.32	0/1300	0.53	0/1743
25	FF	0.32	0/3146	0.56	0/4228
26	G	0.31	0/786	0.49	0/1065
27	GG	0.30	0/2800	0.53	0/3790
28	H	0.32	0/978	0.56	0/1316
29	HH	0.30	0/2425	0.52	0/3271
30	I	0.30	0/533	0.53	0/707
31	II	0.32	0/1251	0.53	0/1682
32	J	0.32	0/974	0.54	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	JJ	0.32	0/1821	0.50	0/2451
34	K	0.30	0/1004	0.58	1/1341 (0.1%)
35	KK	0.30	0/1836	0.49	0/2481
36	L	0.32	0/1118	0.50	0/1497
37	LL	0.31	0/1539	0.53	0/2073
38	M	0.31	0/1204	0.55	0/1612
39	MM	0.31	0/1779	0.55	0/2386
40	N	0.28	0/473	0.52	0/629
41	NN	0.30	0/1374	0.57	0/1842
42	O	0.31	0/750	0.46	0/1008
43	OO	0.31	0/1568	0.59	0/2106
44	P	0.30	0/897	0.57	0/1205
45	PP	0.29	0/1068	0.51	0/1438
46	Pp	0.40	0/19	1.24	0/23
47	Q	0.30	0/1041	0.52	0/1394
48	QQ	0.33	0/1757	0.59	0/2354
49	R	0.35	0/868	0.57	0/1168
50	S	0.30	0/871	0.56	0/1164
51	T	0.29	0/978	0.53	0/1301
52	U	0.27	0/778	0.58	0/1034
53	V	0.33	0/680	0.60	0/901
54	W	0.31	0/618	0.59	0/826
55	X	0.30	0/443	0.65	0/588
56	Y	0.28	0/423	0.54	0/562
57	Z	0.27	0/234	0.70	0/300
58	a	0.31	0/831	0.59	0/1097
59	b	0.31	0/701	0.58	0/934
60	c	0.45	0/37665	0.81	29/58663 (0.0%)
61	d	0.30	0/1623	0.55	0/2222
62	e	0.29	0/1714	0.54	0/2308
63	f	0.30	0/1665	0.54	0/2263
64	g	0.30	0/1622	0.58	1/2180 (0.0%)
65	h	0.28	0/2097	0.54	0/2823
66	i	0.27	0/1591	0.56	0/2151
67	j	0.27	0/1790	0.57	0/2393
68	k	0.28	0/1506	0.56	1/2028 (0.0%)
69	l	0.28	0/1482	0.58	0/1980
70	m	0.27	0/1519	0.54	0/2035
71	n	0.31	0/792	0.57	0/1071
72	o	0.30	0/1172	0.54	0/1580
73	p	0.29	0/1215	0.53	0/1638
74	q	0.29	0/901	0.64	0/1217
75	r	0.30	0/853	0.54	0/1145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	s	0.29	0/1099	0.55	0/1473
77	t	0.32	0/971	0.63	0/1303
78	u	0.27	0/1211	0.58	0/1628
79	v	0.29	0/1130	0.55	0/1517
80	w	0.29	0/810	0.54	0/1095
81	x	0.30	0/693	0.59	0/935
82	y	0.32	0/1038	0.57	0/1395
83	z	0.29	0/1139	0.55	0/1518
All	All	0.43	1/213256 (0.0%)	0.72	72/313108 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	JJ	0	1
36	L	0	1
58	a	0	1
62	e	0	2
66	i	0	2
68	k	0	1
73	p	0	1
74	q	0	2
76	s	0	1
78	u	0	1
83	z	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Cc	1	C	OP3-P	-10.65	1.48	1.61

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	c	94	U	C2-N3-C4	13.64	135.18	127.00
11	AA	406	G	O4'-C1'-N9	9.27	115.61	108.20
11	AA	2269	U	N3-C2-O2	-7.76	116.77	122.20
60	c	1096	C	N1-C2-O2	7.71	123.52	118.90
60	c	1537	C	C2-N1-C1'	7.52	127.07	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2269	U	C2-N1-C1'	7.51	126.71	117.70
60	c	1537	C	N1-C2-O2	7.50	123.40	118.90
11	AA	2269	U	N1-C2-O2	7.34	127.94	122.80
60	c	1535	U	C2-N1-C1'	7.09	126.21	117.70
60	c	94	U	N3-C4-C5	6.90	118.74	114.60
11	AA	2490	C	C2-N1-C1'	6.88	126.37	118.80
34	K	126	LEU	CA-CB-CG	6.82	130.98	115.30
11	AA	835	G	O4'-C1'-N9	6.68	113.54	108.20
11	AA	3278	C	N1-C2-O2	6.48	122.79	118.90
11	AA	2444	C	C2-N1-C1'	6.46	125.91	118.80
11	AA	620	U	C2-N1-C1'	6.44	125.43	117.70
11	AA	620	U	N1-C2-O2	6.43	127.30	122.80
11	AA	620	U	N3-C2-O2	-6.25	117.83	122.20
11	AA	922	U	C2-N1-C1'	6.20	125.14	117.70
60	c	1389	C	C2-N1-C1'	6.20	125.62	118.80
60	c	1096	C	C2-N1-C1'	6.18	125.60	118.80
60	c	1473	U	C2-N1-C1'	6.13	125.06	117.70
11	AA	3278	C	C2-N1-C1'	6.11	125.52	118.80
11	AA	1222	G	O4'-C1'-N9	6.04	113.03	108.20
60	c	852	C	C2-N1-C1'	5.94	125.34	118.80
60	c	1096	C	N3-C2-O2	-5.94	117.75	121.90
2	1	83	LEU	CA-CB-CG	5.92	128.92	115.30
60	c	965	U	C2-N1-C1'	5.90	124.78	117.70
11	AA	1767	C	C2-N1-C1'	5.89	125.28	118.80
64	g	41	VAL	C-N-CA	5.80	136.21	121.70
11	AA	2490	C	N1-C2-O2	5.79	122.37	118.90
11	AA	895	A	N9-C4-C5	-5.78	103.49	105.80
60	c	94	U	N1-C2-N3	5.75	118.35	114.90
11	AA	3181	C	N3-C2-O2	-5.70	117.91	121.90
60	c	1458	G	C4-N9-C1'	5.65	133.85	126.50
60	c	1473	U	N1-C2-O2	5.64	126.75	122.80
60	c	1537	C	N3-C2-O2	-5.62	117.97	121.90
11	AA	895	A	C6-C5-N7	-5.61	128.37	132.30
60	c	453	U	C2-N1-C1'	5.59	124.41	117.70
11	AA	3181	C	N1-C2-O2	5.57	122.24	118.90
11	AA	3057	U	N3-C2-O2	-5.56	118.31	122.20
11	AA	2836	C	N3-C2-O2	-5.52	118.04	121.90
11	AA	2270	A	N7-C8-N9	5.50	116.55	113.80
68	k	38	LEU	CA-CB-CG	5.50	127.96	115.30
60	c	531	C	C2-N1-C1'	5.50	124.85	118.80
11	AA	3278	C	N3-C2-O2	-5.50	118.05	121.90
17	Cc	20	G	O4'-C1'-N9	-5.49	103.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2772	C	N1-C2-O2	5.47	122.18	118.90
11	AA	2772	C	C2-N1-C1'	5.41	124.75	118.80
11	AA	2490	C	C6-N1-C1'	-5.37	114.36	120.80
60	c	610	G	C4-N9-C1'	5.33	133.44	126.50
60	c	1535	U	C6-N1-C1'	-5.31	113.76	121.20
60	c	1537	C	C6-N1-C1'	-5.31	114.43	120.80
11	AA	1496	C	C2-N1-C1'	5.30	124.63	118.80
11	AA	895	A	C4-N9-C1'	5.27	135.78	126.30
60	c	852	C	N1-C2-O2	5.23	122.04	118.90
11	AA	2836	C	C2-N1-C1'	5.21	124.53	118.80
11	AA	895	A	C8-N9-C1'	-5.21	118.33	127.70
60	c	1246	C	C2-N1-C1'	5.21	124.53	118.80
60	c	1389	C	C6-N1-C2	-5.20	118.22	120.30
11	AA	1724	U	O4'-C1'-N1	5.18	112.35	108.20
60	c	852	C	N3-C2-O2	-5.14	118.30	121.90
11	AA	2846	U	C2-N1-C1'	5.13	123.86	117.70
60	c	1535	U	N1-C2-O2	5.12	126.39	122.80
11	AA	2272	G	O4'-C1'-N9	5.11	112.29	108.20
60	c	139	C	C2-N1-C1'	5.10	124.41	118.80
11	AA	2846	U	N3-C2-O2	-5.10	118.63	122.20
11	AA	1232	C	C2-N1-C1'	5.09	124.40	118.80
11	AA	2836	C	C6-N1-C2	-5.09	118.26	120.30
11	AA	922	U	N1-C2-O2	5.09	126.36	122.80
60	c	1003	A	O4'-C1'-N9	5.08	112.27	108.20
60	c	864	U	N3-C2-O2	-5.05	118.67	122.20

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	JJ	232	ARG	Peptide
36	L	102	GLU	Peptide
58	a	7	THR	Peptide
62	e	35	PRO	Peptide
62	e	38	PHE	Peptide
66	i	220	VAL	Peptide
66	i	65	ARG	Peptide
68	k	64	VAL	Peptide
73	p	105	ASN	Peptide
74	q	123	SER	Peptide
74	q	124	ASP	Peptide
76	s	40	GLU	Peptide

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Mol	Chain	Res	Type	Group
78	u	90	ASN	Peptide
83	z	88	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
2	1	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
3	2	95/119 (80%)	87 (92%)	8 (8%)	0	100	100
4	3	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
5	4	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
6	5	51/56 (91%)	51 (100%)	0	0	100	100
7	6	51/63 (81%)	47 (92%)	4 (8%)	0	100	100
8	7	316/319 (99%)	297 (94%)	19 (6%)	0	100	100
9	8	32/152 (21%)	22 (69%)	10 (31%)	0	100	100
10	A	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
12	B	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
15	C	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
18	D	174/189 (92%)	170 (98%)	3 (2%)	1 (1%)	25	14
19	DD	195/312 (62%)	187 (96%)	8 (4%)	0	100	100
21	E	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
22	EE	250/254 (98%)	244 (98%)	6 (2%)	0	100	100
23	Ee	156/165 (94%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	F	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
25	FF	384/387 (99%)	374 (97%)	10 (3%)	0	100	100
26	G	95/121 (78%)	93 (98%)	2 (2%)	0	100	100
27	GG	359/362 (99%)	342 (95%)	17 (5%)	0	100	100
28	H	127/137 (93%)	126 (99%)	1 (1%)	0	100	100
29	HH	294/297 (99%)	284 (97%)	10 (3%)	0	100	100
30	I	61/155 (39%)	61 (100%)	0	0	100	100
31	II	151/176 (86%)	147 (97%)	4 (3%)	0	100	100
32	J	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
33	JJ	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
34	K	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
35	KK	231/256 (90%)	227 (98%)	4 (2%)	0	100	100
36	L	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
37	LL	189/191 (99%)	182 (96%)	7 (4%)	0	100	100
38	M	146/149 (98%)	138 (94%)	7 (5%)	1 (1%)	22	11
39	MM	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
40	N	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
41	NN	167/174 (96%)	159 (95%)	8 (5%)	0	100	100
42	O	95/105 (90%)	95 (100%)	0	0	100	100
43	OO	191/199 (96%)	177 (93%)	13 (7%)	1 (0%)	29	16
44	P	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
45	PP	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
47	Q	125/130 (96%)	125 (100%)	0	0	100	100
48	QQ	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
49	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
50	S	107/121 (88%)	107 (100%)	0	0	100	100
51	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
52	U	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
53	V	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
54	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
55	X	48/51 (94%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	Y	50/128 (39%)	50 (100%)	0	0	100	100
57	Z	23/25 (92%)	23 (100%)	0	0	100	100
58	a	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
59	b	89/92 (97%)	89 (100%)	0	0	100	100
61	d	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
62	e	210/255 (82%)	194 (92%)	16 (8%)	0	100	100
63	f	215/254 (85%)	202 (94%)	13 (6%)	0	100	100
64	g	204/240 (85%)	195 (96%)	9 (4%)	0	100	100
65	h	256/261 (98%)	249 (97%)	7 (3%)	0	100	100
66	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
67	j	217/236 (92%)	208 (96%)	9 (4%)	0	100	100
68	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
69	l	180/200 (90%)	168 (93%)	12 (7%)	0	100	100
70	m	183/197 (93%)	177 (97%)	6 (3%)	0	100	100
71	n	89/105 (85%)	80 (90%)	7 (8%)	2 (2%)	6	1
72	o	140/156 (90%)	132 (94%)	8 (6%)	0	100	100
73	p	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
74	q	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
75	r	100/142 (70%)	96 (96%)	4 (4%)	0	100	100
76	s	135/143 (94%)	127 (94%)	8 (6%)	0	100	100
77	t	119/136 (88%)	101 (85%)	14 (12%)	4 (3%)	3	0
78	u	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
79	v	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
80	w	98/121 (81%)	97 (99%)	1 (1%)	0	100	100
81	x	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
82	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
83	z	142/145 (98%)	129 (91%)	13 (9%)	0	100	100
All	All	10968/12214 (90%)	10515 (96%)	444 (4%)	9 (0%)	54	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
77	t	94	SER

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Mol	Chain	Res	Type
38	M	78	LEU
43	OO	63	VAL
71	n	48	SER
71	n	49	LEU
77	t	85	VAL
18	D	131	ALA
77	t	95	ARG
77	t	83	GLN

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%)	101 (90%)	11 (10%)	8 1
2	1	61/89 (68%)	59 (97%)	2 (3%)	38 26
3	2	83/101 (82%)	77 (93%)	6 (7%)	14 5
4	3	70/71 (99%)	69 (99%)	1 (1%)	67 62
5	4	56/60 (93%)	50 (89%)	6 (11%)	6 1
6	5	47/49 (96%)	39 (83%)	8 (17%)	2 0
7	6	46/54 (85%)	41 (89%)	5 (11%)	6 1
8	7	259/262 (99%)	220 (85%)	39 (15%)	3 0
9	8	30/135 (22%)	28 (93%)	2 (7%)	16 6
10	A	160/162 (99%)	158 (99%)	2 (1%)	69 64
12	B	125/146 (86%)	123 (98%)	2 (2%)	62 56
15	C	150/151 (99%)	149 (99%)	1 (1%)	84 83
18	D	143/154 (93%)	135 (94%)	8 (6%)	21 9
19	DD	167/254 (66%)	155 (93%)	12 (7%)	14 5
21	E	156/156 (100%)	151 (97%)	5 (3%)	39 28
22	EE	193/196 (98%)	191 (99%)	2 (1%)	76 73
23	Ee	129/136 (95%)	122 (95%)	7 (5%)	22 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	F	136/137 (99%)	129 (95%)	7 (5%)	24 12
25	FF	318/323 (98%)	306 (96%)	12 (4%)	33 21
26	G	84/107 (78%)	81 (96%)	3 (4%)	35 23
27	GG	288/289 (100%)	279 (97%)	9 (3%)	40 28
28	H	101/105 (96%)	94 (93%)	7 (7%)	15 6
29	HH	244/245 (100%)	239 (98%)	5 (2%)	55 48
30	I	55/129 (43%)	54 (98%)	1 (2%)	59 51
31	II	133/153 (87%)	129 (97%)	4 (3%)	41 29
32	J	104/118 (88%)	102 (98%)	2 (2%)	57 50
33	JJ	186/205 (91%)	182 (98%)	4 (2%)	52 46
34	K	109/110 (99%)	105 (96%)	4 (4%)	34 22
35	KK	187/208 (90%)	180 (96%)	7 (4%)	34 22
36	L	115/116 (99%)	111 (96%)	4 (4%)	36 24
37	LL	171/171 (100%)	164 (96%)	7 (4%)	30 18
38	M	118/119 (99%)	115 (98%)	3 (2%)	47 39
39	MM	184/187 (98%)	178 (97%)	6 (3%)	38 26
40	N	46/47 (98%)	44 (96%)	2 (4%)	29 17
41	NN	147/150 (98%)	132 (90%)	15 (10%)	7 1
42	O	81/88 (92%)	76 (94%)	5 (6%)	18 8
43	OO	154/159 (97%)	149 (97%)	5 (3%)	39 28
44	P	94/97 (97%)	91 (97%)	3 (3%)	39 28
45	PP	107/109 (98%)	104 (97%)	3 (3%)	43 32
46	Pp	2/2 (100%)	2 (100%)	0	100 100
47	Q	109/111 (98%)	108 (99%)	1 (1%)	78 77
48	QQ	175/176 (99%)	172 (98%)	3 (2%)	60 53
49	R	90/91 (99%)	90 (100%)	0	100 100
50	S	94/103 (91%)	93 (99%)	1 (1%)	73 70
51	T	104/105 (99%)	103 (99%)	1 (1%)	76 73
52	U	81/82 (99%)	79 (98%)	2 (2%)	47 39
53	V	69/71 (97%)	68 (99%)	1 (1%)	67 62
54	W	68/69 (99%)	63 (93%)	5 (7%)	13 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	X	45/46 (98%)	45 (100%)	0	100 100
56	Y	47/116 (40%)	45 (96%)	2 (4%)	29 17
57	Z	23/23 (100%)	22 (96%)	1 (4%)	29 17
58	a	87/91 (96%)	83 (95%)	4 (5%)	27 14
59	b	71/72 (99%)	70 (99%)	1 (1%)	67 62
61	d	165/210 (79%)	160 (97%)	5 (3%)	41 29
62	e	189/224 (84%)	177 (94%)	12 (6%)	18 7
63	f	176/205 (86%)	167 (95%)	9 (5%)	24 12
64	g	167/195 (86%)	154 (92%)	13 (8%)	12 4
65	h	220/222 (99%)	205 (93%)	15 (7%)	16 6
66	i	172/191 (90%)	160 (93%)	12 (7%)	15 6
67	j	188/201 (94%)	179 (95%)	9 (5%)	25 13
68	k	165/170 (97%)	152 (92%)	13 (8%)	12 3
69	l	146/161 (91%)	139 (95%)	7 (5%)	25 13
70	m	158/166 (95%)	144 (91%)	14 (9%)	9 2
71	n	84/98 (86%)	82 (98%)	2 (2%)	49 41
72	o	127/137 (93%)	121 (95%)	6 (5%)	26 13
73	p	127/128 (99%)	122 (96%)	5 (4%)	32 19
74	q	81/105 (77%)	80 (99%)	1 (1%)	71 67
75	r	89/118 (75%)	84 (94%)	5 (6%)	21 9
76	s	114/119 (96%)	105 (92%)	9 (8%)	12 3
77	t	105/124 (85%)	88 (84%)	17 (16%)	2 0
78	u	128/129 (99%)	122 (95%)	6 (5%)	26 13
79	v	115/116 (99%)	108 (94%)	7 (6%)	18 8
80	w	94/114 (82%)	84 (89%)	10 (11%)	6 1
81	x	74/74 (100%)	70 (95%)	4 (5%)	22 10
82	y	110/111 (99%)	108 (98%)	2 (2%)	59 51
83	z	119/120 (99%)	113 (95%)	6 (5%)	24 12
All	All	9327/10257 (91%)	8879 (95%)	448 (5%)	29 13

All (448) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	3	ASP
1	0	8	ARG
1	0	41	ARG
1	0	52	LYS
1	0	53	ASP
1	0	88	THR
1	0	104	SER
1	0	105	ARG
1	0	112	LYS
1	0	125	LEU
1	0	131	ARG
2	1	38	HIS
2	1	90	LYS
3	2	15	ARG
3	2	45	VAL
3	2	52	ASP
3	2	57	SER
3	2	64	LEU
3	2	84	VAL
4	3	2	VAL
5	4	16	LEU
5	4	22	ARG
5	4	26	THR
5	4	30	VAL
5	4	44	VAL
5	4	64	ARG
6	5	10	HIS
6	5	11	PRO
6	5	14	TYR
6	5	16	LYS
6	5	19	ARG
6	5	26	SER
6	5	39	CYS
6	5	46	LYS
7	6	10	ARG
7	6	37	ARG
7	6	46	ASN
7	6	50	VAL
7	6	53	LYS
8	7	26	SER
8	7	41	THR
8	7	54	PHE
8	7	56	VAL

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Mol	Chain	Res	Type
8	7	58	VAL
8	7	60	SER
8	7	64	HIS
8	7	76	ASP
8	7	103	PHE
8	7	109	ASP
8	7	120	SER
8	7	134	TRP
8	7	143	THR
8	7	144	LEU
8	7	167	VAL
8	7	177	MET
8	7	178	VAL
8	7	179	LYS
8	7	191	ASP
8	7	192	PHE
8	7	195	HIS
8	7	203	THR
8	7	213	SER
8	7	221	MET
8	7	223	TRP
8	7	234	LEU
8	7	235	SER
8	7	238	ASP
8	7	243	LEU
8	7	245	PHE
8	7	250	TYR
8	7	258	THR
8	7	263	PHE
8	7	264	SER
8	7	266	ASP
8	7	274	LEU
8	7	297	ASP
8	7	302	PHE
8	7	308	ASN
9	8	130	VAL
9	8	132	LEU
10	A	14	HIS
10	A	180	SER
12	B	118	GLN
12	B	149	VAL
15	C	180	ARG

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Mol	Chain	Res	Type
18	D	69	SER
18	D	91	SER
18	D	116	ASP
18	D	152	GLU
18	D	155	LEU
18	D	170	ARG
18	D	173	ARG
18	D	177	VAL
19	DD	5	ARG
19	DD	8	LYS
19	DD	27	VAL
19	DD	38	MET
19	DD	41	VAL
19	DD	98	ASN
19	DD	128	MET
19	DD	144	LYS
19	DD	147	ARG
19	DD	159	VAL
19	DD	160	ASP
19	DD	167	GLN
21	E	71	LYS
21	E	96	ASP
21	E	104	GLU
21	E	132	THR
21	E	172	TYR
22	EE	137	ILE
22	EE	142	ASP
23	Ee	35	LEU
23	Ee	51	LYS
23	Ee	67	ARG
23	Ee	80	LEU
23	Ee	90	ARG
23	Ee	92	ARG
23	Ee	150	ASP
24	F	18	ASP
24	F	19	PHE
24	F	26	HIS
24	F	27	LEU
24	F	83	ARG
24	F	107	GLU
24	F	139	ARG
25	FF	34	LYS

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Mol	Chain	Res	Type
25	FF	37	ARG
25	FF	38	SER
25	FF	55	THR
25	FF	104	THR
25	FF	146	ARG
25	FF	261	MET
25	FF	300	ARG
25	FF	302	LYS
25	FF	332	ARG
25	FF	369	ARG
25	FF	386	ASP
26	G	24	GLU
26	G	55	THR
26	G	67	SER
27	GG	6	VAL
27	GG	12	THR
27	GG	37	THR
27	GG	82	THR
27	GG	120	TYR
27	GG	141	ARG
27	GG	145	ILE
27	GG	181	VAL
27	GG	338	LYS
28	H	9	THR
28	H	34	LEU
28	H	64	LYS
28	H	72	LYS
28	H	84	SER
28	H	98	ASN
28	H	128	ARG
29	HH	10	SER
29	HH	217	GLU
29	HH	234	ASP
29	HH	272	TYR
29	HH	293	LEU
30	I	1	MET
31	II	12	SER
31	II	15	VAL
31	II	92	SER
31	II	136	GLU
32	J	77	GLU
32	J	97	LYS

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Mol	Chain	Res	Type
33	JJ	30	ARG
33	JJ	39	GLU
33	JJ	46	GLU
33	JJ	52	GLN
34	K	3	LYS
34	K	74	TYR
34	K	115	ARG
34	K	125	LYS
35	KK	40	VAL
35	KK	112	GLU
35	KK	197	VAL
35	KK	203	VAL
35	KK	216	SER
35	KK	231	LYS
35	KK	249	ARG
36	L	87	LEU
36	L	95	VAL
36	L	106	GLN
36	L	116	LYS
37	LL	50	ASN
37	LL	69	ARG
37	LL	92	TYR
37	LL	137	SER
37	LL	139	ASN
37	LL	157	ASN
37	LL	177	ASP
38	M	15	VAL
38	M	60	TYR
38	M	85	ASP
39	MM	4	ARG
39	MM	30	LYS
39	MM	36	LEU
39	MM	101	LYS
39	MM	103	LEU
39	MM	148	VAL
40	N	22	LYS
40	N	31	SER
41	NN	11	ASP
41	NN	13	LYS
41	NN	22	SER
41	NN	34	SER
41	NN	37	LEU

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Mol	Chain	Res	Type
41	NN	40	LEU
41	NN	44	THR
41	NN	54	VAL
41	NN	57	PHE
41	NN	60	ARG
41	NN	81	GLU
41	NN	82	ARG
41	NN	107	ASP
41	NN	112	LEU
41	NN	165	GLN
42	O	12	GLN
42	O	61	MET
42	O	64	LYS
42	O	74	ASN
42	O	99	ASP
43	OO	4	SER
43	OO	5	LYS
43	OO	58	VAL
43	OO	69	VAL
43	OO	138	VAL
44	P	31	ARG
44	P	76	SER
44	P	84	ASP
45	PP	27	GLN
45	PP	82	SER
45	PP	137	LYS
47	Q	67	SER
48	QQ	19	LEU
48	QQ	117	ASN
48	QQ	140	LYS
50	S	49	SER
51	T	40	SER
52	U	36	ARG
52	U	71	LYS
53	V	71	SER
54	W	19	ASP
54	W	24	THR
54	W	36	LYS
54	W	49	SER
54	W	77	ARG
56	Y	80	PRO
56	Y	94	SER

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Mol	Chain	Res	Type
57	Z	19	LYS
58	a	8	ARG
58	a	15	LYS
58	a	24	LYS
58	a	80	ARG
59	b	63	THR
61	d	13	ASP
61	d	35	PRO
61	d	124	THR
61	d	151	SER
61	d	200	ASP
62	e	54	LEU
62	e	58	SER
62	e	78	ASP
62	e	87	ARG
62	e	95	ASN
62	e	131	ASP
62	e	154	SER
62	e	198	GLU
62	e	205	PHE
62	e	213	ARG
62	e	217	LEU
62	e	231	LEU
63	f	51	THR
63	f	52	THR
63	f	54	GLU
63	f	89	GLN
63	f	90	THR
63	f	95	ARG
63	f	147	ASN
63	f	241	ASP
63	f	243	TYR
64	g	35	SER
64	g	44	THR
64	g	65	ARG
64	g	76	ARG
64	g	85	VAL
64	g	116	ARG
64	g	167	PHE
64	g	168	ILE
64	g	178	ARG
64	g	179	GLN

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Mol	Chain	Res	Type
64	g	187	LYS
64	g	195	SER
64	g	207	THR
65	h	68	ARG
65	h	91	THR
65	h	98	ASN
65	h	108	ARG
65	h	116	ASP
65	h	117	GLU
65	h	118	GLU
65	h	120	SER
65	h	146	THR
65	h	176	ASP
65	h	182	TYR
65	h	206	ASP
65	h	219	VAL
65	h	254	ARG
65	h	256	ARG
66	i	25	LEU
66	i	33	VAL
66	i	42	LEU
66	i	43	PHE
66	i	48	PHE
66	i	52	GLU
66	i	63	GLN
66	i	73	THR
66	i	79	ASN
66	i	126	ASP
66	i	176	THR
66	i	206	SER
67	j	1	MET
67	j	36	VAL
67	j	43	ASP
67	j	65	GLN
67	j	71	THR
67	j	119	GLN
67	j	126	ASP
67	j	143	LYS
67	j	202	ARG
68	k	7	LYS
68	k	28	GLU
68	k	37	GLU

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Mol	Chain	Res	Type
68	k	50	ASP
68	k	70	PHE
68	k	77	LEU
68	k	95	GLU
68	k	107	ARG
68	k	131	PHE
68	k	157	LYS
68	k	175	LYS
68	k	181	ILE
68	k	186	PRO
69	l	4	SER
69	l	21	PHE
69	l	58	LEU
69	l	60	ILE
69	l	110	ARG
69	l	113	PHE
69	l	154	SER
70	m	6	ARG
70	m	13	SER
70	m	17	ARG
70	m	25	ASP
70	m	50	SER
70	m	53	ARG
70	m	66	ASP
70	m	74	ASN
70	m	87	SER
70	m	92	LYS
70	m	152	SER
70	m	154	LYS
70	m	157	ASP
70	m	168	ARG
71	n	51	SER
71	n	67	THR
72	o	15	LYS
72	o	31	THR
72	o	33	ARG
72	o	67	ARG
72	o	116	ARG
72	o	138	ASN
73	p	55	ARG
73	p	60	VAL
73	p	103	GLU

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Mol	Chain	Res	Type
73	p	143	SER
73	p	149	LEU
74	q	124	ASP
75	r	17	TYR
75	r	29	SER
75	r	31	GLU
75	r	44	ARG
75	r	64	LYS
76	s	43	ILE
76	s	50	GLU
76	s	55	VAL
76	s	58	ASP
76	s	67	VAL
76	s	68	ARG
76	s	102	LYS
76	s	107	LYS
76	s	136	SER
77	t	5	ARG
77	t	8	THR
77	t	24	LEU
77	t	25	THR
77	t	30	THR
77	t	66	VAL
77	t	72	LYS
77	t	73	LEU
77	t	75	GLU
77	t	77	GLU
77	t	78	ARG
77	t	79	GLU
77	t	81	LYS
77	t	85	VAL
77	t	87	GLU
77	t	91	LEU
77	t	108	ASP
78	u	16	ARG
78	u	40	ARG
78	u	51	ASP
78	u	57	ARG
78	u	75	ASN
78	u	85	PHE
79	v	9	VAL
79	v	89	ARG

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Mol	Chain	Res	Type
79	v	114	VAL
79	v	116	ILE
79	v	122	ARG
79	v	141	GLU
79	v	142	GLU
80	w	28	SER
80	w	30	LYS
80	w	39	SER
80	w	46	GLU
80	w	52	LYS
80	w	53	LYS
80	w	60	THR
80	w	65	ILE
80	w	93	LEU
80	w	107	THR
81	x	10	GLU
81	x	32	VAL
81	x	44	ARG
81	x	50	TYR
82	y	30	SER
82	y	51	GLU
83	z	31	LYS
83	z	41	SER
83	z	66	SER
83	z	82	LYS
83	z	107	PHE
83	z	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
8	7	64	HIS
28	H	47	ASN
55	X	33	ASN
63	f	147	ASN
67	j	65	GLN
68	k	108	GLN
74	q	99	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3185/3396 (93%)	472 (14%)	21 (0%)
13	BB	120/121 (99%)	9 (7%)	1 (0%)
14	Bb	75/76 (98%)	29 (38%)	0
16	CC	157/158 (99%)	21 (13%)	0
17	Cc	76/77 (98%)	19 (25%)	0
20	Dd	12/39 (30%)	3 (25%)	0
60	c	1589/1800 (88%)	283 (17%)	0
All	All	5214/5667 (92%)	836 (16%)	22 (0%)

All (836) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	6	A
11	AA	26	A
11	AA	40	A
11	AA	43	A
11	AA	49	A
11	AA	59	G
11	AA	60	A
11	AA	65	A
11	AA	66	A
11	AA	72	C
11	AA	86	G
11	AA	92	G
11	AA	99	A
11	AA	110	G
11	AA	111	C
11	AA	122	A
11	AA	135	C
11	AA	136	G
11	AA	142	C
11	AA	156	G
11	AA	157	A
11	AA	165	A
11	AA	170	G
11	AA	190	U
11	AA	200	C
11	AA	206	G
11	AA	219	A
11	AA	220	G
11	AA	241	G
11	AA	243	G
11	AA	247	C

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Mol	Chain	Res	Type
11	AA	252	U
11	AA	253	A
11	AA	269	G
11	AA	286	U
11	AA	295	A
11	AA	305	U
11	AA	329	U
11	AA	374	A
11	AA	376	G
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	520	U
11	AA	521	A
11	AA	523	A
11	AA	532	A
11	AA	533	A
11	AA	534	U
11	AA	546	C
11	AA	555	U
11	AA	557	A
11	AA	559	A
11	AA	560	G
11	AA	589	A
11	AA	592	A
11	AA	602	A
11	AA	603	A
11	AA	604	G
11	AA	607	A
11	AA	611	A
11	AA	620	U
11	AA	621	A
11	AA	636	C
11	AA	649	A2M
11	AA	660	A
11	AA	677	A
11	AA	678	G
11	AA	681	U
11	AA	691	A

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Mol	Chain	Res	Type
11	AA	705	A
11	AA	712	G
11	AA	715	A
11	AA	719	U
11	AA	758	C
11	AA	767	U
11	AA	776	U
11	AA	780	A
11	AA	781	G
11	AA	785	G
11	AA	786	A
11	AA	817	A2M
11	AA	830	A
11	AA	849	C
11	AA	861	C
11	AA	874	U
11	AA	879	U
11	AA	880	G
11	AA	896	A
11	AA	897	U
11	AA	907	G
11	AA	908	OMG
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	925	A
11	AA	937	G
11	AA	944	C
11	AA	953	G
11	AA	959	C
11	AA	960	U
11	AA	961	C
11	AA	964	G
11	AA	974	G
11	AA	980	A
11	AA	994	G
11	AA	1006	A
11	AA	1014	U
11	AA	1015	U

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Mol	Chain	Res	Type
11	AA	1016	C
11	AA	1017	C
11	AA	1018	G
11	AA	1020	G
11	AA	1023	C
11	AA	1026	A
11	AA	1027	A
11	AA	1028	U
11	AA	1029	G
11	AA	1032	C
11	AA	1034	U
11	AA	1036	A
11	AA	1037	C
11	AA	1038	C
11	AA	1047	A
11	AA	1064	A
11	AA	1066	G
11	AA	1072	G
11	AA	1081	U
11	AA	1083	G
11	AA	1087	G
11	AA	1096	U
11	AA	1097	G
11	AA	1098	A
11	AA	1103	A
11	AA	1117	G
11	AA	1131	G
11	AA	1144	U
11	AA	1153	A
11	AA	1159	A
11	AA	1160	C
11	AA	1180	A
11	AA	1181	U
11	AA	1182	A
11	AA	1192	C
11	AA	1193	A
11	AA	1196	C
11	AA	1201	C
11	AA	1208	U
11	AA	1209	G
11	AA	1217	A
11	AA	1222	G

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Mol	Chain	Res	Type
11	AA	1230	G
11	AA	1232	C
11	AA	1235	U
11	AA	1236	G
11	AA	1237	G
11	AA	1240	A
11	AA	1244	A
11	AA	1245	A
11	AA	1246	G
11	AA	1249	G
11	AA	1250	G
11	AA	1254	C
11	AA	1257	C
11	AA	1262	G
11	AA	1263	A
11	AA	1265	U
11	AA	1272	C
11	AA	1275	C
11	AA	1276	U
11	AA	1281	G
11	AA	1284	C
11	AA	1285	G
11	AA	1286	A
11	AA	1302	A
11	AA	1307	G
11	AA	1308	A
11	AA	1309	U
11	AA	1313	G
11	AA	1330	A
11	AA	1331	U
11	AA	1345	G
11	AA	1348	U
11	AA	1349	G
11	AA	1351	U
11	AA	1352	A
11	AA	1355	A
11	AA	1356	U
11	AA	1357	G
11	AA	1386	A
11	AA	1392	G
11	AA	1399	A
11	AA	1400	G

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Mol	Chain	Res	Type
11	AA	1425	U
11	AA	1434	G
11	AA	1437	OMC
11	AA	1443	G
11	AA	1446	A
11	AA	1450	OMG
11	AA	1481	A
11	AA	1483	G
11	AA	1508	C
11	AA	1527	C
11	AA	1555	U
11	AA	1556	C
11	AA	1560	G
11	AA	1562	C
11	AA	1563	C
11	AA	1566	A
11	AA	1568	U
11	AA	1569	U
11	AA	1571	A
11	AA	1573	G
11	AA	1579	C
11	AA	1581	C
11	AA	1583	A
11	AA	1587	A
11	AA	1589	A
11	AA	1605	A
11	AA	1629	U
11	AA	1630	U
11	AA	1643	A
11	AA	1645	U
11	AA	1657	C
11	AA	1724	U
11	AA	1741	A
11	AA	1750	A
11	AA	1751	G
11	AA	1759	C
11	AA	1762	C
11	AA	1763	U
11	AA	1765	U
11	AA	1769	G
11	AA	1796	G
11	AA	1797	A

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Mol	Chain	Res	Type
11	AA	1815	U
11	AA	1816	A
11	AA	1817	G
11	AA	1821	U
11	AA	1842	A
11	AA	1878	G
11	AA	1879	A
11	AA	1880	U
11	AA	1893	A
11	AA	1906	G
11	AA	2102	U
11	AA	2112	U
11	AA	2114	C
11	AA	2122	G
11	AA	2131	A
11	AA	2140	U
11	AA	2144	A
11	AA	2158	A
11	AA	2168	A
11	AA	2169	G
11	AA	2170	U
11	AA	2171	G
11	AA	2188	A
11	AA	2204	C
11	AA	2206	G
11	AA	2207	A
11	AA	2209	U
11	AA	2223	A
11	AA	2244	A
11	AA	2254	U
11	AA	2266	U
11	AA	2267	C
11	AA	2268	U
11	AA	2271	A
11	AA	2273	G
11	AA	2279	A
11	AA	2280	A2M
11	AA	2281	A2M
11	AA	2307	G
11	AA	2308	C
11	AA	2310	U
11	AA	2313	A

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Mol	Chain	Res	Type
11	AA	2315	G
11	AA	2334	U
11	AA	2335	G
11	AA	2336	U
11	AA	2363	A
11	AA	2373	A
11	AA	2374	C
11	AA	2375	G
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	2435	G
11	AA	2437	G
11	AA	2438	A
11	AA	2442	G
11	AA	2444	C
11	AA	2445	A
11	AA	2447	A
11	AA	2448	G
11	AA	2449	A
11	AA	2450	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	2467	G
11	AA	2470	C
11	AA	2471	U
11	AA	2472	U
11	AA	2474	G

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Mol	Chain	Res	Type
11	AA	2475	G
11	AA	2477	G
11	AA	2478	C
11	AA	2479	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	2495	C
11	AA	2496	C
11	AA	2499	U
11	AA	2501	U
11	AA	2503	G
11	AA	2511	A
11	AA	2514	U
11	AA	2515	A
11	AA	2550	U
11	AA	2552	C
11	AA	2554	A
11	AA	2560	C
11	AA	2561	A
11	AA	2569	A
11	AA	2570	U
11	AA	2571	U
11	AA	2572	C
11	AA	2573	G
11	AA	2585	G
11	AA	2593	A
11	AA	2606	G
11	AA	2607	G
11	AA	2614	G
11	AA	2629	U
11	AA	2637	A
11	AA	2652	U
11	AA	2656	A
11	AA	2674	A

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Mol	Chain	Res	Type
11	AA	2677	G
11	AA	2678	A
11	AA	2689	A
11	AA	2691	A
11	AA	2696	A
11	AA	2704	A
11	AA	2705	A
11	AA	2713	U
11	AA	2714	G
11	AA	2728	G
11	AA	2729	OMU
11	AA	2753	G
11	AA	2772	C
11	AA	2777	G
11	AA	2778	G
11	AA	2793	OMG
11	AA	2795	U
11	AA	2796	G
11	AA	2799	A
11	AA	2800	G
11	AA	2801	A
11	AA	2802	A
11	AA	2808	A
11	AA	2810	C
11	AA	2814	G
11	AA	2817	A
11	AA	2844	C
11	AA	2845	A
11	AA	2867	C
11	AA	2871	G
11	AA	2872	A
11	AA	2875	U
11	AA	2876	C
11	AA	2887	A
11	AA	2899	C
11	AA	2910	A
11	AA	2914	G
11	AA	2922	OMG
11	AA	2923	U
11	AA	2935	U
11	AA	2936	A
11	AA	2938	G

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Mol	Chain	Res	Type
11	AA	2942	C
11	AA	2947	G
11	AA	2951	G
11	AA	2971	A
11	AA	2972	G
11	AA	2977	G
11	AA	2983	C
11	AA	2990	G
11	AA	2997	G
11	AA	3012	A
11	AA	3056	U
11	AA	3059	G
11	AA	3078	U
11	AA	3080	G
11	AA	3092	C
11	AA	3101	G
11	AA	3104	U
11	AA	3113	A
11	AA	3122	A
11	AA	3129	A
11	AA	3130	A
11	AA	3131	U
11	AA	3142	A
11	AA	3143	C
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	3187	A
11	AA	3207	U
11	AA	3217	C
11	AA	3218	A
11	AA	3219	G
11	AA	3224	G

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Mol	Chain	Res	Type
11	AA	3243	A
11	AA	3247	G
11	AA	3270	U
11	AA	3276	G
11	AA	3277	U
11	AA	3281	U
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	3341	U
11	AA	3345	G
11	AA	3348	G
11	AA	3351	U
11	AA	3352	U
11	AA	3353	G
11	AA	3369	G
11	AA	3378	C
11	AA	3389	U
13	BB	7	G
13	BB	52	G
13	BB	54	U
13	BB	65	G
13	BB	73	C
13	BB	74	C
13	BB	76	A
13	BB	112	G
13	BB	121	U
14	Bb	4	G
14	Bb	5	A
14	Bb	6	U
14	Bb	7	U
14	Bb	8	U
14	Bb	9	A
14	Bb	15	G
14	Bb	16	U
14	Bb	17	U
14	Bb	19	G
14	Bb	20	G
14	Bb	21	A

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Mol	Chain	Res	Type
14	Bb	22	G
14	Bb	24	G
14	Bb	36	A
14	Bb	41	U
14	Bb	42	G
14	Bb	46	G
14	Bb	47	U
14	Bb	48	C
14	Bb	49	C
14	Bb	55	U
14	Bb	58	A
14	Bb	61	C
14	Bb	62	A
14	Bb	64	A
14	Bb	68	U
14	Bb	70	C
14	Bb	75	C
16	CC	23	U
16	CC	34	U
16	CC	35	C
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	86	U
16	CC	87	G
16	CC	91	C
16	CC	95	G
16	CC	104	A
16	CC	105	A
16	CC	106	C
16	CC	113	U
16	CC	125	U
16	CC	126	A
16	CC	152	G
17	Cc	7	G
17	Cc	9	G
17	Cc	12	G
17	Cc	16	C

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Mol	Chain	Res	Type
17	Cc	18	C
17	Cc	19	G
17	Cc	20	G
17	Cc	22	A
17	Cc	23	G
17	Cc	48	U
17	Cc	53	G
17	Cc	56	U
17	Cc	57	C
17	Cc	62	C
17	Cc	63	C
17	Cc	65	G
17	Cc	66	C
17	Cc	68	C
17	Cc	77	A
20	Dd	16	A
20	Dd	24	U
20	Dd	25	U
60	c	2	A
60	c	4	C
60	c	17	C
60	c	26	A
60	c	34	G
60	c	45	U
60	c	47	A
60	c	61	A
60	c	67	A
60	c	68	A
60	c	71	A
60	c	72	A
60	c	78	A
60	c	111	U
60	c	114	C
60	c	127	G
60	c	131	C
60	c	140	A
60	c	145	A
60	c	146	U
60	c	168	A
60	c	176	C
60	c	183	U
60	c	184	C

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Mol	Chain	Res	Type
60	c	261	U
60	c	262	U
60	c	271	A
60	c	272	U
60	c	277	U
60	c	278	U
60	c	279	G
60	c	285	G
60	c	287	G
60	c	299	A
60	c	309	C
60	c	314	C
60	c	316	A
60	c	322	G
60	c	337	G
60	c	338	C
60	c	361	C
60	c	390	G
60	c	400	A
60	c	401	A
60	c	402	C
60	c	404	G
60	c	414	OMC
60	c	419	G
60	c	423	G
60	c	424	C
60	c	426	G
60	c	428	A
60	c	434	G
60	c	439	U
60	c	444	C
60	c	448	C
60	c	455	C
60	c	460	A
60	c	468	A
60	c	475	A
60	c	477	A
60	c	506	A
60	c	511	A
60	c	515	A
60	c	519	C
60	c	524	U

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Mol	Chain	Res	Type
60	c	525	A
60	c	526	A
60	c	527	A
60	c	534	A
60	c	537	G
60	c	538	A
60	c	539	G
60	c	541	A2M
60	c	557	G
60	c	558	U
60	c	565	C
60	c	568	G
60	c	576	G
60	c	578	OMU
60	c	579	A
60	c	582	U
60	c	583	C
60	c	594	A
60	c	606	A
60	c	611	U
60	c	619	A2M
60	c	620	A
60	c	623	A
60	c	624	G
60	c	639	U
60	c	644	C
60	c	645	C
60	c	648	G
60	c	649	U
60	c	650	U
60	c	651	G
60	c	691	C
60	c	692	C
60	c	695	U
60	c	696	C
60	c	745	U
60	c	760	A
60	c	765	G
60	c	766	U
60	c	775	G
60	c	778	G
60	c	780	A

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Mol	Chain	Res	Type
60	c	781	U
60	c	782	U
60	c	783	G
60	c	784	C
60	c	789	A
60	c	793	A
60	c	794	U
60	c	795	U
60	c	809	A
60	c	812	A
60	c	814	A
60	c	820	U
60	c	821	U
60	c	822	U
60	c	859	A
60	c	860	U
60	c	863	A
60	c	895	G
60	c	898	A
60	c	906	A
60	c	913	G
60	c	914	G
60	c	915	A
60	c	933	A
60	c	935	U
60	c	951	A
60	c	960	U
60	c	966	A
60	c	988	A
60	c	992	A
60	c	993	A
60	c	1002	G
60	c	1010	C
60	c	1026	A
60	c	1028	C
60	c	1031	U
60	c	1032	G
60	c	1052	U
60	c	1053	G
60	c	1058	U
60	c	1059	U
60	c	1060	U

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Mol	Chain	Res	Type
60	c	1061	A
60	c	1063	U
60	c	1076	A
60	c	1081	A
60	c	1082	C
60	c	1092	A
60	c	1097	U
60	c	1100	G
60	c	1138	A
60	c	1150	G
60	c	1151	A
60	c	1158	C
60	c	1162	C
60	c	1185	U
60	c	1194	A
60	c	1196	A
60	c	1199	G
60	c	1200	G
60	c	1202	A
60	c	1217	A
60	c	1218	G
60	c	1221	A
60	c	1222	C
60	c	1223	A
60	c	1224	A
60	c	1225	U
60	c	1227	A
60	c	1228	G
60	c	1241	G
60	c	1244	A
60	c	1245	G
60	c	1246	C
60	c	1252	C
60	c	1256	A
60	c	1258	U
60	c	1259	U
60	c	1261	G
60	c	1274	C
60	c	1286	U
60	c	1291	G
60	c	1301	U
60	c	1309	C

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Mol	Chain	Res	Type
60	c	1314	U
60	c	1315	U
60	c	1316	G
60	c	1318	G
60	c	1321	A
60	c	1336	A
60	c	1338	C
60	c	1339	C
60	c	1340	U
60	c	1346	A
60	c	1347	U
60	c	1351	G
60	c	1353	U
60	c	1354	G
60	c	1355	C
60	c	1361	U
60	c	1363	U
60	c	1370	U
60	c	1371	A
60	c	1372	U
60	c	1373	C
60	c	1378	U
60	c	1388	A
60	c	1390	U
60	c	1398	U
60	c	1399	C
60	c	1400	A
60	c	1411	A
60	c	1413	U
60	c	1414	U
60	c	1415	U
60	c	1425	A
60	c	1427	A
60	c	1428	OMG
60	c	1432	U
60	c	1436	A
60	c	1459	C
60	c	1460	A
60	c	1469	A
60	c	1471	A
60	c	1489	U
60	c	1490	C

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Mol	Chain	Res	Type
60	c	1491	U
60	c	1492	A
60	c	1496	U
60	c	1506	G
60	c	1510	U
60	c	1514	U
60	c	1516	A
60	c	1521	G
60	c	1523	G
60	c	1524	A
60	c	1535	U
60	c	1536	G
60	c	1537	C
60	c	1542	G
60	c	1557	U
60	c	1559	A
60	c	1572	OMG
60	c	1573	A
60	c	1575	G7M
60	c	1576	A
60	c	1590	G
60	c	1601	G
60	c	1616	G
60	c	1622	G
60	c	1631	A
60	c	1634	C
60	c	1646	C
60	c	1657	U
60	c	1658	G
60	c	1668	G
60	c	1678	A
60	c	1681	A
60	c	1683	C
60	c	1684	U
60	c	1685	G
60	c	1717	G
60	c	1740	A
60	c	1755	A
60	c	1756	A
60	c	1762	A
60	c	1766	A
60	c	1769	U

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

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	588	G
11	AA	601	U
11	AA	619	A
11	AA	873	C
11	AA	896	A
11	AA	916	G
11	AA	993	G
11	AA	1033	U
11	AA	1348	U
11	AA	1562	C
11	AA	2101	C
11	AA	2253	G
11	AA	2372	A
11	AA	2487	U
11	AA	2490	C
11	AA	2500	A
11	AA	2792	A
11	AA	2922	OMG
11	AA	2971	A
11	AA	3121	U
11	AA	3206	C
13	BB	72	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	2815	11	18,26,27	1.19	2 (11%)	19,38,41	0.91	1 (5%)
11	A2M	AA	2640	11	18,25,26	3.62	8 (44%)	18,36,39	3.26	4 (22%)
60	A2M	c	28	60	18,25,26	3.61	8 (44%)	18,36,39	3.32	3 (16%)
11	OMG	AA	2922	14,11	18,26,27	1.32	2 (11%)	19,38,41	0.94	1 (5%)
60	MA6	c	1781	60	18,26,27	1.08	2 (11%)	19,38,41	3.43	2 (10%)
11	OMG	AA	2793	11	18,26,27	1.26	3 (16%)	19,38,41	0.86	1 (5%)
60	OMU	c	1269	60	19,22,23	2.97	8 (42%)	26,31,34	1.70	5 (19%)
11	OMC	AA	663	11	19,22,23	0.63	0	26,31,34	0.73	0
11	OMC	AA	2197	86,11	19,22,23	0.61	0	26,31,34	0.67	0
11	A2M	AA	2256	11	18,25,26	3.58	7 (38%)	18,36,39	3.50	4 (22%)
11	OMC	AA	2959	11,85	19,22,23	0.64	0	26,31,34	0.64	0
11	A2M	AA	876	11	18,25,26	3.59	7 (38%)	18,36,39	3.38	4 (22%)
11	OMU	AA	2421	11	19,22,23	2.95	8 (42%)	26,31,34	1.75	5 (19%)
60	OMG	c	1126	60	18,26,27	1.19	2 (11%)	19,38,41	0.85	1 (5%)
11	OMG	AA	908	11	18,26,27	1.25	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	1449	11,85	18,25,26	3.58	7 (38%)	18,36,39	3.36	4 (22%)
14	YYG	Bb	37	14,85	31,42,43	2.23	8 (25%)	33,62,65	1.79	10 (30%)
11	OMU	AA	2729	11	19,22,23	2.94	8 (42%)	26,31,34	1.66	5 (19%)
11	OMU	AA	2921	11,85	19,22,23	2.95	8 (42%)	26,31,34	1.71	5 (19%)
60	MA6	c	1782	60	18,26,27	1.06	2 (11%)	19,38,41	3.54	2 (10%)
11	OMG	AA	2791	11	18,26,27	1.22	2 (11%)	19,38,41	0.82	1 (5%)
11	A2M	AA	2220	11	18,25,26	3.60	8 (44%)	18,36,39	3.38	3 (16%)
11	1MA	AA	645	11,85	16,25,26	1.00	2 (12%)	18,37,40	1.11	2 (11%)
60	A2M	c	974	60	18,25,26	3.62	9 (50%)	18,36,39	3.34	3 (16%)
60	OMG	c	562	60	18,26,27	1.16	2 (11%)	19,38,41	0.87	1 (5%)
11	UR3	AA	2634	11	19,22,23	2.79	7 (36%)	26,32,35	1.31	1 (3%)
60	OMG	c	1572	60	18,26,27	1.20	2 (11%)	19,38,41	0.87	1 (5%)
11	OMU	AA	1888	11	19,22,23	3.00	8 (42%)	26,31,34	1.81	6 (23%)
11	A2M	AA	2280	11	18,25,26	3.62	8 (44%)	18,36,39	3.30	3 (16%)
11	A2M	AA	817	11,85	18,25,26	3.59	7 (38%)	18,36,39	3.50	3 (16%)
60	B8N	c	1191	60	24,29,30	3.03	7 (29%)	29,42,45	1.69	5 (17%)
60	OMC	c	1007	60	19,22,23	0.59	0	26,31,34	0.63	0
60	OMC	c	1639	85,60	19,22,23	0.64	0	26,31,34	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OMG	AA	1450	11	18,26,27	1.20	2 (11%)	19,38,41	0.77	1 (5%)
11	OMG	AA	2619	11	18,26,27	1.21	2 (11%)	19,38,41	0.83	1 (5%)
60	A2M	c	436	60	18,25,26	3.62	8 (44%)	18,36,39	3.39	3 (16%)
11	5MC	AA	2870	86,11	18,22,23	0.80	0	26,32,35	0.66	0
60	A2M	c	619	85,60	18,25,26	3.65	8 (44%)	18,36,39	3.50	3 (16%)
11	OMG	AA	2288	11	18,26,27	1.21	2 (11%)	19,38,41	0.81	1 (5%)
11	OMC	AA	2948	11	19,22,23	0.62	0	26,31,34	0.75	1 (3%)
60	OMU	c	578	60	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
60	OMG	c	1271	60	18,26,27	1.18	2 (11%)	19,38,41	0.87	1 (5%)
11	1MA	AA	2142	11,85	16,25,26	1.02	2 (12%)	18,37,40	1.10	2 (11%)
11	A2M	AA	649	11	18,25,26	3.65	7 (38%)	18,36,39	3.26	3 (16%)
60	OMC	c	414	60	19,22,23	0.63	0	26,31,34	0.78	1 (3%)
60	A2M	c	420	60	18,25,26	3.60	8 (44%)	18,36,39	3.30	3 (16%)
60	A2M	c	796	60	18,25,26	3.62	8 (44%)	18,36,39	3.38	3 (16%)
11	OMG	AA	867	86,11	18,26,27	1.27	2 (11%)	19,38,41	0.88	1 (5%)
11	A2M	AA	2946	11,85	18,25,26	3.61	7 (38%)	18,36,39	3.40	3 (16%)
11	A2M	AA	2281	11	18,25,26	3.72	8 (44%)	18,36,39	3.32	4 (22%)
11	OMC	AA	2337	11	19,22,23	0.62	0	26,31,34	0.77	1 (3%)
60	A2M	c	100	85,60	18,25,26	3.63	9 (50%)	18,36,39	3.33	4 (22%)
11	OMU	AA	2347	11	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
11	OMU	AA	2417	11	19,22,23	2.92	8 (42%)	26,31,34	1.75	5 (19%)
11	5MC	AA	2278	11,85	18,22,23	0.63	0	26,32,35	0.60	0
60	4AC	c	1773	60	21,24,25	3.36	10 (47%)	29,34,37	1.55	5 (17%)
60	4AC	c	1280	60	21,24,25	3.40	10 (47%)	29,34,37	1.58	5 (17%)
11	OMU	AA	2724	11	19,22,23	2.95	8 (42%)	26,31,34	1.70	5 (19%)
11	OMG	AA	805	11	18,26,27	1.23	3 (16%)	19,38,41	0.86	1 (5%)
60	OMG	c	1428	85,60	18,26,27	1.20	2 (11%)	19,38,41	0.86	1 (5%)
11	OMU	AA	898	11	19,22,23	2.93	8 (42%)	26,31,34	1.69	5 (19%)
60	A2M	c	541	60	18,25,26	3.58	8 (44%)	18,36,39	3.44	5 (27%)
60	G7M	c	1575	60,17	20,26,27	2.34	7 (35%)	17,39,42	1.33	2 (11%)
11	A2M	AA	807	11	18,25,26	3.60	8 (44%)	18,36,39	3.36	3 (16%)
11	OMC	AA	1437	11,85	19,22,23	0.64	0	26,31,34	0.85	1 (3%)
11	A2M	AA	1133	11,85	18,25,26	3.62	8 (44%)	18,36,39	3.46	3 (16%)
11	OMC	AA	650	11,85	19,22,23	0.62	0	26,31,34	0.63	0

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	2815	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2640	11	-	1/5/27/28	0/3/3/3
60	A2M	c	28	60	-	1/5/27/28	0/3/3/3
11	OMG	AA	2922	14,11	-	2/5/27/28	0/3/3/3
60	MA6	c	1781	60	-	0/7/29/30	0/3/3/3
11	OMG	AA	2793	11	-	0/5/27/28	0/3/3/3
60	OMU	c	1269	60	-	0/9/27/28	0/2/2/2
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2197	86,11	-	4/9/27/28	0/2/2/2
11	A2M	AA	2256	11	-	3/5/27/28	0/3/3/3
11	OMC	AA	2959	11,85	-	0/9/27/28	0/2/2/2
11	A2M	AA	876	11	-	2/5/27/28	0/3/3/3
11	OMU	AA	2421	11	-	0/9/27/28	0/2/2/2
60	OMG	c	1126	60	-	1/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	1449	11,85	-	0/5/27/28	0/3/3/3
14	YYG	Bb	37	14,85	-	9/20/42/43	0/3/4/4
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2921	11,85	-	0/9/27/28	0/2/2/2
60	MA6	c	1782	60	-	3/7/29/30	0/3/3/3
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2220	11	-	0/5/27/28	0/3/3/3
11	1MA	AA	645	11,85	-	0/3/25/26	0/3/3/3
60	A2M	c	974	60	-	0/5/27/28	0/3/3/3
60	OMG	c	562	60	-	0/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
60	OMG	c	1572	60	-	2/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	817	11,85	-	3/5/27/28	0/3/3/3
60	B8N	c	1191	60	-	1/16/34/35	0/2/2/2
60	OMC	c	1007	60	-	0/9/27/28	0/2/2/2
60	OMC	c	1639	85,60	-	0/9/27/28	0/2/2/2
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	OMG	AA	2619	11	-	1/5/27/28	0/3/3/3
60	A2M	c	436	60	-	0/5/27/28	0/3/3/3
11	5MC	AA	2870	86,11	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	A2M	c	619	85,60	-	3/5/27/28	0/3/3/3
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
60	OMU	c	578	60	-	4/9/27/28	0/2/2/2
60	OMG	c	1271	60	-	1/5/27/28	0/3/3/3
11	1MA	AA	2142	11,85	-	0/3/25/26	0/3/3/3
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
60	OMC	c	414	60	-	3/9/27/28	0/2/2/2
60	A2M	c	420	60	-	1/5/27/28	0/3/3/3
60	A2M	c	796	60	-	0/5/27/28	0/3/3/3
11	OMG	AA	867	86,11	-	2/5/27/28	0/3/3/3
11	A2M	AA	2946	11,85	-	0/5/27/28	0/3/3/3
11	A2M	AA	2281	11	-	1/5/27/28	0/3/3/3
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
60	A2M	c	100	85,60	-	2/5/27/28	0/3/3/3
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
11	5MC	AA	2278	11,85	-	0/7/25/26	0/2/2/2
60	4AC	c	1773	60	-	2/11/29/30	0/2/2/2
60	4AC	c	1280	60	-	4/11/29/30	0/2/2/2
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
60	OMG	c	1428	85,60	-	1/5/27/28	0/3/3/3
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
60	A2M	c	541	60	-	3/5/27/28	0/3/3/3
60	G7M	c	1575	60,17	-	2/3/25/26	0/3/3/3
11	A2M	AA	807	11	-	3/5/27/28	0/3/3/3
11	OMC	AA	1437	11,85	-	2/9/27/28	0/2/2/2
11	A2M	AA	1133	11,85	-	0/5/27/28	0/3/3/3
11	OMC	AA	650	11,85	-	0/9/27/28	0/2/2/2

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	796	A2M	C3'-C4'	-8.98	1.30	1.53
60	c	100	A2M	C3'-C4'	-8.92	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.88	1.30	1.53
60	c	619	A2M	C3'-C4'	-8.88	1.30	1.53
60	c	28	A2M	C3'-C4'	-8.88	1.30	1.53
60	c	436	A2M	C3'-C4'	-8.87	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	807	A2M	C3'-C4'	-8.82	1.30	1.53
11	AA	2640	A2M	C3'-C4'	-8.82	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.81	1.30	1.53
11	AA	2220	A2M	C3'-C4'	-8.81	1.30	1.53
60	c	420	A2M	C3'-C4'	-8.79	1.30	1.53
60	c	541	A2M	C3'-C4'	-8.78	1.30	1.53
11	AA	817	A2M	C3'-C4'	-8.77	1.30	1.53
60	c	974	A2M	C3'-C4'	-8.77	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.72	1.30	1.53
11	AA	876	A2M	C3'-C4'	-8.71	1.30	1.53
11	AA	649	A2M	C3'-C4'	-8.67	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.60	1.31	1.53
11	AA	2256	A2M	C3'-C4'	-8.59	1.31	1.53
11	AA	2281	A2M	C3'-C4'	-8.50	1.31	1.53
11	AA	2281	A2M	O4'-C1'	-8.45	1.29	1.41
60	c	619	A2M	O4'-C1'	-7.95	1.30	1.41
60	c	1191	B8N	C4-N3	-7.87	1.25	1.40
11	AA	649	A2M	O4'-C1'	-7.71	1.30	1.41
60	c	1191	B8N	C6-N1	7.71	1.55	1.36
11	AA	2256	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	649	A2M	O4'-C4'	7.63	1.62	1.45
60	c	420	A2M	O4'-C4'	7.61	1.62	1.45
11	AA	2640	A2M	O4'-C4'	7.60	1.62	1.45
60	c	436	A2M	O4'-C4'	7.59	1.62	1.45
11	AA	1133	A2M	O4'-C4'	7.58	1.61	1.45
11	AA	2946	A2M	O4'-C4'	7.58	1.61	1.45
60	c	974	A2M	O4'-C4'	7.58	1.61	1.45
60	c	796	A2M	O4'-C4'	7.56	1.61	1.45
11	AA	2220	A2M	O4'-C4'	7.55	1.61	1.45
11	AA	2280	A2M	O4'-C1'	-7.52	1.30	1.41
11	AA	807	A2M	O4'-C1'	-7.51	1.30	1.41
11	AA	1449	A2M	O4'-C4'	7.51	1.61	1.45
11	AA	2281	A2M	O4'-C4'	7.51	1.61	1.45
60	c	100	A2M	O4'-C4'	7.51	1.61	1.45
11	AA	876	A2M	O4'-C4'	7.48	1.61	1.45
60	c	541	A2M	O4'-C4'	7.47	1.61	1.45
60	c	28	A2M	O4'-C4'	7.43	1.61	1.45
11	AA	2280	A2M	O4'-C4'	7.41	1.61	1.45
11	AA	817	A2M	O4'-C1'	-7.34	1.30	1.41
60	c	974	A2M	O4'-C1'	-7.33	1.30	1.41
11	AA	2256	A2M	O4'-C1'	-7.30	1.30	1.41
60	c	100	A2M	O4'-C1'	-7.30	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2640	A2M	O4'-C1'	-7.27	1.30	1.41
60	c	28	A2M	O4'-C1'	-7.27	1.30	1.41
11	AA	817	A2M	O4'-C4'	7.26	1.61	1.45
11	AA	876	A2M	O4'-C1'	-7.26	1.30	1.41
60	c	436	A2M	O4'-C1'	-7.23	1.31	1.41
11	AA	807	A2M	O4'-C4'	7.21	1.61	1.45
11	AA	1449	A2M	O4'-C1'	-7.21	1.31	1.41
60	c	541	A2M	O4'-C1'	-7.21	1.31	1.41
11	AA	2946	A2M	O4'-C1'	-7.19	1.31	1.41
11	AA	1133	A2M	O4'-C1'	-7.17	1.31	1.41
11	AA	2347	OMU	C2-N1	7.17	1.50	1.38
11	AA	2220	A2M	O4'-C1'	-7.11	1.31	1.41
60	c	420	A2M	O4'-C1'	-7.10	1.31	1.41
14	Bb	37	YYG	C21-N20	7.08	1.52	1.34
60	c	796	A2M	O4'-C1'	-7.06	1.31	1.41
11	AA	1888	OMU	C2-N1	7.02	1.49	1.38
60	c	1280	4AC	C4-N3	7.01	1.45	1.32
60	c	619	A2M	O4'-C4'	6.95	1.60	1.45
60	c	578	OMU	C2-N1	6.93	1.49	1.38
60	c	1773	4AC	C4-N3	6.91	1.44	1.32
60	c	1269	OMU	C2-N1	6.89	1.49	1.38
11	AA	2421	OMU	C2-N1	6.85	1.49	1.38
60	c	1773	4AC	C6-C5	6.84	1.51	1.35
11	AA	2724	OMU	C2-N1	6.81	1.49	1.38
11	AA	2921	OMU	C2-N1	6.78	1.49	1.38
11	AA	898	OMU	C2-N1	6.77	1.49	1.38
11	AA	2729	OMU	C2-N1	6.67	1.49	1.38
60	c	578	OMU	C2-N3	6.62	1.49	1.38
60	c	1280	4AC	C6-C5	6.58	1.50	1.35
11	AA	2634	UR3	C6-C5	6.56	1.50	1.35
11	AA	2634	UR3	C2-N1	6.54	1.47	1.38
60	c	1269	OMU	C2-N3	6.54	1.49	1.38
11	AA	2417	OMU	C2-N1	6.53	1.48	1.38
11	AA	2347	OMU	C2-N3	6.53	1.49	1.38
11	AA	1888	OMU	C2-N3	6.52	1.49	1.38
11	AA	2921	OMU	C2-N3	6.48	1.49	1.38
11	AA	2724	OMU	C2-N3	6.46	1.49	1.38
11	AA	898	OMU	C2-N3	6.45	1.49	1.38
11	AA	2417	OMU	C2-N3	6.39	1.49	1.38
11	AA	2729	OMU	C2-N3	6.38	1.49	1.38
11	AA	2421	OMU	C2-N3	6.34	1.49	1.38
60	c	1191	B8N	C2-N1	5.76	1.56	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	578	OMU	C6-C5	5.61	1.48	1.35
11	AA	2417	OMU	C6-C5	5.61	1.48	1.35
11	AA	1888	OMU	C6-C5	5.59	1.48	1.35
11	AA	2729	OMU	C6-C5	5.59	1.48	1.35
60	c	1269	OMU	C6-C5	5.56	1.48	1.35
11	AA	2724	OMU	C6-C5	5.55	1.48	1.35
11	AA	2921	OMU	C6-C5	5.51	1.47	1.35
11	AA	2421	OMU	C6-C5	5.49	1.47	1.35
11	AA	898	OMU	C6-C5	5.49	1.47	1.35
14	Bb	37	YYG	O23-C21	5.46	1.43	1.34
11	AA	2634	UR3	C2-N3	5.43	1.49	1.39
11	AA	2347	OMU	C6-C5	5.42	1.47	1.35
60	c	1280	4AC	C7-N4	5.30	1.47	1.37
60	c	1773	4AC	C7-N4	5.25	1.46	1.37
60	c	1191	B8N	C6-C5	5.21	1.42	1.34
60	c	1575	G7M	C2-N3	5.20	1.45	1.33
60	c	1280	4AC	C2-N1	5.07	1.51	1.40
60	c	1280	4AC	C4-N4	4.90	1.46	1.39
60	c	1773	4AC	C4-N4	4.88	1.46	1.39
60	c	1773	4AC	C2-N1	4.72	1.50	1.40
60	c	1280	4AC	C2-N3	4.70	1.45	1.36
60	c	1575	G7M	C4-N3	4.70	1.48	1.37
60	c	1773	4AC	C2-N3	4.68	1.45	1.36
60	c	1575	G7M	C2-N2	4.51	1.44	1.34
60	c	578	OMU	C4-N3	4.14	1.46	1.38
60	c	1280	4AC	CM7-C7	4.12	1.59	1.50
60	c	1269	OMU	C4-N3	4.03	1.45	1.38
60	c	1280	4AC	C5-C4	4.02	1.49	1.40
14	Bb	37	YYG	O18-C16	4.01	1.43	1.33
11	AA	2347	OMU	C4-N3	4.01	1.45	1.38
60	c	1773	4AC	C5-C4	3.99	1.49	1.40
11	AA	1888	OMU	C4-N3	3.96	1.45	1.38
11	AA	2724	OMU	C4-N3	3.92	1.45	1.38
11	AA	2729	OMU	C4-N3	3.89	1.45	1.38
11	AA	2921	OMU	C4-N3	3.88	1.45	1.38
11	AA	2421	OMU	C4-N3	3.86	1.45	1.38
11	AA	2417	OMU	C4-N3	3.83	1.45	1.38
11	AA	898	OMU	C4-N3	3.78	1.45	1.38
60	c	1773	4AC	CM7-C7	3.69	1.58	1.50
14	Bb	37	YYG	O6-C6	-3.58	1.17	1.22
60	c	1191	B8N	C1'-C5	3.57	1.58	1.50
11	AA	2922	OMG	C8-N7	-3.37	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	1575	G7M	C6-N1	3.36	1.42	1.37
11	AA	898	OMU	O4-C4	-3.26	1.18	1.24
11	AA	1888	OMU	O4-C4	-3.24	1.18	1.24
11	AA	908	OMG	C8-N7	-3.22	1.29	1.35
11	AA	867	OMG	C8-N7	-3.22	1.29	1.35
11	AA	2634	UR3	C6-N1	3.21	1.45	1.38
11	AA	2921	OMU	O4-C4	-3.21	1.18	1.24
11	AA	2421	OMU	O4-C4	-3.20	1.18	1.24
11	AA	2724	OMU	O4-C4	-3.18	1.18	1.24
11	AA	2417	OMU	O4-C4	-3.18	1.18	1.24
11	AA	2347	OMU	O4-C4	-3.16	1.18	1.24
11	AA	2729	OMU	O4-C4	-3.16	1.18	1.24
60	c	541	A2M	C6-N6	3.13	1.45	1.34
11	AA	2791	OMG	C8-N7	-3.11	1.29	1.35
60	c	1575	G7M	C5-C6	3.11	1.53	1.45
11	AA	2640	A2M	C6-N6	3.10	1.45	1.34
60	c	28	A2M	C6-N6	3.09	1.45	1.34
11	AA	2256	A2M	C6-N6	3.08	1.45	1.34
60	c	796	A2M	C6-N6	3.08	1.45	1.34
60	c	420	A2M	C6-N6	3.08	1.45	1.34
11	AA	1133	A2M	C6-N6	3.07	1.45	1.34
11	AA	2220	A2M	C6-N6	3.07	1.45	1.34
60	c	100	A2M	C6-N6	3.05	1.45	1.34
60	c	619	A2M	C6-N6	3.05	1.45	1.34
11	AA	807	A2M	C6-N6	3.05	1.45	1.34
11	AA	2619	OMG	C8-N7	-3.05	1.29	1.35
11	AA	876	A2M	C6-N6	3.04	1.45	1.34
60	c	436	A2M	C6-N6	3.04	1.45	1.34
11	AA	2280	A2M	C6-N6	3.04	1.45	1.34
11	AA	2946	A2M	C6-N6	3.03	1.45	1.34
11	AA	1449	A2M	C6-N6	3.02	1.45	1.34
11	AA	2815	OMG	C8-N7	-3.02	1.29	1.35
60	c	1269	OMU	O4-C4	-3.01	1.18	1.24
11	AA	817	A2M	C6-N6	3.01	1.45	1.34
60	c	974	A2M	C6-N6	3.01	1.45	1.34
11	AA	2288	OMG	C8-N7	-3.00	1.29	1.35
11	AA	649	A2M	C6-N6	2.99	1.45	1.34
60	c	1428	OMG	C8-N7	-2.98	1.29	1.35
11	AA	2793	OMG	C8-N7	-2.97	1.30	1.35
60	c	619	A2M	C5-C4	-2.96	1.33	1.40
11	AA	817	A2M	O3'-C3'	2.96	1.49	1.43
11	AA	2281	A2M	C5-C4	-2.96	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	805	OMG	C8-N7	-2.95	1.30	1.35
60	c	578	OMU	O4-C4	-2.95	1.18	1.24
14	Bb	37	YYG	C4-N3	-2.95	1.34	1.40
11	AA	2281	A2M	C6-N6	2.94	1.44	1.34
11	AA	2281	A2M	O3'-C3'	2.92	1.49	1.43
11	AA	1450	OMG	C8-N7	-2.89	1.30	1.35
14	Bb	37	YYG	C2-N1	-2.88	1.31	1.37
60	c	541	A2M	O3'-C3'	2.88	1.49	1.43
11	AA	649	A2M	C5-C4	-2.86	1.33	1.40
11	AA	1449	A2M	O3'-C3'	2.86	1.49	1.43
60	c	619	A2M	O3'-C3'	2.86	1.49	1.43
60	c	1271	OMG	C8-N7	-2.86	1.30	1.35
11	AA	2946	A2M	C5-C4	-2.86	1.33	1.40
60	c	1126	OMG	C8-N7	-2.86	1.30	1.35
11	AA	817	A2M	C5-C4	-2.85	1.33	1.40
11	AA	2280	A2M	C5-C4	-2.85	1.33	1.40
60	c	420	A2M	O3'-C3'	2.85	1.49	1.43
60	c	1781	MA6	C5-C4	-2.84	1.33	1.40
11	AA	2220	A2M	O3'-C3'	2.84	1.49	1.43
60	c	562	OMG	C8-N7	-2.84	1.30	1.35
11	AA	807	A2M	C5-C4	-2.83	1.33	1.40
11	AA	2142	1MA	C8-N7	-2.82	1.30	1.35
11	AA	2280	A2M	O3'-C3'	2.82	1.49	1.43
60	c	1782	MA6	C5-C4	-2.81	1.33	1.40
11	AA	1133	A2M	C5-C4	-2.80	1.33	1.40
60	c	28	A2M	C5-C4	-2.80	1.33	1.40
11	AA	1449	A2M	C5-C4	-2.79	1.33	1.40
60	c	796	A2M	O2'-C2'	-2.79	1.35	1.42
11	AA	2640	A2M	C5-C4	-2.79	1.33	1.40
60	c	578	OMU	C6-N1	2.79	1.44	1.38
11	AA	2256	A2M	O3'-C3'	2.78	1.49	1.43
60	c	974	A2M	O3'-C3'	2.77	1.49	1.43
60	c	436	A2M	C5-C4	-2.77	1.33	1.40
60	c	100	A2M	C5-C4	-2.77	1.33	1.40
11	AA	2640	A2M	O3'-C3'	2.77	1.49	1.43
60	c	796	A2M	C5-C4	-2.76	1.33	1.40
11	AA	2256	A2M	C5-C4	-2.76	1.33	1.40
11	AA	2729	OMU	C6-N1	2.76	1.44	1.38
60	c	1269	OMU	C6-N1	2.75	1.44	1.38
60	c	420	A2M	C5-C4	-2.75	1.33	1.40
11	AA	2421	OMU	C6-N1	2.75	1.44	1.38
60	c	28	A2M	O3'-C3'	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	974	A2M	C5-C4	-2.74	1.33	1.40
11	AA	2921	OMU	C6-N1	2.74	1.44	1.38
11	AA	2922	OMG	C5-C6	-2.74	1.41	1.47
11	AA	2417	OMU	C6-N1	2.73	1.44	1.38
11	AA	2724	OMU	C6-N1	2.73	1.44	1.38
14	Bb	37	YYG	C13-C12	2.73	1.58	1.50
60	c	436	A2M	O3'-C3'	2.72	1.49	1.43
11	AA	1888	OMU	C6-N1	2.72	1.44	1.38
11	AA	2220	A2M	C5-C4	-2.72	1.33	1.40
11	AA	645	1MA	C8-N7	-2.72	1.30	1.35
11	AA	1133	A2M	O3'-C3'	2.72	1.49	1.43
11	AA	876	A2M	C5-C4	-2.72	1.33	1.40
60	c	28	A2M	O2'-C2'	-2.71	1.35	1.42
11	AA	876	A2M	O3'-C3'	2.71	1.49	1.43
11	AA	2347	OMU	C6-N1	2.71	1.44	1.38
60	c	796	A2M	O3'-C3'	2.71	1.49	1.43
60	c	100	A2M	O3'-C3'	2.70	1.49	1.43
11	AA	898	OMU	C6-N1	2.70	1.44	1.38
11	AA	2281	A2M	O2'-C2'	-2.69	1.35	1.42
11	AA	2220	A2M	O2'-C2'	-2.69	1.35	1.42
11	AA	2946	A2M	O3'-C3'	2.69	1.49	1.43
11	AA	2946	A2M	O2'-C2'	-2.68	1.35	1.42
60	c	100	A2M	O2'-C2'	-2.68	1.35	1.42
11	AA	1449	A2M	O2'-C2'	-2.68	1.35	1.42
11	AA	2421	OMU	O2-C2	-2.66	1.18	1.23
11	AA	2724	OMU	O2-C2	-2.66	1.18	1.23
11	AA	1133	A2M	O2'-C2'	-2.65	1.35	1.42
11	AA	807	A2M	O3'-C3'	2.65	1.49	1.43
11	AA	2729	OMU	O2-C2	-2.65	1.18	1.23
60	c	1572	OMG	C8-N7	-2.65	1.30	1.35
60	c	974	A2M	O2'-C2'	-2.64	1.35	1.42
11	AA	2417	OMU	O2-C2	-2.64	1.18	1.23
11	AA	876	A2M	O2'-C2'	-2.64	1.35	1.42
11	AA	649	A2M	O3'-C3'	2.63	1.49	1.43
60	c	436	A2M	O2'-C2'	-2.63	1.35	1.42
11	AA	2793	OMG	C5-C6	-2.63	1.42	1.47
11	AA	817	A2M	O2'-C2'	-2.62	1.35	1.42
11	AA	2280	A2M	O2'-C2'	-2.61	1.35	1.42
11	AA	898	OMU	O2-C2	-2.61	1.18	1.23
11	AA	1888	OMU	O2-C2	-2.60	1.18	1.23
11	AA	2921	OMU	O2-C2	-2.59	1.18	1.23
60	c	420	A2M	O2'-C2'	-2.58	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	805	OMG	C5-C6	-2.57	1.42	1.47
60	c	1126	OMG	C5-C6	-2.57	1.42	1.47
11	AA	807	A2M	O2'-C2'	-2.57	1.36	1.42
60	c	1269	OMU	O2-C2	-2.57	1.18	1.23
60	c	619	A2M	O2'-C2'	-2.56	1.36	1.42
60	c	541	A2M	C5-C4	-2.56	1.34	1.40
60	c	1428	OMG	C5-C6	-2.55	1.42	1.47
11	AA	2640	A2M	O2'-C2'	-2.54	1.36	1.42
11	AA	649	A2M	O2'-C2'	-2.53	1.36	1.42
11	AA	2619	OMG	C5-C6	-2.52	1.42	1.47
11	AA	2288	OMG	C5-C6	-2.51	1.42	1.47
11	AA	2347	OMU	O2-C2	-2.51	1.18	1.23
60	c	1575	G7M	C2-N1	2.51	1.43	1.37
60	c	578	OMU	O2-C2	-2.50	1.18	1.23
11	AA	1450	OMG	C5-C6	-2.49	1.42	1.47
60	c	1773	4AC	C6-N1	2.47	1.44	1.38
11	AA	867	OMG	C5-C6	-2.46	1.42	1.47
60	c	1773	4AC	O7-C7	-2.45	1.17	1.23
60	c	1271	OMG	C5-C6	-2.45	1.42	1.47
11	AA	2791	OMG	C5-C6	-2.44	1.42	1.47
11	AA	908	OMG	C5-C6	-2.43	1.42	1.47
14	Bb	37	YYG	C10-C11	2.43	1.54	1.50
60	c	1269	OMU	C5-C4	2.41	1.49	1.43
11	AA	2815	OMG	C5-C6	-2.40	1.42	1.47
11	AA	2142	1MA	C5-C4	-2.38	1.37	1.43
11	AA	645	1MA	C5-C4	-2.38	1.37	1.43
60	c	1572	OMG	C5-C6	-2.38	1.42	1.47
60	c	578	OMU	C5-C4	2.37	1.48	1.43
11	AA	2421	OMU	C5-C4	2.35	1.48	1.43
11	AA	2417	OMU	C5-C4	2.33	1.48	1.43
60	c	1575	G7M	O6-C6	-2.33	1.18	1.23
60	c	541	A2M	O2'-C2'	-2.33	1.36	1.42
60	c	1280	4AC	C6-N1	2.32	1.43	1.38
60	c	562	OMG	C5-C6	-2.32	1.42	1.47
11	AA	2729	OMU	C5-C4	2.32	1.48	1.43
60	c	1280	4AC	O7-C7	-2.31	1.18	1.23
11	AA	2634	UR3	O2-C2	-2.31	1.18	1.22
60	c	1782	MA6	C2-N3	2.29	1.35	1.32
11	AA	1888	OMU	C5-C4	2.28	1.48	1.43
11	AA	2921	OMU	C5-C4	2.27	1.48	1.43
60	c	1781	MA6	C2-N3	2.22	1.35	1.32
11	AA	2281	A2M	O5'-C5'	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2256	A2M	O2'-C2'	-2.19	1.37	1.42
11	AA	2634	UR3	C5-C4	2.19	1.49	1.43
11	AA	2347	OMU	C5-C4	2.18	1.48	1.43
60	c	619	A2M	O5'-C5'	-2.17	1.39	1.44
60	c	1191	B8N	O4-C4	-2.16	1.18	1.23
11	AA	2724	OMU	C5-C4	2.16	1.48	1.43
60	c	1191	B8N	O2-C2	-2.15	1.18	1.22
11	AA	898	OMU	C5-C4	2.15	1.48	1.43
60	c	541	A2M	C2-N3	2.15	1.35	1.32
11	AA	2634	UR3	C4-N3	2.13	1.45	1.40
60	c	974	A2M	O5'-C5'	-2.12	1.39	1.44
11	AA	1133	A2M	O5'-C5'	-2.09	1.39	1.44
11	AA	2220	A2M	C2-N3	2.06	1.35	1.32
60	c	28	A2M	O5'-C5'	-2.06	1.39	1.44
60	c	100	A2M	O5'-C5'	-2.06	1.39	1.44
11	AA	2793	OMG	C5-C4	-2.05	1.37	1.43
11	AA	2280	A2M	C2-N3	2.05	1.35	1.32
60	c	420	A2M	C2-N3	2.04	1.35	1.32
11	AA	807	A2M	O5'-C5'	-2.04	1.39	1.44
60	c	100	A2M	C2-N3	2.03	1.35	1.32
60	c	796	A2M	C2-N3	2.03	1.35	1.32
60	c	436	A2M	C2-N3	2.03	1.35	1.32
60	c	974	A2M	C2-N3	2.02	1.35	1.32
11	AA	2640	A2M	C2-N3	2.01	1.35	1.32
11	AA	805	OMG	C5-C4	-2.01	1.38	1.43

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	c	1782	MA6	N1-C6-N6	-14.10	102.21	117.06
60	c	1781	MA6	N1-C6-N6	-13.64	102.70	117.06
11	AA	817	A2M	C5-C6-N6	11.00	137.06	120.35
11	AA	1133	A2M	C5-C6-N6	10.94	136.97	120.35
60	c	619	A2M	C5-C6-N6	10.88	136.88	120.35
11	AA	2946	A2M	C5-C6-N6	10.72	136.64	120.35
60	c	796	A2M	C5-C6-N6	10.70	136.61	120.35
11	AA	2220	A2M	C5-C6-N6	10.66	136.55	120.35
11	AA	807	A2M	C5-C6-N6	10.62	136.49	120.35
60	c	436	A2M	C5-C6-N6	10.61	136.48	120.35
11	AA	876	A2M	C5-C6-N6	10.54	136.36	120.35
60	c	974	A2M	C5-C6-N6	10.53	136.35	120.35
11	AA	1449	A2M	C5-C6-N6	10.53	136.35	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2256	A2M	C5-C6-N6	10.52	136.33	120.35
60	c	28	A2M	C5-C6-N6	10.45	136.23	120.35
60	c	100	A2M	C5-C6-N6	10.43	136.21	120.35
60	c	541	A2M	C5-C6-N6	10.36	136.09	120.35
60	c	420	A2M	C5-C6-N6	10.34	136.07	120.35
11	AA	2280	A2M	C5-C6-N6	10.31	136.03	120.35
11	AA	2640	A2M	C5-C6-N6	10.26	135.94	120.35
11	AA	649	A2M	C5-C6-N6	10.13	135.74	120.35
11	AA	2281	A2M	C5-C6-N6	10.09	135.68	120.35
11	AA	817	A2M	N6-C6-N1	-7.49	103.02	118.57
60	c	619	A2M	N6-C6-N1	-7.36	103.30	118.57
60	c	436	A2M	N6-C6-N1	-7.27	103.48	118.57
11	AA	1449	A2M	N6-C6-N1	-7.23	103.56	118.57
11	AA	807	A2M	N6-C6-N1	-7.23	103.56	118.57
11	AA	2220	A2M	N6-C6-N1	-7.21	103.60	118.57
11	AA	1133	A2M	N6-C6-N1	-7.20	103.62	118.57
11	AA	2946	A2M	N6-C6-N1	-7.17	103.69	118.57
11	AA	876	A2M	N6-C6-N1	-7.16	103.72	118.57
60	c	796	A2M	N6-C6-N1	-7.13	103.78	118.57
11	AA	2256	A2M	N6-C6-N1	-7.09	103.86	118.57
11	AA	2280	A2M	N6-C6-N1	-7.09	103.87	118.57
60	c	541	A2M	N6-C6-N1	-7.07	103.91	118.57
60	c	100	A2M	N6-C6-N1	-7.05	103.95	118.57
60	c	420	A2M	N6-C6-N1	-7.04	103.95	118.57
60	c	974	A2M	N6-C6-N1	-7.01	104.03	118.57
60	c	28	A2M	N6-C6-N1	-6.99	104.06	118.57
11	AA	2640	A2M	N6-C6-N1	-6.97	104.10	118.57
11	AA	2281	A2M	N6-C6-N1	-6.90	104.25	118.57
11	AA	649	A2M	N6-C6-N1	-6.82	104.41	118.57
60	c	619	A2M	N3-C2-N1	-6.02	119.27	128.68
11	AA	1133	A2M	N3-C2-N1	-5.83	119.56	128.68
60	c	974	A2M	N3-C2-N1	-5.83	119.57	128.68
11	AA	817	A2M	N3-C2-N1	-5.82	119.58	128.68
11	AA	649	A2M	N3-C2-N1	-5.78	119.64	128.68
11	AA	2220	A2M	N3-C2-N1	-5.70	119.76	128.68
60	c	28	A2M	N3-C2-N1	-5.68	119.81	128.68
60	c	420	A2M	N3-C2-N1	-5.67	119.81	128.68
60	c	1782	MA6	N3-C2-N1	-5.65	119.85	128.68
11	AA	2281	A2M	N3-C2-N1	-5.64	119.86	128.68
60	c	1781	MA6	N3-C2-N1	-5.62	119.89	128.68
11	AA	1449	A2M	N3-C2-N1	-5.61	119.91	128.68
60	c	100	A2M	N3-C2-N1	-5.61	119.91	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	876	A2M	N3-C2-N1	-5.58	119.95	128.68
11	AA	2946	A2M	N3-C2-N1	-5.58	119.96	128.68
60	c	436	A2M	N3-C2-N1	-5.57	119.97	128.68
60	c	1773	4AC	CM7-C7-N4	5.49	124.79	115.29
60	c	541	A2M	N3-C2-N1	-5.49	120.10	128.68
11	AA	1888	OMU	C4-N3-C2	-5.49	119.34	126.58
11	AA	807	A2M	N3-C2-N1	-5.48	120.12	128.68
60	c	796	A2M	N3-C2-N1	-5.47	120.13	128.68
11	AA	2421	OMU	C4-N3-C2	-5.44	119.40	126.58
11	AA	2417	OMU	C4-N3-C2	-5.43	119.41	126.58
14	Bb	37	YYG	O23-C21-N20	5.41	120.30	110.80
11	AA	2280	A2M	N3-C2-N1	-5.40	120.24	128.68
60	c	1280	4AC	CM7-C7-N4	5.37	124.58	115.29
60	c	578	OMU	C4-N3-C2	-5.35	119.52	126.58
11	AA	2921	OMU	C4-N3-C2	-5.34	119.54	126.58
60	c	1269	OMU	C4-N3-C2	-5.33	119.54	126.58
11	AA	2256	A2M	N3-C2-N1	-5.33	120.36	128.68
11	AA	2640	A2M	N3-C2-N1	-5.28	120.42	128.68
11	AA	2347	OMU	C4-N3-C2	-5.24	119.67	126.58
11	AA	2729	OMU	C4-N3-C2	-5.20	119.72	126.58
11	AA	2634	UR3	C4-N3-C2	-5.15	119.71	124.56
11	AA	898	OMU	C4-N3-C2	-5.14	119.80	126.58
11	AA	2724	OMU	C4-N3-C2	-5.12	119.82	126.58
60	c	1191	B8N	C5-C4-N3	4.98	125.39	116.17
60	c	1191	B8N	C4-N3-C2	-4.16	120.20	125.46
11	AA	2421	OMU	N3-C2-N1	4.01	120.22	114.89
11	AA	2417	OMU	N3-C2-N1	4.01	120.22	114.89
11	AA	1888	OMU	N3-C2-N1	4.00	120.20	114.89
11	AA	2921	OMU	N3-C2-N1	3.83	119.98	114.89
60	c	1269	OMU	N3-C2-N1	3.77	119.89	114.89
11	AA	2347	OMU	N3-C2-N1	3.70	119.80	114.89
11	AA	2256	A2M	O2'-C2'-C1'	3.68	116.38	109.09
60	c	578	OMU	N3-C2-N1	3.66	119.75	114.89
11	AA	2729	OMU	N3-C2-N1	3.66	119.75	114.89
11	AA	2724	OMU	N3-C2-N1	3.66	119.75	114.89
11	AA	898	OMU	N3-C2-N1	3.63	119.70	114.89
60	c	578	OMU	C5-C4-N3	3.55	120.16	114.84
11	AA	2724	OMU	C5-C4-N3	3.50	120.07	114.84
11	AA	898	OMU	C5-C4-N3	3.48	120.05	114.84
11	AA	2417	OMU	C5-C4-N3	3.47	120.04	114.84
11	AA	2729	OMU	C5-C4-N3	3.44	119.98	114.84
11	AA	1888	OMU	C5-C4-N3	3.42	119.95	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2347	OMU	C5-C4-N3	3.41	119.94	114.84
11	AA	2921	OMU	C5-C4-N3	3.41	119.94	114.84
11	AA	2421	OMU	C5-C4-N3	3.40	119.93	114.84
60	c	1269	OMU	C5-C4-N3	3.37	119.88	114.84
14	Bb	37	YYG	O18-C16-C15	3.25	119.84	111.52
60	c	1575	G7M	C2-N1-C6	-3.19	119.22	125.10
14	Bb	37	YYG	O22-C21-N20	-3.18	119.63	124.85
60	c	541	A2M	C1'-N9-C4	3.15	132.18	126.64
14	Bb	37	YYG	O23-C21-O22	-3.07	120.07	124.58
60	c	1280	4AC	C6-C5-C4	3.05	120.69	116.96
11	AA	2347	OMU	O4-C4-C5	-2.99	119.90	125.16
14	Bb	37	YYG	C8-N7-C5	2.98	108.67	102.99
11	AA	2724	OMU	O4-C4-C5	-2.95	119.98	125.16
60	c	578	OMU	O4-C4-C5	-2.94	120.00	125.16
11	AA	1888	OMU	O4-C4-C5	-2.88	120.10	125.16
60	c	1280	4AC	O7-C7-N4	-2.87	117.18	121.82
60	c	1191	B8N	N3-C2-N1	2.86	120.80	116.76
14	Bb	37	YYG	C5-C6-N1	2.86	118.23	113.96
60	c	541	A2M	O2'-C2'-C1'	2.84	114.73	109.09
11	AA	898	OMU	O4-C4-C5	-2.81	120.21	125.16
11	AA	2921	OMU	O4-C4-C5	-2.76	120.30	125.16
11	AA	2417	OMU	O4-C4-C5	-2.69	120.42	125.16
60	c	1773	4AC	C5-C4-N3	-2.67	118.30	122.59
60	c	1269	OMU	O4-C4-C5	-2.66	120.49	125.16
60	c	1773	4AC	O7-C7-N4	-2.60	117.61	121.82
11	AA	876	A2M	C1'-N9-C4	2.59	131.19	126.64
11	AA	2417	OMU	O2-C2-N1	-2.59	119.34	122.79
11	AA	2815	OMG	O6-C6-C5	2.58	129.41	124.37
11	AA	2421	OMU	O4-C4-C5	-2.52	120.73	125.16
11	AA	2281	A2M	O4'-C1'-C2'	-2.50	102.25	106.59
11	AA	645	1MA	N1-C6-N6	2.50	126.13	119.77
11	AA	2729	OMU	O4-C4-C5	-2.49	120.77	125.16
11	AA	1437	OMC	C1'-N1-C2	2.48	123.96	118.42
60	c	1271	OMG	O6-C6-C5	2.47	129.19	124.37
11	AA	2142	1MA	N1-C6-N6	2.47	126.05	119.77
60	c	1773	4AC	C6-C5-C4	2.46	119.97	116.96
60	c	1280	4AC	C5-C4-N3	-2.44	118.67	122.59
60	c	562	OMG	O6-C6-C5	2.43	129.12	124.37
11	AA	2640	A2M	C1'-N9-C4	2.42	130.90	126.64
60	c	1773	4AC	O7-C7-CM7	-2.40	117.60	122.06
14	Bb	37	YYG	C3-N3-C4	2.38	120.93	116.71
60	c	1428	OMG	O6-C6-C5	2.36	128.97	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2619	OMG	O6-C6-C5	2.34	128.94	124.37
60	c	1572	OMG	O6-C6-C5	2.34	128.93	124.37
11	AA	805	OMG	O6-C6-C5	2.33	128.92	124.37
11	AA	2948	OMC	C1'-N1-C2	2.26	123.47	118.42
60	c	578	OMU	O2-C2-N1	-2.25	119.79	122.79
11	AA	867	OMG	O6-C6-C5	2.25	128.77	124.37
11	AA	2793	OMG	O6-C6-C5	2.24	128.74	124.37
11	AA	908	OMG	O6-C6-C5	2.23	128.72	124.37
60	c	1191	B8N	O4'-C1'-C2'	2.23	108.29	105.14
60	c	1126	OMG	O6-C6-C5	2.21	128.69	124.37
11	AA	2142	1MA	C5-C6-N1	-2.20	110.61	113.90
11	AA	2791	OMG	O6-C6-C5	2.20	128.67	124.37
60	c	1575	G7M	O3'-C3'-C2'	2.20	118.92	111.82
11	AA	2288	OMG	O6-C6-C5	2.18	128.64	124.37
11	AA	2421	OMU	O2-C2-N1	-2.18	119.89	122.79
11	AA	2921	OMU	O2-C2-N1	-2.17	119.90	122.79
11	AA	1888	OMU	O2-C2-N1	-2.17	119.91	122.79
11	AA	1450	OMG	O6-C6-C5	2.16	128.59	124.37
60	c	1191	B8N	O4-C4-N3	-2.16	116.31	119.98
14	Bb	37	YYG	C3-N3-C2	-2.16	118.12	120.13
11	AA	2347	OMU	C1'-N1-C2	2.15	121.47	117.57
60	c	414	OMC	C1'-N1-C2	2.14	123.21	118.42
11	AA	2729	OMU	O2-C2-N1	-2.12	119.97	122.79
14	Bb	37	YYG	O6-C6-C5	-2.12	120.42	124.17
11	AA	2922	OMG	O6-C6-C5	2.12	128.50	124.37
60	c	1269	OMU	O2-C2-N1	-2.10	120.00	122.79
11	AA	645	1MA	C5-C6-N1	-2.09	110.78	113.90
60	c	100	A2M	C1'-N9-C4	2.09	130.31	126.64
11	AA	898	OMU	O2-C2-N1	-2.07	120.03	122.79
11	AA	2337	OMC	C1'-N1-C2	2.07	123.03	118.42
60	c	1280	4AC	O7-C7-CM7	-2.06	118.24	122.06
11	AA	1888	OMU	C2'-C1'-N1	-2.03	110.28	114.22
14	Bb	37	YYG	O18-C16-O17	-2.02	119.89	123.84
11	AA	2724	OMU	C1'-N1-C2	2.01	121.21	117.57
11	AA	1449	A2M	C1'-N9-C4	2.01	130.16	126.64

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	1437	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C2
11	AA	2197	OMC	C2'-C1'-N1-C6
11	AA	2256	A2M	C1'-C2'-O2'-CM'
11	AA	2417	OMU	C1'-C2'-O2'-CM2
11	AA	2619	OMG	C1'-C2'-O2'-CM2
11	AA	2640	A2M	C1'-C2'-O2'-CM'
11	AA	2724	OMU	C1'-C2'-O2'-CM2
11	AA	2922	OMG	C3'-C4'-C5'-O5'
14	Bb	37	YYG	C12-C13-C14-C15
14	Bb	37	YYG	C14-C15-N20-C21
14	Bb	37	YYG	O22-C21-N20-C15
14	Bb	37	YYG	O23-C21-N20-C15
14	Bb	37	YYG	N20-C21-O23-C24
14	Bb	37	YYG	O22-C21-O23-C24
60	c	100	A2M	C1'-C2'-O2'-CM'
60	c	414	OMC	C3'-C4'-C5'-O5'
60	c	414	OMC	O4'-C4'-C5'-O5'
60	c	420	A2M	C1'-C2'-O2'-CM'
60	c	541	A2M	O4'-C4'-C5'-O5'
60	c	541	A2M	C3'-C4'-C5'-O5'
60	c	541	A2M	C1'-C2'-O2'-CM'
60	c	619	A2M	C1'-C2'-O2'-CM'
60	c	1271	OMG	C1'-C2'-O2'-CM2
60	c	1280	4AC	O4'-C4'-C5'-O5'
60	c	1280	4AC	C3'-C4'-C5'-O5'
60	c	1572	OMG	O4'-C4'-C5'-O5'
60	c	1782	MA6	O4'-C4'-C5'-O5'
14	Bb	37	YYG	O17-C16-O18-C19
14	Bb	37	YYG	C15-C16-O18-C19
11	AA	1450	OMG	C3'-C4'-C5'-O5'
60	c	578	OMU	O4'-C4'-C5'-O5'
60	c	619	A2M	O4'-C4'-C5'-O5'
60	c	619	A2M	C3'-C4'-C5'-O5'
60	c	1572	OMG	C3'-C4'-C5'-O5'
60	c	1575	G7M	C3'-C4'-C5'-O5'
60	c	1782	MA6	C3'-C4'-C5'-O5'
60	c	1575	G7M	O4'-C4'-C5'-O5'
11	AA	817	A2M	C3'-C2'-O2'-CM'
11	AA	908	OMG	C3'-C2'-O2'-CM2
11	AA	2870	5MC	C2'-C1'-N1-C6
11	AA	867	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	AA	2922	OMG	O4'-C4'-C5'-O5'
11	AA	2256	A2M	O4'-C4'-C5'-O5'
60	c	100	A2M	O4'-C4'-C5'-O5'
11	AA	2870	5MC	O4'-C1'-N1-C6
60	c	1280	4AC	O7-C7-N4-C4
60	c	1280	4AC	CM7-C7-N4-C4
60	c	1773	4AC	O7-C7-N4-C4
60	c	1773	4AC	CM7-C7-N4-C4
11	AA	867	OMG	O4'-C4'-C5'-O5'
60	c	28	A2M	C1'-C2'-O2'-CM'
11	AA	2870	5MC	C2'-C1'-N1-C2
60	c	1191	B8N	C31-C32-C33-N34
60	c	1428	OMG	C4'-C5'-O5'-P
11	AA	807	A2M	C3'-C2'-O2'-CM'
11	AA	807	A2M	C3'-C4'-C5'-O5'
60	c	578	OMU	C3'-C4'-C5'-O5'
11	AA	817	A2M	C4'-C5'-O5'-P
11	AA	2197	OMC	O4'-C1'-N1-C2
11	AA	2870	5MC	O4'-C1'-N1-C2
11	AA	2256	A2M	C3'-C4'-C5'-O5'
11	AA	2197	OMC	O4'-C1'-N1-C6
60	c	1126	OMG	C3'-C4'-C5'-O5'
11	AA	2280	A2M	C3'-C4'-C5'-O5'
11	AA	2281	A2M	O4'-C4'-C5'-O5'
60	c	1782	MA6	C4'-C5'-O5'-P
60	c	578	OMU	C2'-C1'-N1-C6
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	876	A2M	C1'-C2'-O2'-CM'
14	Bb	37	YYG	N20-C15-C16-O17
60	c	578	OMU	O4'-C1'-N1-C6
11	AA	876	A2M	C3'-C2'-O2'-CM'
11	AA	807	A2M	O4'-C4'-C5'-O5'
11	AA	2280	A2M	O4'-C4'-C5'-O5'
11	AA	1437	OMC	O4'-C4'-C5'-O5'
11	AA	817	A2M	O4'-C4'-C5'-O5'
60	c	414	OMC	C2'-C1'-N1-C2

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 315 ligands modelled in this entry, 311 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
87	SPD	AA	3620	-	9,9,9	0.28	0	8,8,8	0.76	0
87	SPD	AA	3619	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPD	c	1965	-	9,9,9	0.29	0	8,8,8	0.81	0
87	SPD	AA	3618	-	9,9,9	0.31	0	8,8,8	0.81	0

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
87	SPD	AA	3620	-	-	4/7/7/7	-
87	SPD	AA	3619	-	-	0/7/7/7	-
87	SPD	c	1965	-	-	1/7/7/7	-
87	SPD	AA	3618	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	AA	3620	SPD	C3-C4-C5-N6
87	AA	3620	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
87	AA	3620	SPD	C4-C5-N6-C7
87	AA	3618	SPD	N1-C2-C3-C4
87	c	1965	SPD	C2-C3-C4-C5
87	AA	3618	SPD	C7-C8-C9-N10
87	AA	3620	SPD	N1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16563. 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.