



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 10:44 PM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

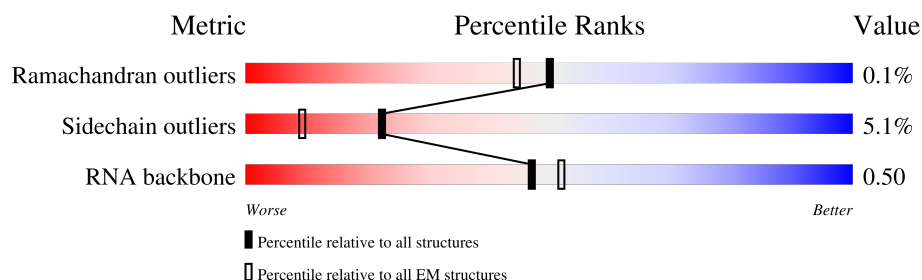
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





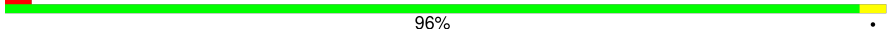

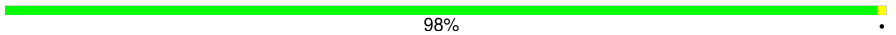
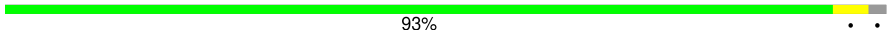

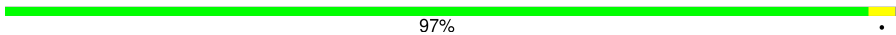

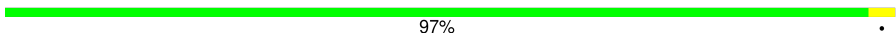
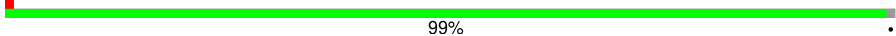




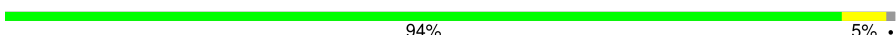
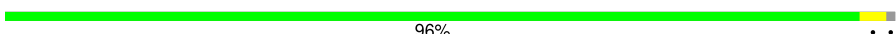



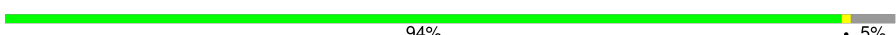
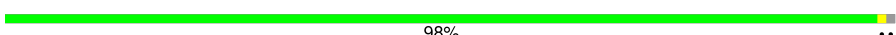

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	413	
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

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

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

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

## 2 Entry composition

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

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

- Molecule 1 is a protein called Ribosomal protein L8.

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

- Molecule 2 is a protein called Ribosomal protein L3.

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

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

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

- Molecule 4 is a protein called Ribosomal\_L18\_c domain-containing protein.

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 11 is a protein called eL13.

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



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

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called Ribosomal protein L18.

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

There are 12 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 17 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

There are 11 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 21 is a protein called Ribosomal protein L23.

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

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

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

- Molecule 23 is a protein called eL23.

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

- Molecule 24 is a protein called uL24.

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

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

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

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

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

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

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

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

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

- Molecule 33 is a protein called eL35.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	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 37 is a protein called eL39.

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

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

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

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

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

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

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

- Molecule 45 is a protein called NC.

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

- Molecule 46 is a RNA chain called P\_tRNA.

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

- Molecule 47 is a RNA chain called E\_tRNA.

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

- Molecule 48 is a RNA chain called 28S\_rRNA.

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

- Molecule 49 is a RNA chain called 5S\_rRNA.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 50 is a RNA chain called 5.8S\_rRNA.

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

- Molecule 51 is a RNA chain called 18S\_rRNA.

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

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

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called Ribosomal protein S3.

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 57 is a protein called uS7.



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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	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 61 is a protein called uS4.

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

- Molecule 62 is a protein called S10\_pectin domain-containing protein.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	138	Total	C	N	O	S	0	0
			1075	674	206	192	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 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

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

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

- Molecule 77 is a protein called eS25.

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	28	ARG	CYS	conflict	UNP G1TFE8
aa	56	ALA	VAL	conflict	UNP G1TFE8
aa	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

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

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

- Molecule 85 is a RNA chain called mRNA.

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

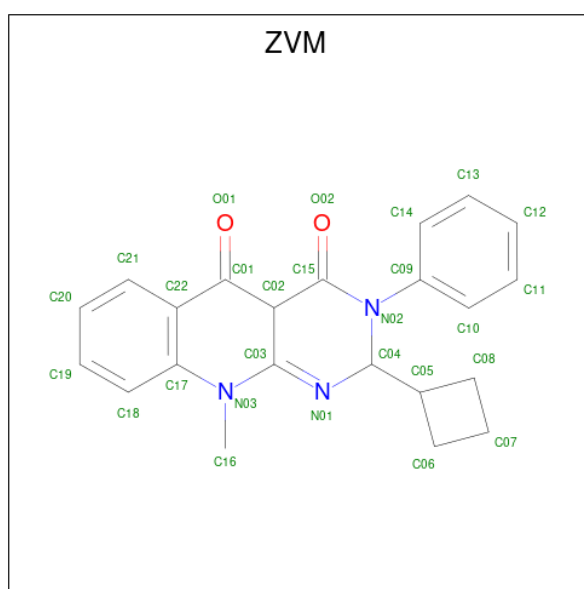
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0

*Continued on next page...*

Continued from previous page...

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

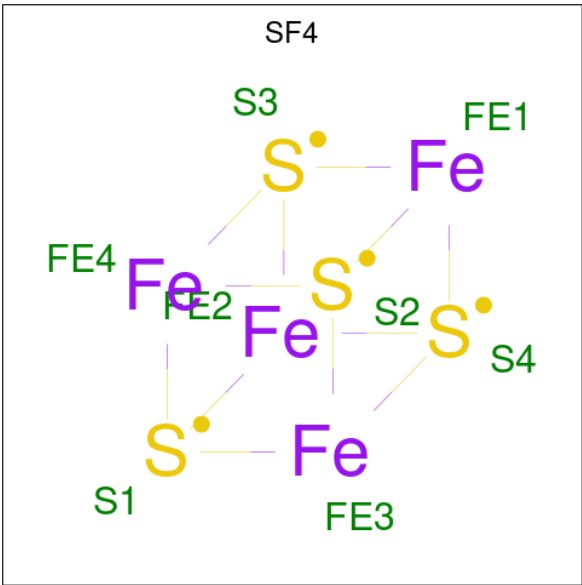
- Molecule 90 is (2S,4aS)-2-cyclobutyl-10-methyl-3-phenyl-2,10-dihydropyrimido[4,5-b]quinoline-4,5(3H,4aH)-dione (three-letter code: ZVM) (formula: C<sub>22</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 91 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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

- Molecule 92 is water.

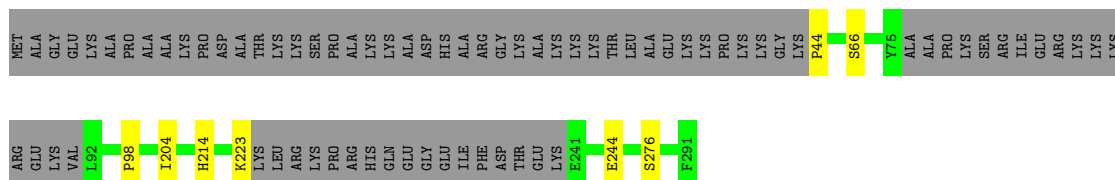
Mol	Chain	Residues	Atoms		AltConf
92	A	6	Total	O	0
			6	6	
92	B	2	Total	O	0
			2	2	
92	C	1	Total	O	0
			1	1	
92	F	1	Total	O	0
			1	1	
92	I	1	Total	O	0
			1	1	
92	L	1	Total	O	0
			1	1	
92	N	4	Total	O	0
			4	4	
92	Q	1	Total	O	0
			1	1	
92	R	1	Total	O	0
			1	1	
92	V	2	Total	O	0
			2	2	

Continued on next page...


*Continued from previous page...*

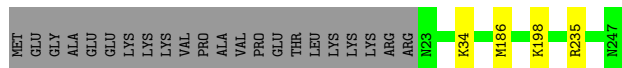
Mol	Chain	Residues	Atoms		AltConf
92	X	2	Total 2	O 2	0
92	a	5	Total 5	O 5	0
92	e	5	Total 5	O 5	0
92	j	1	Total 1	O 1	0
92	o	2	Total 2	O 2	0
92	5	723	Total 723	O 723	0
92	7	13	Total 13	O 13	0
92	8	8	Total 8	O 8	0
92	9	173	Total 173	O 173	0
92	II	1	Total 1	O 1	0
92	OO	1	Total 1	O 1	0
92	XX	1	Total 1	O 1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





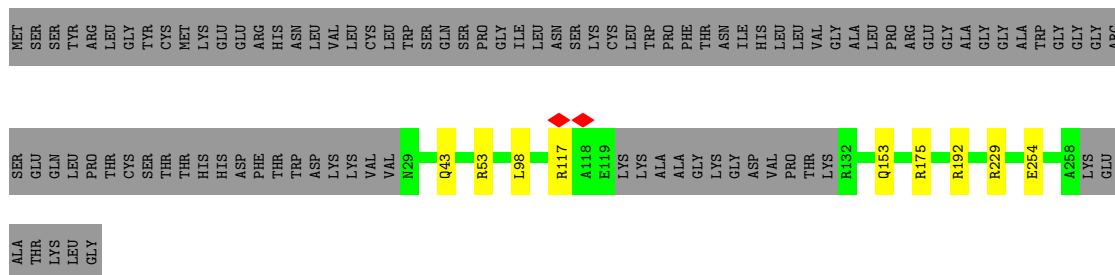
• Molecule 6: 60S ribosomal protein L7

Chain F:  89% • 9%



• Molecule 7: 60S ribosomal protein L7a

Chain G:  66% • 32%



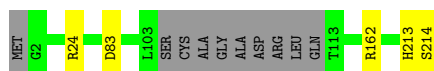
• Molecule 8: 60S ribosomal protein L9

Chain H:  97% • •




• Molecule 9: 60S ribosomal protein L10

Chain I:  93% • 5%



• Molecule 10: 60S ribosomal protein L11

Chain J:  89% • 6%



• Molecule 11: eL13

Chain L:  96% •



A diagram of a protein structure represented as a horizontal bar. The bar is divided into segments by vertical lines. The segments are colored: the first and last segments are red, and the middle segments are yellow. The residues are labeled as follows: M1 (red), R29 (yellow), K53 (yellow), M93 (yellow), T102 (yellow), K164 (yellow), and F176 (red).

Chain T: 

Chain U:  73% 23%

MET	ALA	PRO	VAL	LYS	LEU	VAL	ALA	LYS	GLY	GLY	LYS	LYS	LYS	LYS	GLN	L18	K67	K93	R101	E108	F115	TLE	ASN	GLN	ASP	GLU	GLU	GLU	GLU	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain V:  92% • 7%

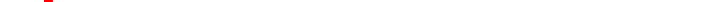
MET  
SER  
LYS  
ARG  
GLY  
ARG  
GLY  
GLY  
SER  
SER  
G11  
K109  
A140

Chain W:  39% 60%

[illegible]

Chain X:  73% 26%

MET	ALA	PRO	LYS	ALA	LYS	GLU	ALA	PRO	PRO	ALA	ALA	PRO	PRO	LYS	VAL	GLU	ALA	LYS	ALA	LYS	LYS	LEU	LYS	ALA	LYS	LYS	ALA	ALA	VAL	LEU	LYS	GLY	VAL	HIS	SER	HIS	LYS	LYS	LYS	LYS	I40	R63	D143	I155	T16
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----

Chain Y:  89% 8%

- |      |
|------|
| MET  |
| A2   |
| K11  |
| L129 |
| ARG  |
| SER  |
| GLU  |
| GLU  |
| ASN  |
| GLU  |

- Molecule 31: eL33

Chain f:  98% ..



- Molecule 32: 60S ribosomal protein L34

Chain g:  94% ..



- Molecule 33: eL35

Chain h:  94% 5% ..




- Molecule 34: 60S ribosomal protein L36

Chain i:  94% ..




- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: 60S ribosomal protein L38

Chain k:  89% 7% ..



- Molecule 37: eL39

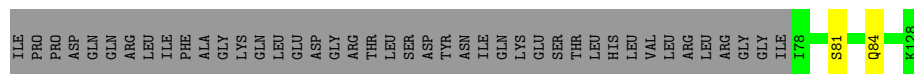
Chain l:  92% ..





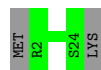
- Molecule 38: Ubiquitin A-52 residue ribosomal protein fusion product 1

Chain m:  53% 45%



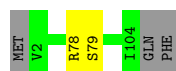
- Molecule 39: eL41

Chain n:  92% 8%



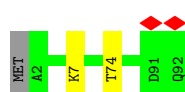
- Molecule 40: eL42

Chain o:  95%




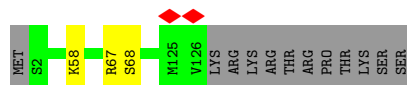
- Molecule 41: eL43

Chain p:  97%



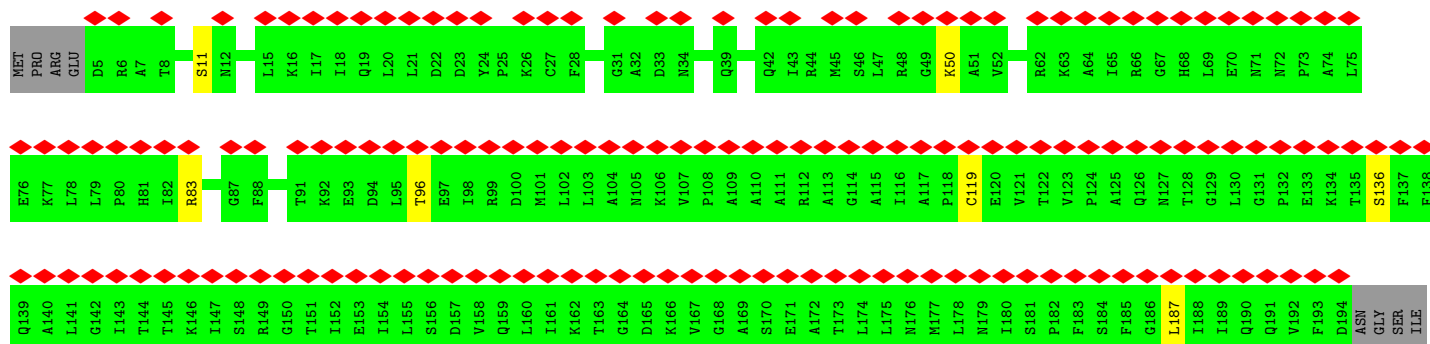
- Molecule 42: eL28

Chain r:  89% 9%

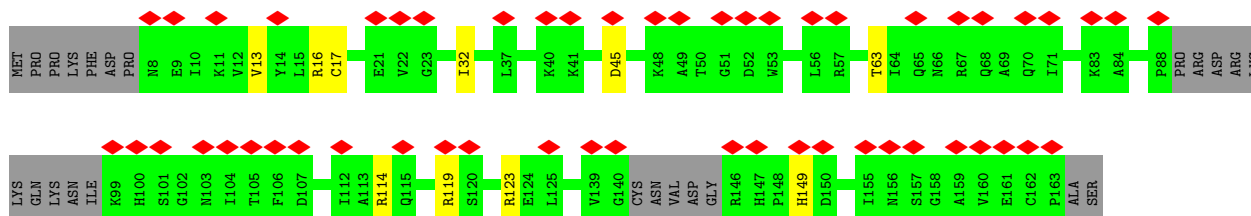
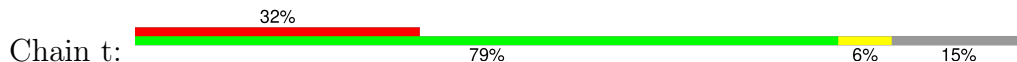


- Molecule 43: 60S acidic ribosomal protein P0

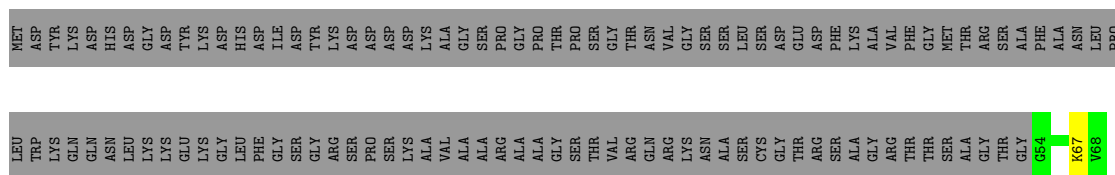
Chain s:  50% 58% 40%



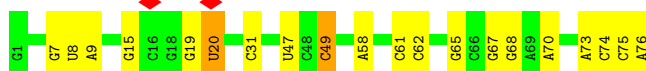
- Molecule 44: 60S ribosomal protein L12



- Molecule 45: NC



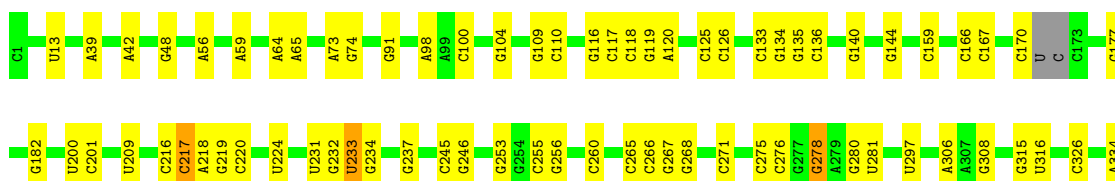
- Molecule 46: P tRNA



- Molecule 47: E tRNA

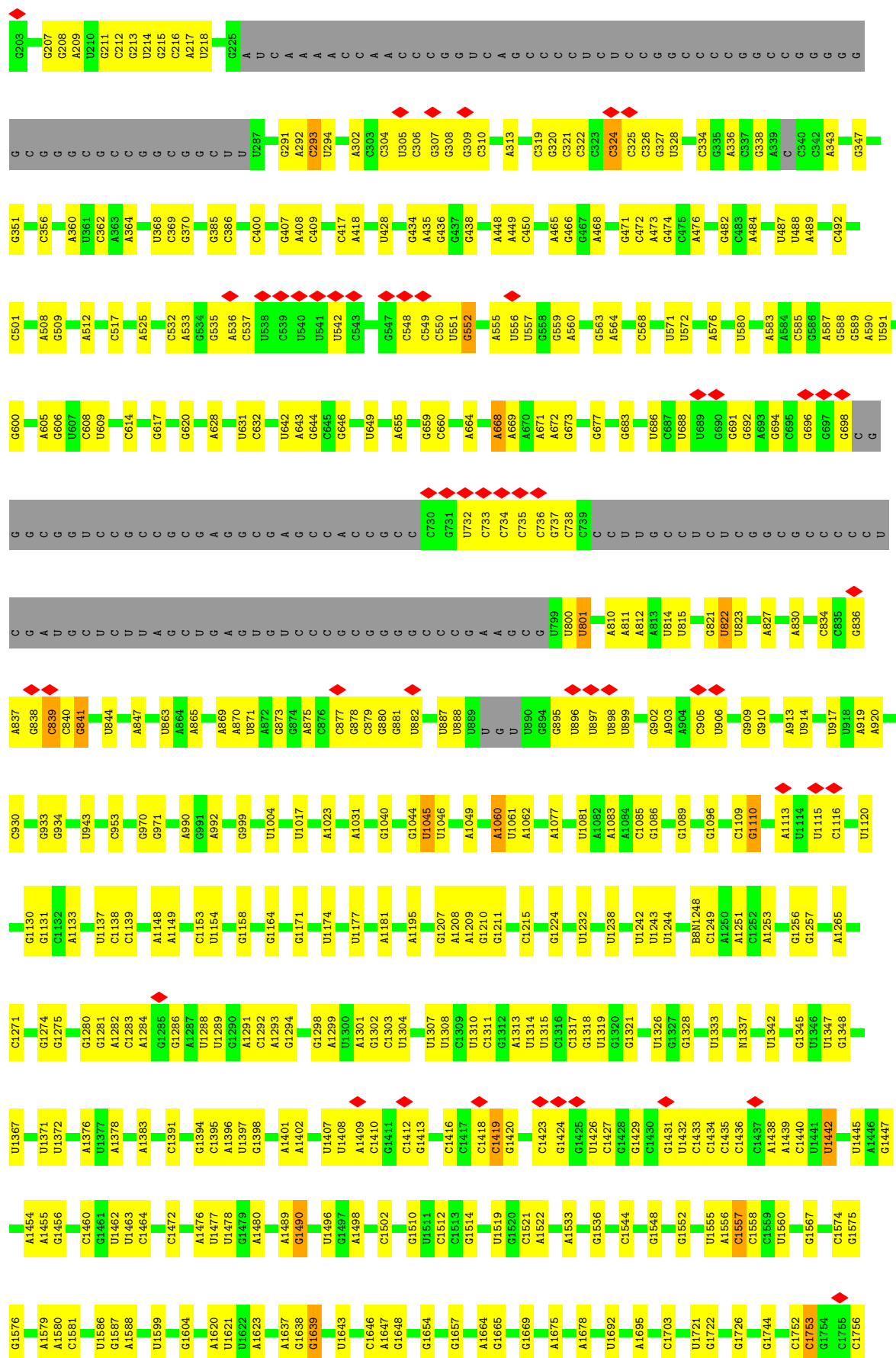


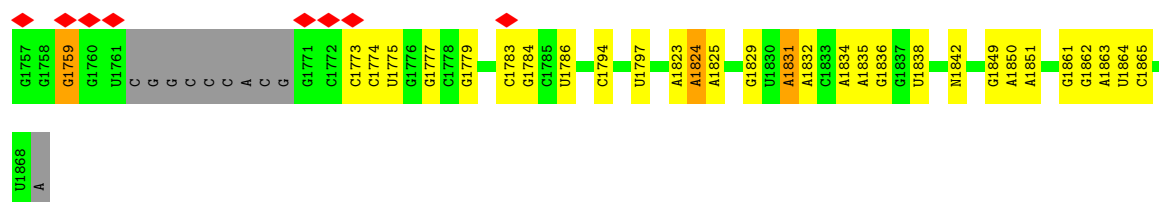
- Molecule 48: 28S rRNA



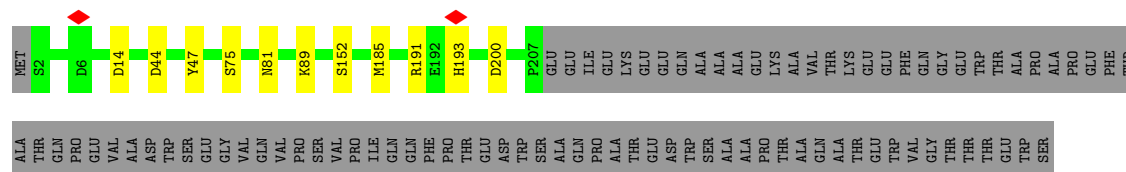




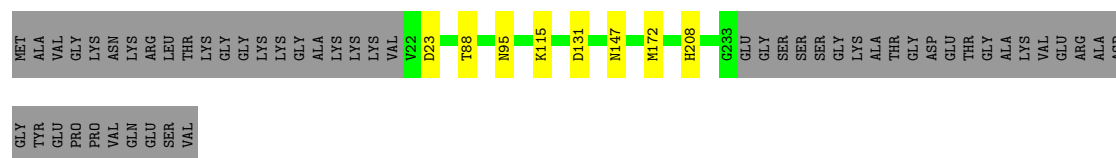
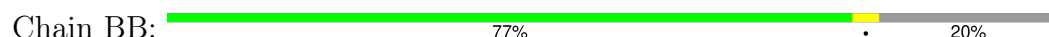




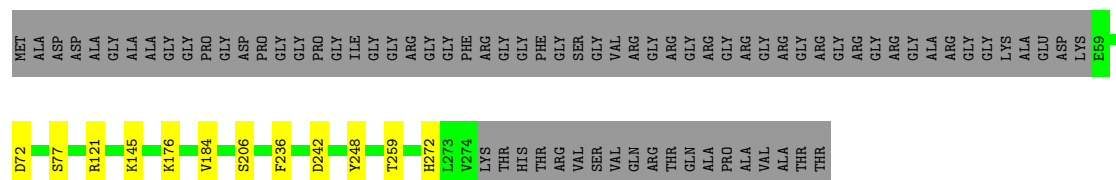
- Molecule 52: uS2 (SA)



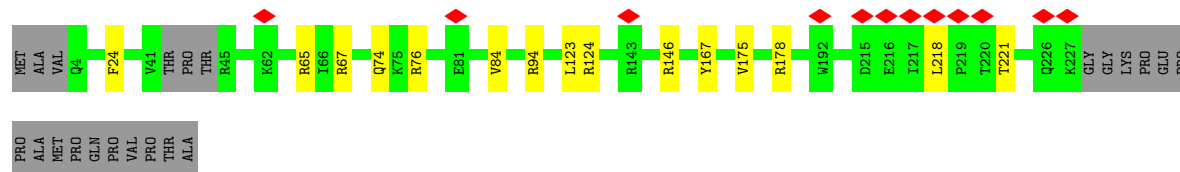
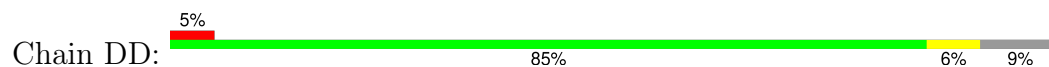
- Molecule 53: eS1



- Molecule 54: uS5



- Molecule 55: Ribosomal protein S3



- Molecule 56: eS4 (S4 X isoform)





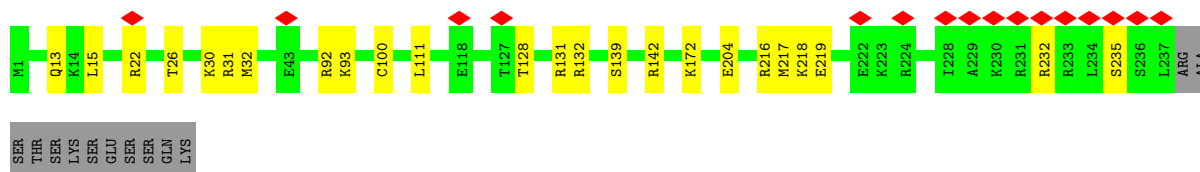
• Molecule 57: uS7

Chain FF: 81% 7% 11%



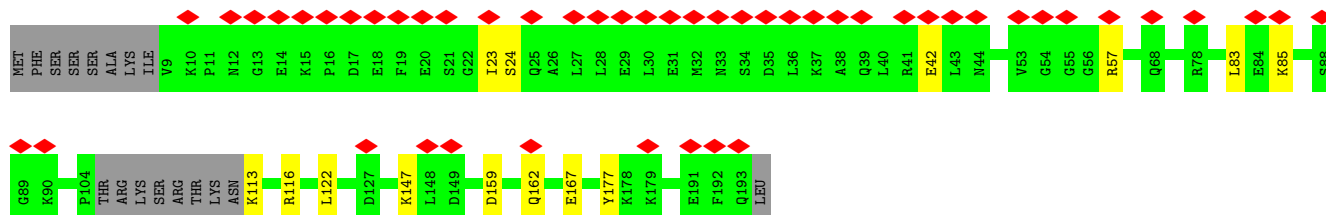
• Molecule 58: eS6

Chain GG: 6% 86% 10% 5%



• Molecule 59: eS7

Chain HH: 25% 84% 7% 9%



• Molecule 60: eS8

Chain II: 5% 93% 6%



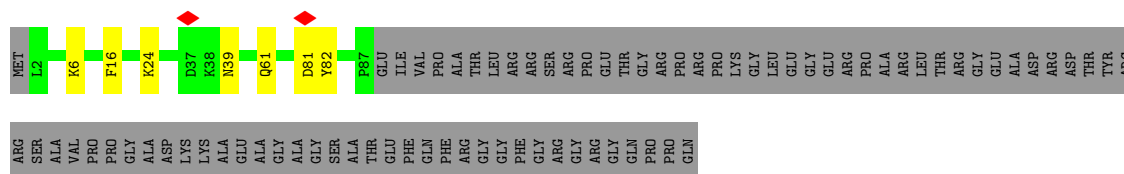
• Molecule 61: uS4

Chain JJ: 91% 5% 5%

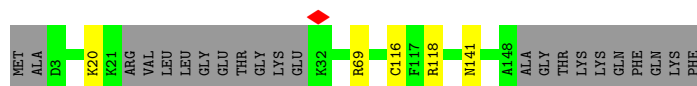
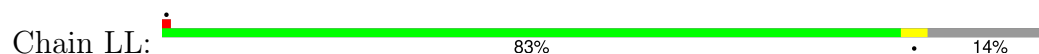


• Molecule 62: S10\_pectin domain-containing protein

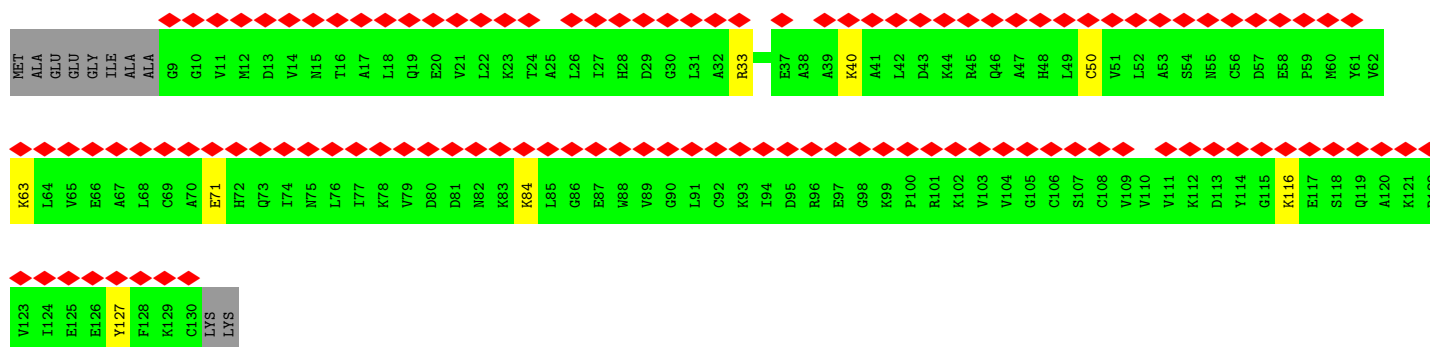
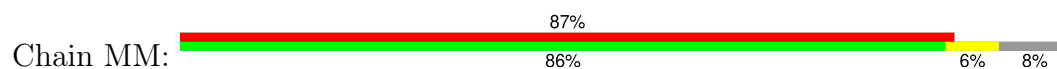
Chain KK: 48% 48%



• Molecule 63: uS17



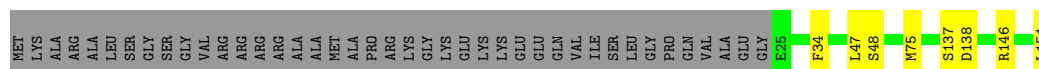
• Molecule 64: eS12



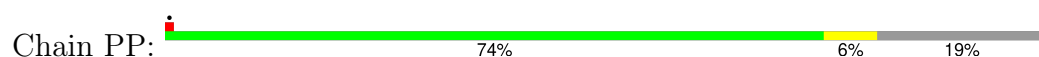
• Molecule 65: uS15



• Molecule 66: uS11



• Molecule 67: uS19






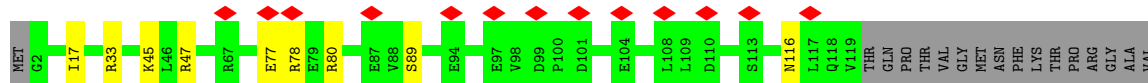
- Molecule 68: uS9

Chain QQ:  92%




- Molecule 69: eS17

Chain RR:  10% 81% 7% 13%



- Molecule 70: uS13

Chain SS:  86% 7% 8%




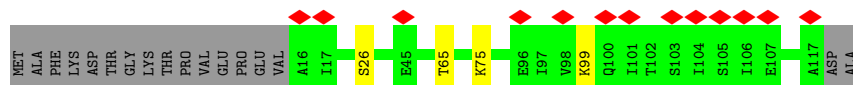
- Molecule 71: eS19

Chain TT:  92% 5%



- Molecule 72: uS10

Chain UU:  11% 82% 14%



- Molecule 73: eS21

Chain VV:  93% 5%



- Molecule 74: uS8

Chain WW:  95%



- Molecule 75: uS12

Chain XX:  95%



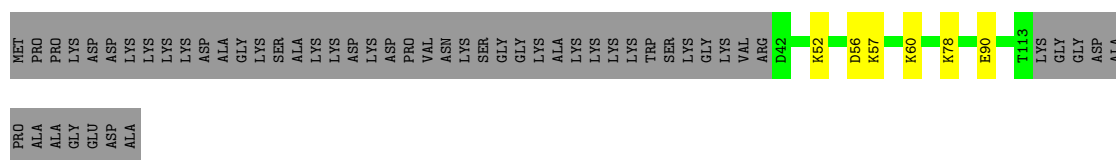
- Molecule 76: 40S ribosomal protein S24

Chain YY:  89% 5% 5%




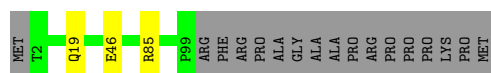
- Molecule 77: eS25

Chain ZZ:  53% 5% 42%



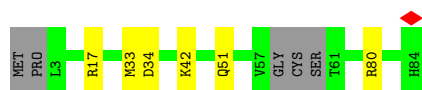
- Molecule 78: 40S ribosomal protein S26

Chain aa:  83% 15%




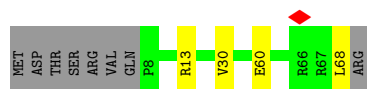
- Molecule 79: eS27

Chain bb:  87% 7% 6%




- Molecule 80: eS28

Chain cc:  83% 6% 12%

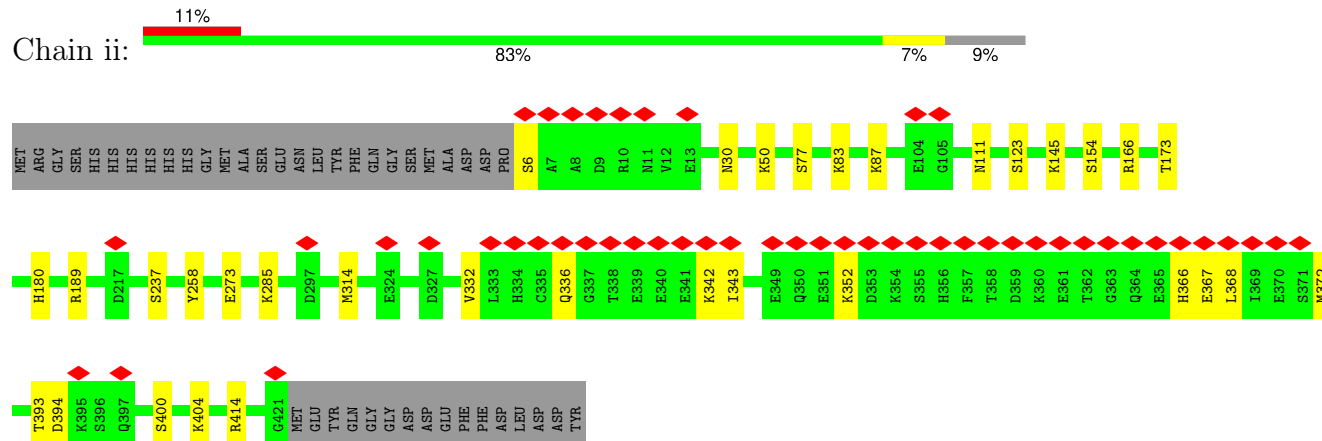


- Molecule 81: uS14

Chain dd:  84% 11% 5%



- Molecule 86: Eukaryotic peptide chain release factor subunit 1



- Molecule 87: ATP binding cassette subfamily E member 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, OMC, OMU, B8N, 6MZ, ZVM, G7M, SF4, MA6, 1MA, UR3, 2MG, 5MC, UY1, MG, ZN, 4AC, B9B, A2M

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

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

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

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

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

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

All (13) bond length outliers are listed below:

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



All (172) bond angle outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

## 5.2 Too-close contacts [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	A	242/257 (94%)	226 (93%)	16 (7%)	0	100	100
2	B	392/403 (97%)	376 (96%)	16 (4%)	0	100	100
3	C	360/413 (87%)	348 (97%)	12 (3%)	0	100	100
4	D	287/297 (97%)	270 (94%)	16 (6%)	1 (0%)	37	56
5	E	209/291 (72%)	189 (90%)	20 (10%)	0	100	100
6	F	223/247 (90%)	218 (98%)	5 (2%)	0	100	100
7	G	214/319 (67%)	202 (94%)	12 (6%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	200/214 (94%)	193 (96%)	7 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	165/178 (93%)	151 (92%)	13 (8%)	1 (1%)	22	39
11	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
12	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
13	N	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
14	O	196/203 (97%)	187 (95%)	8 (4%)	1 (0%)	25	44
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
16	Q	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
17	R	177/196 (90%)	172 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	96/128 (75%)	88 (92%)	8 (8%)	0	100	100
21	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
22	W	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
23	X	114/156 (73%)	108 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
25	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
26	a	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	19	35
27	b	73/245 (30%)	70 (96%)	3 (4%)	0	100	100
28	c	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
29	d	96/125 (77%)	94 (98%)	2 (2%)	0	100	100
30	e	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
31	f	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
32	g	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
33	h	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
34	i	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
35	j	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
36	k	66/70 (94%)	60 (91%)	5 (8%)	1 (2%)	8	16
37	l	47/51 (92%)	45 (96%)	2 (4%)	0	100	100
38	m	49/93 (53%)	47 (96%)	2 (4%)	0	100	100
39	n	21/25 (84%)	21 (100%)	0	0	100	100
40	o	101/106 (95%)	95 (94%)	6 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
42	r	123/137 (90%)	113 (92%)	10 (8%)	0	100	100
43	s	188/318 (59%)	163 (87%)	25 (13%)	0	100	100
44	t	135/165 (82%)	113 (84%)	21 (16%)	1 (1%)	19	35
45	1	13/130 (10%)	11 (85%)	2 (15%)	0	100	100
52	AA	204/295 (69%)	189 (93%)	15 (7%)	0	100	100
53	BB	210/264 (80%)	200 (95%)	10 (5%)	0	100	100
54	CC	214/293 (73%)	202 (94%)	12 (6%)	0	100	100
55	DD	217/243 (89%)	196 (90%)	21 (10%)	0	100	100
56	EE	257/263 (98%)	231 (90%)	26 (10%)	0	100	100
57	FF	177/204 (87%)	163 (92%)	13 (7%)	1 (1%)	22	39
58	GG	235/249 (94%)	205 (87%)	29 (12%)	1 (0%)	30	49
59	HH	173/194 (89%)	146 (84%)	27 (16%)	0	100	100
60	II	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
61	JJ	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
62	KK	84/165 (51%)	76 (90%)	8 (10%)	0	100	100
63	LL	132/158 (84%)	125 (95%)	7 (5%)	0	100	100
64	MM	120/132 (91%)	91 (76%)	29 (24%)	0	100	100
65	NN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
66	OO	125/168 (74%)	121 (97%)	4 (3%)	0	100	100
67	PP	115/145 (79%)	106 (92%)	9 (8%)	0	100	100
68	QQ	138/146 (94%)	128 (93%)	10 (7%)	0	100	100
69	RR	116/135 (86%)	106 (91%)	10 (9%)	0	100	100
70	SS	138/152 (91%)	130 (94%)	8 (6%)	0	100	100
71	TT	136/145 (94%)	124 (91%)	12 (9%)	0	100	100
72	UU	100/119 (84%)	89 (89%)	11 (11%)	0	100	100
73	VV	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
76	YY	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
77	ZZ	70/125 (56%)	64 (91%)	6 (9%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	aa	96/115 (84%)	86 (90%)	10 (10%)	0	100	100
79	bb	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
80	cc	59/69 (86%)	54 (92%)	5 (8%)	0	100	100
81	dd	51/56 (91%)	45 (88%)	6 (12%)	0	100	100
82	ee	43/133 (32%)	37 (86%)	6 (14%)	0	100	100
83	ff	59/156 (38%)	49 (83%)	10 (17%)	0	100	100
84	gg	300/317 (95%)	252 (84%)	48 (16%)	0	100	100
86	ii	414/459 (90%)	380 (92%)	33 (8%)	1 (0%)	44	64
87	jj	574/599 (96%)	529 (92%)	44 (8%)	1 (0%)	44	64
All	All	12249/14542 (84%)	11407 (93%)	832 (7%)	10 (0%)	50	69

All (10) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/199 (94%)	181 (97%)	6 (3%)	34	60
2	B	336/348 (97%)	326 (97%)	10 (3%)	36	63
3	C	302/337 (90%)	291 (96%)	11 (4%)	30	56

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	245/250 (98%)	237 (97%)	8 (3%)	33	59
5	E	191/251 (76%)	183 (96%)	8 (4%)	25	49
6	F	196/215 (91%)	192 (98%)	4 (2%)	50	75
7	G	189/272 (70%)	180 (95%)	9 (5%)	21	43
8	H	169/171 (99%)	165 (98%)	4 (2%)	44	70
9	I	174/181 (96%)	169 (97%)	5 (3%)	37	64
10	J	140/149 (94%)	133 (95%)	7 (5%)	20	41
11	L	175/176 (99%)	168 (96%)	7 (4%)	27	51
12	M	117/161 (73%)	116 (99%)	1 (1%)	75	90
13	N	171/172 (99%)	168 (98%)	3 (2%)	54	78
14	O	170/173 (98%)	162 (95%)	8 (5%)	22	44
15	P	134/163 (82%)	130 (97%)	4 (3%)	36	63
16	Q	164/165 (99%)	159 (97%)	5 (3%)	36	63
17	R	158/175 (90%)	151 (96%)	7 (4%)	24	47
18	S	157/157 (100%)	152 (97%)	5 (3%)	34	60
19	T	139/140 (99%)	139 (100%)	0	100	100
20	U	88/114 (77%)	84 (96%)	4 (4%)	23	46
21	V	100/107 (94%)	99 (99%)	1 (1%)	73	88
22	W	55/126 (44%)	53 (96%)	2 (4%)	30	56
23	X	104/134 (78%)	102 (98%)	2 (2%)	52	77
24	Y	124/135 (92%)	119 (96%)	5 (4%)	27	51
25	Z	117/118 (99%)	110 (94%)	7 (6%)	16	33
26	a	119/120 (99%)	115 (97%)	4 (3%)	32	58
27	b	62/184 (34%)	60 (97%)	2 (3%)	34	60
28	c	80/98 (82%)	73 (91%)	7 (9%)	8	17
29	d	91/110 (83%)	90 (99%)	1 (1%)	70	87
30	e	114/121 (94%)	113 (99%)	1 (1%)	75	90
31	f	88/89 (99%)	87 (99%)	1 (1%)	70	87
32	g	98/100 (98%)	94 (96%)	4 (4%)	26	50
33	h	109/110 (99%)	103 (94%)	6 (6%)	18	37
34	i	86/89 (97%)	83 (96%)	3 (4%)	31	57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	j	73/80 (91%)	67 (92%)	6 (8%)	9	19
36	k	63/65 (97%)	57 (90%)	6 (10%)	7	14
37	l	46/48 (96%)	44 (96%)	2 (4%)	25	48
38	m	47/84 (56%)	45 (96%)	2 (4%)	25	48
39	n	22/24 (92%)	22 (100%)	0	100	100
40	o	91/94 (97%)	89 (98%)	2 (2%)	47	73
41	p	74/75 (99%)	72 (97%)	2 (3%)	40	67
42	r	109/121 (90%)	106 (97%)	3 (3%)	38	65
43	s	159/258 (62%)	152 (96%)	7 (4%)	24	47
44	t	115/137 (84%)	106 (92%)	9 (8%)	10	21
45	1	13/102 (13%)	12 (92%)	1 (8%)	10	22
52	AA	172/244 (70%)	161 (94%)	11 (6%)	14	30
53	BB	193/231 (84%)	185 (96%)	8 (4%)	26	50
54	CC	182/225 (81%)	170 (93%)	12 (7%)	14	28
55	DD	185/202 (92%)	170 (92%)	15 (8%)	9	20
56	EE	222/225 (99%)	210 (95%)	12 (5%)	18	37
57	FF	154/170 (91%)	140 (91%)	14 (9%)	7	16
58	GG	207/218 (95%)	184 (89%)	23 (11%)	5	10
59	HH	158/174 (91%)	144 (91%)	14 (9%)	8	17
60	II	178/180 (99%)	166 (93%)	12 (7%)	13	28
61	JJ	161/168 (96%)	152 (94%)	9 (6%)	17	36
62	KK	78/136 (57%)	71 (91%)	7 (9%)	8	16
63	LL	125/142 (88%)	121 (97%)	4 (3%)	34	60
64	MM	102/108 (94%)	94 (92%)	8 (8%)	10	21
65	NN	130/131 (99%)	123 (95%)	7 (5%)	18	37
66	OO	100/130 (77%)	92 (92%)	8 (8%)	10	20
67	PP	106/130 (82%)	97 (92%)	9 (8%)	8	18
68	QQ	116/121 (96%)	111 (96%)	5 (4%)	25	48
69	RR	107/121 (88%)	98 (92%)	9 (8%)	9	19
70	SS	122/132 (92%)	112 (92%)	10 (8%)	9	19
71	TT	109/115 (95%)	104 (95%)	5 (5%)	23	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	UU	93/107 (87%)	89 (96%)	4 (4%)	25	48
73	VV	65/67 (97%)	61 (94%)	4 (6%)	15	31
74	WW	112/113 (99%)	107 (96%)	5 (4%)	23	46
75	XX	113/115 (98%)	108 (96%)	5 (4%)	24	47
76	YY	107/112 (96%)	100 (94%)	7 (6%)	14	29
77	ZZ	64/103 (62%)	58 (91%)	6 (9%)	7	15
78	aa	85/98 (87%)	82 (96%)	3 (4%)	31	57
79	bb	72/76 (95%)	66 (92%)	6 (8%)	9	19
80	cc	54/62 (87%)	50 (93%)	4 (7%)	11	23
81	dd	47/49 (96%)	41 (87%)	6 (13%)	3	7
82	ee	39/106 (37%)	36 (92%)	3 (8%)	10	22
83	ff	59/140 (42%)	54 (92%)	5 (8%)	8	18
84	gg	263/275 (96%)	238 (90%)	25 (10%)	7	14
86	ii	358/394 (91%)	326 (91%)	32 (9%)	8	17
87	jj	508/526 (97%)	485 (96%)	23 (4%)	23	46
All	All	10707/12344 (87%)	10165 (95%)	542 (5%)	22	40

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

### 5.3.3 RNA ⓘ

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



All (1170) RNA backbone outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

All (111) RNA pucker outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
48	OMG	5	4499	48	19,26,27	2.47	8 (42%)	21,38,41	1.51	4 (19%)
48	OMC	5	2422	48,88	19,22,23	2.93	8 (42%)	25,31,34	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	OMG	5	4494	48	19,26,27	2.27	8 (42%)	21,38,41	1.44	5 (23%)
48	OMG	5	2876	48	19,26,27	2.37	8 (42%)	21,38,41	1.38	3 (14%)
51	OMU	9	116	51	19,22,23	2.80	6 (31%)	25,31,34	1.78	5 (20%)
50	OMG	8	75	50	19,26,27	2.33	8 (42%)	21,38,41	1.48	5 (23%)
48	6MZ	5	4220	48	17,25,26	1.38	1 (5%)	15,36,39	2.33	3 (20%)
48	A2M	5	3830	48	18,25,26	4.29	6 (33%)	20,36,39	3.36	5 (25%)
48	A2M	5	3825	48	18,25,26	4.40	6 (33%)	20,36,39	3.08	4 (20%)
48	OMC	5	2351	48	19,22,23	2.74	8 (42%)	25,31,34	0.82	0
51	A2M	9	668	51,88	18,25,26	4.35	5 (27%)	20,36,39	3.65	7 (35%)
48	A2M	5	1871	48,88	18,25,26	4.28	6 (33%)	20,36,39	3.28	4 (20%)
48	PSU	5	4579	48	17,20,22	1.05	1 (5%)	21,28,33	1.89	4 (19%)
48	A2M	5	4571	48	18,25,26	4.48	7 (38%)	20,36,39	3.46	4 (20%)
48	OMG	5	3627	48	19,26,27	2.38	8 (42%)	21,38,41	1.48	3 (14%)
48	OMG	5	4623	48	19,26,27	2.44	8 (42%)	21,38,41	1.56	4 (19%)
48	A2M	5	1326	48	18,25,26	4.34	7 (38%)	20,36,39	3.33	4 (20%)
48	OMC	5	3869	48	19,22,23	2.83	7 (36%)	25,31,34	0.76	0
51	MA6	9	1850	51	19,26,27	1.74	2 (10%)	18,38,41	4.28	4 (22%)
51	PSU	9	1692	51	17,20,22	1.14	1 (5%)	21,28,33	1.78	3 (14%)
51	OMC	9	1703	51	19,22,23	2.96	8 (42%)	25,31,34	0.80	0
48	OMC	5	2365	48	19,22,23	2.84	8 (42%)	25,31,34	0.67	0
48	PSU	5	3851	48	17,20,22	1.09	2 (11%)	21,28,33	2.06	4 (19%)
48	OMC	5	2824	48	19,22,23	2.84	8 (42%)	25,31,34	0.95	1 (4%)
51	PSU	9	109	51	17,20,22	1.20	1 (5%)	21,28,33	2.02	4 (19%)
48	2MG	5	1517	48	18,26,27	2.27	7 (38%)	16,38,41	2.49	5 (31%)
51	PSU	9	822	51	17,20,22	1.23	3 (17%)	21,28,33	2.24	6 (28%)
51	PSU	9	1045	51	17,20,22	1.15	2 (11%)	21,28,33	2.14	5 (23%)
51	OMC	9	174	51	19,22,23	2.91	8 (42%)	25,31,34	0.95	0
48	OMG	5	2364	48	19,26,27	2.38	8 (42%)	21,38,41	1.51	3 (14%)
51	PSU	9	609	51	17,20,22	1.08	1 (5%)	21,28,33	2.01	4 (19%)
48	A2M	5	3760	48,88	18,25,26	4.46	6 (33%)	20,36,39	3.38	3 (15%)
48	PSU	5	1781	48	17,20,22	1.13	2 (11%)	21,28,33	1.96	5 (23%)
48	B9B	5	237	48	20,28,29	1.70	2 (10%)	19,40,43	2.13	6 (31%)
51	A2M	9	1678	51	18,25,26	4.37	6 (33%)	20,36,39	3.58	4 (20%)
48	A2M	5	3724	48	18,25,26	4.48	6 (33%)	20,36,39	3.18	4 (20%)
48	PSU	5	4296	48	17,20,22	1.20	2 (11%)	21,28,33	1.96	3 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	OMG	9	509	51,88	19,26,27	2.35	8 (42%)	21,38,41	1.38	4 (19%)
51	A2M	9	512	51	18,25,26	4.40	5 (27%)	20,36,39	3.66	4 (20%)
51	OMG	9	683	51	19,26,27	2.49	8 (42%)	21,38,41	1.69	4 (19%)
48	A2M	5	3785	48	18,25,26	4.13	6 (33%)	20,36,39	3.64	5 (25%)
48	OMC	5	3841	48	19,22,23	2.82	8 (42%)	25,31,34	0.90	0
48	OMU	5	4227	48	19,22,23	2.83	7 (36%)	25,31,34	1.85	5 (20%)
48	5MC	5	4447	48,88	19,22,23	3.54	8 (42%)	26,32,35	1.14	2 (7%)
48	PSU	5	4423	48	17,20,22	1.00	1 (5%)	21,28,33	1.98	4 (19%)
48	PSU	5	3639	48	17,20,22	1.16	1 (5%)	21,28,33	1.91	4 (19%)
48	OMG	5	2424	48	19,26,27	2.35	8 (42%)	21,38,41	1.48	4 (19%)
48	OMC	5	3701	48,88	19,22,23	2.76	8 (42%)	25,31,34	1.04	1 (4%)
48	OMG	5	4618	48	19,26,27	2.34	8 (42%)	21,38,41	1.60	5 (23%)
48	PSU	5	1683	48,88	17,20,22	1.23	1 (5%)	21,28,33	2.02	4 (19%)
51	PSU	9	686	51	17,20,22	1.02	2 (11%)	21,28,33	2.29	6 (28%)
51	A2M	9	166	51	18,25,26	4.31	5 (27%)	20,36,39	3.35	4 (20%)
51	6MZ	9	1832	51,88	17,25,26	1.22	1 (5%)	15,36,39	2.34	2 (13%)
48	PSU	5	3920	48	17,20,22	1.05	1 (5%)	21,28,33	2.18	5 (23%)
51	OMG	9	436	51	19,26,27	2.43	8 (42%)	21,38,41	1.49	4 (19%)
51	PSU	9	649	51	17,20,22	1.06	1 (5%)	21,28,33	1.89	4 (19%)
51	PSU	9	1232	51	17,20,22	1.20	1 (5%)	21,28,33	1.93	3 (14%)
48	OMC	5	2861	48	19,22,23	2.94	8 (42%)	25,31,34	0.84	1 (4%)
48	PSU	5	4403	48	17,20,22	1.10	1 (5%)	21,28,33	1.88	4 (19%)
48	A2M	5	2363	48,88	18,25,26	4.39	5 (27%)	20,36,39	3.39	4 (20%)
48	OMG	5	3899	48	19,26,27	2.34	8 (42%)	21,38,41	1.42	3 (14%)
51	OMU	9	121	51	19,22,23	2.72	6 (31%)	25,31,34	1.90	6 (24%)
51	A2M	9	1383	51	18,25,26	4.47	6 (33%)	20,36,39	3.67	5 (25%)
48	PSU	5	4521	48,88	17,20,22	1.24	2 (11%)	21,28,33	2.25	7 (33%)
48	PSU	5	4442	48	17,20,22	1.09	1 (5%)	21,28,33	2.09	5 (23%)
48	A2M	5	400	48	18,25,26	4.35	8 (44%)	20,36,39	3.12	5 (25%)
51	PSU	9	1347	51	17,20,22	1.08	1 (5%)	21,28,33	2.00	5 (23%)
51	PSU	9	1643	51	17,20,22	1.03	1 (5%)	21,28,33	2.08	4 (19%)
51	PSU	9	1174	51	17,20,22	1.11	1 (5%)	21,28,33	2.07	4 (19%)
48	PSU	5	2508	48	17,20,22	1.07	1 (5%)	21,28,33	1.92	4 (19%)
48	A2M	5	1534	48,88	18,25,26	4.45	6 (33%)	20,36,39	3.42	6 (30%)
51	PSU	9	572	51	17,20,22	1.08	1 (5%)	21,28,33	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	A2M	9	27	51	18,25,26	4.31	5 (27%)	20,36,39	3.32	3 (15%)
48	A2M	5	2787	48	18,25,26	4.30	7 (38%)	20,36,39	3.24	4 (20%)
51	PSU	9	1445	51	17,20,22	1.05	1 (5%)	21,28,33	1.84	4 (19%)
48	PSU	5	3715	48	17,20,22	1.13	3 (17%)	21,28,33	2.10	6 (28%)
48	5MC	5	3782	48,88	19,22,23	3.55	8 (42%)	26,32,35	1.14	2 (7%)
51	OMG	9	1490	51,88	19,26,27	2.32	7 (36%)	21,38,41	1.33	4 (19%)
48	PSU	5	1860	48	17,20,22	1.03	1 (5%)	21,28,33	1.92	4 (19%)
48	PSU	5	4628	48	17,20,22	1.22	2 (11%)	21,28,33	2.19	6 (28%)
48	UY1	5	3818	48,88	19,22,23	4.33	9 (47%)	21,31,34	2.11	5 (23%)
48	PSU	5	4500	48	17,20,22	1.11	3 (17%)	21,28,33	2.07	5 (23%)
48	PSU	5	4457	48	17,20,22	1.15	1 (5%)	21,28,33	1.77	3 (14%)
48	OMC	5	4536	48	19,22,23	2.77	8 (42%)	25,31,34	0.86	0
51	PSU	9	1046	51	17,20,22	1.13	1 (5%)	21,28,33	1.92	5 (23%)
48	OMG	5	1316	48	19,26,27	2.37	8 (42%)	21,38,41	1.59	3 (14%)
48	OMG	5	1625	48,88	19,26,27	2.51	8 (42%)	21,38,41	1.71	4 (19%)
48	OMU	5	2837	48	19,22,23	2.84	6 (31%)	25,31,34	2.02	6 (24%)
48	PSU	5	4293	48	17,20,22	1.22	2 (11%)	21,28,33	1.88	4 (19%)
48	OMG	5	4392	48	19,26,27	2.27	8 (42%)	21,38,41	1.45	4 (19%)
51	OMU	9	172	51	19,22,23	2.85	7 (36%)	25,31,34	1.82	5 (20%)
51	A2M	9	159	51	18,25,26	4.48	7 (38%)	20,36,39	3.37	4 (20%)
48	PSU	5	4420	48	17,20,22	1.13	1 (5%)	21,28,33	2.06	4 (19%)
48	PSU	5	3695	48	17,20,22	1.05	1 (5%)	21,28,33	1.97	4 (19%)
48	UR3	5	4530	48	19,22,23	2.64	8 (42%)	26,32,35	1.50	4 (15%)
48	OMG	5	4228	48	19,26,27	2.33	8 (42%)	21,38,41	1.42	3 (14%)
51	OMU	9	1442	51	19,22,23	2.84	6 (31%)	25,31,34	1.83	4 (16%)
51	PSU	9	814	51	17,20,22	1.08	1 (5%)	21,28,33	2.05	5 (23%)
48	1MA	5	1322	48,88	17,25,26	3.52	5 (29%)	17,37,40	1.93	3 (17%)
51	PSU	9	1177	51	17,20,22	1.08	1 (5%)	21,28,33	1.77	4 (19%)
51	PSU	9	1238	51	17,20,22	1.22	2 (11%)	21,28,33	2.00	4 (19%)
48	PSU	5	1677	48	17,20,22	1.25	2 (11%)	21,28,33	2.17	4 (19%)
51	A2M	9	99	51,88	18,25,26	4.46	6 (33%)	20,36,39	3.36	4 (20%)
51	PSU	9	119	51	17,20,22	1.08	1 (5%)	21,28,33	2.02	5 (23%)
51	4AC	9	1842	51	21,24,25	3.00	10 (47%)	28,34,37	1.08	2 (7%)
48	OMU	5	4620	48	19,22,23	2.83	7 (36%)	25,31,34	1.87	5 (20%)
51	PSU	9	815	51	17,20,22	1.06	1 (5%)	21,28,33	2.17	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	PSU	9	1081	51	17,20,22	1.14	1 (5%)	21,28,33	2.03	6 (28%)
48	PSU	5	4299	48	17,20,22	1.00	1 (5%)	21,28,33	1.94	3 (14%)
48	OMG	5	1522	48	19,26,27	2.38	8 (42%)	21,38,41	1.50	4 (19%)
51	A2M	9	468	51	18,25,26	4.44	7 (38%)	20,36,39	3.33	4 (20%)
48	OMG	5	3792	48	19,26,27	2.29	7 (36%)	21,38,41	1.41	4 (19%)
48	OMC	5	4456	48	19,22,23	2.80	8 (42%)	25,31,34	0.77	0
51	OMG	9	644	51	19,26,27	2.35	7 (36%)	21,38,41	1.33	3 (14%)
48	OMG	5	4196	48,46	19,26,27	2.41	8 (42%)	21,38,41	1.44	4 (19%)
48	PSU	5	4532	48	17,20,22	1.12	1 (5%)	21,28,33	1.76	3 (14%)
51	4AC	9	1337	51	21,24,25	3.09	10 (47%)	28,34,37	1.03	1 (3%)
48	OMC	5	3887	48	19,22,23	2.78	7 (36%)	25,31,34	0.77	1 (4%)
51	OMU	9	1326	51	19,22,23	2.81	7 (36%)	25,31,34	1.95	5 (20%)
48	PSU	5	3762	48	17,20,22	1.14	1 (5%)	21,28,33	2.13	5 (23%)
48	PSU	5	3853	48	17,20,22	1.21	1 (5%)	21,28,33	2.19	5 (23%)
51	A2M	9	484	51	18,25,26	4.46	5 (27%)	20,36,39	3.56	3 (15%)
48	A2M	5	398	48	18,25,26	4.49	7 (38%)	20,36,39	3.29	3 (15%)
48	OMG	5	4637	48	19,26,27	2.35	8 (42%)	21,38,41	1.49	4 (19%)
51	OMG	9	1328	51	19,26,27	2.36	8 (42%)	21,38,41	1.41	4 (19%)
48	PSU	5	1862	48	17,20,22	1.11	1 (5%)	21,28,33	1.99	5 (23%)
51	B8N	9	1248	51	25,29,30	3.40	8 (32%)	28,42,45	2.31	7 (25%)
51	PSU	9	1004	51	17,20,22	1.13	1 (5%)	21,28,33	1.99	4 (19%)
51	OMC	9	1391	51	19,22,23	2.96	8 (42%)	25,31,34	0.97	1 (4%)
48	A2M	5	1524	48	18,25,26	4.25	6 (33%)	20,36,39	3.63	4 (20%)
48	PSU	5	3734	48	17,20,22	1.19	2 (11%)	21,28,33	1.93	5 (23%)
51	PSU	9	1244	51	17,20,22	1.17	1 (5%)	21,28,33	2.06	5 (23%)
51	PSU	9	105	51	17,20,22	1.14	1 (5%)	21,28,33	2.00	4 (19%)
51	MA6	9	1851	51	19,26,27	1.59	3 (15%)	18,38,41	4.96	4 (22%)
48	PSU	5	3764	48	17,20,22	1.18	1 (5%)	21,28,33	2.04	5 (23%)
51	PSU	9	801	51	17,20,22	1.25	2 (11%)	21,28,33	1.67	4 (19%)
48	A2M	5	3867	48	18,25,26	4.29	6 (33%)	20,36,39	3.26	3 (15%)
51	OMC	9	517	51	19,22,23	2.99	8 (42%)	25,31,34	0.82	0
48	OMU	5	4498	48	19,22,23	2.81	8 (42%)	25,31,34	1.93	5 (20%)
51	PSU	9	1367	51	17,20,22	1.15	1 (5%)	21,28,33	1.90	4 (19%)
48	PSU	5	1792	48	17,20,22	1.03	1 (5%)	21,28,33	1.89	3 (14%)
48	OMU	5	4306	48	19,22,23	2.86	7 (36%)	25,31,34	1.85	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	PSU	5	2632	48	17,20,22	1.15	1 (5%)	21,28,33	1.97	4 (19%)
48	OMU	5	3925	48	19,22,23	2.81	7 (36%)	25,31,34	1.88	4 (16%)
51	OMU	9	428	51	19,22,23	2.87	7 (36%)	25,31,34	1.79	5 (20%)
51	PSU	9	34	51	17,20,22	1.16	1 (5%)	21,28,33	1.96	4 (19%)
48	PSU	5	4552	48	17,20,22	1.16	1 (5%)	21,28,33	1.93	4 (19%)
48	OMC	5	3808	48	19,22,23	2.74	8 (42%)	25,31,34	0.65	0
48	A2M	5	4523	48,88	18,25,26	4.30	6 (33%)	20,36,39	3.43	4 (20%)
48	OMG	5	373	48	19,26,27	2.36	8 (42%)	21,38,41	1.53	3 (14%)
51	G7M	9	1639	51,46	20,26,27	2.64	8 (40%)	16,39,42	1.10	2 (12%)
48	OMC	5	1340	48	19,22,23	2.97	8 (42%)	25,31,34	1.01	2 (8%)
48	OMC	5	2804	48	19,22,23	2.79	8 (42%)	25,31,34	0.72	0
48	A2M	5	3718	48	18,25,26	4.47	6 (33%)	20,36,39	3.42	5 (25%)
48	PSU	5	1782	48	17,20,22	1.10	1 (5%)	21,28,33	2.01	5 (23%)
51	PSU	9	218	51	17,20,22	1.13	1 (5%)	21,28,33	2.28	7 (33%)
48	PSU	5	4361	48	17,20,22	1.11	1 (5%)	21,28,33	2.01	5 (23%)
48	OMG	5	4370	48	19,26,27	2.35	8 (42%)	21,38,41	1.51	4 (19%)
48	PSU	5	4353	48	17,20,22	1.12	2 (11%)	21,28,33	2.11	5 (23%)
51	PSU	9	863	51	17,20,22	0.99	1 (5%)	21,28,33	1.93	3 (14%)
51	A2M	9	1031	51	18,25,26	4.40	6 (33%)	20,36,39	3.24	4 (20%)
48	A2M	5	2815	48	18,25,26	4.30	6 (33%)	20,36,39	3.34	4 (20%)
48	PSU	5	1744	48,88	17,20,22	0.96	1 (5%)	21,28,33	2.01	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	5	4499	48	-	1/5/27/28	0/3/3/3
48	OMC	5	2422	48,88	-	0/9/27/28	0/2/2/2
48	OMG	5	4494	48	-	1/5/27/28	0/3/3/3
48	OMG	5	2876	48	-	0/5/27/28	0/3/3/3
51	OMU	9	116	51	-	0/9/27/28	0/2/2/2
50	OMG	8	75	50	-	0/5/27/28	0/3/3/3
48	6MZ	5	4220	48	-	0/5/27/28	0/3/3/3
48	A2M	5	3830	48	-	0/5/27/28	0/3/3/3
48	A2M	5	3825	48	-	0/5/27/28	0/3/3/3
48	OMC	5	2351	48	-	1/9/27/28	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	9	668	51,88	-	2/5/27/28	0/3/3/3
48	A2M	5	1871	48,88	-	0/5/27/28	0/3/3/3
48	PSU	5	4579	48	-	0/6/24/26	0/2/2/2
48	A2M	5	4571	48	-	0/5/27/28	0/3/3/3
48	OMG	5	3627	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4623	48	-	0/5/27/28	0/3/3/3
48	A2M	5	1326	48	-	1/5/27/28	0/3/3/3
48	OMC	5	3869	48	-	0/9/27/28	0/2/2/2
51	MA6	9	1850	51	-	0/7/29/30	0/3/3/3
51	PSU	9	1692	51	-	0/6/24/26	0/2/2/2
51	OMC	9	1703	51	-	2/9/27/28	0/2/2/2
48	OMC	5	2365	48	-	0/9/27/28	0/2/2/2
48	PSU	5	3851	48	-	1/6/24/26	0/2/2/2
48	OMC	5	2824	48	-	0/9/27/28	0/2/2/2
51	PSU	9	109	51	-	0/6/24/26	0/2/2/2
48	2MG	5	1517	48	-	0/5/27/28	0/3/3/3
51	PSU	9	822	51	-	2/6/24/26	0/2/2/2
51	PSU	9	1045	51	-	2/6/24/26	0/2/2/2
51	OMC	9	174	51	-	0/9/27/28	0/2/2/2
48	OMG	5	2364	48	-	3/5/27/28	0/3/3/3
51	PSU	9	609	51	-	0/6/24/26	0/2/2/2
48	A2M	5	3760	48,88	-	3/5/27/28	0/3/3/3
48	PSU	5	1781	48	-	2/6/24/26	0/2/2/2
48	B9B	5	237	48	-	2/7/29/30	0/3/3/3
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
48	A2M	5	3724	48	-	0/5/27/28	0/3/3/3
48	PSU	5	4296	48	-	0/6/24/26	0/2/2/2
51	OMG	9	509	51,88	-	0/5/27/28	0/3/3/3
51	A2M	9	512	51	-	1/5/27/28	0/3/3/3
51	OMG	9	683	51	-	3/5/27/28	0/3/3/3
48	A2M	5	3785	48	-	2/5/27/28	0/3/3/3
48	OMC	5	3841	48	-	0/9/27/28	0/2/2/2
48	OMU	5	4227	48	-	0/9/27/28	0/2/2/2
48	5MC	5	4447	48,88	-	4/7/25/26	0/2/2/2
48	PSU	5	4423	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3639	48	-	0/6/24/26	0/2/2/2
48	OMG	5	2424	48	-	3/5/27/28	0/3/3/3
48	OMC	5	3701	48,88	-	4/9/27/28	0/2/2/2
48	OMG	5	4618	48	-	0/5/27/28	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	5	1683	48,88	-	0/6/24/26	0/2/2/2
51	PSU	9	686	51	-	0/6/24/26	0/2/2/2
51	A2M	9	166	51	-	2/5/27/28	0/3/3/3
51	6MZ	9	1832	51,88	-	2/5/27/28	0/3/3/3
48	PSU	5	3920	48	-	0/6/24/26	0/2/2/2
51	OMG	9	436	51	-	0/5/27/28	0/3/3/3
51	PSU	9	649	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1232	51	-	0/6/24/26	0/2/2/2
48	OMC	5	2861	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4403	48	-	0/6/24/26	0/2/2/2
48	A2M	5	2363	48,88	-	0/5/27/28	0/3/3/3
48	OMG	5	3899	48	-	0/5/27/28	0/3/3/3
51	OMU	9	121	51	-	1/9/27/28	0/2/2/2
51	A2M	9	1383	51	-	0/5/27/28	0/3/3/3
48	PSU	5	4521	48,88	-	0/6/24/26	0/2/2/2
48	PSU	5	4442	48	-	0/6/24/26	0/2/2/2
48	A2M	5	400	48	-	0/5/27/28	0/3/3/3
51	PSU	9	1347	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1643	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1174	51	-	0/6/24/26	0/2/2/2
48	PSU	5	2508	48	-	0/6/24/26	0/2/2/2
48	A2M	5	1534	48,88	-	2/5/27/28	0/3/3/3
51	PSU	9	572	51	-	0/6/24/26	0/2/2/2
51	A2M	9	27	51	-	0/5/27/28	0/3/3/3
48	A2M	5	2787	48	-	0/5/27/28	0/3/3/3
51	PSU	9	1445	51	-	1/6/24/26	0/2/2/2
48	PSU	5	3715	48	-	0/6/24/26	0/2/2/2
48	5MC	5	3782	48,88	-	0/7/25/26	0/2/2/2
51	OMG	9	1490	51,88	-	2/5/27/28	0/3/3/3
48	PSU	5	1860	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4628	48	-	0/6/24/26	0/2/2/2
48	UY1	5	3818	48,88	-	3/9/27/28	0/2/2/2
48	PSU	5	4500	48	-	2/6/24/26	0/2/2/2
48	PSU	5	4457	48	-	0/6/24/26	0/2/2/2
48	OMC	5	4536	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1046	51	-	0/6/24/26	0/2/2/2
48	OMG	5	1316	48	-	0/5/27/28	0/3/3/3
48	OMG	5	1625	48,88	-	1/5/27/28	0/3/3/3
48	OMU	5	2837	48	-	1/9/27/28	0/2/2/2
48	PSU	5	4293	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4392	48	-	0/5/27/28	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMU	9	172	51	-	2/9/27/28	0/2/2/2
51	A2M	9	159	51	-	0/5/27/28	0/3/3/3
48	PSU	5	4420	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3695	48	-	0/6/24/26	0/2/2/2
48	UR3	5	4530	48	-	0/7/25/26	0/2/2/2
48	OMG	5	4228	48	-	1/5/27/28	0/3/3/3
51	OMU	9	1442	51	-	2/9/27/28	0/2/2/2
51	PSU	9	814	51	-	0/6/24/26	0/2/2/2
48	1MA	5	1322	48,88	-	0/3/25/26	0/3/3/3
51	PSU	9	1177	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1238	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1677	48	-	0/6/24/26	0/2/2/2
51	A2M	9	99	51,88	-	2/5/27/28	0/3/3/3
51	PSU	9	119	51	-	0/6/24/26	0/2/2/2
51	4AC	9	1842	51	-	0/11/29/30	0/2/2/2
48	OMU	5	4620	48	-	0/9/27/28	0/2/2/2
51	PSU	9	815	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1081	51	-	0/6/24/26	0/2/2/2
48	PSU	5	4299	48	-	0/6/24/26	0/2/2/2
48	OMG	5	1522	48	-	0/5/27/28	0/3/3/3
51	A2M	9	468	51	-	1/5/27/28	0/3/3/3
48	OMG	5	3792	48	-	2/5/27/28	0/3/3/3
48	OMC	5	4456	48	-	0/9/27/28	0/2/2/2
51	OMG	9	644	51	-	1/5/27/28	0/3/3/3
48	OMG	5	4196	48,46	-	0/5/27/28	0/3/3/3
48	PSU	5	4532	48	-	0/6/24/26	0/2/2/2
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
48	OMC	5	3887	48	-	0/9/27/28	0/2/2/2
51	OMU	9	1326	51	-	0/9/27/28	0/2/2/2
48	PSU	5	3762	48	-	0/6/24/26	0/2/2/2
48	PSU	5	3853	48	-	0/6/24/26	0/2/2/2
51	A2M	9	484	51	-	0/5/27/28	0/3/3/3
48	A2M	5	398	48	-	0/5/27/28	0/3/3/3
48	OMG	5	4637	48	-	0/5/27/28	0/3/3/3
51	OMG	9	1328	51	-	1/5/27/28	0/3/3/3
48	PSU	5	1862	48	-	0/6/24/26	0/2/2/2
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
51	PSU	9	1004	51	-	0/6/24/26	0/2/2/2
51	OMC	9	1391	51	-	0/9/27/28	0/2/2/2
48	A2M	5	1524	48	-	1/5/27/28	0/3/3/3
48	PSU	5	3734	48	-	0/6/24/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PSU	9	1244	51	-	0/6/24/26	0/2/2/2
51	PSU	9	105	51	-	0/6/24/26	0/2/2/2
51	MA6	9	1851	51	-	3/7/29/30	0/3/3/3
48	PSU	5	3764	48	-	0/6/24/26	0/2/2/2
51	PSU	9	801	51	-	2/6/24/26	0/2/2/2
48	A2M	5	3867	48	-	1/5/27/28	0/3/3/3
51	OMC	9	517	51	-	0/9/27/28	0/2/2/2
48	OMU	5	4498	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1367	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1792	48	-	0/6/24/26	0/2/2/2
48	OMU	5	4306	48	-	0/9/27/28	0/2/2/2
48	PSU	5	2632	48	-	0/6/24/26	0/2/2/2
48	OMU	5	3925	48	-	0/9/27/28	0/2/2/2
51	OMU	9	428	51	-	4/9/27/28	0/2/2/2
51	PSU	9	34	51	-	4/6/24/26	0/2/2/2
48	PSU	5	4552	48	-	0/6/24/26	0/2/2/2
48	OMC	5	3808	48	-	0/9/27/28	0/2/2/2
48	A2M	5	4523	48,88	-	0/5/27/28	0/3/3/3
48	OMG	5	373	48	-	1/5/27/28	0/3/3/3
51	G7M	9	1639	51,46	-	2/3/25/26	0/3/3/3
48	OMC	5	1340	48	-	0/9/27/28	0/2/2/2
48	OMC	5	2804	48	-	0/9/27/28	0/2/2/2
48	A2M	5	3718	48	-	0/5/27/28	0/3/3/3
48	PSU	5	1782	48	-	0/6/24/26	0/2/2/2
51	PSU	9	218	51	-	0/6/24/26	0/2/2/2
48	PSU	5	4361	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4370	48	-	0/5/27/28	0/3/3/3
48	PSU	5	4353	48	-	0/6/24/26	0/2/2/2
51	PSU	9	863	51	-	2/6/24/26	0/2/2/2
51	A2M	9	1031	51	-	1/5/27/28	0/3/3/3
48	A2M	5	2815	48	-	2/5/27/28	0/3/3/3
48	PSU	5	1744	48,88	-	0/6/24/26	0/2/2/2

All (776) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1383	A2M	O4'-C1'	16.64	1.62	1.40
48	5	3724	A2M	O4'-C1'	16.59	1.62	1.40
51	9	99	A2M	O4'-C1'	16.56	1.62	1.40
48	5	398	A2M	O4'-C1'	16.55	1.62	1.40
51	9	159	A2M	O4'-C1'	16.48	1.62	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3718	A2M	O4'-C1'	16.47	1.62	1.40
51	9	484	A2M	O4'-C1'	16.47	1.62	1.40
48	5	3760	A2M	O4'-C1'	16.39	1.62	1.40
48	5	4571	A2M	O4'-C1'	16.24	1.62	1.40
51	9	468	A2M	O4'-C1'	16.22	1.62	1.40
51	9	1031	A2M	O4'-C1'	16.20	1.62	1.40
51	9	512	A2M	O4'-C1'	16.19	1.62	1.40
48	5	1534	A2M	O4'-C1'	16.16	1.62	1.40
48	5	3825	A2M	O4'-C1'	16.15	1.62	1.40
48	5	2363	A2M	O4'-C1'	16.10	1.62	1.40
51	9	1678	A2M	O4'-C1'	16.03	1.61	1.40
51	9	27	A2M	O4'-C1'	15.77	1.61	1.40
51	9	166	A2M	O4'-C1'	15.77	1.61	1.40
48	5	400	A2M	O4'-C1'	15.77	1.61	1.40
48	5	2815	A2M	O4'-C1'	15.70	1.61	1.40
48	5	1326	A2M	O4'-C1'	15.69	1.61	1.40
48	5	2787	A2M	O4'-C1'	15.66	1.61	1.40
48	5	4523	A2M	O4'-C1'	15.64	1.61	1.40
51	9	668	A2M	O4'-C1'	15.64	1.61	1.40
48	5	3830	A2M	O4'-C1'	15.62	1.61	1.40
48	5	3867	A2M	O4'-C1'	15.53	1.61	1.40
48	5	1871	A2M	O4'-C1'	15.51	1.61	1.40
48	5	1524	A2M	O4'-C1'	15.26	1.60	1.40
48	5	3785	A2M	O4'-C1'	15.08	1.60	1.40
48	5	1322	1MA	C2-N3	12.84	1.44	1.28
48	5	3818	UY1	C6-C5	11.34	1.47	1.35
48	5	3818	UY1	C2-N1	9.65	1.49	1.36
48	5	3782	5MC	C6-C5	9.13	1.49	1.34
48	5	4447	5MC	C6-C5	8.73	1.48	1.34
51	9	1248	B8N	C4-C5	8.03	1.65	1.47
51	9	1248	B8N	C6-N1	7.54	1.54	1.36
51	9	1248	B8N	C4-N3	-7.46	1.27	1.40
51	9	1442	OMU	C2-N1	7.14	1.49	1.38
51	9	668	A2M	O4'-C4'	-7.11	1.29	1.45
48	5	2837	OMU	C2-N1	7.10	1.49	1.38
48	5	4530	UR3	C2-N1	7.04	1.48	1.38
48	5	3818	UY1	C2-N3	7.00	1.49	1.37
48	5	1524	A2M	O4'-C4'	-6.87	1.29	1.45
48	5	4620	OMU	C2-N1	6.84	1.49	1.38
48	5	4571	A2M	O4'-C4'	-6.83	1.29	1.45
48	5	1534	A2M	O4'-C4'	-6.78	1.29	1.45
51	9	428	OMU	C2-N1	6.74	1.49	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	428	OMU	C2-N3	6.66	1.49	1.38
48	5	3867	A2M	O4'-C4'	-6.65	1.30	1.45
51	9	116	OMU	C2-N1	6.64	1.48	1.38
48	5	3925	OMU	C2-N1	6.63	1.48	1.38
51	9	1391	OMC	C2-N3	6.60	1.49	1.36
48	5	4306	OMU	C2-N1	6.60	1.48	1.38
48	5	4227	OMU	C2-N1	6.58	1.48	1.38
51	9	1248	B8N	C2-N1	6.57	1.58	1.39
48	5	400	A2M	O4'-C4'	-6.52	1.30	1.45
48	5	2815	A2M	O4'-C4'	-6.52	1.30	1.45
51	9	172	OMU	C2-N3	6.51	1.49	1.38
51	9	1639	G7M	C2-N2	6.50	1.49	1.34
48	5	2363	A2M	O4'-C4'	-6.49	1.30	1.45
48	5	1340	OMC	C2-N3	6.45	1.49	1.36
48	5	1326	A2M	O4'-C4'	-6.44	1.30	1.45
48	5	1871	A2M	O4'-C4'	-6.44	1.30	1.45
48	5	3760	A2M	O4'-C4'	-6.44	1.30	1.45
51	9	159	A2M	O4'-C4'	-6.43	1.30	1.45
51	9	517	OMC	C2-N3	6.43	1.49	1.36
51	9	1031	A2M	O4'-C4'	-6.43	1.30	1.45
51	9	27	A2M	O4'-C4'	-6.40	1.30	1.45
48	5	3782	5MC	C5-C4	6.40	1.49	1.44
51	9	484	A2M	O4'-C4'	-6.39	1.30	1.45
51	9	172	OMU	C2-N1	6.38	1.48	1.38
48	5	3718	A2M	O4'-C4'	-6.38	1.30	1.45
48	5	2422	OMC	C2-N3	6.35	1.49	1.36
48	5	3887	OMC	C2-N3	6.35	1.48	1.36
51	9	468	A2M	O4'-C4'	-6.34	1.30	1.45
48	5	4498	OMU	C2-N1	6.34	1.48	1.38
51	9	1326	OMU	C2-N1	6.33	1.48	1.38
48	5	398	A2M	O4'-C4'	-6.33	1.30	1.45
48	5	2787	A2M	O4'-C4'	-6.32	1.30	1.45
51	9	1337	4AC	C6-C5	6.31	1.49	1.35
51	9	1703	OMC	C2-N3	6.31	1.48	1.36
48	5	4523	A2M	O4'-C4'	-6.31	1.31	1.45
51	9	121	OMU	C2-N1	6.29	1.48	1.38
51	9	517	OMC	C6-C5	6.27	1.49	1.35
48	5	2861	OMC	C2-N3	6.24	1.48	1.36
48	5	3830	A2M	O4'-C4'	-6.23	1.31	1.45
51	9	1442	OMU	C2-N3	6.23	1.48	1.38
51	9	99	A2M	O4'-C4'	-6.20	1.31	1.45
51	9	512	A2M	O4'-C4'	-6.18	1.31	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3825	A2M	O4'-C4'	-6.16	1.31	1.45
51	9	116	OMU	C2-N3	6.16	1.48	1.38
51	9	1678	A2M	O4'-C4'	-6.15	1.31	1.45
48	5	4447	5MC	C4-N3	6.15	1.44	1.34
51	9	166	A2M	O4'-C4'	-6.14	1.31	1.45
51	9	1326	OMU	C2-N3	6.14	1.48	1.38
48	5	1340	OMC	C6-C5	6.14	1.49	1.35
51	9	121	OMU	C2-N3	6.14	1.48	1.38
48	5	2837	OMU	C2-N3	6.13	1.48	1.38
48	5	3724	A2M	O4'-C4'	-6.11	1.31	1.45
48	5	4498	OMU	C2-N3	6.10	1.48	1.38
48	5	4620	OMU	C2-N3	6.10	1.48	1.38
48	5	3785	A2M	O4'-C4'	-6.08	1.31	1.45
51	9	174	OMC	C2-N3	6.06	1.48	1.36
51	9	1383	A2M	O4'-C4'	-6.05	1.31	1.45
51	9	174	OMC	C6-C5	6.04	1.49	1.35
48	5	2804	OMC	C2-N3	6.04	1.48	1.36
51	9	1391	OMC	C6-C5	6.03	1.49	1.35
48	5	4227	OMU	C2-N3	6.03	1.48	1.38
48	5	4536	OMC	C6-C5	6.01	1.49	1.35
48	5	2365	OMC	C2-N3	6.01	1.48	1.36
48	5	3925	OMU	C2-N3	6.01	1.48	1.38
48	5	3841	OMC	C2-N3	6.00	1.48	1.36
51	9	1337	4AC	C4-N3	5.97	1.42	1.32
51	9	1842	4AC	C4-N3	5.95	1.42	1.32
48	5	3869	OMC	C6-C5	5.94	1.48	1.35
48	5	3841	OMC	C6-C5	5.92	1.48	1.35
48	5	4306	OMU	C6-C5	5.91	1.48	1.35
51	9	1703	OMC	C6-C5	5.90	1.48	1.35
48	5	2365	OMC	C6-C5	5.88	1.48	1.35
48	5	2861	OMC	C6-C5	5.88	1.48	1.35
48	5	4306	OMU	C2-N3	5.88	1.48	1.38
51	9	172	OMU	C6-C5	5.87	1.48	1.35
48	5	4456	OMC	C2-N3	5.87	1.48	1.36
48	5	2824	OMC	C2-N3	5.85	1.48	1.36
51	9	1842	4AC	C6-C5	5.84	1.48	1.35
48	5	2422	OMC	C6-C5	5.84	1.48	1.35
48	5	2351	OMC	C6-C5	5.80	1.48	1.35
48	5	3701	OMC	C6-C5	5.79	1.48	1.35
51	9	116	OMU	C6-C5	5.78	1.48	1.35
48	5	2824	OMC	C6-C5	5.77	1.48	1.35
48	5	4447	5MC	C2-N3	5.75	1.47	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1326	OMU	C6-C5	5.74	1.48	1.35
48	5	3869	OMC	C2-N3	5.73	1.47	1.36
51	9	1248	B8N	C6-C5	5.70	1.43	1.35
48	5	3808	OMC	C2-N3	5.69	1.47	1.36
48	5	2804	OMC	C6-C5	5.66	1.48	1.35
48	5	4536	OMC	C2-N3	5.66	1.47	1.36
48	5	4456	OMC	C6-C5	5.65	1.48	1.35
48	5	4498	OMU	C6-C5	5.64	1.48	1.35
48	5	4227	OMU	C6-C5	5.64	1.48	1.35
48	5	3925	OMU	C6-C5	5.64	1.48	1.35
51	9	436	OMG	C2-N3	5.63	1.46	1.33
48	5	4620	OMU	C6-C5	5.62	1.48	1.35
51	9	1850	MA6	C6-C5	-5.57	1.36	1.44
48	5	3808	OMC	C6-C5	5.57	1.48	1.35
48	5	3701	OMC	C2-N3	5.54	1.47	1.36
48	5	4530	UR3	C6-C5	5.52	1.47	1.35
51	9	428	OMU	C6-C5	5.52	1.47	1.35
51	9	683	OMG	C2-N3	5.51	1.46	1.33
48	5	2351	OMC	C2-N3	5.51	1.47	1.36
51	9	1442	OMU	C6-C5	5.48	1.47	1.35
48	5	4196	OMG	C2-N3	5.45	1.46	1.33
48	5	237	B9B	C2-N2	5.40	1.44	1.33
48	5	1625	OMG	C2-N3	5.40	1.46	1.33
48	5	4447	5MC	C5-C4	5.38	1.48	1.44
48	5	3782	5MC	C4-N3	5.36	1.42	1.34
48	5	3887	OMC	C6-C5	5.35	1.47	1.35
48	5	3818	UY1	C1'-C5	-5.35	1.38	1.50
48	5	4499	OMG	C2-N3	5.35	1.46	1.33
48	5	2837	OMU	C6-C5	5.31	1.47	1.35
51	9	509	OMG	C2-N3	5.30	1.46	1.33
51	9	1337	4AC	C2-N3	5.29	1.46	1.36
48	5	4623	OMG	C2-N3	5.27	1.46	1.33
51	9	121	OMU	C6-C5	5.25	1.47	1.35
51	9	1328	OMG	C2-N3	5.23	1.46	1.33
48	5	3782	5MC	C2-N3	5.18	1.46	1.36
51	9	1639	G7M	C2-N3	5.16	1.45	1.33
48	5	373	OMG	C2-N3	5.14	1.45	1.33
48	5	4499	OMG	C4-N3	5.14	1.49	1.37
48	5	4637	OMG	C2-N3	5.11	1.45	1.33
48	5	2876	OMG	C2-N3	5.11	1.45	1.33
51	9	509	OMG	C4-N3	5.09	1.49	1.37
51	9	683	OMG	C4-N3	5.09	1.49	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1842	4AC	C2-N3	5.07	1.46	1.36
48	5	1517	2MG	C2-N2	5.07	1.44	1.33
51	9	436	OMG	C4-N3	5.07	1.49	1.37
48	5	3627	OMG	C2-N3	5.06	1.45	1.33
48	5	4370	OMG	C2-N3	5.05	1.45	1.33
48	5	2364	OMG	C2-N3	5.04	1.45	1.33
51	9	644	OMG	C2-N3	5.04	1.45	1.33
48	5	2424	OMG	C2-N3	5.02	1.45	1.33
48	5	2876	OMG	C4-N3	5.02	1.49	1.37
48	5	3899	OMG	C2-N3	5.01	1.45	1.33
48	5	1316	OMG	C2-N3	5.00	1.45	1.33
48	5	4623	OMG	C4-N3	4.99	1.49	1.37
48	5	4637	OMG	C4-N3	4.98	1.49	1.37
48	5	4392	OMG	C2-N3	4.98	1.45	1.33
50	8	75	OMG	C2-N3	4.97	1.45	1.33
48	5	1340	OMC	C4-N4	4.97	1.45	1.33
48	5	3792	OMG	C2-N3	4.95	1.45	1.33
48	5	1625	OMG	C4-N3	4.94	1.49	1.37
48	5	4196	OMG	C4-N3	4.93	1.49	1.37
51	9	1391	OMC	C4-N4	4.89	1.45	1.33
51	9	1703	OMC	C2-N1	4.87	1.50	1.40
48	5	3899	OMG	C4-N3	4.87	1.49	1.37
48	5	373	OMG	C4-N3	4.87	1.49	1.37
48	5	4618	OMG	C2-N3	4.85	1.45	1.33
48	5	1522	OMG	C2-N3	4.85	1.45	1.33
48	5	4494	OMG	C2-N3	4.85	1.45	1.33
51	9	1337	4AC	C4-N4	4.84	1.47	1.39
51	9	644	OMG	C4-N3	4.81	1.48	1.37
51	9	1703	OMC	C4-N3	4.81	1.44	1.34
51	9	1639	G7M	C4-N3	4.78	1.48	1.37
48	5	4370	OMG	C4-N3	4.78	1.48	1.37
51	9	517	OMC	C4-N3	4.76	1.44	1.34
48	5	1522	OMG	C4-N3	4.76	1.48	1.37
48	5	4220	6MZ	C6-C5	-4.75	1.37	1.44
48	5	3887	OMC	C4-N3	4.73	1.43	1.34
48	5	3627	OMG	C4-N3	4.73	1.48	1.37
48	5	4228	OMG	C4-N3	4.72	1.48	1.37
51	9	174	OMC	C4-N3	4.71	1.43	1.34
51	9	1851	MA6	C6-C5	-4.69	1.37	1.44
51	9	1328	OMG	C4-N3	4.68	1.48	1.37
48	5	3818	UY1	C6-N1	4.67	1.44	1.36
48	5	2422	OMC	C4-N3	4.67	1.43	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4228	OMG	C2-N3	4.65	1.44	1.33
48	5	2364	OMG	C4-N3	4.65	1.48	1.37
48	5	1625	OMG	C2-N2	4.64	1.45	1.34
48	5	3792	OMG	C4-N3	4.64	1.48	1.37
48	5	2861	OMC	C4-N3	4.62	1.43	1.34
48	5	1316	OMG	C4-N3	4.60	1.48	1.37
48	5	237	B9B	O6-C6	4.60	1.40	1.34
51	9	1490	OMG	C2-N3	4.59	1.44	1.33
48	5	2424	OMG	C4-N3	4.56	1.48	1.37
51	9	1703	OMC	C4-N4	4.55	1.44	1.33
51	9	1490	OMG	C4-N3	4.53	1.48	1.37
48	5	3869	OMC	C4-N4	4.53	1.44	1.33
48	5	2365	OMC	C4-N3	4.52	1.43	1.34
51	9	644	OMG	C2-N2	4.51	1.44	1.34
48	5	4618	OMG	C4-N3	4.51	1.48	1.37
48	5	4196	OMG	C2-N2	4.50	1.44	1.34
48	5	3869	OMC	C4-N3	4.50	1.43	1.34
48	5	4392	OMG	C4-N3	4.50	1.48	1.37
50	8	75	OMG	C4-N3	4.50	1.48	1.37
51	9	517	OMC	C4-N4	4.49	1.44	1.33
48	5	4456	OMC	C4-N3	4.48	1.43	1.34
48	5	2861	OMC	C2-N1	4.46	1.49	1.40
48	5	4456	OMC	C4-N4	4.46	1.44	1.33
48	5	2824	OMC	C4-N4	4.45	1.44	1.33
51	9	174	OMC	C4-N4	4.45	1.44	1.33
48	5	2422	OMC	C2-N1	4.44	1.49	1.40
48	5	4499	OMG	C2-N2	4.44	1.44	1.34
51	9	683	OMG	C2-N2	4.44	1.44	1.34
48	5	2861	OMC	C4-N4	4.44	1.44	1.33
51	9	1391	OMC	C4-N3	4.43	1.43	1.34
51	9	436	OMG	C2-N2	4.43	1.44	1.34
48	5	2365	OMC	C4-N4	4.42	1.44	1.33
48	5	4623	OMG	C2-N2	4.42	1.44	1.34
51	9	517	OMC	C2-N1	4.41	1.49	1.40
48	5	4530	UR3	C2-N3	4.41	1.47	1.39
48	5	4494	OMG	C4-N3	4.40	1.47	1.37
48	5	2422	OMC	C4-N4	4.38	1.44	1.33
48	5	2424	OMG	C2-N2	4.38	1.44	1.34
51	9	1842	4AC	C7-N4	4.37	1.46	1.37
51	9	1490	OMG	C2-N2	4.37	1.44	1.34
48	5	3887	OMC	C4-N4	4.37	1.44	1.33
48	5	3701	OMC	C4-N3	4.36	1.43	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3841	OMC	C4-N4	4.34	1.44	1.33
48	5	1340	OMC	C4-N3	4.34	1.43	1.34
50	8	75	OMG	C2-N2	4.34	1.44	1.34
48	5	2364	OMG	C2-N2	4.34	1.44	1.34
48	5	4447	5MC	C6-N1	4.34	1.45	1.38
48	5	373	OMG	C2-N2	4.32	1.44	1.34
51	9	509	OMG	C2-N2	4.32	1.44	1.34
51	9	1328	OMG	C2-N2	4.30	1.44	1.34
51	9	174	OMC	C2-N1	4.29	1.49	1.40
48	5	4370	OMG	C2-N2	4.29	1.44	1.34
48	5	2824	OMC	C2-N1	4.28	1.49	1.40
48	5	2804	OMC	C4-N4	4.28	1.44	1.33
48	5	3899	OMG	C2-N2	4.27	1.44	1.34
51	9	1391	OMC	C2-N1	4.27	1.49	1.40
48	5	3808	OMC	C2-N1	4.27	1.49	1.40
48	5	4536	OMC	C4-N4	4.26	1.44	1.33
48	5	2351	OMC	C4-N3	4.25	1.43	1.34
48	5	3841	OMC	C4-N3	4.24	1.42	1.34
48	5	4228	OMG	C2-N2	4.23	1.44	1.34
48	5	3701	OMC	C2-N1	4.23	1.48	1.40
48	5	3627	OMG	C2-N2	4.21	1.44	1.34
48	5	4618	OMG	C2-N2	4.20	1.44	1.34
48	5	2804	OMC	C4-N3	4.20	1.42	1.34
48	5	2824	OMC	C4-N3	4.19	1.42	1.34
48	5	3808	OMC	C4-N3	4.18	1.42	1.34
48	5	3792	OMG	C2-N2	4.18	1.44	1.34
48	5	3782	5MC	C6-N1	4.17	1.45	1.38
48	5	4494	OMG	C2-N2	4.17	1.43	1.34
48	5	3808	OMC	C4-N4	4.15	1.44	1.33
51	9	1842	4AC	C4-N4	4.11	1.46	1.39
51	9	1337	4AC	C7-N4	4.08	1.45	1.37
48	5	1522	OMG	C2-N2	4.08	1.43	1.34
48	5	2876	OMG	C2-N2	4.08	1.43	1.34
48	5	2351	OMC	C2-N1	4.07	1.48	1.40
48	5	2351	OMC	C4-N4	4.05	1.43	1.33
48	5	3701	OMC	C4-N4	4.05	1.43	1.33
48	5	4536	OMC	C2-N1	4.03	1.48	1.40
48	5	4536	OMC	C4-N3	4.01	1.42	1.34
48	5	2804	OMC	C2-N1	4.01	1.48	1.40
48	5	1316	OMG	C2-N2	4.01	1.43	1.34
51	9	1639	G7M	C6-N1	4.00	1.43	1.37
48	5	4447	5MC	C4-N4	3.99	1.44	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3782	5MC	C4-N4	3.98	1.44	1.34
48	5	1340	OMC	C2-N1	3.97	1.48	1.40
48	5	4637	OMG	C2-N2	3.96	1.43	1.34
48	5	3841	OMC	C2-N1	3.94	1.48	1.40
51	9	1842	4AC	C2-N1	3.92	1.48	1.40
51	9	1832	6MZ	C6-C5	-3.90	1.38	1.44
48	5	4293	PSU	C6-C5	3.85	1.39	1.35
48	5	3734	PSU	C6-C5	3.85	1.39	1.35
48	5	2365	OMC	C2-N1	3.82	1.48	1.40
48	5	1517	2MG	C2-N1	3.82	1.42	1.36
48	5	1517	2MG	C6-N1	3.81	1.43	1.37
48	5	3869	OMC	C2-N1	3.80	1.48	1.40
48	5	3887	OMC	C2-N1	3.80	1.48	1.40
48	5	4456	OMC	C2-N1	3.79	1.48	1.40
51	9	1248	B8N	O4-C4	-3.76	1.15	1.23
48	5	4392	OMG	C2-N2	3.76	1.43	1.34
48	5	4306	OMU	O2-C2	-3.76	1.16	1.23
51	9	801	PSU	C6-C5	3.73	1.39	1.35
48	5	4447	5MC	C2-N1	3.72	1.47	1.40
48	5	1683	PSU	C6-C5	3.71	1.39	1.35
48	5	3782	5MC	C2-N1	3.70	1.47	1.40
51	9	1337	4AC	C5-C4	3.65	1.49	1.41
51	9	1842	4AC	C5-C4	3.64	1.49	1.41
48	5	4456	OMC	O2-C2	-3.64	1.16	1.23
48	5	2824	OMC	O2-C2	-3.64	1.16	1.23
48	5	4420	PSU	C6-C5	3.63	1.39	1.35
48	5	3853	PSU	C6-C5	3.62	1.39	1.35
48	5	1625	OMG	C6-N1	3.61	1.43	1.37
48	5	4296	PSU	C6-C5	3.60	1.39	1.35
48	5	1862	PSU	C6-C5	3.58	1.39	1.35
48	5	4457	PSU	C6-C5	3.58	1.39	1.35
48	5	2861	OMC	O2-C2	-3.58	1.17	1.23
51	9	1238	PSU	C6-C5	3.57	1.39	1.35
48	5	4306	OMU	O4-C4	-3.56	1.17	1.24
48	5	4628	PSU	C6-C5	3.56	1.39	1.35
51	9	109	PSU	C6-C5	3.55	1.39	1.35
51	9	822	PSU	C6-C5	3.54	1.39	1.35
51	9	34	PSU	C6-C5	3.54	1.39	1.35
48	5	3869	OMC	O2-C2	-3.53	1.17	1.23
48	5	4536	OMC	O2-C2	-3.52	1.17	1.23
48	5	2632	PSU	C6-C5	3.52	1.39	1.35
51	9	1692	PSU	C6-C5	3.52	1.39	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1244	PSU	C6-C5	3.51	1.39	1.35
48	5	1322	1MA	C2-N1	3.51	1.43	1.35
51	9	1367	PSU	C6-C5	3.51	1.39	1.35
48	5	1322	1MA	C4-N3	3.50	1.48	1.37
48	5	4620	OMU	O2-C2	-3.47	1.16	1.23
48	5	3925	OMU	O4-C4	-3.46	1.17	1.24
48	5	4521	PSU	C6-C5	3.46	1.39	1.35
48	5	3701	OMC	O2-C2	-3.46	1.17	1.23
51	9	105	PSU	C6-C5	3.45	1.39	1.35
51	9	1232	PSU	C6-C5	3.45	1.39	1.35
48	5	2804	OMC	O2-C2	-3.45	1.17	1.23
51	9	1442	OMU	C4-N3	3.44	1.44	1.38
51	9	1850	MA6	C6-N6	3.43	1.45	1.37
48	5	3764	PSU	C6-C5	3.43	1.39	1.35
51	9	428	OMU	C4-N3	3.43	1.44	1.38
48	5	3925	OMU	O2-C2	-3.42	1.17	1.23
48	5	1782	PSU	C6-C5	3.41	1.39	1.35
48	5	1517	2MG	C4-N3	3.40	1.45	1.37
51	9	1004	PSU	C6-C5	3.40	1.39	1.35
51	9	609	PSU	C6-C5	3.39	1.39	1.35
51	9	1326	OMU	C4-N3	3.39	1.44	1.38
48	5	4227	OMU	O2-C2	-3.39	1.17	1.23
51	9	1490	OMG	C5-C4	-3.39	1.34	1.43
48	5	2837	OMU	O2-C2	-3.38	1.17	1.23
51	9	1174	PSU	C6-C5	3.38	1.39	1.35
51	9	1045	PSU	C6-C5	3.38	1.39	1.35
48	5	1340	OMC	O2-C2	-3.38	1.17	1.23
48	5	3841	OMC	O2-C2	-3.37	1.17	1.23
51	9	1046	PSU	C6-C5	3.37	1.39	1.35
48	5	2365	OMC	O2-C2	-3.37	1.17	1.23
51	9	468	A2M	O3'-C3'	-3.37	1.34	1.43
51	9	1842	4AC	O2-C2	-3.37	1.17	1.23
51	9	218	PSU	C6-C5	3.37	1.39	1.35
51	9	1177	PSU	C6-C5	3.37	1.39	1.35
51	9	572	PSU	C6-C5	3.36	1.39	1.35
51	9	121	OMU	O4-C4	-3.36	1.18	1.24
48	5	3808	OMC	O2-C2	-3.35	1.17	1.23
48	5	4532	PSU	C6-C5	3.35	1.39	1.35
48	5	3782	5MC	O2-C2	-3.35	1.17	1.23
51	9	1639	G7M	C5-C6	3.34	1.54	1.45
51	9	1851	MA6	C6-N6	3.34	1.45	1.37
51	9	1337	4AC	O2-C2	-3.33	1.17	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	172	OMU	C4-N3	3.32	1.44	1.38
51	9	166	A2M	C6-N6	3.32	1.46	1.34
48	5	2351	OMC	O2-C2	-3.32	1.17	1.23
48	5	2364	OMG	C5-C6	3.32	1.54	1.47
48	5	4552	PSU	C6-C5	3.32	1.39	1.35
51	9	174	OMC	O2-C2	-3.32	1.17	1.23
51	9	1081	PSU	C6-C5	3.30	1.38	1.35
51	9	1326	OMU	O2-C2	-3.29	1.17	1.23
48	5	4498	OMU	O4-C4	-3.29	1.18	1.24
51	9	1337	4AC	C6-N1	3.28	1.45	1.38
48	5	1677	PSU	C6-C5	3.27	1.38	1.35
48	5	2422	OMC	O2-C2	-3.26	1.17	1.23
48	5	4498	OMU	C4-N3	3.26	1.44	1.38
51	9	1337	4AC	C2-N1	3.26	1.46	1.40
48	5	4498	OMU	O2-C2	-3.25	1.17	1.23
48	5	4623	OMG	C5-C4	-3.25	1.35	1.43
48	5	4620	OMU	O4-C4	-3.24	1.18	1.24
48	5	2424	OMG	C5-C4	-3.24	1.35	1.43
51	9	1490	OMG	C6-N1	3.24	1.42	1.37
48	5	3762	PSU	C6-C5	3.24	1.38	1.35
48	5	3792	OMG	C5-C4	-3.23	1.35	1.43
51	9	649	PSU	C6-C5	3.23	1.38	1.35
51	9	512	A2M	O2'-C2'	3.22	1.50	1.42
48	5	3639	PSU	C6-C5	3.22	1.38	1.35
48	5	3869	OMC	C6-N1	3.21	1.45	1.38
48	5	4442	PSU	C6-C5	3.21	1.38	1.35
51	9	1678	A2M	O2'-C2'	3.21	1.50	1.42
48	5	1860	PSU	C6-C5	3.20	1.38	1.35
48	5	3627	OMG	C5-C6	3.19	1.53	1.47
48	5	4571	A2M	C6-N6	3.19	1.45	1.34
48	5	4361	PSU	C6-C5	3.19	1.38	1.35
51	9	815	PSU	C6-C5	3.18	1.38	1.35
48	5	1522	OMG	C6-N1	3.18	1.42	1.37
48	5	2861	OMC	C6-N1	3.18	1.45	1.38
51	9	1678	A2M	C6-N6	3.17	1.45	1.34
48	5	4447	5MC	O2-C2	-3.17	1.17	1.23
48	5	2422	OMC	C6-N1	3.17	1.45	1.38
48	5	1326	A2M	O2'-C2'	3.17	1.50	1.42
51	9	1391	OMC	C6-N1	3.17	1.45	1.38
48	5	1781	PSU	C6-C5	3.17	1.38	1.35
51	9	1328	OMG	C6-N1	3.16	1.42	1.37
48	5	3825	A2M	C6-N6	3.16	1.45	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4392	OMG	C5-C4	-3.16	1.35	1.43
48	5	4499	OMG	C6-N1	3.16	1.42	1.37
48	5	2508	PSU	C6-C5	3.15	1.38	1.35
48	5	4618	OMG	C5-C4	-3.15	1.35	1.43
51	9	119	PSU	C6-C5	3.15	1.38	1.35
51	9	683	OMG	C6-N1	3.14	1.42	1.37
48	5	373	OMG	C5-C4	-3.13	1.35	1.43
48	5	1316	OMG	C5-C6	3.13	1.53	1.47
48	5	2824	OMC	C6-N1	3.13	1.45	1.38
51	9	1643	PSU	C6-C5	3.12	1.38	1.35
51	9	517	OMC	C6-N1	3.12	1.45	1.38
48	5	3841	OMC	C6-N1	3.12	1.45	1.38
48	5	1322	1MA	C5-C4	-3.12	1.35	1.43
48	5	4227	OMU	C4-N3	3.11	1.43	1.38
51	9	1445	PSU	C6-C5	3.11	1.38	1.35
48	5	2424	OMG	C6-N1	3.11	1.42	1.37
48	5	4227	OMU	O4-C4	-3.11	1.18	1.24
48	5	4618	OMG	C6-N1	3.11	1.42	1.37
48	5	1340	OMC	C6-N1	3.11	1.45	1.38
51	9	1328	OMG	C5-C4	-3.10	1.35	1.43
51	9	1347	PSU	C6-C5	3.10	1.38	1.35
50	8	75	OMG	C6-N1	3.10	1.42	1.37
48	5	2837	OMU	O4-C4	-3.10	1.18	1.24
48	5	4228	OMG	C5-C6	3.09	1.53	1.47
48	5	4353	PSU	C6-C5	3.09	1.38	1.35
51	9	116	OMU	C4-N3	3.09	1.43	1.38
48	5	1522	OMG	C5-C4	-3.09	1.35	1.43
48	5	398	A2M	C6-N6	3.08	1.45	1.34
48	5	2365	OMC	C6-N1	3.08	1.45	1.38
51	9	468	A2M	C6-N6	3.08	1.45	1.34
48	5	2351	OMC	C6-N1	3.08	1.45	1.38
48	5	4571	A2M	O3'-C3'	-3.07	1.35	1.43
48	5	4523	A2M	O3'-C3'	-3.07	1.35	1.43
48	5	4637	OMG	C5-C4	-3.07	1.35	1.43
48	5	1677	PSU	O4'-C1'	-3.06	1.39	1.43
48	5	1316	OMG	C5-C4	-3.05	1.35	1.43
48	5	1522	OMG	C5-C6	3.05	1.53	1.47
48	5	3718	A2M	O2'-C2'	3.04	1.50	1.42
48	5	4392	OMG	C5-C6	3.04	1.53	1.47
51	9	1391	OMC	O2-C2	-3.04	1.18	1.23
48	5	3887	OMC	O2-C2	-3.04	1.18	1.23
48	5	2364	OMG	C5-C4	-3.03	1.35	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	814	PSU	C6-C5	3.03	1.38	1.35
51	9	121	OMU	O2-C2	-3.03	1.17	1.23
48	5	1316	OMG	C6-N1	3.03	1.42	1.37
48	5	4623	OMG	C6-N1	3.03	1.42	1.37
51	9	1703	OMC	C6-N1	3.03	1.45	1.38
48	5	3724	A2M	C6-N6	3.03	1.44	1.34
48	5	4571	A2M	O2'-C2'	3.03	1.50	1.42
48	5	4403	PSU	C6-C5	3.02	1.38	1.35
48	5	4370	OMG	C5-C4	-3.02	1.35	1.43
51	9	512	A2M	C6-N6	3.02	1.44	1.34
48	5	3701	OMC	C6-N1	3.01	1.45	1.38
51	9	159	A2M	O3'-C3'	-3.01	1.35	1.43
48	5	1517	2MG	C5-C4	-3.01	1.35	1.43
48	5	4494	OMG	C5-C4	-3.01	1.35	1.43
51	9	484	A2M	C6-N6	3.01	1.44	1.34
51	9	668	A2M	C6-N6	3.00	1.44	1.34
51	9	174	OMC	C6-N1	3.00	1.45	1.38
51	9	159	A2M	C6-N6	3.00	1.44	1.34
48	5	3760	A2M	C6-N6	3.00	1.44	1.34
48	5	3818	UY1	C4-N3	3.00	1.44	1.38
51	9	166	A2M	O3'-C3'	-3.00	1.35	1.43
48	5	3627	OMG	C6-N1	2.99	1.42	1.37
51	9	27	A2M	C6-N6	2.99	1.44	1.34
51	9	1383	A2M	O2'-C2'	2.99	1.50	1.42
48	5	4499	OMG	C5-C4	-2.98	1.35	1.43
51	9	517	OMC	O2-C2	-2.98	1.18	1.23
48	5	4500	PSU	C6-C5	2.97	1.38	1.35
48	5	2363	A2M	O2'-C2'	2.96	1.49	1.42
48	5	1524	A2M	C6-N6	2.96	1.44	1.34
51	9	172	OMU	O2-C2	-2.96	1.17	1.23
48	5	1625	OMG	C5-C4	-2.95	1.35	1.43
48	5	2804	OMC	C6-N1	2.95	1.45	1.38
51	9	484	A2M	O2'-C2'	2.94	1.49	1.42
48	5	3808	OMC	C6-N1	2.93	1.45	1.38
48	5	1534	A2M	O2'-C2'	2.93	1.49	1.42
51	9	172	OMU	O4-C4	-2.93	1.18	1.24
51	9	428	OMU	O4-C4	-2.93	1.18	1.24
48	5	2876	OMG	C5-C6	2.93	1.53	1.47
51	9	644	OMG	C5-C6	2.93	1.53	1.47
51	9	683	OMG	C5-C6	2.93	1.53	1.47
48	5	3867	A2M	C6-N6	2.93	1.44	1.34
48	5	1326	A2M	O3'-C3'	-2.93	1.35	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3760	A2M	O2'-C2'	2.92	1.49	1.42
48	5	2837	OMU	C4-N3	2.92	1.43	1.38
51	9	1383	A2M	C6-N6	2.92	1.44	1.34
51	9	683	OMG	C5-C4	-2.92	1.35	1.43
51	9	159	A2M	O2'-C2'	2.92	1.49	1.42
48	5	4536	OMC	C6-N1	2.92	1.45	1.38
48	5	4579	PSU	C6-C5	2.91	1.38	1.35
48	5	3627	OMG	C5-C4	-2.91	1.35	1.43
48	5	398	A2M	O3'-C3'	-2.91	1.35	1.43
51	9	116	OMU	O2-C2	-2.91	1.17	1.23
48	5	2787	A2M	C6-N6	2.91	1.44	1.34
48	5	1524	A2M	O2'-C2'	2.90	1.49	1.42
51	9	512	A2M	O3'-C3'	-2.90	1.35	1.43
51	9	863	PSU	C6-C5	2.90	1.38	1.35
48	5	3899	OMG	C5-C4	-2.89	1.35	1.43
48	5	1871	A2M	C6-N6	2.89	1.44	1.34
51	9	436	OMG	C5-C4	-2.89	1.35	1.43
51	9	1442	OMU	O4-C4	-2.89	1.18	1.24
48	5	1534	A2M	C6-N6	2.89	1.44	1.34
48	5	1792	PSU	C6-C5	2.89	1.38	1.35
48	5	4196	OMG	C5-C4	-2.89	1.35	1.43
48	5	3760	A2M	O3'-C3'	-2.89	1.35	1.43
48	5	3851	PSU	C6-C5	2.88	1.38	1.35
48	5	3887	OMC	C6-N1	2.88	1.44	1.38
48	5	3830	A2M	O3'-C3'	-2.87	1.35	1.43
51	9	1031	A2M	C6-N6	2.87	1.44	1.34
48	5	4523	A2M	C6-N6	2.87	1.44	1.34
51	9	686	PSU	C6-C5	2.87	1.38	1.35
51	9	668	A2M	O3'-C3'	-2.87	1.35	1.43
48	5	400	A2M	C6-N6	2.87	1.44	1.34
48	5	3724	A2M	O3'-C3'	-2.86	1.35	1.43
51	9	166	A2M	O2'-C2'	2.85	1.49	1.42
48	5	2363	A2M	O3'-C3'	-2.85	1.35	1.43
48	5	4618	OMG	C5-C6	2.85	1.53	1.47
51	9	668	A2M	O2'-C2'	2.85	1.49	1.42
48	5	2815	A2M	O2'-C2'	2.85	1.49	1.42
48	5	3867	A2M	O3'-C3'	-2.85	1.35	1.43
48	5	1534	A2M	O3'-C3'	-2.84	1.35	1.43
48	5	4228	OMG	C5-C4	-2.84	1.36	1.43
48	5	2363	A2M	C6-N6	2.84	1.44	1.34
48	5	3818	UY1	O2-C2	-2.84	1.17	1.23
51	9	99	A2M	C6-N6	2.84	1.44	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3825	A2M	O2'-C2'	2.84	1.49	1.42
48	5	3792	OMG	C6-N1	2.84	1.42	1.37
48	5	1326	A2M	C6-N6	2.84	1.44	1.34
51	9	1842	4AC	C6-N1	2.84	1.44	1.38
50	8	75	OMG	C5-C4	-2.83	1.36	1.43
48	5	2815	A2M	C6-N6	2.83	1.44	1.34
50	8	75	OMG	C5-C6	2.83	1.53	1.47
48	5	3920	PSU	C6-C5	2.82	1.38	1.35
51	9	1703	OMC	O2-C2	-2.82	1.18	1.23
48	5	3718	A2M	C6-N6	2.82	1.44	1.34
51	9	121	OMU	C4-N3	2.82	1.43	1.38
48	5	2787	A2M	O2'-C2'	2.82	1.49	1.42
48	5	398	A2M	O2'-C2'	2.81	1.49	1.42
48	5	4637	OMG	C5-C6	2.81	1.53	1.47
48	5	3785	A2M	C6-N6	2.80	1.44	1.34
48	5	4423	PSU	C6-C5	2.80	1.38	1.35
48	5	3830	A2M	O2'-C2'	2.80	1.49	1.42
51	9	1326	OMU	O4-C4	-2.79	1.19	1.24
51	9	1383	A2M	O3'-C3'	-2.79	1.36	1.43
48	5	4228	OMG	C6-N1	2.79	1.42	1.37
48	5	4523	A2M	O2'-C2'	2.78	1.49	1.42
51	9	116	OMU	O4-C4	-2.78	1.19	1.24
48	5	3899	OMG	C6-N1	2.77	1.42	1.37
48	5	2787	A2M	O3'-C3'	-2.77	1.36	1.43
51	9	644	OMG	C6-N1	2.77	1.42	1.37
48	5	4530	UR3	C6-N1	2.77	1.44	1.38
48	5	4196	OMG	C6-N1	2.77	1.42	1.37
48	5	1744	PSU	C6-C5	2.76	1.38	1.35
48	5	3899	OMG	C5-C6	2.76	1.52	1.47
48	5	3715	PSU	C6-C5	2.76	1.38	1.35
51	9	27	A2M	O2'-C2'	2.76	1.49	1.42
51	9	99	A2M	O2'-C2'	2.76	1.49	1.42
48	5	4370	OMG	C5-C6	2.76	1.52	1.47
48	5	4370	OMG	C6-N1	2.75	1.42	1.37
51	9	468	A2M	O2'-C2'	2.75	1.49	1.42
51	9	1490	OMG	C5-C6	2.75	1.52	1.47
48	5	4456	OMC	C6-N1	2.75	1.44	1.38
48	5	2876	OMG	C5-C4	-2.74	1.36	1.43
48	5	3818	UY1	O4-C4	-2.74	1.18	1.23
51	9	1639	G7M	C2-N1	2.74	1.44	1.37
48	5	3695	PSU	C6-C5	2.73	1.38	1.35
48	5	4299	PSU	C6-C5	2.73	1.38	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1871	A2M	O2'-C2'	2.73	1.49	1.42
51	9	428	OMU	O2-C2	-2.72	1.18	1.23
48	5	400	A2M	O3'-C3'	-2.72	1.36	1.43
48	5	3830	A2M	C6-N6	2.71	1.43	1.34
48	5	3724	A2M	O2'-C2'	2.70	1.49	1.42
48	5	2815	A2M	O3'-C3'	-2.69	1.36	1.43
51	9	99	A2M	O3'-C3'	-2.69	1.36	1.43
48	5	3825	A2M	O3'-C3'	-2.69	1.36	1.43
48	5	373	OMG	O6-C6	-2.69	1.17	1.23
48	5	2876	OMG	C6-N1	2.69	1.41	1.37
48	5	4530	UR3	O2-C2	-2.69	1.17	1.22
51	9	436	OMG	C6-N1	2.68	1.41	1.37
48	5	400	A2M	O2'-C2'	2.68	1.49	1.42
48	5	3867	A2M	O2'-C2'	2.67	1.49	1.42
48	5	1871	A2M	O3'-C3'	-2.67	1.36	1.43
48	5	2364	OMG	C6-N1	2.67	1.41	1.37
51	9	1031	A2M	O3'-C3'	-2.66	1.36	1.43
48	5	2424	OMG	C5-C6	2.66	1.52	1.47
48	5	1522	OMG	O6-C6	-2.66	1.17	1.23
48	5	1524	A2M	O3'-C3'	-2.66	1.36	1.43
48	5	3718	A2M	O3'-C3'	-2.65	1.36	1.43
51	9	27	A2M	O3'-C3'	-2.65	1.36	1.43
51	9	509	OMG	C5-C4	-2.65	1.36	1.43
48	5	4494	OMG	C6-N1	2.63	1.41	1.37
48	5	4623	OMG	C5-C6	2.62	1.52	1.47
51	9	1442	OMU	O2-C2	-2.62	1.18	1.23
51	9	644	OMG	C2-N1	2.62	1.44	1.37
51	9	1031	A2M	O2'-C2'	2.61	1.49	1.42
51	9	644	OMG	C5-C4	-2.61	1.36	1.43
51	9	484	A2M	O3'-C3'	-2.61	1.36	1.43
48	5	4618	OMG	O6-C6	-2.61	1.17	1.23
48	5	3785	A2M	O2'-C2'	2.60	1.49	1.42
48	5	4494	OMG	C5-C6	2.60	1.52	1.47
48	5	4499	OMG	C2-N1	2.60	1.43	1.37
48	5	1316	OMG	O6-C6	-2.60	1.17	1.23
48	5	373	OMG	C5-C6	2.59	1.52	1.47
51	9	1842	4AC	O7-C7	-2.59	1.17	1.23
48	5	1322	1MA	C6-N1	2.58	1.44	1.41
48	5	4530	UR3	O4-C4	-2.58	1.18	1.23
48	5	3818	UY1	O4'-C1'	-2.57	1.40	1.43
48	5	4637	OMG	C6-N1	2.56	1.41	1.37
48	5	1871	A2M	C1'-N9	-2.56	1.43	1.49

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4196	OMG	O6-C6	-2.54	1.17	1.23
48	5	4392	OMG	O6-C6	-2.54	1.17	1.23
48	5	4196	OMG	C5-C6	2.53	1.52	1.47
51	9	509	OMG	O6-C6	-2.53	1.17	1.23
48	5	1625	OMG	O6-C6	-2.53	1.17	1.23
51	9	509	OMG	C6-N1	2.52	1.41	1.37
51	9	1248	B8N	C32-C33	2.52	1.58	1.53
48	5	4494	OMG	O6-C6	-2.51	1.17	1.23
51	9	1703	OMC	C5-C4	2.50	1.48	1.42
51	9	1678	A2M	O3'-C3'	-2.49	1.36	1.43
48	5	4623	OMG	O6-C6	-2.48	1.17	1.23
48	5	4370	OMG	O6-C6	-2.45	1.17	1.23
48	5	4306	OMU	C4-N3	2.45	1.42	1.38
50	8	75	OMG	C2-N1	2.45	1.43	1.37
51	9	517	OMC	C5-C4	2.44	1.48	1.42
48	5	2365	OMC	C5-C4	2.43	1.48	1.42
51	9	1337	4AC	O7-C7	-2.43	1.17	1.23
48	5	2364	OMG	O6-C6	-2.42	1.17	1.23
48	5	4499	OMG	C5-C6	2.42	1.52	1.47
51	9	1328	OMG	C5-C6	2.42	1.52	1.47
51	9	1031	A2M	C1'-N9	-2.42	1.43	1.49
48	5	398	A2M	C2-N3	2.41	1.35	1.32
48	5	3925	OMU	C4-N3	2.41	1.42	1.38
48	5	4620	OMU	C4-N3	2.41	1.42	1.38
48	5	2364	OMG	C2-N1	2.41	1.43	1.37
48	5	4228	OMG	O6-C6	-2.40	1.17	1.23
48	5	2876	OMG	C2-N1	2.40	1.43	1.37
48	5	3830	A2M	C1'-N9	-2.40	1.44	1.49
48	5	1522	OMG	C2-N1	2.40	1.43	1.37
48	5	4637	OMG	O6-C6	-2.38	1.17	1.23
51	9	1678	A2M	C1'-N9	-2.38	1.44	1.49
48	5	4571	A2M	C1'-N9	-2.37	1.44	1.49
48	5	3627	OMG	O6-C6	-2.37	1.17	1.23
48	5	2424	OMG	O6-C6	-2.36	1.17	1.23
51	9	436	OMG	O6-C6	-2.36	1.17	1.23
48	5	3792	OMG	O6-C6	-2.35	1.17	1.23
51	9	1328	OMG	C2-N1	2.34	1.43	1.37
51	9	683	OMG	C2-N1	2.33	1.43	1.37
48	5	4228	OMG	C2-N1	2.33	1.43	1.37
48	5	4456	OMC	C5-C4	2.33	1.48	1.42
51	9	436	OMG	C2-N1	2.32	1.43	1.37
48	5	2876	OMG	O6-C6	-2.32	1.17	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3715	PSU	C4-C5	-2.32	1.37	1.44
51	9	174	OMC	C5-C4	2.32	1.48	1.42
48	5	2824	OMC	C5-C4	2.31	1.48	1.42
51	9	159	A2M	C1'-N9	-2.30	1.44	1.49
48	5	1625	OMG	C2-N1	2.30	1.43	1.37
51	9	801	PSU	O4'-C1'	-2.29	1.40	1.43
48	5	4392	OMG	C6-N1	2.28	1.41	1.37
48	5	1340	OMC	C5-C4	2.28	1.48	1.42
48	5	1534	A2M	C1'-N9	-2.27	1.44	1.49
48	5	4499	OMG	O6-C6	-2.27	1.18	1.23
51	9	468	A2M	C1'-N9	-2.27	1.44	1.49
48	5	3899	OMG	O6-C6	-2.27	1.18	1.23
48	5	4618	OMG	C2-N1	2.27	1.43	1.37
48	5	1517	2MG	O6-C6	-2.26	1.18	1.23
51	9	436	OMG	C5-C6	2.26	1.51	1.47
48	5	4370	OMG	C2-N1	2.26	1.43	1.37
48	5	1316	OMG	C2-N1	2.25	1.43	1.37
48	5	3724	A2M	C1'-N9	-2.25	1.44	1.49
48	5	3627	OMG	C2-N1	2.25	1.43	1.37
48	5	2422	OMC	C5-C4	2.24	1.48	1.42
48	5	400	A2M	C2-N3	2.23	1.35	1.32
48	5	4494	OMG	C2-N1	2.23	1.43	1.37
48	5	3867	A2M	C1'-N9	-2.23	1.44	1.49
48	5	1625	OMG	C5-C6	2.23	1.51	1.47
48	5	2787	A2M	C2-N3	2.23	1.35	1.32
51	9	1490	OMG	O6-C6	-2.22	1.18	1.23
48	5	2861	OMC	C5-C4	2.22	1.48	1.42
50	8	75	OMG	O6-C6	-2.22	1.18	1.23
51	9	1328	OMG	O6-C6	-2.21	1.18	1.23
48	5	4500	PSU	O4'-C1'	-2.21	1.40	1.43
48	5	373	OMG	C2-N1	2.21	1.43	1.37
48	5	3715	PSU	O4'-C1'	-2.21	1.40	1.43
48	5	1524	A2M	C1'-N9	-2.20	1.44	1.49
51	9	159	A2M	C2-N3	2.20	1.35	1.32
48	5	2804	OMC	C5-C4	2.19	1.48	1.42
48	5	3792	OMG	C5-C6	2.19	1.51	1.47
48	5	1517	2MG	CM2-N2	2.18	1.49	1.45
48	5	3841	OMC	C5-C4	2.18	1.48	1.42
48	5	3760	A2M	C2-N3	2.18	1.35	1.32
48	5	4637	OMG	C2-N1	2.18	1.42	1.37
51	9	1238	PSU	C4-C5	-2.18	1.38	1.44
51	9	683	OMG	O6-C6	-2.17	1.18	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	2351	OMC	C5-C4	2.17	1.48	1.42
48	5	3825	A2M	C2-N3	2.15	1.35	1.32
48	5	3701	OMC	C5-C4	2.15	1.47	1.42
48	5	373	OMG	C6-N1	2.15	1.41	1.37
51	9	1851	MA6	C2-N3	2.15	1.35	1.32
51	9	428	OMU	C6-N1	2.14	1.43	1.38
51	9	822	PSU	O4'-C1'	-2.14	1.40	1.43
48	5	400	A2M	C1'-N9	-2.13	1.44	1.49
48	5	2424	OMG	C2-N1	2.13	1.42	1.37
51	9	822	PSU	C4-C5	-2.13	1.38	1.44
48	5	3925	OMU	C5-C4	2.12	1.48	1.43
48	5	3785	A2M	O3'-C3'	-2.12	1.37	1.43
51	9	509	OMG	C2-N1	2.12	1.42	1.37
48	5	4523	A2M	C1'-N9	-2.11	1.44	1.49
48	5	3851	PSU	O4'-C1'	-2.11	1.40	1.43
51	9	99	A2M	C1'-N9	-2.10	1.44	1.49
51	9	1326	OMU	C5-C4	2.10	1.48	1.43
51	9	468	A2M	C2-N3	2.10	1.35	1.32
48	5	3808	OMC	C5-C4	2.10	1.47	1.42
51	9	172	OMU	C5-C4	2.10	1.48	1.43
48	5	3718	A2M	C1'-N9	-2.10	1.44	1.49
48	5	3734	PSU	C4-C5	-2.09	1.38	1.44
48	5	1326	A2M	C1'-N9	-2.09	1.44	1.49
48	5	4392	OMG	C2-N1	2.09	1.42	1.37
48	5	4571	A2M	C2-N3	2.08	1.35	1.32
48	5	4530	UR3	C5-C4	2.08	1.49	1.43
48	5	4536	OMC	C5-C4	2.07	1.47	1.42
48	5	2815	A2M	C1'-N9	-2.07	1.44	1.49
48	5	3899	OMG	C2-N1	2.07	1.42	1.37
48	5	4623	OMG	C2-N1	2.07	1.42	1.37
48	5	4530	UR3	C4-N3	2.06	1.44	1.40
51	9	1639	G7M	C8-N7	2.06	1.36	1.33
48	5	4227	OMU	C5-C4	2.06	1.48	1.43
51	9	1383	A2M	C1'-N9	-2.05	1.44	1.49
48	5	4306	OMU	C6-N1	2.05	1.43	1.38
51	9	1639	G7M	O6-C6	-2.05	1.18	1.23
51	9	509	OMG	C5-C6	2.04	1.51	1.47
51	9	1248	B8N	O35-C34	2.04	1.28	1.22
51	9	1391	OMC	C5-C4	2.04	1.47	1.42
48	5	4293	PSU	C4-C5	-2.04	1.38	1.44
48	5	1781	PSU	C4-C5	-2.04	1.38	1.44
48	5	4628	PSU	C4-C5	-2.04	1.38	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4353	PSU	C4-C5	-2.03	1.38	1.44
48	5	400	A2M	C5-N7	-2.03	1.32	1.39
48	5	398	A2M	C1'-N9	-2.03	1.44	1.49
48	5	4521	PSU	O4'-C1'	-2.02	1.41	1.43
48	5	4498	OMU	C5-C4	2.02	1.48	1.43
48	5	4620	OMU	C6-N1	2.02	1.42	1.38
48	5	4296	PSU	C4-C5	-2.02	1.38	1.44
48	5	4196	OMG	C2-N1	2.02	1.42	1.37
48	5	2787	A2M	C1'-N9	-2.02	1.44	1.49
48	5	1326	A2M	C5-N7	-2.01	1.32	1.39
51	9	686	PSU	C4-C5	-2.01	1.38	1.44
48	5	4500	PSU	C4-C5	-2.01	1.38	1.44
48	5	3785	A2M	C1'-N9	-2.00	1.45	1.49
48	5	4498	OMU	C6-N1	2.00	1.42	1.38
51	9	1045	PSU	C4-C5	-2.00	1.38	1.44

All (617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1851	MA6	N1-C6-N6	-16.80	97.42	116.83
51	9	1850	MA6	N1-C6-N6	-13.95	100.72	116.83
51	9	512	A2M	C5-C6-N6	11.97	138.54	120.31
51	9	484	A2M	C5-C6-N6	11.70	138.13	120.31
51	9	1678	A2M	C5-C6-N6	11.45	137.75	120.31
48	5	4523	A2M	C5-C6-N6	11.26	137.47	120.31
51	9	1383	A2M	C5-C6-N6	11.15	137.29	120.31
48	5	2363	A2M	C5-C6-N6	11.14	137.28	120.31
48	5	3760	A2M	C5-C6-N6	11.10	137.22	120.31
48	5	4571	A2M	C5-C6-N6	11.09	137.20	120.31
51	9	27	A2M	C5-C6-N6	11.06	137.16	120.31
51	9	159	A2M	C5-C6-N6	10.98	137.04	120.31
51	9	668	A2M	C5-C6-N6	10.98	137.04	120.31
51	9	99	A2M	C5-C6-N6	10.90	136.92	120.31
48	5	3718	A2M	C5-C6-N6	10.89	136.90	120.31
48	5	1524	A2M	C5-C6-N6	10.85	136.85	120.31
48	5	1534	A2M	C5-C6-N6	10.80	136.76	120.31
51	9	166	A2M	C5-C6-N6	10.74	136.67	120.31
48	5	3830	A2M	C5-C6-N6	10.72	136.63	120.31
51	9	468	A2M	C5-C6-N6	10.70	136.62	120.31
48	5	2815	A2M	C5-C6-N6	10.70	136.61	120.31
48	5	1326	A2M	C5-C6-N6	10.68	136.58	120.31
48	5	398	A2M	C5-C6-N6	10.62	136.50	120.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3867	A2M	C5-C6-N6	10.60	136.46	120.31
48	5	1871	A2M	C5-C6-N6	10.47	136.26	120.31
48	5	3785	A2M	C5-C6-N6	10.47	136.26	120.31
51	9	1031	A2M	C5-C6-N6	10.36	136.09	120.31
48	5	3724	A2M	C5-C6-N6	10.18	135.82	120.31
48	5	3825	A2M	C5-C6-N6	10.09	135.68	120.31
48	5	2787	A2M	C5-C6-N6	10.05	135.63	120.31
51	9	1851	MA6	C1'-N9-C4	-9.96	109.14	126.64
48	5	400	A2M	C5-C6-N6	9.45	134.70	120.31
51	9	1850	MA6	C1'-N9-C4	-9.00	110.83	126.64
51	9	512	A2M	N6-C6-N1	-7.67	101.95	118.33
51	9	484	A2M	N6-C6-N1	-7.62	102.06	118.33
51	9	1678	A2M	N6-C6-N1	-7.54	102.23	118.33
48	5	3760	A2M	N6-C6-N1	-7.37	102.59	118.33
48	5	4571	A2M	N6-C6-N1	-7.37	102.59	118.33
48	5	2363	A2M	N6-C6-N1	-7.34	102.65	118.33
51	9	1383	A2M	N6-C6-N1	-7.30	102.74	118.33
48	5	1517	2MG	N1-C2-N2	7.24	123.96	116.56
48	5	4523	A2M	N6-C6-N1	-7.23	102.89	118.33
51	9	99	A2M	N6-C6-N1	-7.23	102.89	118.33
51	9	668	A2M	N6-C6-N1	-7.21	102.93	118.33
48	5	398	A2M	N6-C6-N1	-7.19	102.98	118.33
51	9	159	A2M	N6-C6-N1	-7.18	103.00	118.33
48	5	3718	A2M	N6-C6-N1	-7.06	103.26	118.33
51	9	166	A2M	N3-C2-N1	-7.04	119.11	128.67
48	5	2815	A2M	N6-C6-N1	-7.01	103.36	118.33
51	9	468	A2M	N6-C6-N1	-6.99	103.41	118.33
51	9	27	A2M	N6-C6-N1	-6.97	103.44	118.33
48	5	3785	A2M	N6-C6-N1	-6.97	103.45	118.33
51	9	484	A2M	N3-C2-N1	-6.94	119.26	128.67
48	5	3867	A2M	N6-C6-N1	-6.93	103.54	118.33
48	5	3830	A2M	N6-C6-N1	-6.89	103.61	118.33
51	9	512	A2M	N3-C2-N1	-6.85	119.38	128.67
48	5	1524	A2M	N6-C6-N1	-6.83	103.74	118.33
48	5	1534	A2M	N6-C6-N1	-6.83	103.75	118.33
48	5	3830	A2M	N3-C2-N1	-6.82	119.41	128.67
51	9	1832	6MZ	N3-C2-N1	-6.78	119.46	128.67
48	5	1524	A2M	C4'-O4'-C1'	-6.77	103.72	109.92
48	5	1871	A2M	N3-C2-N1	-6.77	119.48	128.67
48	5	3724	A2M	N6-C6-N1	-6.77	103.88	118.33
51	9	1031	A2M	N3-C2-N1	-6.70	119.58	128.67
51	9	1031	A2M	N6-C6-N1	-6.69	104.04	118.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2787	A2M	N6-C6-N1	-6.68	104.06	118.33
48	5	1326	A2M	N6-C6-N1	-6.67	104.08	118.33
51	9	166	A2M	N6-C6-N1	-6.64	104.16	118.33
48	5	3867	A2M	N3-C2-N1	-6.63	119.67	128.67
51	9	1851	MA6	N3-C2-N1	-6.59	119.73	128.67
48	5	1326	A2M	N3-C2-N1	-6.57	119.75	128.67
51	9	1383	A2M	N3-C2-N1	-6.56	119.76	128.67
48	5	4571	A2M	N3-C2-N1	-6.55	119.78	128.67
48	5	2815	A2M	N3-C2-N1	-6.54	119.80	128.67
51	9	468	A2M	N3-C2-N1	-6.50	119.85	128.67
48	5	4523	A2M	N3-C2-N1	-6.48	119.87	128.67
51	9	668	A2M	N3-C2-N1	-6.48	119.88	128.67
48	5	1524	A2M	N3-C2-N1	-6.43	119.94	128.67
48	5	3718	A2M	N3-C2-N1	-6.40	119.99	128.67
48	5	1871	A2M	N6-C6-N1	-6.37	104.72	118.33
48	5	1534	A2M	N3-C2-N1	-6.37	120.03	128.67
48	5	4220	6MZ	N3-C2-N1	-6.32	120.09	128.67
51	9	27	A2M	N3-C2-N1	-6.32	120.10	128.67
51	9	1678	A2M	N3-C2-N1	-6.26	120.17	128.67
48	5	3825	A2M	N6-C6-N1	-6.26	104.97	118.33
48	5	2787	A2M	N3-C2-N1	-6.25	120.19	128.67
48	5	3760	A2M	N3-C2-N1	-6.19	120.26	128.67
48	5	398	A2M	N3-C2-N1	-6.18	120.28	128.67
48	5	2363	A2M	N3-C2-N1	-6.15	120.32	128.67
48	5	3785	A2M	N3-C2-N1	-6.14	120.33	128.67
48	5	3724	A2M	N3-C2-N1	-6.13	120.35	128.67
51	9	99	A2M	N3-C2-N1	-6.11	120.37	128.67
48	5	4498	OMU	C4-N3-C2	-6.11	119.03	126.61
51	9	1326	OMU	C4-N3-C2	-6.04	119.11	126.61
51	9	159	A2M	N3-C2-N1	-6.04	120.47	128.67
51	9	1850	MA6	N3-C2-N1	-6.04	120.48	128.67
48	5	237	B9B	N3-C2-N1	-6.00	119.59	127.21
51	9	1248	B8N	C1'-C5-C4	5.99	126.70	117.61
48	5	2837	OMU	C4-N3-C2	-5.99	119.18	126.61
48	5	400	A2M	N3-C2-N1	-5.91	120.66	128.67
48	5	400	A2M	N6-C6-N1	-5.87	105.79	118.33
48	5	4521	PSU	N1-C2-N3	5.82	121.31	115.17
48	5	3925	OMU	C4-N3-C2	-5.82	119.39	126.61
51	9	218	PSU	N1-C2-N3	5.80	121.29	115.17
48	5	4227	OMU	C4-N3-C2	-5.79	119.43	126.61
51	9	686	PSU	C4-N3-C2	-5.78	118.40	126.37
48	5	3825	A2M	N3-C2-N1	-5.75	120.86	128.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4620	OMU	C4-N3-C2	-5.63	119.62	126.61
48	5	4306	OMU	C4-N3-C2	-5.62	119.64	126.61
48	5	3762	PSU	C4-N3-C2	-5.59	118.67	126.37
48	5	3853	PSU	N1-C2-N3	5.58	121.05	115.17
51	9	218	PSU	C4-N3-C2	-5.58	118.69	126.37
48	5	4628	PSU	N1-C2-N3	5.56	121.03	115.17
51	9	172	OMU	C4-N3-C2	-5.56	119.71	126.61
51	9	1442	OMU	C4-N3-C2	-5.54	119.73	126.61
51	9	121	OMU	C4-N3-C2	-5.54	119.73	126.61
48	5	4220	6MZ	C2-N1-C6	5.53	120.89	116.60
48	5	1677	PSU	N1-C2-N3	5.49	120.96	115.17
48	5	1677	PSU	C4-N3-C2	-5.46	118.85	126.37
48	5	1683	PSU	N1-C2-N3	5.46	120.92	115.17
51	9	1174	PSU	N1-C2-N3	5.46	120.92	115.17
51	9	822	PSU	N1-C2-N3	5.45	120.91	115.17
48	5	4442	PSU	N1-C2-N3	5.44	120.91	115.17
51	9	1045	PSU	N1-C2-N3	5.44	120.90	115.17
48	5	4353	PSU	N1-C2-N3	5.43	120.90	115.17
51	9	1643	PSU	C4-N3-C2	-5.43	118.89	126.37
48	5	4628	PSU	C4-N3-C2	-5.43	118.89	126.37
51	9	1248	B8N	C5-C4-N3	5.43	126.00	116.15
51	9	428	OMU	C4-N3-C2	-5.42	119.88	126.61
51	9	686	PSU	N1-C2-N3	5.41	120.87	115.17
48	5	3851	PSU	N1-C2-N3	5.40	120.86	115.17
51	9	1832	6MZ	C2-N1-C6	5.38	120.78	116.60
48	5	3920	PSU	C4-N3-C2	-5.38	118.97	126.37
48	5	3920	PSU	N1-C2-N3	5.36	120.83	115.17
51	9	109	PSU	N1-C2-N3	5.36	120.82	115.17
48	5	3762	PSU	N1-C2-N3	5.32	120.78	115.17
51	9	105	PSU	N1-C2-N3	5.32	120.78	115.17
51	9	1045	PSU	C4-N3-C2	-5.31	119.06	126.37
51	9	1643	PSU	N1-C2-N3	5.30	120.76	115.17
48	5	4361	PSU	N1-C2-N3	5.29	120.75	115.17
51	9	116	OMU	C4-N3-C2	-5.29	120.04	126.61
51	9	1248	B8N	C4-N3-C2	-5.28	119.12	125.62
51	9	815	PSU	N1-C2-N3	5.27	120.73	115.17
48	5	3764	PSU	N1-C2-N3	5.27	120.72	115.17
51	9	1244	PSU	C4-N3-C2	-5.27	119.12	126.37
51	9	1081	PSU	N1-C2-N3	5.26	120.71	115.17
48	5	3853	PSU	C4-N3-C2	-5.24	119.15	126.37
48	5	3764	PSU	C4-N3-C2	-5.22	119.17	126.37
51	9	814	PSU	C4-N3-C2	-5.22	119.19	126.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3785	A2M	O4'-C1'-N9	5.21	115.65	108.75
48	5	4423	PSU	C4-N3-C2	-5.20	119.20	126.37
51	9	34	PSU	N1-C2-N3	5.20	120.65	115.17
48	5	4361	PSU	C4-N3-C2	-5.19	119.23	126.37
51	9	822	PSU	C4-N3-C2	-5.19	119.23	126.37
51	9	109	PSU	C4-N3-C2	-5.18	119.23	126.37
51	9	815	PSU	C4-N3-C2	-5.18	119.23	126.37
48	5	4299	PSU	C4-N3-C2	-5.17	119.25	126.37
51	9	1347	PSU	C4-N3-C2	-5.17	119.25	126.37
48	5	4296	PSU	N1-C2-N3	5.16	120.61	115.17
51	9	1004	PSU	N1-C2-N3	5.15	120.60	115.17
48	5	4552	PSU	C4-N3-C2	-5.15	119.28	126.37
51	9	1174	PSU	C4-N3-C2	-5.15	119.28	126.37
48	5	1683	PSU	C4-N3-C2	-5.15	119.28	126.37
51	9	814	PSU	N1-C2-N3	5.14	120.59	115.17
48	5	4420	PSU	N1-C2-N3	5.13	120.58	115.17
48	5	2632	PSU	N1-C2-N3	5.12	120.56	115.17
51	9	1244	PSU	N1-C2-N3	5.12	120.56	115.17
48	5	1782	PSU	N1-C2-N3	5.11	120.56	115.17
48	5	3695	PSU	N1-C2-N3	5.11	120.56	115.17
48	5	3785	A2M	C4'-O4'-C1'	-5.10	105.25	109.92
51	9	609	PSU	N1-C2-N3	5.10	120.55	115.17
48	5	3695	PSU	C4-N3-C2	-5.08	119.38	126.37
48	5	3851	PSU	C4-N3-C2	-5.08	119.38	126.37
48	5	1860	PSU	N1-C2-N3	5.06	120.51	115.17
51	9	119	PSU	C4-N3-C2	-5.06	119.41	126.37
51	9	1232	PSU	N1-C2-N3	5.05	120.50	115.17
48	5	1744	PSU	C4-N3-C2	-5.04	119.43	126.37
48	5	4423	PSU	N1-C2-N3	5.03	120.47	115.17
48	5	4442	PSU	C4-N3-C2	-5.03	119.44	126.37
48	5	1781	PSU	C4-N3-C2	-5.02	119.45	126.37
48	5	4521	PSU	C4-N3-C2	-5.02	119.45	126.37
48	5	4500	PSU	N1-C2-N3	5.02	120.46	115.17
51	9	119	PSU	N1-C2-N3	5.02	120.46	115.17
48	5	4353	PSU	C4-N3-C2	-5.02	119.46	126.37
48	5	4579	PSU	C4-N3-C2	-5.02	119.46	126.37
51	9	649	PSU	C4-N3-C2	-5.01	119.47	126.37
48	5	4420	PSU	C4-N3-C2	-5.00	119.48	126.37
48	5	1862	PSU	N1-C2-N3	5.00	120.44	115.17
51	9	1238	PSU	C4-N3-C2	-5.00	119.49	126.37
48	5	1744	PSU	N1-C2-N3	4.99	120.44	115.17
51	9	1383	A2M	C4'-O4'-C1'	-4.98	105.36	109.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4293	PSU	C4-N3-C2	-4.98	119.52	126.37
48	5	1792	PSU	C4-N3-C2	-4.97	119.52	126.37
51	9	105	PSU	C4-N3-C2	-4.97	119.52	126.37
48	5	1782	PSU	C4-N3-C2	-4.97	119.52	126.37
51	9	1081	PSU	C4-N3-C2	-4.97	119.52	126.37
48	5	2632	PSU	C4-N3-C2	-4.96	119.53	126.37
51	9	1046	PSU	N1-C2-N3	4.96	120.40	115.17
48	5	4403	PSU	C4-N3-C2	-4.96	119.54	126.37
51	9	609	PSU	C4-N3-C2	-4.96	119.55	126.37
51	9	1004	PSU	C4-N3-C2	-4.95	119.55	126.37
48	5	4457	PSU	C4-N3-C2	-4.94	119.56	126.37
51	9	863	PSU	C4-N3-C2	-4.94	119.57	126.37
48	5	3639	PSU	N1-C2-N3	4.92	120.36	115.17
48	5	4296	PSU	C4-N3-C2	-4.92	119.60	126.37
48	5	3734	PSU	N1-C2-N3	4.92	120.35	115.17
48	5	1862	PSU	C4-N3-C2	-4.91	119.61	126.37
48	5	4403	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	572	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	1238	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	1347	PSU	N1-C2-N3	4.90	120.34	115.17
48	5	4552	PSU	N1-C2-N3	4.89	120.33	115.17
48	5	2508	PSU	C4-N3-C2	-4.89	119.63	126.37
48	5	4500	PSU	C4-N3-C2	-4.88	119.64	126.37
48	5	3639	PSU	C4-N3-C2	-4.88	119.65	126.37
48	5	2508	PSU	N1-C2-N3	4.87	120.30	115.17
51	9	1232	PSU	C4-N3-C2	-4.86	119.68	126.37
48	5	4532	PSU	C4-N3-C2	-4.85	119.69	126.37
51	9	1367	PSU	C4-N3-C2	-4.84	119.70	126.37
48	5	4299	PSU	N1-C2-N3	4.80	120.23	115.17
48	5	3818	UY1	N1-C2-N3	4.80	120.23	115.17
48	5	4530	UR3	C4-N3-C2	-4.80	120.72	124.58
48	5	1781	PSU	N1-C2-N3	4.79	120.22	115.17
51	9	649	PSU	N1-C2-N3	4.78	120.21	115.17
51	9	1367	PSU	N1-C2-N3	4.78	120.21	115.17
48	5	4579	PSU	N1-C2-N3	4.76	120.19	115.17
48	5	1860	PSU	C4-N3-C2	-4.75	119.83	126.37
48	5	1792	PSU	N1-C2-N3	4.74	120.17	115.17
51	9	1692	PSU	C4-N3-C2	-4.74	119.84	126.37
48	5	4293	PSU	N1-C2-N3	4.74	120.17	115.17
48	5	3734	PSU	C4-N3-C2	-4.73	119.85	126.37
51	9	668	A2M	O4'-C1'-N9	-4.73	102.47	108.75
48	5	3818	UY1	C4-N3-C2	-4.73	119.86	126.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	572	PSU	C4-N3-C2	-4.73	119.86	126.37
51	9	1046	PSU	C4-N3-C2	-4.72	119.87	126.37
48	5	1322	1MA	N1-C2-N3	-4.71	120.00	125.90
48	5	3715	PSU	N1-C2-N3	4.67	120.09	115.17
51	9	1177	PSU	N1-C2-N3	4.65	120.07	115.17
51	9	34	PSU	C4-N3-C2	-4.64	119.98	126.37
51	9	1445	PSU	N1-C2-N3	4.61	120.03	115.17
51	9	863	PSU	N1-C2-N3	4.60	120.02	115.17
51	9	1177	PSU	C4-N3-C2	-4.57	120.08	126.37
51	9	1692	PSU	N1-C2-N3	4.55	119.97	115.17
48	5	3715	PSU	C4-N3-C2	-4.50	120.17	126.37
48	5	4306	OMU	N3-C2-N1	4.50	120.75	114.89
51	9	1445	PSU	C4-N3-C2	-4.43	120.27	126.37
51	9	1326	OMU	N3-C2-N1	4.34	120.54	114.89
48	5	237	B9B	C2-N3-C4	4.34	120.16	115.48
48	5	4532	PSU	N1-C2-N3	4.33	119.74	115.17
51	9	801	PSU	N1-C2-N3	4.29	119.70	115.17
48	5	4457	PSU	N1-C2-N3	4.29	119.69	115.17
48	5	4420	PSU	O2-C2-N1	-4.25	118.40	122.79
51	9	815	PSU	O2-C2-N1	-4.23	118.43	122.79
51	9	801	PSU	C4-N3-C2	-4.21	120.57	126.37
48	5	3925	OMU	C5-C4-N3	4.20	120.68	114.80
48	5	4498	OMU	C5-C4-N3	4.17	120.64	114.80
51	9	863	PSU	O2-C2-N1	-4.14	118.52	122.79
51	9	116	OMU	N3-C2-N1	4.13	120.27	114.89
48	5	3853	PSU	O2-C2-N1	-4.08	118.58	122.79
48	5	4620	OMU	C5-C4-N3	4.08	120.51	114.80
48	5	4227	OMU	C5-C4-N3	4.04	120.46	114.80
48	5	3715	PSU	O2-C2-N1	-4.03	118.64	122.79
48	5	3818	UY1	C6-C5-C4	4.01	120.88	118.17
51	9	686	PSU	O2-C2-N1	-4.00	118.66	122.79
51	9	1442	OMU	N3-C2-N1	4.00	120.09	114.89
48	5	1322	1MA	C5-C6-N1	3.98	119.67	113.95
48	5	4498	OMU	N3-C2-N1	3.95	120.04	114.89
51	9	1248	B8N	N3-C2-N1	3.93	121.52	116.72
51	9	428	OMU	C5-C4-N3	3.93	120.30	114.80
48	5	2837	OMU	C5-C4-N3	3.92	120.30	114.80
51	9	572	PSU	O2-C2-N1	-3.90	118.76	122.79
48	5	2837	OMU	N3-C2-N1	3.89	119.95	114.89
51	9	121	OMU	C5-C4-N3	3.86	120.21	114.80
51	9	1643	PSU	O2-C2-N1	-3.85	118.82	122.79
48	5	4620	OMU	N3-C2-N1	3.82	119.87	114.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3925	OMU	N3-C2-N1	3.81	119.85	114.89
48	5	4227	OMU	N3-C2-N1	3.80	119.84	114.89
48	5	4306	OMU	C5-C4-N3	3.77	120.07	114.80
48	5	4623	OMG	C5-C6-N1	3.75	121.22	114.07
51	9	609	PSU	O2-C2-N1	-3.74	118.93	122.79
48	5	4500	PSU	O2-C2-N1	-3.74	118.94	122.79
51	9	172	OMU	C5-C4-N3	3.71	120.00	114.80
48	5	400	A2M	C4'-O4'-C1'	-3.70	106.54	109.92
48	5	3715	PSU	C6-C5-C4	3.70	120.67	118.17
48	5	1517	2MG	C8-N7-C5	3.68	108.81	102.55
51	9	172	OMU	N3-C2-N1	3.68	119.68	114.89
51	9	1326	OMU	C5-C4-N3	3.64	119.90	114.80
48	5	4521	PSU	C6-C5-C4	3.62	120.61	118.17
48	5	2364	OMG	C8-N7-C5	3.61	108.69	102.55
48	5	373	OMG	C8-N7-C5	3.60	108.67	102.55
48	5	4370	OMG	C8-N7-C5	3.59	108.66	102.55
51	9	683	OMG	C8-N7-C5	3.56	108.62	102.55
48	5	3627	OMG	C8-N7-C5	3.54	108.58	102.55
48	5	3899	OMG	C8-N7-C5	3.54	108.57	102.55
48	5	3782	5MC	C5-C6-N1	-3.53	119.47	123.31
48	5	4530	UR3	C5-C4-N3	3.53	119.69	115.04
48	5	1862	PSU	O2-C2-N1	-3.53	119.14	122.79
48	5	4628	PSU	O2-C2-N1	-3.53	119.15	122.79
51	9	121	OMU	N3-C2-N1	3.52	119.48	114.89
51	9	428	OMU	O4-C4-C5	-3.51	119.11	125.16
48	5	3818	UY1	C6-N1-C2	-3.50	119.44	122.69
51	9	1678	A2M	C4'-O4'-C1'	-3.50	106.72	109.92
48	5	4637	OMG	C8-N7-C5	3.49	108.48	102.55
48	5	1625	OMG	O6-C6-C5	-3.47	117.45	124.32
51	9	218	PSU	C6-C5-C4	3.46	120.51	118.17
48	5	1316	OMG	C8-N7-C5	3.45	108.43	102.55
48	5	4623	OMG	C2-N1-C6	-3.45	118.79	125.11
48	5	1677	PSU	O2-C2-N1	-3.45	119.23	122.79
48	5	4447	5MC	C5-C6-N1	-3.45	119.57	123.31
51	9	116	OMU	C5-C4-N3	3.43	119.61	114.80
48	5	4392	OMG	C2-N1-C6	-3.43	118.83	125.11
48	5	4618	OMG	C8-N7-C5	3.43	108.39	102.55
48	5	3762	PSU	O2-C2-N1	-3.42	119.26	122.79
48	5	1625	OMG	C2-N1-C6	-3.42	118.85	125.11
51	9	822	PSU	C6-C5-C4	3.42	120.48	118.17
48	5	3920	PSU	O2-C2-N1	-3.41	119.27	122.79
48	5	4521	PSU	O2-C2-N1	-3.41	119.27	122.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1625	OMG	C5-C6-N1	3.41	120.57	114.07
51	9	1174	PSU	O2-C2-N1	-3.38	119.30	122.79
48	5	4499	OMG	C5-C6-N1	3.38	120.52	114.07
48	5	2876	OMG	C8-N7-C5	3.38	108.31	102.55
48	5	2424	OMG	C2-N1-C6	-3.34	118.99	125.11
48	5	1517	2MG	N2-C2-N3	-3.33	116.26	120.51
48	5	2876	OMG	C2-N1-C6	-3.33	119.01	125.11
51	9	436	OMG	C5-C6-N1	3.32	120.41	114.07
51	9	683	OMG	C2-N1-C6	-3.31	119.06	125.11
48	5	4196	OMG	C5-C6-N1	3.30	120.37	114.07
51	9	683	OMG	C5-C6-N1	3.30	120.36	114.07
48	5	1316	OMG	C5-C6-N1	3.30	120.36	114.07
48	5	2364	OMG	C2-N1-C6	-3.29	119.08	125.11
48	5	4228	OMG	C8-N7-C5	3.29	108.15	102.55
48	5	1744	PSU	O2-C2-N1	-3.28	119.41	122.79
51	9	436	OMG	C2-N1-C6	-3.28	119.11	125.11
50	8	75	OMG	C8-N7-C5	3.27	108.11	102.55
48	5	4392	OMG	C5-C6-N1	3.26	120.29	114.07
48	5	1522	OMG	C8-N7-C5	3.26	108.09	102.55
51	9	822	PSU	O2-C2-N1	-3.25	119.43	122.79
48	5	1782	PSU	O2-C2-N1	-3.25	119.43	122.79
51	9	1442	OMU	C5-C4-N3	3.25	119.35	114.80
48	5	1792	PSU	O2-C2-N1	-3.24	119.45	122.79
51	9	119	PSU	O2-C2-N1	-3.24	119.45	122.79
48	5	1625	OMG	C8-N7-C5	3.23	108.05	102.55
51	9	509	OMG	C5-C6-N1	3.23	120.22	114.07
48	5	4353	PSU	C6-C5-C4	3.22	120.34	118.17
51	9	1442	OMU	O4-C4-C5	-3.21	119.63	125.16
51	9	34	PSU	C6-N1-C2	-3.21	119.72	122.69
48	5	4499	OMG	C2-N1-C6	-3.21	119.24	125.11
48	5	4370	OMG	C5-C6-N1	3.20	120.19	114.07
51	9	428	OMU	N3-C2-N1	3.20	119.06	114.89
51	9	683	OMG	CM2-O2'-C2'	3.18	122.65	114.47
50	8	75	OMG	C2-N1-C6	-3.18	119.28	125.11
48	5	237	B9B	N2-C2-N3	3.18	122.75	117.79
51	9	668	A2M	C4'-O4'-C1'	-3.18	107.02	109.92
48	5	4618	OMG	C5-C6-N1	3.17	120.11	114.07
48	5	4618	OMG	C2-N1-C6	-3.16	119.32	125.11
50	8	75	OMG	C5-C6-N1	3.16	120.11	114.07
51	9	644	OMG	C8-N7-C5	3.16	107.92	102.55
48	5	4196	OMG	C8-N7-C5	3.15	107.92	102.55
48	5	4423	PSU	O2-C2-N1	-3.15	119.54	122.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4637	OMG	C2-N1-C6	-3.15	119.35	125.11
48	5	1522	OMG	C5-C6-N1	3.14	120.07	114.07
48	5	1517	2MG	C5-C6-N1	3.13	120.04	114.07
48	5	4370	OMG	C2-N1-C6	-3.13	119.38	125.11
48	5	2424	OMG	C5-C6-N1	3.12	120.03	114.07
48	5	4637	OMG	C5-C6-N1	3.12	120.02	114.07
48	5	4571	A2M	C4'-O4'-C1'	-3.12	107.07	109.92
48	5	373	OMG	C5-C6-N1	3.10	119.98	114.07
48	5	4392	OMG	C8-N7-C5	3.09	107.81	102.55
48	5	2364	OMG	C5-C6-N1	3.09	119.96	114.07
51	9	436	OMG	C8-N7-C5	3.08	107.79	102.55
48	5	4196	OMG	C2-N1-C6	-3.08	119.47	125.11
48	5	2424	OMG	C8-N7-C5	3.08	107.79	102.55
48	5	373	OMG	C2-N1-C6	-3.08	119.47	125.11
48	5	4499	OMG	C8-N7-C5	3.06	107.77	102.55
51	9	686	PSU	C6-C5-C4	3.06	120.24	118.17
51	9	99	A2M	C4'-O4'-C1'	-3.06	107.12	109.92
48	5	4494	OMG	C8-N7-C5	3.05	107.75	102.55
51	9	1328	OMG	C2-N1-C6	-3.05	119.53	125.11
48	5	3627	OMG	C5-C6-N1	3.05	119.88	114.07
48	5	4442	PSU	O2-C2-N1	-3.05	119.65	122.79
51	9	1328	OMG	C5-C6-N1	3.04	119.87	114.07
51	9	509	OMG	C2-N1-C6	-3.04	119.55	125.11
48	5	4623	OMG	C8-N7-C5	3.03	107.71	102.55
48	5	3851	PSU	O2-C2-N1	-3.03	119.66	122.79
51	9	218	PSU	O2-C2-N1	-3.02	119.67	122.79
48	5	1522	OMG	C2-N1-C6	-3.02	119.58	125.11
51	9	1328	OMG	C8-N7-C5	3.02	107.69	102.55
51	9	1490	OMG	C8-N7-C5	3.01	107.68	102.55
48	5	4500	PSU	C6-C5-C4	3.01	120.21	118.17
48	5	1322	1MA	C8-N7-C5	3.00	107.65	102.55
48	5	4494	OMG	C2-N1-C6	-2.99	119.63	125.11
48	5	3851	PSU	C6-N1-C2	-2.97	119.93	122.69
51	9	1248	B8N	O4-C4-N3	-2.96	115.18	119.99
51	9	1326	OMU	O2-C2-N1	-2.96	118.95	122.80
51	9	1445	PSU	C6-N1-C2	-2.95	119.95	122.69
48	5	1316	OMG	C2-N1-C6	-2.95	119.72	125.11
48	5	3920	PSU	C6-C5-C4	2.94	120.16	118.17
48	5	1860	PSU	O2-C2-N1	-2.93	119.77	122.79
51	9	644	OMG	C2-N1-C6	-2.93	119.75	125.11
51	9	1850	MA6	C2-N1-C6	2.93	119.71	116.84
48	5	2837	OMU	O2-C2-N1	-2.92	118.99	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	814	PSU	O2-C2-N1	-2.92	119.78	122.79
48	5	3627	OMG	C2-N1-C6	-2.91	119.78	125.11
51	9	159	A2M	C4'-O4'-C1'	-2.91	107.26	109.92
48	5	4498	OMU	O4-C4-C5	-2.90	120.16	125.16
51	9	1045	PSU	O2-C2-N1	-2.90	119.80	122.79
48	5	4494	OMG	C5-C6-N1	2.89	119.58	114.07
48	5	4499	OMG	O6-C6-C5	-2.88	118.61	124.32
51	9	116	OMU	O2-C2-N1	-2.88	119.05	122.80
51	9	1238	PSU	C6-C5-C4	2.87	120.11	118.17
51	9	105	PSU	C6-N1-C2	-2.85	120.05	122.69
48	5	3899	OMG	C5-C6-N1	2.85	119.51	114.07
48	5	3792	OMG	C5-C6-N1	2.84	119.50	114.07
51	9	1842	4AC	O2-C2-N3	-2.83	117.86	122.33
48	5	3718	A2M	O4'-C1'-N9	2.83	112.50	108.75
48	5	3792	OMG	C8-N7-C5	2.83	107.37	102.55
51	9	1004	PSU	O2-C2-N1	-2.83	119.87	122.79
48	5	4228	OMG	C5-C6-N1	2.83	119.46	114.07
51	9	1244	PSU	O2-C2-N1	-2.81	119.89	122.79
48	5	4498	OMU	O2-C2-N1	-2.81	119.14	122.80
51	9	1045	PSU	C6-C5-C4	2.80	120.06	118.17
48	5	2815	A2M	C4'-O4'-C1'	-2.80	107.36	109.92
48	5	4228	OMG	C2-N1-C6	-2.80	119.99	125.11
48	5	2837	OMU	C2'-C1'-N1	-2.79	108.94	114.24
48	5	4579	PSU	O2-C2-N1	-2.79	119.91	122.79
51	9	649	PSU	O2-C2-N1	-2.79	119.91	122.79
48	5	3853	PSU	C6-N1-C2	-2.78	120.11	122.69
51	9	822	PSU	C6-N1-C2	-2.78	120.11	122.69
51	9	1326	OMU	O4-C4-C5	-2.78	120.37	125.16
51	9	1639	G7M	C2-N1-C6	-2.78	120.03	125.11
51	9	436	OMG	O6-C6-C5	-2.77	118.82	124.32
51	9	121	OMU	O4-C4-C5	-2.77	120.39	125.16
51	9	1851	MA6	C2-N1-C6	2.77	119.55	116.84
51	9	815	PSU	C6-N1-C2	-2.76	120.13	122.69
51	9	644	OMG	C5-C6-N1	2.76	119.34	114.07
48	5	2837	OMU	O4-C4-C5	-2.76	120.40	125.16
48	5	3639	PSU	O2-C2-N1	-2.76	119.95	122.79
48	5	1683	PSU	C6-N1-C2	-2.75	120.14	122.69
48	5	3724	A2M	C4'-O4'-C1'	-2.74	107.42	109.92
51	9	34	PSU	O2-C2-N1	-2.73	119.97	122.79
48	5	1534	A2M	C4'-O4'-C1'	-2.72	107.43	109.92
48	5	4353	PSU	C6-N1-C2	-2.72	120.17	122.69
48	5	1683	PSU	O2-C2-N1	-2.72	119.98	122.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1031	A2M	C4'-O4'-C1'	-2.71	107.44	109.92
48	5	1871	A2M	C4'-O4'-C1'	-2.71	107.44	109.92
48	5	3825	A2M	C4'-O4'-C1'	-2.70	107.45	109.92
48	5	2876	OMG	C5-C6-N1	2.68	119.19	114.07
48	5	3792	OMG	O6-C6-C5	-2.68	119.01	124.32
51	9	1232	PSU	C6-N1-C2	-2.68	120.20	122.69
48	5	1781	PSU	O2-C2-N1	-2.68	120.03	122.79
48	5	2632	PSU	C6-N1-C2	-2.68	120.21	122.69
48	5	3899	OMG	C2-N1-C6	-2.67	120.22	125.11
48	5	2632	PSU	O2-C2-N1	-2.67	120.03	122.79
48	5	4637	OMG	O6-C6-C5	-2.67	119.03	124.32
51	9	1046	PSU	O2-C2-N1	-2.67	120.04	122.79
51	9	109	PSU	C6-N1-C2	-2.66	120.22	122.69
51	9	1244	PSU	C6-C5-C4	2.65	119.97	118.17
51	9	1174	PSU	C6-N1-C2	-2.65	120.23	122.69
48	5	4521	PSU	C6-N1-C2	-2.64	120.24	122.69
48	5	4628	PSU	C6-C5-C4	2.64	119.96	118.17
51	9	121	OMU	CM2-O2'-C2'	2.64	121.24	114.47
48	5	4442	PSU	C6-C5-C4	2.63	119.95	118.17
48	5	2787	A2M	O4'-C1'-N9	-2.61	105.29	108.75
48	5	3764	PSU	O2-C2-N1	-2.60	120.11	122.79
48	5	4623	OMG	O6-C6-C5	-2.60	119.17	124.32
48	5	3792	OMG	C2-N1-C6	-2.60	120.35	125.11
48	5	2424	OMG	O6-C6-C5	-2.60	119.17	124.32
48	5	3925	OMU	O4-C4-C5	-2.59	120.70	125.16
51	9	1046	PSU	C6-N1-C2	-2.59	120.29	122.69
48	5	1860	PSU	C6-N1-C2	-2.58	120.30	122.69
48	5	4530	UR3	C6-N1-C2	-2.58	119.69	121.80
48	5	3695	PSU	C6-N1-C2	-2.56	120.31	122.69
51	9	1490	OMG	C5-C6-N1	2.56	118.95	114.07
48	5	1782	PSU	C6-C5-C4	2.56	119.90	118.17
48	5	4361	PSU	O2-C2-N1	-2.55	120.15	122.79
51	9	509	OMG	C8-N7-C5	2.55	106.89	102.55
48	5	4442	PSU	C6-N1-C2	-2.54	120.33	122.69
51	9	572	PSU	C6-N1-C2	-2.54	120.33	122.69
48	5	4620	OMU	O4-C4-C5	-2.53	120.79	125.16
51	9	1347	PSU	O2-C2-N1	-2.52	120.19	122.79
48	5	4500	PSU	C6-N1-C2	-2.52	120.36	122.69
48	5	4299	PSU	O2-C2-N1	-2.52	120.19	122.79
48	5	400	A2M	O4'-C1'-N9	-2.52	105.41	108.75
51	9	1367	PSU	C6-N1-C2	-2.51	120.36	122.69
48	5	4227	OMU	O4-C4-C5	-2.51	120.84	125.16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	172	OMU	O4-C4-C5	-2.51	120.84	125.16
51	9	428	OMU	O2-C2-N1	-2.50	119.54	122.80
51	9	815	PSU	C6-C5-C4	2.50	119.86	118.17
51	9	801	PSU	C6-N1-C2	-2.49	120.38	122.69
51	9	1445	PSU	O2-C2-N1	-2.48	120.23	122.79
51	9	172	OMU	O2-C2-N1	-2.48	119.57	122.80
48	5	2824	OMC	O2-C2-N3	-2.48	118.42	122.33
51	9	1177	PSU	C6-N1-C2	-2.48	120.39	122.69
51	9	468	A2M	C5'-C4'-C3'	-2.47	106.31	115.21
48	5	4353	PSU	O2-C2-N1	-2.47	120.24	122.79
51	9	1692	PSU	O2-C2-N1	-2.46	120.25	122.79
51	9	116	OMU	O4-C4-C5	-2.46	120.92	125.16
48	5	4552	PSU	O2-C2-N1	-2.46	120.25	122.79
48	5	4227	OMU	O2-C2-N1	-2.46	119.60	122.80
51	9	509	OMG	O6-C6-C5	-2.46	119.45	124.32
51	9	801	PSU	O2-C2-N1	-2.45	120.26	122.79
51	9	1248	B8N	C31-N3-C4	2.45	120.64	117.18
48	5	4447	5MC	CM5-C5-C6	-2.44	119.55	122.85
48	5	3715	PSU	C6-N1-C2	-2.43	120.43	122.69
48	5	4420	PSU	C6-N1-C2	-2.42	120.44	122.69
51	9	1081	PSU	C6-C5-C4	2.42	119.81	118.17
51	9	1328	OMG	O6-C6-C5	-2.41	119.55	124.32
48	5	237	B9B	C1'-N9-C4	-2.41	122.41	126.64
51	9	609	PSU	C6-N1-C2	-2.41	120.46	122.69
48	5	1517	2MG	O6-C6-C5	-2.40	119.55	124.32
51	9	1004	PSU	C6-N1-C2	-2.40	120.46	122.69
48	5	4296	PSU	C6-N1-C2	-2.40	120.47	122.69
48	5	3734	PSU	C6-C5-C4	2.39	119.78	118.17
51	9	119	PSU	C6-N1-C2	-2.38	120.49	122.69
51	9	512	A2M	C4'-O4'-C1'	-2.37	107.75	109.92
51	9	1367	PSU	O2-C2-N1	-2.37	120.34	122.79
51	9	1045	PSU	C6-N1-C2	-2.37	120.49	122.69
48	5	4293	PSU	C6-N1-C2	-2.36	120.50	122.69
51	9	1490	OMG	O6-C6-C5	-2.35	119.65	124.32
48	5	3764	PSU	C6-N1-C2	-2.35	120.52	122.69
51	9	1347	PSU	C6-N1-C2	-2.35	120.52	122.69
48	5	3718	A2M	C1'-N9-C4	-2.34	122.53	126.64
48	5	4457	PSU	O2-C2-N1	-2.34	120.38	122.79
48	5	237	B9B	O6-C6-N1	-2.33	118.24	120.23
48	5	3734	PSU	C6-N1-C2	-2.33	120.53	122.69
48	5	1340	OMC	C5-C4-N3	-2.33	117.39	121.32
48	5	1781	PSU	C6-C5-C4	2.32	119.74	118.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	822	PSU	O4'-C1'-C2'	2.32	108.36	105.15
48	5	3695	PSU	O2-C2-N1	-2.31	120.40	122.79
51	9	814	PSU	C6-N1-C2	-2.31	120.55	122.69
48	5	3762	PSU	C6-N1-C2	-2.30	120.56	122.69
48	5	3701	OMC	O2-C2-N3	-2.29	118.72	122.33
48	5	3734	PSU	O2-C2-N1	-2.29	120.43	122.79
51	9	1490	OMG	C2-N1-C6	-2.27	120.95	125.11
51	9	1081	PSU	O4'-C1'-C2'	2.27	108.29	105.15
51	9	1081	PSU	O2-C2-N1	-2.26	120.45	122.79
51	9	1177	PSU	O2-C2-N1	-2.26	120.46	122.79
48	5	4392	OMG	O6-C6-C5	-2.26	119.84	124.32
48	5	2508	PSU	O2-C2-N1	-2.26	120.46	122.79
48	5	4618	OMG	O6-C6-C5	-2.26	119.85	124.32
48	5	1862	PSU	C6-C5-C4	2.26	119.70	118.17
51	9	1383	A2M	C2'-C3'-C4'	-2.26	97.14	101.99
51	9	814	PSU	C6-C5-C4	2.25	119.69	118.17
48	5	3715	PSU	O4'-C1'-C2'	2.25	108.26	105.15
51	9	1081	PSU	C6-N1-C2	-2.24	120.61	122.69
51	9	218	PSU	C5-C6-N1	-2.24	119.03	122.14
51	9	218	PSU	C6-N1-C2	-2.24	120.61	122.69
48	5	2508	PSU	C6-N1-C2	-2.22	120.63	122.69
48	5	4618	OMG	N2-C2-N1	2.21	121.44	116.76
48	5	237	B9B	C61-O6-C6	2.21	121.41	117.65
51	9	1238	PSU	C5-C6-N1	-2.20	119.09	122.14
48	5	3818	UY1	O4'-C1'-C2'	2.20	108.41	104.56
48	5	4628	PSU	C6-N1-C2	-2.19	120.66	122.69
51	9	1639	G7M	N2-C2-N1	2.19	121.38	116.76
51	9	119	PSU	C6-C5-C4	2.18	119.64	118.17
51	9	1248	B8N	O4-C4-C5	-2.18	118.81	122.58
48	5	3639	PSU	C6-N1-C2	-2.18	120.67	122.69
51	9	649	PSU	C6-N1-C2	-2.18	120.67	122.69
48	5	3920	PSU	C6-N1-C2	-2.18	120.67	122.69
48	5	4306	OMU	O2-C2-N1	-2.18	119.96	122.80
48	5	4494	OMG	N2-C2-N1	2.17	121.35	116.76
48	5	3782	5MC	CM5-C5-C6	-2.16	119.92	122.85
48	5	1534	A2M	C2'-C1'-N9	2.16	117.36	112.56
51	9	109	PSU	O2-C2-N1	-2.16	120.56	122.79
51	9	1244	PSU	C6-N1-C2	-2.16	120.69	122.69
48	5	4579	PSU	C6-N1-C2	-2.15	120.69	122.69
51	9	668	A2M	C2'-C1'-N9	2.15	117.33	112.56
51	9	1643	PSU	C6-N1-C2	-2.14	120.70	122.69
48	5	1744	PSU	C6-N1-C2	-2.14	120.71	122.69

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1782	PSU	C6-N1-C2	-2.13	120.71	122.69
48	5	4552	PSU	C6-N1-C2	-2.13	120.72	122.69
51	9	668	A2M	C3'-C2'-C1'	2.13	106.88	102.81
50	8	75	OMG	N2-C2-N1	2.12	121.23	116.76
48	5	2861	OMC	O2-C2-N3	-2.11	119.01	122.33
48	5	4423	PSU	C6-N1-C2	-2.10	120.74	122.69
51	9	1391	OMC	O2-C2-N3	-2.10	119.02	122.33
48	5	1677	PSU	C6-C5-C4	2.10	119.59	118.17
48	5	1522	OMG	N2-C2-N1	2.10	121.19	116.76
50	8	75	OMG	O6-C6-C5	-2.10	120.16	124.32
51	9	1347	PSU	O4-C4-C5	-2.10	118.80	124.01
48	5	2363	A2M	C4'-O4'-C1'	-2.10	108.01	109.92
48	5	4361	PSU	C6-N1-C2	-2.09	120.75	122.69
51	9	1046	PSU	O4'-C1'-C2'	2.09	108.05	105.15
48	5	4220	6MZ	C6-C5-C4	2.08	119.89	117.68
51	9	105	PSU	O2-C2-N1	-2.08	120.64	122.79
48	5	4530	UR3	C1'-N1-C2	2.08	120.44	117.04
48	5	4403	PSU	C6-N1-C2	-2.07	120.77	122.69
51	9	121	OMU	C1'-N1-C2	2.07	121.32	117.59
48	5	4403	PSU	O4'-C1'-C2'	2.07	108.02	105.15
48	5	4293	PSU	O4-C4-C5	-2.07	118.87	124.01
48	5	4521	PSU	C5-C6-N1	-2.06	119.28	122.14
48	5	4521	PSU	O4'-C1'-C2'	2.06	108.01	105.15
48	5	4628	PSU	O4'-C1'-C2'	2.06	108.00	105.15
51	9	1337	4AC	C5-C4-N4	2.06	126.41	122.94
48	5	4196	OMG	O6-C6-C5	-2.06	120.24	124.32
48	5	3887	OMC	C2'-C1'-N1	-2.05	110.34	114.24
51	9	686	PSU	O4-C4-C5	-2.05	118.91	124.01
48	5	1862	PSU	C6-N1-C2	-2.05	120.79	122.69
48	5	4523	A2M	C4'-O4'-C1'	-2.04	108.06	109.92
48	5	4532	PSU	O2-C2-N1	-2.04	120.69	122.79
48	5	1340	OMC	C6-C5-C4	2.04	120.87	117.53
51	9	1842	4AC	C6-C5-C4	2.04	119.45	117.00
48	5	1326	A2M	C4'-O4'-C1'	-2.03	108.06	109.92
48	5	3762	PSU	C6-C5-C4	2.03	119.54	118.17
48	5	4361	PSU	C6-C5-C4	2.03	119.54	118.17
48	5	1781	PSU	C6-N1-C2	-2.03	120.81	122.69
48	5	4494	OMG	O6-C6-C5	-2.03	120.31	124.32
48	5	3853	PSU	O4'-C1'-C2'	2.02	107.95	105.15
48	5	3830	A2M	C2'-C1'-N9	-2.02	108.07	112.56
51	9	166	A2M	C4'-O4'-C1'	-2.02	108.07	109.92
48	5	4370	OMG	N2-C2-N1	2.02	121.02	116.76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	686	PSU	C6-N1-C2	-2.02	120.82	122.69
51	9	218	PSU	O4'-C1'-C2'	2.01	107.94	105.15
48	5	3830	A2M	C4'-O4'-C1'	-2.01	108.09	109.92
48	5	3764	PSU	C6-C5-C4	2.01	119.53	118.17
48	5	4620	OMU	O2-C2-N1	-2.00	120.19	122.80
48	5	1534	A2M	O4'-C1'-N9	-2.00	106.09	108.75

There are no chirality outliers.

All (96) torsion outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
51	9	1639	G7M	C3'-C4'-C5'-O5'
51	9	1703	OMC	O4'-C4'-C5'-O5'
48	5	3818	UY1	O4'-C4'-C5'-O5'
51	9	668	A2M	O4'-C4'-C5'-O5'
51	9	668	A2M	C3'-C4'-C5'-O5'
51	9	1045	PSU	O4'-C4'-C5'-O5'
51	9	1851	MA6	C3'-C4'-C5'-O5'
48	5	3760	A2M	O4'-C4'-C5'-O5'
48	5	3785	A2M	O4'-C4'-C5'-O5'
48	5	3785	A2M	C3'-C4'-C5'-O5'
48	5	3818	UY1	C3'-C4'-C5'-O5'
51	9	99	A2M	C3'-C4'-C5'-O5'
51	9	172	OMU	O4'-C4'-C5'-O5'
51	9	801	PSU	O4'-C4'-C5'-O5'
48	5	4447	5MC	C2'-C1'-N1-C6
51	9	428	OMU	C2'-C1'-N1-C6
48	5	2364	OMG	C3'-C4'-C5'-O5'
51	9	172	OMU	C3'-C4'-C5'-O5'
51	9	1442	OMU	C3'-C4'-C5'-O5'
51	9	1490	OMG	O4'-C4'-C5'-O5'
48	5	3818	UY1	C4'-C5'-O5'-P
48	5	1625	OMG	C3'-C2'-O2'-CM2
48	5	2815	A2M	C3'-C4'-C5'-O5'
51	9	512	A2M	O4'-C4'-C5'-O5'
51	9	1248	B8N	C32-C33-C34-O35
48	5	1534	A2M	C4'-C5'-O5'-P
51	9	1832	6MZ	N1-C6-N6-C9
48	5	4447	5MC	O4'-C1'-N1-C6
48	5	3792	OMG	C3'-C4'-C5'-O5'
51	9	683	OMG	C3'-C4'-C5'-O5'
51	9	1832	6MZ	C5-C6-N6-C9
51	9	1248	B8N	N3-C31-C32-C33
51	9	1248	B8N	C32-C33-C34-O36
51	9	428	OMU	O4'-C1'-N1-C6
51	9	1490	OMG	C4'-C5'-O5'-P
48	5	4447	5MC	O4'-C1'-N1-C2
48	5	4447	5MC	C2'-C1'-N1-C2
48	5	1524	A2M	C3'-C2'-O2'-CM'
51	9	1031	A2M	C3'-C2'-O2'-CM'
48	5	1326	A2M	C4'-C5'-O5'-P
51	9	34	PSU	O4'-C1'-C5-C4
51	9	1445	PSU	O4'-C1'-C5-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
51	9	468	A2M	C3'-C4'-C5'-O5'
48	5	3701	OMC	O4'-C1'-N1-C6
48	5	3792	OMG	O4'-C4'-C5'-O5'
51	9	644	OMG	C4'-C5'-O5'-P
48	5	3851	PSU	C3'-C4'-C5'-O5'
48	5	4499	OMG	C3'-C2'-O2'-CM2
51	9	1851	MA6	C4'-C5'-O5'-P
51	9	428	OMU	C2'-C1'-N1-C2
48	5	3701	OMC	O4'-C1'-N1-C2
48	5	2364	OMG	C1'-C2'-O2'-CM2
48	5	2837	OMU	C3'-C4'-C5'-O5'
51	9	863	PSU	C3'-C4'-C5'-O5'
51	9	1703	OMC	C3'-C4'-C5'-O5'
51	9	34	PSU	O4'-C1'-C5-C6
51	9	428	OMU	O4'-C1'-N1-C2
48	5	3867	A2M	C3'-C4'-C5'-O5'
48	5	3760	A2M	C3'-C2'-O2'-CM'
48	5	4494	OMG	C3'-C2'-O2'-CM2
48	5	1534	A2M	O4'-C4'-C5'-O5'
51	9	683	OMG	O4'-C4'-C5'-O5'
51	9	863	PSU	O4'-C4'-C5'-O5'
48	5	373	OMG	C4'-C5'-O5'-P
48	5	2351	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
90	ZVM	ii	501	88	30,31,31	4.96	21 (70%)	32,46,46	3.11	7 (21%)
91	SF4	jj	602	87	0,12,12	-	-	-		
91	SF4	jj	601	87	0,12,12	-	-	-		

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

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

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	ii	501	ZVM	O01-C01	12.83	1.39	1.22
90	ii	501	ZVM	O02-C15	9.69	1.39	1.22
90	ii	501	ZVM	C13-C14	8.13	1.52	1.38
90	ii	501	ZVM	C10-C09	7.54	1.53	1.39
90	ii	501	ZVM	C03-N01	7.44	1.38	1.27
90	ii	501	ZVM	C12-C11	6.49	1.52	1.38
90	ii	501	ZVM	C04-N02	-5.99	1.42	1.47
90	ii	501	ZVM	C03-N03	5.42	1.47	1.37
90	ii	501	ZVM	C05-C04	5.30	1.59	1.54
90	ii	501	ZVM	C02-C03	-4.97	1.40	1.52
90	ii	501	ZVM	C08-C05	-4.27	1.45	1.54
90	ii	501	ZVM	C17-N03	4.25	1.49	1.40
90	ii	501	ZVM	C11-C10	-4.19	1.31	1.38
90	ii	501	ZVM	C14-C09	-4.16	1.31	1.39
90	ii	501	ZVM	C21-C22	-4.06	1.33	1.39
90	ii	501	ZVM	C06-C05	-3.93	1.45	1.54
90	ii	501	ZVM	C12-C13	-2.98	1.31	1.38
90	ii	501	ZVM	C15-N02	2.98	1.40	1.36
90	ii	501	ZVM	C02-C01	-2.56	1.46	1.51
90	ii	501	ZVM	C07-C06	2.18	1.65	1.53
90	ii	501	ZVM	C07-C08	2.12	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	ii	501	ZVM	C05-C04-N01	11.95	121.33	109.91
90	ii	501	ZVM	O01-C01-C02	-9.29	118.89	126.79
90	ii	501	ZVM	C05-C04-N02	4.49	119.42	111.94
90	ii	501	ZVM	N02-C04-N01	4.29	119.25	113.37
90	ii	501	ZVM	C21-C22-C17	2.77	121.99	118.81
90	ii	501	ZVM	C22-C01-C02	2.70	120.36	116.72
90	ii	501	ZVM	C02-C15-N02	2.48	119.16	116.89

All (2) chirality outliers are listed below:

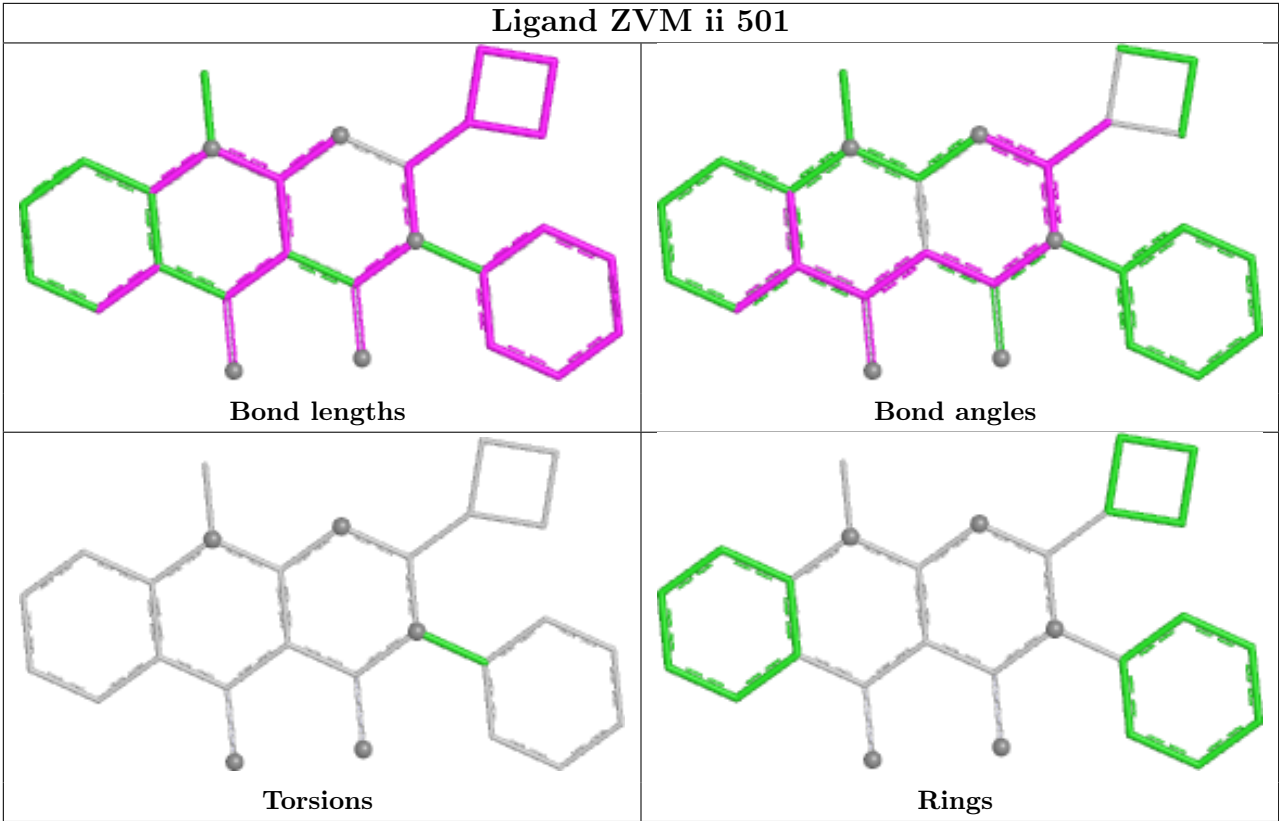
Mol	Chain	Res	Type	Atom
90	ii	501	ZVM	C04
90	ii	501	ZVM	C02

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	23
51	9	3
47	3	2
46	2	1

All chain breaks are listed below:

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

Continued on next page...

*Continued from previous page...*

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



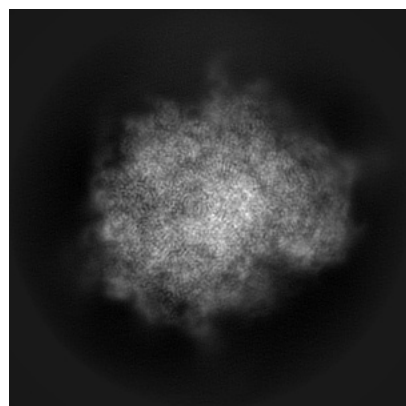
## 6 Map visualisation [i](#)

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

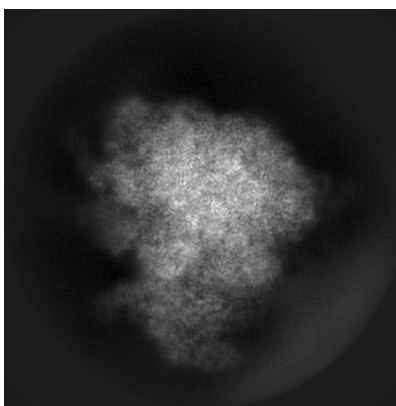
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

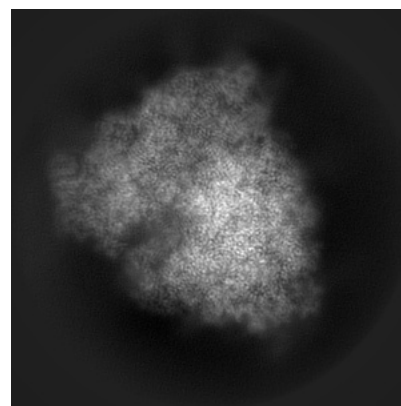
#### 6.1.1 Primary map



X

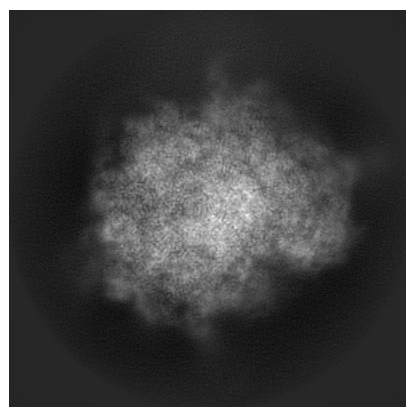


Y

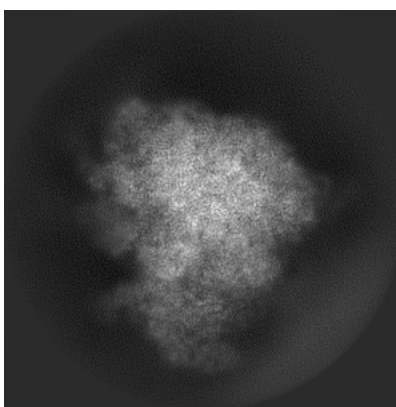


Z

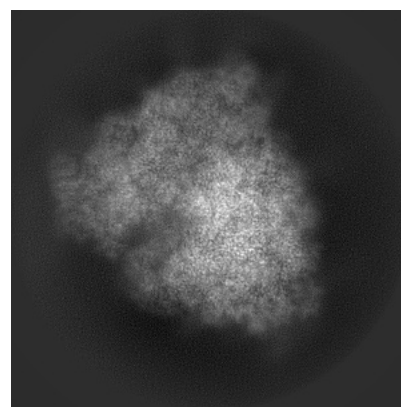
#### 6.1.2 Raw map



X



Y

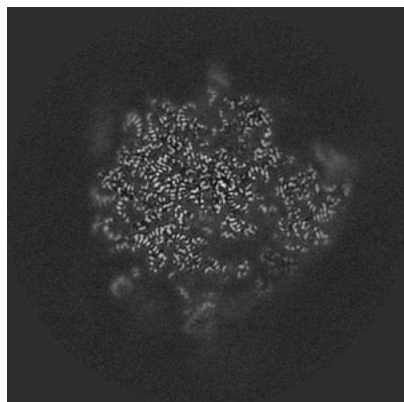


Z

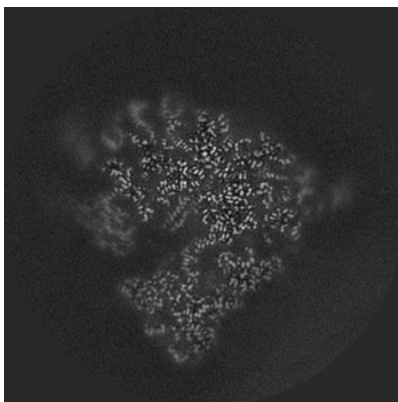
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

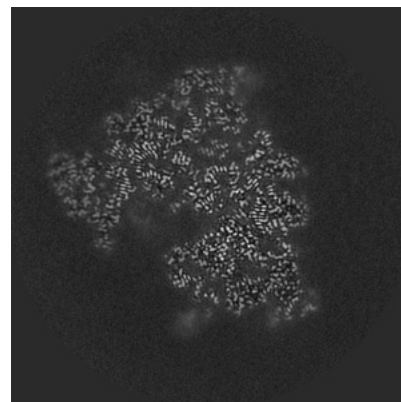
### 6.2.1 Primary map



X Index: 240

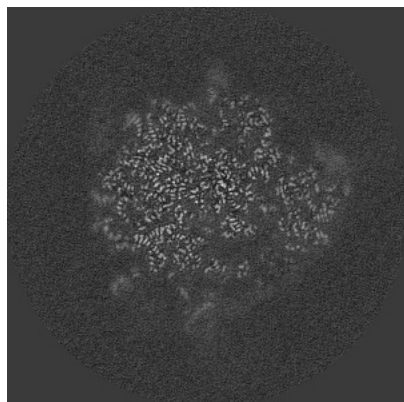


Y Index: 240

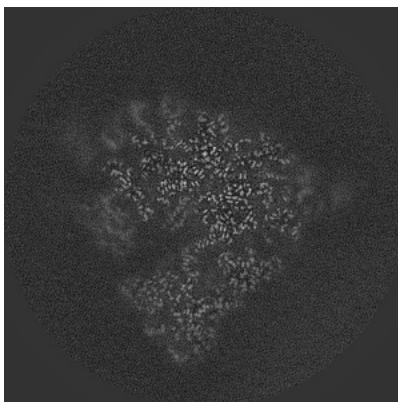


Z Index: 240

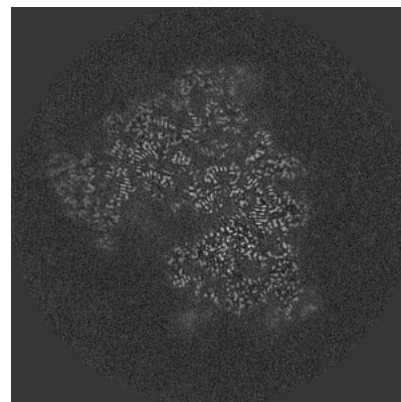
### 6.2.2 Raw map



X Index: 240



Y Index: 240

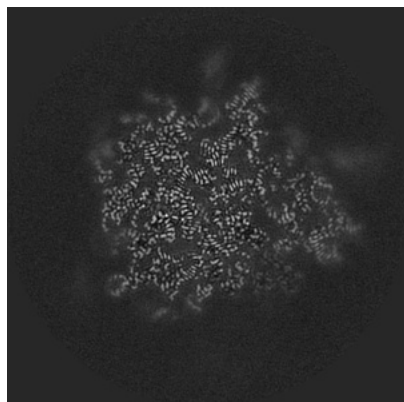


Z Index: 240

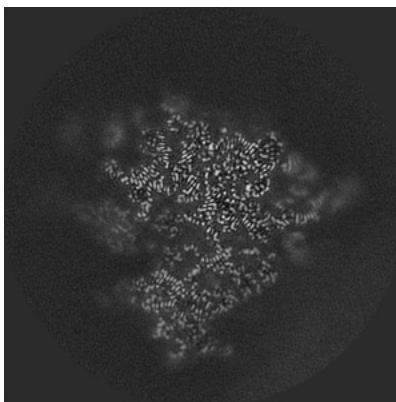
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

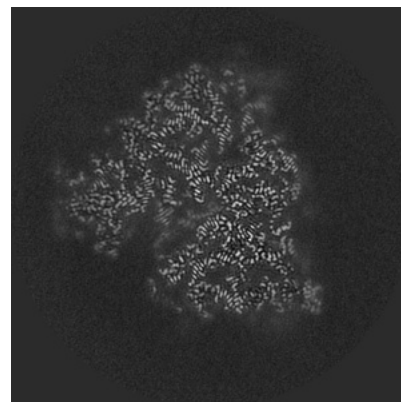
### 6.3.1 Primary map



X Index: 261

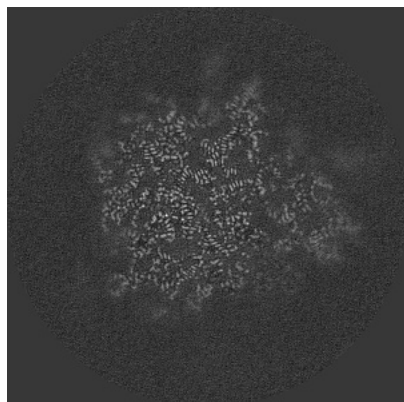


Y Index: 250

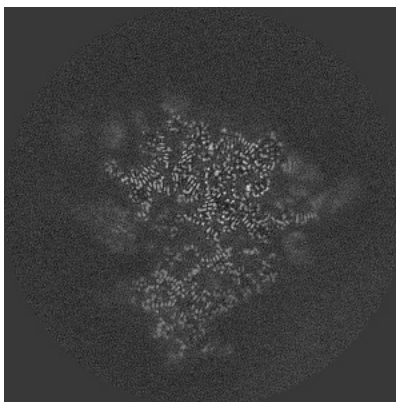


Z Index: 227

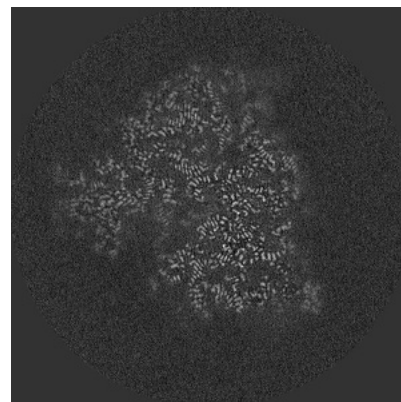
### 6.3.2 Raw map



X Index: 261



Y Index: 250

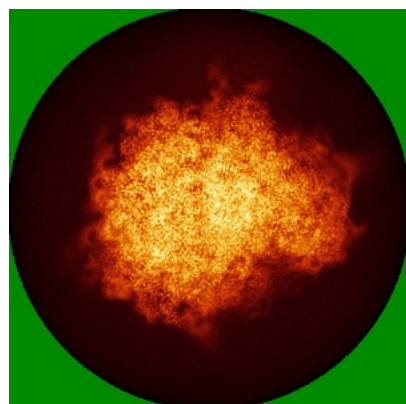


Z Index: 228

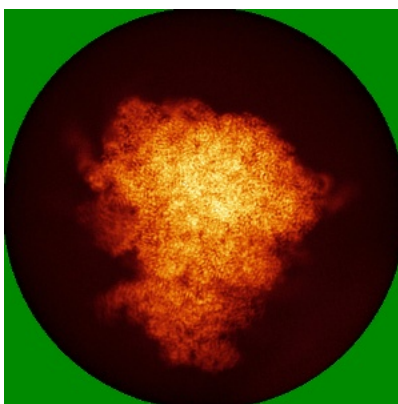
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

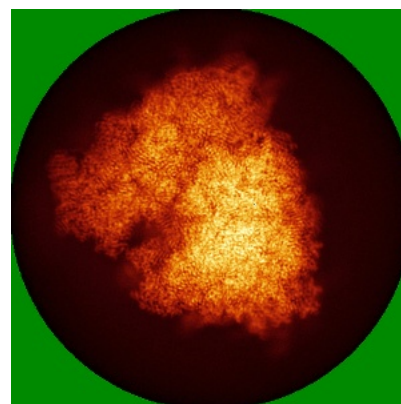
### 6.4.1 Primary map



X

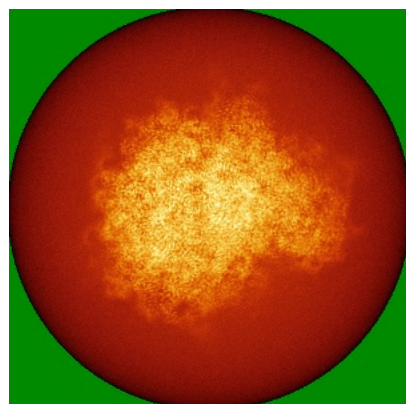


Y

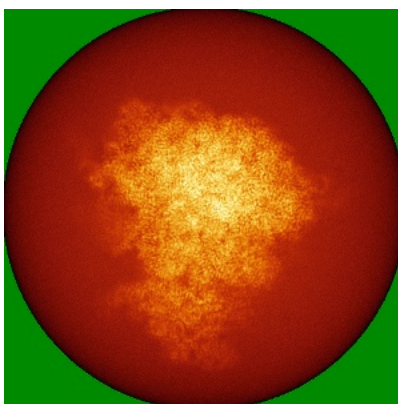


Z

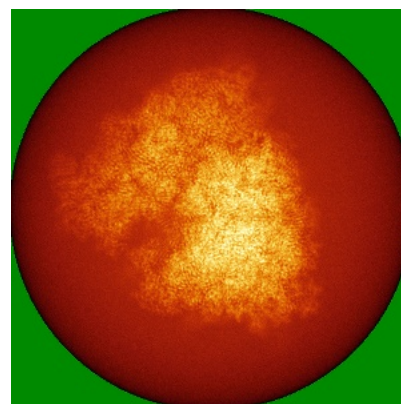
### 6.4.2 Raw map



X



Y



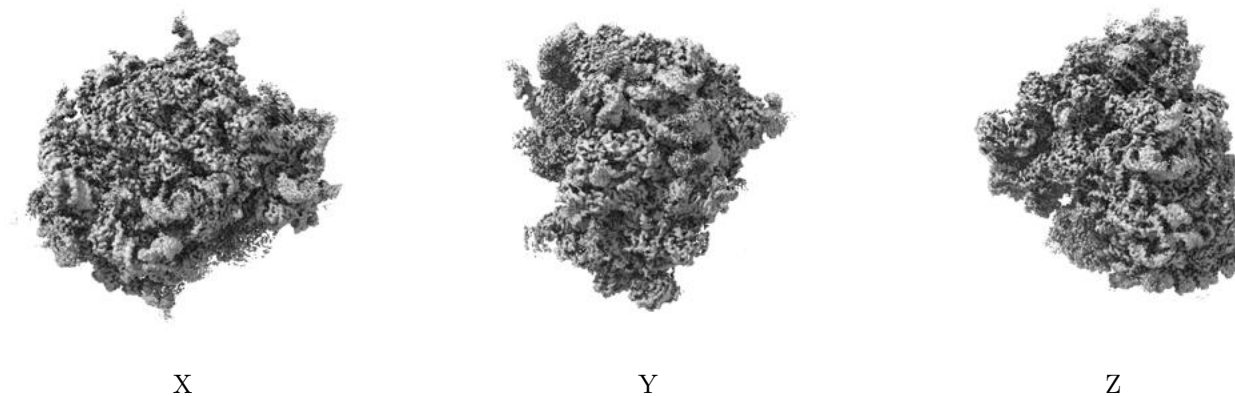
Z

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



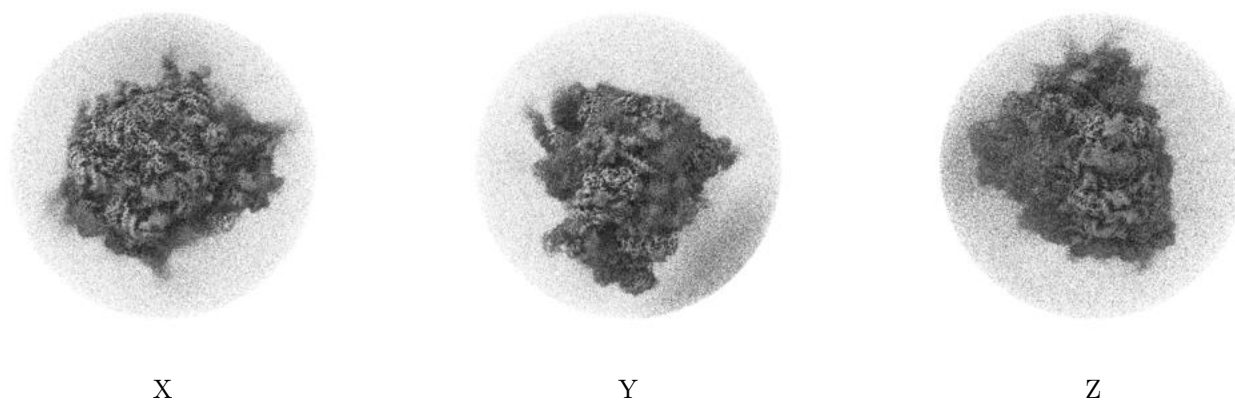
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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

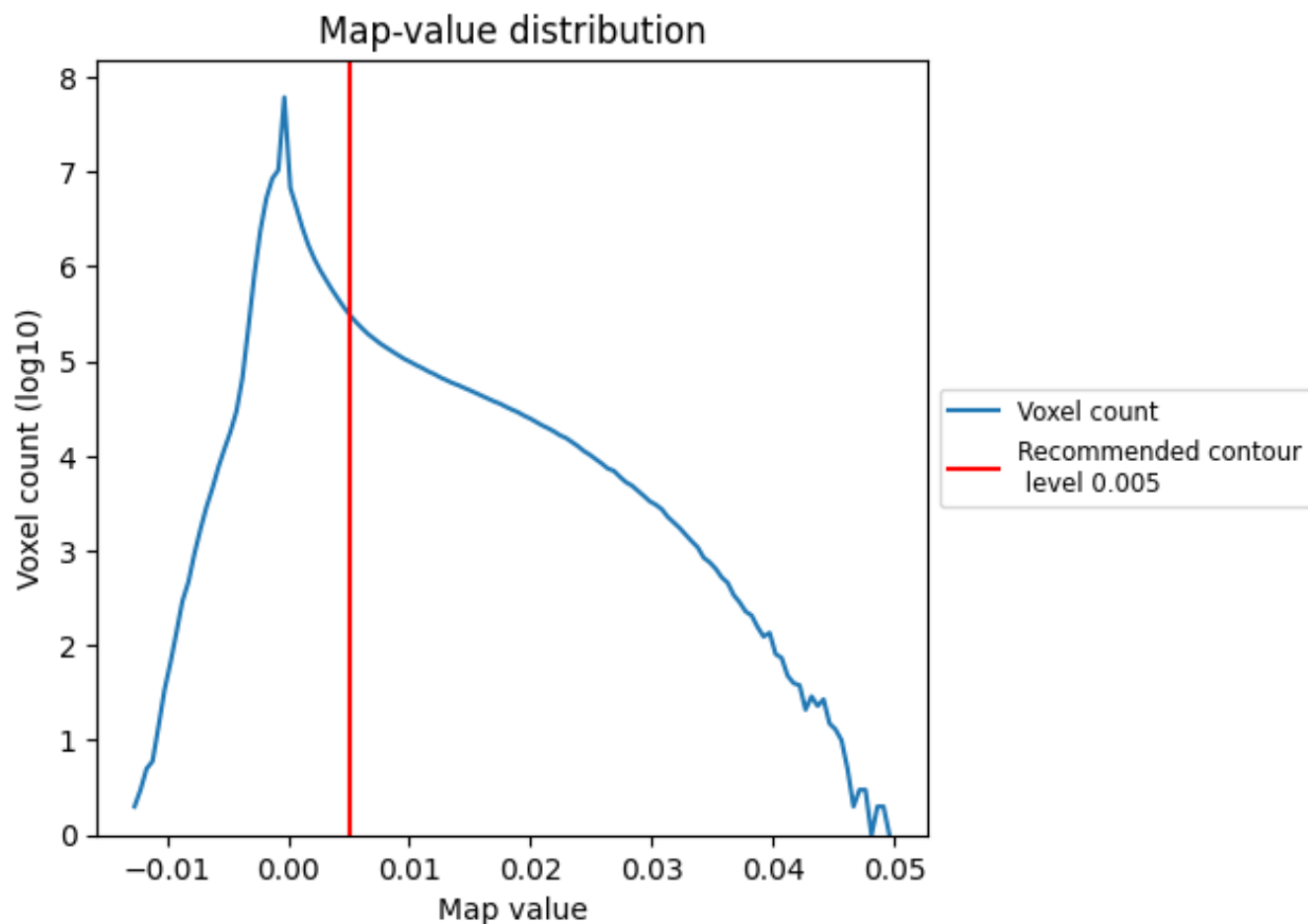
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

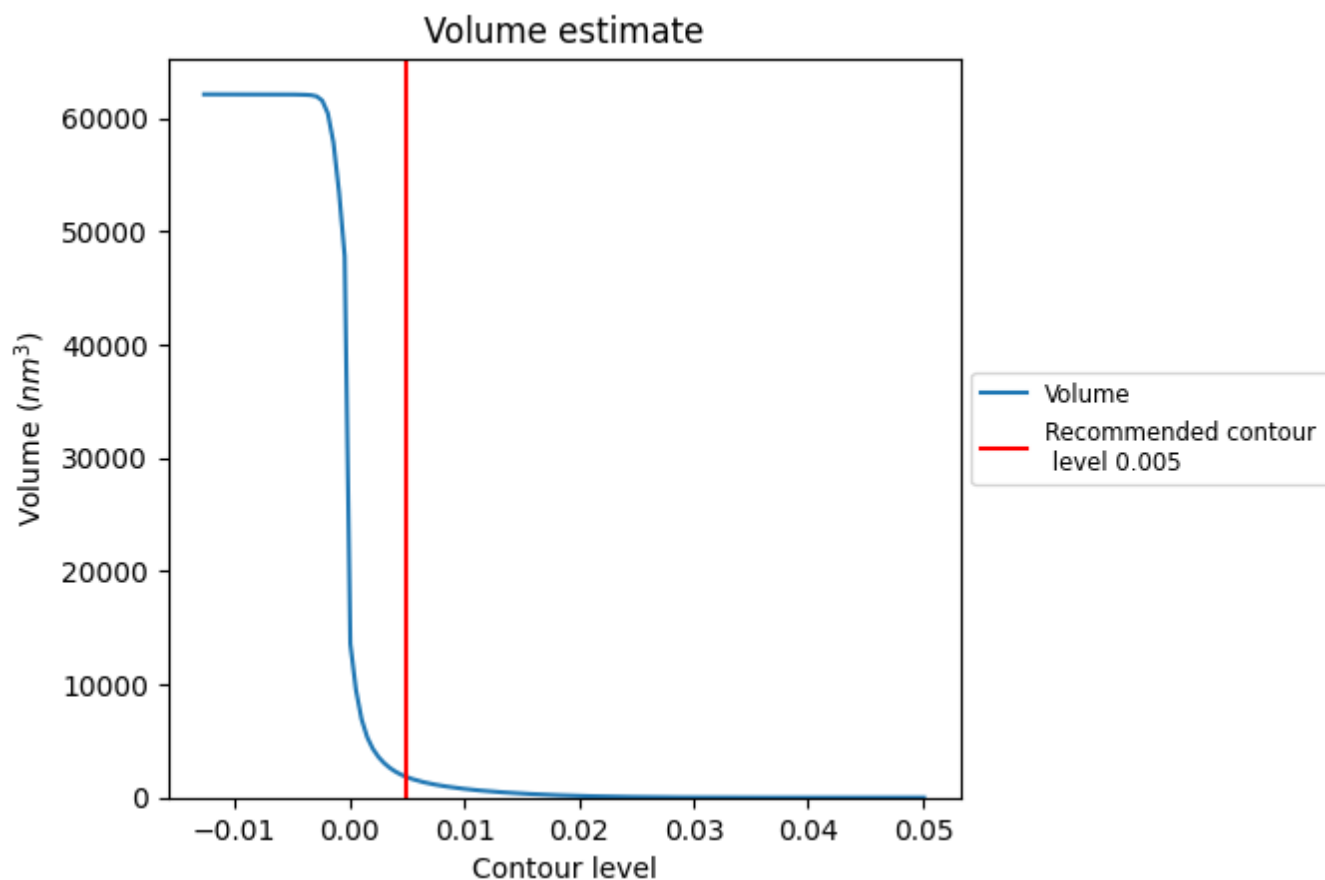
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

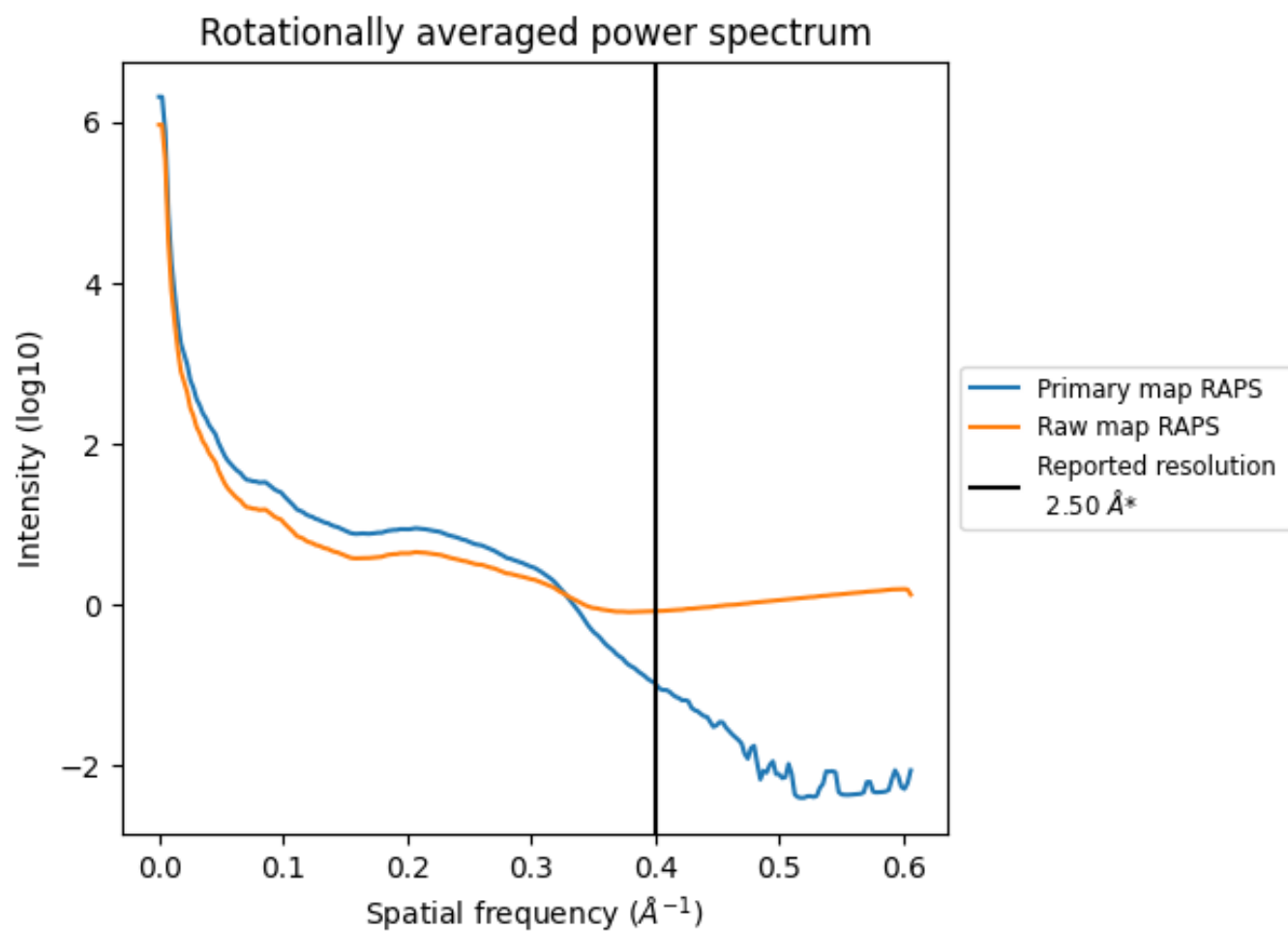
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1812  $\text{nm}^3$ ; this corresponds to an approximate mass of 1637 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



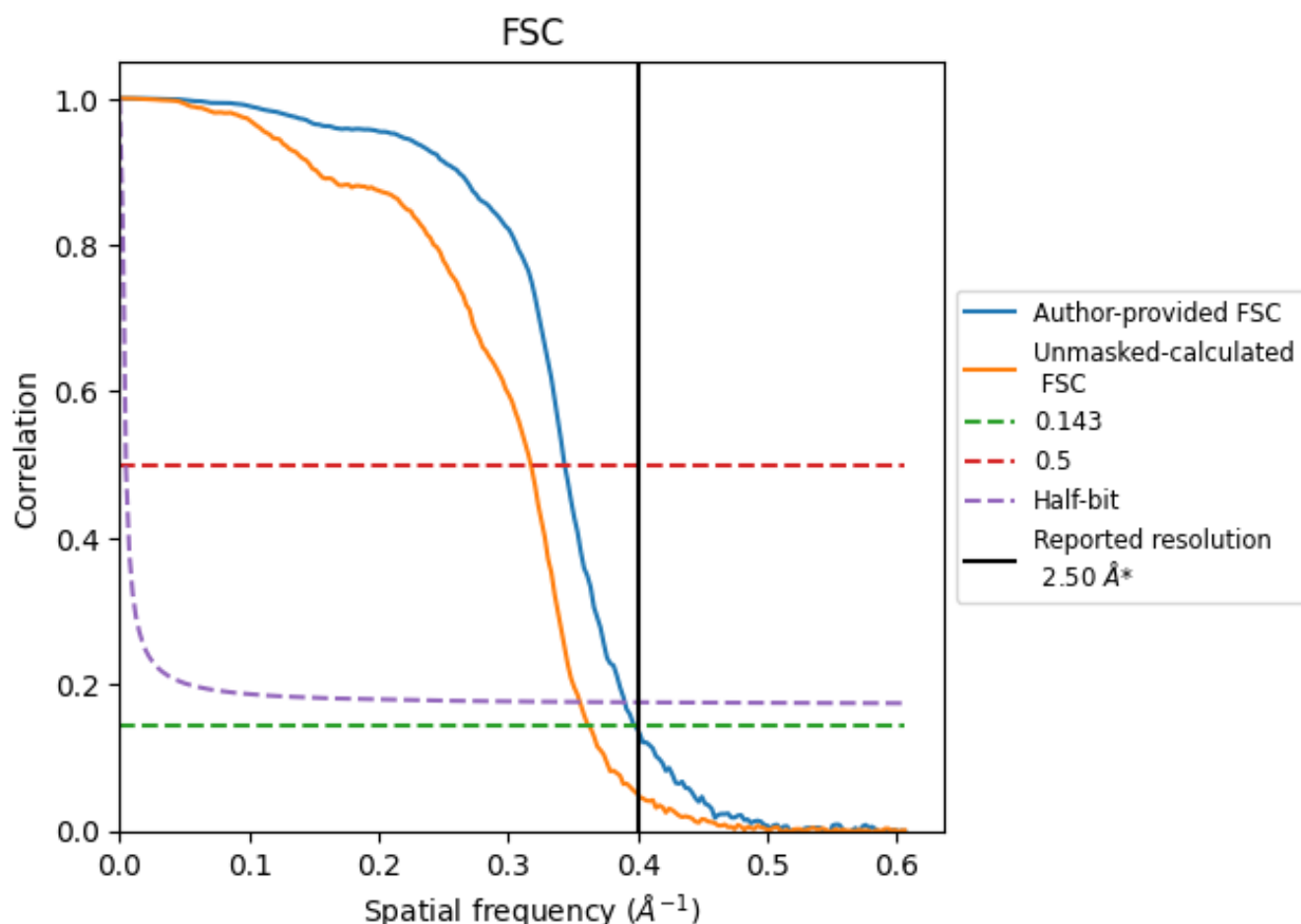
\*Reported resolution corresponds to spatial frequency of 0.400  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

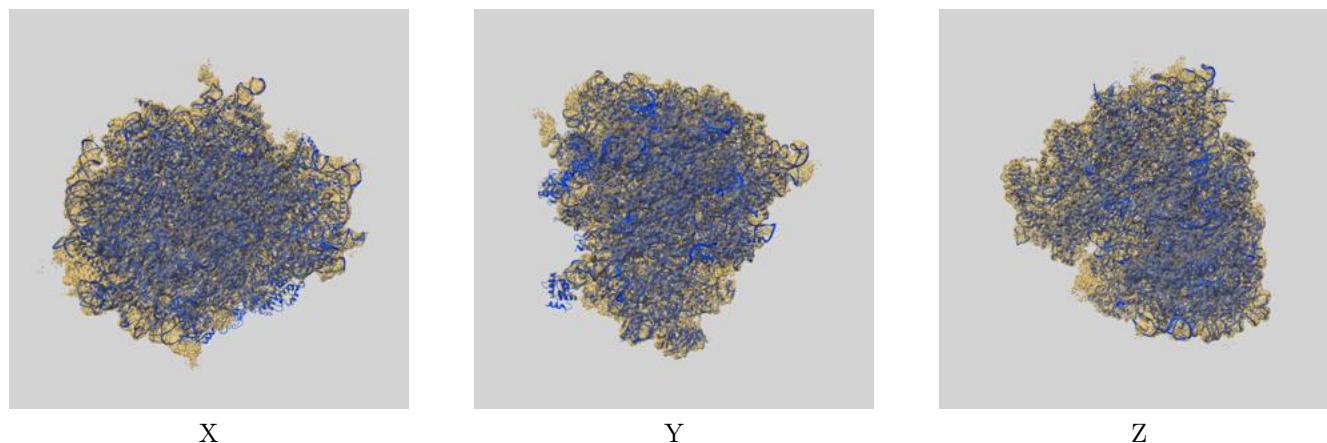
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.91	2.56
Unmasked-calculated*	2.76	3.15	2.81

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

## 9 Map-model fit [i](#)

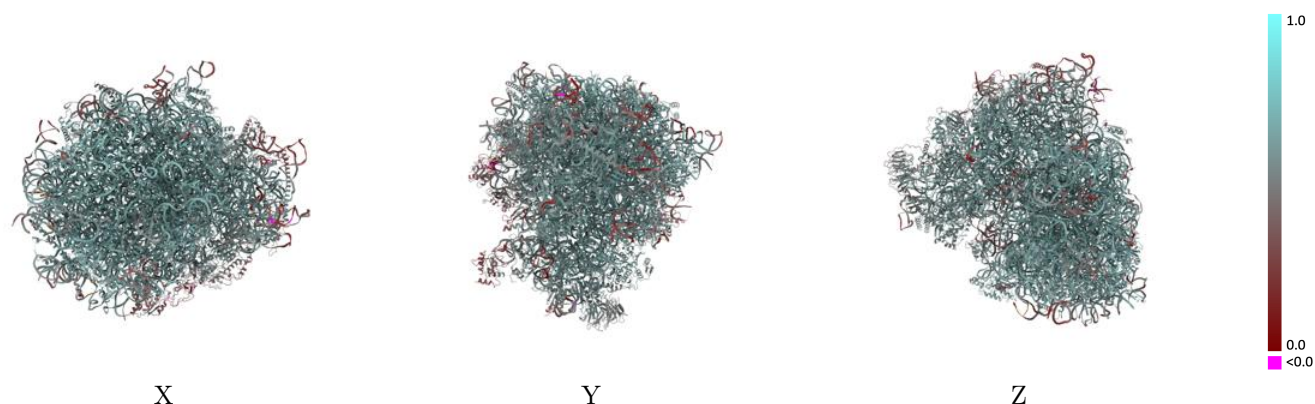
This section contains information regarding the fit between EMDB map EMD-40344 and PDB model 8SCB. Per-residue inclusion information can be found in section [3](#) on page [27](#).

### 9.1 Map-model overlay [i](#)



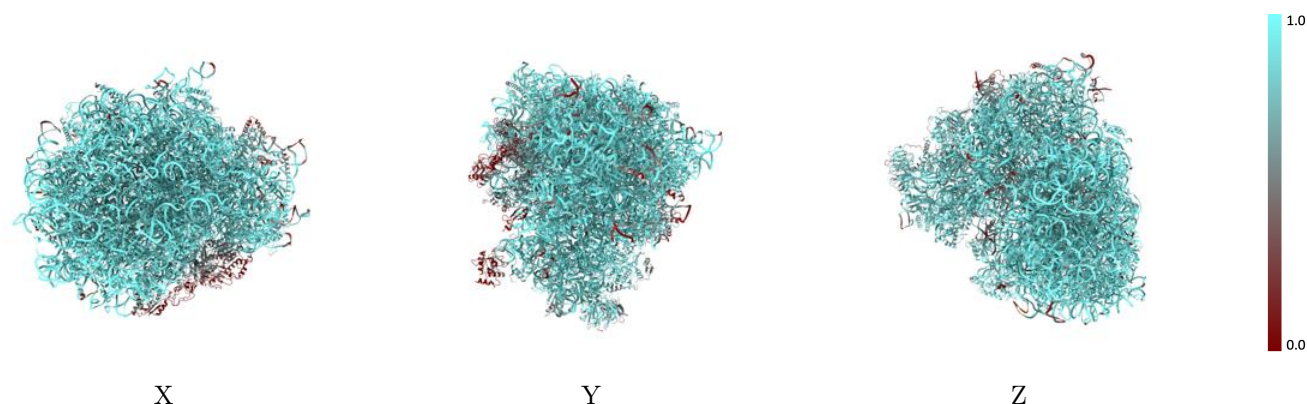
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



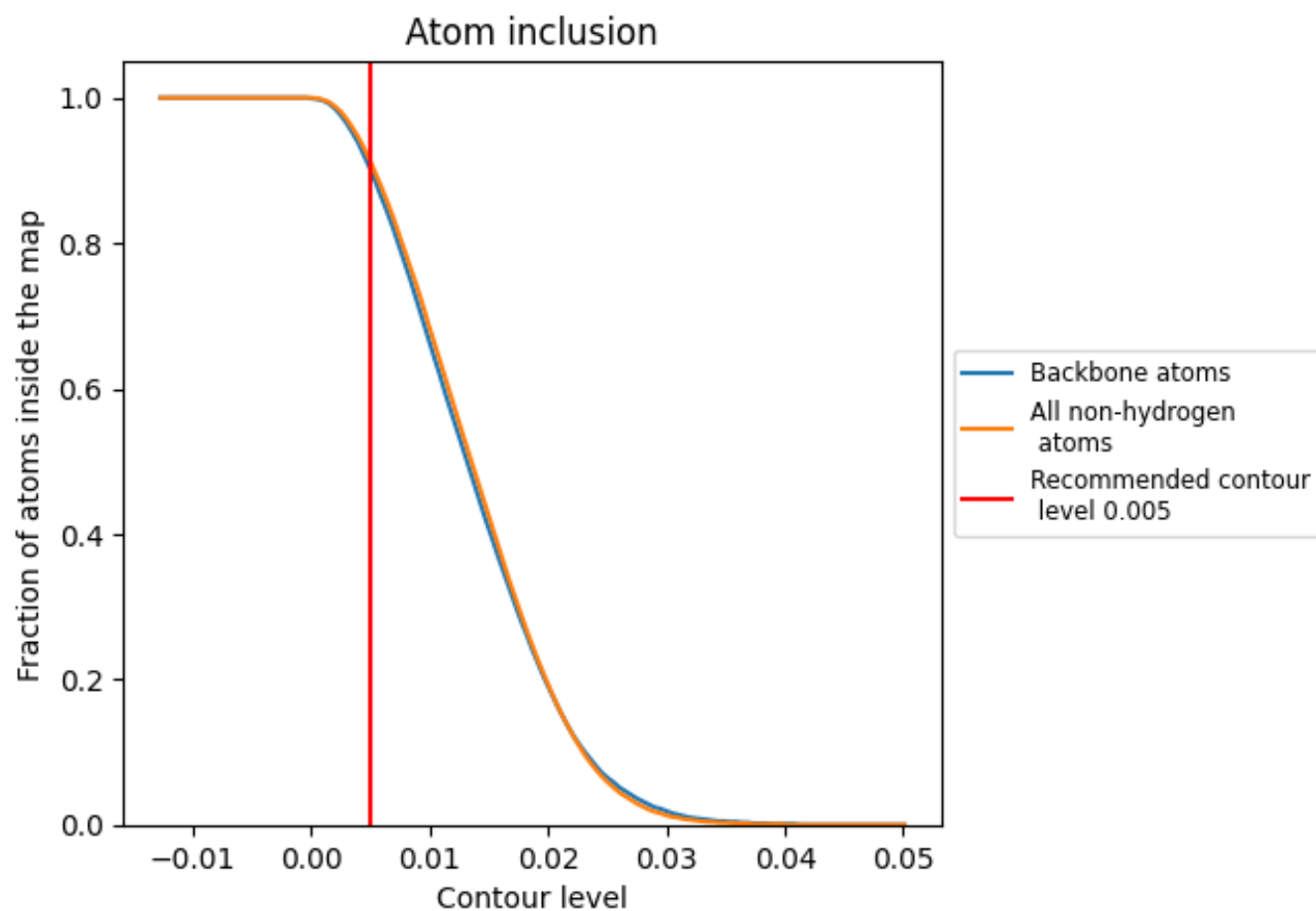
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

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

























*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
O	 0.9690	 0.6370
OO	 0.9570	 0.6170
P	 0.9640	 0.6460
PP	 0.8780	 0.5590
Q	 0.9730	 0.6490
QQ	 0.9080	 0.5780
R	 0.9000	 0.6030
RR	 0.7450	 0.5440
S	 0.9760	 0.6450
SS	 0.8830	 0.5660
T	 0.9440	 0.6210
TT	 0.9120	 0.5790
U	 0.8820	 0.5490
UU	 0.7490	 0.5170
V	 0.9730	 0.6440
VV	 0.8760	 0.5780
W	 0.9490	 0.6300
WW	 0.9550	 0.6150
X	 0.9530	 0.6240
XX	 0.9590	 0.6230
Y	 0.9390	 0.6220
YY	 0.8960	 0.5620
Z	 0.9460	 0.6140
ZZ	 0.8430	 0.5540
a	 0.9660	 0.6480
aa	 0.9420	 0.6160
b	 0.8450	 0.5830
bb	 0.8470	 0.5730
c	 0.9440	 0.6220
cc	 0.8400	 0.5680
d	 0.9650	 0.6330
dd	 0.9490	 0.5990
e	 0.9830	 0.6530
ee	 0.9060	 0.5680
f	 0.9790	 0.6560
ff	 0.2530	 0.3490
g	 0.9350	 0.6170
gg	 0.7550	 0.5030
h	 0.9380	 0.6160
hh	 0.9920	 0.6100
i	 0.9210	 0.6070
ii	 0.7390	 0.5290

*Continued on next page...*

*Continued from previous page...*

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