Full wwPDB EM Validation Report

Apr 16, 2024 – 04:05 am BST

PDB ID	:	7OYD
EMDB ID	:	EMD-13114
Title	:	Cryo-EM structure of a rabbit 80S ribosome with zebrafish Dap1b
Authors	:	Leesch, F.; Lorenzo-Orts, L.; Grishkovskaya, I.; Kandolf, S.; Belacic, K.; Meinhart, A.; Haselbach, D.; Pauli, A.
Deposited on	:	2021-06-24
Resolution	:	2.30 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:

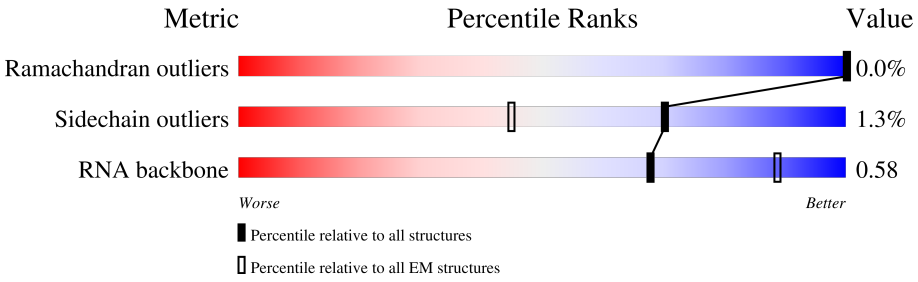
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 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	x	217	74% · 25%
2	5	3740	74% 15% · 10%
3	8	156	83% 10% 8%
4	9	1786	67% 25% · 5%
5	A	257	95% · ·
6	AA	295	73% · 26%
7	Aa	115	87% · 12%
8	B	403	97% · ·
9	BB	264	78% · 19%

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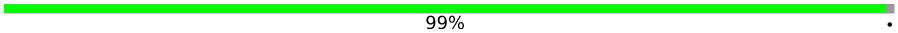
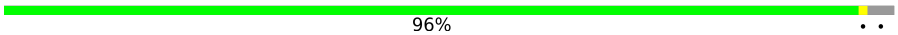
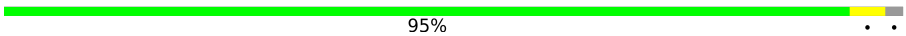
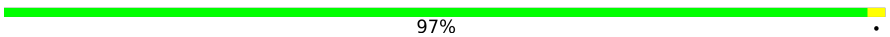
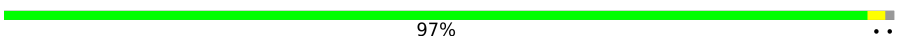
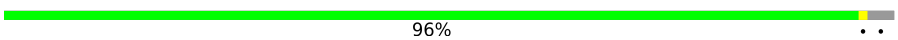
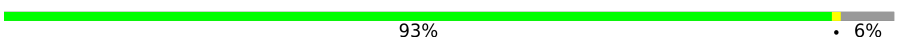
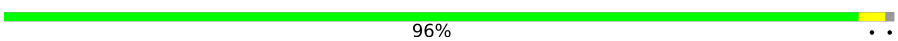
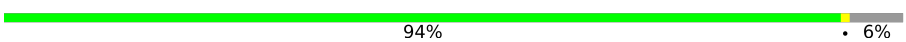
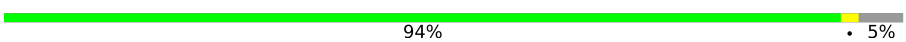
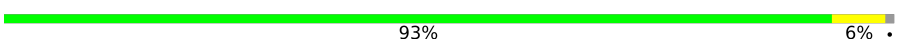
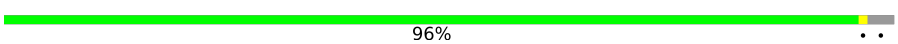
Mol	Chain	Length	Quality of chain
10	Bb	84	
11	C	413	
12	CC	293	
13	Cc	69	
14	D	297	
15	DD	243	
16	Dd	56	
17	E	291	
18	EE	263	
19	Ee	133	
20	F	249	
21	FF	204	
22	G	266	
23	GG	249	
24	Gg	317	
25	H	192	
26	HH	432	
27	I	214	
28	II	208	
29	J	178	
30	JJ	194	
31	K	120	
32	KK	165	
33	L	211	
34	LL	158	

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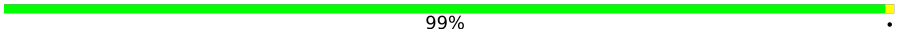
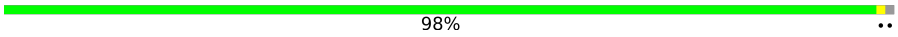
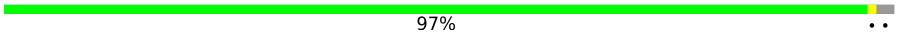
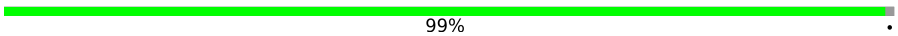
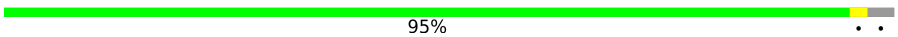
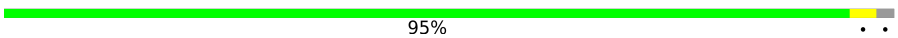
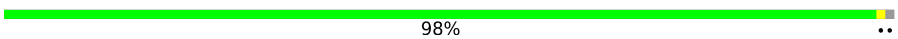
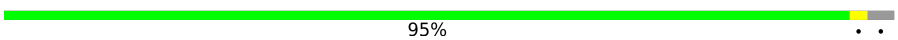
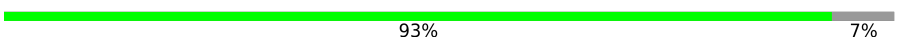
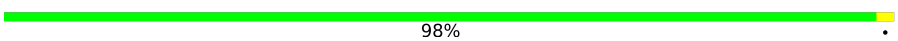
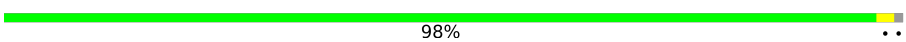
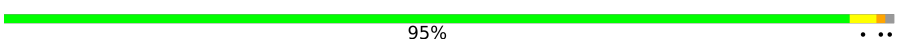
Mol	Chain	Length	Quality of chain
35	M	218	
36	N	204	
37	NN	151	
38	O	203	
39	OO	151	
40	P	187	
41	PP	145	
42	Q	188	
43	QQ	146	
44	R	196	
45	RR	135	
46	S	224	
47	SS	152	
48	T	160	
49	TT	145	
50	U	141	
51	UU	119	
52	V	140	
53	VV	83	
54	W	157	
55	WW	130	
56	X	156	
57	XX	143	
58	Y	145	
59	YY	133	

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Mol	Chain	Length	Quality of chain
60	Z	136	99%
61	ZZ	124	60% 40%
62	a	148	99%
63	b	245	40% 60%
64	c	115	82% 18%
65	d	125	85% 15%
66	e	157	82% 18%
67	f	110	99%
68	g	117	94% 5%
69	h	123	98%
70	i	105	96%
71	j	97	89% 11%
72	k	70	97%
73	l	51	98%
74	m	128	40% 60%
75	n	25	100%
76	o	106	95%
77	p	92	99%
78	r	137	89% 10%
79	s	318	61% 38%
80	s1	109	16% 83%
81	t	154	79% 18%
82	v	858	83% 15%
83	w	407	8% 92%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 213014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	x	163	1291	832	225	228	6	0	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	3358	72165	32204	13226	23377	3358	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	144	3072	1370	547	1011	144	0	0

- Molecule 4 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	9	1698	36291	16217	6509	11868	1697	0	0

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	247	1891	1185	388	312	6	0	0

- Molecule 6 is a protein called 40S ribosomal protein SA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 7 is a protein called 40S ribosomal protein S26-like.

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

- Molecule 8 is a protein called Ribosomal protein L3.

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

- Molecule 9 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 10 is a protein called 40S ribosomal protein S27.

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

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	358	Total	C	N	O	S	0	0
			2856	1797	572	473	14		

- Molecule 12 is a protein called 40S ribosomal protein S2.

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

- Molecule 13 is a protein called 40S ribosomal protein S28.

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

- Molecule 14 is a protein called 60S ribosomal protein L5.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 15 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 16 is a protein called 40S ribosomal protein S29.

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

- Molecule 17 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	213	Total	C	N	O	S	0	0
			1710	1103	325	279	3		

- Molecule 18 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17

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

- Molecule 19 is a protein called 40S ribosomal protein S30.

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

- Molecule 20 is a protein called 60S ribosomal protein L7.

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

- Molecule 21 is a protein called Ribosomal protein S5.

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

- Molecule 22 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	215	Total	C	N	O	S	0	0
			1747	1115	337	291	4		

- Molecule 23 is a protein called 40S ribosomal protein S6.

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

- Molecule 24 is a protein called RACK1.

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

- Molecule 25 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H	186	Total	C	N	O	S	0	0
			1484	933	277	268	6		

- Molecule 26 is a protein called 40S ribosomal protein S7.

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

- Molecule 27 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	202	Total	C	N	O	S	0	0
			1640	1041	317	269	13		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 29 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	168	Total	C	N	O	S	0	0
			1344	850	251	237	6		

- Molecule 30 is a protein called 40S ribosomal protein S9.

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

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	K	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 32 is a protein called S10_plectin domain-containing protein.

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

- Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	205	Total	C	N	O	S	0	0
			1658	1037	346	271	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 34 is a protein called 40S ribosomal protein S11.

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

- Molecule 35 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	M	135	Total	C	N	O	S	0	0
			1117	715	217	178	7		

- Molecule 36 is a protein called Ribosomal protein L15.

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

- Molecule 37 is a protein called 40S ribosomal protein S13.

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

- Molecule 38 is a protein called 60S ribosomal protein L13a.

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

- Molecule 39 is a protein called 40S ribosomal protein S14-like.

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

- Molecule 40 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	152	Total	C	N	O	S	0	0
			1233	772	240	212	9		

- Molecule 41 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	PP	125	Total	C	N	O	S	0	0
			1025	652	192	174	7		

- Molecule 42 is a protein called Ribosomal protein L18.

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

- Molecule 43 is a protein called Ribosomal protein S16.

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

- Molecule 44 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	R	166	Total	C	N	O	S	0	0
			1383	859	298	217	9		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 45 is a protein called 40S ribosomal protein eS17.

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

- Molecule 46 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S	176	Total	C	N	O	S	0	0
			1456	927	282	236	11		

- Molecule 47 is a protein called 40S ribosomal protein uS13.

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

- Molecule 48 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	158	Total	C	N	O	S	0	0
			1292	820	251	215	6		

- Molecule 49 is a protein called 40S ribosomal protein S19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 50 is a protein called 60S ribosomal protein L22-like.

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

- Molecule 51 is a protein called 40S ribosomal protein uS10.

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

- Molecule 52 is a protein called Ribosomal protein L23.

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

- Molecule 53 is a protein called 40S ribosomal protein S21.

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

- Molecule 54 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 55 is a protein called Ribosomal protein S15a.

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

- Molecule 56 is a protein called 60S ribosomal protein L23a.

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

- Molecule 57 is a protein called 40S ribosomal protein S23.

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

- Molecule 58 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 59 is a protein called 40S ribosomal protein S24.

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

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

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

- Molecule 61 is a protein called 40S ribosomal protein S25.

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

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b	98	Total	C	N	O	S	0	0
			806	498	182	123	3		

- Molecule 64 is a protein called 60S ribosomal protein L30.

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

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	d	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 66 is a protein called 60S ribosomal protein L32.

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

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	h	121	Total	C	N	O	S	0	0
			1008	637	203	167	1		

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	i	101	Total	C	N	O	S	0	0
			821	514	174	128	5		

- Molecule 71 is a protein called Ribosomal protein L37.

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

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 73 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 74 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 75 is a protein called 60s ribosomal protein l41.

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

- Molecule 76 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	o	102	Total	C	N	O	S	0	0
			834	522	171	135	6		

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r	123	Total	C	N	O	S	0	0
			986	611	204	166	5		

- Molecule 79 is a protein called 60S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	s	196	Total	C	N	O	S	0	0
			1501	953	263	276	9		

- Molecule 80 is a protein called Dap1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	s1	18	Total	C	N	O	S	0	0
			150	96	30	23	1		

- Molecule 81 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	t	126	Total	C	N	O	S	0	0
			961	603	168	182	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	36	SER	GLY	conflict	UNP P10160

- Molecule 82 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	v	726	Total 5669	C 3611	N 972	O 1046	S 40	0	0

- Molecule 83 is a protein called SERPINE1 mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	w	32	Total 252	C 148	N 55	O 49	0	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	195	Total 195	Mg 195	0
84	8	2	Total 2	Mg 2	0
84	I	1	Total 1	Mg 1	0
84	P	1	Total 1	Mg 1	0
84	g	1	Total 1	Mg 1	0
84	v	1	Total 1	Mg 1	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

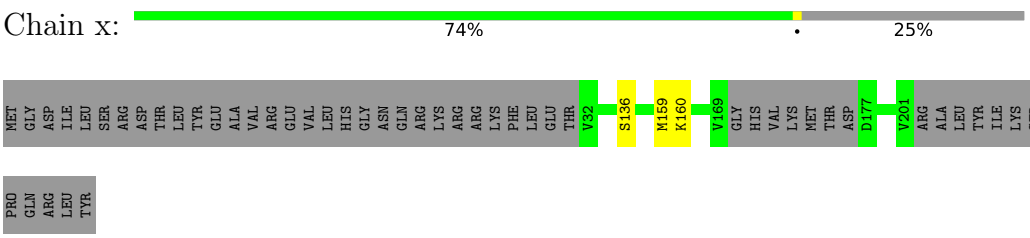
Mol	Chain	Residues	Atoms		AltConf
85	Aa	1	Total 1	Zn 1	0
85	KK	1	Total 1	Zn 1	0
85	g	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0
85	m	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0

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.

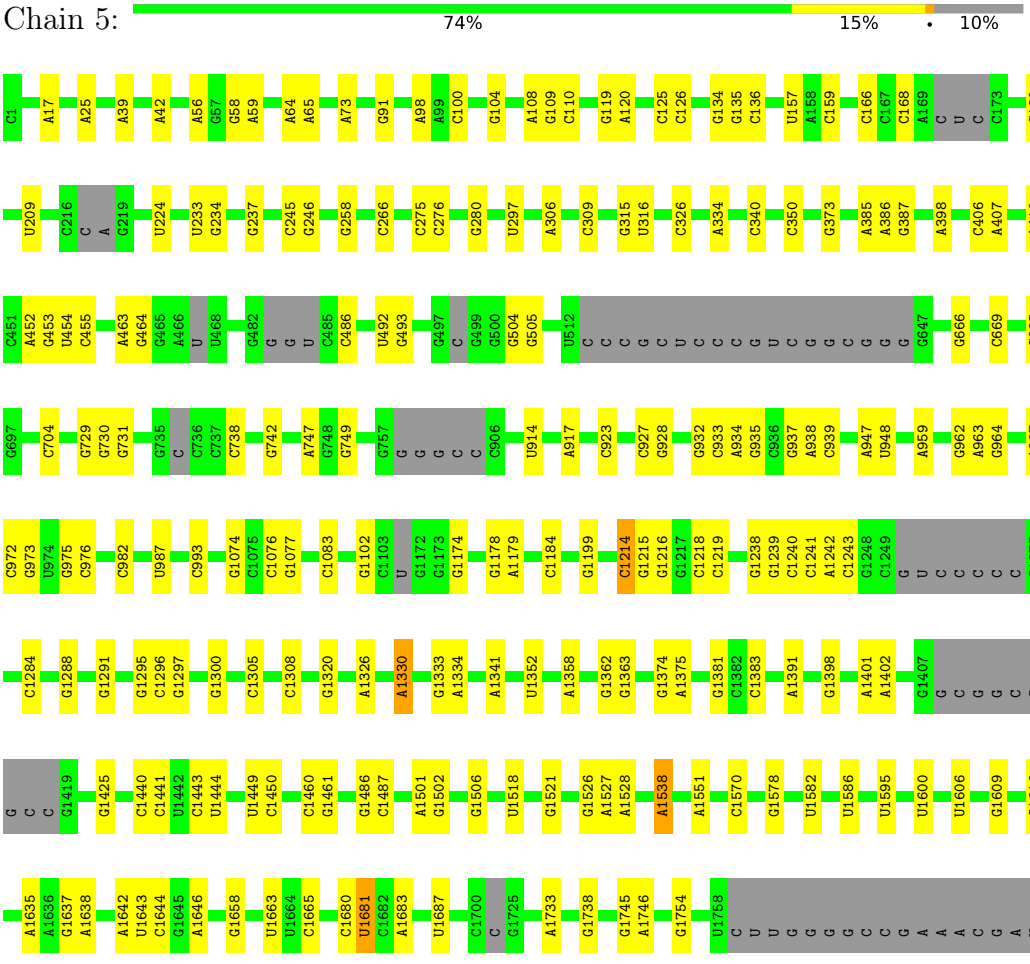
- Molecule 1: Ribosomal protein uL1

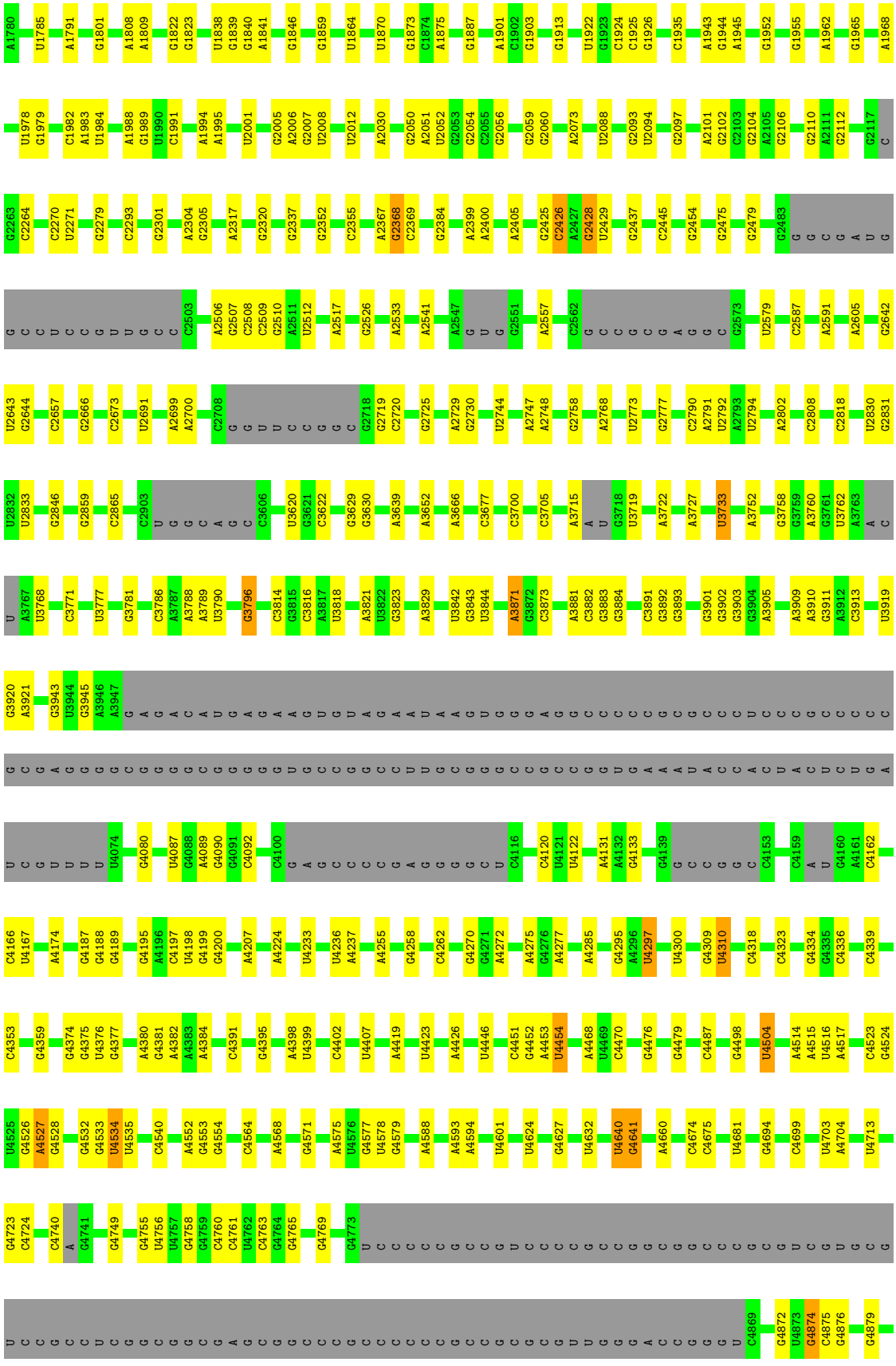
Chain x:

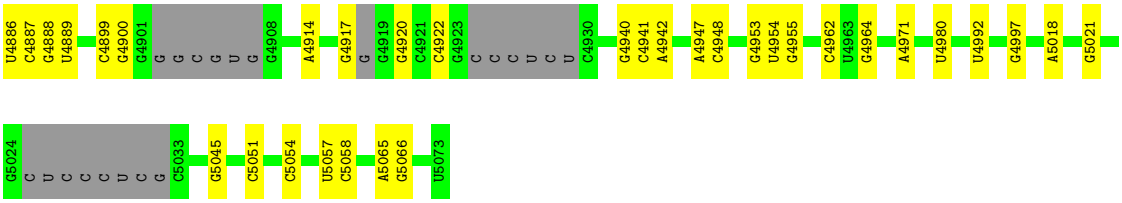


- Molecule 2: 28S rRNA

Chain 5:

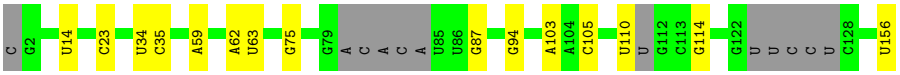






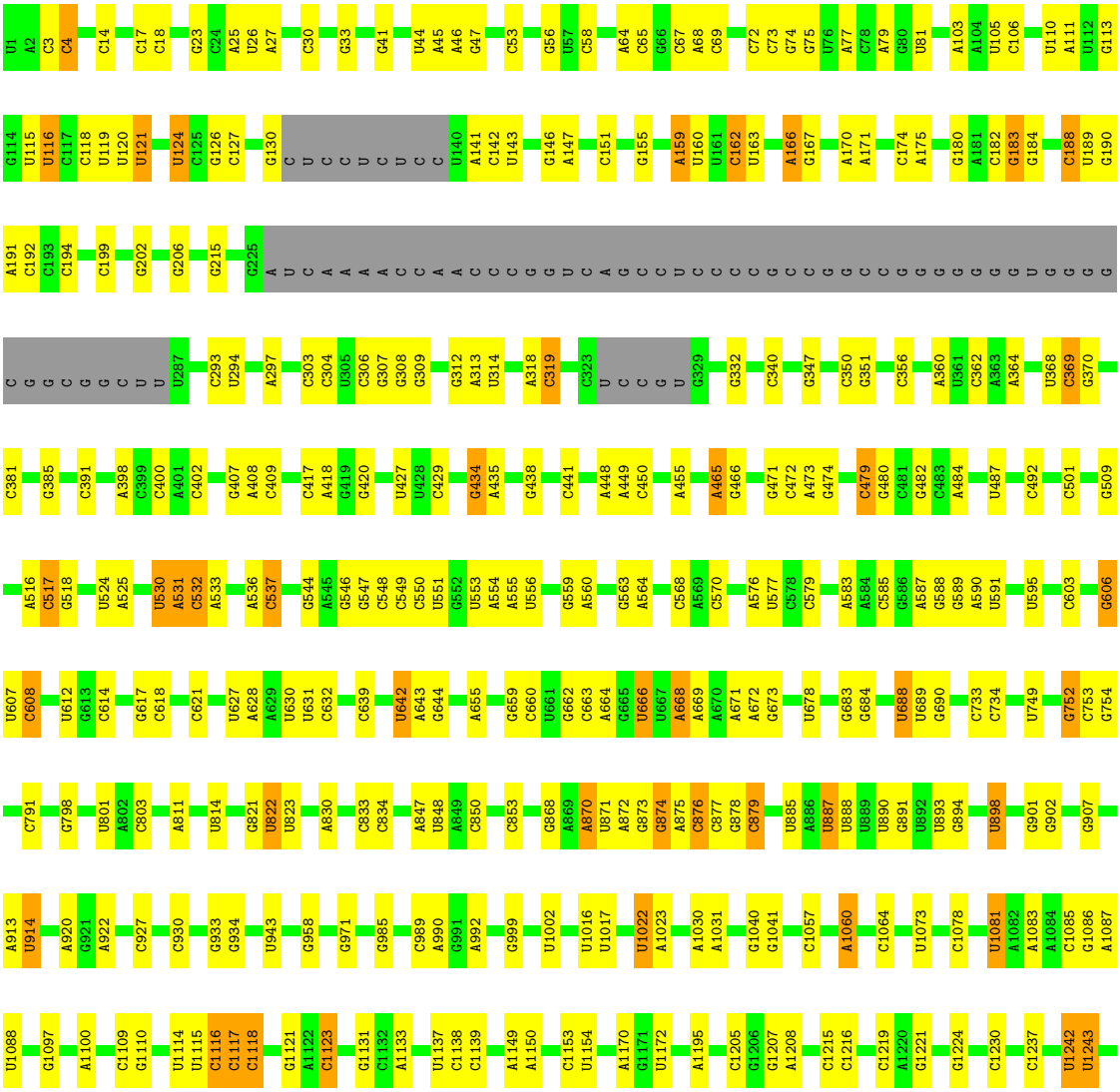
• Molecule 3: 5.8S rRNA

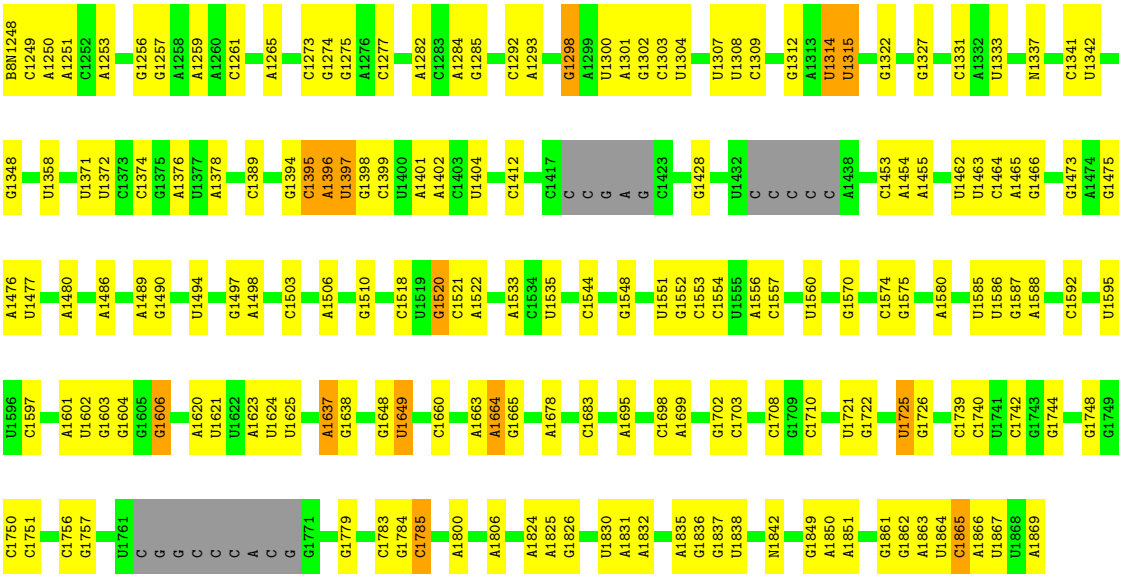
Chain 8:



• Molecule 4: 18S rRNA

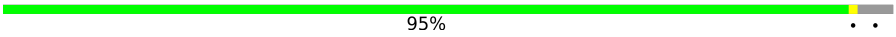
Chain 9:

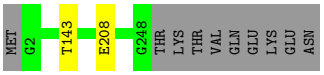




• Molecule 5: 60S ribosomal protein L8

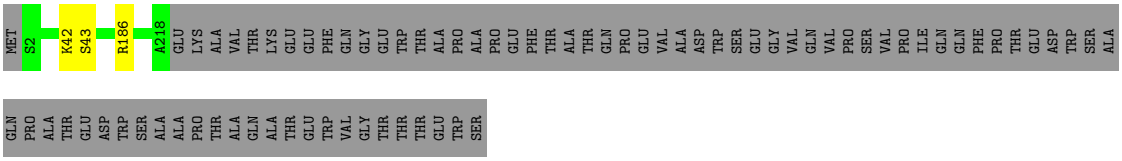
Chain A:





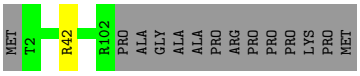
• Molecule 6: 40S ribosomal protein SA

Chain AA:



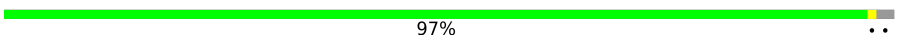
• Molecule 7: 40S ribosomal protein S26-like

Chain Aa:



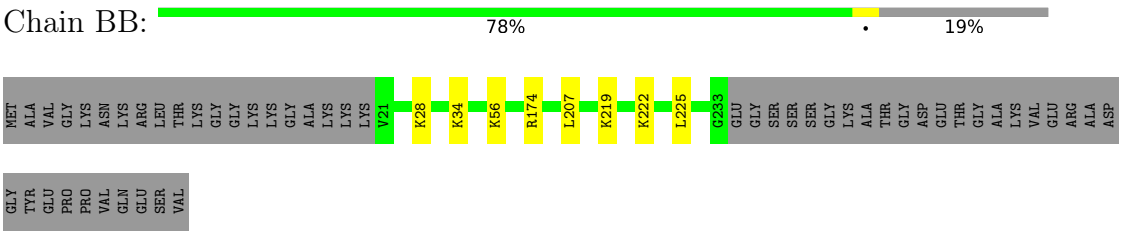
• Molecule 8: Ribosomal protein L3

Chain B:



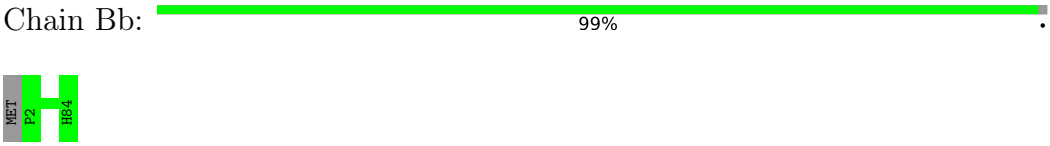
• Molecule 9: 40S ribosomal protein S3a

Chain BB:



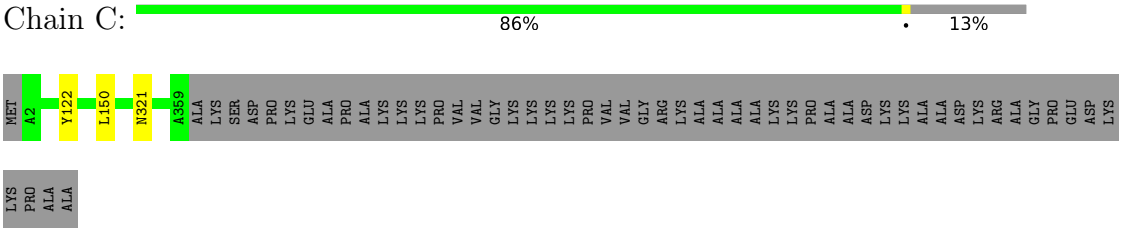
• Molecule 10: 40S ribosomal protein S27

Chain Bb:



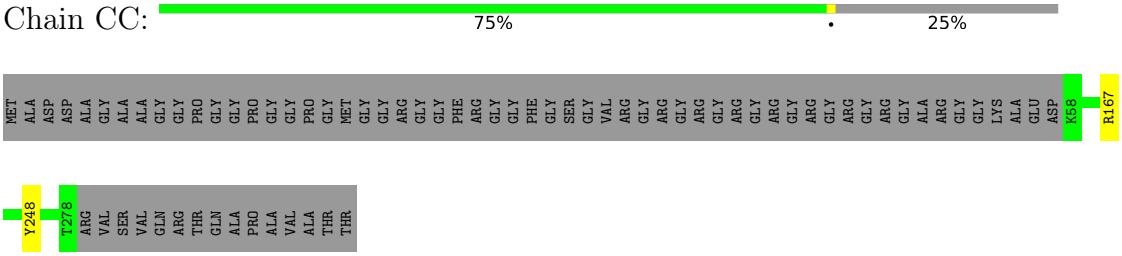
• Molecule 11: 60S ribosomal protein L4

Chain C:



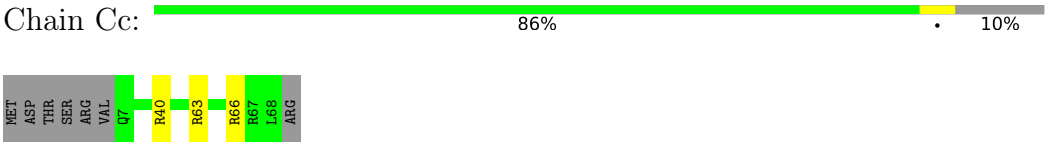
• Molecule 12: 40S ribosomal protein S2

Chain CC:



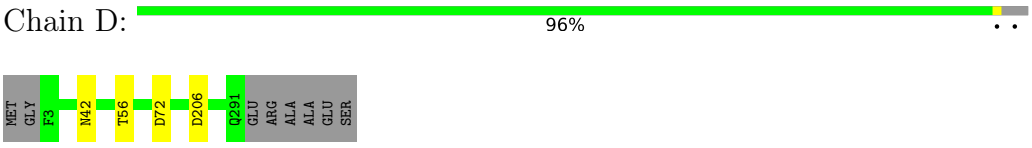
• Molecule 13: 40S ribosomal protein S28

Chain Cc:



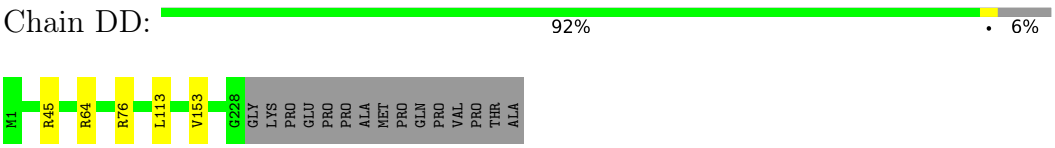
• Molecule 14: 60S ribosomal protein L5

Chain D:



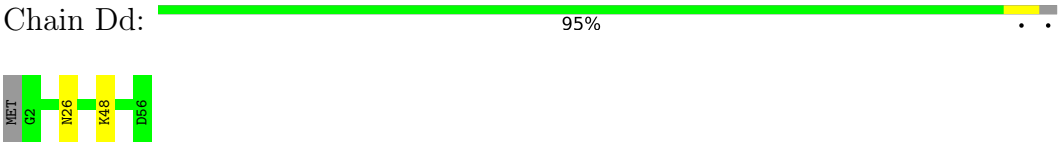
• Molecule 15: Ribosomal protein S3

Chain DD:



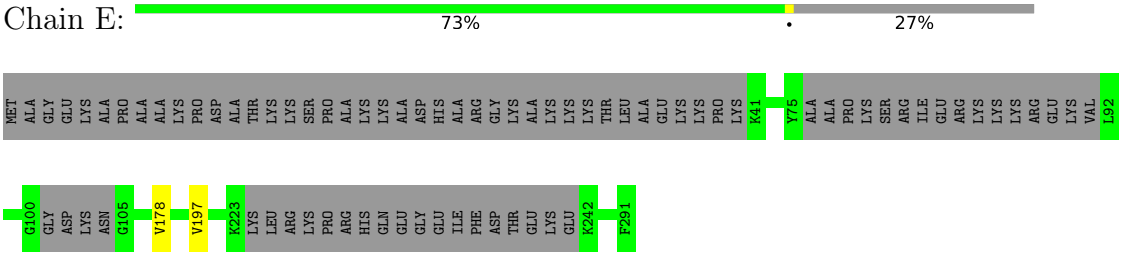
• Molecule 16: 40S ribosomal protein S29

Chain Dd:



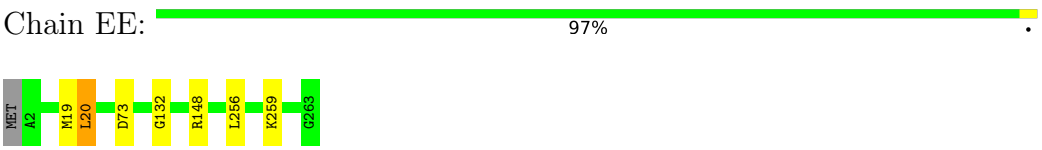
• Molecule 17: 60S ribosomal protein L6

Chain E:



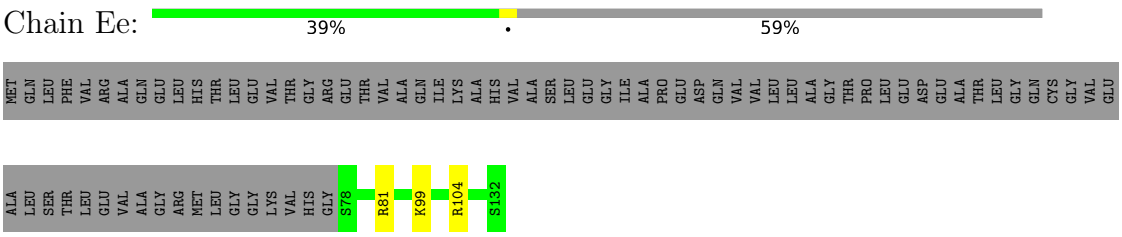
• Molecule 18: 40S ribosomal protein S4

Chain EE:



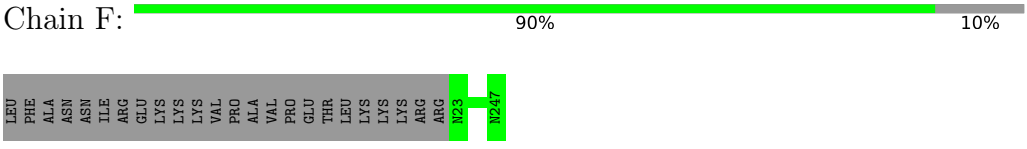
• Molecule 19: 40S ribosomal protein S30

Chain Ee:



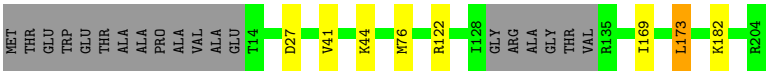
• Molecule 20: 60S ribosomal protein L7

Chain F:



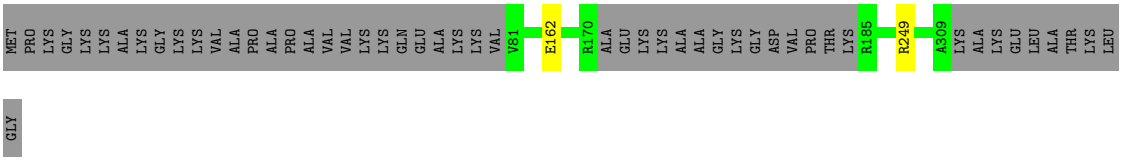
• Molecule 21: Ribosomal protein S5

Chain FF:



• Molecule 22: 60S ribosomal protein L7a

Chain G:

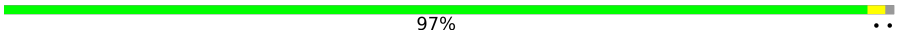


• Molecule 23: 40S ribosomal protein S6

Chain GG:

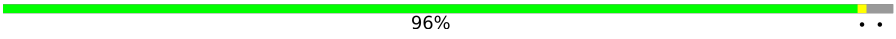
• Molecule 24: RACK1

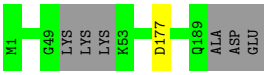
Chain Gg:



• Molecule 25: 60S ribosomal protein L9

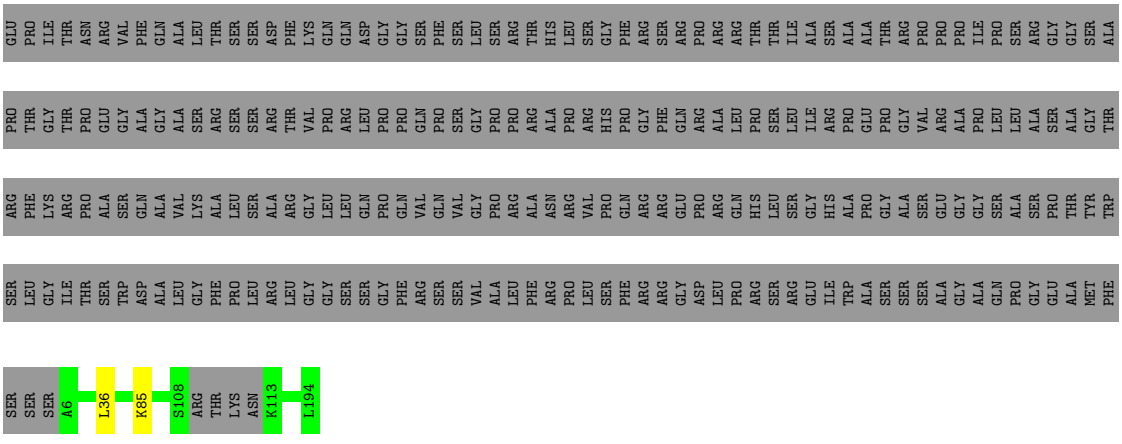
Chain H:





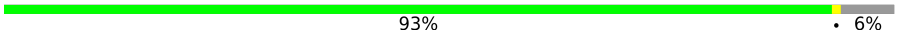
• Molecule 26: 40S ribosomal protein S7

Chain HH:



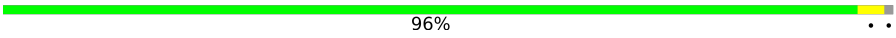
• Molecule 27: 60S ribosomal protein L10

Chain I:



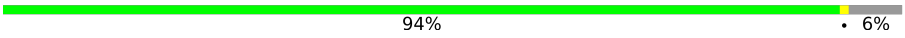
• Molecule 28: 40S ribosomal protein S8

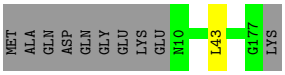
Chain II:



• Molecule 29: 60S ribosomal protein L11

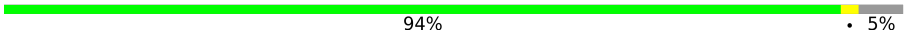
Chain J:

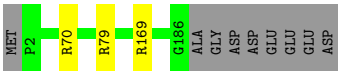




• Molecule 30: 40S ribosomal protein S9

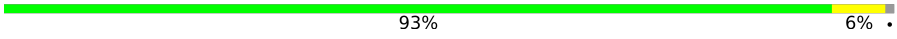
Chain JJ:

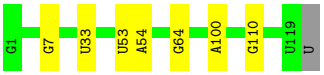




• Molecule 31: 5S rRNA

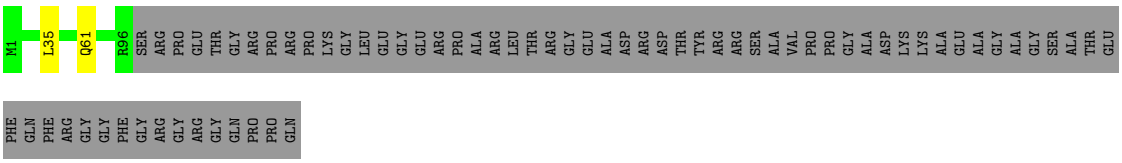
Chain K:





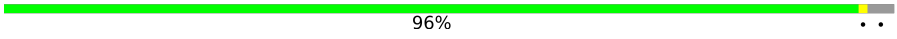
• Molecule 32: S10_plectin domain-containing protein

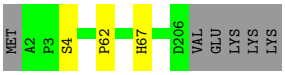
Chain KK:



• Molecule 33: 60S ribosomal protein L13

Chain L:



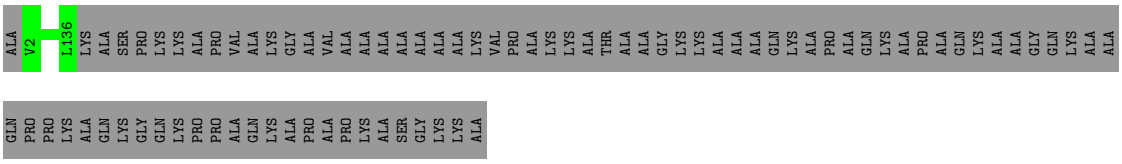


• Molecule 34: 40S ribosomal protein S11

Chain LL:

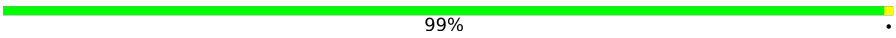
• Molecule 35: 60S ribosomal protein L14

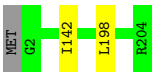
Chain M:



• Molecule 36: Ribosomal protein L15

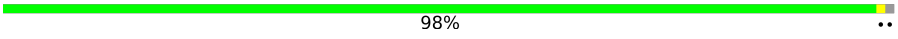
Chain N:

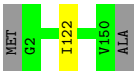




• Molecule 37: 40S ribosomal protein S13

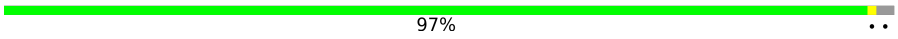
Chain NN:

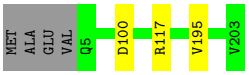




• Molecule 38: 60S ribosomal protein L13a

Chain O:



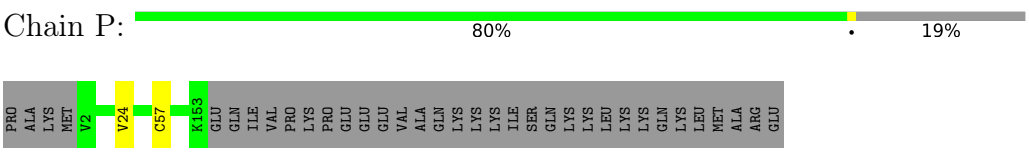


• Molecule 39: 40S ribosomal protein S14-like

Chain OO:

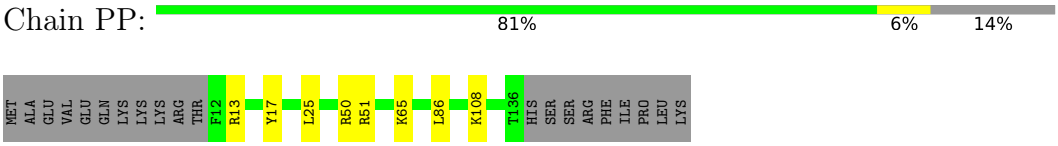
• Molecule 40: 60S ribosomal protein L17

Chain P:



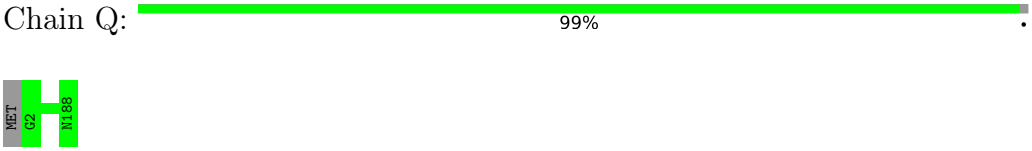
• Molecule 41: 40S ribosomal protein uS19

Chain PP:



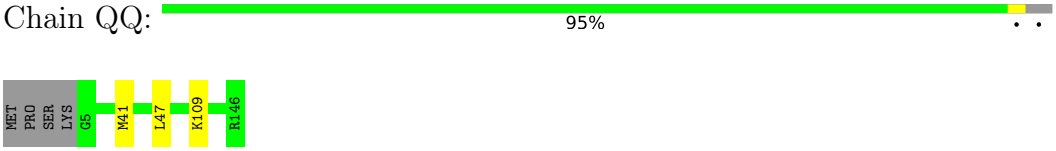
• Molecule 42: Ribosomal protein L18

Chain Q:



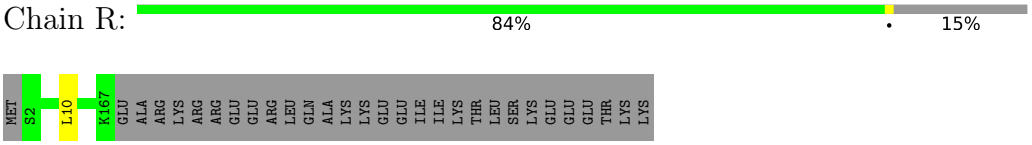
• Molecule 43: Ribosomal protein S16

Chain QQ:



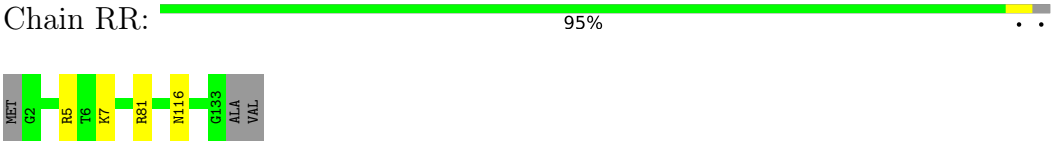
• Molecule 44: Ribosomal protein L19

Chain R:



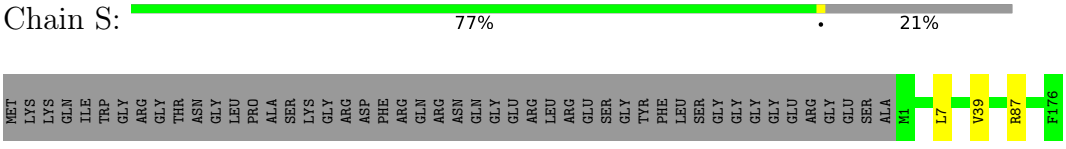
• Molecule 45: 40S ribosomal protein eS17

Chain RR:



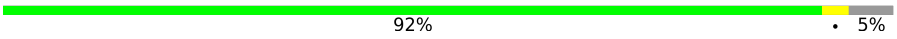
• Molecule 46: 60S ribosomal protein L18a

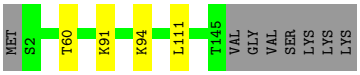
Chain S:



• Molecule 47: 40S ribosomal protein uS13

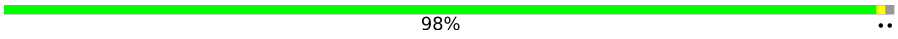
Chain SS:





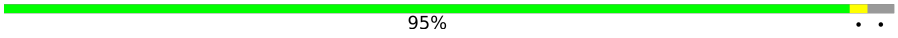
• Molecule 48: 60S ribosomal protein L21

Chain T:



• Molecule 49: 40S ribosomal protein S19

Chain TT:



• Molecule 50: 60S ribosomal protein L22-like

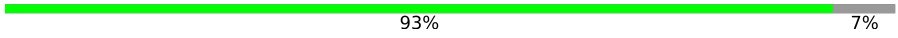
Chain U:

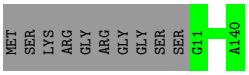
• Molecule 51: 40S ribosomal protein uS10

Chain UU:

• Molecule 52: Ribosomal protein L23

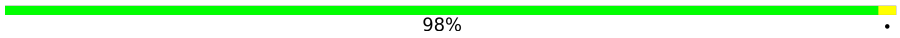
Chain V:

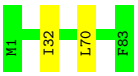




• Molecule 53: 40S ribosomal protein S21

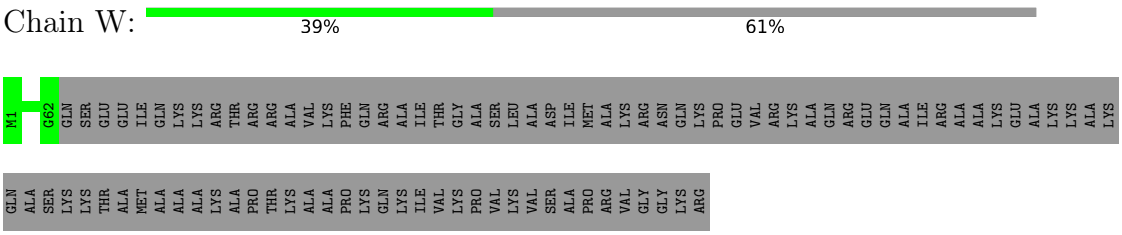
Chain VV:





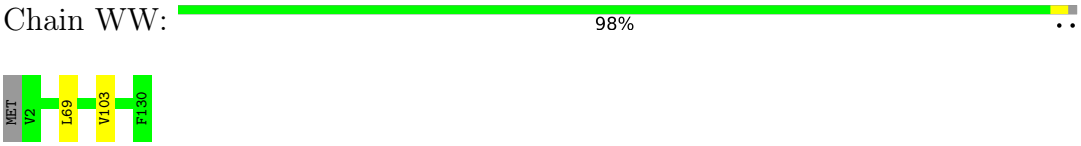
• Molecule 54: Ribosomal protein L24

Chain W:



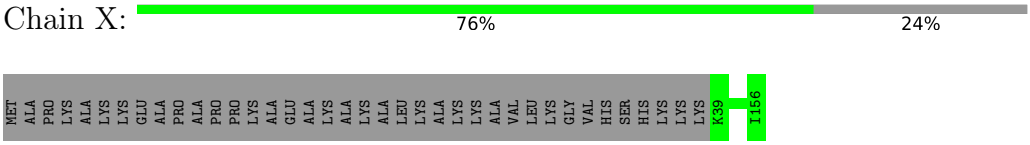
• Molecule 55: Ribosomal protein S15a

Chain WW:



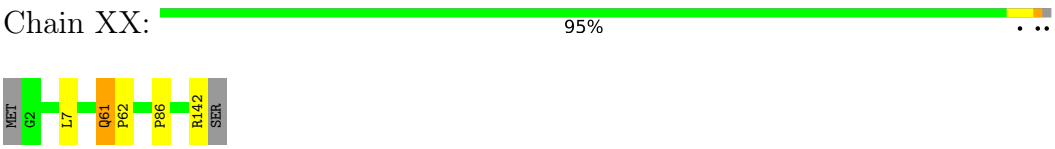
• Molecule 56: 60S ribosomal protein L23a

Chain X:



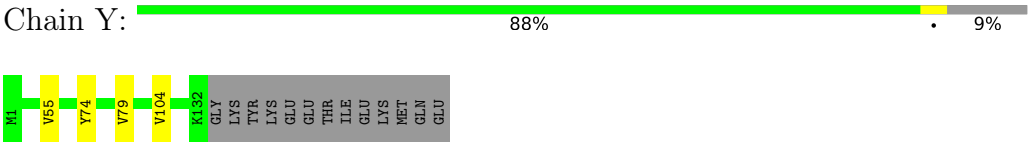
• Molecule 57: 40S ribosomal protein S23

Chain XX:



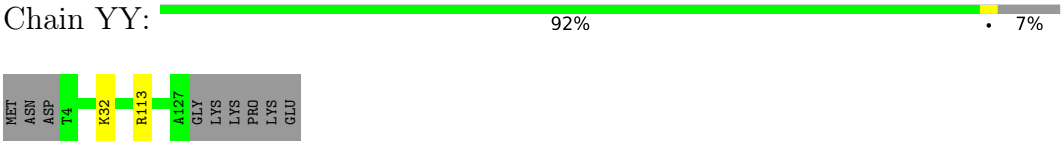
• Molecule 58: Ribosomal protein L26

Chain Y:



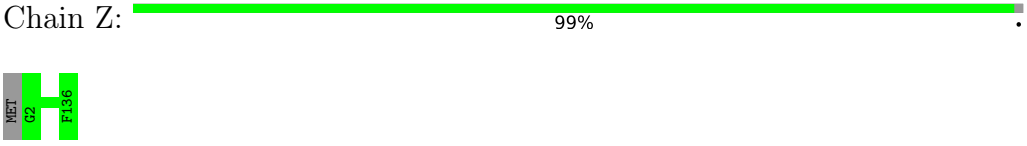
• Molecule 59: 40S ribosomal protein S24

Chain YY:



• Molecule 60: 60S ribosomal protein L27

Chain Z:

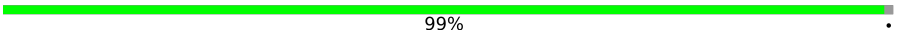


• Molecule 61: 40S ribosomal protein S25

Chain ZZ:

• Molecule 62: 60S ribosomal protein L27a

Chain a:

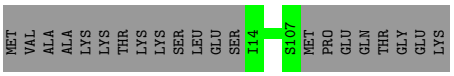


• Molecule 63: 60S ribosomal protein L29

Chain b:

• Molecule 64: 60S ribosomal protein L30

Chain c:



• Molecule 65: 60S ribosomal protein L31

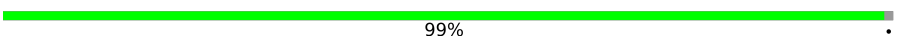
Chain d:

• Molecule 66: 60S ribosomal protein L32

Chain e:

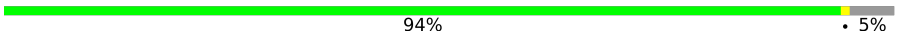
• Molecule 67: 60S ribosomal protein L35a

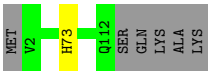
Chain f:



• Molecule 68: 60S ribosomal protein L34

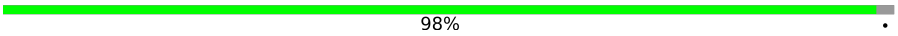
Chain g:





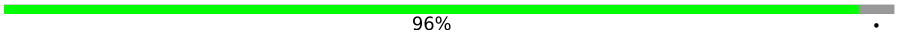
• Molecule 69: 60S ribosomal protein L35

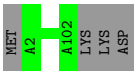
Chain h:



• Molecule 70: 60S ribosomal protein L36

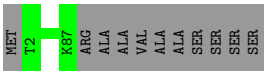
Chain i:





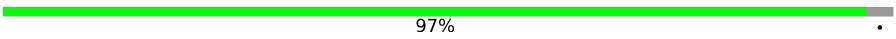
• Molecule 71: Ribosomal protein L37

Chain j:



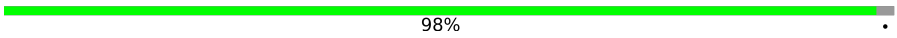
• Molecule 72: 60S ribosomal protein L38

Chain k:



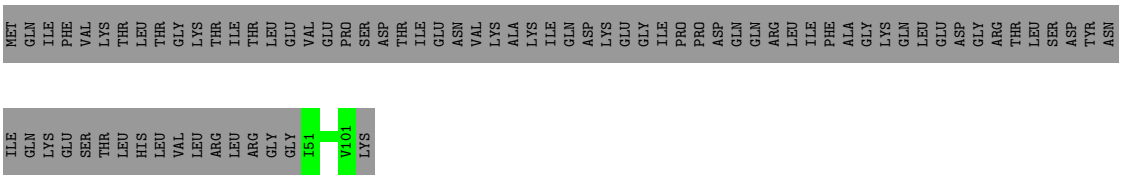
• Molecule 73: 60S ribosomal protein L39-like

Chain l:



• Molecule 74: Ubiquitin-60S ribosomal protein L40

Chain m:



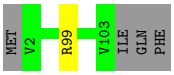
• Molecule 75: 60s ribosomal protein l41

Chain n: 100%

There are no outlier residues recorded for this chain.

• Molecule 76: 60S ribosomal protein L36a-like

Chain o: 95%



• Molecule 77: 60S ribosomal protein L37a

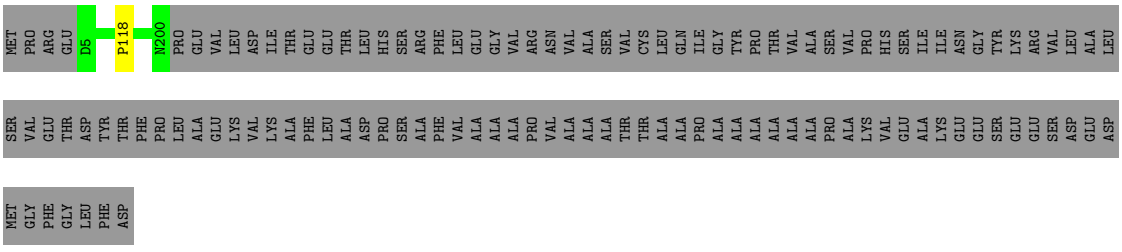
Chain p: 99%

• Molecule 78: 60S ribosomal protein L28

Chain r: 89% 10%

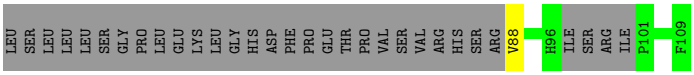
• Molecule 79: 60S ribosomal protein L10E

Chain s: 61% 38%



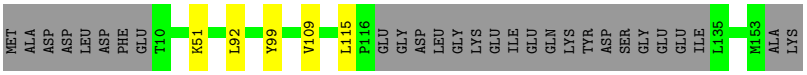
• Molecule 80: Dap1b

Chain s1: 16% 83%



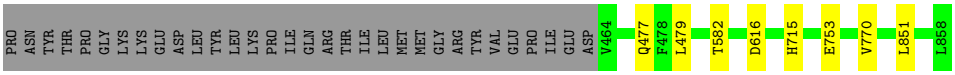
• Molecule 81: Eukaryotic translation initiation factor 5A-1

Chain t:



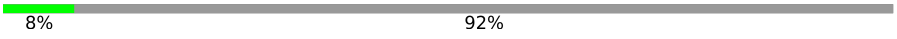
• Molecule 82: Elongation factor 2

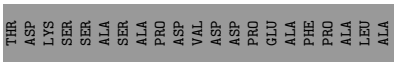
Chain v:



• Molecule 83: SERPINE1 mRNA binding protein 1

Chain w:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479754	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, OMG, B8T, OMU, 2MG, 7MG, 1MA, M7A, A2M, UR3, B8W, 6MZ, P4U, ZN, DDE, B9B, MA6, E3C, E7G, PSU, B9H, BGH, B8K, B8H, 5MC, B8N, B8Q, I4U, E6G, MHG, MG, 5MU, 5CT, MLZ, P7G, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	x	0.30	0/1311	0.44	0/1762
2	5	0.22	0/78172	0.71	7/121809 (0.0%)
3	8	0.21	0/3406	0.69	0/5301
4	9	0.64	0/39723	1.15	275/61870 (0.4%)
5	A	0.25	0/1929	0.44	0/2586
6	AA	0.40	0/1747	0.63	0/2374
7	Aa	0.37	0/828	0.56	0/1109
8	B	0.24	0/3240	0.43	0/4339
9	BB	0.37	0/1756	0.72	4/2350 (0.2%)
10	Bb	0.33	0/665	0.59	0/891
11	C	0.23	0/2899	0.40	0/3895
12	CC	0.47	0/1753	0.64	0/2369
13	Cc	0.32	0/490	0.61	0/656
14	D	0.25	0/2407	0.40	0/3224
15	DD	0.39	0/1796	0.65	0/2417
16	Dd	0.41	0/470	0.61	0/623
17	E	0.24	0/1743	0.42	0/2337
18	EE	0.38	0/2118	0.70	5/2849 (0.2%)
19	Ee	0.36	0/447	0.55	0/587
20	F	0.24	0/1911	0.38	0/2549
21	FF	0.35	0/1492	0.68	2/2005 (0.1%)
22	G	0.23	0/1778	0.39	0/2397
23	GG	0.32	0/1946	0.68	3/2590 (0.1%)
24	Gg	0.32	0/2493	0.64	2/3394 (0.1%)
25	H	0.23	0/1502	0.42	0/2020
26	HH	0.37	0/1510	0.67	1/2022 (0.0%)
27	I	0.24	0/1678	0.40	0/2239
28	II	0.36	0/1715	0.65	0/2287
29	J	0.24	0/1367	0.40	0/1829
30	JJ	0.39	0/1550	0.63	0/2069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	K	0.19	0/2836	0.68	0/4421
32	KK	0.39	0/834	0.65	1/1125 (0.1%)
33	L	0.23	0/1689	0.41	0/2261
34	LL	0.44	0/1195	0.60	0/1597
35	M	0.24	0/1138	0.38	0/1521
36	N	0.30	0/1746	0.44	0/2338
37	NN	0.36	0/1226	0.58	0/1649
38	O	0.24	0/1662	0.38	0/2222
39	OO	0.33	0/1029	0.63	0/1380
40	P	0.23	0/1259	0.40	0/1688
41	PP	0.34	0/1045	0.66	2/1396 (0.1%)
42	Q	0.24	0/1539	0.42	0/2054
43	QQ	0.33	0/1146	0.66	1/1534 (0.1%)
44	R	0.22	0/1399	0.37	0/1851
45	RR	0.33	0/1082	0.62	0/1452
46	S	0.25	0/1495	0.42	0/2005
47	SS	0.32	0/1208	0.67	0/1618
48	T	0.24	0/1320	0.40	0/1763
49	TT	0.30	0/1115	0.59	0/1493
50	U	0.24	0/814	0.40	0/1092
51	UU	0.33	0/805	0.61	0/1081
52	V	0.25	0/987	0.42	0/1324
53	VV	0.41	0/643	0.61	0/860
54	W	0.25	0/532	0.40	0/708
55	WW	0.48	0/1051	0.69	1/1406 (0.1%)
56	X	0.23	0/984	0.40	0/1323
57	XX	0.46	0/1116	0.64	1/1490 (0.1%)
58	Y	0.23	0/1119	0.40	0/1488
59	YY	0.33	0/1028	0.56	0/1366
60	Z	0.25	0/1130	0.40	0/1507
61	ZZ	0.31	0/604	0.69	0/810
62	a	0.24	0/1191	0.43	0/1590
63	b	0.23	0/819	0.35	0/1081
64	c	0.24	0/742	0.39	0/995
65	d	0.23	0/894	0.41	0/1204
66	e	0.23	0/1071	0.40	0/1429
67	f	0.25	0/895	0.45	0/1198
68	g	0.24	0/892	0.41	0/1189
69	h	0.22	0/1016	0.38	0/1341
70	i	0.23	0/832	0.37	0/1101
71	j	0.24	0/720	0.44	0/952
72	k	0.24	0/565	0.39	0/750
73	l	0.21	0/459	0.41	0/608

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	m	0.23	0/415	0.41	0/550
75	n	0.20	0/240	0.32	0/305
76	o	0.28	0/847	0.44	0/1117
77	p	0.23	0/718	0.42	0/953
78	r	0.23	0/1002	0.41	0/1344
79	s	0.24	0/1523	0.42	0/2055
80	s1	0.21	0/154	0.37	0/205
81	t	0.34	0/958	0.60	0/1288
82	v	0.24	0/5758	0.41	0/7779
83	w	0.23	0/257	0.43	0/339
All	All	0.36	0/224586	0.75	305/327945 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	AA	0	2
15	DD	0	1
18	EE	0	1
21	FF	0	1
24	Gg	0	1
28	II	0	1
41	PP	0	1
47	SS	0	1
51	UU	0	1
53	VV	0	1
57	XX	0	1
All	All	0	12

There are no bond length outliers.

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	1116	C	N1-C2-O2	12.77	126.56	118.90
4	9	1116	C	C2-N1-C1'	11.82	131.81	118.80
4	9	501	C	N1-C2-O2	11.01	125.50	118.90
4	9	501	C	C2-N1-C1'	10.28	130.11	118.80
4	9	1116	C	N3-C2-O2	-10.12	114.81	121.90
4	9	1016	U	N1-C2-O2	10.01	129.81	122.80
4	9	1453	C	N1-C2-O2	9.93	124.86	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	356	C	N1-C2-O2	9.91	124.85	118.90
4	9	1453	C	C2-N1-C1'	9.88	129.67	118.80
4	9	1520	G	N3-C4-C5	-9.81	123.69	128.60
4	9	356	C	C2-N1-C1'	9.72	129.49	118.80
4	9	1139	C	N1-C2-O2	9.68	124.70	118.90
4	9	1016	U	C2-N1-C1'	9.57	129.19	117.70
4	9	293	C	N1-C2-O2	9.52	124.61	118.90
4	9	1016	U	N3-C2-O2	-9.18	115.78	122.20
4	9	1139	C	C2-N1-C1'	9.18	128.90	118.80
4	9	501	C	N3-C2-O2	-9.17	115.48	121.90
4	9	1139	C	N3-C2-O2	-9.05	115.57	121.90
4	9	1303	C	N1-C2-O2	8.98	124.29	118.90
4	9	1292	C	N1-C2-O2	8.69	124.11	118.90
4	9	1303	C	C2-N1-C1'	8.69	128.36	118.80
4	9	1116	C	C6-N1-C1'	-8.37	110.75	120.80
4	9	194	C	N3-C2-O2	-8.36	116.05	121.90
4	9	1520	G	C8-N9-C4	-8.30	103.08	106.40
4	9	501	C	C6-N1-C2	-8.22	117.01	120.30
4	9	1624	U	C2-N1-C1'	8.08	127.39	117.70
4	9	1242	U	N1-C2-O2	8.02	128.42	122.80
4	9	1520	G	C4-N9-C1'	7.96	136.85	126.50
4	9	356	C	N3-C2-O2	-7.92	116.36	121.90
4	9	293	C	N3-C2-O2	-7.85	116.41	121.90
4	9	1535	U	C2-N1-C1'	7.84	127.11	117.70
4	9	914	U	C2-N1-C1'	7.84	127.11	117.70
4	9	1453	C	N3-C2-O2	-7.83	116.42	121.90
4	9	801	U	N3-C2-O2	-7.69	116.82	122.20
4	9	1520	G	C2-N3-C4	7.64	115.72	111.90
4	9	1315	U	N3-C2-O2	-7.60	116.88	122.20
4	9	801	U	N1-C2-O2	7.56	128.09	122.80
23	GG	68	LEU	CA-CB-CG	7.54	132.64	115.30
4	9	1389	C	N1-C2-O2	7.50	123.40	118.90
4	9	183	G	C2-N3-C4	7.47	115.64	111.90
4	9	853	C	C2-N1-C1'	7.44	126.98	118.80
4	9	1261	C	N1-C2-O2	7.43	123.36	118.90
4	9	356	C	C6-N1-C1'	-7.42	111.89	120.80
4	9	369	C	N1-C2-O2	7.42	123.35	118.90
9	BB	219	LYS	C-N-CA	7.41	140.23	121.70
4	9	1123	C	C2-N1-C1'	7.38	126.92	118.80
2	5	1214	C	C2-N1-C1'	7.35	126.89	118.80
4	9	369	C	C2-N1-C1'	7.34	126.88	118.80
4	9	632	C	C6-N1-C2	-7.34	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	293	C	C2-N1-C1'	7.29	126.81	118.80
2	5	1214	C	N1-C2-O2	7.25	123.25	118.90
4	9	1396	A	O4'-C1'-N9	7.25	114.00	108.20
4	9	570	C	N1-C2-O2	7.23	123.24	118.90
4	9	1116	C	C6-N1-C2	-7.15	117.44	120.30
32	KK	35	LEU	CA-CB-CG	7.11	131.66	115.30
4	9	914	U	N1-C2-O2	7.06	127.74	122.80
4	9	579	C	N1-C2-O2	7.05	123.13	118.90
4	9	1277	C	C5-C6-N1	7.03	124.52	121.00
4	9	1242	U	C2-N1-C1'	7.02	126.12	117.70
9	BB	34	LYS	C-N-CA	6.97	139.12	121.70
4	9	1756	C	C2-N1-C1'	6.94	126.44	118.80
4	9	1595	U	N3-C2-O2	-6.93	117.35	122.20
4	9	1595	U	N1-C2-O2	6.92	127.64	122.80
4	9	1660	C	C2-N1-C1'	6.90	126.39	118.80
4	9	1315	U	N1-C2-O2	6.86	127.60	122.80
4	9	1331	C	N1-C2-O2	6.84	123.01	118.90
4	9	1242	U	N3-C2-O2	-6.84	117.41	122.20
4	9	1520	G	N3-C4-N9	6.81	130.08	126.00
4	9	1389	C	C2-N1-C1'	6.80	126.28	118.80
4	9	188	C	C2-N1-C1'	6.79	126.27	118.80
4	9	1453	C	C6-N1-C1'	-6.75	112.69	120.80
4	9	1595	U	C2-N1-C1'	6.75	125.80	117.70
21	FF	27	ASP	CB-CG-OD1	6.75	124.37	118.30
4	9	18	C	C5-C6-N1	6.73	124.36	121.00
4	9	183	G	N3-C4-C5	-6.69	125.26	128.60
4	9	1117	C	N1-C2-O2	6.67	122.91	118.90
4	9	1453	C	C6-N1-C2	-6.66	117.63	120.30
4	9	501	C	C6-N1-C1'	-6.66	112.81	120.80
4	9	1535	U	N1-C2-O2	6.65	127.45	122.80
4	9	1303	C	C6-N1-C1'	-6.64	112.83	120.80
4	9	914	U	N3-C2-O2	-6.64	117.55	122.20
4	9	618	C	O5'-P-OP1	-6.64	99.73	105.70
4	9	876	C	C2-N1-C1'	6.63	126.10	118.80
4	9	876	C	N1-C2-O2	6.62	122.87	118.90
4	9	801	U	C2-N1-C1'	6.62	125.64	117.70
2	5	1643	U	C2-N1-C1'	6.61	125.63	117.70
4	9	570	C	N3-C2-O2	-6.59	117.29	121.90
4	9	1453	C	C5-C6-N1	6.58	124.29	121.00
4	9	4	C	C5-C6-N1	6.57	124.28	121.00
4	9	632	C	C5-C6-N1	6.55	124.27	121.00
4	9	17	C	C6-N1-C2	-6.50	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	1592	C	N3-C2-O2	-6.50	117.35	121.90
4	9	1292	C	N3-C2-O2	-6.49	117.36	121.90
4	9	319	C	O5'-P-OP1	6.48	118.47	110.70
4	9	1139	C	C6-N1-C2	-6.48	117.71	120.30
43	QQ	47	LEU	CA-CB-CG	6.47	130.17	115.30
4	9	1395	C	OP1-P-O3'	6.46	119.42	105.20
4	9	340	C	N1-C2-O2	6.44	122.77	118.90
4	9	752	G	P-O3'-C3'	6.44	127.43	119.70
4	9	1303	C	N3-C2-O2	-6.41	117.42	121.90
4	9	1172	U	N1-C2-O2	6.39	127.28	122.80
4	9	4	C	C2-N1-C1'	6.38	125.82	118.80
4	9	1606	G	O4'-C1'-N9	6.37	113.30	108.20
4	9	1750	C	N1-C2-O2	6.37	122.72	118.90
4	9	1123	C	C6-N1-C2	-6.35	117.76	120.30
4	9	1412	C	C6-N1-C2	-6.34	117.76	120.30
4	9	1261	C	N3-C2-O2	-6.33	117.47	121.90
4	9	1637	A	P-O3'-C3'	6.33	127.29	119.70
4	9	1624	U	N1-C2-O2	6.30	127.21	122.80
18	EE	20	LEU	CA-CB-CG	6.29	129.77	115.30
4	9	734	C	C2-N1-C1'	6.27	125.70	118.80
4	9	853	C	N3-C2-O2	-6.27	117.51	121.90
4	9	402	C	N1-C2-O2	6.23	122.64	118.90
4	9	1057	C	C2-N1-C1'	6.21	125.64	118.80
55	WW	69	LEU	CA-CB-CG	6.21	129.59	115.30
4	9	930	C	N1-C2-O2	6.20	122.62	118.90
4	9	1739	C	N1-C2-O2	6.19	122.61	118.90
4	9	1016	U	C6-N1-C1'	-6.18	112.55	121.20
24	Gg	89	LEU	CA-CB-CG	6.18	129.52	115.30
4	9	1139	C	C6-N1-C1'	-6.18	113.38	120.80
4	9	853	C	N1-C2-O2	6.18	122.61	118.90
4	9	314	U	N3-C2-O2	-6.17	117.88	122.20
4	9	1277	C	C6-N1-C2	-6.17	117.83	120.30
4	9	688	U	P-O3'-C3'	6.15	127.08	119.70
4	9	887	U	C2-N1-C1'	6.15	125.08	117.70
4	9	303	C	N1-C2-O2	6.13	122.58	118.90
4	9	1078	C	C2-N1-C1'	6.13	125.54	118.80
4	9	1396	A	O5'-P-OP1	-6.13	100.19	105.70
4	9	199	C	N1-C2-O2	6.12	122.57	118.90
4	9	1389	C	N3-C2-O2	-6.10	117.63	121.90
4	9	870	A	P-O3'-C3'	6.09	127.01	119.70
4	9	479	C	P-O3'-C3'	6.08	126.99	119.70
4	9	501	C	C5-C6-N1	6.06	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	531	A	OP1-P-O3'	6.06	118.53	105.20
4	9	887	U	N1-C2-O2	6.05	127.04	122.80
9	BB	207	LEU	CA-CB-CG	6.05	129.22	115.30
2	5	1214	C	N3-C2-O2	-6.04	117.67	121.90
4	9	162	C	C6-N1-C2	-6.04	117.88	120.30
4	9	1123	C	N1-C2-O2	6.04	122.52	118.90
4	9	1123	C	C5-C6-N1	6.02	124.01	121.00
4	9	1116	C	C5-C6-N1	6.02	124.01	121.00
4	9	1520	G	N7-C8-N9	6.02	116.11	113.10
4	9	124	U	N3-C2-O2	-6.01	117.99	122.20
4	9	570	C	C2-N1-C1'	6.00	125.40	118.80
4	9	124	U	N1-C2-O2	5.96	126.97	122.80
4	9	630	U	C2-N1-C1'	5.95	124.84	117.70
4	9	632	C	C2-N1-C1'	5.94	125.34	118.80
4	9	1624	U	N3-C2-O2	-5.93	118.05	122.20
4	9	1261	C	C2-N1-C1'	5.93	125.32	118.80
4	9	914	U	C6-N1-C1'	-5.92	112.92	121.20
4	9	1535	U	N3-C2-O2	-5.90	118.07	122.20
23	GG	185	LEU	CA-CB-CG	5.89	128.85	115.30
4	9	1395	C	P-O3'-C3'	5.89	126.77	119.70
4	9	1660	C	N1-C2-O2	5.87	122.42	118.90
4	9	303	C	C6-N1-C2	-5.83	117.97	120.30
4	9	194	C	N1-C2-O2	5.82	122.39	118.90
4	9	293	C	C6-N1-C2	-5.82	117.97	120.30
4	9	402	C	C6-N1-C2	-5.82	117.97	120.30
4	9	1230	C	C5-C6-N1	5.79	123.89	121.00
4	9	1535	U	C5-C6-N1	5.79	125.59	122.70
4	9	853	C	C6-N1-C2	-5.78	117.99	120.30
4	9	927	C	N3-C2-O2	-5.77	117.86	121.90
4	9	1649	U	N1-C2-O2	5.75	126.83	122.80
4	9	1756	C	C6-N1-C2	-5.74	118.00	120.30
4	9	1002	U	N1-C2-O2	5.74	126.82	122.80
4	9	1292	C	C6-N1-C2	-5.73	118.01	120.30
4	9	579	C	N3-C2-O2	-5.73	117.89	121.90
4	9	1624	U	O4'-C1'-N1	5.71	112.77	108.20
4	9	1277	C	C2-N1-C1'	5.71	125.08	118.80
4	9	1016	U	C5-C6-N1	5.70	125.55	122.70
4	9	577	U	N3-C2-O2	-5.69	118.22	122.20
4	9	391	C	C6-N1-C2	-5.68	118.03	120.30
4	9	1172	U	C2-N1-C1'	5.68	124.52	117.70
4	9	1725	U	C2-N1-C1'	5.68	124.51	117.70
4	9	1397	U	N1-C2-O2	5.67	126.77	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	1708	C	C6-N1-C2	-5.66	118.04	120.30
4	9	1503	C	C6-N1-C2	-5.65	118.04	120.30
18	EE	256	LEU	CA-CB-CG	5.65	128.30	115.30
4	9	65	C	C6-N1-C2	-5.65	118.04	120.30
4	9	1751	C	N1-C2-O2	5.65	122.29	118.90
4	9	1389	C	C6-N1-C2	-5.65	118.04	120.30
4	9	427	U	C2-N1-C1'	5.64	124.47	117.70
4	9	1172	U	N3-C2-O2	-5.64	118.25	122.20
23	GG	133	LEU	CA-CB-CG	5.63	128.26	115.30
4	9	958	G	C4-N9-C1'	5.62	133.81	126.50
4	9	124	U	C2-N1-C1'	5.62	124.44	117.70
4	9	1740	C	N3-C2-O2	-5.62	117.97	121.90
4	9	465	A	P-O3'-C3'	5.61	126.44	119.70
4	9	1149	A	C2-N3-C4	5.61	113.41	110.60
21	FF	173	LEU	CA-CB-CG	5.61	128.20	115.30
4	9	1298	G	C4-N9-C1'	5.60	133.78	126.50
4	9	1865	C	C6-N1-C2	-5.60	118.06	120.30
4	9	1518	C	C2-N1-C1'	5.60	124.96	118.80
4	9	1315	U	C2-N1-C1'	5.58	124.39	117.70
4	9	303	C	N3-C2-O2	-5.57	118.00	121.90
4	9	1060	A	O4'-C1'-N9	5.55	112.64	108.20
4	9	1002	U	N3-C2-O2	-5.55	118.32	122.20
4	9	930	C	C2-N1-C1'	5.54	124.89	118.80
4	9	1118	C	C2-N1-C1'	5.54	124.89	118.80
4	9	183	G	C4-N9-C1'	5.53	133.69	126.50
4	9	369	C	N3-C2-O2	-5.53	118.03	121.90
4	9	183	G	O4'-C1'-N9	5.53	112.62	108.20
4	9	434	G	P-O3'-C3'	5.52	126.33	119.70
4	9	874	G	P-O3'-C3'	5.52	126.32	119.70
4	9	876	C	C5-C6-N1	5.49	123.75	121.00
4	9	628	A	C2-N3-C4	5.47	113.34	110.60
4	9	1592	C	N1-C2-O2	5.47	122.18	118.90
18	EE	19	MET	CG-SD-CE	-5.47	91.45	100.20
4	9	1551	U	C2-N1-C1'	5.46	124.26	117.70
4	9	659	G	C4-N9-C1'	5.46	133.60	126.50
4	9	733	C	C6-N1-C2	-5.46	118.11	120.30
4	9	402	C	C5-C6-N1	5.46	123.73	121.00
4	9	524	U	N3-C2-O2	-5.46	118.38	122.20
4	9	1664	A	P-O3'-C3'	5.45	126.24	119.70
4	9	1756	C	N1-C2-O2	5.45	122.17	118.90
4	9	1303	C	O4'-C1'-N1	5.45	112.56	108.20
4	9	577	U	N1-C2-O2	5.44	126.61	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	927	C	N1-C2-O2	5.44	122.17	118.90
4	9	530	U	C2-N1-C1'	5.44	124.23	117.70
4	9	630	U	N3-C2-O2	-5.43	118.40	122.20
4	9	1750	C	N3-C2-O2	-5.43	118.10	121.90
4	9	151	C	C2-N1-C1'	5.42	124.76	118.80
4	9	570	C	C6-N1-C2	-5.42	118.13	120.30
4	9	118	C	N1-C2-O2	5.41	122.14	118.90
4	9	369	C	C6-N1-C1'	-5.40	114.32	120.80
18	EE	19	MET	CA-CB-CG	-5.39	104.13	113.30
4	9	887	U	N3-C2-O2	-5.38	118.43	122.20
4	9	1397	U	N3-C2-O2	-5.38	118.43	122.20
41	PP	86	LEU	CA-CB-CG	5.38	127.68	115.30
4	9	663	C	C5-C6-N1	5.37	123.69	121.00
4	9	630	U	N1-C2-O2	5.36	126.55	122.80
4	9	958	G	O4'-C1'-N9	5.35	112.48	108.20
4	9	1314	U	O4'-C1'-N1	5.35	112.48	108.20
4	9	1520	G	C8-N9-C1'	-5.34	120.06	127.00
4	9	1117	C	N3-C2-O2	-5.34	118.16	121.90
4	9	595	U	C2-N1-C1'	5.33	124.10	117.70
4	9	1785	C	C2-N1-C1'	5.33	124.66	118.80
2	5	1643	U	N1-C2-O2	5.33	126.53	122.80
4	9	1725	U	N1-C2-O2	5.33	126.53	122.80
4	9	850	C	N1-C2-O2	5.32	122.09	118.90
4	9	124	U	C5-C6-N1	5.32	125.36	122.70
4	9	1412	C	C2-N1-C1'	5.31	124.64	118.80
4	9	4	C	C6-N1-C2	-5.30	118.18	120.30
4	9	183	G	C8-N9-C4	-5.30	104.28	106.40
4	9	848	U	N3-C2-O2	-5.30	118.49	122.20
4	9	1620	A	O4'-C1'-N9	5.29	112.43	108.20
4	9	606	G	C4-N9-C1'	5.29	133.37	126.50
4	9	142	C	N1-C2-O2	5.28	122.07	118.90
4	9	733	C	N1-C2-O2	5.28	122.07	118.90
4	9	53	C	C6-N1-C2	-5.28	118.19	120.30
4	9	791	C	N1-C2-O2	5.27	122.06	118.90
2	5	1214	C	C6-N1-C2	-5.27	118.19	120.30
4	9	642	U	P-O3'-C3'	5.26	126.01	119.70
4	9	427	U	N3-C2-O2	-5.25	118.52	122.20
4	9	1837	G	N3-C4-N9	-5.24	122.85	126.00
2	5	100	C	C2-N1-C1'	5.24	124.57	118.80
26	HH	36	LEU	CA-CB-CG	5.24	127.34	115.30
4	9	1660	C	C6-N1-C1'	-5.23	114.53	120.80
4	9	1412	C	C5-C6-N1	5.22	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	532	C	P-O3'-C3'	5.22	125.97	119.70
41	PP	25	LEU	CA-CB-CG	5.22	127.31	115.30
4	9	1022	U	C2-N1-C1'	5.22	123.97	117.70
4	9	537	C	N1-C2-O2	5.22	122.03	118.90
4	9	1237	C	C6-N1-C2	-5.22	118.21	120.30
4	9	105	U	N3-C2-O2	-5.22	118.55	122.20
4	9	606	G	C4-C5-N7	5.21	112.88	110.80
4	9	199	C	N3-C2-O2	-5.19	118.27	121.90
4	9	1078	C	C6-N1-C2	-5.19	118.22	120.30
4	9	438	G	N3-C4-C5	-5.19	126.01	128.60
4	9	579	C	C2-N1-C1'	5.18	124.50	118.80
4	9	30	C	C6-N1-C2	-5.18	118.23	120.30
4	9	1624	U	C6-N1-C1'	-5.18	113.95	121.20
57	XX	7	LEU	CA-CB-CG	5.17	127.18	115.30
4	9	608	C	C5-C6-N1	5.16	123.58	121.00
4	9	1064	C	C6-N1-C2	-5.16	118.24	120.30
4	9	1331	C	N3-C2-O2	-5.14	118.30	121.90
4	9	1518	C	N3-C2-O2	-5.13	118.31	121.90
4	9	1551	U	N3-C2-O2	-5.13	118.61	122.20
4	9	639	C	C6-N1-C2	-5.13	118.25	120.30
4	9	1520	G	C6-N1-C2	-5.13	122.02	125.10
4	9	803	C	C6-N1-C2	-5.12	118.25	120.30
4	9	106	C	C6-N1-C2	-5.11	118.25	120.30
18	EE	73	ASP	CB-CG-OD1	5.11	122.90	118.30
4	9	1205	C	C6-N1-C2	-5.10	118.26	120.30
4	9	853	C	O4'-C1'-N1	5.10	112.28	108.20
9	BB	225	LEU	CA-CB-CG	5.09	127.01	115.30
4	9	151	C	N1-C2-O2	5.09	121.95	118.90
4	9	1230	C	C6-N1-C2	-5.09	118.27	120.30
4	9	1073	U	N3-C2-O2	-5.08	118.65	122.20
4	9	879	C	N1-C2-O2	5.07	121.94	118.90
4	9	391	C	C2-N1-C1'	5.07	124.37	118.80
4	9	659	G	C8-N9-C1'	-5.07	120.42	127.00
24	Gg	32	LEU	CA-CB-CG	5.05	126.93	115.30
4	9	1242	U	C6-N1-C1'	-5.04	114.14	121.20
4	9	1057	C	N1-C2-O2	5.04	121.92	118.90
4	9	1261	C	C6-N1-C2	-5.04	118.28	120.30
4	9	1725	U	N3-C2-O2	-5.04	118.67	122.20
4	9	585	C	C2-N1-C1'	5.03	124.34	118.80
4	9	1624	U	C5-C6-N1	5.03	125.22	122.70
4	9	898	U	N3-C2-O2	-5.02	118.69	122.20
4	9	1389	C	C5-C6-N1	5.02	123.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	188	C	C6-N1-C1'	-5.02	114.78	120.80
4	9	585	C	C6-N1-C2	-5.01	118.30	120.30
4	9	749	U	N3-C2-O2	-5.01	118.69	122.20
4	9	666	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AA	42	LYS	Peptide
6	AA	43	SER	Peptide
15	DD	153	VAL	Peptide
18	EE	132	GLY	Peptide
21	FF	41	VAL	Peptide
24	Gg	135	LEU	Peptide
28	II	92	ARG	Peptide
41	PP	17	TYR	Peptide
47	SS	60	THR	Peptide
51	UU	107	GLU	Peptide
53	VV	32	ILE	Peptide
57	XX	61	GLN	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	x	159/217 (73%)	151 (95%)	8 (5%)	0	100	100
5	A	245/257 (95%)	233 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AA	215/295 (73%)	206 (96%)	9 (4%)	0	100	100
7	Aa	99/115 (86%)	89 (90%)	10 (10%)	0	100	100
8	B	392/403 (97%)	382 (97%)	10 (3%)	0	100	100
9	BB	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
10	Bb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
11	C	355/413 (86%)	344 (97%)	11 (3%)	0	100	100
12	CC	219/293 (75%)	205 (94%)	14 (6%)	0	100	100
13	Cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
14	D	287/297 (97%)	281 (98%)	6 (2%)	0	100	100
15	DD	226/243 (93%)	216 (96%)	10 (4%)	0	100	100
16	Dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
17	E	205/291 (70%)	197 (96%)	8 (4%)	0	100	100
18	EE	260/263 (99%)	244 (94%)	16 (6%)	0	100	100
19	Ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
20	F	223/249 (90%)	216 (97%)	7 (3%)	0	100	100
21	FF	181/204 (89%)	162 (90%)	19 (10%)	0	100	100
22	G	211/266 (79%)	208 (99%)	3 (1%)	0	100	100
23	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
24	Gg	311/317 (98%)	281 (90%)	30 (10%)	0	100	100
25	H	182/192 (95%)	179 (98%)	3 (2%)	0	100	100
26	HH	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
27	I	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
28	II	204/208 (98%)	185 (91%)	19 (9%)	0	100	100
29	J	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
30	JJ	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
32	KK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
33	L	203/211 (96%)	198 (98%)	4 (2%)	1 (0%)	29	35
34	LL	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
35	M	133/218 (61%)	130 (98%)	3 (2%)	0	100	100
36	N	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
37	NN	147/151 (97%)	138 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	O	197/203 (97%)	193 (98%)	4 (2%)	0	100	100
39	OO	134/151 (89%)	123 (92%)	11 (8%)	0	100	100
40	P	150/187 (80%)	147 (98%)	3 (2%)	0	100	100
41	PP	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
42	Q	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
43	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
44	R	164/196 (84%)	162 (99%)	2 (1%)	0	100	100
45	RR	130/135 (96%)	121 (93%)	9 (7%)	0	100	100
46	S	174/224 (78%)	168 (97%)	6 (3%)	0	100	100
47	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
48	T	156/160 (98%)	151 (97%)	5 (3%)	0	100	100
49	TT	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
50	U	96/141 (68%)	93 (97%)	3 (3%)	0	100	100
51	UU	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
52	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
53	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
54	W	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
55	WW	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
56	X	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
57	XX	139/143 (97%)	132 (95%)	4 (3%)	3 (2%)	6	5
58	Y	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
59	YY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
60	Z	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
61	ZZ	73/124 (59%)	70 (96%)	3 (4%)	0	100	100
62	a	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
63	b	94/245 (38%)	92 (98%)	2 (2%)	0	100	100
64	c	92/115 (80%)	91 (99%)	1 (1%)	0	100	100
65	d	104/125 (83%)	101 (97%)	3 (3%)	0	100	100
66	e	126/157 (80%)	122 (97%)	4 (3%)	0	100	100
67	f	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
68	g	109/117 (93%)	107 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	h	119/123 (97%)	119 (100%)	0	0	100	100
70	i	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
71	j	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
72	k	66/70 (94%)	66 (100%)	0	0	100	100
73	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
74	m	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
75	n	23/25 (92%)	23 (100%)	0	0	100	100
76	o	100/106 (94%)	98 (98%)	2 (2%)	0	100	100
77	p	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
78	r	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
79	s	194/318 (61%)	185 (95%)	8 (4%)	1 (0%)	29	35
80	s1	14/109 (13%)	13 (93%)	1 (7%)	0	100	100
81	t	121/154 (79%)	117 (97%)	4 (3%)	0	100	100
82	v	711/858 (83%)	684 (96%)	27 (4%)	0	100	100
83	w	30/407 (7%)	28 (93%)	2 (7%)	0	100	100
All	All	12093/14939 (81%)	11610 (96%)	478 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	XX	62	PRO
57	XX	61	GLN
57	XX	86	PRO
79	s	118	PRO
33	L	62	PRO

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	x	146/195 (75%)	143 (98%)	3 (2%)	53	70
5	A	189/199 (95%)	187 (99%)	2 (1%)	73	86
6	AA	180/245 (74%)	179 (99%)	1 (1%)	86	94
7	Aa	88/98 (90%)	87 (99%)	1 (1%)	73	86
8	B	342/348 (98%)	338 (99%)	4 (1%)	71	84
9	BB	194/231 (84%)	190 (98%)	4 (2%)	53	70
10	Bb	75/76 (99%)	75 (100%)	0	100	100
11	C	298/336 (89%)	295 (99%)	3 (1%)	76	87
12	CC	187/224 (84%)	185 (99%)	2 (1%)	73	86
13	Cc	55/62 (89%)	52 (94%)	3 (6%)	21	30
14	D	245/250 (98%)	241 (98%)	4 (2%)	62	78
15	DD	190/202 (94%)	186 (98%)	4 (2%)	53	70
16	Dd	48/49 (98%)	46 (96%)	2 (4%)	30	42
17	E	189/251 (75%)	187 (99%)	2 (1%)	73	86
18	EE	224/225 (100%)	221 (99%)	3 (1%)	69	82
19	Ee	46/106 (43%)	43 (94%)	3 (6%)	17	23
20	F	196/218 (90%)	196 (100%)	0	100	100
21	FF	158/170 (93%)	152 (96%)	6 (4%)	33	47
22	G	188/224 (84%)	186 (99%)	2 (1%)	73	86
23	GG	207/218 (95%)	199 (96%)	8 (4%)	32	46
24	Gg	272/275 (99%)	268 (98%)	4 (2%)	65	79
25	H	166/171 (97%)	165 (99%)	1 (1%)	86	94
26	HH	165/360 (46%)	164 (99%)	1 (1%)	86	94
27	I	172/181 (95%)	169 (98%)	3 (2%)	60	76
28	II	178/180 (99%)	173 (97%)	5 (3%)	43	60
29	J	141/149 (95%)	140 (99%)	1 (1%)	84	92
30	JJ	161/168 (96%)	158 (98%)	3 (2%)	57	73
32	KK	87/136 (64%)	86 (99%)	1 (1%)	73	86
33	L	170/176 (97%)	168 (99%)	2 (1%)	71	84
34	LL	130/142 (92%)	128 (98%)	2 (2%)	65	79
35	M	115/160 (72%)	115 (100%)	0	100	100
36	N	171/172 (99%)	169 (99%)	2 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	NN	130/131 (99%)	129 (99%)	1 (1%)	81 91
38	O	171/174 (98%)	168 (98%)	3 (2%)	59 75
39	OO	106/119 (89%)	105 (99%)	1 (1%)	78 89
40	P	133/165 (81%)	131 (98%)	2 (2%)	65 79
41	PP	111/130 (85%)	106 (96%)	5 (4%)	27 39
42	Q	164/165 (99%)	164 (100%)	0	100 100
43	QQ	117/121 (97%)	115 (98%)	2 (2%)	60 76
44	R	147/175 (84%)	146 (99%)	1 (1%)	84 92
45	RR	119/121 (98%)	115 (97%)	4 (3%)	37 51
46	S	156/192 (81%)	153 (98%)	3 (2%)	57 73
47	SS	125/132 (95%)	122 (98%)	3 (2%)	49 66
48	T	139/140 (99%)	137 (99%)	2 (1%)	67 81
49	TT	111/115 (96%)	108 (97%)	3 (3%)	44 61
50	U	88/127 (69%)	88 (100%)	0	100 100
51	UU	92/107 (86%)	92 (100%)	0	100 100
52	V	100/107 (94%)	100 (100%)	0	100 100
53	VV	67/67 (100%)	66 (98%)	1 (2%)	65 79
54	W	54/126 (43%)	54 (100%)	0	100 100
55	WW	112/113 (99%)	111 (99%)	1 (1%)	78 89
56	X	106/133 (80%)	106 (100%)	0	100 100
57	XX	113/115 (98%)	112 (99%)	1 (1%)	78 89
58	Y	123/135 (91%)	119 (97%)	4 (3%)	38 53
59	YY	107/115 (93%)	105 (98%)	2 (2%)	57 73
60	Z	117/118 (99%)	117 (100%)	0	100 100
61	ZZ	66/102 (65%)	66 (100%)	0	100 100
62	a	119/120 (99%)	119 (100%)	0	100 100
63	b	80/184 (44%)	79 (99%)	1 (1%)	69 82
64	c	80/98 (82%)	80 (100%)	0	100 100
65	d	97/110 (88%)	97 (100%)	0	100 100
66	e	114/141 (81%)	114 (100%)	0	100 100
67	f	88/89 (99%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	g	95/100 (95%)	94 (99%)	1 (1%)	73 86
69	h	109/110 (99%)	109 (100%)	0	100 100
70	i	85/89 (96%)	85 (100%)	0	100 100
71	j	73/80 (91%)	73 (100%)	0	100 100
72	k	63/65 (97%)	63 (100%)	0	100 100
73	l	47/48 (98%)	47 (100%)	0	100 100
74	m	46/115 (40%)	46 (100%)	0	100 100
75	n	24/24 (100%)	24 (100%)	0	100 100
76	o	90/94 (96%)	89 (99%)	1 (1%)	73 86
77	p	74/75 (99%)	74 (100%)	0	100 100
78	r	107/121 (88%)	106 (99%)	1 (1%)	78 89
79	s	163/258 (63%)	163 (100%)	0	100 100
80	s1	18/97 (19%)	17 (94%)	1 (6%)	21 29
81	t	105/128 (82%)	101 (96%)	4 (4%)	33 47
82	v	619/729 (85%)	610 (98%)	9 (2%)	65 79
83	w	26/327 (8%)	26 (100%)	0	100 100
All	All	10569/12644 (84%)	10430 (99%)	139 (1%)	70 82

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	136	SER
1	x	159	MET
1	x	160	LYS
5	A	143	THR
5	A	208	GLU
6	AA	186	ARG
7	Aa	42	ARG
8	B	162	VAL
8	B	195	ASP
8	B	207	VAL
8	B	371	THR
9	BB	28	LYS
9	BB	56	LYS
9	BB	174	ARG
9	BB	222	LYS

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Mol	Chain	Res	Type
11	C	122	TYR
11	C	150	LEU
11	C	321	ASN
12	CC	167	ARG
12	CC	248	TYR
13	Cc	40	ARG
13	Cc	63	ARG
13	Cc	66	ARG
14	D	42	ASN
14	D	56	THR
14	D	72	ASP
14	D	206	ASP
15	DD	45	ARG
15	DD	64	ARG
15	DD	76	ARG
15	DD	113	LEU
16	Dd	26	ASN
16	Dd	48	LYS
17	E	178	VAL
17	E	197	VAL
18	EE	20	LEU
18	EE	148	ARG
18	EE	259	LYS
19	Ee	81	ARG
19	Ee	99	LYS
19	Ee	104	ARG
21	FF	44	LYS
21	FF	76	MET
21	FF	122	ARG
21	FF	169	ILE
21	FF	173	LEU
21	FF	182	LYS
22	G	162	GLU
22	G	249	ARG
23	GG	14	LYS
23	GG	22	ARG
23	GG	25	ARG
23	GG	79	LYS
23	GG	185	LEU
23	GG	203	LYS
23	GG	224	ARG
23	GG	231	ARG

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Mol	Chain	Res	Type
24	Gg	8	ARG
24	Gg	99	ARG
24	Gg	280	LYS
24	Gg	285	GLN
25	H	177	ASP
26	HH	85	LYS
27	I	96	VAL
27	I	126	VAL
27	I	202	ASN
28	II	5	ARG
28	II	47	ARG
28	II	74	ARG
28	II	84	ASN
28	II	165	GLN
29	J	43	LEU
30	JJ	70	ARG
30	JJ	79	ARG
30	JJ	169	ARG
32	KK	61	GLN
33	L	4	SER
33	L	67	HIS
34	LL	12	LYS
34	LL	22	ARG
36	N	142	ILE
36	N	198	LEU
37	NN	122	ILE
38	O	100	ASP
38	O	117	ARG
38	O	195	VAL
39	OO	146	ARG
40	P	24	VAL
40	P	57	CYS
41	PP	13	ARG
41	PP	50	ARG
41	PP	51	ARG
41	PP	65	LYS
41	PP	108	LYS
43	QQ	41	MET
43	QQ	109	LYS
44	R	10	LEU
45	RR	5	ARG
45	RR	7	LYS

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Mol	Chain	Res	Type
45	RR	81	ARG
45	RR	116	ASN
46	S	7	LEU
46	S	39	VAL
46	S	87	ARG
47	SS	91	LYS
47	SS	94	LYS
47	SS	111	LEU
48	T	38	ASP
48	T	72	VAL
49	TT	43	LYS
49	TT	62	ARG
49	TT	75	MET
53	VV	70	LEU
55	WW	103	VAL
57	XX	142	ARG
58	Y	55	VAL
58	Y	74	TYR
58	Y	79	VAL
58	Y	104	VAL
59	YY	32	LYS
59	YY	113	ARG
63	b	8	THR
68	g	73	HIS
76	o	99	ARG
78	r	103	HIS
80	s1	88	VAL
81	t	92	LEU
81	t	99	TYR
81	t	109	VAL
81	t	115	LEU
82	v	4	PHE
82	v	81	LEU
82	v	477	GLN
82	v	479	LEU
82	v	582	THR
82	v	616	ASP
82	v	753	GLU
82	v	770	VAL
82	v	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	71	GLN
1	x	94	ASN
1	x	96	ASN
1	x	188	ASN
5	A	95	GLN
8	B	138	GLN
8	B	209	GLN
8	B	213	GLN
8	B	258	HIS
8	B	354	GLN
10	Bb	26	GLN
11	C	276	ASN
11	C	321	ASN
12	CC	113	GLN
14	D	42	ASN
14	D	111	ASN
14	D	122	GLN
14	D	138	GLN
14	D	175	HIS
14	D	275	GLN
14	D	282	GLN
14	D	291	GLN
16	Dd	26	ASN
17	E	131	HIS
17	E	170	GLN
17	E	193	HIS
17	E	253	GLN
18	EE	36	HIS
20	F	23	ASN
20	F	115	GLN
20	F	205	ASN
22	G	91	ASN
22	G	96	GLN
22	G	99	GLN
22	G	134	ASN
22	G	143	GLN
22	G	259	GLN
23	GG	81	HIS
25	H	98	HIS
25	H	189	GLN
28	II	99	ASN
29	J	42	GLN
29	J	98	ASN

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Mol	Chain	Res	Type
29	J	110	GLN
32	KK	28	HIS
33	L	15	HIS
33	L	19	GLN
33	L	67	HIS
34	LL	83	GLN
35	M	56	GLN
35	M	131	GLN
36	N	87	HIS
36	N	90	ASN
36	N	109	HIS
36	N	145	ASN
36	N	199	GLN
37	NN	5	HIS
38	O	180	GLN
40	P	25	HIS
40	P	28	ASN
40	P	56	GLN
40	P	137	ASN
43	QQ	80	GLN
43	QQ	142	GLN
44	R	39	GLN
44	R	40	GLN
44	R	75	HIS
48	T	77	ASN
48	T	127	GLN
49	TT	12	GLN
50	U	41	GLN
50	U	44	GLN
52	V	84	GLN
53	VV	29	HIS
53	VV	82	ASN
55	WW	56	HIS
56	X	93	ASN
56	X	108	GLN
57	XX	46	HIS
57	XX	92	ASN
58	Y	43	ASN
58	Y	96	HIS
58	Y	127	GLN
59	YY	19	GLN
62	a	28	HIS

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Mol	Chain	Res	Type
63	b	27	GLN
63	b	60	ASN
63	b	61	ASN
63	b	101	HIS
64	c	33	GLN
64	c	40	GLN
65	d	121	ASN
66	e	23	HIS
66	e	57	ASN
66	e	68	HIS
68	g	110	GLN
69	h	107	GLN
70	i	15	HIS
70	i	80	HIS
71	j	13	ASN
71	j	28	HIS
71	j	57	ASN
72	k	28	ASN
72	k	58	GLN
73	l	17	GLN
73	l	25	GLN
74	m	58	GLN
77	p	33	GLN
78	r	45	HIS
78	r	95	HIS
79	s	39	GLN
81	t	22	GLN
81	t	96	GLN
81	t	104	GLN
82	v	87	ASN
82	v	138	GLN
82	v	684	GLN
82	v	720	GLN
83	w	206	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	3290/3740 (87%)	480 (14%)	38 (1%)
3	8	140/156 (89%)	14 (10%)	0
31	K	118/120 (98%)	7 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	9	1670/1786 (93%)	387 (23%)	18 (1%)
All	All	5218/5802 (89%)	888 (17%)	56 (1%)

All (888) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	5	17	A
2	5	25	A
2	5	39	A
2	5	42	A
2	5	56	A
2	5	58	G
2	5	59	A
2	5	64	A
2	5	65	A
2	5	73	A
2	5	91	G
2	5	98	A
2	5	104	G
2	5	108	A
2	5	109	G
2	5	110	C
2	5	119	G
2	5	120	A
2	5	126	C
2	5	134	G
2	5	135	G
2	5	136	C
2	5	157	U
2	5	159	C
2	5	166	C
2	5	168	C
2	5	180	C
2	5	182	G
2	5	200	U
2	5	209	U
2	5	224	U
2	5	233	U
2	5	234	G
2	5	246	G
2	5	258	G
2	5	266	C

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Mol	Chain	Res	Type
2	5	276	C
2	5	280	G
2	5	297	U
2	5	306	A
2	5	309	C
2	5	315	G
2	5	316	U
2	5	326	C
2	5	334	A
2	5	340	C
2	5	350	C
2	5	386	A
2	5	387	G
2	5	407	A
2	5	410	A
2	5	412	G
2	5	450	G
2	5	452	A
2	5	453	G
2	5	454	U
2	5	455	C
2	5	463	A
2	5	464	G
2	5	486	C
2	5	492	U
2	5	493	G
2	5	505	G
2	5	666	G
2	5	669	C
2	5	685	C
2	5	686	A
2	5	704	C
2	5	730	G
2	5	731	G
2	5	738	C
2	5	742	G
2	5	747	A
2	5	749	G
2	5	914	U
2	5	917	A
2	5	923	C
2	5	927	C

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Mol	Chain	Res	Type
2	5	928	G
2	5	933	C
2	5	934	A
2	5	935	G
2	5	937	G
2	5	939	C
2	5	947	A
2	5	948	U
2	5	959	A
2	5	962	G
2	5	963	A
2	5	964	G
2	5	967	A
2	5	969	A
2	5	970	C
2	5	972	C
2	5	973	G
2	5	976	C
2	5	982	C
2	5	987	U
2	5	993	C
2	5	1074	G
2	5	1076	C
2	5	1077	G
2	5	1083	C
2	5	1102	G
2	5	1174	G
2	5	1179	A
2	5	1184	C
2	5	1199	G
2	5	1214	C
2	5	1215	G
2	5	1216	G
2	5	1218	C
2	5	1219	C
2	5	1238	G
2	5	1239	G
2	5	1241	C
2	5	1243	C
2	5	1277	G
2	5	1279	G
2	5	1284	C

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Mol	Chain	Res	Type
2	5	1288	G
2	5	1291	G
2	5	1296	C
2	5	1297	G
2	5	1300	G
2	5	1305	C
2	5	1308	C
2	5	1330	A2M
2	5	1334	A
2	5	1341	A
2	5	1358	A
2	5	1362	G
2	5	1363	G
2	5	1375	A
2	5	1381	G
2	5	1383	C
2	5	1391	A
2	5	1398	G
2	5	1401	A
2	5	1402	A
2	5	1425	G
2	5	1440	C
2	5	1441	C
2	5	1443	C
2	5	1444	U
2	5	1449	U
2	5	1450	C
2	5	1461	G
2	5	1486	G
2	5	1487	C
2	5	1501	A
2	5	1502	G
2	5	1506	G
2	5	1518	U
2	5	1527	A
2	5	1538	A2M
2	5	1551	A
2	5	1570	C
2	5	1582	U
2	5	1595	U
2	5	1600	U
2	5	1606	U

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Mol	Chain	Res	Type
2	5	1616	G
2	5	1617	A
2	5	1628	G
2	5	1629	OMG
2	5	1635	A
2	5	1637	G
2	5	1638	A
2	5	1642	A
2	5	1644	C
2	5	1646	A
2	5	1658	G
2	5	1665	C
2	5	1680	C
2	5	1681	PSU
2	5	1683	A
2	5	1733	A
2	5	1738	G
2	5	1745	G
2	5	1746	A
2	5	1754	G
2	5	1785	U
2	5	1791	A
2	5	1808	A
2	5	1809	A
2	5	1823	G
2	5	1838	U
2	5	1839	G
2	5	1840	G
2	5	1841	A
2	5	1846	G
2	5	1859	G
2	5	1873	G
2	5	1901	A
2	5	1903	G
2	5	1922	U
2	5	1924	C
2	5	1925	C
2	5	1926	G
2	5	1935	C
2	5	1944	G
2	5	1945	A
2	5	1952	G

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Mol	Chain	Res	Type
2	5	1955	G
2	5	1962	A
2	5	1965	G
2	5	1968	A
2	5	1978	U
2	5	1979	G
2	5	1982	C
2	5	1984	U
2	5	1988	A
2	5	1989	G
2	5	1991	C
2	5	1994	A
2	5	1995	A
2	5	2001	U
2	5	2005	G
2	5	2006	A
2	5	2007	G
2	5	2008	U
2	5	2012	U
2	5	2030	A
2	5	2050	G
2	5	2051	A
2	5	2052	U
2	5	2056	G
2	5	2059	G
2	5	2060	G
2	5	2073	A
2	5	2088	U
2	5	2094	U
2	5	2097	G
2	5	2101	A
2	5	2102	G
2	5	2104	G
2	5	2106	G
2	5	2110	G
2	5	2112	G
2	5	2264	C
2	5	2271	U
2	5	2279	G
2	5	2293	C
2	5	2304	A
2	5	2305	G

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Mol	Chain	Res	Type
2	5	2317	A
2	5	2320	G
2	5	2337	G
2	5	2352	G
2	5	2355	C
2	5	2368	OMG
2	5	2399	A
2	5	2400	A
2	5	2425	G
2	5	2426	OMC
2	5	2428	OMG
2	5	2429	U
2	5	2437	G
2	5	2445	C
2	5	2454	G
2	5	2475	G
2	5	2479	G
2	5	2506	A
2	5	2507	G
2	5	2508	C
2	5	2509	C
2	5	2510	G
2	5	2517	A
2	5	2533	A
2	5	2541	A
2	5	2557	A
2	5	2579	U
2	5	2587	C
2	5	2591	A
2	5	2605	A
2	5	2642	G
2	5	2644	G
2	5	2657	C
2	5	2666	G
2	5	2673	C
2	5	2691	U
2	5	2699	A
2	5	2700	A
2	5	2719	G
2	5	2720	C
2	5	2725	G
2	5	2729	A

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Mol	Chain	Res	Type
2	5	2730	G
2	5	2744	U
2	5	2747	A
2	5	2748	A
2	5	2768	A
2	5	2773	U
2	5	2791	A
2	5	2792	U
2	5	2794	U
2	5	2802	A
2	5	2818	C
2	5	2830	U
2	5	2831	G
2	5	2833	U
2	5	2846	G
2	5	2859	G
2	5	3620	U
2	5	3622	C
2	5	3629	G
2	5	3630	G
2	5	3639	A
2	5	3652	A
2	5	3666	A
2	5	3677	C
2	5	3700	C
2	5	3715	A
2	5	3733	PSU
2	5	3752	A
2	5	3758	G
2	5	3760	A
2	5	3762	U
2	5	3771	C
2	5	3777	U
2	5	3781	G
2	5	3788	A
2	5	3790	U
2	5	3796	OMG
2	5	3814	C
2	5	3816	C
2	5	3818	U
2	5	3821	A
2	5	3823	G

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Mol	Chain	Res	Type
2	5	3842	U
2	5	3843	G
2	5	3844	U
2	5	3871	A2M
2	5	3881	A
2	5	3882	C
2	5	3883	G
2	5	3893	G
2	5	3902	G
2	5	3905	A
2	5	3909	A
2	5	3910	A
2	5	3911	G
2	5	3919	U
2	5	3920	G
2	5	3921	A
2	5	3943	G
2	5	3945	G
2	5	4080	G
2	5	4089	A
2	5	4090	G
2	5	4092	C
2	5	4120	C
2	5	4122	U
2	5	4131	A
2	5	4162	C
2	5	4166	C
2	5	4167	U
2	5	4174	A
2	5	4187	G
2	5	4188	G
2	5	4195	G
2	5	4197	C
2	5	4199	G
2	5	4207	A
2	5	4233	U
2	5	4237	A
2	5	4255	A
2	5	4258	G
2	5	4262	C
2	5	4270	G
2	5	4272	A

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Mol	Chain	Res	Type
2	5	4275	A
2	5	4277	A
2	5	4285	A
2	5	4295	G
2	5	4297	PSU
2	5	4309	G
2	5	4310	OMU
2	5	4318	C
2	5	4323	C
2	5	4334	G
2	5	4336	C
2	5	4353	C
2	5	4376	U
2	5	4377	G
2	5	4380	A
2	5	4381	G
2	5	4382	A
2	5	4384	A
2	5	4391	C
2	5	4395	G
2	5	4398	A
2	5	4399	U
2	5	4402	C
2	5	4423	U
2	5	4426	A
2	5	4452	G
2	5	4453	A
2	5	4454	PSU
2	5	4468	A
2	5	4470	C
2	5	4479	G
2	5	4504	PSU
2	5	4514	A
2	5	4515	A
2	5	4516	U
2	5	4517	A
2	5	4523	C
2	5	4524	G
2	5	4526	G
2	5	4527	A2M
2	5	4528	G
2	5	4532	G

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Mol	Chain	Res	Type
2	5	4534	UR3
2	5	4552	A
2	5	4553	G
2	5	4564	C
2	5	4571	G
2	5	4577	G
2	5	4578	U
2	5	4579	G
2	5	4588	A
2	5	4593	A
2	5	4594	A
2	5	4640	PSU
2	5	4641	OMG
2	5	4660	A
2	5	4674	C
2	5	4681	U
2	5	4699	C
2	5	4704	A
2	5	4713	U
2	5	4723	G
2	5	4724	C
2	5	4740	C
2	5	4749	G
2	5	4755	G
2	5	4756	U
2	5	4758	G
2	5	4760	C
2	5	4761	C
2	5	4763	C
2	5	4765	G
2	5	4769	G
2	5	4872	G
2	5	4874	OMG
2	5	4875	C
2	5	4879	G
2	5	4886	U
2	5	4887	C
2	5	4889	U
2	5	4899	C
2	5	4900	G
2	5	4914	A
2	5	4917	G

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Mol	Chain	Res	Type
2	5	4920	G
2	5	4922	C
2	5	4941	C
2	5	4942	A
2	5	4947	A
2	5	4948	C
2	5	4953	G
2	5	4954	U
2	5	4955	G
2	5	4962	C
2	5	4964	G
2	5	4971	A
2	5	4980	U
2	5	4992	U
2	5	4997	G
2	5	5018	A
2	5	5021	G
2	5	5045	G
2	5	5051	C
2	5	5054	C
2	5	5057	U
2	5	5058	C
2	5	5065	A
2	5	5066	G
3	8	23	C
3	8	34	U
3	8	35	C
3	8	59	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	87	G
3	8	94	G
3	8	103	A
3	8	105	C
3	8	110	U
3	8	114	G
3	8	156	U
4	9	3	C
4	9	4	C
4	9	14	C
4	9	23	G

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Mol	Chain	Res	Type
4	9	25	A
4	9	26	U
4	9	33	G
4	9	41	G
4	9	44	U
4	9	45	A
4	9	46	A
4	9	47	G
4	9	56	G
4	9	58	C
4	9	64	A
4	9	67	C
4	9	68	A
4	9	69	C
4	9	72	C
4	9	73	C
4	9	74	G
4	9	75	G
4	9	77	A
4	9	79	A
4	9	81	U
4	9	103	A
4	9	110	U
4	9	111	A
4	9	113	G
4	9	115	U
4	9	116	OMU
4	9	120	U
4	9	121	OMU
4	9	124	U
4	9	126	G
4	9	127	C
4	9	130	G
4	9	141	A
4	9	143	U
4	9	146	G
4	9	147	A
4	9	155	G
4	9	159	A2M
4	9	160	U
4	9	162	C
4	9	163	U

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Mol	Chain	Res	Type
4	9	166	A2M
4	9	167	G
4	9	170	A
4	9	171	A
4	9	175	A
4	9	180	G
4	9	182	C
4	9	183	G
4	9	184	G
4	9	188	C
4	9	189	U
4	9	190	G
4	9	191	A
4	9	192	C
4	9	202	G
4	9	206	G
4	9	215	G
4	9	294	U
4	9	297	A
4	9	304	C
4	9	306	C
4	9	307	G
4	9	308	G
4	9	309	G
4	9	312	G
4	9	313	A
4	9	318	A
4	9	319	C
4	9	332	G
4	9	347	G
4	9	350	C
4	9	351	G
4	9	360	A
4	9	362	C
4	9	364	A
4	9	368	U
4	9	369	C
4	9	370	G
4	9	381	C
4	9	385	G
4	9	398	A
4	9	400	C

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Mol	Chain	Res	Type
4	9	407	G
4	9	408	A
4	9	409	C
4	9	417	C
4	9	418	A
4	9	420	G
4	9	429	C
4	9	435	A
4	9	441	C
4	9	448	A
4	9	449	A
4	9	450	C
4	9	455	A
4	9	465	A
4	9	466	G
4	9	471	G
4	9	472	C
4	9	473	A
4	9	474	G
4	9	480	G
4	9	482	G
4	9	487	U
4	9	492	C
4	9	516	A
4	9	517	OMC
4	9	518	G
4	9	525	A
4	9	530	U
4	9	531	A
4	9	532	C
4	9	533	A
4	9	536	A
4	9	537	C
4	9	544	G
4	9	546	G
4	9	547	G
4	9	548	C
4	9	549	C
4	9	550	C
4	9	551	U
4	9	554	A
4	9	555	A

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Mol	Chain	Res	Type
4	9	556	U
4	9	559	G
4	9	560	A
4	9	563	G
4	9	564	A
4	9	576	A
4	9	583	A
4	9	587	A
4	9	588	G
4	9	589	G
4	9	590	A
4	9	591	U
4	9	603	C
4	9	606	G
4	9	607	U
4	9	608	C
4	9	614	C
4	9	617	G
4	9	621	C
4	9	627	U
4	9	631	U
4	9	643	A
4	9	655	A
4	9	660	C
4	9	662	G
4	9	664	A
4	9	666	U
4	9	668	A2M
4	9	669	A
4	9	671	A
4	9	672	A
4	9	673	G
4	9	678	U
4	9	684	G
4	9	688	U
4	9	689	U
4	9	690	G
4	9	752	G
4	9	753	C
4	9	754	G
4	9	798	G
4	9	811	A

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Mol	Chain	Res	Type
4	9	821	G
4	9	822	PSU
4	9	830	A
4	9	833	C
4	9	834	C
4	9	847	A
4	9	868	G
4	9	870	A
4	9	871	U
4	9	872	A
4	9	873	G
4	9	875	A
4	9	876	C
4	9	877	C
4	9	878	G
4	9	879	C
4	9	885	U
4	9	887	U
4	9	888	U
4	9	890	U
4	9	891	G
4	9	893	U
4	9	894	G
4	9	898	U
4	9	901	G
4	9	902	G
4	9	907	G
4	9	913	A
4	9	914	U
4	9	920	A
4	9	922	A
4	9	933	G
4	9	934	G
4	9	943	U
4	9	971	G
4	9	985	G
4	9	989	C
4	9	990	A
4	9	992	A
4	9	999	G
4	9	1017	U
4	9	1022	U

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Mol	Chain	Res	Type
4	9	1023	A
4	9	1030	A
4	9	1040	G
4	9	1041	G
4	9	1060	A
4	9	1081	PSU
4	9	1083	A
4	9	1085	C
4	9	1086	G
4	9	1087	A
4	9	1088	U
4	9	1097	G
4	9	1100	A
4	9	1109	C
4	9	1110	G
4	9	1114	U
4	9	1115	U
4	9	1116	C
4	9	1117	C
4	9	1118	C
4	9	1121	G
4	9	1123	C
4	9	1131	G
4	9	1133	A
4	9	1138	C
4	9	1150	A
4	9	1153	C
4	9	1154	U
4	9	1170	A
4	9	1195	A
4	9	1207	G
4	9	1208	A
4	9	1215	C
4	9	1216	C
4	9	1221	G
4	9	1224	G
4	9	1242	U
4	9	1243	PSU
4	9	1249	C
4	9	1250	A
4	9	1251	A
4	9	1253	A

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Mol	Chain	Res	Type
4	9	1256	G
4	9	1257	G
4	9	1259	A
4	9	1265	A
4	9	1273	C
4	9	1274	G
4	9	1275	G
4	9	1282	A
4	9	1284	A
4	9	1285	G
4	9	1293	A
4	9	1298	G
4	9	1300	U
4	9	1301	A
4	9	1302	G
4	9	1304	U
4	9	1307	U
4	9	1308	U
4	9	1309	C
4	9	1312	G
4	9	1314	U
4	9	1315	U
4	9	1322	G
4	9	1327	G
4	9	1333	U
4	9	1341	C
4	9	1342	U
4	9	1348	G
4	9	1358	U
4	9	1371	U
4	9	1372	U
4	9	1376	A
4	9	1378	A
4	9	1395	C
4	9	1396	A
4	9	1397	U
4	9	1398	G
4	9	1399	C
4	9	1401	A
4	9	1402	A
4	9	1404	U
4	9	1428	G

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Mol	Chain	Res	Type
4	9	1454	A
4	9	1455	A
4	9	1462	U
4	9	1463	U
4	9	1464	C
4	9	1465	A
4	9	1466	G
4	9	1473	G
4	9	1475	G
4	9	1476	A
4	9	1477	U
4	9	1480	A
4	9	1486	A
4	9	1489	A
4	9	1490	G
4	9	1494	U
4	9	1497	G
4	9	1498	A
4	9	1506	A
4	9	1510	G
4	9	1521	C
4	9	1522	A
4	9	1533	A
4	9	1544	C
4	9	1548	G
4	9	1552	G
4	9	1553	C
4	9	1554	C
4	9	1556	A
4	9	1557	C
4	9	1560	U
4	9	1570	G
4	9	1574	C
4	9	1575	G
4	9	1580	A
4	9	1585	U
4	9	1586	U
4	9	1587	G
4	9	1588	A
4	9	1597	C
4	9	1601	A
4	9	1602	U

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Mol	Chain	Res	Type
4	9	1603	G
4	9	1604	G
4	9	1606	G
4	9	1621	U
4	9	1623	A
4	9	1625	U
4	9	1637	A
4	9	1638	G
4	9	1648	G
4	9	1649	U
4	9	1663	A
4	9	1664	A
4	9	1665	G
4	9	1683	C
4	9	1695	A
4	9	1698	C
4	9	1699	A
4	9	1702	G
4	9	1721	U
4	9	1722	G
4	9	1725	U
4	9	1726	G
4	9	1742	C
4	9	1744	G
4	9	1748	G
4	9	1757	G
4	9	1779	G
4	9	1783	C
4	9	1784	G
4	9	1785	C
4	9	1800	A
4	9	1824	A
4	9	1825	A
4	9	1826	G
4	9	1831	A
4	9	1835	A
4	9	1836	G
4	9	1838	U
4	9	1849	G
4	9	1861	G
4	9	1862	G
4	9	1863	A

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Mol	Chain	Res	Type
4	9	1864	U
4	9	1865	C
4	9	1866	A
4	9	1867	U
4	9	1869	A
31	K	7	G
31	K	33	U
31	K	53	U
31	K	54	A
31	K	64	G
31	K	100	A
31	K	110	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	125	C
2	5	134	G
2	5	245	C
2	5	275	C
2	5	385	A
2	5	406	C
2	5	504	G
2	5	932	G
2	5	938	A
2	5	975	G
2	5	1076	C
2	5	1178	G
2	5	1215	G
2	5	1240	C
2	5	1242	A
2	5	1295	G
2	5	1333	G
2	5	1374	G
2	5	1443	C
2	5	1449	U
2	5	1637	G
2	5	1808	A
2	5	1822	G
2	5	1943	A
2	5	1983	A
2	5	2050	G

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Mol	Chain	Res	Type
2	5	2093	G
2	5	2270	C
2	5	2506	A
2	5	2643	U
2	5	2699	A
2	5	3892	G
2	5	4236	U
2	5	4452	G
2	5	4703	U
2	5	4888	G
2	5	4940	G
2	5	4953	G
4	9	110	U
4	9	434	G
4	9	465	A
4	9	479	C
4	9	532	C
4	9	553	U
4	9	642	U
4	9	688	U
4	9	752	G
4	9	870	A
4	9	874	G
4	9	1137	U
4	9	1394	G
4	9	1395	C
4	9	1489	A
4	9	1520	G
4	9	1637	A
4	9	1664	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	6MZ	9	1832	4	18,25,26	2.24	3 (16%)	16,36,39	1.53	1 (6%)
4	A2M	9	27	4	18,25,26	4.68	9 (50%)	18,36,39	2.69	4 (22%)
2	OMC	5	3705	2,84	19,22,23	3.31	8 (42%)	26,31,34	0.75	0
4	M7A	9	1806	4	20,25,26	2.04	3 (15%)	28,37,40	3.72	8 (28%)
2	OMG	5	1887	2	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
2	A2M	5	4575	2	18,25,26	4.50	7 (38%)	18,36,39	2.83	3 (16%)
4	B8Q	9	1219	4	17,22,23	2.92	4 (23%)	22,32,35	2.34	7 (31%)
4	E3C	9	568	4	18,23,24	3.37	6 (33%)	21,33,36	2.23	5 (23%)
2	PSU	5	4535	2	18,21,22	4.93	7 (38%)	22,30,33	1.81	5 (22%)
4	4AC	9	1842	4	21,24,25	3.13	10 (47%)	29,34,37	1.18	4 (13%)
2	5MC	5	3786	2	18,22,23	3.91	7 (38%)	26,32,35	1.03	2 (7%)
2	A2M	5	3829	2	18,25,26	4.49	7 (38%)	18,36,39	2.79	3 (16%)
4	OMC	9	1710	4	19,22,23	2.94	7 (36%)	26,31,34	0.92	1 (3%)
2	A2M	5	2367	2,84	18,25,26	4.49	7 (38%)	18,36,39	2.86	3 (16%)
2	OMG	5	4374	2	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)
2	5MC	5	4451	2	18,22,23	3.93	7 (38%)	26,32,35	1.05	1 (3%)
2	OMG	5	4200	2	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)
2	OMG	5	2054	2	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
2	A2M	5	1330	2	18,25,26	4.44	7 (38%)	18,36,39	2.80	3 (16%)
2	A2M	5	3789	2	18,25,26	4.36	8 (44%)	18,36,39	2.83	3 (16%)
2	A2M	5	3727	2,70	18,25,26	4.51	7 (38%)	18,36,39	2.84	3 (16%)
2	B8Q	5	1460	2	17,22,23	2.93	5 (29%)	22,32,35	2.08	4 (18%)
2	2MG	5	1521	2	18,26,27	2.76	7 (38%)	16,38,41	1.48	4 (25%)
2	A2M	5	3871	2	18,25,26	4.46	7 (38%)	18,36,39	2.78	3 (16%)
2	B8H	5	4300	2	19,22,23	6.53	6 (31%)	22,32,35	2.34	5 (22%)
2	OMU	5	4310	2	19,22,23	3.03	8 (42%)	26,31,34	1.71	5 (19%)
2	PSU	5	2512	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)
2	OMG	5	1320	2	18,26,27	2.60	8 (44%)	19,38,41	1.58	5 (26%)
2	B9H	5	2790	2	20,25,26	2.95	5 (25%)	22,35,38	1.47	3 (13%)
4	OMC	9	174	4	19,22,23	2.95	7 (36%)	26,31,34	0.81	1 (3%)
2	E6G	5	4359	2	20,27,28	2.04	3 (15%)	22,39,42	2.16	7 (31%)
2	PSU	5	4640	2,65	18,21,22	4.96	7 (38%)	22,30,33	1.89	5 (22%)
2	1MA	5	1326	2,84	16,25,26	4.04	4 (25%)	18,37,40	1.77	3 (16%)
2	PSU	5	4407	2	18,21,22	4.92	7 (38%)	22,30,33	1.76	5 (22%)
4	PSU	9	1081	4	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMG	5	2777	2	18,26,27	2.60	8 (44%)	19,38,41	1.57	4 (21%)
2	PSU	5	4504	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)
4	B8N	9	1248	4	24,29,30	2.79	6 (25%)	29,42,45	1.75	5 (17%)
2	PSU	5	4297	2	18,21,22	4.91	7 (38%)	22,30,33	1.86	5 (22%)
4	PSU	9	822	4	18,21,22	1.03	2 (11%)	22,30,33	1.93	5 (22%)
2	PSU	5	3768	2	18,21,22	4.97	7 (38%)	22,30,33	1.71	6 (27%)
4	OMG	9	683	4	18,26,27	2.48	8 (44%)	19,38,41	1.55	4 (21%)
2	PSU	5	4446	2	18,21,22	4.95	7 (38%)	22,30,33	1.86	5 (22%)
2	5MC	5	4339	2	18,22,23	3.92	7 (38%)	26,32,35	1.04	2 (7%)
2	B8W	5	2384	2	18,26,27	2.03	2 (11%)	21,38,41	2.23	5 (23%)
2	OMG	5	1629	2	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)
2	PSU	5	1586	2	18,21,22	4.95	7 (38%)	22,30,33	1.85	5 (22%)
2	OMC	5	2865	2	19,22,23	3.33	8 (42%)	26,31,34	0.69	0
2	OMG	5	4498	2	18,26,27	2.57	8 (44%)	19,38,41	1.51	4 (21%)
2	OMC	5	4540	2	19,22,23	3.34	8 (42%)	26,31,34	0.74	0
2	UR3	5	4534	2	19,22,23	3.20	7 (36%)	26,32,35	1.31	3 (11%)
2	E7G	5	1801	2	24,27,28	3.87	11 (45%)	30,40,43	2.22	10 (33%)
2	OMG	5	4641	2	18,26,27	2.57	8 (44%)	19,38,41	1.55	4 (21%)
4	5MC	9	1374	4	18,22,23	3.69	7 (38%)	26,32,35	1.34	4 (15%)
2	PSU	5	1687	2	18,21,22	4.91	7 (38%)	22,30,33	1.84	5 (22%)
2	B8W	5	4533	2,84	18,26,27	2.00	2 (11%)	21,38,41	2.55	7 (33%)
2	OMG	5	3796	2	18,26,27	2.57	8 (44%)	19,38,41	1.51	4 (21%)
2	PSU	5	4632	2	18,21,22	4.90	7 (38%)	22,30,33	1.93	5 (22%)
4	OMC	9	1703	4	19,22,23	2.94	7 (36%)	26,31,34	0.83	1 (3%)
4	PSU	9	1243	4	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
2	P7G	5	1913	2	24,28,29	4.23	11 (45%)	27,41,44	1.56	3 (11%)
2	B9B	5	237	2	21,28,29	1.99	3 (14%)	23,40,43	1.91	5 (21%)
4	PSU	9	612	4	18,21,22	0.99	1 (5%)	22,30,33	1.74	4 (18%)
2	2MG	5	729	2	18,26,27	2.75	6 (33%)	16,38,41	1.36	3 (18%)
2	B8W	5	4476	2	18,26,27	2.03	2 (11%)	21,38,41	2.78	8 (38%)
2	OMG	5	4627	2	18,26,27	2.58	8 (44%)	19,38,41	1.56	4 (21%)
2	B8K	5	4694	2	24,28,29	3.38	11 (45%)	30,42,45	2.33	11 (36%)
4	UR3	9	1830	4	19,22,23	2.69	6 (31%)	26,32,35	1.57	4 (15%)
4	MA6	9	1850	4	18,26,27	1.02	1 (5%)	19,38,41	2.74	2 (10%)
4	OMU	9	116	4	19,22,23	2.88	7 (36%)	26,31,34	1.75	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MA6	9	1851	4	18,26,27	0.98	1 (5%)	19,38,41	2.62	2 (10%)
4	PSU	9	119	4	18,21,22	0.94	1 (5%)	22,30,33	1.60	5 (22%)
2	UR3	5	4601	2	19,22,23	3.21	7 (36%)	26,32,35	1.29	2 (7%)
4	A2M	9	668	4	18,25,26	4.68	8 (44%)	18,36,39	2.70	5 (27%)
2	5MU	5	4087	2	19,22,23	4.98	7 (36%)	28,32,35	3.62	9 (32%)
2	A2M	5	1538	2,84	18,25,26	4.49	7 (38%)	18,36,39	2.89	3 (16%)
2	B8T	5	4487	2	19,22,23	3.25	8 (42%)	26,31,34	0.85	1 (3%)
2	A2M	5	2405	2,84	18,25,26	4.48	7 (38%)	18,36,39	2.84	3 (16%)
4	A2M	9	1031	4	18,25,26	4.75	8 (44%)	18,36,39	2.78	4 (22%)
2	OMC	5	3913	2	19,22,23	3.34	8 (42%)	26,31,34	0.71	0
4	A2M	9	1678	4	18,25,26	4.81	9 (50%)	18,36,39	2.59	3 (16%)
2	OMG	5	1526	2	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)
2	PSU	5	3733	2	18,21,22	4.95	7 (38%)	22,30,33	1.82	5 (22%)
2	OMC	5	2808	2	19,22,23	3.33	8 (42%)	26,31,34	0.71	0
2	6MZ	5	4224	2	18,25,26	2.19	3 (16%)	16,36,39	2.05	4 (25%)
4	4AC	9	1337	4	21,24,25	3.19	9 (42%)	29,34,37	1.23	3 (10%)
2	P7G	5	3884	2	24,28,29	4.14	11 (45%)	27,41,44	1.60	3 (11%)
2	2MG	5	4876	2	18,26,27	2.72	7 (38%)	16,38,41	1.55	4 (25%)
2	A2M	5	3722	2	18,25,26	4.49	7 (38%)	18,36,39	2.85	3 (16%)
2	A2M	5	1875	2,84	18,25,26	4.51	7 (38%)	18,36,39	2.87	3 (16%)
2	B8K	5	3901	2	24,28,29	3.30	11 (45%)	30,42,45	2.28	11 (36%)
2	PSU	5	1681	2	18,21,22	4.95	8 (44%)	22,30,33	1.88	5 (22%)
2	PSU	5	3719	2	18,21,22	4.94	7 (38%)	22,30,33	1.86	5 (22%)
82	DDE	v	715	82	14,20,21	1.02	1 (7%)	14,28,30	1.09	1 (7%)
2	OMG	5	373	2	18,26,27	2.55	8 (44%)	19,38,41	1.56	4 (21%)
2	7MG	5	1609	2	22,26,27	3.92	10 (45%)	29,39,42	2.03	9 (31%)
4	PSU	9	823	4	18,21,22	1.09	1 (5%)	22,30,33	1.83	4 (18%)
2	1MA	5	4419	2	16,25,26	4.01	4 (25%)	18,37,40	1.71	3 (16%)
2	7MG	5	2526	2	22,26,27	3.92	10 (45%)	29,39,42	2.04	9 (31%)
2	B8H	5	1864	2	19,22,23	6.50	6 (31%)	22,32,35	2.35	5 (22%)
4	A2M	9	159	4	18,25,26	4.83	9 (50%)	18,36,39	2.75	4 (22%)
4	A2M	9	484	4	18,25,26	4.71	9 (50%)	18,36,39	2.71	3 (16%)
2	A2M	5	398	2	18,25,26	4.49	7 (38%)	18,36,39	2.86	3 (16%)
2	MHG	5	4375	2	29,32,33	3.95	11 (37%)	34,46,49	2.29	10 (29%)
2	M7A	5	4568	2	20,25,26	2.02	3 (15%)	28,37,40	3.67	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMC	5	2369	2	19,22,23	3.34	8 (42%)	26,31,34	0.75	0
11	MLZ	C	333	11	8,9,10	0.77	0	4,9,11	0.67	0
4	OMU	9	121	4	19,22,23	2.96	8 (42%)	26,31,34	1.77	5 (19%)
2	OMG	5	4874	2	18,26,27	2.59	8 (44%)	19,38,41	1.53	4 (21%)
2	P4U	5	1352	2	21,24,25	4.09	7 (33%)	27,33,36	0.98	1 (3%)
2	OMC	5	2426	2,40,84	19,22,23	3.35	8 (42%)	26,31,34	0.76	0
2	7MG	5	4554	2	22,26,27	3.95	10 (45%)	29,39,42	1.99	9 (31%)
74	MLZ	m	72	74	8,9,10	0.76	0	4,9,11	0.64	0
4	5MU	9	814	4	19,22,23	4.87	7 (36%)	28,32,35	3.59	12 (42%)
4	OMG	9	509	4	18,26,27	2.46	8 (44%)	19,38,41	1.46	4 (21%)
2	B8T	5	4675	2	19,22,23	3.25	8 (42%)	26,31,34	0.91	1 (3%)
2	OMC	5	3891	2	19,22,23	3.34	8 (42%)	26,31,34	0.72	0
81	5CT	t	51	81	13,14,15	0.66	0	9,15,17	1.20	1 (11%)
2	OMC	5	3873	2	19,22,23	3.34	8 (42%)	26,31,34	0.74	0
2	BGH	5	3903	2,84	25,29,30	4.62	18 (72%)	31,43,46	2.35	12 (38%)
2	OMU	5	4624	2,52	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
4	A2M	9	166	4	18,25,26	4.79	9 (50%)	18,36,39	2.78	4 (22%)
2	B8W	5	4133	2	18,26,27	2.06	2 (11%)	21,38,41	2.34	6 (28%)
4	OMC	9	517	4	19,22,23	2.84	7 (36%)	26,31,34	0.64	0
2	B8W	5	4189	2	18,26,27	2.04	2 (11%)	21,38,41	2.43	6 (28%)
2	OMG	5	2428	2	18,26,27	2.58	8 (44%)	19,38,41	1.48	4 (21%)
2	PSU	5	4454	2,84	18,21,22	4.95	7 (38%)	22,30,33	1.84	5 (22%)
2	B9B	5	2758	2,84	21,28,29	1.98	3 (14%)	23,40,43	1.87	4 (17%)
2	I4U	5	4198	2	21,24,25	3.61	8 (38%)	27,34,37	1.00	1 (3%)
4	OMG	9	644	4	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
3	OMU	8	14	2,3	19,22,23	3.00	8 (42%)	26,31,34	1.69	4 (15%)
2	B9B	5	1578	2	21,28,29	1.98	3 (14%)	23,40,43	1.85	5 (21%)
2	UR3	5	1870	2	19,22,23	3.20	7 (36%)	26,32,35	1.27	3 (11%)
2	A2M	5	4527	2,84	18,25,26	4.50	7 (38%)	18,36,39	2.81	3 (16%)
2	E7G	5	2301	2	24,27,28	3.86	11 (45%)	30,40,43	2.24	10 (33%)
2	I4U	5	1663	2	21,24,25	3.63	9 (42%)	27,34,37	0.95	1 (3%)
2	OMG	5	2368	2	18,26,27	2.57	8 (44%)	19,38,41	1.55	4 (21%)
2	A2M	5	1528	2	18,25,26	4.47	7 (38%)	18,36,39	2.87	3 (16%)

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
4	6MZ	9	1832	4	-	2/5/27/28	0/3/3/3
4	A2M	9	27	4	-	0/5/27/28	0/3/3/3
2	OMC	5	3705	2,84	-	4/9/27/28	0/2/2/2
4	M7A	9	1806	4	-	0/7/37/38	0/3/3/3
2	OMG	5	1887	2	-	0/5/27/28	0/3/3/3
2	A2M	5	4575	2	-	0/5/27/28	0/3/3/3
4	B8Q	9	1219	4	-	0/7/42/43	0/2/2/2
4	E3C	9	568	4	-	4/9/44/45	0/2/2/2
2	PSU	5	4535	2	-	2/7/25/26	0/2/2/2
4	4AC	9	1842	4	-	0/11/29/30	0/2/2/2
2	5MC	5	3786	2	-	0/7/25/26	0/2/2/2
2	A2M	5	3829	2	-	0/5/27/28	0/3/3/3
4	OMC	9	1710	4	-	0/9/27/28	0/2/2/2
2	A2M	5	2367	2,84	-	1/5/27/28	0/3/3/3
2	OMG	5	4374	2	-	0/5/27/28	0/3/3/3
2	5MC	5	4451	2	-	4/7/25/26	0/2/2/2
2	OMG	5	4200	2	-	0/5/27/28	0/3/3/3
2	OMG	5	2054	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1330	2	-	1/5/27/28	0/3/3/3
2	A2M	5	3789	2	-	2/5/27/28	0/3/3/3
2	A2M	5	3727	2,70	-	1/5/27/28	0/3/3/3
2	B8Q	5	1460	2	-	0/7/42/43	0/2/2/2
2	2MG	5	1521	2	-	0/5/27/28	0/3/3/3
2	A2M	5	3871	2	-	3/5/27/28	0/3/3/3
2	B8H	5	4300	2	-	0/7/25/26	0/2/2/2
2	OMU	5	4310	2	-	0/9/27/28	0/2/2/2
2	PSU	5	2512	2	-	0/7/25/26	0/2/2/2
2	OMG	5	1320	2	-	0/5/27/28	0/3/3/3
2	B9H	5	2790	2	-	1/12/47/48	0/2/2/2
4	OMC	9	174	4	-	0/9/27/28	0/2/2/2
2	E6G	5	4359	2	-	2/6/28/29	0/3/3/3
2	PSU	5	4640	2,65	-	3/7/25/26	0/2/2/2
2	1MA	5	1326	2,84	-	0/3/25/26	0/3/3/3
2	PSU	5	4407	2	-	2/7/25/26	0/2/2/2
4	PSU	9	1081	4	-	3/7/25/26	0/2/2/2
2	OMG	5	2777	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4504	2	-	3/7/25/26	0/2/2/2
4	B8N	9	1248	4	-	3/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	4297	2	-	2/7/25/26	0/2/2/2
4	PSU	9	822	4	-	2/7/25/26	0/2/2/2
2	PSU	5	3768	2	-	4/7/25/26	0/2/2/2
4	OMG	9	683	4	-	2/5/27/28	0/3/3/3
2	PSU	5	4446	2	-	0/7/25/26	0/2/2/2
2	5MC	5	4339	2	-	0/7/25/26	0/2/2/2
2	B8W	5	2384	2	-	4/5/27/28	0/3/3/3
2	OMG	5	1629	2	-	0/5/27/28	0/3/3/3
2	PSU	5	1586	2	-	0/7/25/26	0/2/2/2
2	OMC	5	2865	2	-	0/9/27/28	0/2/2/2
2	OMG	5	4498	2	-	0/5/27/28	0/3/3/3
2	OMC	5	4540	2	-	0/9/27/28	0/2/2/2
2	UR3	5	4534	2	-	2/7/25/26	0/2/2/2
2	E7G	5	1801	2	-	2/9/39/40	0/3/3/3
2	OMG	5	4641	2	-	3/5/27/28	0/3/3/3
4	5MC	9	1374	4	-	0/7/25/26	0/2/2/2
2	PSU	5	1687	2	-	0/7/25/26	0/2/2/2
2	B8W	5	4533	2,84	-	2/5/27/28	0/3/3/3
2	OMG	5	3796	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4632	2	-	0/7/25/26	0/2/2/2
4	OMC	9	1703	4	-	2/9/27/28	0/2/2/2
4	PSU	9	1243	4	-	2/7/25/26	0/2/2/2
2	P7G	5	1913	2	-	2/10/40/41	0/3/3/3
2	B9B	5	237	2	-	2/7/29/30	0/3/3/3
4	PSU	9	612	4	-	0/7/25/26	0/2/2/2
2	2MG	5	729	2	-	1/5/27/28	0/3/3/3
2	B8W	5	4476	2	-	2/5/27/28	0/3/3/3
2	OMG	5	4627	2	-	0/5/27/28	0/3/3/3
2	B8K	5	4694	2	-	0/11/41/42	0/3/3/3
4	UR3	9	1830	4	-	4/7/25/26	0/2/2/2
4	MA6	9	1850	4	-	1/7/29/30	0/3/3/3
4	OMU	9	116	4	-	3/9/27/28	0/2/2/2
4	MA6	9	1851	4	-	3/7/29/30	0/3/3/3
4	PSU	9	119	4	-	2/7/25/26	0/2/2/2
2	UR3	5	4601	2	-	0/7/25/26	0/2/2/2
4	A2M	9	668	4	-	4/5/27/28	0/3/3/3
2	5MU	5	4087	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	5	1538	2,84	-	2/5/27/28	0/3/3/3
2	B8T	5	4487	2	-	0/7/27/28	0/2/2/2
2	A2M	5	2405	2,84	-	2/5/27/28	0/3/3/3
4	A2M	9	1031	4	-	0/5/27/28	0/3/3/3
2	OMC	5	3913	2	-	0/9/27/28	0/2/2/2
4	A2M	9	1678	4	-	0/5/27/28	0/3/3/3
2	OMG	5	1526	2	-	0/5/27/28	0/3/3/3
2	PSU	5	3733	2	-	2/7/25/26	0/2/2/2
2	OMC	5	2808	2	-	0/9/27/28	0/2/2/2
2	6MZ	5	4224	2	-	0/5/27/28	0/3/3/3
4	4AC	9	1337	4	-	0/11/29/30	0/2/2/2
2	P7G	5	3884	2	-	2/10/40/41	0/3/3/3
2	2MG	5	4876	2	-	0/5/27/28	0/3/3/3
2	A2M	5	3722	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1875	2,84	-	0/5/27/28	0/3/3/3
2	B8K	5	3901	2	-	3/11/41/42	0/3/3/3
2	PSU	5	1681	2	-	2/7/25/26	0/2/2/2
2	PSU	5	3719	2	-	0/7/25/26	0/2/2/2
82	DDE	v	715	82	-	16/20/21/23	0/1/1/1
2	OMG	5	373	2	-	1/5/27/28	0/3/3/3
2	7MG	5	1609	2	-	0/7/37/38	0/3/3/3
4	PSU	9	823	4	-	0/7/25/26	0/2/2/2
2	1MA	5	4419	2	-	2/3/25/26	0/3/3/3
2	7MG	5	2526	2	-	0/7/37/38	0/3/3/3
2	B8H	5	1864	2	-	0/7/25/26	0/2/2/2
4	A2M	9	159	4	-	3/5/27/28	0/3/3/3
4	A2M	9	484	4	-	0/5/27/28	0/3/3/3
2	A2M	5	398	2	-	2/5/27/28	0/3/3/3
2	MHG	5	4375	2	-	7/16/46/47	0/3/3/3
2	M7A	5	4568	2	-	0/7/37/38	0/3/3/3
2	OMC	5	2369	2	-	0/9/27/28	0/2/2/2
11	MLZ	C	333	11	-	0/7/8/10	-
4	OMU	9	121	4	-	2/9/27/28	0/2/2/2
2	OMG	5	4874	2	-	4/5/27/28	0/3/3/3
2	P4U	5	1352	2	-	3/10/29/30	0/2/2/2
2	OMC	5	2426	2,40,84	-	1/9/27/28	0/2/2/2
2	7MG	5	4554	2	-	0/7/37/38	0/3/3/3
74	MLZ	m	72	74	-	0/7/8/10	-
4	5MU	9	814	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	9	509	4	-	0/5/27/28	0/3/3/3
2	B8T	5	4675	2	-	1/7/27/28	0/2/2/2
2	OMC	5	3891	2	-	0/9/27/28	0/2/2/2
81	5CT	t	51	81	-	5/13/14/16	-
2	OMC	5	3873	2	-	0/9/27/28	0/2/2/2
2	BGH	5	3903	2,84	-	2/13/43/44	0/3/3/3
2	OMU	5	4624	2,52	-	1/9/27/28	0/2/2/2
4	A2M	9	166	4	-	2/5/27/28	0/3/3/3
2	B8W	5	4133	2	-	2/5/27/28	0/3/3/3
4	OMC	9	517	4	-	2/9/27/28	0/2/2/2
2	B8W	5	4189	2	-	2/5/27/28	0/3/3/3
2	OMG	5	2428	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4454	2,84	-	3/7/25/26	0/2/2/2
2	B9B	5	2758	2,84	-	2/7/29/30	0/3/3/3
2	I4U	5	4198	2	-	2/9/29/30	0/2/2/2
4	OMG	9	644	4	-	1/5/27/28	0/3/3/3
3	OMU	8	14	2,3	-	1/9/27/28	0/2/2/2
2	B9B	5	1578	2	-	2/7/29/30	0/3/3/3
2	UR3	5	1870	2	-	0/7/25/26	0/2/2/2
2	A2M	5	4527	2,84	-	3/5/27/28	0/3/3/3
2	E7G	5	2301	2	-	1/9/39/40	0/3/3/3
2	I4U	5	1663	2	-	1/9/29/30	0/2/2/2
2	OMG	5	2368	2	-	2/5/27/28	0/3/3/3
2	A2M	5	1528	2	-	1/5/27/28	0/3/3/3

All (920) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	166	A2M	O4'-C1'	16.42	1.64	1.41
4	9	159	A2M	O4'-C1'	16.40	1.64	1.41
4	9	1678	A2M	O4'-C1'	16.34	1.63	1.41
2	5	1875	A2M	O4'-C1'	16.24	1.63	1.41
2	5	4527	A2M	O4'-C1'	16.22	1.63	1.41
2	5	3727	A2M	O4'-C1'	16.19	1.63	1.41
2	5	3722	A2M	O4'-C1'	16.17	1.63	1.41
2	5	4575	A2M	O4'-C1'	16.14	1.63	1.41
2	5	2367	A2M	O4'-C1'	16.14	1.63	1.41
2	5	2405	A2M	O4'-C1'	16.13	1.63	1.41
2	5	398	A2M	O4'-C1'	16.12	1.63	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3829	A2M	O4'-C1'	16.12	1.63	1.41
2	5	1538	A2M	O4'-C1'	16.11	1.63	1.41
4	9	1031	A2M	O4'-C1'	16.10	1.63	1.41
2	5	1528	A2M	O4'-C1'	15.97	1.63	1.41
2	5	1330	A2M	O4'-C1'	15.93	1.63	1.41
2	5	3871	A2M	O4'-C1'	15.92	1.63	1.41
4	9	484	A2M	O4'-C1'	15.89	1.63	1.41
4	9	27	A2M	O4'-C1'	15.69	1.63	1.41
2	5	3789	A2M	O4'-C1'	15.51	1.62	1.41
4	9	668	A2M	O4'-C1'	15.40	1.62	1.41
2	5	4300	B8H	C4-N3	-14.95	1.11	1.38
2	5	1864	B8H	C4-N3	-14.87	1.11	1.38
2	5	1326	1MA	C2-N3	14.71	1.46	1.29
2	5	4419	1MA	C2-N3	14.58	1.46	1.29
2	5	4300	B8H	C4-C5	13.89	1.83	1.44
2	5	1864	B8H	C4-C5	13.85	1.83	1.44
2	5	4300	B8H	C6-C5	-13.49	1.16	1.34
2	5	1864	B8H	C6-C5	-13.39	1.16	1.34
2	5	4300	B8H	C6-N1	12.78	1.68	1.36
2	5	1864	B8H	C6-N1	12.72	1.67	1.36
2	5	3768	PSU	C6-C5	11.99	1.49	1.35
2	5	4087	5MU	C2-N1	11.95	1.57	1.38
2	5	4640	PSU	C2-N1	11.87	1.52	1.36
2	5	4407	PSU	C6-C5	11.85	1.49	1.35
2	5	2512	PSU	C6-C5	11.80	1.49	1.35
2	5	4454	PSU	C6-C5	11.79	1.49	1.35
2	5	1681	PSU	C2-N1	11.79	1.52	1.36
2	5	2512	PSU	C2-N1	11.78	1.52	1.36
2	5	3733	PSU	C6-C5	11.77	1.49	1.35
2	5	4640	PSU	C6-C5	11.76	1.49	1.35
2	5	4446	PSU	C6-C5	11.76	1.49	1.35
2	5	4504	PSU	C2-N1	11.75	1.52	1.36
2	5	3719	PSU	C2-N1	11.75	1.52	1.36
2	5	4504	PSU	C6-C5	11.75	1.49	1.35
2	5	1687	PSU	C6-C5	11.73	1.49	1.35
2	5	4535	PSU	C2-N1	11.73	1.52	1.36
2	5	1586	PSU	C2-N1	11.72	1.52	1.36
2	5	4407	PSU	C2-N1	11.72	1.52	1.36
2	5	4454	PSU	C2-N1	11.72	1.52	1.36
2	5	3768	PSU	C2-N1	11.72	1.52	1.36
2	5	1913	P7G	C8-N9	11.72	1.52	1.46
2	5	4446	PSU	C2-N1	11.70	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4632	PSU	C6-C5	11.69	1.48	1.35
2	5	1586	PSU	C6-C5	11.69	1.48	1.35
2	5	3719	PSU	C6-C5	11.68	1.48	1.35
2	5	3733	PSU	C2-N1	11.65	1.52	1.36
2	5	4297	PSU	C6-C5	11.61	1.48	1.35
2	5	1687	PSU	C2-N1	11.59	1.52	1.36
2	5	4297	PSU	C2-N1	11.58	1.52	1.36
2	5	4535	PSU	C6-C5	11.55	1.48	1.35
2	5	4632	PSU	C2-N1	11.52	1.52	1.36
2	5	1681	PSU	C6-C5	11.50	1.48	1.35
4	9	814	5MU	C2-N1	11.44	1.56	1.38
2	5	1663	I4U	C4-N3	11.27	1.45	1.31
2	5	4198	I4U	C4-N3	11.23	1.45	1.31
2	5	3884	P7G	C8-N9	10.97	1.52	1.46
2	5	1352	P4U	C4-N3	10.78	1.45	1.31
2	5	4087	5MU	C6-N1	10.70	1.56	1.38
2	5	4087	5MU	C4-C5	10.33	1.61	1.44
4	9	814	5MU	C6-N1	10.28	1.55	1.38
2	5	3903	BGH	O4'-C4'	10.19	1.67	1.45
2	5	4375	MHG	C8-N9	10.16	1.51	1.46
2	5	4451	5MC	C6-C5	10.15	1.51	1.34
2	5	3786	5MC	C6-C5	10.06	1.51	1.34
2	5	4339	5MC	C6-C5	10.01	1.51	1.34
2	5	3903	BGH	C3'-C4'	-9.70	1.28	1.53
2	5	4554	7MG	C8-N9	9.68	1.51	1.46
2	5	2301	E7G	C8-N9	9.62	1.51	1.46
4	9	814	5MU	C4-C5	9.50	1.60	1.44
4	9	1374	5MC	C6-C5	9.37	1.50	1.34
2	5	1801	E7G	C8-N9	9.34	1.51	1.46
2	5	2526	7MG	C8-N9	9.27	1.51	1.46
2	5	1609	7MG	C8-N9	9.21	1.51	1.46
2	5	4694	B8K	C8-N9	8.79	1.50	1.46
2	5	1870	UR3	C2-N1	8.76	1.51	1.38
2	5	4601	UR3	C2-N1	8.70	1.51	1.38
2	5	4534	UR3	C2-N1	8.64	1.50	1.38
2	5	2790	B9H	C2-N3	8.52	1.48	1.37
4	9	568	E3C	C2-N3	8.49	1.48	1.37
2	5	3733	PSU	C2-N3	8.48	1.52	1.37
2	5	1913	P7G	C5-N7	8.45	1.45	1.35
4	9	814	5MU	C4-N3	-8.45	1.23	1.38
2	5	4535	PSU	C2-N3	8.44	1.52	1.37
2	5	4454	PSU	C2-N3	8.42	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4446	PSU	C2-N3	8.42	1.51	1.37
2	5	3719	PSU	C2-N3	8.38	1.51	1.37
2	5	4504	PSU	C2-N3	8.38	1.51	1.37
2	5	4297	PSU	C2-N3	8.38	1.51	1.37
4	9	1219	B8Q	C6-C5	8.37	1.52	1.33
2	5	1586	PSU	C2-N3	8.37	1.51	1.37
2	5	4632	PSU	C2-N3	8.36	1.51	1.37
2	5	1681	PSU	C2-N3	8.36	1.51	1.37
2	5	1687	PSU	C2-N3	8.33	1.51	1.37
2	5	3768	PSU	C2-N3	8.33	1.51	1.37
2	5	4640	PSU	C2-N3	8.27	1.51	1.37
2	5	3884	P7G	C5-N7	8.26	1.44	1.35
2	5	2512	PSU	C2-N3	8.23	1.51	1.37
2	5	3901	B8K	C8-N9	8.22	1.50	1.46
2	5	4375	MHG	C5-N7	8.22	1.44	1.35
2	5	3903	BGH	C8-N9	8.20	1.50	1.46
4	9	1832	6MZ	C6-N6	8.14	1.48	1.35
2	5	4407	PSU	C2-N3	8.14	1.51	1.37
2	5	1801	E7G	C5-N7	8.11	1.44	1.35
2	5	4224	6MZ	C6-N6	8.04	1.48	1.35
2	5	2301	E7G	C5-N7	7.97	1.44	1.35
4	9	668	A2M	O4'-C4'	-7.96	1.27	1.45
4	9	568	E3C	C2-N1	7.95	1.50	1.38
4	9	1248	B8N	C4-N3	-7.93	1.25	1.40
2	5	2526	7MG	C5-N7	7.90	1.44	1.35
2	5	4554	7MG	C5-N7	7.90	1.44	1.35
2	5	4375	MHG	C2-N3	7.88	1.47	1.31
2	5	4133	B8W	C2-N2	7.88	1.49	1.33
2	5	1609	7MG	C5-N7	7.87	1.44	1.35
2	5	1460	B8Q	C6-C5	7.81	1.50	1.33
2	5	2384	B8W	C2-N2	7.77	1.49	1.33
2	5	4476	B8W	C2-N2	7.75	1.49	1.33
2	5	4189	B8W	C2-N2	7.75	1.49	1.33
2	5	4533	B8W	C2-N2	7.70	1.49	1.33
4	9	484	A2M	O4'-C4'	-7.59	1.28	1.45
4	9	159	A2M	O4'-C4'	-7.54	1.28	1.45
4	9	1678	A2M	O4'-C4'	-7.47	1.28	1.45
4	9	1031	A2M	O4'-C4'	-7.42	1.28	1.45
4	9	27	A2M	O4'-C4'	-7.35	1.28	1.45
2	5	1352	P4U	C2-N3	7.31	1.51	1.36
2	5	1870	UR3	C6-C5	7.31	1.52	1.35
2	5	4601	UR3	C6-C5	7.31	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4534	UR3	C6-C5	7.29	1.52	1.35
4	9	1248	B8N	C6-N1	7.22	1.54	1.36
4	9	166	A2M	O4'-C4'	-7.22	1.28	1.45
2	5	1352	P4U	C6-C5	7.06	1.51	1.35
2	5	4339	5MC	C4-N3	7.04	1.46	1.34
4	9	1830	UR3	C2-N1	7.04	1.48	1.38
2	5	1352	P4U	O4-C4	7.00	1.43	1.35
2	5	1528	A2M	O4'-C4'	-7.00	1.29	1.45
2	5	3871	A2M	O4'-C4'	-6.97	1.29	1.45
2	5	3786	5MC	C4-N3	6.97	1.45	1.34
3	8	14	OMU	C2-N1	6.95	1.49	1.38
2	5	4087	5MU	C4-N3	-6.95	1.25	1.38
2	5	4375	MHG	C8-N7	6.92	1.52	1.45
2	5	4310	OMU	C2-N1	6.91	1.49	1.38
2	5	4451	5MC	C4-N3	6.91	1.45	1.34
2	5	4675	B8T	C4-N3	6.90	1.44	1.32
2	5	1538	A2M	O4'-C4'	-6.89	1.29	1.45
2	5	4487	B8T	C4-N3	6.88	1.44	1.32
2	5	4310	OMU	C2-N3	6.87	1.50	1.38
2	5	4624	OMU	C2-N1	6.86	1.49	1.38
2	5	4575	A2M	O4'-C4'	-6.85	1.29	1.45
2	5	4624	OMU	C2-N3	6.80	1.50	1.38
2	5	2790	B9H	C6-C5	6.80	1.48	1.33
4	9	121	OMU	C2-N1	6.80	1.49	1.38
2	5	3727	A2M	O4'-C4'	-6.78	1.29	1.45
2	5	1875	A2M	O4'-C4'	-6.77	1.29	1.45
2	5	2367	A2M	O4'-C4'	-6.76	1.29	1.45
4	9	1842	4AC	C4-N3	6.75	1.44	1.32
2	5	4375	MHG	C2-N1	6.72	1.47	1.36
2	5	4527	A2M	O4'-C4'	-6.72	1.30	1.45
2	5	3829	A2M	O4'-C4'	-6.71	1.30	1.45
2	5	4087	5MU	C6-C5	6.71	1.45	1.34
2	5	1330	A2M	O4'-C4'	-6.70	1.30	1.45
3	8	14	OMU	C2-N3	6.68	1.49	1.38
2	5	3789	A2M	O4'-C4'	-6.68	1.30	1.45
2	5	2405	A2M	O4'-C4'	-6.68	1.30	1.45
2	5	3722	A2M	O4'-C4'	-6.67	1.30	1.45
2	5	398	A2M	O4'-C4'	-6.66	1.30	1.45
4	9	116	OMU	C2-N3	6.64	1.49	1.38
2	5	1460	B8Q	C2-N3	6.63	1.46	1.35
4	9	568	E3C	C6-C5	6.62	1.48	1.33
2	5	3786	5MC	C2-N3	6.60	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1352	P4U	C5-C4	6.60	1.51	1.43
2	5	4339	5MC	C2-N3	6.59	1.49	1.36
4	9	116	OMU	C2-N1	6.59	1.49	1.38
4	9	1337	4AC	C4-N3	6.58	1.44	1.32
2	5	4451	5MC	C2-N3	6.57	1.49	1.36
2	5	3903	BGH	C2-N3	6.55	1.49	1.33
2	5	1586	PSU	C6-N1	6.55	1.47	1.36
2	5	4640	PSU	C6-N1	6.54	1.47	1.36
2	5	4504	PSU	C6-N1	6.53	1.47	1.36
2	5	3719	PSU	C6-N1	6.52	1.47	1.36
2	5	2512	PSU	C6-N1	6.51	1.47	1.36
4	9	1374	5MC	C4-N3	6.51	1.45	1.34
4	9	121	OMU	C2-N3	6.50	1.49	1.38
2	5	3733	PSU	C6-N1	6.50	1.47	1.36
2	5	3768	PSU	C6-N1	6.49	1.47	1.36
2	5	1681	PSU	C6-N1	6.48	1.47	1.36
2	5	4446	PSU	C6-N1	6.46	1.47	1.36
2	5	4198	I4U	C6-C5	6.44	1.50	1.35
2	5	4297	PSU	C6-N1	6.44	1.46	1.36
2	5	4540	OMC	C6-C5	6.43	1.50	1.35
2	5	1663	I4U	C6-C5	6.43	1.50	1.35
2	5	4535	PSU	C6-N1	6.43	1.46	1.36
2	5	3705	OMC	C6-C5	6.42	1.50	1.35
2	5	3891	OMC	C2-N3	6.41	1.49	1.36
2	5	2369	OMC	C6-C5	6.38	1.49	1.35
2	5	2426	OMC	C6-C5	6.38	1.49	1.35
2	5	4454	PSU	C6-N1	6.38	1.46	1.36
2	5	4407	PSU	C6-N1	6.37	1.46	1.36
2	5	3873	OMC	C2-N3	6.37	1.49	1.36
2	5	3913	OMC	C6-C5	6.36	1.49	1.35
2	5	2369	OMC	C2-N3	6.36	1.49	1.36
2	5	2865	OMC	C6-C5	6.36	1.49	1.35
4	9	1703	OMC	C6-C5	6.34	1.49	1.35
2	5	2426	OMC	C2-N3	6.34	1.49	1.36
2	5	2865	OMC	C2-N3	6.34	1.49	1.36
2	5	3873	OMC	C6-C5	6.34	1.49	1.35
2	5	4632	PSU	C6-N1	6.33	1.46	1.36
4	9	1219	B8Q	C2-N3	6.32	1.46	1.35
2	5	2808	OMC	C2-N3	6.32	1.49	1.36
2	5	4540	OMC	C2-N3	6.32	1.49	1.36
2	5	3891	OMC	C6-C5	6.31	1.49	1.35
2	5	4487	B8T	C2-N3	6.31	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3913	OMC	C2-N3	6.30	1.49	1.36
2	5	1687	PSU	C6-N1	6.30	1.46	1.36
2	5	2808	OMC	C6-C5	6.29	1.49	1.35
4	9	174	OMC	C6-C5	6.28	1.49	1.35
2	5	4675	B8T	C2-N3	6.28	1.49	1.36
2	5	3705	OMC	C2-N3	6.27	1.49	1.36
2	5	3884	P7G	C4-N3	6.26	1.48	1.37
2	5	1913	P7G	C4-N3	6.25	1.48	1.37
4	9	1710	OMC	C6-C5	6.23	1.49	1.35
4	9	1710	OMC	C2-N3	6.21	1.48	1.36
2	5	4300	B8H	C2-N3	6.20	1.49	1.38
4	9	174	OMC	C2-N3	6.20	1.48	1.36
2	5	1864	B8H	C2-N3	6.19	1.49	1.38
2	5	2790	B9H	C2-N1	6.18	1.47	1.38
2	5	4675	B8T	C6-C5	6.18	1.49	1.35
2	5	4487	B8T	C6-C5	6.17	1.49	1.35
2	5	3873	OMC	C4-N3	6.16	1.46	1.34
2	5	2369	OMC	C4-N3	6.16	1.46	1.34
2	5	3891	OMC	C4-N3	6.16	1.46	1.34
2	5	2808	OMC	C4-N3	6.16	1.46	1.34
4	9	1337	4AC	C6-C5	6.13	1.49	1.35
2	5	1801	E7G	C8-N7	6.09	1.51	1.45
2	5	4359	E6G	O6-C6	6.08	1.40	1.35
2	5	3913	OMC	C4-N3	6.08	1.46	1.34
2	5	2426	OMC	C4-N3	6.08	1.46	1.34
2	5	3884	P7G	C4-N9	6.07	1.44	1.35
2	5	4540	OMC	C4-N3	6.06	1.46	1.34
4	9	517	OMC	C2-N3	6.06	1.48	1.36
2	5	4554	7MG	C4-N3	6.05	1.48	1.34
2	5	237	B9B	O6-C6	6.05	1.40	1.35
4	9	1703	OMC	C2-N3	6.04	1.48	1.36
2	5	3705	OMC	C4-N3	6.03	1.46	1.34
2	5	2865	OMC	C4-N3	6.01	1.46	1.34
2	5	2758	B9B	O6-C6	6.01	1.40	1.35
2	5	1913	P7G	C8-N7	5.99	1.51	1.45
4	9	1830	UR3	C6-C5	5.98	1.48	1.35
4	9	517	OMC	C6-C5	5.97	1.48	1.35
2	5	2526	7MG	C4-N3	5.96	1.48	1.34
4	9	814	5MU	C6-C5	5.96	1.44	1.34
2	5	1609	7MG	C4-N3	5.94	1.48	1.34
2	5	1578	B9B	O6-C6	5.93	1.40	1.35
2	5	1609	7MG	C2-N3	5.92	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	1374	5MC	C2-N3	5.92	1.48	1.36
2	5	1913	P7G	C2-N1	5.91	1.47	1.33
2	5	2301	E7G	C8-N7	5.91	1.51	1.45
2	5	2426	OMC	C4-N4	5.91	1.47	1.33
2	5	1609	7MG	C4-N9	5.90	1.44	1.37
2	5	2865	OMC	C4-N4	5.90	1.47	1.33
4	9	1337	4AC	C2-N3	5.89	1.48	1.36
2	5	3884	P7G	C8-N7	5.89	1.51	1.45
2	5	2808	OMC	C4-N4	5.89	1.47	1.33
2	5	2369	OMC	C4-N4	5.88	1.47	1.33
2	5	2526	7MG	C2-N3	5.88	1.47	1.33
2	5	3913	OMC	C4-N4	5.88	1.47	1.33
2	5	4554	7MG	C2-N3	5.87	1.47	1.33
4	9	1842	4AC	C2-N3	5.86	1.48	1.36
2	5	4601	UR3	C2-N3	5.86	1.50	1.39
2	5	2301	E7G	C2-N3	5.86	1.47	1.33
2	5	3884	P7G	C2-N1	5.85	1.47	1.33
2	5	4540	OMC	C4-N4	5.85	1.47	1.33
2	5	1801	E7G	C2-N3	5.85	1.47	1.33
4	9	1806	M7A	C4-N9	5.83	1.49	1.38
2	5	3891	OMC	C4-N4	5.82	1.47	1.33
2	5	3873	OMC	C4-N4	5.82	1.47	1.33
2	5	4876	2MG	C2-N1	5.82	1.46	1.36
2	5	1913	P7G	C4-N9	5.81	1.43	1.35
2	5	2526	7MG	C4-N9	5.81	1.44	1.37
2	5	4534	UR3	C2-N3	5.81	1.50	1.39
4	9	1703	OMC	C4-N3	5.80	1.46	1.34
2	5	3705	OMC	C4-N4	5.79	1.47	1.33
4	9	1842	4AC	C6-C5	5.78	1.48	1.35
2	5	3903	BGH	C4-N3	5.76	1.48	1.34
2	5	729	2MG	C2-N1	5.76	1.45	1.36
2	5	237	B9B	C2-N2	5.75	1.45	1.33
2	5	3901	B8K	C2-N3	5.74	1.47	1.33
2	5	1578	B9B	C2-N2	5.74	1.45	1.33
2	5	4694	B8K	C2-N3	5.73	1.47	1.33
2	5	1521	2MG	C2-N1	5.72	1.45	1.36
2	5	4375	MHG	C2-N2	5.72	1.46	1.33
2	5	4568	M7A	C4-N9	5.72	1.48	1.38
2	5	4694	B8K	C4-N3	5.71	1.47	1.34
4	9	1710	OMC	C4-N3	5.71	1.46	1.34
2	5	4310	OMU	C6-C5	5.71	1.48	1.35
2	5	4359	E6G	C2-N2	5.71	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4554	7MG	C4-N9	5.70	1.44	1.37
2	5	3901	B8K	C4-N3	5.70	1.47	1.34
2	5	1870	UR3	C2-N3	5.70	1.50	1.39
2	5	2758	B9B	C2-N2	5.70	1.45	1.33
4	9	121	OMU	C6-C5	5.69	1.48	1.35
4	9	174	OMC	C4-N3	5.69	1.45	1.34
2	5	1663	I4U	C2-N3	5.68	1.47	1.36
2	5	1801	E7G	C4-N9	5.67	1.44	1.37
2	5	4624	OMU	C6-C5	5.67	1.48	1.35
2	5	3903	BGH	C4-N9	5.65	1.44	1.37
3	8	14	OMU	C6-C5	5.65	1.48	1.35
2	5	4198	I4U	C2-N3	5.65	1.47	1.36
4	9	517	OMC	C4-N3	5.61	1.45	1.34
2	5	1801	E7G	C4-N3	5.59	1.47	1.34
2	5	2301	E7G	C4-N3	5.57	1.47	1.34
2	5	729	2MG	C4-N3	5.52	1.50	1.37
2	5	1521	2MG	C2-N2	5.49	1.45	1.33
2	5	2301	E7G	C4-N9	5.48	1.44	1.37
2	5	4375	MHG	C4-N3	5.48	1.47	1.34
2	5	729	2MG	C2-N2	5.45	1.45	1.33
2	5	1629	OMG	C2-N3	5.45	1.46	1.33
2	5	2428	OMG	C2-N3	5.42	1.46	1.33
2	5	1521	2MG	C4-N3	5.39	1.50	1.37
2	5	4374	OMG	C2-N3	5.38	1.46	1.33
2	5	4874	OMG	C2-N3	5.38	1.46	1.33
2	5	3796	OMG	C2-N3	5.35	1.46	1.33
2	5	4627	OMG	C2-N3	5.35	1.46	1.33
2	5	4200	OMG	C2-N3	5.35	1.46	1.33
2	5	2777	OMG	C2-N3	5.34	1.46	1.33
4	9	644	OMG	C2-N3	5.32	1.46	1.33
4	9	116	OMU	C6-C5	5.31	1.47	1.35
2	5	1526	OMG	C2-N3	5.30	1.46	1.33
2	5	4498	OMG	C2-N3	5.29	1.46	1.33
4	9	1248	B8N	C2-N1	5.29	1.55	1.39
2	5	4641	OMG	C2-N3	5.28	1.46	1.33
2	5	2054	OMG	C2-N3	5.28	1.46	1.33
2	5	1887	OMG	C2-N3	5.26	1.46	1.33
2	5	1320	OMG	C2-N3	5.23	1.45	1.33
2	5	4876	2MG	C2-N2	5.23	1.45	1.33
2	5	4375	MHG	C4-N9	5.23	1.43	1.37
2	5	373	OMG	C2-N3	5.22	1.45	1.33
4	9	509	OMG	C2-N3	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2368	OMG	C2-N3	5.20	1.45	1.33
2	5	4694	B8K	C4-N9	5.20	1.43	1.37
2	5	4876	2MG	C4-N3	5.18	1.49	1.37
2	5	4451	5MC	C6-N1	5.16	1.46	1.38
2	5	2426	OMC	C2-N1	5.13	1.51	1.40
2	5	4339	5MC	C4-N4	5.09	1.47	1.34
2	5	3901	B8K	C4-N9	5.08	1.43	1.37
2	5	3786	5MC	C4-N4	5.06	1.47	1.34
2	5	4451	5MC	C4-N4	5.06	1.47	1.34
2	5	3913	OMC	C2-N1	5.05	1.50	1.40
2	5	3873	OMC	C2-N1	5.05	1.50	1.40
2	5	3891	OMC	C2-N1	5.04	1.50	1.40
2	5	3786	5MC	C6-N1	5.04	1.46	1.38
2	5	1629	OMG	C4-N3	5.02	1.49	1.37
2	5	4339	5MC	C6-N1	5.02	1.46	1.38
2	5	2428	OMG	C4-N3	5.01	1.49	1.37
2	5	4540	OMC	C2-N1	5.01	1.50	1.40
2	5	2865	OMC	C2-N1	4.98	1.50	1.40
2	5	2808	OMC	C2-N1	4.96	1.50	1.40
2	5	1887	OMG	C4-N3	4.95	1.49	1.37
2	5	3903	BGH	O4'-C1'	-4.94	1.30	1.42
2	5	3705	OMC	C2-N1	4.94	1.50	1.40
2	5	2777	OMG	C4-N3	4.93	1.49	1.37
2	5	2368	OMG	C4-N3	4.93	1.49	1.37
2	5	4374	OMG	C4-N3	4.92	1.49	1.37
4	9	1830	UR3	C2-N3	4.92	1.48	1.39
2	5	3884	P7G	C2-N2	4.92	1.45	1.34
2	5	4200	OMG	C4-N3	4.91	1.49	1.37
2	5	4641	OMG	C4-N3	4.91	1.49	1.37
2	5	2526	7MG	C2-N2	4.91	1.45	1.34
2	5	1352	P4U	C2-N1	4.91	1.50	1.40
2	5	4498	OMG	C4-N3	4.91	1.49	1.37
2	5	4874	OMG	C4-N3	4.90	1.49	1.37
2	5	3796	OMG	C4-N3	4.90	1.49	1.37
2	5	1526	OMG	C4-N3	4.90	1.49	1.37
2	5	2369	OMC	C2-N1	4.90	1.50	1.40
2	5	1913	P7G	C2-N2	4.90	1.45	1.34
2	5	2054	OMG	C4-N3	4.90	1.49	1.37
2	5	4694	B8K	C2-N2	4.88	1.45	1.34
2	5	1320	OMG	C4-N3	4.88	1.49	1.37
4	9	683	OMG	C2-N3	4.88	1.45	1.33
2	5	373	OMG	C4-N3	4.87	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4554	7MG	C2-N2	4.87	1.45	1.34
2	5	4627	OMG	C4-N3	4.86	1.49	1.37
4	9	1374	5MC	C2-N1	4.86	1.50	1.40
4	9	1337	4AC	C7-N4	4.85	1.46	1.37
2	5	1609	7MG	C2-N2	4.85	1.45	1.34
2	5	3901	B8K	C2-N2	4.83	1.45	1.34
2	5	1326	1MA	C2-N1	4.80	1.44	1.35
4	9	1374	5MC	C4-N4	4.77	1.46	1.34
2	5	4874	OMG	C2-N2	4.77	1.45	1.34
4	9	509	OMG	C4-N3	4.75	1.48	1.37
2	5	2428	OMG	C2-N2	4.75	1.45	1.34
2	5	2777	OMG	C2-N2	4.74	1.45	1.34
4	9	1248	B8N	C6-C5	4.73	1.41	1.34
2	5	4568	M7A	C6-N6	4.72	1.46	1.34
2	5	1887	OMG	C2-N2	4.72	1.45	1.34
2	5	4419	1MA	C2-N1	4.71	1.44	1.35
2	5	1801	E7G	C2-N2	4.71	1.45	1.34
2	5	4200	OMG	C2-N2	4.71	1.45	1.34
2	5	1320	OMG	C2-N2	4.70	1.45	1.34
4	9	683	OMG	C2-N2	4.70	1.45	1.34
2	5	4487	B8T	C4-N4	4.70	1.45	1.35
4	9	1842	4AC	C7-N4	4.69	1.45	1.37
2	5	1629	OMG	C2-N2	4.69	1.45	1.34
2	5	4374	OMG	C2-N2	4.68	1.45	1.34
2	5	2368	OMG	C2-N2	4.66	1.45	1.34
2	5	2301	E7G	C2-N2	4.66	1.45	1.34
2	5	4498	OMG	C2-N2	4.65	1.45	1.34
2	5	2054	OMG	C2-N2	4.65	1.45	1.34
2	5	3796	OMG	C2-N2	4.65	1.45	1.34
2	5	3903	BGH	C5-C6	4.65	1.55	1.43
4	9	1031	A2M	O3'-C3'	-4.64	1.32	1.43
2	5	4297	PSU	C4-N3	4.64	1.47	1.38
2	5	1526	OMG	C2-N2	4.63	1.45	1.34
4	9	683	OMG	C4-N3	4.63	1.48	1.37
4	9	166	A2M	O3'-C3'	-4.63	1.32	1.43
2	5	4675	B8T	C4-N4	4.63	1.45	1.35
2	5	4627	OMG	C2-N2	4.61	1.45	1.34
2	5	3768	PSU	C4-N3	4.61	1.47	1.38
2	5	4641	OMG	C2-N2	4.61	1.45	1.34
4	9	27	A2M	O3'-C3'	-4.60	1.32	1.43
2	5	373	OMG	C2-N2	4.60	1.45	1.34
4	9	159	A2M	O3'-C3'	-4.60	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4535	PSU	C4-N3	4.57	1.47	1.38
2	5	4675	B8T	C2-N1	4.56	1.49	1.40
4	9	1678	A2M	C6-N6	4.56	1.50	1.34
2	5	1586	PSU	C4-N3	4.55	1.47	1.38
2	5	4446	PSU	C4-N3	4.55	1.47	1.38
4	9	644	OMG	C4-N3	4.55	1.48	1.37
2	5	4504	PSU	C4-N3	4.55	1.47	1.38
4	9	166	A2M	C6-N6	4.54	1.50	1.34
4	9	1219	B8Q	C2-N1	4.54	1.45	1.38
2	5	3733	PSU	C4-N3	4.54	1.47	1.38
4	9	668	A2M	C6-N6	4.53	1.50	1.34
4	9	27	A2M	C6-N6	4.52	1.50	1.34
4	9	1031	A2M	C6-N6	4.52	1.50	1.34
4	9	159	A2M	C6-N6	4.52	1.50	1.34
2	5	1681	PSU	C4-N3	4.52	1.47	1.38
4	9	1337	4AC	C4-N4	4.52	1.46	1.39
2	5	3786	5MC	C2-N1	4.50	1.49	1.40
2	5	4487	B8T	C2-N1	4.50	1.49	1.40
2	5	4339	5MC	C2-N1	4.50	1.49	1.40
2	5	2512	PSU	C4-N3	4.49	1.47	1.38
2	5	3719	PSU	C4-N3	4.49	1.47	1.38
4	9	1806	M7A	C6-N6	4.48	1.45	1.34
2	5	4407	PSU	C4-N3	4.48	1.47	1.38
4	9	668	A2M	O3'-C3'	-4.48	1.32	1.43
2	5	4454	PSU	C4-N3	4.48	1.47	1.38
2	5	1663	I4U	C2-N1	4.48	1.49	1.40
2	5	1687	PSU	C4-N3	4.48	1.47	1.38
4	9	484	A2M	C6-N6	4.47	1.50	1.34
4	9	1374	5MC	C6-N1	4.46	1.45	1.38
4	9	1678	A2M	O3'-C3'	-4.46	1.32	1.43
2	5	4451	5MC	C2-N1	4.45	1.49	1.40
2	5	4632	PSU	C4-N3	4.44	1.47	1.38
4	9	644	OMG	C2-N2	4.44	1.44	1.34
4	9	509	OMG	C2-N2	4.42	1.44	1.34
2	5	4640	PSU	C4-N3	4.42	1.47	1.38
2	5	1460	B8Q	C2-N1	4.36	1.44	1.38
2	5	3903	BGH	C6-N1	4.34	1.46	1.38
2	5	4198	I4U	C2-N1	4.29	1.49	1.40
2	5	4198	I4U	O4-C4	4.24	1.43	1.35
2	5	1663	I4U	O4-C4	4.23	1.43	1.35
4	9	484	A2M	O3'-C3'	-4.19	1.33	1.43
2	5	1609	7MG	C2-N1	4.18	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4554	7MG	C2-N1	4.15	1.47	1.37
4	9	1842	4AC	C4-N4	4.14	1.45	1.39
2	5	2526	7MG	C2-N1	4.14	1.47	1.37
2	5	4310	OMU	C4-N3	4.12	1.45	1.38
2	5	1521	2MG	C6-N1	4.11	1.44	1.37
2	5	4624	OMU	C4-N3	4.06	1.45	1.38
2	5	4632	PSU	C1'-C5	-4.04	1.41	1.50
2	5	3727	A2M	C6-N6	4.03	1.48	1.34
4	9	1806	M7A	C5-N7	4.01	1.49	1.39
2	5	4454	PSU	C1'-C5	-4.01	1.41	1.50
2	5	3901	B8K	C5-N7	4.00	1.46	1.39
2	5	4575	A2M	C6-N6	4.00	1.48	1.34
2	5	1586	PSU	C1'-C5	-3.99	1.41	1.50
2	5	3722	A2M	C6-N6	3.99	1.48	1.34
2	5	398	A2M	C6-N6	3.99	1.48	1.34
2	5	1538	A2M	C6-N6	3.99	1.48	1.34
2	5	3733	PSU	C1'-C5	-3.99	1.41	1.50
2	5	2405	A2M	C6-N6	3.98	1.48	1.34
2	5	4535	PSU	C1'-C5	-3.98	1.41	1.50
2	5	3871	A2M	C6-N6	3.97	1.48	1.34
2	5	2512	PSU	C1'-C5	-3.97	1.41	1.50
2	5	4640	PSU	C1'-C5	-3.97	1.41	1.50
2	5	2367	A2M	C6-N6	3.97	1.48	1.34
2	5	4504	PSU	C1'-C5	-3.97	1.41	1.50
3	8	14	OMU	C4-N3	3.96	1.45	1.38
2	5	1528	A2M	C6-N6	3.96	1.48	1.34
2	5	3884	P7G	C2-N3	3.96	1.47	1.37
2	5	4694	B8K	C5-N7	3.96	1.46	1.39
2	5	1875	A2M	C6-N6	3.95	1.48	1.34
2	5	3829	A2M	C6-N6	3.95	1.48	1.34
2	5	2865	OMC	C6-N1	3.95	1.47	1.38
2	5	1681	PSU	C1'-C5	-3.95	1.41	1.50
4	9	174	OMC	C4-N4	3.95	1.43	1.33
2	5	1687	PSU	C1'-C5	-3.94	1.41	1.50
2	5	4527	A2M	C6-N6	3.94	1.48	1.34
2	5	4297	PSU	C1'-C5	-3.94	1.41	1.50
2	5	2369	OMC	C6-N1	3.93	1.47	1.38
2	5	2808	OMC	C6-N1	3.93	1.47	1.38
2	5	4876	2MG	C5-C6	3.93	1.55	1.47
2	5	3719	PSU	C1'-C5	-3.92	1.41	1.50
2	5	4540	OMC	C6-N1	3.91	1.47	1.38
2	5	4446	PSU	C1'-C5	-3.91	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4694	B8K	C5-C6	3.90	1.53	1.43
2	5	4876	2MG	C6-N1	3.90	1.43	1.37
2	5	3891	OMC	C6-N1	3.90	1.47	1.38
2	5	1609	7MG	C5-C6	3.90	1.53	1.43
2	5	3913	OMC	C6-N1	3.90	1.47	1.38
2	5	1330	A2M	C6-N6	3.90	1.48	1.34
2	5	3903	BGH	C2-N1	3.90	1.47	1.37
4	9	1710	OMC	C4-N4	3.88	1.43	1.33
2	5	3903	BGH	O2'-C2'	-3.88	1.32	1.42
4	9	1703	OMC	C4-N4	3.88	1.43	1.33
2	5	2426	OMC	C6-N1	3.87	1.47	1.38
2	5	1913	P7G	C2-N3	3.87	1.47	1.37
2	5	1320	OMG	C6-N1	3.87	1.43	1.37
2	5	3901	B8K	C5-C6	3.87	1.53	1.43
2	5	1521	2MG	C5-C6	3.86	1.55	1.47
2	5	3873	OMC	C6-N1	3.86	1.47	1.38
4	9	1337	4AC	C2-N1	3.85	1.48	1.40
4	9	1710	OMC	C2-N1	3.84	1.48	1.40
2	5	3705	OMC	C6-N1	3.84	1.47	1.38
2	5	4554	7MG	C5-C6	3.83	1.53	1.43
2	5	3789	A2M	C6-N6	3.83	1.48	1.34
2	5	2777	OMG	C6-N1	3.82	1.43	1.37
2	5	2526	7MG	C5-C6	3.82	1.53	1.43
2	5	4568	M7A	C5-N7	3.81	1.48	1.39
2	5	4198	I4U	C5-C4	3.80	1.48	1.43
2	5	2368	OMG	C6-N1	3.79	1.43	1.37
4	9	116	OMU	C4-N3	3.79	1.45	1.38
2	5	4627	OMG	C6-N1	3.79	1.43	1.37
2	5	4874	OMG	C6-N1	3.78	1.43	1.37
2	5	729	2MG	C5-C6	3.77	1.55	1.47
4	9	1703	OMC	C2-N1	3.77	1.48	1.40
4	9	1842	4AC	C2-N1	3.77	1.48	1.40
4	9	517	OMC	C4-N4	3.77	1.42	1.33
2	5	729	2MG	C6-N1	3.77	1.43	1.37
4	9	1337	4AC	C5-C4	3.77	1.48	1.40
2	5	4675	B8T	C5-C4	3.77	1.48	1.40
4	9	174	OMC	C2-N1	3.76	1.48	1.40
2	5	1526	OMG	C6-N1	3.76	1.43	1.37
2	5	3796	OMG	C6-N1	3.76	1.43	1.37
2	5	4641	OMG	C6-N1	3.76	1.43	1.37
2	5	1887	OMG	C6-N1	3.75	1.43	1.37
2	5	4487	B8T	C5-C4	3.74	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	121	OMU	C4-N3	3.73	1.45	1.38
2	5	2301	E7G	C2-N1	3.73	1.46	1.37
2	5	1663	I4U	C5-C4	3.73	1.48	1.43
2	5	1801	E7G	C2-N1	3.72	1.46	1.37
2	5	4374	OMG	C6-N1	3.71	1.43	1.37
2	5	2428	OMG	C6-N1	3.71	1.43	1.37
2	5	4200	OMG	C6-N1	3.70	1.43	1.37
2	5	2054	OMG	C6-N1	3.70	1.43	1.37
2	5	4498	OMG	C6-N1	3.70	1.43	1.37
2	5	1629	OMG	C6-N1	3.69	1.43	1.37
2	5	3884	P7G	C5-C4	3.65	1.44	1.37
2	5	373	OMG	C6-N1	3.64	1.43	1.37
2	5	3901	B8K	C2-N1	3.63	1.46	1.37
2	5	3903	BGH	C5-N7	3.63	1.45	1.39
2	5	4407	PSU	C1'-C5	-3.62	1.41	1.50
4	9	174	OMC	C6-N1	3.61	1.46	1.38
2	5	1913	P7G	C6-N1	3.60	1.44	1.38
2	5	1326	1MA	C4-N3	3.60	1.48	1.37
2	5	4419	1MA	C4-N3	3.59	1.48	1.37
2	5	4694	B8K	C2-N1	3.58	1.46	1.37
4	9	1842	4AC	C5-C4	3.57	1.48	1.40
2	5	3768	PSU	C1'-C5	-3.57	1.42	1.50
2	5	2526	7MG	C6-N1	3.52	1.45	1.38
2	5	4375	MHG	C6-N1	3.51	1.45	1.38
2	5	3884	P7G	C6-N1	3.51	1.44	1.38
2	5	1801	E7G	C5-C6	3.51	1.52	1.43
2	5	1609	7MG	O6-C6	-3.49	1.16	1.23
2	5	4375	MHG	C5-C6	3.48	1.52	1.43
4	9	517	OMC	C6-N1	3.48	1.46	1.38
4	9	1710	OMC	C6-N1	3.47	1.46	1.38
2	5	1913	P7G	C5-C4	3.46	1.44	1.37
2	5	4554	7MG	O6-C6	-3.45	1.17	1.23
2	5	2301	E7G	C5-C6	3.45	1.52	1.43
2	5	1609	7MG	C6-N1	3.44	1.45	1.38
4	9	683	OMG	C6-N1	3.44	1.43	1.37
2	5	2526	7MG	O6-C6	-3.44	1.17	1.23
4	9	1678	A2M	O2'-C2'	3.43	1.51	1.42
4	9	484	A2M	O2'-C2'	3.43	1.51	1.42
4	9	517	OMC	C2-N1	3.41	1.47	1.40
4	9	644	OMG	C6-N1	3.36	1.42	1.37
4	9	166	A2M	O2'-C2'	3.36	1.51	1.42
4	9	668	A2M	O2'-C2'	3.34	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4554	7MG	C6-N1	3.34	1.45	1.38
4	9	1243	PSU	C6-C5	3.33	1.39	1.35
2	5	4487	B8T	C6-N1	3.31	1.46	1.38
2	5	2301	E7G	C6-N1	3.31	1.45	1.38
4	9	509	OMG	C6-N1	3.30	1.42	1.37
4	9	159	A2M	O2'-C2'	3.29	1.51	1.42
4	9	1703	OMC	C6-N1	3.29	1.45	1.38
4	9	1678	A2M	C2-N3	3.29	1.37	1.32
4	9	27	A2M	C2-N3	3.27	1.37	1.32
2	5	1801	E7G	C6-N1	3.26	1.44	1.38
2	5	1526	OMG	C5-C6	3.26	1.54	1.47
2	5	3901	B8K	C6-N1	3.25	1.44	1.38
4	9	668	A2M	C5-C4	-3.23	1.32	1.40
2	5	4675	B8T	C6-N1	3.23	1.45	1.38
4	9	166	A2M	C2-N3	3.22	1.37	1.32
2	5	4694	B8K	C71-N7	3.21	1.46	1.39
4	9	159	A2M	C2-N3	3.21	1.37	1.32
2	5	4694	B8K	C6-N1	3.21	1.44	1.38
2	5	3913	OMC	O2-C2	-3.20	1.17	1.23
2	5	4407	PSU	C4-C5	3.19	1.53	1.44
2	5	1352	P4U	C6-N1	3.19	1.45	1.38
2	5	4641	OMG	C5-C6	3.18	1.53	1.47
2	5	3705	OMC	O2-C2	-3.18	1.17	1.23
4	9	1031	A2M	O2'-C2'	3.18	1.50	1.42
2	5	2777	OMG	C5-C6	3.18	1.53	1.47
2	5	3768	PSU	C4-C5	3.17	1.53	1.44
2	5	2368	OMG	C5-C6	3.17	1.53	1.47
2	5	4627	OMG	C5-C6	3.16	1.53	1.47
4	9	1081	PSU	C6-C5	3.16	1.39	1.35
2	5	4498	OMG	C5-C6	3.16	1.53	1.47
4	9	1703	OMC	O2-C2	-3.15	1.17	1.23
2	5	2426	OMC	O2-C2	-3.15	1.17	1.23
4	9	823	PSU	C6-C5	3.14	1.39	1.35
2	5	4198	I4U	C6-N1	3.14	1.45	1.38
4	9	568	E3C	C4-N3	3.13	1.53	1.48
2	5	2865	OMC	O2-C2	-3.13	1.17	1.23
2	5	2369	OMC	O2-C2	-3.12	1.17	1.23
2	5	3796	OMG	C5-C6	3.12	1.53	1.47
2	5	4200	OMG	C5-C6	3.11	1.53	1.47
2	5	4540	OMC	O2-C2	-3.11	1.17	1.23
2	5	1320	OMG	C5-C6	3.11	1.53	1.47
2	5	3873	OMC	O2-C2	-3.11	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2808	OMC	O2-C2	-3.10	1.18	1.23
4	9	683	OMG	C5-C4	-3.10	1.35	1.43
2	5	4874	OMG	C5-C6	3.09	1.53	1.47
2	5	1663	I4U	C6-N1	3.09	1.45	1.38
2	5	3891	OMC	O2-C2	-3.08	1.18	1.23
2	5	373	OMG	C5-C6	3.08	1.53	1.47
2	5	1913	P7G	O6-C6	-3.08	1.18	1.23
2	5	3903	BGH	C2-N2	3.08	1.41	1.34
2	5	3901	B8K	C71-N7	3.08	1.46	1.39
4	9	1374	5MC	O2-C2	-3.07	1.18	1.23
4	9	668	A2M	C2-N3	3.07	1.37	1.32
2	5	4374	OMG	C5-C6	3.07	1.53	1.47
2	5	2054	OMG	C5-C6	3.07	1.53	1.47
4	9	1337	4AC	C6-N1	3.06	1.45	1.38
4	9	484	A2M	C2-N3	3.06	1.37	1.32
2	5	3789	A2M	C5-C4	-3.06	1.32	1.40
2	5	1629	OMG	C5-C6	3.06	1.53	1.47
4	9	1842	4AC	C6-N1	3.05	1.45	1.38
2	5	4601	UR3	O4-C4	-3.05	1.17	1.23
2	5	1870	UR3	O4-C4	-3.05	1.17	1.23
2	5	2428	OMG	C5-C6	3.04	1.53	1.47
2	5	4534	UR3	O4-C4	-3.04	1.17	1.23
2	5	1687	PSU	C4-C5	3.03	1.52	1.44
4	9	568	E3C	C6-N1	3.03	1.45	1.38
2	5	1875	A2M	C5-C4	-3.02	1.32	1.40
4	9	119	PSU	C6-C5	3.01	1.38	1.35
4	9	116	OMU	O4-C4	-3.01	1.18	1.24
4	9	121	OMU	O4-C4	-3.00	1.18	1.24
2	5	4535	PSU	C4-C5	3.00	1.52	1.44
3	8	14	OMU	O4-C4	-3.00	1.18	1.24
2	5	3884	P7G	O6-C6	-3.00	1.19	1.23
2	5	4446	PSU	C4-C5	3.00	1.52	1.44
2	5	1681	PSU	C4-C5	2.99	1.52	1.44
2	5	1330	A2M	C5-C4	-2.99	1.33	1.40
2	5	3829	A2M	C5-C4	-2.99	1.33	1.40
2	5	2367	A2M	C5-C4	-2.99	1.33	1.40
2	5	4694	B8K	O6-C6	-2.98	1.17	1.23
4	9	159	A2M	C5-C4	-2.98	1.33	1.40
2	5	2512	PSU	C4-C5	2.97	1.52	1.44
2	5	1538	A2M	C5-C4	-2.97	1.33	1.40
4	9	1710	OMC	O2-C2	-2.96	1.18	1.23
2	5	3871	A2M	C5-C4	-2.96	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4504	PSU	C4-C5	2.95	1.52	1.44
2	5	1528	A2M	C5-C4	-2.95	1.33	1.40
4	9	1031	A2M	C5-C4	-2.95	1.33	1.40
2	5	4575	A2M	C5-C4	-2.95	1.33	1.40
2	5	1887	OMG	C5-C6	2.95	1.53	1.47
2	5	1586	PSU	C4-C5	2.95	1.52	1.44
4	9	1031	A2M	C2-N3	2.94	1.36	1.32
4	9	517	OMC	O2-C2	-2.94	1.18	1.23
4	9	27	A2M	O2'-C2'	2.94	1.50	1.42
4	9	27	A2M	C5-C4	-2.94	1.33	1.40
2	5	4310	OMU	O4-C4	-2.93	1.18	1.24
2	5	3722	A2M	C5-C4	-2.93	1.33	1.40
2	5	4624	OMU	O4-C4	-2.93	1.18	1.24
2	5	3719	PSU	C4-C5	2.93	1.52	1.44
2	5	4632	PSU	C4-C5	2.93	1.52	1.44
2	5	4454	PSU	C4-C5	2.93	1.52	1.44
3	8	14	OMU	C6-N1	2.92	1.45	1.38
2	5	3727	A2M	C5-C4	-2.92	1.33	1.40
2	5	4297	PSU	C4-C5	2.92	1.52	1.44
4	9	644	OMG	C5-C4	-2.92	1.35	1.43
2	5	2405	A2M	C5-C4	-2.92	1.33	1.40
2	5	398	A2M	C5-C4	-2.91	1.33	1.40
2	5	3733	PSU	C4-C5	2.90	1.52	1.44
2	5	4527	A2M	C5-C4	-2.89	1.33	1.40
2	5	3901	B8K	O6-C6	-2.89	1.18	1.23
2	5	4640	PSU	C4-C5	2.89	1.52	1.44
4	9	822	PSU	C6-C5	2.87	1.38	1.35
2	5	3903	BGH	O3'-C3'	2.87	1.49	1.43
4	9	1842	4AC	O2-C2	-2.87	1.18	1.23
2	5	3705	OMC	C5-C4	2.86	1.49	1.42
4	9	174	OMC	O2-C2	-2.85	1.18	1.23
2	5	4310	OMU	C6-N1	2.84	1.44	1.38
4	9	1337	4AC	O2-C2	-2.83	1.18	1.23
2	5	3913	OMC	C5-C4	2.83	1.49	1.42
2	5	4624	OMU	C6-N1	2.82	1.44	1.38
2	5	398	A2M	C2-N3	2.81	1.36	1.32
2	5	1330	A2M	O2'-C2'	2.81	1.49	1.42
2	5	3727	A2M	O2'-C2'	2.81	1.49	1.42
2	5	3789	A2M	C2-N3	2.81	1.36	1.32
2	5	4527	A2M	O2'-C2'	2.81	1.49	1.42
2	5	4575	A2M	O2'-C2'	2.81	1.49	1.42
2	5	398	A2M	O2'-C2'	2.81	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1538	A2M	O2'-C2'	2.80	1.49	1.42
2	5	3722	A2M	O2'-C2'	2.79	1.49	1.42
2	5	4498	OMG	C2-N1	2.79	1.44	1.37
2	5	2368	OMG	C2-N1	2.79	1.44	1.37
2	5	4189	B8W	C5-C4	-2.79	1.33	1.40
2	5	3829	A2M	O2'-C2'	2.79	1.49	1.42
2	5	1528	A2M	O2'-C2'	2.79	1.49	1.42
4	9	121	OMU	O2-C2	-2.79	1.18	1.23
2	5	1320	OMG	C2-N1	2.79	1.44	1.37
2	5	3891	OMC	C5-C4	2.78	1.49	1.42
2	5	1875	A2M	O2'-C2'	2.78	1.49	1.42
4	9	484	A2M	C5-C4	-2.78	1.33	1.40
4	9	1832	6MZ	C5-C4	-2.78	1.33	1.40
2	5	2865	OMC	C5-C4	2.78	1.49	1.42
2	5	2369	OMC	C5-C4	2.78	1.49	1.42
2	5	2405	A2M	O2'-C2'	2.78	1.49	1.42
4	9	1830	UR3	C6-N1	2.78	1.44	1.38
2	5	373	OMG	C5-C4	-2.77	1.36	1.43
2	5	2808	OMC	C5-C4	2.77	1.49	1.42
2	5	2777	OMG	C2-N1	2.77	1.44	1.37
2	5	3796	OMG	C2-N1	2.77	1.44	1.37
2	5	4874	OMG	C2-N1	2.77	1.44	1.37
2	5	2367	A2M	O2'-C2'	2.77	1.49	1.42
2	5	1460	B8Q	O2-C2	-2.77	1.17	1.22
2	5	4200	OMG	C2-N1	2.77	1.44	1.37
2	5	3786	5MC	O2-C2	-2.77	1.18	1.23
2	5	3727	A2M	C2-N3	2.76	1.36	1.32
2	5	4359	E6G	C5-C4	-2.76	1.33	1.40
4	9	814	5MU	O4-C4	-2.76	1.18	1.23
2	5	3873	OMC	C5-C4	2.76	1.49	1.42
2	5	3789	A2M	O2'-C2'	2.75	1.49	1.42
2	5	2367	A2M	C2-N3	2.74	1.36	1.32
2	5	1578	B9B	C5-C4	-2.74	1.33	1.40
4	9	683	OMG	C5-C6	2.74	1.53	1.47
2	5	4451	5MC	O2-C2	-2.74	1.18	1.23
4	9	1219	B8Q	O2-C2	-2.74	1.17	1.22
2	5	2426	OMC	C5-C4	2.74	1.49	1.42
2	5	4527	A2M	C2-N3	2.73	1.36	1.32
2	5	4627	OMG	C2-N1	2.73	1.44	1.37
4	9	166	A2M	C5-C4	-2.73	1.33	1.40
2	5	1681	PSU	O4'-C1'	-2.73	1.40	1.43
2	5	4339	5MC	O2-C2	-2.73	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1887	OMG	C2-N1	2.73	1.44	1.37
2	5	237	B9B	C5-C4	-2.73	1.33	1.40
2	5	2054	OMG	C2-N1	2.73	1.44	1.37
2	5	1320	OMG	C5-C4	-2.72	1.36	1.43
2	5	4575	A2M	C2-N3	2.72	1.36	1.32
2	5	1538	A2M	C2-N3	2.72	1.36	1.32
2	5	1629	OMG	C2-N1	2.72	1.44	1.37
2	5	373	OMG	C2-N1	2.71	1.44	1.37
2	5	1526	OMG	C2-N1	2.71	1.44	1.37
2	5	3727	A2M	O3'-C3'	-2.71	1.36	1.43
2	5	3871	A2M	O2'-C2'	2.71	1.49	1.42
2	5	3722	A2M	C2-N3	2.71	1.36	1.32
2	5	4641	OMG	C2-N1	2.71	1.44	1.37
2	5	4540	OMC	C5-C4	2.71	1.49	1.42
2	5	2054	OMG	C5-C4	-2.70	1.36	1.43
2	5	3829	A2M	C2-N3	2.70	1.36	1.32
2	5	1875	A2M	O3'-C3'	-2.69	1.36	1.43
2	5	3903	BGH	O6-C6	-2.69	1.18	1.23
2	5	2428	OMG	C2-N1	2.69	1.44	1.37
2	5	4374	OMG	C2-N1	2.69	1.44	1.37
2	5	3871	A2M	C2-N3	2.69	1.36	1.32
4	9	509	OMG	C5-C6	2.69	1.52	1.47
2	5	2368	OMG	C5-C4	-2.69	1.36	1.43
2	5	1330	A2M	O3'-C3'	-2.69	1.36	1.43
2	5	1887	OMG	C5-C4	-2.69	1.36	1.43
2	5	2758	B9B	C5-C4	-2.68	1.33	1.40
2	5	2777	OMG	C5-C4	-2.68	1.36	1.43
2	5	3829	A2M	O3'-C3'	-2.67	1.36	1.43
2	5	1875	A2M	C2-N3	2.67	1.36	1.32
4	9	509	OMG	C5-C4	-2.67	1.36	1.43
2	5	2405	A2M	C2-N3	2.67	1.36	1.32
4	9	644	OMG	C5-C6	2.66	1.52	1.47
2	5	1526	OMG	C5-C4	-2.66	1.36	1.43
4	9	121	OMU	C6-N1	2.65	1.44	1.38
2	5	4641	OMG	C5-C4	-2.65	1.36	1.43
2	5	398	A2M	O3'-C3'	-2.65	1.36	1.43
2	5	2405	A2M	O3'-C3'	-2.65	1.36	1.43
2	5	1870	UR3	C6-N1	2.65	1.44	1.38
2	5	4133	B8W	C5-C4	-2.65	1.33	1.40
2	5	4476	B8W	C5-C4	-2.64	1.33	1.40
2	5	4575	A2M	O3'-C3'	-2.64	1.36	1.43
2	5	2384	B8W	C5-C4	-2.64	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4627	OMG	C5-C4	-2.64	1.36	1.43
2	5	4601	UR3	C6-N1	2.63	1.44	1.38
2	5	1538	A2M	O3'-C3'	-2.63	1.36	1.43
2	5	1528	A2M	C2-N3	2.63	1.36	1.32
4	9	1678	A2M	C5-C4	-2.63	1.34	1.40
2	5	4200	OMG	C5-C4	-2.62	1.36	1.43
2	5	4374	OMG	C5-C4	-2.61	1.36	1.43
2	5	4675	B8T	O2-C2	-2.61	1.18	1.23
2	5	4874	OMG	C5-C4	-2.61	1.36	1.43
2	5	1460	B8Q	C4-N3	-2.60	1.44	1.48
2	5	1801	E7G	O6-C6	-2.60	1.18	1.23
2	5	3871	A2M	O3'-C3'	-2.60	1.36	1.43
2	5	3796	OMG	C5-C4	-2.60	1.36	1.43
2	5	4487	B8T	O2-C2	-2.60	1.18	1.23
2	5	3722	A2M	O3'-C3'	-2.59	1.36	1.43
2	5	2367	A2M	O3'-C3'	-2.59	1.36	1.43
2	5	1330	A2M	C2-N3	2.59	1.36	1.32
2	5	4527	A2M	O3'-C3'	-2.58	1.36	1.43
2	5	1528	A2M	O3'-C3'	-2.57	1.36	1.43
2	5	4198	I4U	O4-C41	-2.56	1.41	1.47
2	5	2301	E7G	O6-C6	-2.56	1.18	1.23
2	5	4534	UR3	C6-N1	2.55	1.44	1.38
2	5	4498	OMG	C5-C4	-2.55	1.36	1.43
4	9	1850	MA6	C5-C4	-2.55	1.34	1.40
4	9	814	5MU	O2-C2	-2.54	1.18	1.23
2	5	1663	I4U	O4-C41	-2.54	1.41	1.47
2	5	4533	B8W	C5-C4	-2.52	1.34	1.40
2	5	3903	BGH	C71-N7	2.52	1.45	1.39
2	5	729	2MG	CM2-N2	-2.51	1.41	1.45
2	5	3903	BGH	C5-C4	2.50	1.46	1.38
2	5	1326	1MA	C5-C4	-2.50	1.36	1.43
4	9	1851	MA6	C5-C4	-2.50	1.34	1.40
2	5	1629	OMG	C5-C4	-2.49	1.36	1.43
4	9	116	OMU	O2-C2	-2.49	1.18	1.23
4	9	612	PSU	C6-C5	2.49	1.38	1.35
2	5	1870	UR3	C5-C4	2.49	1.50	1.43
4	9	509	OMG	C2-N1	2.49	1.43	1.37
2	5	4601	UR3	C5-C4	2.48	1.50	1.43
2	5	4224	6MZ	C2-N3	2.48	1.36	1.32
3	8	14	OMU	O2-C2	-2.47	1.18	1.23
2	5	2428	OMG	C5-C4	-2.47	1.36	1.43
4	9	683	OMG	C2-N1	2.47	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2790	B9H	C6-N1	2.46	1.43	1.38
2	5	4534	UR3	C5-C4	2.46	1.50	1.43
2	5	4876	2MG	CM2-N2	-2.46	1.41	1.45
2	5	4419	1MA	C5-C4	-2.45	1.36	1.43
2	5	4375	MHG	O6-C6	-2.42	1.19	1.23
2	5	4601	UR3	C4-N3	2.42	1.46	1.40
4	9	1832	6MZ	C2-N3	2.42	1.36	1.32
2	5	3789	A2M	O3'-C3'	-2.41	1.37	1.43
4	9	116	OMU	C6-N1	2.41	1.43	1.38
2	5	4310	OMU	O2-C2	-2.40	1.18	1.23
2	5	4534	UR3	C4-N3	2.40	1.46	1.40
4	9	644	OMG	O6-C6	-2.39	1.18	1.23
2	5	4224	6MZ	C5-C4	-2.39	1.34	1.40
2	5	1870	UR3	C4-N3	2.39	1.46	1.40
4	9	644	OMG	C2-N1	2.39	1.43	1.37
4	9	509	OMG	O6-C6	-2.38	1.18	1.23
2	5	4310	OMU	C5-C4	2.36	1.48	1.43
2	5	4624	OMU	O2-C2	-2.36	1.18	1.23
3	8	14	OMU	C5-C4	2.35	1.48	1.43
2	5	1887	OMG	O6-C6	-2.35	1.18	1.23
2	5	1320	OMG	O6-C6	-2.35	1.18	1.23
4	9	159	A2M	C5'-C4'	2.33	1.58	1.51
4	9	683	OMG	O6-C6	-2.33	1.18	1.23
4	9	1830	UR3	O2-C2	-2.31	1.18	1.22
2	5	4374	OMG	O6-C6	-2.30	1.18	1.23
4	9	1830	UR3	O4-C4	-2.30	1.18	1.23
2	5	4087	5MU	O4-C4	-2.29	1.19	1.23
2	5	1526	OMG	O6-C6	-2.29	1.18	1.23
4	9	484	A2M	C3'-C4'	2.28	1.58	1.53
2	5	373	OMG	O6-C6	-2.27	1.18	1.23
2	5	1629	OMG	O6-C6	-2.26	1.18	1.23
2	5	4200	OMG	O6-C6	-2.26	1.18	1.23
2	5	4087	5MU	O2-C2	-2.25	1.18	1.23
4	9	1678	A2M	C3'-C4'	2.25	1.58	1.53
4	9	1678	A2M	C5'-C4'	2.25	1.58	1.51
2	5	4641	OMG	O6-C6	-2.25	1.18	1.23
2	5	4624	OMU	C5-C4	2.25	1.48	1.43
4	9	121	OMU	C5-C4	2.24	1.48	1.43
4	9	1248	B8N	O4-C4	-2.24	1.18	1.23
2	5	2054	OMG	O6-C6	-2.23	1.18	1.23
82	v	715	DDE	CD2-NE2	2.23	1.39	1.36
2	5	4627	OMG	O6-C6	-2.23	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3789	A2M	C3'-C4'	2.22	1.58	1.53
2	5	2368	OMG	O6-C6	-2.22	1.18	1.23
2	5	2777	OMG	O6-C6	-2.21	1.18	1.23
2	5	3796	OMG	O6-C6	-2.21	1.18	1.23
2	5	2428	OMG	O6-C6	-2.21	1.18	1.23
2	5	1521	2MG	CM2-N2	-2.20	1.41	1.45
2	5	4498	OMG	O6-C6	-2.19	1.18	1.23
2	5	4874	OMG	O6-C6	-2.19	1.18	1.23
2	5	1864	B8H	O2-C2	-2.16	1.19	1.23
2	5	4300	B8H	O2-C2	-2.15	1.19	1.23
4	9	1842	4AC	O7-C7	-2.15	1.18	1.23
4	9	27	A2M	O5'-C5'	-2.15	1.39	1.44
4	9	668	A2M	O5'-C5'	-2.15	1.39	1.44
4	9	568	E3C	O2-C2	-2.12	1.18	1.22
4	9	166	A2M	C3'-C4'	2.10	1.58	1.53
4	9	484	A2M	C5'-C4'	2.09	1.58	1.51
4	9	1248	B8N	O2-C2	-2.06	1.18	1.22
2	5	1663	I4U	O2-C2	-2.06	1.19	1.23
4	9	822	PSU	O4'-C1'	-2.05	1.41	1.43
4	9	27	A2M	C5'-C4'	2.05	1.58	1.51
2	5	2790	B9H	O2-C2	-2.05	1.18	1.22
4	9	166	A2M	C5'-C4'	2.05	1.58	1.51
4	9	1031	A2M	O5'-C5'	-2.03	1.39	1.44
2	5	3903	BGH	C3'-C2'	2.02	1.57	1.52
2	5	1521	2MG	C5-C4	-2.01	1.37	1.43
2	5	4876	2MG	C5-C4	-2.01	1.38	1.43
4	9	159	A2M	C3'-C4'	2.01	1.58	1.53

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	1806	M7A	C5-C6-N6	12.77	145.55	123.74
2	5	4568	M7A	C5-C6-N6	12.30	144.75	123.74
2	5	4087	5MU	C5-C4-N3	12.06	125.61	115.31
4	9	814	5MU	C5-C4-N3	11.64	125.25	115.31
4	9	1806	M7A	N6-C6-N1	-10.95	94.37	118.35
2	5	4568	M7A	N6-C6-N1	-10.58	95.18	118.35
4	9	1850	MA6	N1-C6-N6	-10.13	106.39	117.06
2	5	4087	5MU	C5-C6-N1	-9.99	113.06	123.34
4	9	814	5MU	C5-C6-N1	-9.81	113.24	123.34
4	9	1851	MA6	N1-C6-N6	-9.62	106.93	117.06
2	5	3722	A2M	C5-C6-N6	8.73	133.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	1538	A2M	C5-C6-N6	8.72	133.60	120.35
2	5	398	A2M	C5-C6-N6	8.71	133.59	120.35
2	5	2367	A2M	C5-C6-N6	8.67	133.53	120.35
2	5	2405	A2M	C5-C6-N6	8.58	133.39	120.35
2	5	1875	A2M	C5-C6-N6	8.58	133.39	120.35
2	5	1528	A2M	C5-C6-N6	8.57	133.38	120.35
2	5	4575	A2M	C5-C6-N6	8.57	133.37	120.35
2	5	1330	A2M	C5-C6-N6	8.56	133.37	120.35
2	5	3727	A2M	C5-C6-N6	8.52	133.30	120.35
2	5	3871	A2M	C5-C6-N6	8.49	133.25	120.35
2	5	3829	A2M	C5-C6-N6	8.43	133.16	120.35
2	5	4527	A2M	C5-C6-N6	8.42	133.15	120.35
2	5	3789	A2M	C5-C6-N6	8.27	132.93	120.35
4	9	1031	A2M	C5-C6-N6	8.06	132.60	120.35
4	9	484	A2M	C5-C6-N6	7.98	132.47	120.35
4	9	159	A2M	C5-C6-N6	7.87	132.32	120.35
4	9	166	A2M	C5-C6-N6	7.64	131.96	120.35
4	9	668	A2M	C5-C6-N6	7.53	131.79	120.35
4	9	27	A2M	C5-C6-N6	7.32	131.48	120.35
4	9	1678	A2M	C5-C6-N6	7.30	131.45	120.35
2	5	4476	B8W	O6-C6-C5	6.92	125.91	116.01
2	5	1864	B8H	C4-N3-C2	-6.70	118.67	127.35
2	5	4300	B8H	C4-N3-C2	-6.70	118.67	127.35
2	5	4375	MHG	C2-N3-C4	6.56	120.17	112.04
2	5	3884	P7G	C4-C5-N7	6.48	110.09	106.67
2	5	1913	P7G	C4-C5-N7	6.47	110.08	106.67
2	5	4533	B8W	O6-C6-C5	6.34	125.07	116.01
4	9	166	A2M	N3-C2-N1	-6.13	119.09	128.68
4	9	568	E3C	C1'-N1-C2	6.04	127.19	116.99
2	5	1864	B8H	N3-C2-N1	5.95	121.57	115.14
2	5	1460	B8Q	N3-C2-N1	5.91	124.08	117.13
2	5	398	A2M	N6-C6-N1	-5.91	106.31	118.57
2	5	2367	A2M	N6-C6-N1	-5.91	106.32	118.57
2	5	1538	A2M	N6-C6-N1	-5.90	106.32	118.57
2	5	2301	E7G	C4-C5-N7	5.90	110.16	104.91
4	9	1806	M7A	N3-C2-N1	-5.87	119.42	128.60
2	5	3722	A2M	N6-C6-N1	-5.85	106.44	118.57
4	9	1031	A2M	N3-C2-N1	-5.85	119.54	128.68
2	5	2405	A2M	N6-C6-N1	-5.85	106.44	118.57
2	5	3789	A2M	N6-C6-N1	-5.84	106.44	118.57
2	5	1528	A2M	N6-C6-N1	-5.83	106.47	118.57
2	5	4575	A2M	N6-C6-N1	-5.83	106.47	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	3727	A2M	N6-C6-N1	-5.81	106.52	118.57
2	5	1875	A2M	N6-C6-N1	-5.80	106.54	118.57
2	5	4300	B8H	N3-C2-N1	5.79	121.39	115.14
2	5	1330	A2M	N6-C6-N1	-5.77	106.59	118.57
2	5	3829	A2M	N6-C6-N1	-5.74	106.67	118.57
4	9	1850	MA6	N3-C2-N1	-5.69	119.78	128.68
4	9	1851	MA6	N3-C2-N1	-5.68	119.80	128.68
2	5	3871	A2M	N6-C6-N1	-5.68	106.78	118.57
4	9	484	A2M	N3-C2-N1	-5.66	119.83	128.68
4	9	1678	A2M	N3-C2-N1	-5.66	119.83	128.68
4	9	27	A2M	N3-C2-N1	-5.66	119.84	128.68
2	5	4527	A2M	N6-C6-N1	-5.65	106.84	118.57
2	5	1875	A2M	N3-C2-N1	-5.62	119.90	128.68
2	5	4568	M7A	N3-C2-N1	-5.59	119.86	128.60
2	5	1801	E7G	C4-C5-N7	5.57	109.87	104.91
2	5	4694	B8K	C5-C6-N1	5.57	120.81	110.99
4	9	1832	6MZ	N3-C2-N1	-5.57	119.98	128.68
4	9	159	A2M	N3-C2-N1	-5.56	119.99	128.68
2	5	4224	6MZ	N3-C2-N1	-5.53	120.04	128.68
2	5	3727	A2M	N3-C2-N1	-5.52	120.06	128.68
2	5	3789	A2M	N3-C2-N1	-5.51	120.07	128.68
4	9	668	A2M	N3-C2-N1	-5.51	120.07	128.68
2	5	1528	A2M	N3-C2-N1	-5.50	120.08	128.68
2	5	1538	A2M	N3-C2-N1	-5.50	120.08	128.68
2	5	2367	A2M	N3-C2-N1	-5.50	120.09	128.68
2	5	4375	MHG	C4-C5-N7	5.48	109.79	104.91
2	5	4476	B8W	N3-C2-N1	-5.48	119.91	127.22
2	5	398	A2M	N3-C2-N1	-5.46	120.14	128.68
2	5	4359	E6G	N3-C2-N1	-5.45	119.95	127.22
2	5	1460	B8Q	C31-N3-C4	5.44	122.45	114.25
2	5	2405	A2M	N3-C2-N1	-5.44	120.18	128.68
2	5	3829	A2M	N3-C2-N1	-5.44	120.18	128.68
2	5	4575	A2M	N3-C2-N1	-5.44	120.18	128.68
2	5	3903	BGH	C5-C6-N1	5.43	120.56	110.99
2	5	4527	A2M	N3-C2-N1	-5.42	120.21	128.68
4	9	159	A2M	N6-C6-N1	-5.40	107.36	118.57
2	5	2758	B9B	N3-C2-N1	-5.38	120.05	127.22
4	9	1031	A2M	N6-C6-N1	-5.37	107.42	118.57
2	5	3722	A2M	N3-C2-N1	-5.36	120.29	128.68
2	5	1578	B9B	N3-C2-N1	-5.35	120.08	127.22
2	5	3901	B8K	C5-C6-N1	5.35	120.42	110.99
2	5	1330	A2M	N3-C2-N1	-5.35	120.32	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	2790	B9H	C31-N3-C2	5.35	123.89	117.21
4	9	1219	B8Q	N3-C2-N1	5.34	123.41	117.13
2	5	3871	A2M	N3-C2-N1	-5.34	120.33	128.68
2	5	237	B9B	N3-C2-N1	-5.34	120.10	127.22
3	8	14	OMU	C4-N3-C2	-5.32	119.57	126.58
2	5	1326	1MA	N1-C2-N3	-5.31	119.83	126.02
4	9	484	A2M	N6-C6-N1	-5.27	107.63	118.57
4	9	121	OMU	C4-N3-C2	-5.27	119.63	126.58
2	5	4189	B8W	N3-C2-N1	-5.25	120.21	127.22
2	5	4310	OMU	C4-N3-C2	-5.25	119.65	126.58
4	9	166	A2M	N6-C6-N1	-5.23	107.72	118.57
4	9	668	A2M	N6-C6-N1	-5.17	107.85	118.57
2	5	4419	1MA	N1-C2-N3	-5.15	120.02	126.02
2	5	4133	B8W	N3-C2-N1	-5.13	120.38	127.22
2	5	4189	B8W	N2-C2-N3	5.11	126.12	117.79
2	5	4189	B8W	O6-C6-C5	5.10	123.29	116.01
4	9	116	OMU	C4-N3-C2	-5.09	119.86	126.58
2	5	4624	OMU	C4-N3-C2	-5.09	119.87	126.58
4	9	1248	B8N	C5-C4-N3	5.09	125.59	116.17
2	5	4476	B8W	N2-C2-N3	5.07	126.06	117.79
2	5	2384	B8W	N3-C2-N1	-5.07	120.46	127.22
4	9	1219	B8Q	C31-N3-C4	5.07	121.89	114.25
2	5	4133	B8W	O6-C6-C5	5.02	123.19	116.01
2	5	2384	B8W	N2-C2-N3	5.02	125.97	117.79
4	9	27	A2M	N6-C6-N1	-5.02	108.16	118.57
2	5	1801	E7G	C5-C6-N1	5.01	119.82	110.99
4	9	814	5MU	N3-C2-N1	5.00	121.53	114.89
2	5	4533	B8W	N3-C2-N1	-4.99	120.56	127.22
4	9	1678	A2M	N6-C6-N1	-4.98	108.24	118.57
2	5	2301	E7G	C5-C6-N1	4.98	119.77	110.99
4	9	1243	PSU	N1-C2-N3	4.96	120.75	115.13
2	5	2526	7MG	C5-C6-N1	4.96	119.73	110.99
2	5	4375	MHG	C5-C6-N1	4.96	119.72	110.99
2	5	4087	5MU	C4-N3-C2	-4.95	120.94	127.35
2	5	1609	7MG	C5-C6-N1	4.95	119.71	110.99
2	5	4533	B8W	N2-C2-N3	4.94	125.85	117.79
2	5	4133	B8W	N2-C2-N3	4.93	125.83	117.79
2	5	4568	M7A	C4-N9-C1'	-4.89	114.98	126.60
2	5	4087	5MU	O4-C4-C5	-4.89	119.24	124.90
4	9	822	PSU	C4-N3-C2	-4.89	119.30	126.34
2	5	4554	7MG	C5-C6-N1	4.88	119.59	110.99
4	9	822	PSU	N1-C2-N3	4.88	120.65	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	4694	B8K	C4-C5-N7	4.86	109.23	104.91
4	9	814	5MU	O4-C4-C5	-4.81	119.32	124.90
2	5	4568	M7A	N3-C4-N9	4.79	132.92	126.87
4	9	1219	B8Q	O2-C2-N3	-4.77	115.94	122.95
2	5	4601	UR3	C4-N3-C2	-4.75	120.09	124.56
2	5	3901	B8K	C4-C5-N7	4.75	109.13	104.91
2	5	4454	PSU	C4-N3-C2	-4.74	119.50	126.34
2	5	3903	BGH	C2-N3-C4	4.72	120.72	112.30
4	9	1806	M7A	N3-C4-N9	4.71	132.82	126.87
2	5	4640	PSU	C4-N3-C2	-4.71	119.56	126.34
4	9	814	5MU	C4-N3-C2	-4.69	121.28	127.35
2	5	1681	PSU	C4-N3-C2	-4.68	119.60	126.34
2	5	4534	UR3	C4-N3-C2	-4.66	120.18	124.56
2	5	2512	PSU	C4-N3-C2	-4.65	119.64	126.34
4	9	823	PSU	C4-N3-C2	-4.65	119.64	126.34
2	5	4632	PSU	C4-N3-C2	-4.62	119.68	126.34
4	9	1081	PSU	N1-C2-N3	4.62	120.36	115.13
2	5	3719	PSU	C4-N3-C2	-4.62	119.69	126.34
4	9	823	PSU	N1-C2-N3	4.61	120.36	115.13
2	5	4694	B8K	C2-N3-C4	4.61	120.52	112.30
2	5	1687	PSU	C4-N3-C2	-4.61	119.70	126.34
2	5	4446	PSU	C4-N3-C2	-4.61	119.70	126.34
2	5	1586	PSU	C4-N3-C2	-4.60	119.71	126.34
2	5	4297	PSU	C4-N3-C2	-4.58	119.73	126.34
4	9	568	E3C	O2-C2-N3	-4.58	116.27	122.07
2	5	3901	B8K	C2-N3-C4	4.55	120.41	112.30
2	5	3903	BGH	C4-C5-N7	4.55	108.96	104.91
2	5	4504	PSU	C4-N3-C2	-4.55	119.79	126.34
2	5	4407	PSU	C4-N3-C2	-4.55	119.79	126.34
4	9	1219	B8Q	C1'-N1-C2	4.55	124.66	116.99
2	5	4535	PSU	C4-N3-C2	-4.54	119.80	126.34
4	9	1248	B8N	C4-N3-C2	-4.51	119.76	125.46
2	5	1801	E7G	C2-N3-C4	4.49	120.30	112.30
2	5	1870	UR3	C4-N3-C2	-4.49	120.33	124.56
2	5	4087	5MU	N3-C2-N1	4.49	120.85	114.89
4	9	612	PSU	C4-N3-C2	-4.47	119.90	126.34
2	5	3733	PSU	C4-N3-C2	-4.46	119.92	126.34
2	5	2526	7MG	C2-N3-C4	4.46	120.24	112.30
2	5	2301	E7G	C2-N3-C4	4.45	120.22	112.30
2	5	4632	PSU	N1-C2-N3	4.44	120.16	115.13
4	9	1243	PSU	C4-N3-C2	-4.43	119.95	126.34
2	5	1609	7MG	C2-N3-C4	4.41	120.15	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	1081	PSU	C4-N3-C2	-4.37	120.04	126.34
2	5	4554	7MG	C2-N3-C4	4.36	120.07	112.30
2	5	2384	B8W	O6-C6-C5	4.33	122.20	116.01
2	5	4476	B8W	C2-N3-C4	4.33	120.30	115.36
4	9	612	PSU	N1-C2-N3	4.33	120.03	115.13
2	5	4359	E6G	O6-C6-N1	4.32	123.86	120.12
2	5	2512	PSU	N1-C2-N3	4.29	119.99	115.13
2	5	3768	PSU	C4-N3-C2	-4.27	120.18	126.34
2	5	4189	B8W	C2-N3-C4	4.25	120.21	115.36
2	5	4446	PSU	N1-C2-N3	4.22	119.91	115.13
2	5	4133	B8W	C2-N3-C4	4.22	120.17	115.36
2	5	4504	PSU	N1-C2-N3	4.21	119.90	115.13
4	9	1830	UR3	C4-N3-C2	-4.21	120.60	124.56
4	9	1830	UR3	C1'-N1-C2	4.20	124.08	116.99
2	5	4454	PSU	N1-C2-N3	4.19	119.88	115.13
2	5	4640	PSU	N1-C2-N3	4.19	119.87	115.13
2	5	2384	B8W	C2-N3-C4	4.18	120.13	115.36
2	5	1687	PSU	N1-C2-N3	4.18	119.86	115.13
2	5	237	B9B	C2-N3-C4	4.17	120.12	115.36
2	5	4297	PSU	N1-C2-N3	4.17	119.85	115.13
2	5	1586	PSU	N1-C2-N3	4.17	119.85	115.13
2	5	2758	B9B	C2-N3-C4	4.16	120.11	115.36
2	5	4359	E6G	C2-N3-C4	4.15	120.10	115.36
2	5	4694	B8K	C72-C71-N7	4.15	125.11	118.86
2	5	1681	PSU	N1-C2-N3	4.14	119.82	115.13
2	5	3719	PSU	N1-C2-N3	4.14	119.82	115.13
2	5	4533	B8W	C2-N3-C4	4.13	120.08	115.36
2	5	1326	1MA	C5-C6-N1	4.13	120.06	113.90
2	5	4535	PSU	N1-C2-N3	4.13	119.81	115.13
2	5	4476	B8W	O6-C6-N1	-4.12	113.32	119.03
2	5	4419	1MA	C5-C6-N1	4.11	120.03	113.90
2	5	4224	6MZ	C2-N1-C6	4.10	120.10	116.59
2	5	2301	E7G	C5-C4-N3	-4.09	120.33	128.13
2	5	4407	PSU	N1-C2-N3	4.09	119.76	115.13
2	5	1801	E7G	C5-C4-N3	-4.07	120.37	128.13
4	9	121	OMU	N3-C2-N1	4.07	120.29	114.89
2	5	3733	PSU	N1-C2-N3	4.07	119.74	115.13
2	5	1578	B9B	C2-N3-C4	4.06	119.99	115.36
2	5	2526	7MG	C5-C4-N3	-4.02	120.47	128.13
2	5	1609	7MG	C5-C4-N3	-4.01	120.49	128.13
2	5	4087	5MU	C5M-C5-C6	-3.99	117.52	122.85
4	9	568	E3C	C31-N3-C2	3.98	122.55	117.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	3901	B8K	C72-C71-N7	3.94	124.78	118.86
2	5	3768	PSU	N1-C2-N3	3.92	119.57	115.13
2	5	4554	7MG	C5-C4-N3	-3.85	120.79	128.13
4	9	119	PSU	N1-C2-N3	3.85	119.49	115.13
3	8	14	OMU	N3-C2-N1	3.82	119.96	114.89
2	5	4087	5MU	C5M-C5-C4	3.82	122.97	118.77
2	5	4310	OMU	N3-C2-N1	3.81	119.95	114.89
2	5	4375	MHG	C5-C4-N3	-3.80	120.88	128.13
2	5	4375	MHG	C2-N1-C6	-3.80	120.11	124.48
2	5	237	B9B	O6-C6-N1	-3.80	116.85	120.12
4	9	568	E3C	C6-N1-C2	-3.73	118.45	121.79
2	5	4624	OMU	N3-C2-N1	3.70	119.81	114.89
4	9	119	PSU	C4-N3-C2	-3.67	121.06	126.34
2	5	1460	B8Q	O2-C2-N3	-3.65	117.58	122.95
2	5	3903	BGH	C72-C71-N7	3.65	124.35	118.86
2	5	4451	5MC	C5-C6-N1	-3.64	119.59	123.34
2	5	4198	I4U	C5-C4-N3	-3.59	119.45	124.91
4	9	1374	5MC	O2-C2-N3	-3.56	116.54	122.33
4	9	116	OMU	N3-C2-N1	3.55	119.60	114.89
2	5	4694	B8K	C5-C4-N3	-3.55	121.37	128.13
2	5	1352	P4U	C5-C4-N3	-3.54	119.52	124.91
2	5	4694	B8K	C5-C4-N9	3.54	110.94	106.35
2	5	3903	BGH	C2'-C1'-N9	-3.54	106.94	114.14
2	5	3903	BGH	C5-C4-N9	3.53	110.94	106.35
2	5	1521	2MG	C5-C6-N1	3.53	120.19	113.95
2	5	4300	B8H	C5-C4-N3	3.49	124.48	116.58
4	9	683	OMG	C5-C6-N1	3.49	120.12	113.95
2	5	1887	OMG	C5-C6-N1	3.47	120.07	113.95
2	5	4533	B8W	O6-C6-N1	-3.47	114.22	119.03
2	5	4627	OMG	C5-C6-N1	3.46	120.07	113.95
2	5	2054	OMG	C5-C6-N1	3.46	120.07	113.95
2	5	3901	B8K	C5-C4-N3	-3.46	121.54	128.13
4	9	644	OMG	C5-C6-N1	3.46	120.06	113.95
2	5	4641	OMG	C5-C6-N1	3.45	120.05	113.95
3	8	14	OMU	C5-C4-N3	3.45	120.00	114.84
2	5	1864	B8H	C5-C4-N3	3.45	124.38	116.58
2	5	2777	OMG	C5-C6-N1	3.44	120.03	113.95
4	9	1806	M7A	C4-N9-C1'	-3.44	118.43	126.60
4	9	814	5MU	C5M-C5-C6	-3.44	118.26	122.85
2	5	2368	OMG	C5-C6-N1	3.44	120.02	113.95
2	5	4200	OMG	C5-C6-N1	3.43	120.00	113.95
2	5	3901	B8K	C5-C4-N9	3.43	110.80	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	373	OMG	C5-C6-N1	3.43	120.00	113.95
2	5	1629	OMG	C5-C6-N1	3.42	120.00	113.95
2	5	4876	2MG	C5-C6-N1	3.42	119.99	113.95
4	9	116	OMU	C5-C4-N3	3.42	119.95	114.84
2	5	2428	OMG	C5-C6-N1	3.42	119.98	113.95
2	5	4876	2MG	CM2-N2-C2	-3.41	116.32	123.86
2	5	4339	5MC	C5-C6-N1	-3.41	119.83	123.34
2	5	3796	OMG	C5-C6-N1	3.40	119.96	113.95
2	5	4640	PSU	C6-C5-C4	3.40	120.58	118.20
2	5	4568	M7A	C2-N3-C4	3.40	119.78	111.75
2	5	4374	OMG	C5-C6-N1	3.39	119.95	113.95
4	9	121	OMU	C5-C4-N3	3.39	119.91	114.84
2	5	1663	I4U	C5-C4-N3	-3.39	119.76	124.91
2	5	4874	OMG	C5-C6-N1	3.38	119.92	113.95
2	5	1526	OMG	C5-C6-N1	3.38	119.91	113.95
2	5	4498	OMG	C5-C6-N1	3.37	119.91	113.95
2	5	4454	PSU	C6-C5-C4	3.37	120.55	118.20
2	5	3903	BGH	C5-C4-N3	-3.36	121.72	128.13
2	5	729	2MG	C5-C6-N1	3.36	119.88	113.95
4	9	1806	M7A	C2-N3-C4	3.36	119.68	111.75
2	5	1320	OMG	C5-C6-N1	3.36	119.88	113.95
2	5	4632	PSU	C6-C5-C4	3.35	120.54	118.20
4	9	509	OMG	C5-C6-N1	3.34	119.85	113.95
2	5	4504	PSU	C6-C5-C4	3.32	120.52	118.20
2	5	4310	OMU	C5-C4-N3	3.30	119.78	114.84
2	5	3786	5MC	C5-C6-N1	-3.29	119.95	123.34
2	5	2758	B9B	O6-C6-N1	-3.28	117.29	120.12
2	5	4375	MHG	C5-C4-N9	3.27	110.60	106.35
2	5	1578	B9B	O6-C6-N1	-3.27	117.31	120.12
2	5	4624	OMU	C5-C4-N3	3.26	119.72	114.84
4	9	116	OMU	O4-C4-C5	-3.24	119.46	125.16
4	9	1374	5MC	C5-C6-N1	-3.24	120.00	123.34
4	9	644	OMG	C2-N1-C6	-3.24	119.13	125.10
2	5	3719	PSU	C6-C5-C4	3.23	120.45	118.20
2	5	4535	PSU	C6-C5-C4	3.22	120.45	118.20
2	5	4694	B8K	N9-C8-N7	3.21	107.64	103.33
2	5	3901	B8K	N9-C8-N7	3.19	107.61	103.33
4	9	509	OMG	C2-N1-C6	-3.18	119.23	125.10
2	5	1681	PSU	C6-C5-C4	3.18	120.42	118.20
2	5	1864	B8H	O2-C2-N1	-3.17	119.30	122.87
2	5	4632	PSU	C6-N1-C2	-3.17	119.44	122.68
2	5	1609	7MG	C4-C5-N7	3.16	109.92	105.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	2526	7MG	C4-C5-N7	3.16	109.92	105.53
4	9	1248	B8N	N3-C2-N1	3.14	121.20	116.76
2	5	4554	7MG	C4-C5-N7	3.13	109.88	105.53
2	5	1586	PSU	C6-C5-C4	3.13	120.39	118.20
4	9	1830	UR3	C6-N1-C2	-3.13	118.99	121.79
4	9	822	PSU	O2-C2-N1	-3.12	119.35	122.79
2	5	4300	B8H	O2-C2-N1	-3.11	119.37	122.87
2	5	4554	7MG	C5-C4-N9	3.11	110.38	106.35
2	5	2512	PSU	C6-C5-C4	3.09	120.36	118.20
2	5	4446	PSU	C6-C5-C4	3.09	120.36	118.20
2	5	2526	7MG	C5-C4-N9	3.08	110.34	106.35
2	5	2368	OMG	C8-N7-C5	3.06	108.82	102.99
2	5	1609	7MG	C5-C4-N9	3.05	110.30	106.35
2	5	3733	PSU	C6-C5-C4	3.02	120.31	118.20
2	5	4641	OMG	C8-N7-C5	3.02	108.74	102.99
2	5	4297	PSU	C6-C5-C4	3.01	120.30	118.20
2	5	3733	PSU	C6-N1-C2	-3.01	119.61	122.68
2	5	3903	BGH	N9-C8-N7	3.00	107.35	103.33
2	5	1801	E7G	C5-C4-N9	3.00	110.24	106.35
2	5	1687	PSU	C6-C5-C4	2.99	120.29	118.20
2	5	373	OMG	C8-N7-C5	2.98	108.67	102.99
2	5	4359	E6G	N2-C2-N3	2.98	122.65	117.79
4	9	568	E3C	C1'-N1-C6	-2.98	114.35	120.84
2	5	4504	PSU	C6-N1-C2	-2.97	119.65	122.68
2	5	4297	PSU	C6-N1-C2	-2.96	119.65	122.68
4	9	612	PSU	O2-C2-N1	-2.96	119.53	122.79
2	5	1526	OMG	C8-N7-C5	2.95	108.61	102.99
2	5	4535	PSU	C6-N1-C2	-2.95	119.67	122.68
2	5	2428	OMG	C2-N1-C6	-2.95	119.67	125.10
2	5	1629	OMG	C2-N1-C6	-2.94	119.68	125.10
2	5	2054	OMG	C2-N1-C6	-2.93	119.69	125.10
2	5	4446	PSU	C6-N1-C2	-2.93	119.68	122.68
4	9	1337	4AC	C5-C4-N3	-2.93	117.87	122.59
2	5	2512	PSU	C6-N1-C2	-2.93	119.69	122.68
2	5	3768	PSU	C6-N1-C2	-2.93	119.69	122.68
4	9	1806	M7A	C71-N7-C5	-2.93	112.77	124.01
2	5	1320	OMG	C8-N7-C5	2.93	108.56	102.99
2	5	2054	OMG	C8-N7-C5	2.92	108.55	102.99
2	5	2777	OMG	C8-N7-C5	2.92	108.55	102.99
4	9	814	5MU	C1'-N1-C2	2.91	122.84	117.57
2	5	4498	OMG	C8-N7-C5	2.91	108.54	102.99
2	5	3796	OMG	C2-N1-C6	-2.91	119.74	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	4641	OMG	C2-N1-C6	-2.91	119.74	125.10
2	5	2301	E7G	C5-C4-N9	2.90	110.11	106.35
2	5	4224	6MZ	C9-N6-C6	-2.90	120.38	122.87
2	5	1586	PSU	C6-N1-C2	-2.90	119.72	122.68
2	5	4874	OMG	C8-N7-C5	2.90	108.51	102.99
2	5	4200	OMG	C8-N7-C5	2.88	108.48	102.99
2	5	4200	OMG	C2-N1-C6	-2.88	119.80	125.10
2	5	2368	OMG	C2-N1-C6	-2.88	119.80	125.10
2	5	3796	OMG	C8-N7-C5	2.87	108.46	102.99
2	5	4627	OMG	C8-N7-C5	2.87	108.46	102.99
2	5	4374	OMG	C8-N7-C5	2.87	108.45	102.99
4	9	1219	B8Q	C6-N1-C2	-2.87	119.22	121.79
4	9	1842	4AC	C6-C5-C4	2.86	120.47	116.96
2	5	1887	OMG	C8-N7-C5	2.86	108.44	102.99
2	5	4359	E6G	C61-O6-C6	-2.86	114.73	117.56
2	5	2526	7MG	O6-C6-C5	-2.85	120.55	127.54
2	5	1526	OMG	C2-N1-C6	-2.85	119.85	125.10
2	5	4627	OMG	C2-N1-C6	-2.85	119.85	125.10
2	5	1887	OMG	C2-N1-C6	-2.85	119.86	125.10
2	5	2777	OMG	C2-N1-C6	-2.84	119.86	125.10
2	5	1801	E7G	O6-C6-C5	-2.84	120.58	127.54
2	5	1609	7MG	O6-C6-C5	-2.83	120.59	127.54
4	9	1248	B8N	C31-N3-C4	2.83	121.48	117.31
2	5	4310	OMU	O4-C4-C5	-2.83	120.18	125.16
2	5	3719	PSU	C6-N1-C2	-2.83	119.79	122.68
2	5	373	OMG	C2-N1-C6	-2.83	119.89	125.10
2	5	4554	7MG	O6-C6-C5	-2.83	120.61	127.54
2	5	4498	OMG	C2-N1-C6	-2.82	119.90	125.10
4	9	683	OMG	C2-N1-C6	-2.82	119.91	125.10
2	5	4375	MHG	O6-C6-C5	-2.81	120.65	127.54
2	5	4874	OMG	C2-N1-C6	-2.81	119.93	125.10
2	5	4374	OMG	C2-N1-C6	-2.81	119.93	125.10
2	5	4224	6MZ	C1'-N9-C4	-2.80	121.72	126.64
2	5	2301	E7G	O6-C6-C5	-2.80	120.67	127.54
4	9	814	5MU	O2-C2-N3	-2.80	116.28	121.50
2	5	4407	PSU	C6-N1-C2	-2.80	119.82	122.68
2	5	1629	OMG	C8-N7-C5	2.80	108.32	102.99
2	5	2428	OMG	C8-N7-C5	2.79	108.30	102.99
2	5	4624	OMU	O4-C4-C5	-2.78	120.27	125.16
4	9	116	OMU	C1'-N1-C2	2.78	122.61	117.57
2	5	1681	PSU	C6-N1-C2	-2.78	119.84	122.68
2	5	2301	E7G	C2-N1-C6	-2.78	120.03	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	1687	PSU	C6-N1-C2	-2.78	119.84	122.68
4	9	814	5MU	C5M-C5-C4	2.75	121.79	118.77
2	5	1609	7MG	C2-N1-C6	-2.75	120.09	125.10
3	8	14	OMU	O4-C4-C5	-2.74	120.34	125.16
2	5	4568	M7A	C71-N7-C5	-2.74	113.50	124.01
2	5	2526	7MG	C2-N1-C6	-2.74	120.11	125.10
2	5	2301	E7G	N9-C4-N3	2.73	129.55	125.47
4	9	1842	4AC	C5-C4-N3	-2.73	118.21	122.59
4	9	119	PSU	O2-C2-N1	-2.72	119.79	122.79
2	5	4640	PSU	C6-N1-C2	-2.72	119.90	122.68
2	5	1320	OMG	C2-N1-C6	-2.72	120.09	125.10
2	5	1801	E7G	C2-N1-C6	-2.71	120.15	125.10
4	9	119	PSU	C6-N1-C2	-2.71	119.91	122.68
4	9	121	OMU	O4-C4-C5	-2.70	120.41	125.16
2	5	3903	BGH	C6-C5-C4	-2.69	117.07	122.62
4	9	1243	PSU	C6-N1-C2	-2.68	119.94	122.68
4	9	823	PSU	O2-C2-N1	-2.68	119.84	122.79
2	5	4454	PSU	C6-N1-C2	-2.67	119.96	122.68
4	9	1243	PSU	O2-C2-N1	-2.66	119.86	122.79
2	5	4876	2MG	C8-N7-C5	2.66	108.06	102.99
4	9	1337	4AC	C6-C5-C4	2.66	120.21	116.96
2	5	4300	B8H	O4-C4-N3	-2.65	115.04	120.12
2	5	4632	PSU	O2-C2-N1	-2.65	119.88	122.79
2	5	4189	B8W	O6-C6-N1	-2.64	115.36	119.03
2	5	4675	B8T	C6-C5-C4	2.64	120.19	116.96
2	5	4087	5MU	O2-C2-N1	-2.64	119.28	122.79
2	5	4297	PSU	O2-C2-N1	-2.64	119.89	122.79
2	5	1521	2MG	C8-N7-C5	2.63	108.00	102.99
2	5	4568	M7A	C5-C4-N3	-2.63	120.45	126.62
2	5	1801	E7G	N9-C4-N3	2.63	129.40	125.47
4	9	27	A2M	C3'-C2'-C1'	2.63	107.83	102.89
2	5	4535	PSU	O2-C2-N1	-2.61	119.92	122.79
2	5	4419	1MA	C8-N7-C5	2.60	107.94	102.99
4	9	644	OMG	C8-N7-C5	2.60	107.94	102.99
4	9	683	OMG	C8-N7-C5	2.59	107.93	102.99
4	9	509	OMG	C8-N7-C5	2.59	107.93	102.99
2	5	4087	5MU	O4-C4-N3	-2.59	115.16	120.12
2	5	1326	1MA	C8-N7-C5	2.59	107.92	102.99
2	5	1460	B8Q	C31-N3-C2	2.58	121.54	117.79
2	5	4375	MHG	N1-C2-N3	-2.58	119.96	123.95
2	5	729	2MG	C8-N7-C5	2.57	107.89	102.99
2	5	4694	B8K	C2-N1-C6	-2.57	120.41	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	1864	B8H	O4-C4-N3	-2.56	115.20	120.12
2	5	4694	B8K	C6-C5-C4	-2.54	117.38	122.62
2	5	4504	PSU	O2-C2-N1	-2.54	119.99	122.79
4	9	814	5MU	C6-N1-C2	-2.54	118.73	121.30
2	5	1687	PSU	O2-C2-N1	-2.53	120.01	122.79
4	9	1081	PSU	O2-C2-N1	-2.52	120.02	122.79
4	9	1081	PSU	C6-N1-C2	-2.50	120.12	122.68
2	5	1609	7MG	N9-C8-N7	2.50	106.96	103.38
2	5	1609	7MG	N9-C4-N3	2.50	129.21	125.47
4	9	644	OMG	O6-C6-C5	-2.50	119.50	124.37
2	5	2526	7MG	N9-C4-N3	2.49	129.19	125.47
2	5	3903	BGH	C2-N1-C6	-2.49	120.55	125.10
2	5	4359	E6G	C2-N1-C6	2.48	120.06	116.08
2	5	3901	B8K	C6-C5-C4	-2.48	117.52	122.62
2	5	4554	7MG	C2-N1-C6	-2.47	120.59	125.10
4	9	1219	B8Q	C31-N3-C2	2.47	121.38	117.79
2	5	2301	E7G	C8-N7-C71	2.47	126.39	120.50
2	5	4133	B8W	O6-C6-N1	-2.47	115.60	119.03
2	5	3884	P7G	N9-C8-N7	2.46	106.90	103.38
4	9	1710	OMC	O2-C2-N3	-2.46	118.33	122.33
4	9	814	5MU	O4-C4-N3	-2.45	115.41	120.12
2	5	4487	B8T	C6-C5-C4	2.45	119.96	116.96
2	5	3733	PSU	O2-C2-N1	-2.45	120.09	122.79
2	5	4446	PSU	O2-C2-N1	-2.45	120.09	122.79
2	5	1586	PSU	O2-C2-N1	-2.43	120.11	122.79
4	9	822	PSU	O4'-C1'-C2'	2.43	108.57	105.14
2	5	1887	OMG	O6-C6-C5	-2.41	119.66	124.37
2	5	4476	B8W	C4-C5-N7	-2.41	106.89	109.40
2	5	1681	PSU	O2-C2-N1	-2.39	120.16	122.79
2	5	4476	B8W	C2-N1-C6	2.39	119.92	116.08
2	5	2758	B9B	C2-N1-C6	2.39	119.92	116.08
4	9	668	A2M	C3'-C2'-C1'	2.39	107.38	102.89
2	5	237	B9B	C2-N1-C6	2.39	119.92	116.08
2	5	2301	E7G	N9-C8-N7	2.38	106.79	103.38
2	5	2526	7MG	N9-C8-N7	2.38	106.78	103.38
2	5	1521	2MG	O6-C6-C5	-2.38	119.73	124.37
2	5	1913	P7G	N9-C8-N7	2.38	106.78	103.38
4	9	1806	M7A	C5-C4-N3	-2.37	121.06	126.62
4	9	166	A2M	C5'-C4'-C3'	-2.37	106.30	115.18
2	5	4407	PSU	O2-C2-N1	-2.37	120.19	122.79
2	5	2384	B8W	N2-C2-N1	-2.37	113.57	117.25
4	9	121	OMU	C1'-N1-C2	2.36	121.84	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	3901	B8K	C2-N1-C6	-2.36	120.80	125.10
2	5	4533	B8W	N2-C2-N1	-2.36	113.59	117.25
2	5	3719	PSU	O2-C2-N1	-2.35	120.20	122.79
2	5	1578	B9B	C2-N1-C6	2.35	119.85	116.08
2	5	1801	E7G	N9-C8-N7	2.34	106.73	103.38
2	5	4454	PSU	O2-C2-N1	-2.33	120.22	122.79
4	9	1842	4AC	O7-C7-CM7	-2.33	117.73	122.06
2	5	1320	OMG	O6-C6-C5	-2.32	119.85	124.37
2	5	4189	B8W	N2-C2-N1	-2.31	113.66	117.25
2	5	4534	UR3	C6-N1-C2	-2.31	119.72	121.79
4	9	814	5MU	C6-C5-C4	2.29	119.95	118.03
2	5	2512	PSU	O2-C2-N1	-2.29	120.27	122.79
4	9	159	A2M	O4'-C4'-C3'	-2.29	100.59	105.11
4	9	683	OMG	O6-C6-C5	-2.28	119.92	124.37
2	5	4359	E6G	C1'-N9-C4	-2.28	122.64	126.64
4	9	823	PSU	C6-N1-C2	-2.28	120.36	122.68
2	5	3796	OMG	O6-C6-C5	-2.27	119.94	124.37
2	5	1578	B9B	N2-C2-N1	2.27	120.78	117.25
2	5	1801	E7G	C8-N7-C71	2.26	125.88	120.50
2	5	2777	OMG	O6-C6-C5	-2.25	119.98	124.37
2	5	4554	7MG	N9-C4-N3	2.25	128.83	125.47
4	9	509	OMG	O6-C6-C5	-2.25	119.99	124.37
4	9	1337	4AC	O7-C7-CM7	-2.24	117.90	122.06
2	5	3786	5MC	CM5-C5-C6	-2.24	119.86	122.85
2	5	4200	OMG	O6-C6-C5	-2.23	120.01	124.37
2	5	2054	OMG	O6-C6-C5	-2.23	120.02	124.37
2	5	729	2MG	O6-C6-C5	-2.22	120.03	124.37
2	5	4133	B8W	N2-C2-N1	-2.22	113.80	117.25
2	5	3884	P7G	C5-C4-N3	-2.22	120.09	124.00
2	5	1629	OMG	O6-C6-C5	-2.21	120.06	124.37
4	9	1830	UR3	O2-C2-N3	-2.20	118.23	121.34
2	5	4374	OMG	O6-C6-C5	-2.20	120.07	124.37
2	5	4310	OMU	O2-C2-N1	-2.20	119.86	122.79
2	5	4627	OMG	O6-C6-C5	-2.19	120.08	124.37
2	5	373	OMG	O6-C6-C5	-2.19	120.10	124.37
2	5	2428	OMG	O6-C6-C5	-2.18	120.11	124.37
4	9	822	PSU	C6-N1-C2	-2.18	120.45	122.68
2	5	4498	OMG	O6-C6-C5	-2.18	120.11	124.37
2	5	4534	UR3	C1'-N1-C2	2.18	120.67	116.99
2	5	3901	B8K	O6-C6-C5	-2.18	122.19	127.54
2	5	4694	B8K	O6-C6-C5	-2.18	122.19	127.54
2	5	3768	PSU	C6-C5-C4	2.18	119.72	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	4876	2MG	O6-C6-C5	-2.17	120.13	124.37
4	9	1374	5MC	O2-C2-N1	2.17	123.38	118.89
4	9	1219	B8Q	C1'-N1-C6	-2.17	116.11	120.84
82	v	715	DDE	CBW-CBI-NAD	2.16	118.03	115.28
2	5	1521	2MG	CM2-N2-C2	-2.15	119.10	123.86
2	5	3901	B8K	N1-C2-N3	-2.15	119.31	123.32
2	5	4554	7MG	N9-C8-N7	2.15	106.45	103.38
2	5	4601	UR3	C6-N1-C2	-2.14	119.87	121.79
2	5	3768	PSU	O2-C2-N1	-2.14	120.44	122.79
2	5	4874	OMG	O6-C6-C5	-2.14	120.20	124.37
4	9	1248	B8N	O4'-C1'-C2'	2.12	108.14	105.14
2	5	4375	MHG	N9-C8-N7	2.12	106.41	103.38
2	5	3903	BGH	N1-C2-N3	-2.11	119.38	123.32
2	5	4339	5MC	CM5-C5-C6	-2.11	120.03	122.85
4	9	612	PSU	O4'-C1'-C2'	2.11	108.12	105.14
2	5	3903	BGH	O6-C6-C5	-2.11	122.37	127.54
2	5	237	B9B	N2-C2-N1	2.11	120.53	117.25
2	5	1870	UR3	C1'-N1-C2	2.10	120.54	116.99
4	9	668	A2M	C5'-C4'-C3'	-2.10	107.30	115.18
2	5	2368	OMG	O6-C6-C5	-2.10	120.27	124.37
4	9	1842	4AC	N4-C4-N3	2.09	117.37	113.85
4	9	1703	OMC	O2-C2-N3	-2.09	118.92	122.33
2	5	2790	B9H	O2-C2-N1	-2.08	117.84	122.72
2	5	4624	OMU	O2-C2-N1	-2.08	120.02	122.79
2	5	3768	PSU	O4'-C1'-C2'	2.08	108.08	105.14
2	5	4641	OMG	O6-C6-C5	-2.07	120.32	124.37
2	5	1870	UR3	C6-N1-C2	-2.07	119.93	121.79
2	5	4476	B8W	N2-C2-N1	-2.07	114.03	117.25
2	5	1526	OMG	O6-C6-C5	-2.07	120.33	124.37
2	5	2790	B9H	C6-N1-C2	-2.07	119.94	121.79
2	5	4407	PSU	C6-C5-C4	2.05	119.63	118.20
2	5	4375	MHG	N9-C4-N3	2.04	128.52	125.47
4	9	1081	PSU	O4'-C1'-C2'	2.04	108.02	105.14
2	5	4694	B8K	N1-C2-N3	-2.04	119.52	123.32
2	5	4533	B8W	C2-N1-C6	2.03	119.34	116.08
4	9	1031	A2M	C5'-C4'-C3'	-2.03	107.58	115.18
4	9	1374	5MC	CM5-C5-C6	-2.02	120.15	122.85
4	9	174	OMC	O2-C2-N3	-2.02	119.05	122.33
2	5	1913	P7G	C5-C4-N3	-2.01	120.45	124.00
2	5	1320	OMG	N1-C2-N3	-2.01	119.56	123.32
2	5	4640	PSU	O2-C2-N1	-2.01	120.58	122.79
81	t	51	5CT	C4-C3-C2	-2.00	109.25	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	9	119	PSU	O4-C4-N3	-2.00	116.28	120.12

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	8	14	OMU	C1'-C2'-O2'-CM2
81	t	51	5CT	NZ-C1-C2-C3
2	5	237	B9B	C5-C6-O6-C61
2	5	237	B9B	N1-C6-O6-C61
2	5	1352	P4U	N3-C4-O4-C41
2	5	1352	P4U	C3'-C4'-C5'-O5'
2	5	1352	P4U	O4'-C4'-C5'-O5'
2	5	1578	B9B	C5-C6-O6-C61
2	5	1578	B9B	N1-C6-O6-C61
2	5	2368	OMG	O4'-C4'-C5'-O5'
2	5	2384	B8W	C5-C6-O6-C61
2	5	2384	B8W	C3'-C4'-C5'-O5'
2	5	2384	B8W	O4'-C4'-C5'-O5'
2	5	2428	OMG	O4'-C4'-C5'-O5'
2	5	2428	OMG	C3'-C4'-C5'-O5'
2	5	2758	B9B	C5-C6-O6-C61
2	5	2758	B9B	N1-C6-O6-C61
2	5	3705	OMC	C2'-C1'-N1-C6
2	5	3727	A2M	C1'-C2'-O2'-CM'
2	5	3768	PSU	O4'-C1'-C5-C4
2	5	3768	PSU	O4'-C1'-C5-C6
2	5	3789	A2M	O4'-C4'-C5'-O5'
2	5	3796	OMG	O4'-C4'-C5'-O5'
2	5	3796	OMG	C3'-C4'-C5'-O5'
2	5	3871	A2M	O4'-C4'-C5'-O5'
2	5	3871	A2M	C3'-C4'-C5'-O5'
2	5	3901	B8K	O4'-C4'-C5'-O5'
2	5	3903	BGH	C3'-C4'-C5'-O5'
2	5	4133	B8W	C5-C6-O6-C61
2	5	4133	B8W	N1-C6-O6-C61
2	5	4189	B8W	C5-C6-O6-C61
2	5	4189	B8W	N1-C6-O6-C61
2	5	4359	E6G	C5-C6-O6-C61
2	5	4359	E6G	N1-C6-O6-C61
2	5	4375	MHG	O4'-C4'-C5'-O5'
2	5	4407	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
2	5	4407	PSU	O4'-C1'-C5-C6
2	5	4476	B8W	C5-C6-O6-C61
2	5	4476	B8W	N1-C6-O6-C61
2	5	4527	A2M	O4'-C4'-C5'-O5'
2	5	4533	B8W	C5-C6-O6-C61
2	5	4533	B8W	N1-C6-O6-C61
2	5	4534	UR3	O4'-C4'-C5'-O5'
2	5	4534	UR3	C3'-C4'-C5'-O5'
2	5	4624	OMU	C1'-C2'-O2'-CM2
2	5	4640	PSU	C3'-C4'-C5'-O5'
2	5	4641	OMG	O4'-C4'-C5'-O5'
2	5	4874	OMG	O4'-C4'-C5'-O5'
2	5	4874	OMG	C3'-C4'-C5'-O5'
4	9	116	OMU	C1'-C2'-O2'-CM2
4	9	116	OMU	C3'-C4'-C5'-O5'
4	9	116	OMU	O4'-C4'-C5'-O5'
4	9	121	OMU	C3'-C4'-C5'-O5'
4	9	121	OMU	O4'-C4'-C5'-O5'
4	9	159	A2M	C3'-C4'-C5'-O5'
4	9	166	A2M	C3'-C4'-C5'-O5'
4	9	568	E3C	O4'-C1'-N1-C2
4	9	568	E3C	O4'-C1'-N1-C6
4	9	1248	B8N	N3-C31-C32-C33
4	9	1830	UR3	O4'-C1'-N1-C2
4	9	1832	6MZ	C5-C6-N6-C9
4	9	1832	6MZ	N1-C6-N6-C9
4	9	1851	MA6	O4'-C4'-C5'-O5'
4	9	1851	MA6	C3'-C4'-C5'-O5'
82	v	715	DDE	O-C-CA-CB
82	v	715	DDE	CA-CB-CG-ND1
2	5	2368	OMG	C3'-C4'-C5'-O5'
2	5	2405	A2M	C3'-C4'-C5'-O5'
2	5	3733	PSU	O4'-C4'-C5'-O5'
2	5	3768	PSU	C3'-C4'-C5'-O5'
2	5	3768	PSU	O4'-C4'-C5'-O5'
2	5	3789	A2M	C3'-C4'-C5'-O5'
2	5	3884	P7G	O4'-C4'-C5'-O5'
2	5	3901	B8K	C3'-C4'-C5'-O5'
2	5	3903	BGH	O4'-C4'-C5'-O5'
2	5	4454	PSU	C3'-C4'-C5'-O5'
2	5	4454	PSU	O4'-C4'-C5'-O5'
2	5	4504	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	5	4504	PSU	O4'-C4'-C5'-O5'
2	5	4527	A2M	C3'-C4'-C5'-O5'
2	5	4641	OMG	C3'-C4'-C5'-O5'
4	9	159	A2M	O4'-C4'-C5'-O5'
4	9	668	A2M	O4'-C4'-C5'-O5'
4	9	668	A2M	C3'-C4'-C5'-O5'
4	9	1081	PSU	O4'-C4'-C5'-O5'
2	5	2384	B8W	N1-C6-O6-C61
4	9	1830	UR3	O4'-C1'-N1-C6
2	5	1801	E7G	O4'-C4'-C5'-O5'
2	5	2405	A2M	O4'-C4'-C5'-O5'
2	5	3733	PSU	C3'-C4'-C5'-O5'
2	5	3884	P7G	C3'-C4'-C5'-O5'
2	5	4297	PSU	C3'-C4'-C5'-O5'
2	5	4640	PSU	O4'-C4'-C5'-O5'
4	9	119	PSU	O4'-C4'-C5'-O5'
4	9	166	A2M	O4'-C4'-C5'-O5'
4	9	568	E3C	C3'-C4'-C5'-O5'
4	9	568	E3C	O4'-C4'-C5'-O5'
4	9	683	OMG	O4'-C4'-C5'-O5'
4	9	1081	PSU	C3'-C4'-C5'-O5'
4	9	1703	OMC	O4'-C4'-C5'-O5'
4	9	1830	UR3	O4'-C4'-C5'-O5'
4	9	1830	UR3	C3'-C4'-C5'-O5'
2	5	4874	OMG	C3'-C2'-O2'-CM2
2	5	4451	5MC	C2'-C1'-N1-C6
2	5	3705	OMC	C2'-C1'-N1-C2
81	t	51	5CT	NZ-C1-C2-O1
4	9	517	OMC	C3'-C4'-C5'-O5'
2	5	1801	E7G	C3'-C4'-C5'-O5'
2	5	4297	PSU	O4'-C4'-C5'-O5'
2	5	4419	1MA	C3'-C4'-C5'-O5'
4	9	1243	PSU	O4'-C4'-C5'-O5'
2	5	4375	MHG	C72-C73-C74-C76
2	5	398	A2M	O4'-C4'-C5'-O5'
4	9	517	OMC	O4'-C4'-C5'-O5'
4	9	683	OMG	C3'-C4'-C5'-O5'
2	5	1913	P7G	C72-C71-N7-C8
82	v	715	DDE	N-CA-CB-CG
4	9	1851	MA6	C5-C6-N6-C9
2	5	4375	MHG	C2'-C1'-N9-C8
2	5	4451	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	5	2790	B9H	C32-C31-N3-C2
2	5	4375	MHG	C75-C73-C74-C76
82	v	715	DDE	NAD-CBI-CBW-NCB
82	v	715	DDE	OAG-CBI-CBW-NCB
2	5	4527	A2M	C1'-C2'-O2'-CM'
2	5	4641	OMG	C1'-C2'-O2'-CM2
4	9	668	A2M	C1'-C2'-O2'-CM'
81	t	51	5CT	C2-C1-NZ-CE
2	5	4451	5MC	O4'-C1'-N1-C6
2	5	4504	PSU	C4'-C5'-O5'-P
4	9	644	OMG	C4'-C5'-O5'-P
2	5	4198	I4U	O4'-C4'-C5'-O5'
82	v	715	DDE	CAU-CBW-NCB-CAB
82	v	715	DDE	CAU-CBW-NCB-CAC
82	v	715	DDE	CAU-CBW-NCB-CAA
2	5	3705	OMC	O4'-C1'-N1-C6
82	v	715	DDE	C-CA-CB-CG
2	5	373	OMG	C4'-C5'-O5'-P
4	9	159	A2M	C4'-C5'-O5'-P
4	9	119	PSU	C3'-C4'-C5'-O5'
4	9	822	PSU	C3'-C4'-C5'-O5'
2	5	4451	5MC	O4'-C1'-N1-C2
82	v	715	DDE	CAT-CAU-CBW-CBI
2	5	4375	MHG	C72-C71-N7-C5
2	5	1538	A2M	C4'-C5'-O5'-P
4	9	1850	MA6	C5-C6-N6-C9
2	5	4419	1MA	O4'-C4'-C5'-O5'
4	9	1703	OMC	C3'-C4'-C5'-O5'
2	5	3705	OMC	O4'-C1'-N1-C2
2	5	1330	A2M	C4'-C5'-O5'-P
2	5	3901	B8K	C4'-C5'-O5'-P
4	9	1081	PSU	C4'-C5'-O5'-P
2	5	1528	A2M	C3'-C2'-O2'-CM'
2	5	2367	A2M	C3'-C2'-O2'-CM'
82	v	715	DDE	CE1-CAT-CAU-CBW
2	5	2301	E7G	C72-C71-N7-C8
2	5	729	2MG	O4'-C4'-C5'-O5'
2	5	4375	MHG	C72-C71-N7-C8
2	5	1681	PSU	O4'-C1'-C5-C4
2	5	4454	PSU	O4'-C1'-C5-C4
2	5	4535	PSU	O4'-C1'-C5-C4
4	9	1248	B8N	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
4	9	668	A2M	C3'-C2'-O2'-CM'
4	9	1243	PSU	C3'-C4'-C5'-O5'
82	v	715	DDE	CBI-CBW-NCB-CAB
82	v	715	DDE	CBI-CBW-NCB-CAC
82	v	715	DDE	CBI-CBW-NCB-CAA
81	t	51	5CT	C-CA-CB-CG
2	5	1913	P7G	C72-C71-N7-C5
2	5	4375	MHG	O4'-C1'-N9-C8
2	5	4198	I4U	C3'-C4'-C5'-O5'
4	9	822	PSU	O4'-C4'-C5'-O5'
82	v	715	DDE	CAU-CAT-CE1-ND1
2	5	1681	PSU	O4'-C1'-C5-C6
2	5	4535	PSU	O4'-C1'-C5-C6
2	5	4640	PSU	O4'-C1'-C5-C6
4	9	1248	B8N	C31-C32-C33-N34
2	5	3871	A2M	C4'-C5'-O5'-P
2	5	398	A2M	C3'-C4'-C5'-O5'
2	5	1538	A2M	O4'-C4'-C5'-O5'
2	5	2426	OMC	O4'-C4'-C5'-O5'
2	5	2777	OMG	O4'-C4'-C5'-O5'
2	5	1663	I4U	C42-C41-O4-C4
81	t	51	5CT	CD-CE-NZ-C1
82	v	715	DDE	CA-CB-CG-CD2
2	5	4675	B8T	C4'-C5'-O5'-P
2	5	4874	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 208 ligands modelled in this entry, 208 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	9	12
2	5	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1223:G	O3'	1237:G	P	24.58
1	9	834:C	O3'	841:G	P	17.65
1	9	697:G	O3'	729:C	P	17.13
1	9	756:C	O3'	788:G	P	17.02
1	5	994:U	O3'	1068:G	P	16.68
1	5	182:G	O3'	189:G	P	16.36
1	5	1368:U	O3'	1372:A	P	14.19
1	5	4733:A	O3'	4739:G	P	11.77
1	5	1184:C	O3'	1187:C	P	10.43
1	9	745:C	O3'	749:U	P	9.60
1	5	4744:G	O3'	4747:G	P	6.60
1	5	500:G	O3'	504:G	P	5.76
1	9	798:G	O3'	799:U	P	5.40
1	9	322:C	O3'	323:C	P	4.79
1	9	304:C	O3'	305:U	P	4.65
1	9	736:C	O3'	743:U	P	4.64
1	9	309:G	O3'	310:C	P	3.69
1	5	1243:C	O3'	1248:G	P	3.40
1	5	751:G	O3'	752:G	P	3.29
1	9	902:G	O3'	903:A	P	3.24
1	9	903:A	O3'	904:A	P	3.22
1	9	1295:A	O3'	1296:U	P	3.17
1	5	267:G	O3'	268:G	P	3.07

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13114. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

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

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

9 Map-model fit

This section was not generated.