



Full wwPDB EM Validation Report ⓘ

Mar 18, 2024 – 03:58 PM JST

PDB ID : 8JIV
EMDB ID : EMD-36331
Title : Atomic structure of wheat ribosome reveals unique features of the plant ribosomes
Authors : Mishra, R.K.; Sharma, P.; Hussain, T.
Deposited on : 2023-05-28
Resolution : 2.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

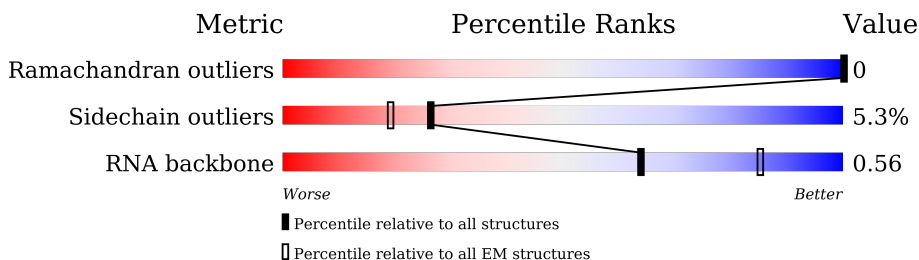
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	Aa	3391	
2	Ab	119	
3	Ac	158	
4	CA	261	
5	CB	385	
6	CC	405	
7	CD	307	
8	CE	232	

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Mol	Chain	Length	Quality of chain
9	CF	244	19% 93%
10	CG	258	16% 83% 14%
11	CH	189	13% 95%
12	CI	217	16% 89% 5% 6%
13	CJ	180	54% 87% 6% 7%
14	CL	208	7% 91% 5%
15	CM	135	19% 88% 10%
16	CN	204	96%
17	CO	206	15% 94% 5%
18	CP	170	86% 10%
19	CQ	188	96%
20	CR	206	71% 28%
21	CS	178	10% 94%
22	CT	164	12% 93%
23	CU	129	44% 74% 22%
24	CV	136	88% 6% 6%
25	CW	161	37% 62%
26	CX	152	72% 24%
27	CY	127	5% 94% 6%
28	CZ	137	10% 88% 8%
29	Ca	145	95%
30	Cb	60	78% 18%
31	Cc	112	16% 81% 15%
32	Cd	123	78% 19%
33	Ce	133	91% 6%

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Mol	Chain	Length	Quality of chain
34	Cf	111	<p>6% 89% 10%</p>
35	Cg	119	<p>86% 11%</p>
36	Ch	124	<p>86% 7% 6%</p>
37	Ci	111	<p>8% 86% 11%</p>
38	Cj	93	<p>88% 8%</p>
39	Ck	69	<p>38% 91% 7%</p>
40	Cl	51	<p>92% 6%</p>
41	Cm	129	<p>37% 61%</p>
42	Co	105	<p>88% 6% 7%</p>
43	Cp	92	<p>91% 5%</p>
44	Cr	147	<p>16% 85% 7% 8%</p>

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 116711 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 RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Aa	2863	61426	27432	11224	19907	2863	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	1	G	-	conflict	GB 2123606587

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	Ab	119	2541	1135	458	830	118	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	Ac	152	3248	1451	589	1057	151	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ac	?	-	C	deletion	GB AF438188.1

- Molecule 4 is a protein called Ribosomal protein L2 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CA	245	1874	1169	384	314	7	0	0

- Molecule 5 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CB	384	3052	1941	569	525	17	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CC	376	2845	1801	541	495	8	0	0

- Molecule 7 is a protein called Ribosomal protein L5 eukaryotic C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CD	271	2158	1360	397	396	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CE	175	1317	843	235	237	2	0	0

- Molecule 9 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CF	234	1879	1208	354	312	5	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CG	221	1749	1132	323	288	6	0	0

- Molecule 11 is a protein called Ribosomal protein L6 alpha-beta domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	CH	186	1426	908	258	253	7	0	0

- Molecule 12 is a protein called Ribosomal protein L10e/L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CI	204	Total	C	N	O	S	0	0
			1599	1013	313	264	9		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CJ	167	Total	C	N	O	S	0	0
			1314	830	248	229	7		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CL	200	Total	C	N	O	S	0	0
			1596	1000	318	272	6		

- Molecule 15 is a protein called Ribosomal protein L14e domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CM	122	Total	C	N	O	S	0	0
			963	618	176	164	5		

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	203	Total	C	N	O	S	0	0
			1719	1078	370	268	3		

- Molecule 17 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CO	205	Total	C	N	O	S	0	0
			1633	1036	318	269	10		

- Molecule 18 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	153	Total	C	N	O	S	0	0
			1235	770	245	215	5		

- Molecule 19 is a protein called Ribosomal protein L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CQ	187	1477	929	294	248	6	0	0

- Molecule 20 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CR	148	1227	769	256	194	8	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	CS	175	1471	946	273	244	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	CT	159	1260	797	246	214	3	0	0

- Molecule 23 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	CU	101	800	511	139	148	2	0	0

- Molecule 24 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	CV	128	956	605	176	166	9	0	0

- Molecule 25 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	CW	61	507	328	96	79	4	0	0

- Molecule 26 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	CX	116	931	597	164	168	2	0	0

- Molecule 27 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	CY	127	1012	627	212	170	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CZ	126	1008	655	188	161	4	0	0

- Molecule 29 is a protein called Ribosomal protein L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ca	141	1104	711	215	174	4	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Cb	49	409	249	92	67	1	0	0

- Molecule 31 is a protein called Ribosomal protein L7Ae/L30e/S12e/Gadd45 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Cc	95	730	465	126	134	5	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Cd	100	784	497	155	130	2	0	0

- Molecule 33 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ce	125	Total	C	N	O	S	0	0
			1017	644	201	167	5		

- Molecule 34 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Cf	110	Total	C	N	O	S	0	0
			879	553	168	155	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cg	106	Total	C	N	O	S	0	0
			858	541	176	140	1		

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Ch	116	Total	C	N	O	0	0
			938	590	189	159		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ci	99	Total	C	N	O	S	0	0
			798	502	165	129	2		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Cj	86	Total	C	N	O	S	0	0
			696	426	153	111	6		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ck	68	Total	C	N	O	S	0	0
			556	350	108	96	2		

- Molecule 40 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cl	50	Total	C	N	O	S	0	0
			451	286	99	65	1		

- Molecule 41 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Cm	50	Total	C	N	O	S	0	0
			408	254	87	62	5		

- Molecule 42 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Co	98	Total	C	N	O	S	0	0
			795	499	157	134	5		

- Molecule 43 is a protein called 60S ribosomal protein L37a, expressed.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Cp	89	Total	C	N	O	S	0	0
			684	429	130	119	6		

- Molecule 44 is a protein called Ribosomal L28e/Mak16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Cr	135	Total	C	N	O	S	0	0
			1064	674	196	190	4		

- Molecule 45 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
45	Aa	64	Total	K	0
			64	64	
45	Ac	1	Total	K	0
			1	1	
45	CA	2	Total	K	0
			2	2	
45	CI	1	Total	K	0
			1	1	
45	CL	2	Total	K	0
			2	2	
45	Cg	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
45	Co	1	Total	K	0
			1	1	

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	Aa	227	Total	Mg	0
			227	227	
46	Ab	4	Total	Mg	0
			4	4	
46	Ac	3	Total	Mg	0
			3	3	
46	CB	1	Total	Mg	0
			1	1	
46	CI	1	Total	Mg	0
			1	1	
46	CL	1	Total	Mg	0
			1	1	
46	CP	1	Total	Mg	0
			1	1	
46	CR	1	Total	Mg	0
			1	1	
46	CV	1	Total	Mg	0
			1	1	
46	Cj	2	Total	Mg	0
			2	2	

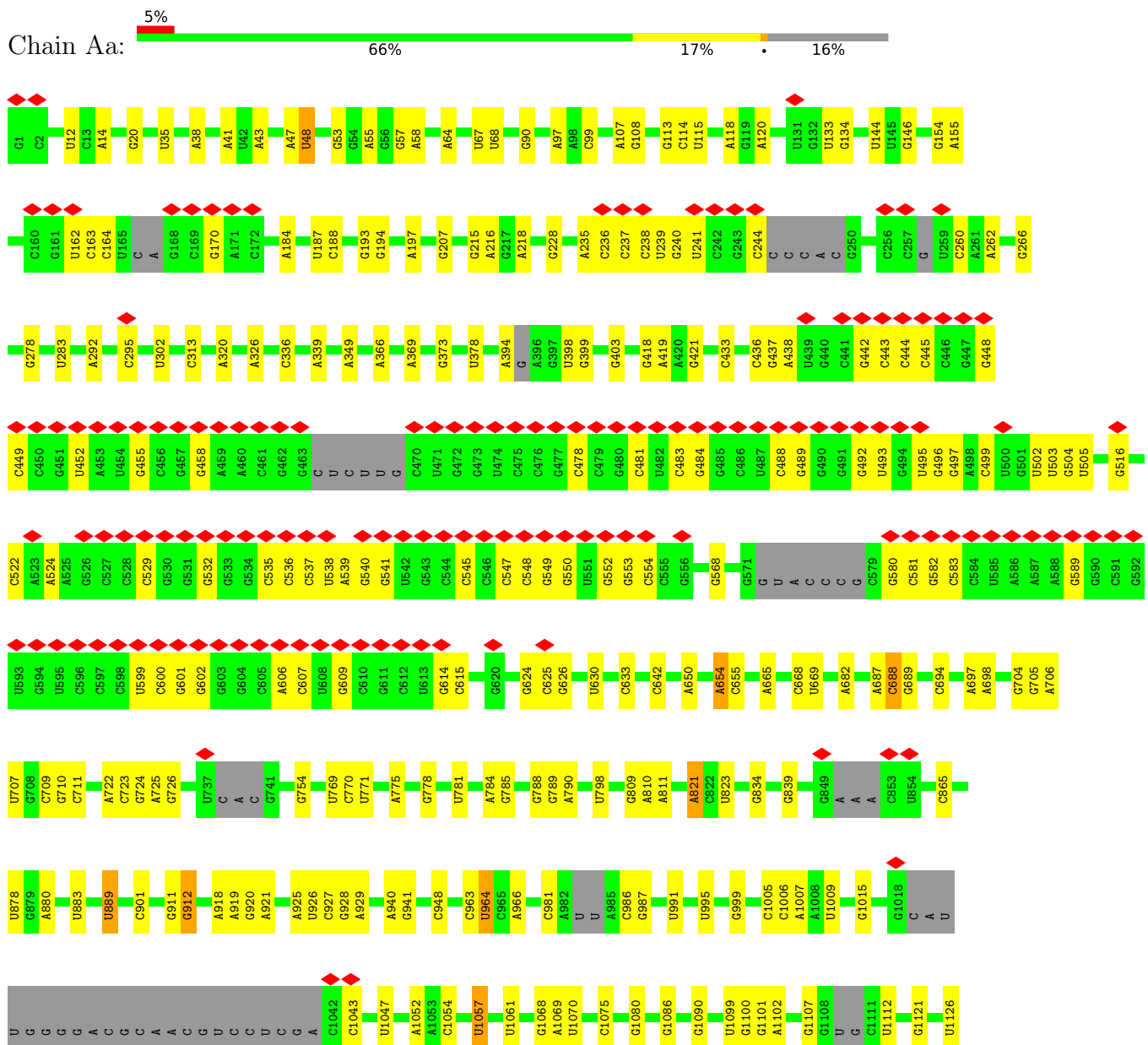
- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

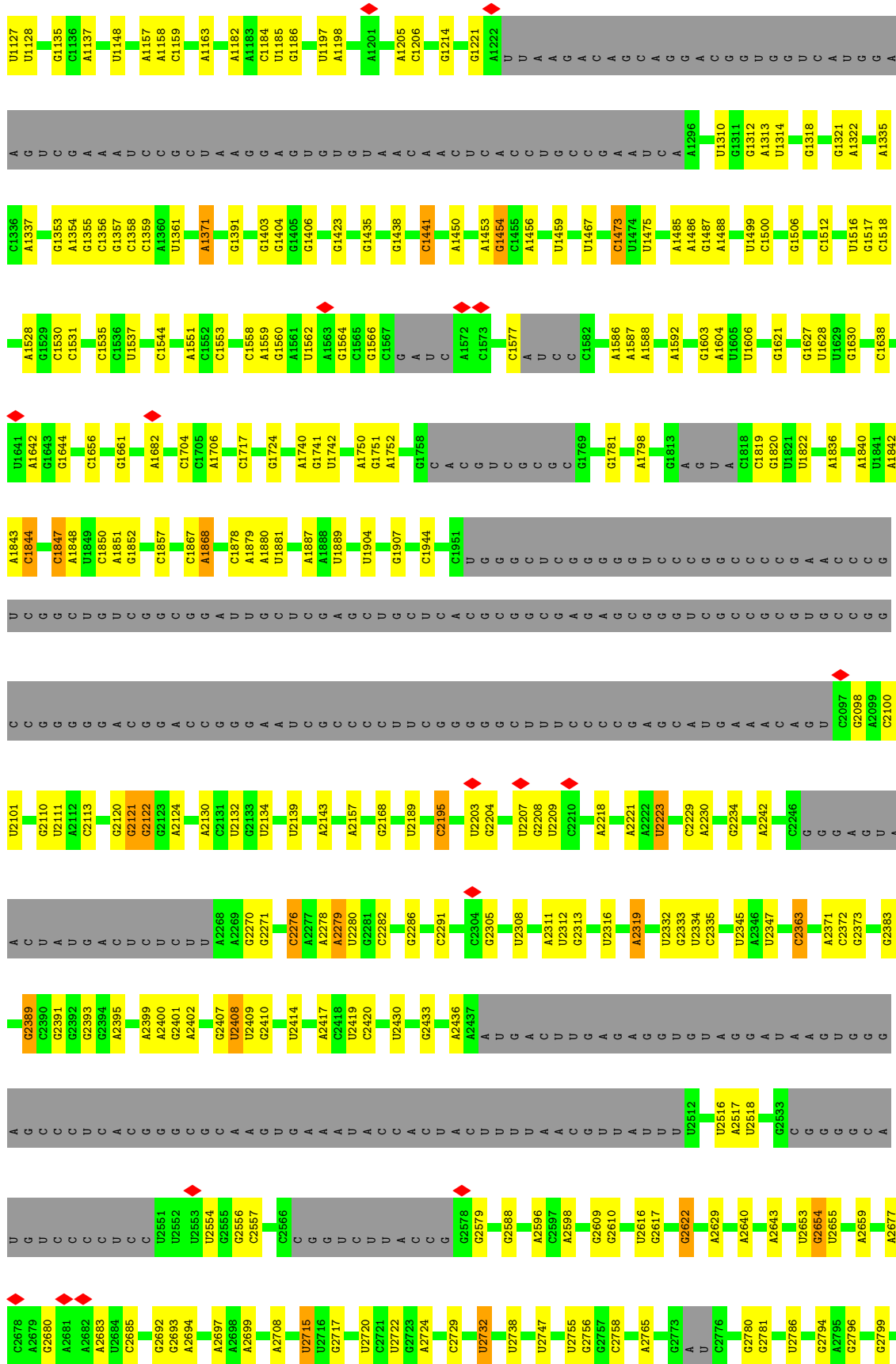
Mol	Chain	Residues	Atoms		AltConf
47	Cj	1	Total	Zn	0
			1	1	
47	Cm	1	Total	Zn	0
			1	1	
47	Co	1	Total	Zn	0
			1	1	

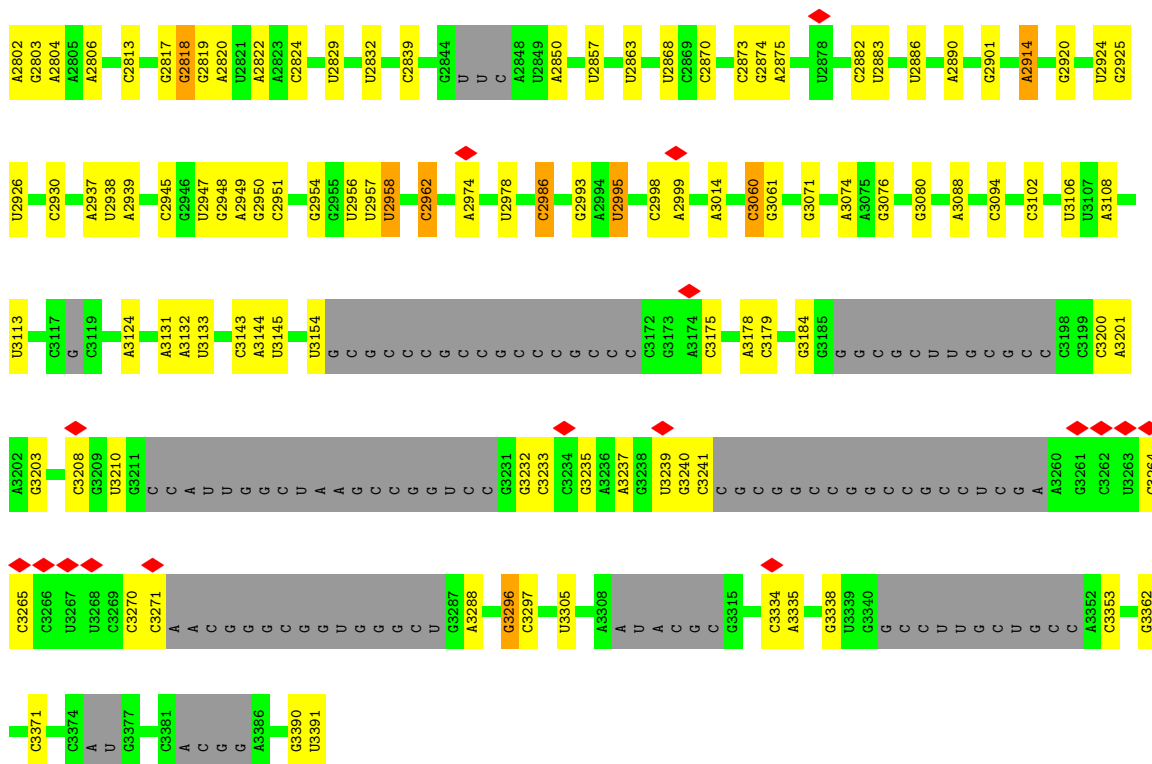
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

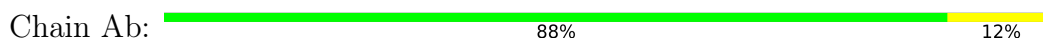
• Molecule 1: 25S rRNA



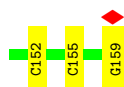
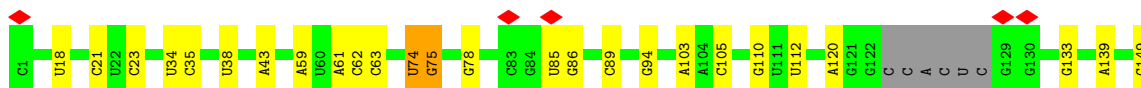
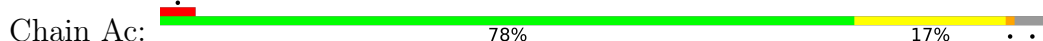




• Molecule 2: 5S rRNA



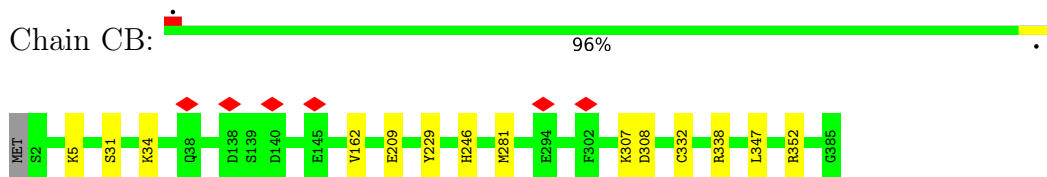
• Molecule 3: 5.8S rRNA



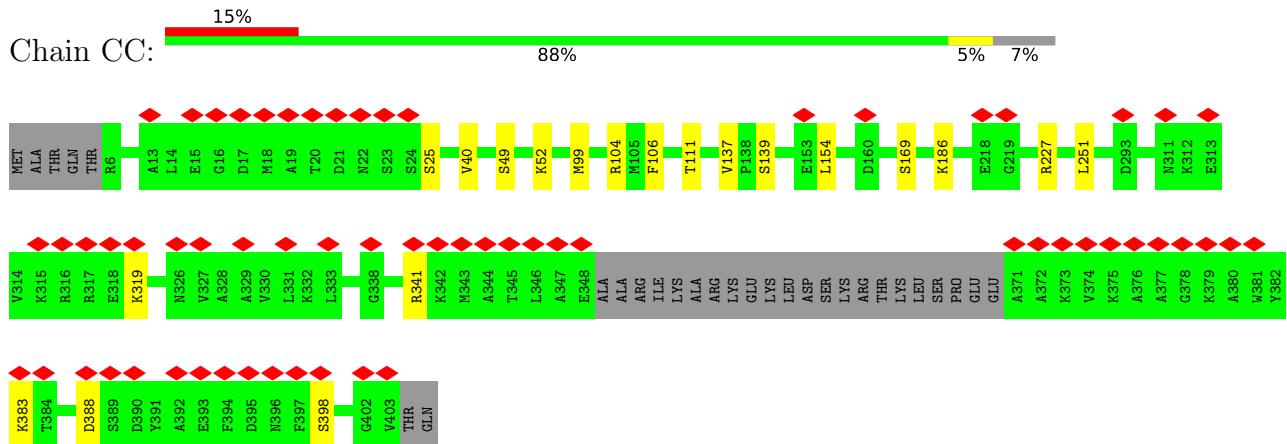
• Molecule 4: Ribosomal protein L2 C-terminal domain-containing protein



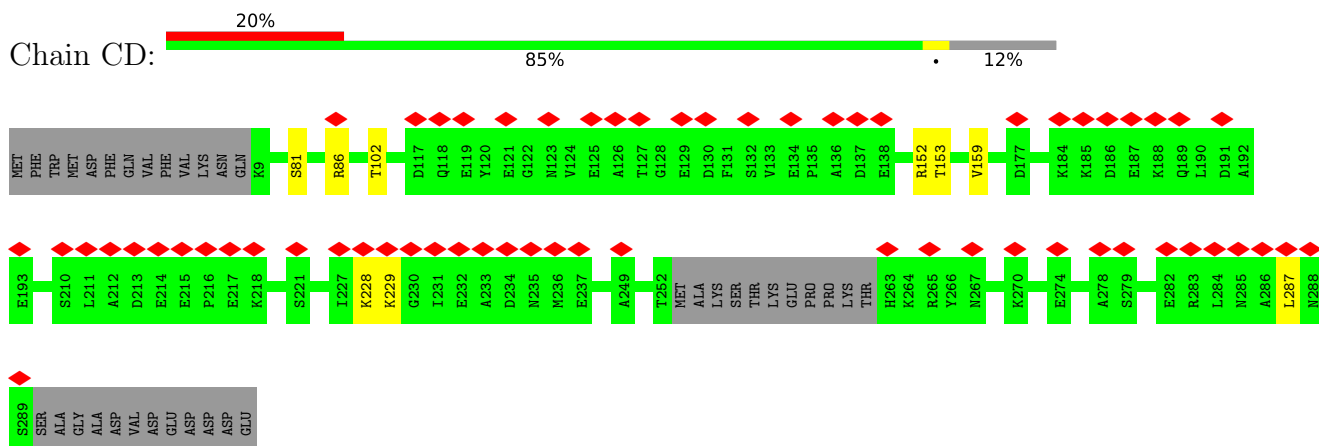
• Molecule 5: Ribosomal protein L3



- Molecule 6: 60S ribosomal protein L4 C-terminal domain-containing protein



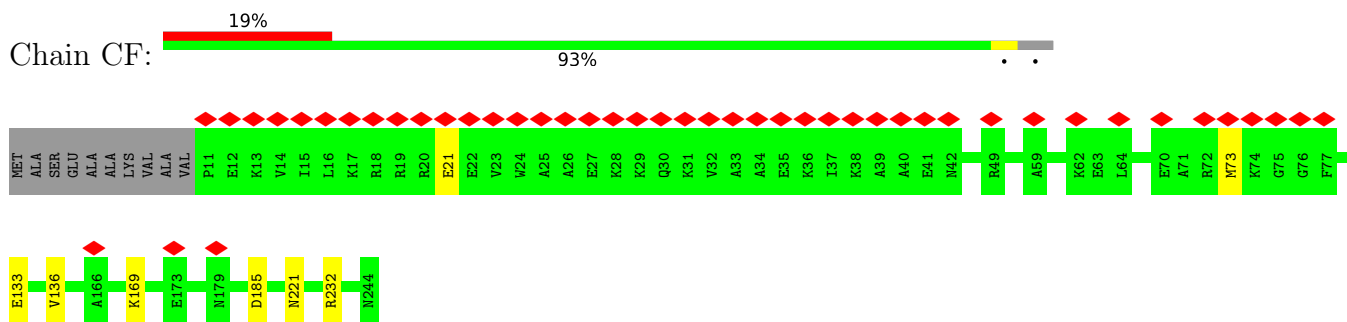
- Molecule 7: Ribosomal protein L5 eukaryotic C-terminal domain-containing protein



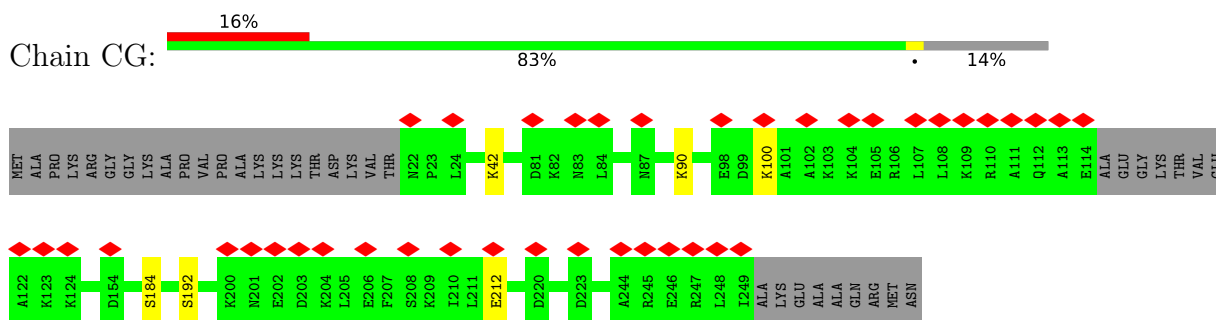
- Molecule 8: 60S ribosomal protein L6



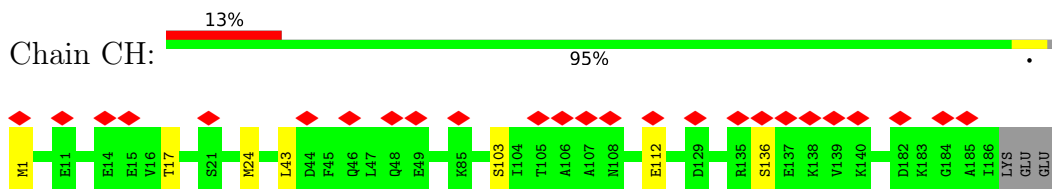
- Molecule 9: 60S ribosomal protein uL30



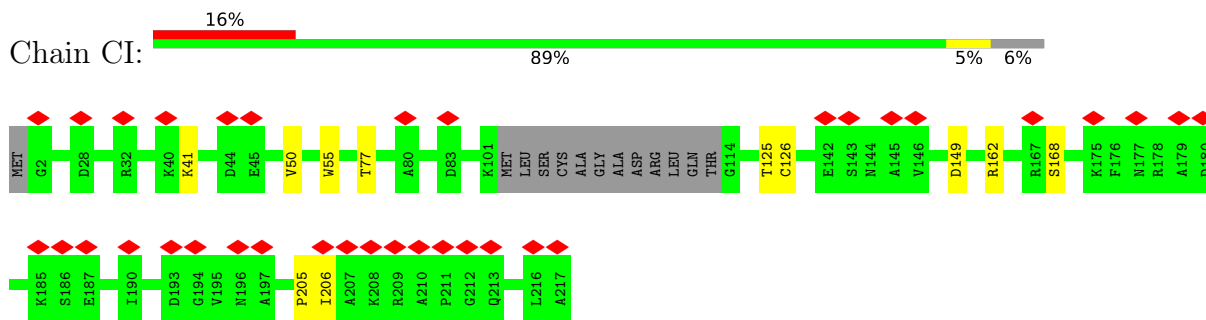
- Molecule 10: 60S ribosomal protein L7a



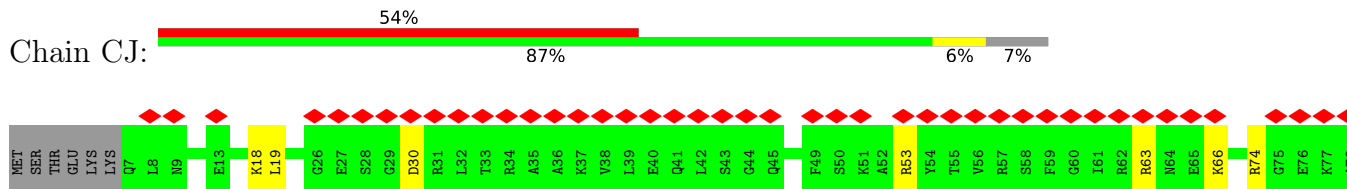
- Molecule 11: Ribosomal protein L6 alpha-beta domain-containing protein

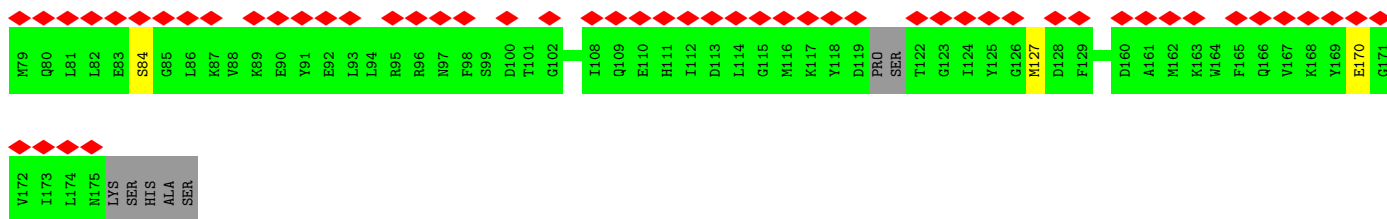


- Molecule 12: Ribosomal protein L10e/L16 domain-containing protein

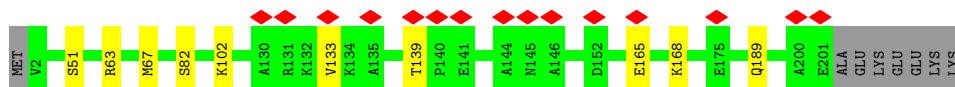
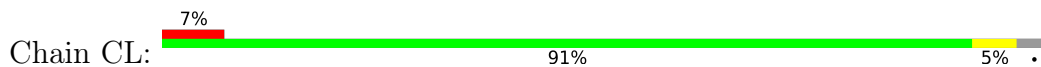


- Molecule 13: 60S ribosomal protein L11

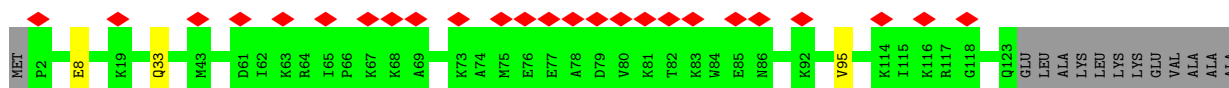
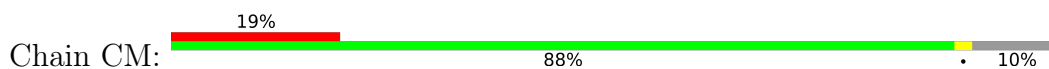




- Molecule 14: 60S ribosomal protein L13



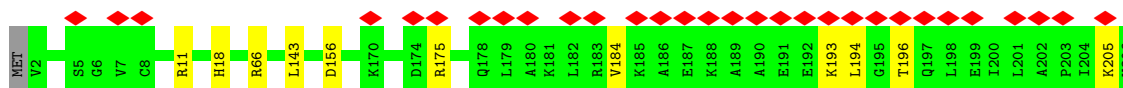
- Molecule 15: Ribosomal protein L14e domain-containing protein



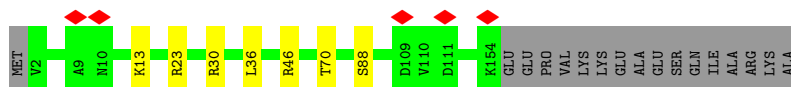
- Molecule 16: Ribosomal protein L15



- Molecule 17: Ribosomal protein L13a

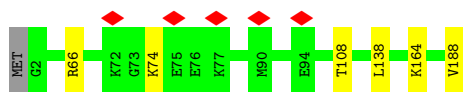


- Molecule 18: 60S ribosomal protein uL22

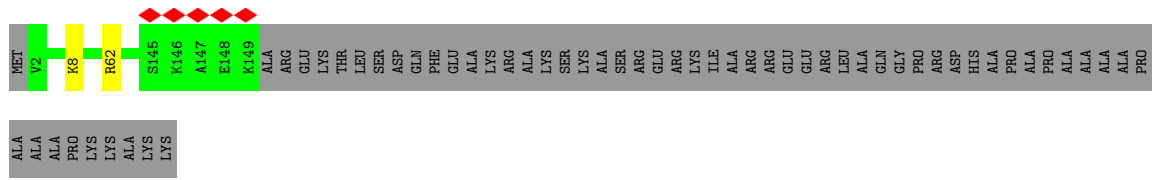


- Molecule 19: Ribosomal protein L18e/L15P domain-containing protein

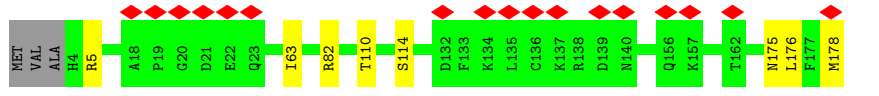




• Molecule 20: Ribosomal protein L19



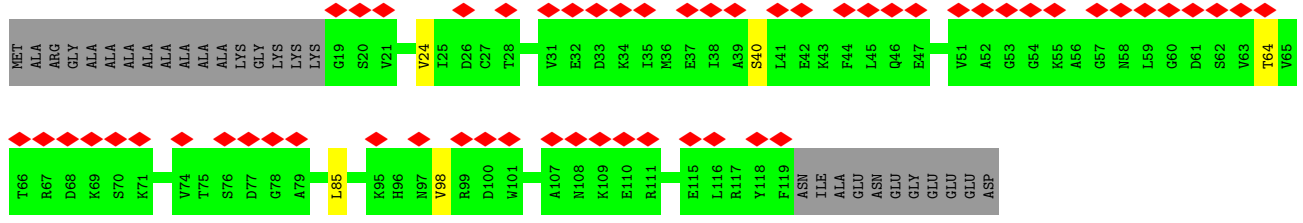
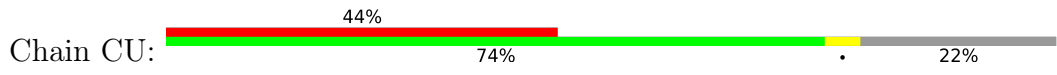
• Molecule 21: 60S ribosomal protein L18a



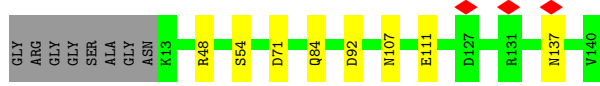
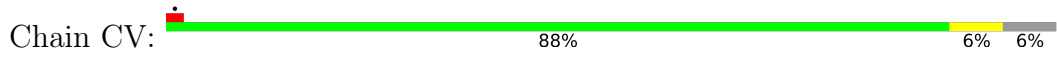
• Molecule 22: 60S ribosomal protein L21



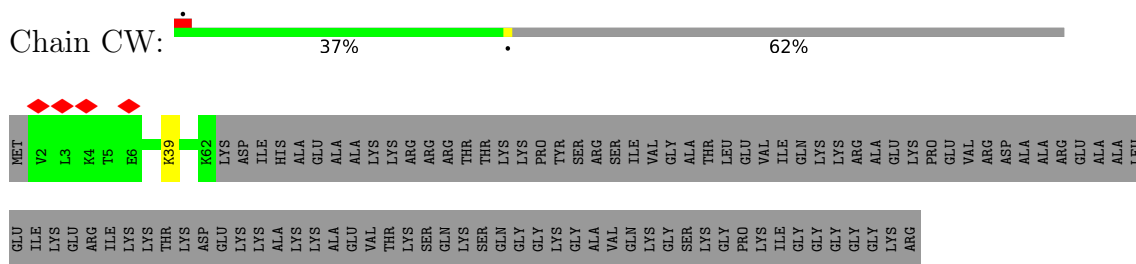
• Molecule 23: Genome assembly, chromosome: II



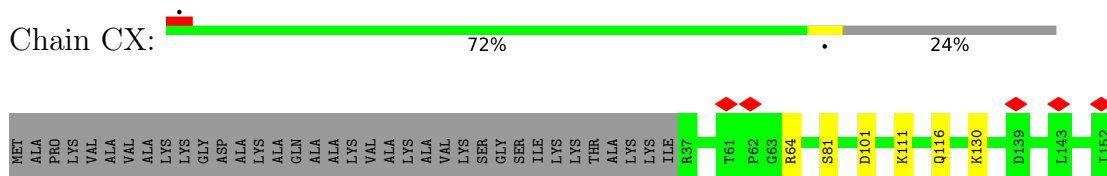
• Molecule 24: Ribosomal protein L17



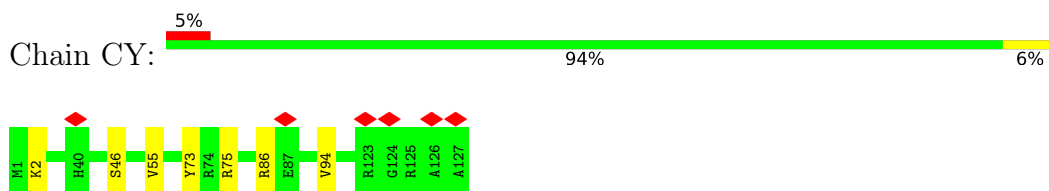
• Molecule 25: TRASH domain-containing protein



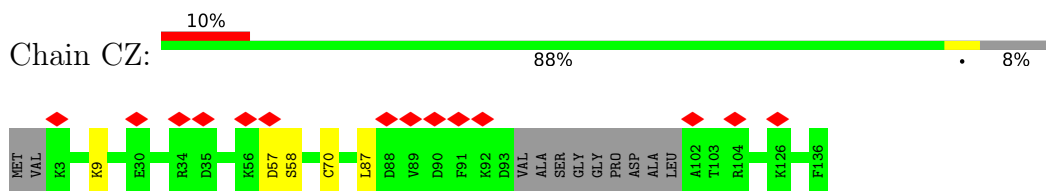
• Molecule 26: Genome assembly, chromosome: II



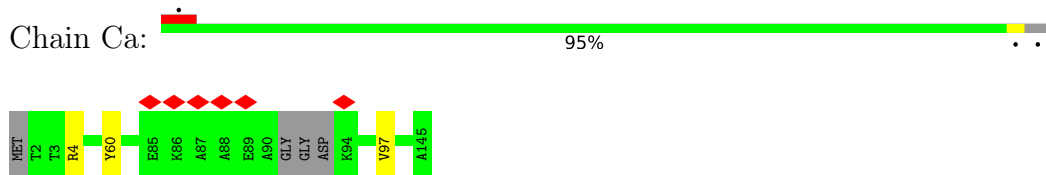
• Molecule 27: KOW domain-containing protein



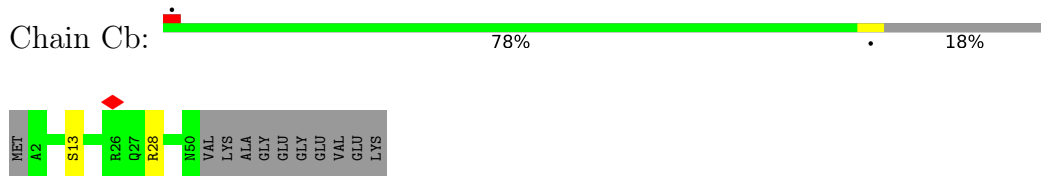
• Molecule 28: 60S ribosomal protein L27



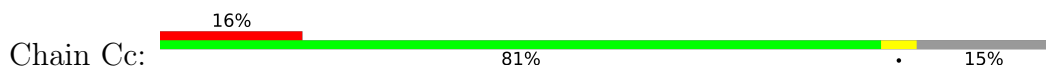
• Molecule 29: Ribosomal protein L18e/L15P domain-containing protein

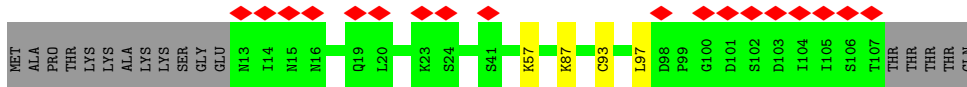


• Molecule 30: 60S ribosomal protein L29

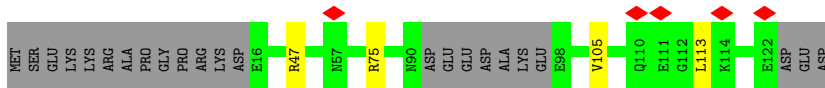
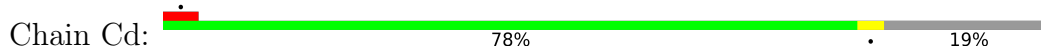


• Molecule 31: Ribosomal protein L7Ae/L30e/S12e/Gadd45 domain-containing protein

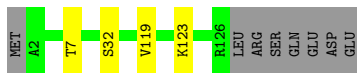




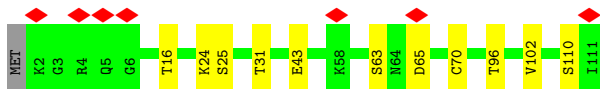
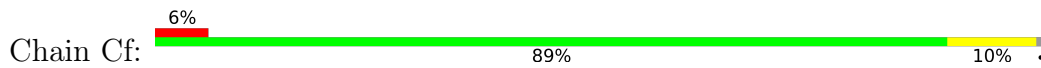
- Molecule 32: 60S ribosomal protein L31



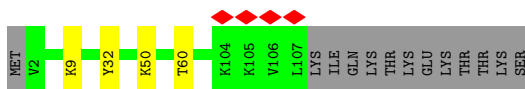
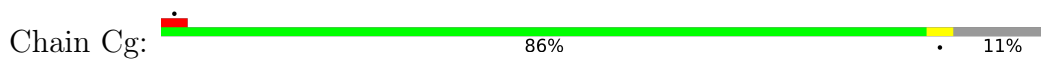
- Molecule 33: 60S ribosomal protein eL32



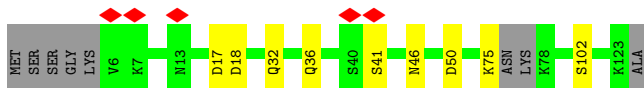
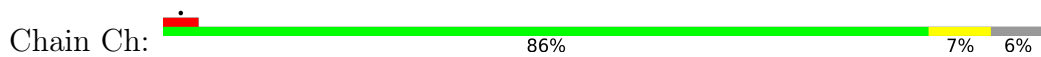
- Molecule 34: 60S ribosomal protein eL33



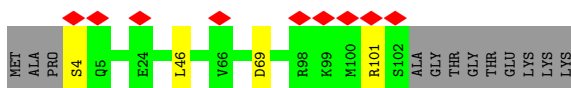
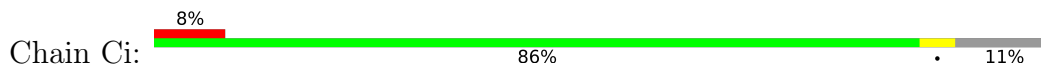
- Molecule 35: 60S ribosomal protein L34



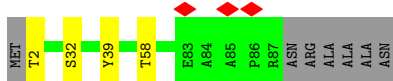
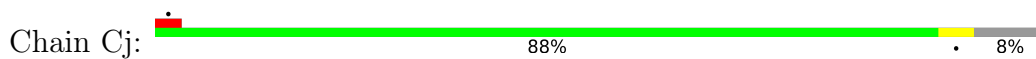
- Molecule 36: 60S ribosomal protein L35



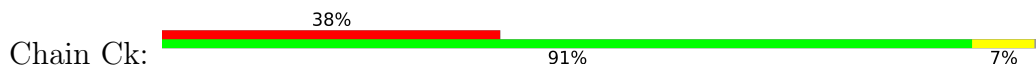
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: Ribosomal protein L37



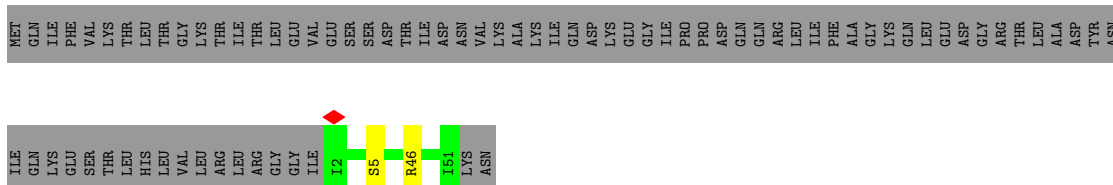
- Molecule 39: 60S ribosomal protein L38



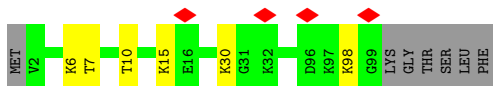
- Molecule 40: Ribosomal protein L39



- Molecule 41: Ubiquitin-like domain-containing protein



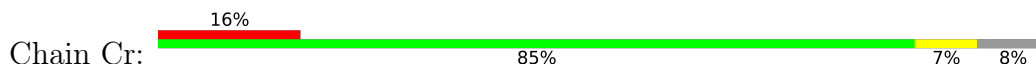
- Molecule 42: Genome assembly, chromosome: II

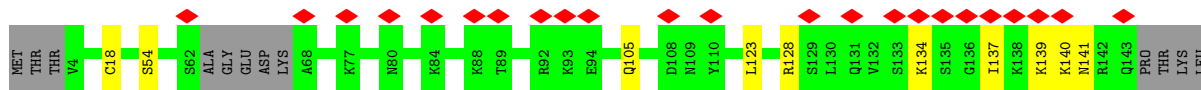


- Molecule 43: 60S ribosomal protein L37a, expressed



- Molecule 44: Ribosomal L28e/Mak16 domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105563	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 ($e^-/\text{\AA}^2$)	44.60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.721	Depositor
Minimum map value	-0.345	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 1MA, A2M, MLZ, UR3, PSU, OMU, MG, OMC, HIC, ZN, 5MC, K

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	Aa	0.60	0/65943	0.87	40/102798 (0.0%)
2	Ab	0.49	0/2842	0.82	2/4430 (0.0%)
3	Ac	0.57	0/3534	0.83	0/5507
4	CA	0.32	0/1920	0.58	0/2584
5	CB	0.31	0/3106	0.54	0/4162
6	CC	0.30	0/2902	0.54	1/3923 (0.0%)
7	CD	0.30	0/2199	0.51	0/2962
8	CE	0.27	0/1340	0.51	0/1810
9	CF	0.31	0/1914	0.52	0/2568
10	CG	0.29	0/1782	0.49	0/2396
11	CH	0.27	0/1445	0.51	0/1944
12	CI	0.48	2/1634 (0.1%)	0.87	4/2194 (0.2%)
13	CJ	0.28	0/1332	0.55	0/1783
14	CL	0.30	0/1625	0.54	0/2179
15	CM	0.28	0/976	0.51	0/1309
16	CN	0.33	0/1759	0.61	0/2354
17	CO	0.29	0/1661	0.54	0/2226
18	CP	0.31	0/1258	0.56	0/1689
19	CQ	0.30	0/1500	0.56	0/2007
20	CR	0.29	0/1245	0.53	0/1646
21	CS	0.31	0/1509	0.52	0/2029
22	CT	0.31	0/1288	0.54	0/1737
23	CU	0.28	0/812	0.50	0/1091
24	CV	0.31	0/972	0.56	0/1310
25	CW	0.31	0/520	0.51	0/694
26	CX	0.30	0/946	0.51	0/1271
27	CY	0.28	0/1025	0.58	0/1373
28	CZ	0.30	0/1027	0.51	0/1367
29	Ca	0.33	0/1132	0.50	0/1510
30	Cb	0.30	0/417	0.54	0/551
31	Cc	0.31	0/741	0.48	0/999
32	Cd	0.29	0/794	0.55	0/1065

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ce	0.31	0/1036	0.54	0/1387
34	Cf	0.33	0/896	0.57	0/1201
35	Cg	0.34	0/873	0.59	0/1170
36	Ch	0.29	0/947	0.57	0/1263
37	Ci	0.27	0/809	0.57	0/1070
38	Cj	0.33	0/710	0.67	0/943
39	Ck	0.28	0/564	0.52	0/754
40	Cl	0.30	0/463	0.61	0/616
41	Cm	0.29	0/414	0.55	0/548
42	Co	0.33	0/797	0.48	0/1049
43	Cp	0.32	0/693	0.55	0/920
44	Cr	0.28	0/1082	0.47	0/1455
All	All	0.50	2/122384 (0.0%)	0.76	47/179844 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	CI	205	PRO	CG-CD	-11.64	1.12	1.50
12	CI	205	PRO	CB-CG	-7.89	1.10	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	CI	205	PRO	CB-CG-CD	18.83	179.94	106.50
12	CI	205	PRO	N-CD-CG	-17.29	77.27	103.20
12	CI	205	PRO	CA-CB-CG	-16.85	71.98	104.00
1	Aa	545	C	N3-C2-O2	-8.96	115.63	121.90
12	CI	205	PRO	CA-N-CD	-8.91	99.03	111.50
1	Aa	545	C	N1-C2-O2	7.94	123.67	118.90
1	Aa	688	C	O4'-C1'-N1	7.53	114.22	108.20
1	Aa	709	C	N3-C2-O2	-7.12	116.91	121.90
1	Aa	403	G	O4'-C1'-N9	6.89	113.72	108.20
1	Aa	2557	C	C2-N1-C1'	6.64	126.11	118.80
1	Aa	2729	C	N3-C2-O2	-6.46	117.37	121.90
2	Ab	79	A	C2-N3-C4	-6.36	107.42	110.60
1	Aa	115	U	N3-C2-O2	-6.35	117.75	122.20
1	Aa	926	U	C2-N1-C1'	6.33	125.30	117.70
1	Aa	711	C	N1-C2-O2	6.28	122.67	118.90
1	Aa	926	U	N1-C2-O2	6.24	127.17	122.80
1	Aa	926	U	N3-C2-O2	-6.14	117.90	122.20
1	Aa	115	U	N1-C2-O2	6.10	127.07	122.80
1	Aa	709	C	N1-C2-O2	6.02	122.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	839	G	O4'-C1'-N9	5.99	112.99	108.20
1	Aa	99	C	C2-N1-C1'	5.90	125.29	118.80
1	Aa	711	C	N3-C2-O2	-5.83	117.82	121.90
1	Aa	115	U	C2-N1-C1'	5.81	124.67	117.70
1	Aa	568	G	N3-C2-N2	-5.78	115.85	119.90
1	Aa	2229	C	C2-N1-C1'	5.77	125.14	118.80
1	Aa	2986	C	C2-N1-C1'	5.76	125.14	118.80
1	Aa	633	C	N3-C2-O2	-5.74	117.88	121.90
1	Aa	1112	U	C2-N1-C1'	5.70	124.54	117.70
1	Aa	545	C	C6-N1-C2	-5.66	118.04	120.30
1	Aa	2729	C	C6-N1-C2	-5.54	118.08	120.30
1	Aa	1544	C	C2-N1-C1'	5.53	124.88	118.80
1	Aa	633	C	C2-N1-C1'	5.45	124.80	118.80
1	Aa	568	G	N3-C4-N9	-5.40	122.76	126.00
1	Aa	711	C	C2-N1-C1'	5.31	124.64	118.80
1	Aa	2270	G	O4'-C1'-N9	5.24	112.39	108.20
1	Aa	3060	C	C2-N1-C1'	5.23	124.55	118.80
2	Ab	93	U	C2-N1-C1'	5.21	123.96	117.70
1	Aa	499	C	N3-C2-O2	-5.19	118.27	121.90
1	Aa	1499	U	C5-C6-N1	-5.14	120.13	122.70
1	Aa	2998	C	C2-N1-C1'	5.13	124.45	118.80
6	CC	154	LEU	CA-CB-CG	-5.13	103.51	115.30
1	Aa	3179	C	C2-N1-C1'	5.11	124.42	118.80
1	Aa	3179	C	N1-C2-O2	5.11	121.97	118.90
1	Aa	1544	C	N3-C2-O2	-5.06	118.36	121.90
1	Aa	709	C	C2-N1-C1'	5.05	124.36	118.80
1	Aa	99	C	C6-N1-C2	-5.04	118.28	120.30
1	Aa	504	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

There are no planarity outliers.

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CA	243/261 (93%)	233 (96%)	10 (4%)	0	100	100
5	CB	381/385 (99%)	372 (98%)	9 (2%)	0	100	100
6	CC	372/405 (92%)	347 (93%)	25 (7%)	0	100	100
7	CD	267/307 (87%)	258 (97%)	9 (3%)	0	100	100
8	CE	169/232 (73%)	151 (89%)	18 (11%)	0	100	100
9	CF	232/244 (95%)	223 (96%)	9 (4%)	0	100	100
10	CG	217/258 (84%)	203 (94%)	14 (6%)	0	100	100
11	CH	184/189 (97%)	176 (96%)	8 (4%)	0	100	100
12	CI	200/217 (92%)	193 (96%)	7 (4%)	0	100	100
13	CJ	163/180 (91%)	158 (97%)	5 (3%)	0	100	100
14	CL	198/208 (95%)	192 (97%)	6 (3%)	0	100	100
15	CM	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
16	CN	201/204 (98%)	188 (94%)	13 (6%)	0	100	100
17	CO	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
18	CP	151/170 (89%)	146 (97%)	5 (3%)	0	100	100
19	CQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
20	CR	146/206 (71%)	144 (99%)	2 (1%)	0	100	100
21	CS	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
22	CT	157/164 (96%)	153 (98%)	4 (2%)	0	100	100
23	CU	99/129 (77%)	96 (97%)	3 (3%)	0	100	100
24	CV	126/136 (93%)	124 (98%)	2 (2%)	0	100	100
25	CW	59/161 (37%)	58 (98%)	1 (2%)	0	100	100
26	CX	114/152 (75%)	110 (96%)	4 (4%)	0	100	100
27	CY	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
28	CZ	122/137 (89%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Ca	137/145 (94%)	130 (95%)	7 (5%)	0	100	100
30	Cb	47/60 (78%)	42 (89%)	5 (11%)	0	100	100
31	Cc	93/112 (83%)	85 (91%)	8 (9%)	0	100	100
32	Cd	96/123 (78%)	96 (100%)	0	0	100	100
33	Ce	123/133 (92%)	119 (97%)	4 (3%)	0	100	100
34	Cf	108/111 (97%)	105 (97%)	3 (3%)	0	100	100
35	Cg	104/119 (87%)	102 (98%)	2 (2%)	0	100	100
36	Ch	112/124 (90%)	105 (94%)	7 (6%)	0	100	100
37	Ci	97/111 (87%)	87 (90%)	10 (10%)	0	100	100
38	Cj	84/93 (90%)	77 (92%)	7 (8%)	0	100	100
39	Ck	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
40	Cl	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	Cm	48/129 (37%)	47 (98%)	1 (2%)	0	100	100
42	Co	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
43	Cp	87/92 (95%)	83 (95%)	4 (5%)	0	100	100
44	Cr	131/147 (89%)	125 (95%)	6 (5%)	0	100	100
All	All	6083/6903 (88%)	5827 (96%)	256 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CA	189/199 (95%)	182 (96%)	7 (4%)	34	59
5	CB	319/331 (96%)	306 (96%)	13 (4%)	30	56
6	CC	284/329 (86%)	265 (93%)	19 (7%)	16	32
7	CD	216/258 (84%)	207 (96%)	9 (4%)	30	54
8	CE	132/197 (67%)	123 (93%)	9 (7%)	16	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CF	189/205 (92%)	181 (96%)	8 (4%)	30	54
10	CG	185/222 (83%)	179 (97%)	6 (3%)	39	63
11	CH	150/163 (92%)	143 (95%)	7 (5%)	26	50
12	CI	162/178 (91%)	152 (94%)	10 (6%)	18	35
13	CJ	134/156 (86%)	124 (92%)	10 (8%)	13	28
14	CL	164/178 (92%)	154 (94%)	10 (6%)	18	36
15	CM	100/115 (87%)	97 (97%)	3 (3%)	41	65
16	CN	177/178 (99%)	170 (96%)	7 (4%)	31	57
17	CO	170/173 (98%)	159 (94%)	11 (6%)	17	33
18	CP	130/144 (90%)	123 (95%)	7 (5%)	22	42
19	CQ	155/159 (98%)	149 (96%)	6 (4%)	32	58
20	CR	130/173 (75%)	128 (98%)	2 (2%)	65	82
21	CS	156/160 (98%)	148 (95%)	8 (5%)	24	45
22	CT	133/141 (94%)	126 (95%)	7 (5%)	22	43
23	CU	86/104 (83%)	81 (94%)	5 (6%)	20	38
24	CV	99/105 (94%)	91 (92%)	8 (8%)	11	24
25	CW	53/132 (40%)	52 (98%)	1 (2%)	57	77
26	CX	103/128 (80%)	97 (94%)	6 (6%)	20	38
27	CY	109/113 (96%)	102 (94%)	7 (6%)	17	34
28	CZ	102/114 (90%)	97 (95%)	5 (5%)	25	47
29	Ca	111/114 (97%)	108 (97%)	3 (3%)	44	69
30	Cb	43/51 (84%)	41 (95%)	2 (5%)	26	50
31	Cc	82/98 (84%)	78 (95%)	4 (5%)	25	47
32	Cd	83/108 (77%)	79 (95%)	4 (5%)	25	49
33	Ce	109/121 (90%)	105 (96%)	4 (4%)	34	59
34	Cf	94/96 (98%)	83 (88%)	11 (12%)	5	10
35	Cg	93/107 (87%)	89 (96%)	4 (4%)	29	54
36	Ch	99/109 (91%)	90 (91%)	9 (9%)	9	19
37	Ci	86/94 (92%)	82 (95%)	4 (5%)	26	50
38	Cj	72/77 (94%)	68 (94%)	4 (6%)	21	40
39	Ck	62/64 (97%)	57 (92%)	5 (8%)	11	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Cl	47/48 (98%)	44 (94%)	3 (6%)	17	34
41	Cm	44/115 (38%)	42 (96%)	2 (4%)	27	51
42	Co	86/92 (94%)	80 (93%)	6 (7%)	15	30
43	Cp	69/73 (94%)	64 (93%)	5 (7%)	14	29
44	Cr	119/132 (90%)	109 (92%)	10 (8%)	11	23
All	All	5126/5854 (88%)	4855 (95%)	271 (5%)	26	43

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CA	14	SER
4	CA	70	LYS
4	CA	76	PHE
4	CA	122	ASP
4	CA	147	ARG
4	CA	228	ASP
4	CA	245	ARG
5	CB	5	LYS
5	CB	31	SER
5	CB	34	LYS
5	CB	162	VAL
5	CB	209	GLU
5	CB	229	TYR
5	CB	281	MET
5	CB	307	LYS
5	CB	308	ASP
5	CB	332	CYS
5	CB	338	ARG
5	CB	347	LEU
5	CB	352	ARG
6	CC	25	SER
6	CC	40	VAL
6	CC	49	SER
6	CC	52	LYS
6	CC	99	MET
6	CC	104	ARG
6	CC	106	PHE
6	CC	111	THR
6	CC	137	VAL
6	CC	139	SER

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Mol	Chain	Res	Type
6	CC	169	SER
6	CC	186	LYS
6	CC	227	ARG
6	CC	251	LEU
6	CC	319	LYS
6	CC	341	ARG
6	CC	383	LYS
6	CC	388	ASP
6	CC	398	SER
7	CD	81	SER
7	CD	86	ARG
7	CD	102	THR
7	CD	152	ARG
7	CD	153	THR
7	CD	159	VAL
7	CD	228	LYS
7	CD	229	LYS
7	CD	287	LEU
8	CE	54	ASP
8	CE	60	THR
8	CE	61	VAL
8	CE	136	LYS
8	CE	140	GLN
8	CE	175	ASP
8	CE	185	ASP
8	CE	195	VAL
8	CE	219	PHE
9	CF	21	GLU
9	CF	73	MET
9	CF	133	GLU
9	CF	136	VAL
9	CF	169	LYS
9	CF	185	ASP
9	CF	221	ASN
9	CF	232	ARG
10	CG	42	LYS
10	CG	90	LYS
10	CG	100	LYS
10	CG	184	SER
10	CG	192	SER
10	CG	212	GLU
11	CH	1	MET

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Mol	Chain	Res	Type
11	CH	17	THR
11	CH	24	MET
11	CH	43	LEU
11	CH	103	SER
11	CH	112	GLU
11	CH	136	SER
12	CI	41	LYS
12	CI	50	VAL
12	CI	55	TRP
12	CI	77	THR
12	CI	125	THR
12	CI	126	CYS
12	CI	149	ASP
12	CI	162	ARG
12	CI	168	SER
12	CI	206	ILE
13	CJ	18	LYS
13	CJ	19	LEU
13	CJ	30	ASP
13	CJ	53	ARG
13	CJ	63	ARG
13	CJ	66	LYS
13	CJ	74	ARG
13	CJ	84	SER
13	CJ	127	MET
13	CJ	170	GLU
14	CL	51	SER
14	CL	63	ARG
14	CL	67	MET
14	CL	82	SER
14	CL	102	LYS
14	CL	133	VAL
14	CL	139	THR
14	CL	165	GLU
14	CL	168	LYS
14	CL	189	GLN
15	CM	8	GLU
15	CM	33	GLN
15	CM	95	VAL
16	CN	8	SER
16	CN	118	SER
16	CN	126	THR

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Mol	Chain	Res	Type
16	CN	128	LYS
16	CN	155	VAL
16	CN	180	ARG
16	CN	199	SER
17	CO	11	ARG
17	CO	18	HIS
17	CO	66	ARG
17	CO	143	LEU
17	CO	156	ASP
17	CO	175	ARG
17	CO	184	VAL
17	CO	193	LYS
17	CO	194	LEU
17	CO	196	THR
17	CO	205	LYS
18	CP	13	LYS
18	CP	23	ARG
18	CP	30	ARG
18	CP	36	LEU
18	CP	46	ARG
18	CP	70	THR
18	CP	88	SER
19	CQ	66	ARG
19	CQ	74	LYS
19	CQ	108	THR
19	CQ	138	LEU
19	CQ	164	LYS
19	CQ	188	VAL
20	CR	8	LYS
20	CR	62	ARG
21	CS	5	ARG
21	CS	63	ILE
21	CS	82	ARG
21	CS	110	THR
21	CS	114	SER
21	CS	175	ASN
21	CS	176	LEU
21	CS	178	MET
22	CT	9	SER
22	CT	10	ARG
22	CT	17	ARG
22	CT	83	ARG

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Mol	Chain	Res	Type
22	CT	104	GLU
22	CT	127	SER
22	CT	150	THR
23	CU	24	VAL
23	CU	40	SER
23	CU	64	THR
23	CU	85	LEU
23	CU	98	VAL
24	CV	48	ARG
24	CV	54	SER
24	CV	71	ASP
24	CV	84	GLN
24	CV	92	ASP
24	CV	107	ASN
24	CV	111	GLU
24	CV	137	ASN
25	CW	39	LYS
26	CX	64	ARG
26	CX	81	SER
26	CX	101	ASP
26	CX	111	LYS
26	CX	116	GLN
26	CX	130	LYS
27	CY	2	LYS
27	CY	46	SER
27	CY	55	VAL
27	CY	73	TYR
27	CY	75	ARG
27	CY	86	ARG
27	CY	94	VAL
28	CZ	9	LYS
28	CZ	57	ASP
28	CZ	58	SER
28	CZ	70	CYS
28	CZ	87	LEU
29	Ca	4	ARG
29	Ca	60	TYR
29	Ca	97	VAL
30	Cb	13	SER
30	Cb	28	ARG
31	Cc	57	LYS
31	Cc	87	LYS

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Mol	Chain	Res	Type
31	Cc	93	CYS
31	Cc	97	LEU
32	Cd	47	ARG
32	Cd	75	ARG
32	Cd	105	VAL
32	Cd	113	LEU
33	Ce	7	THR
33	Ce	32	SER
33	Ce	119	VAL
33	Ce	123	LYS
34	Cf	16	THR
34	Cf	24	LYS
34	Cf	25	SER
34	Cf	31	THR
34	Cf	43	GLU
34	Cf	63	SER
34	Cf	65	ASP
34	Cf	70	CYS
34	Cf	96	THR
34	Cf	102	VAL
34	Cf	110	SER
35	Cg	9	LYS
35	Cg	32	TYR
35	Cg	50	LYS
35	Cg	60	THR
36	Ch	17	ASP
36	Ch	18	ASP
36	Ch	32	GLN
36	Ch	36	GLN
36	Ch	41	SER
36	Ch	46	ASN
36	Ch	50	ASP
36	Ch	75	LYS
36	Ch	102	SER
37	Ci	4	SER
37	Ci	46	LEU
37	Ci	69	ASP
37	Ci	101	ARG
38	Cj	2	THR
38	Cj	32	SER
38	Cj	39	TYR
38	Cj	58	THR

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Mol	Chain	Res	Type
39	Ck	9	LYS
39	Ck	10	ASP
39	Ck	50	THR
39	Ck	51	ASP
39	Ck	55	LYS
40	Cl	5	LYS
40	Cl	38	ASN
40	Cl	49	LEU
41	Cm	5	SER
41	Cm	46	ARG
42	Co	6	LYS
42	Co	7	THR
42	Co	10	THR
42	Co	15	LYS
42	Co	30	LYS
42	Co	98	LYS
43	Cp	17	VAL
43	Cp	31	GLN
43	Cp	39	GLN
43	Cp	76	THR
43	Cp	77	MET
44	Cr	18	CYS
44	Cr	54	SER
44	Cr	105	GLN
44	Cr	123	LEU
44	Cr	128	ARG
44	Cr	134	LYS
44	Cr	137	ILE
44	Cr	139	LYS
44	Cr	140	LYS
44	Cr	141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
15	CM	16	ASN
15	CM	33	GLN
21	CS	10	GLN
29	Ca	66	ASN
31	Cc	77	ASN
36	Ch	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	2829/3391 (83%)	515 (18%)	0
2	Ab	118/119 (99%)	12 (10%)	0
3	Ac	150/158 (94%)	27 (18%)	0
All	All	3097/3668 (84%)	554 (17%)	0

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	12	U
1	Aa	14	A
1	Aa	20	G
1	Aa	38	A
1	Aa	41	A
1	Aa	43	A
1	Aa	47	A
1	Aa	48	OMU
1	Aa	53	G
1	Aa	55	A
1	Aa	57	G
1	Aa	58	A
1	Aa	64	A
1	Aa	67	U
1	Aa	90	G
1	Aa	97	A
1	Aa	107	A
1	Aa	108	G
1	Aa	113	G
1	Aa	114	C
1	Aa	118	A
1	Aa	120	A
1	Aa	133	U
1	Aa	134	G
1	Aa	146	G
1	Aa	154	G
1	Aa	155	A
1	Aa	162	U
1	Aa	163	C
1	Aa	164	C
1	Aa	170	G
1	Aa	184	A
1	Aa	187	U

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Mol	Chain	Res	Type
1	Aa	188	C
1	Aa	193	G
1	Aa	194	G
1	Aa	197	A
1	Aa	207	G
1	Aa	215	G
1	Aa	216	A
1	Aa	218	A
1	Aa	228	G
1	Aa	235	A
1	Aa	236	C
1	Aa	237	C
1	Aa	238	C
1	Aa	239	U
1	Aa	240	G
1	Aa	241	U
1	Aa	244	C
1	Aa	260	C
1	Aa	262	A
1	Aa	266	G
1	Aa	278	G
1	Aa	283	U
1	Aa	292	A
1	Aa	295	C
1	Aa	302	U
1	Aa	313	C
1	Aa	320	A
1	Aa	326	A
1	Aa	336	C
1	Aa	339	A
1	Aa	349	A
1	Aa	366	A
1	Aa	373	G
1	Aa	394	A
1	Aa	398	U
1	Aa	399	G
1	Aa	418	G
1	Aa	419	A
1	Aa	421	G
1	Aa	433	C
1	Aa	436	C
1	Aa	437	G

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Mol	Chain	Res	Type
1	Aa	438	A
1	Aa	442	G
1	Aa	443	C
1	Aa	444	C
1	Aa	445	C
1	Aa	448	G
1	Aa	449	C
1	Aa	452	U
1	Aa	455	G
1	Aa	458	G
1	Aa	478	C
1	Aa	481	C
1	Aa	483	C
1	Aa	484	G
1	Aa	488	C
1	Aa	489	G
1	Aa	492	G
1	Aa	493	U
1	Aa	495	U
1	Aa	496	G
1	Aa	497	G
1	Aa	502	U
1	Aa	503	U
1	Aa	505	U
1	Aa	516	G
1	Aa	522	C
1	Aa	524	A
1	Aa	529	C
1	Aa	532	G
1	Aa	535	C
1	Aa	536	C
1	Aa	537	C
1	Aa	538	U
1	Aa	539	A
1	Aa	540	G
1	Aa	541	G
1	Aa	547	C
1	Aa	548	C
1	Aa	549	G
1	Aa	550	G
1	Aa	552	G
1	Aa	553	G

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Mol	Chain	Res	Type
1	Aa	554	C
1	Aa	580	G
1	Aa	581	C
1	Aa	582	G
1	Aa	583	C
1	Aa	589	G
1	Aa	599	U
1	Aa	600	C
1	Aa	601	G
1	Aa	602	G
1	Aa	606	A
1	Aa	607	C
1	Aa	609	G
1	Aa	614	G
1	Aa	615	C
1	Aa	624	G
1	Aa	625	C
1	Aa	626	G
1	Aa	630	U
1	Aa	642	C
1	Aa	654	A2M
1	Aa	655	C
1	Aa	665	A
1	Aa	682	A
1	Aa	687	A
1	Aa	688	C
1	Aa	689	G
1	Aa	694	C
1	Aa	697	A
1	Aa	698	A
1	Aa	704	G
1	Aa	705	G
1	Aa	706	A
1	Aa	707	U
1	Aa	710	G
1	Aa	722	A
1	Aa	723	C
1	Aa	724	G
1	Aa	725	A
1	Aa	726	G
1	Aa	754	G
1	Aa	769	U

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Mol	Chain	Res	Type
1	Aa	770	C
1	Aa	771	U
1	Aa	775	A
1	Aa	778	G
1	Aa	781	U
1	Aa	784	A
1	Aa	785	G
1	Aa	788	G
1	Aa	789	G
1	Aa	790	A
1	Aa	810	A
1	Aa	821	A2M
1	Aa	834	G
1	Aa	865	C
1	Aa	878	U
1	Aa	883	U
1	Aa	889	PSU
1	Aa	901	C
1	Aa	911	G
1	Aa	912	OMG
1	Aa	918	A
1	Aa	919	A
1	Aa	920	G
1	Aa	921	A
1	Aa	925	A
1	Aa	927	C
1	Aa	928	G
1	Aa	929	A
1	Aa	941	G
1	Aa	948	C
1	Aa	963	C
1	Aa	964	PSU
1	Aa	966	A
1	Aa	981	C
1	Aa	986	C
1	Aa	987	G
1	Aa	991	U
1	Aa	999	G
1	Aa	1005	C
1	Aa	1006	C
1	Aa	1007	A
1	Aa	1015	G

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Mol	Chain	Res	Type
1	Aa	1043	C
1	Aa	1052	A
1	Aa	1054	C
1	Aa	1057	PSU
1	Aa	1068	G
1	Aa	1069	A
1	Aa	1070	U
1	Aa	1075	C
1	Aa	1080	G
1	Aa	1086	G
1	Aa	1090	G
1	Aa	1099	U
1	Aa	1100	G
1	Aa	1101	G
1	Aa	1102	A
1	Aa	1107	G
1	Aa	1121	G
1	Aa	1135	G
1	Aa	1148	U
1	Aa	1157	A
1	Aa	1158	A
1	Aa	1159	C
1	Aa	1163	A
1	Aa	1182	A
1	Aa	1184	C
1	Aa	1185	U
1	Aa	1186	G
1	Aa	1197	U
1	Aa	1198	A
1	Aa	1205	A
1	Aa	1206	C
1	Aa	1214	G
1	Aa	1221	G
1	Aa	1310	U
1	Aa	1312	G
1	Aa	1313	A
1	Aa	1314	U
1	Aa	1318	G
1	Aa	1321	G
1	Aa	1322	A
1	Aa	1335	A
1	Aa	1337	A

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Mol	Chain	Res	Type
1	Aa	1353	G
1	Aa	1354	A
1	Aa	1355	G
1	Aa	1356	C
1	Aa	1357	G
1	Aa	1358	C
1	Aa	1359	C
1	Aa	1361	U
1	Aa	1371	A2M
1	Aa	1391	G
1	Aa	1403	G
1	Aa	1404	G
1	Aa	1406	G
1	Aa	1423	G
1	Aa	1435	G
1	Aa	1438	G
1	Aa	1441	OMC
1	Aa	1450	A
1	Aa	1454	OMG
1	Aa	1456	A
1	Aa	1459	U
1	Aa	1473	OMC
1	Aa	1485	A
1	Aa	1486	A
1	Aa	1487	G
1	Aa	1488	A
1	Aa	1500	C
1	Aa	1506	G
1	Aa	1516	U
1	Aa	1517	G
1	Aa	1518	C
1	Aa	1528	A
1	Aa	1531	C
1	Aa	1535	C
1	Aa	1537	U
1	Aa	1551	A
1	Aa	1553	C
1	Aa	1558	C
1	Aa	1559	A
1	Aa	1560	G
1	Aa	1562	U
1	Aa	1564	G

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Mol	Chain	Res	Type
1	Aa	1566	G
1	Aa	1577	C
1	Aa	1586	A
1	Aa	1587	A
1	Aa	1588	A
1	Aa	1592	A
1	Aa	1603	G
1	Aa	1604	A
1	Aa	1606	U
1	Aa	1621	G
1	Aa	1627	G
1	Aa	1628	U
1	Aa	1630	G
1	Aa	1638	C
1	Aa	1642	A
1	Aa	1644	G
1	Aa	1656	C
1	Aa	1661	G
1	Aa	1682	A
1	Aa	1704	C
1	Aa	1706	A
1	Aa	1717	C
1	Aa	1724	G
1	Aa	1740	A
1	Aa	1741	G
1	Aa	1742	U
1	Aa	1750	A
1	Aa	1751	G
1	Aa	1752	A
1	Aa	1781	G
1	Aa	1798	A
1	Aa	1819	C
1	Aa	1820	G
1	Aa	1822	U
1	Aa	1836	A
1	Aa	1840	A
1	Aa	1842	A
1	Aa	1843	A
1	Aa	1844	OMC
1	Aa	1847	OMC
1	Aa	1848	A
1	Aa	1850	C

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Mol	Chain	Res	Type
1	Aa	1851	A
1	Aa	1867	C
1	Aa	1868	A2M
1	Aa	1878	C
1	Aa	1879	A
1	Aa	1880	A
1	Aa	1881	U
1	Aa	1887	A
1	Aa	1907	G
1	Aa	1944	C
1	Aa	2098	G
1	Aa	2100	C
1	Aa	2101	U
1	Aa	2110	G
1	Aa	2113	C
1	Aa	2120	G
1	Aa	2121	OMG
1	Aa	2122	OMG
1	Aa	2130	A
1	Aa	2139	U
1	Aa	2143	A
1	Aa	2157	A
1	Aa	2168	G
1	Aa	2195	OMC
1	Aa	2203	U
1	Aa	2204	G
1	Aa	2207	U
1	Aa	2208	G
1	Aa	2221	A
1	Aa	2223	PSU
1	Aa	2230	A
1	Aa	2242	A
1	Aa	2271	G
1	Aa	2276	5MC
1	Aa	2278	A
1	Aa	2279	A2M
1	Aa	2280	U
1	Aa	2282	C
1	Aa	2305	G
1	Aa	2308	U
1	Aa	2311	A
1	Aa	2313	G

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Mol	Chain	Res	Type
1	Aa	2319	A2M
1	Aa	2332	U
1	Aa	2333	G
1	Aa	2334	U
1	Aa	2363	OMC
1	Aa	2371	A
1	Aa	2372	C
1	Aa	2373	G
1	Aa	2383	G
1	Aa	2389	OMG
1	Aa	2391	G
1	Aa	2395	A
1	Aa	2399	A
1	Aa	2400	A
1	Aa	2401	G
1	Aa	2402	A
1	Aa	2408	OMU
1	Aa	2409	U
1	Aa	2410	G
1	Aa	2417	A
1	Aa	2420	C
1	Aa	2433	G
1	Aa	2436	A
1	Aa	2516	U
1	Aa	2517	A
1	Aa	2554	U
1	Aa	2556	G
1	Aa	2579	G
1	Aa	2588	G
1	Aa	2596	A
1	Aa	2598	A
1	Aa	2609	G
1	Aa	2610	G
1	Aa	2617	G
1	Aa	2622	OMG
1	Aa	2629	A
1	Aa	2640	A
1	Aa	2654	OMG
1	Aa	2655	U
1	Aa	2659	A
1	Aa	2677	A
1	Aa	2680	G

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Mol	Chain	Res	Type
1	Aa	2683	A
1	Aa	2692	G
1	Aa	2693	G
1	Aa	2694	A
1	Aa	2697	A
1	Aa	2699	A
1	Aa	2708	A
1	Aa	2715	PSU
1	Aa	2717	G
1	Aa	2722	U
1	Aa	2724	A
1	Aa	2732	OMU
1	Aa	2755	U
1	Aa	2756	G
1	Aa	2758	C
1	Aa	2765	A
1	Aa	2780	G
1	Aa	2781	G
1	Aa	2786	U
1	Aa	2799	G
1	Aa	2802	A
1	Aa	2803	G
1	Aa	2804	A
1	Aa	2806	A
1	Aa	2813	C
1	Aa	2817	G
1	Aa	2818	OMG
1	Aa	2819	G
1	Aa	2820	A
1	Aa	2822	A
1	Aa	2824	C
1	Aa	2832	U
1	Aa	2850	A
1	Aa	2863	U
1	Aa	2870	C
1	Aa	2874	G
1	Aa	2875	A
1	Aa	2890	A
1	Aa	2901	G
1	Aa	2914	A2M
1	Aa	2930	C
1	Aa	2938	U

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Mol	Chain	Res	Type
1	Aa	2939	A
1	Aa	2945	C
1	Aa	2948	G
1	Aa	2950	G
1	Aa	2954	G
1	Aa	2957	U
1	Aa	2958	PSU
1	Aa	2962	OMC
1	Aa	2974	A
1	Aa	2986	C
1	Aa	2993	G
1	Aa	2995	PSU
1	Aa	2999	A
1	Aa	3014	A
1	Aa	3060	C
1	Aa	3061	G
1	Aa	3071	G
1	Aa	3074	A
1	Aa	3076	G
1	Aa	3080	G
1	Aa	3088	A
1	Aa	3094	C
1	Aa	3102	C
1	Aa	3106	U
1	Aa	3124	A
1	Aa	3131	A
1	Aa	3132	A
1	Aa	3133	U
1	Aa	3143	C
1	Aa	3144	A
1	Aa	3145	U
1	Aa	3154	U
1	Aa	3175	C
1	Aa	3178	A
1	Aa	3184	G
1	Aa	3200	C
1	Aa	3201	A
1	Aa	3203	G
1	Aa	3208	C
1	Aa	3210	U
1	Aa	3232	G
1	Aa	3233	C

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Mol	Chain	Res	Type
1	Aa	3235	G
1	Aa	3237	A
1	Aa	3239	U
1	Aa	3240	G
1	Aa	3241	C
1	Aa	3264	C
1	Aa	3265	C
1	Aa	3270	C
1	Aa	3271	C
1	Aa	3288	A
1	Aa	3296	OMG
1	Aa	3297	C
1	Aa	3334	C
1	Aa	3335	A
1	Aa	3338	G
1	Aa	3353	C
1	Aa	3362	G
1	Aa	3371	C
1	Aa	3390	G
1	Aa	3391	U
2	Ab	2	G
2	Ab	38	U
2	Ab	42	A
2	Ab	48	G
2	Ab	49	A
2	Ab	53	U
2	Ab	54	A
2	Ab	63	U
2	Ab	64	G
2	Ab	89	G
2	Ab	100	A
2	Ab	110	G
3	Ac	21	C
3	Ac	23	C
3	Ac	34	U
3	Ac	35	C
3	Ac	38	U
3	Ac	59	A
3	Ac	61	A
3	Ac	62	C
3	Ac	63	C
3	Ac	74	PSU

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Mol	Chain	Res	Type
3	Ac	75	OMG
3	Ac	78	G
3	Ac	85	U
3	Ac	86	G
3	Ac	89	C
3	Ac	94	G
3	Ac	103	A
3	Ac	105	C
3	Ac	110	G
3	Ac	112	U
3	Ac	120	A
3	Ac	133	G
3	Ac	139	A
3	Ac	149	G
3	Ac	152	C
3	Ac	155	C
3	Ac	159	G

There are no RNA pucker outliers to report.

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

122 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
1	A2M	Aa	3108	1	18,25,26	3.61	7 (38%)	18,36,39	3.46	3 (16%)
1	OMG	Aa	2121	1	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)
1	OMG	Aa	912	1,45	18,26,27	2.39	8 (44%)	19,38,41	1.50	4 (21%)
1	PSU	Aa	2926	46,1	18,21,22	4.28	7 (38%)	22,30,33	1.81	4 (18%)
1	PSU	Aa	2616	1	18,21,22	4.15	7 (38%)	22,30,33	1.79	5 (22%)
1	OMU	Aa	2924	1	19,22,23	3.02	8 (42%)	26,31,34	1.90	6 (23%)
1	PSU	Aa	2715	1	18,21,22	4.20	8 (44%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	Aa	821	46,1	18,25,26	3.61	7 (38%)	18,36,39	3.36	3 (16%)
1	OMG	Aa	2122	1	18,26,27	2.42	8 (44%)	19,38,41	1.63	3 (15%)
1	PSU	Aa	1467	1	18,21,22	4.16	7 (38%)	22,30,33	1.79	4 (18%)
1	PSU	Aa	2947	46,1,45	18,21,22	4.10	7 (38%)	22,30,33	1.87	5 (22%)
1	OMC	Aa	2882	1	19,22,23	2.87	8 (42%)	26,31,34	0.87	1 (3%)
1	OMG	Aa	2794	1	18,26,27	2.42	8 (44%)	19,38,41	1.57	4 (21%)
1	PSU	Aa	2518	1	18,21,22	4.15	7 (38%)	22,30,33	1.75	4 (18%)
1	PSU	Aa	2132	46,1,45	18,21,22	4.12	7 (38%)	22,30,33	1.79	5 (22%)
1	A2M	Aa	2643	1	18,25,26	3.57	7 (38%)	18,36,39	3.51	3 (16%)
1	OMC	Aa	1512	46,1	19,22,23	2.86	8 (42%)	26,31,34	0.84	0
1	PSU	Aa	1127	1	18,21,22	4.13	7 (38%)	22,30,33	1.81	5 (22%)
1	PSU	Aa	2868	1	18,21,22	4.16	7 (38%)	22,30,33	1.79	4 (18%)
1	OMU	Aa	2111	1	19,22,23	2.98	8 (42%)	26,31,34	1.83	5 (19%)
1	PSU	Aa	2978	1	18,21,22	4.05	7 (38%)	22,30,33	1.86	5 (22%)
1	PSU	Aa	2430	1	18,21,22	4.09	7 (38%)	22,30,33	1.99	5 (22%)
1	A2M	Aa	1371	46,1	18,25,26	3.59	7 (38%)	18,36,39	3.42	4 (22%)
1	OMC	Aa	1530	1,45	19,22,23	2.86	8 (42%)	26,31,34	0.66	0
1	OMG	Aa	2407	46,1	18,26,27	2.39	8 (44%)	19,38,41	1.65	4 (21%)
1	1MA	Aa	650	46,1	16,25,26	4.01	5 (31%)	18,37,40	1.84	3 (16%)
1	OMG	Aa	2920	1	18,26,27	2.39	8 (44%)	19,38,41	1.54	4 (21%)
3	PSU	Ac	18	3,1	18,21,22	4.11	7 (38%)	22,30,33	2.00	5 (22%)
1	PSU	Aa	2209	46,1	18,21,22	4.20	7 (38%)	22,30,33	1.75	5 (22%)
1	PSU	Aa	1126	1	18,21,22	4.10	7 (38%)	22,30,33	1.76	4 (18%)
1	PSU	Aa	2414	46,1	18,21,22	4.04	7 (38%)	22,30,33	2.03	5 (22%)
1	OMC	Aa	2962	1	19,22,23	2.93	8 (42%)	26,31,34	0.75	0
1	OMU	Aa	3305	1	19,22,23	3.01	7 (36%)	26,31,34	2.17	8 (30%)
1	OMC	Aa	2363	1	19,22,23	2.86	8 (42%)	26,31,34	1.40	3 (11%)
1	A2M	Aa	654	1	18,25,26	3.70	7 (38%)	18,36,39	3.40	4 (22%)
1	A2M	Aa	2218	1	18,25,26	3.61	8 (44%)	18,36,39	3.52	5 (27%)
1	A2M	Aa	2279	1	18,25,26	3.67	8 (44%)	18,36,39	3.43	4 (22%)
1	A2M	Aa	369	1	18,25,26	3.55	7 (38%)	18,36,39	3.29	4 (22%)
1	A2M	Aa	2319	1	18,25,26	3.62	8 (44%)	18,36,39	3.34	3 (16%)
1	OMG	Aa	2286	1	18,26,27	2.44	8 (44%)	19,38,41	1.50	4 (21%)
1	OMC	Aa	2951	1	19,22,23	2.91	8 (42%)	26,31,34	0.70	0
1	A2M	Aa	2949	46,1	18,25,26	3.58	7 (38%)	18,36,39	3.47	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	Aa	940	1	18,25,26	3.62	8 (44%)	18,36,39	3.50	4 (22%)
3	OMG	Ac	75	3	18,26,27	2.43	8 (44%)	19,38,41	1.48	4 (21%)
1	OMC	Aa	1847	1	19,22,23	2.97	8 (42%)	26,31,34	0.97	1 (3%)
1	OMU	Aa	1061	1	19,22,23	3.02	8 (42%)	26,31,34	1.94	7 (26%)
1	A2M	Aa	811	1	18,25,26	3.61	7 (38%)	18,36,39	3.32	4 (22%)
1	PSU	Aa	995	1	18,21,22	4.11	7 (38%)	22,30,33	1.82	4 (18%)
1	OMC	Aa	2195	1,45	19,22,23	2.88	8 (42%)	26,31,34	0.87	0
1	PSU	Aa	68	1	18,21,22	4.07	8 (44%)	22,30,33	2.06	6 (27%)
1	OMU	Aa	669	1	19,22,23	3.00	7 (36%)	26,31,34	2.10	7 (26%)
1	OMC	Aa	1441	1	19,22,23	2.86	8 (42%)	26,31,34	1.19	3 (11%)
1	OMG	Aa	2234	1	18,26,27	2.44	8 (44%)	19,38,41	1.50	4 (21%)
1	OMC	Aa	2839	1	19,22,23	2.95	8 (42%)	26,31,34	1.16	3 (11%)
1	PSU	Aa	378	1	18,21,22	4.13	7 (38%)	22,30,33	1.72	2 (9%)
1	OMC	Aa	1844	1	19,22,23	2.88	8 (42%)	26,31,34	1.39	3 (11%)
1	PSU	Aa	2223	1	18,21,22	4.14	7 (38%)	22,30,33	1.88	5 (22%)
1	OMC	Aa	2291	1	19,22,23	2.95	8 (42%)	26,31,34	1.18	3 (11%)
1	OMU	Aa	2345	1,45	19,22,23	2.99	8 (42%)	26,31,34	1.90	6 (23%)
1	OMG	Aa	2389	1	18,26,27	2.38	8 (44%)	19,38,41	1.45	3 (15%)
1	OMU	Aa	2653	1	19,22,23	3.00	8 (42%)	26,31,34	1.98	6 (23%)
1	OMG	Aa	809	1	18,26,27	2.40	8 (44%)	19,38,41	1.47	4 (21%)
1	5MC	Aa	2276	46,1	18,22,23	3.50	7 (38%)	26,32,35	1.04	3 (11%)
1	PSU	Aa	1904	46,1,45	18,21,22	4.03	7 (38%)	22,30,33	1.94	5 (22%)
1	PSU	Aa	964	1	18,21,22	4.27	8 (44%)	22,30,33	1.86	4 (18%)
1	PSU	Aa	35	1	18,21,22	4.17	7 (38%)	22,30,33	1.96	5 (22%)
1	5MC	Aa	2873	1,45	18,22,23	3.41	7 (38%)	26,32,35	1.23	3 (11%)
1	OMC	Aa	1473	1	19,22,23	2.91	8 (42%)	26,31,34	0.81	0
1	OMG	Aa	2393	1	18,26,27	2.42	8 (44%)	19,38,41	1.57	3 (15%)
1	PSU	Aa	2347	46,1	18,21,22	4.12	7 (38%)	22,30,33	1.63	4 (18%)
1	PSU	Aa	1128	1	18,21,22	4.18	7 (38%)	22,30,33	1.95	5 (22%)
42	MLZ	Co	55	42	8,9,10	0.63	0	4,9,11	0.97	0
1	A2M	Aa	1868	46,1	18,25,26	3.60	8 (44%)	18,36,39	3.40	4 (22%)
1	OMG	Aa	3296	46,1	18,26,27	2.41	8 (44%)	19,38,41	1.68	5 (26%)
1	A2M	Aa	1453	46,1	18,25,26	3.57	7 (38%)	18,36,39	3.56	3 (16%)
1	OMU	Aa	48	1	19,22,23	2.97	8 (42%)	26,31,34	1.75	4 (15%)
1	PSU	Aa	1047	1	18,21,22	4.17	7 (38%)	22,30,33	1.79	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	Aa	2720	1	19,22,23	2.97	8 (42%)	26,31,34	2.02	7 (26%)
1	A2M	Aa	2937	1	18,25,26	3.60	7 (38%)	18,36,39	3.46	3 (16%)
1	PSU	Aa	2829	1	18,21,22	4.02	7 (38%)	22,30,33	1.85	5 (22%)
1	PSU	Aa	823	1	18,21,22	4.06	7 (38%)	22,30,33	1.83	5 (22%)
1	PSU	Aa	2134	1	18,21,22	4.12	7 (38%)	22,30,33	1.72	3 (13%)
1	OMU	Aa	2419	1	19,22,23	2.97	8 (42%)	26,31,34	1.75	4 (15%)
1	OMU	Aa	798	1	19,22,23	2.90	8 (42%)	26,31,34	1.87	5 (19%)
1	OMU	Aa	2408	1	19,22,23	2.89	8 (42%)	26,31,34	2.22	8 (30%)
1	OMC	Aa	2335	1	19,22,23	2.84	8 (42%)	26,31,34	0.81	0
1	OMU	Aa	2732	1	19,22,23	2.95	8 (42%)	26,31,34	1.83	5 (19%)
1	OMG	Aa	2818	1	18,26,27	2.41	8 (44%)	19,38,41	1.59	4 (21%)
3	A2M	Ac	43	3	18,25,26	3.61	7 (38%)	18,36,39	3.43	3 (16%)
1	PSU	Aa	1009	1,45	18,21,22	4.20	7 (38%)	22,30,33	1.77	3 (13%)
1	PSU	Aa	1475	1	18,21,22	4.12	7 (38%)	22,30,33	1.92	5 (22%)
1	PSU	Aa	2316	46,1	18,21,22	4.23	7 (38%)	22,30,33	1.88	4 (18%)
1	OMG	Aa	1852	1	18,26,27	2.36	8 (44%)	19,38,41	1.46	4 (21%)
1	OMG	Aa	1454	1	18,26,27	2.38	8 (44%)	19,38,41	1.52	3 (15%)
3	PSU	Ac	74	3	18,21,22	4.17	7 (38%)	22,30,33	1.74	3 (13%)
1	OMU	Aa	1889	1,45	19,22,23	2.95	8 (42%)	26,31,34	1.88	4 (15%)
1	A2M	Aa	880	1	18,25,26	3.59	7 (38%)	18,36,39	3.45	4 (22%)
1	OMU	Aa	2886	1	19,22,23	3.02	8 (42%)	26,31,34	1.76	5 (19%)
1	PSU	Aa	2857	1	18,21,22	4.20	7 (38%)	22,30,33	1.71	4 (18%)
1	PSU	Aa	2883	1	18,21,22	4.08	7 (38%)	22,30,33	1.69	4 (18%)
1	PSU	Aa	2747	1	18,21,22	4.14	7 (38%)	22,30,33	1.93	5 (22%)
1	PSU	Aa	3113	1	18,21,22	4.15	7 (38%)	22,30,33	1.82	4 (18%)
1	A2M	Aa	2914	1	18,25,26	3.60	7 (38%)	18,36,39	3.50	3 (16%)
1	PSU	Aa	2312	46,1,45	18,21,22	4.23	7 (38%)	22,30,33	1.96	5 (22%)
1	A2M	Aa	1137	46,1	18,25,26	3.65	8 (44%)	18,36,39	3.43	3 (16%)
5	HIC	CB	246	5	8,11,12	1.90	1 (12%)	6,14,16	0.66	0
1	PSU	Aa	889	1	18,21,22	4.16	7 (38%)	22,30,33	1.69	3 (13%)
1	OMG	Aa	2622	1	18,26,27	2.40	8 (44%)	19,38,41	1.51	4 (21%)
1	OMC	Aa	2685	1	19,22,23	2.93	8 (42%)	26,31,34	0.81	0
1	OMU	Aa	144	1	19,22,23	2.92	8 (42%)	26,31,34	1.67	5 (19%)
1	PSU	Aa	1057	1	18,21,22	4.16	7 (38%)	22,30,33	1.72	3 (13%)
1	OMC	Aa	1857	1	19,22,23	2.84	8 (42%)	26,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	Aa	2796	1	18,26,27	2.39	8 (44%)	19,38,41	1.48	3 (15%)
1	OMC	Aa	668	1	19,22,23	2.86	8 (42%)	26,31,34	0.72	0
1	A2M	Aa	2124	1	18,25,26	3.61	8 (44%)	18,36,39	3.35	4 (22%)
1	PSU	Aa	2958	1	18,21,22	4.08	7 (38%)	22,30,33	1.69	4 (18%)
1	OMG	Aa	2654	1	18,26,27	2.39	8 (44%)	19,38,41	1.55	5 (26%)
1	OMU	Aa	2738	1	19,22,23	2.98	8 (42%)	26,31,34	1.66	4 (15%)
1	PSU	Aa	2189	1	18,21,22	4.18	7 (38%)	22,30,33	1.74	4 (18%)
1	PSU	Aa	2995	1	18,21,22	4.07	7 (38%)	22,30,33	1.84	5 (22%)
1	OMG	Aa	2925	1	18,26,27	2.41	8 (44%)	19,38,41	1.46	3 (15%)
1	UR3	Aa	2956	1	19,22,23	2.81	6 (31%)	26,32,35	1.27	3 (11%)

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
1	A2M	Aa	3108	1	-	0/5/27/28	0/3/3/3
1	OMG	Aa	2121	1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	912	1,45	-	3/5/27/28	0/3/3/3
1	PSU	Aa	2926	46,1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	2616	1	-	2/7/25/26	0/2/2/2
1	OMU	Aa	2924	1	-	2/9/27/28	0/2/2/2
1	PSU	Aa	2715	1	-	5/7/25/26	0/2/2/2
1	A2M	Aa	821	46,1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	2122	1	-	2/5/27/28	0/3/3/3
1	PSU	Aa	1467	1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	2947	46,1,45	-	2/7/25/26	0/2/2/2
1	OMC	Aa	2882	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	2794	1	-	3/5/27/28	0/3/3/3
1	PSU	Aa	2518	1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	2132	46,1,45	-	3/7/25/26	0/2/2/2
1	A2M	Aa	2643	1	-	1/5/27/28	0/3/3/3
1	OMC	Aa	1512	46,1	-	2/9/27/28	0/2/2/2
1	PSU	Aa	1127	1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	2868	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	Aa	2111	1	-	2/9/27/28	0/2/2/2
1	PSU	Aa	2978	1	-	0/7/25/26	0/2/2/2
1	PSU	Aa	2430	1	-	0/7/25/26	0/2/2/2
1	A2M	Aa	1371	46,1	-	2/5/27/28	0/3/3/3
1	OMC	Aa	1530	1,45	-	0/9/27/28	0/2/2/2
1	OMG	Aa	2407	46,1	-	1/5/27/28	0/3/3/3
1	1MA	Aa	650	46,1	-	0/3/25/26	0/3/3/3
1	OMG	Aa	2920	1	-	0/5/27/28	0/3/3/3
3	PSU	Ac	18	3,1	-	0/7/25/26	0/2/2/2
1	PSU	Aa	2209	46,1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	1126	1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	2414	46,1	-	3/7/25/26	0/2/2/2
1	OMC	Aa	2962	1	-	2/9/27/28	0/2/2/2
1	OMU	Aa	3305	1	-	2/9/27/28	0/2/2/2
1	OMC	Aa	2363	1	-	4/9/27/28	0/2/2/2
1	A2M	Aa	654	1	-	0/5/27/28	0/3/3/3
1	A2M	Aa	2218	1	-	0/5/27/28	0/3/3/3
1	A2M	Aa	2279	1	-	1/5/27/28	0/3/3/3
1	A2M	Aa	369	1	-	1/5/27/28	0/3/3/3
1	A2M	Aa	2319	1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	2286	1	-	0/5/27/28	0/3/3/3
1	OMC	Aa	2951	1	-	0/9/27/28	0/2/2/2
1	A2M	Aa	2949	46,1	-	1/5/27/28	0/3/3/3
1	A2M	Aa	940	1	-	0/5/27/28	0/3/3/3
3	OMG	Ac	75	3	-	2/5/27/28	0/3/3/3
1	OMC	Aa	1847	1	-	6/9/27/28	0/2/2/2
1	OMU	Aa	1061	1	-	2/9/27/28	0/2/2/2
1	A2M	Aa	811	1	-	0/5/27/28	0/3/3/3
1	PSU	Aa	995	1	-	2/7/25/26	0/2/2/2
1	OMC	Aa	2195	1,45	-	6/9/27/28	0/2/2/2
1	PSU	Aa	68	1	-	3/7/25/26	0/2/2/2
1	OMU	Aa	669	1	-	2/9/27/28	0/2/2/2
1	OMC	Aa	1441	1	-	3/9/27/28	0/2/2/2
1	OMG	Aa	2234	1	-	0/5/27/28	0/3/3/3
1	OMC	Aa	2839	1	-	3/9/27/28	0/2/2/2
1	PSU	Aa	378	1	-	2/7/25/26	0/2/2/2
1	OMC	Aa	1844	1	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	Aa	2223	1	-	2/7/25/26	0/2/2/2
1	OMC	Aa	2291	1	-	2/9/27/28	0/2/2/2
1	OMU	Aa	2345	1,45	-	2/9/27/28	0/2/2/2
1	OMG	Aa	2389	1	-	2/5/27/28	0/3/3/3
1	OMU	Aa	2653	1	-	2/9/27/28	0/2/2/2
1	OMG	Aa	809	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	2276	46,1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	1904	46,1,45	-	0/7/25/26	0/2/2/2
1	PSU	Aa	964	1	-	1/7/25/26	0/2/2/2
1	PSU	Aa	35	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	2873	1,45	-	4/7/25/26	0/2/2/2
1	OMC	Aa	1473	1	-	2/9/27/28	0/2/2/2
1	OMG	Aa	2393	1	-	0/5/27/28	0/3/3/3
1	PSU	Aa	2347	46,1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	1128	1	-	3/7/25/26	0/2/2/2
42	MLZ	Co	55	42	-	1/7/8/10	-
1	A2M	Aa	1868	46,1	-	2/5/27/28	0/3/3/3
1	OMG	Aa	3296	46,1	-	2/5/27/28	0/3/3/3
1	A2M	Aa	1453	46,1	-	0/5/27/28	0/3/3/3
1	OMU	Aa	48	1	-	3/9/27/28	0/2/2/2
1	PSU	Aa	1047	1	-	2/7/25/26	0/2/2/2
1	OMU	Aa	2720	1	-	2/9/27/28	0/2/2/2
1	A2M	Aa	2937	1	-	0/5/27/28	0/3/3/3
1	PSU	Aa	2829	1	-	3/7/25/26	0/2/2/2
1	PSU	Aa	823	1	-	0/7/25/26	0/2/2/2
1	PSU	Aa	2134	1	-	3/7/25/26	0/2/2/2
1	OMU	Aa	2419	1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	798	1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	2408	1	-	5/9/27/28	0/2/2/2
1	OMC	Aa	2335	1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	2732	1	-	2/9/27/28	0/2/2/2
1	OMG	Aa	2818	1	-	2/5/27/28	0/3/3/3
3	A2M	Ac	43	3	-	0/5/27/28	0/3/3/3
1	PSU	Aa	1009	1,45	-	2/7/25/26	0/2/2/2
1	PSU	Aa	1475	1	-	0/7/25/26	0/2/2/2
1	PSU	Aa	2316	46,1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	1852	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	1454	1	-	3/5/27/28	0/3/3/3
3	PSU	Ac	74	3	-	5/7/25/26	0/2/2/2
1	OMU	Aa	1889	1,45	-	0/9/27/28	0/2/2/2
1	A2M	Aa	880	1	-	0/5/27/28	0/3/3/3
1	OMU	Aa	2886	1	-	3/9/27/28	0/2/2/2
1	PSU	Aa	2857	1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	2883	1	-	0/7/25/26	0/2/2/2
1	PSU	Aa	2747	1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	3113	1	-	2/7/25/26	0/2/2/2
1	A2M	Aa	2914	1	-	2/5/27/28	0/3/3/3
1	PSU	Aa	2312	46,1,45	-	1/7/25/26	0/2/2/2
1	A2M	Aa	1137	46,1	-	0/5/27/28	0/3/3/3
5	HIC	CB	246	5	-	1/5/6/8	0/1/1/1
1	PSU	Aa	889	1	-	5/7/25/26	0/2/2/2
1	OMG	Aa	2622	1	-	3/5/27/28	0/3/3/3
1	OMC	Aa	2685	1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	144	1	-	1/9/27/28	0/2/2/2
1	PSU	Aa	1057	1	-	4/7/25/26	0/2/2/2
1	OMC	Aa	1857	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	2796	1	-	1/5/27/28	0/3/3/3
1	OMC	Aa	668	1	-	0/9/27/28	0/2/2/2
1	A2M	Aa	2124	1	-	0/5/27/28	0/3/3/3
1	PSU	Aa	2958	1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	2654	1	-	2/5/27/28	0/3/3/3
1	OMU	Aa	2738	1	-	0/9/27/28	0/2/2/2
1	PSU	Aa	2189	1	-	2/7/25/26	0/2/2/2
1	PSU	Aa	2995	1	-	5/7/25/26	0/2/2/2
1	OMG	Aa	2925	1	-	0/5/27/28	0/3/3/3
1	UR3	Aa	2956	1	-	1/7/25/26	0/2/2/2

All (900) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	650	1MA	C2-N3	14.25	1.46	1.29
1	Aa	2316	PSU	C6-C5	11.47	1.48	1.35
1	Aa	2926	PSU	C6-C5	11.38	1.48	1.35
1	Aa	964	PSU	C6-C5	11.12	1.48	1.35
1	Aa	2209	PSU	C6-C5	11.08	1.48	1.35
1	Aa	35	PSU	C6-C5	11.06	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1057	PSU	C6-C5	11.05	1.48	1.35
1	Aa	2857	PSU	C6-C5	11.01	1.48	1.35
1	Aa	889	PSU	C6-C5	11.00	1.48	1.35
1	Aa	1128	PSU	C6-C5	10.99	1.48	1.35
1	Aa	1009	PSU	C6-C5	10.99	1.48	1.35
1	Aa	2312	PSU	C6-C5	10.98	1.48	1.35
3	Ac	74	PSU	C6-C5	10.97	1.48	1.35
1	Aa	2715	PSU	C6-C5	10.96	1.48	1.35
1	Aa	2134	PSU	C6-C5	10.95	1.48	1.35
1	Aa	1047	PSU	C6-C5	10.93	1.48	1.35
1	Aa	2223	PSU	C6-C5	10.91	1.48	1.35
1	Aa	2189	PSU	C6-C5	10.89	1.48	1.35
1	Aa	1475	PSU	C6-C5	10.89	1.48	1.35
1	Aa	1127	PSU	C6-C5	10.88	1.48	1.35
1	Aa	2132	PSU	C6-C5	10.88	1.48	1.35
1	Aa	2947	PSU	C6-C5	10.88	1.48	1.35
1	Aa	2747	PSU	C6-C5	10.88	1.48	1.35
1	Aa	2868	PSU	C6-C5	10.85	1.47	1.35
1	Aa	995	PSU	C6-C5	10.84	1.47	1.35
1	Aa	378	PSU	C6-C5	10.84	1.47	1.35
1	Aa	2430	PSU	C6-C5	10.83	1.47	1.35
1	Aa	1126	PSU	C6-C5	10.82	1.47	1.35
1	Aa	1467	PSU	C6-C5	10.82	1.47	1.35
1	Aa	3113	PSU	C6-C5	10.78	1.47	1.35
1	Aa	2616	PSU	C6-C5	10.77	1.47	1.35
1	Aa	2347	PSU	C6-C5	10.75	1.47	1.35
1	Aa	2958	PSU	C6-C5	10.71	1.47	1.35
3	Ac	18	PSU	C6-C5	10.70	1.47	1.35
1	Aa	2518	PSU	C6-C5	10.68	1.47	1.35
1	Aa	1904	PSU	C6-C5	10.66	1.47	1.35
1	Aa	823	PSU	C6-C5	10.64	1.47	1.35
1	Aa	2414	PSU	C6-C5	10.59	1.47	1.35
1	Aa	2978	PSU	C6-C5	10.53	1.47	1.35
1	Aa	2995	PSU	C6-C5	10.52	1.47	1.35
1	Aa	2883	PSU	C6-C5	10.51	1.47	1.35
1	Aa	2829	PSU	C6-C5	10.45	1.47	1.35
1	Aa	68	PSU	C6-C5	10.23	1.47	1.35
1	Aa	2518	PSU	C2-N1	9.69	1.49	1.36
1	Aa	1009	PSU	C2-N1	9.63	1.49	1.36
1	Aa	964	PSU	C2-N1	9.50	1.49	1.36
1	Aa	2316	PSU	C2-N1	9.48	1.49	1.36
1	Aa	2189	PSU	C2-N1	9.46	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1128	PSU	C2-N1	9.46	1.49	1.36
1	Aa	1467	PSU	C2-N1	9.46	1.49	1.36
1	Aa	2926	PSU	C2-N1	9.45	1.49	1.36
1	Aa	2209	PSU	C2-N1	9.44	1.49	1.36
1	Aa	2857	PSU	C2-N1	9.42	1.49	1.36
1	Aa	2747	PSU	C2-N1	9.41	1.49	1.36
1	Aa	2715	PSU	C2-N1	9.40	1.49	1.36
1	Aa	2868	PSU	C2-N1	9.39	1.49	1.36
1	Aa	2347	PSU	C2-N1	9.38	1.49	1.36
1	Aa	2414	PSU	C2-N1	9.37	1.49	1.36
1	Aa	1047	PSU	C2-N1	9.35	1.49	1.36
1	Aa	2312	PSU	C2-N1	9.34	1.49	1.36
1	Aa	3113	PSU	C2-N1	9.34	1.49	1.36
1	Aa	889	PSU	C2-N1	9.33	1.49	1.36
3	Ac	74	PSU	C2-N1	9.31	1.49	1.36
1	Aa	35	PSU	C2-N1	9.31	1.49	1.36
1	Aa	823	PSU	C2-N1	9.30	1.49	1.36
1	Aa	2134	PSU	C2-N1	9.29	1.49	1.36
1	Aa	378	PSU	C2-N1	9.27	1.49	1.36
1	Aa	995	PSU	C2-N1	9.25	1.49	1.36
3	Ac	18	PSU	C2-N1	9.23	1.49	1.36
1	Aa	1126	PSU	C2-N1	9.22	1.49	1.36
1	Aa	2873	5MC	C6-C5	9.21	1.49	1.34
1	Aa	1127	PSU	C2-N1	9.20	1.49	1.36
1	Aa	2132	PSU	C2-N1	9.17	1.49	1.36
1	Aa	2829	PSU	C2-N1	9.16	1.49	1.36
1	Aa	2616	PSU	C2-N1	9.13	1.49	1.36
1	Aa	2995	PSU	C2-N1	9.11	1.49	1.36
1	Aa	1137	A2M	C3'-C4'	-9.11	1.29	1.53
1	Aa	2223	PSU	C2-N1	9.11	1.49	1.36
1	Aa	2947	PSU	C2-N1	9.10	1.49	1.36
1	Aa	2883	PSU	C2-N1	9.10	1.49	1.36
1	Aa	1475	PSU	C2-N1	9.06	1.49	1.36
1	Aa	2430	PSU	C2-N1	9.06	1.49	1.36
1	Aa	68	PSU	C2-N1	9.06	1.49	1.36
1	Aa	1057	PSU	C2-N1	9.05	1.49	1.36
1	Aa	2978	PSU	C2-N1	9.03	1.48	1.36
1	Aa	654	A2M	C3'-C4'	-9.01	1.30	1.53
1	Aa	2958	PSU	C2-N1	9.00	1.48	1.36
1	Aa	2319	A2M	C3'-C4'	-9.00	1.30	1.53
1	Aa	2276	5MC	C6-C5	8.99	1.49	1.34
1	Aa	1904	PSU	C2-N1	8.96	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	3108	A2M	C3'-C4'	-8.91	1.30	1.53
1	Aa	821	A2M	C3'-C4'	-8.86	1.30	1.53
1	Aa	2218	A2M	C3'-C4'	-8.85	1.30	1.53
1	Aa	940	A2M	C3'-C4'	-8.84	1.30	1.53
1	Aa	1868	A2M	C3'-C4'	-8.83	1.30	1.53
1	Aa	811	A2M	C3'-C4'	-8.83	1.30	1.53
1	Aa	2124	A2M	C3'-C4'	-8.80	1.30	1.53
1	Aa	2914	A2M	C3'-C4'	-8.80	1.30	1.53
1	Aa	1453	A2M	C3'-C4'	-8.77	1.30	1.53
1	Aa	2937	A2M	C3'-C4'	-8.76	1.30	1.53
1	Aa	2949	A2M	C3'-C4'	-8.72	1.30	1.53
1	Aa	369	A2M	C3'-C4'	-8.71	1.30	1.53
3	Ac	43	A2M	C3'-C4'	-8.65	1.30	1.53
1	Aa	2643	A2M	C3'-C4'	-8.63	1.30	1.53
1	Aa	880	A2M	C3'-C4'	-8.61	1.31	1.53
1	Aa	1371	A2M	C3'-C4'	-8.54	1.31	1.53
1	Aa	2279	A2M	C3'-C4'	-8.30	1.31	1.53
1	Aa	2279	A2M	O4'-C1'	-8.27	1.29	1.41
1	Aa	2124	A2M	O4'-C4'	7.73	1.62	1.45
1	Aa	2218	A2M	O4'-C4'	7.71	1.62	1.45
3	Ac	43	A2M	O4'-C4'	7.71	1.62	1.45
1	Aa	2949	A2M	O4'-C4'	7.69	1.62	1.45
1	Aa	654	A2M	O4'-C4'	7.68	1.62	1.45
1	Aa	3108	A2M	O4'-C4'	7.67	1.62	1.45
1	Aa	3305	OMU	C2-N1	7.67	1.50	1.38
1	Aa	2319	A2M	O4'-C4'	7.64	1.62	1.45
1	Aa	654	A2M	O4'-C1'	-7.62	1.30	1.41
1	Aa	669	OMU	C2-N1	7.58	1.50	1.38
1	Aa	2643	A2M	O4'-C4'	7.56	1.61	1.45
1	Aa	1137	A2M	O4'-C4'	7.56	1.61	1.45
1	Aa	2279	A2M	O4'-C4'	7.55	1.61	1.45
1	Aa	1371	A2M	O4'-C4'	7.55	1.61	1.45
1	Aa	1868	A2M	O4'-C4'	7.53	1.61	1.45
1	Aa	880	A2M	O4'-C4'	7.53	1.61	1.45
1	Aa	2345	OMU	C2-N1	7.52	1.50	1.38
1	Aa	940	A2M	O4'-C4'	7.51	1.61	1.45
1	Aa	2653	OMU	C2-N1	7.47	1.50	1.38
1	Aa	1453	A2M	O4'-C4'	7.46	1.61	1.45
1	Aa	2937	A2M	O4'-C4'	7.46	1.61	1.45
1	Aa	811	A2M	O4'-C1'	-7.46	1.30	1.41
1	Aa	1061	OMU	C2-N1	7.44	1.50	1.38
1	Aa	2924	OMU	C2-N1	7.43	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2914	A2M	O4'-C1'	-7.42	1.30	1.41
1	Aa	940	A2M	O4'-C1'	-7.41	1.30	1.41
1	Aa	880	A2M	O4'-C1'	-7.39	1.30	1.41
1	Aa	2720	OMU	C2-N1	7.39	1.50	1.38
1	Aa	821	A2M	O4'-C4'	7.39	1.61	1.45
1	Aa	1371	A2M	O4'-C1'	-7.38	1.30	1.41
1	Aa	369	A2M	O4'-C4'	7.37	1.61	1.45
1	Aa	2419	OMU	C2-N1	7.36	1.50	1.38
3	Ac	43	A2M	O4'-C1'	-7.35	1.30	1.41
1	Aa	1137	A2M	O4'-C1'	-7.32	1.30	1.41
1	Aa	811	A2M	O4'-C4'	7.31	1.61	1.45
1	Aa	2914	A2M	O4'-C4'	7.30	1.61	1.45
1	Aa	2937	A2M	O4'-C1'	-7.28	1.30	1.41
1	Aa	68	PSU	C2-N3	7.27	1.50	1.37
1	Aa	821	A2M	O4'-C1'	-7.27	1.30	1.41
1	Aa	2312	PSU	C2-N3	7.24	1.49	1.37
1	Aa	2886	OMU	C2-N1	7.21	1.50	1.38
1	Aa	1868	A2M	O4'-C1'	-7.20	1.31	1.41
1	Aa	2643	A2M	O4'-C1'	-7.19	1.31	1.41
1	Aa	1453	A2M	O4'-C1'	-7.19	1.31	1.41
1	Aa	369	A2M	O4'-C1'	-7.17	1.31	1.41
1	Aa	2926	PSU	C2-N3	7.15	1.49	1.37
1	Aa	964	PSU	C2-N3	7.13	1.49	1.37
1	Aa	48	OMU	C2-N1	7.12	1.49	1.38
1	Aa	2223	PSU	C2-N3	7.08	1.49	1.37
1	Aa	1047	PSU	C2-N3	7.03	1.49	1.37
1	Aa	2408	OMU	C2-N1	7.01	1.49	1.38
1	Aa	1475	PSU	C2-N3	7.01	1.49	1.37
1	Aa	2218	A2M	O4'-C1'	-6.99	1.31	1.41
1	Aa	2124	A2M	O4'-C1'	-6.99	1.31	1.41
1	Aa	2319	A2M	O4'-C1'	-6.99	1.31	1.41
3	Ac	18	PSU	C2-N3	6.98	1.49	1.37
1	Aa	1128	PSU	C2-N3	6.96	1.49	1.37
1	Aa	3108	A2M	O4'-C1'	-6.96	1.31	1.41
1	Aa	2978	PSU	C2-N3	6.94	1.49	1.37
1	Aa	1127	PSU	C2-N3	6.92	1.49	1.37
1	Aa	2189	PSU	C2-N3	6.91	1.49	1.37
1	Aa	2616	PSU	C2-N3	6.91	1.49	1.37
1	Aa	1889	OMU	C2-N1	6.90	1.49	1.38
1	Aa	2715	PSU	C2-N3	6.88	1.49	1.37
1	Aa	2949	A2M	O4'-C1'	-6.88	1.31	1.41
1	Aa	2209	PSU	C2-N3	6.87	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	35	PSU	C2-N3	6.87	1.49	1.37
1	Aa	2958	PSU	C2-N3	6.87	1.49	1.37
1	Aa	2883	PSU	C2-N3	6.85	1.49	1.37
1	Aa	1057	PSU	C2-N3	6.85	1.49	1.37
1	Aa	2111	OMU	C2-N1	6.80	1.49	1.38
1	Aa	2316	PSU	C2-N3	6.78	1.49	1.37
1	Aa	2738	OMU	C2-N1	6.77	1.49	1.38
1	Aa	1904	PSU	C2-N3	6.76	1.49	1.37
1	Aa	2956	UR3	C2-N1	6.75	1.48	1.38
1	Aa	1467	PSU	C2-N3	6.75	1.49	1.37
1	Aa	2995	PSU	C2-N3	6.75	1.49	1.37
1	Aa	798	OMU	C2-N1	6.74	1.49	1.38
1	Aa	1009	PSU	C2-N3	6.74	1.49	1.37
1	Aa	2430	PSU	C2-N3	6.74	1.49	1.37
1	Aa	2132	PSU	C2-N3	6.73	1.49	1.37
1	Aa	2732	OMU	C2-N1	6.73	1.49	1.38
3	Ac	74	PSU	C2-N3	6.71	1.49	1.37
1	Aa	2857	PSU	C2-N3	6.69	1.49	1.37
1	Aa	378	PSU	C2-N3	6.65	1.48	1.37
1	Aa	2868	PSU	C2-N3	6.64	1.48	1.37
1	Aa	2956	UR3	C6-C5	6.61	1.50	1.35
1	Aa	144	OMU	C2-N1	6.60	1.49	1.38
1	Aa	995	PSU	C2-N3	6.59	1.48	1.37
1	Aa	2732	OMU	C2-N3	6.59	1.49	1.38
1	Aa	3305	OMU	C2-N3	6.57	1.49	1.38
1	Aa	2111	OMU	C2-N3	6.57	1.49	1.38
1	Aa	3113	PSU	C2-N3	6.56	1.48	1.37
1	Aa	2947	PSU	C2-N3	6.55	1.48	1.37
1	Aa	2738	OMU	C2-N3	6.53	1.49	1.38
1	Aa	823	PSU	C2-N3	6.52	1.48	1.37
1	Aa	1126	PSU	C2-N3	6.50	1.48	1.37
1	Aa	2747	PSU	C2-N3	6.48	1.48	1.37
1	Aa	2886	OMU	C2-N3	6.46	1.49	1.38
1	Aa	2345	OMU	C2-N3	6.41	1.49	1.38
1	Aa	1061	OMU	C2-N3	6.40	1.49	1.38
1	Aa	2347	PSU	C2-N3	6.39	1.48	1.37
1	Aa	144	OMU	C2-N3	6.37	1.49	1.38
1	Aa	48	OMU	C2-N3	6.36	1.49	1.38
1	Aa	669	OMU	C2-N3	6.34	1.49	1.38
1	Aa	1889	OMU	C2-N3	6.32	1.49	1.38
1	Aa	2653	OMU	C2-N3	6.31	1.49	1.38
1	Aa	2829	PSU	C2-N3	6.30	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2518	PSU	C2-N3	6.30	1.48	1.37
1	Aa	2720	OMU	C2-N3	6.29	1.49	1.38
1	Aa	2134	PSU	C2-N3	6.28	1.48	1.37
1	Aa	2419	OMU	C2-N3	6.27	1.49	1.38
1	Aa	2924	OMU	C2-N3	6.25	1.49	1.38
1	Aa	798	OMU	C2-N3	6.25	1.49	1.38
1	Aa	889	PSU	C2-N3	6.24	1.48	1.37
1	Aa	1847	OMC	C2-N3	6.20	1.48	1.36
1	Aa	2685	OMC	C2-N3	6.19	1.48	1.36
1	Aa	2414	PSU	C2-N3	6.18	1.48	1.37
1	Aa	2276	5MC	C4-N3	6.15	1.44	1.34
1	Aa	1441	OMC	C2-N3	6.12	1.48	1.36
1	Aa	2291	OMC	C2-N3	6.11	1.48	1.36
1	Aa	2195	OMC	C6-C5	6.11	1.49	1.35
1	Aa	2839	OMC	C2-N3	6.10	1.48	1.36
1	Aa	2962	OMC	C2-N3	6.10	1.48	1.36
1	Aa	668	OMC	C2-N3	6.07	1.48	1.36
1	Aa	1473	OMC	C2-N3	6.02	1.48	1.36
1	Aa	1847	OMC	C6-C5	6.01	1.49	1.35
1	Aa	2951	OMC	C2-N3	5.98	1.48	1.36
1	Aa	1512	OMC	C2-N3	5.96	1.48	1.36
1	Aa	2335	OMC	C2-N3	5.96	1.48	1.36
1	Aa	2291	OMC	C6-C5	5.94	1.48	1.35
1	Aa	1530	OMC	C2-N3	5.93	1.48	1.36
1	Aa	2685	OMC	C6-C5	5.91	1.48	1.35
1	Aa	2408	OMU	C2-N3	5.89	1.48	1.38
1	Aa	1844	OMC	C2-N3	5.88	1.48	1.36
1	Aa	2839	OMC	C6-C5	5.87	1.48	1.35
1	Aa	2882	OMC	C6-C5	5.87	1.48	1.35
1	Aa	1473	OMC	C6-C5	5.86	1.48	1.35
1	Aa	2195	OMC	C2-N3	5.84	1.48	1.36
1	Aa	1530	OMC	C6-C5	5.82	1.48	1.35
1	Aa	2882	OMC	C2-N3	5.81	1.48	1.36
1	Aa	2962	OMC	C6-C5	5.80	1.48	1.35
1	Aa	1857	OMC	C2-N3	5.80	1.48	1.36
1	Aa	2363	OMC	C2-N3	5.78	1.48	1.36
1	Aa	2276	5MC	C2-N3	5.77	1.48	1.36
1	Aa	1512	OMC	C6-C5	5.76	1.48	1.35
1	Aa	2951	OMC	C6-C5	5.72	1.48	1.35
1	Aa	1857	OMC	C6-C5	5.70	1.48	1.35
1	Aa	668	OMC	C6-C5	5.70	1.48	1.35
1	Aa	2335	OMC	C6-C5	5.68	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2363	OMC	C6-C5	5.64	1.48	1.35
1	Aa	2111	OMU	C6-C5	5.62	1.48	1.35
1	Aa	2924	OMU	C6-C5	5.62	1.48	1.35
1	Aa	144	OMU	C6-C5	5.61	1.48	1.35
1	Aa	2956	UR3	C2-N3	5.59	1.49	1.39
1	Aa	2419	OMU	C6-C5	5.57	1.48	1.35
1	Aa	1844	OMC	C6-C5	5.55	1.48	1.35
1	Aa	2738	OMU	C6-C5	5.51	1.47	1.35
1	Aa	1441	OMC	C6-C5	5.49	1.47	1.35
1	Aa	2234	OMG	C2-N3	5.48	1.46	1.33
1	Aa	2873	5MC	C4-N3	5.46	1.43	1.34
1	Aa	1061	OMU	C6-C5	5.46	1.47	1.35
1	Aa	798	OMU	C6-C5	5.44	1.47	1.35
1	Aa	1889	OMU	C6-C5	5.43	1.47	1.35
1	Aa	48	OMU	C6-C5	5.39	1.47	1.35
1	Aa	2286	OMG	C2-N3	5.37	1.46	1.33
1	Aa	2886	OMU	C6-C5	5.37	1.47	1.35
1	Aa	2653	OMU	C6-C5	5.36	1.47	1.35
1	Aa	2720	OMU	C6-C5	5.36	1.47	1.35
3	Ac	75	OMG	C2-N3	5.35	1.46	1.33
1	Aa	2732	OMU	C6-C5	5.35	1.47	1.35
1	Aa	669	OMU	C6-C5	5.32	1.47	1.35
1	Aa	2121	OMG	C2-N3	5.32	1.46	1.33
1	Aa	2345	OMU	C6-C5	5.32	1.47	1.35
1	Aa	2408	OMU	C6-C5	5.32	1.47	1.35
1	Aa	912	OMG	C2-N3	5.28	1.46	1.33
1	Aa	2794	OMG	C2-N3	5.25	1.45	1.33
1	Aa	2873	5MC	C2-N3	5.25	1.47	1.36
1	Aa	2389	OMG	C2-N3	5.25	1.45	1.33
1	Aa	2796	OMG	C2-N3	5.24	1.45	1.33
1	Aa	2925	OMG	C2-N3	5.24	1.45	1.33
1	Aa	2393	OMG	C2-N3	5.23	1.45	1.33
1	Aa	1852	OMG	C2-N3	5.22	1.45	1.33
1	Aa	2857	PSU	C6-N1	5.21	1.44	1.36
1	Aa	3113	PSU	C6-N1	5.21	1.44	1.36
1	Aa	2818	OMG	C2-N3	5.21	1.45	1.33
1	Aa	2622	OMG	C2-N3	5.21	1.45	1.33
1	Aa	2407	OMG	C2-N3	5.20	1.45	1.33
1	Aa	3296	OMG	C2-N3	5.19	1.45	1.33
1	Aa	2122	OMG	C2-N3	5.18	1.45	1.33
1	Aa	2518	PSU	C6-N1	5.18	1.44	1.36
1	Aa	2920	OMG	C2-N3	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2312	PSU	C6-N1	5.17	1.44	1.36
1	Aa	809	OMG	C2-N3	5.15	1.45	1.33
1	Aa	964	PSU	C6-N1	5.11	1.44	1.36
1	Aa	1467	PSU	C6-N1	5.08	1.44	1.36
1	Aa	2715	PSU	C6-N1	5.08	1.44	1.36
1	Aa	2616	PSU	C6-N1	5.08	1.44	1.36
1	Aa	2347	PSU	C6-N1	5.08	1.44	1.36
1	Aa	1454	OMG	C2-N3	5.07	1.45	1.33
1	Aa	1057	PSU	C6-N1	5.06	1.44	1.36
1	Aa	1844	OMC	C2-N1	5.06	1.51	1.40
3	Ac	74	PSU	C6-N1	5.05	1.44	1.36
1	Aa	2209	PSU	C6-N1	5.04	1.44	1.36
1	Aa	2654	OMG	C2-N3	5.03	1.45	1.33
1	Aa	3305	OMU	C6-C5	5.03	1.46	1.35
1	Aa	2747	PSU	C6-N1	5.01	1.44	1.36
1	Aa	2868	PSU	C6-N1	5.00	1.44	1.36
1	Aa	2926	PSU	C6-N1	5.00	1.44	1.36
1	Aa	1009	PSU	C6-N1	5.00	1.44	1.36
1	Aa	2958	PSU	C6-N1	4.98	1.44	1.36
1	Aa	889	PSU	C6-N1	4.97	1.44	1.36
1	Aa	1441	OMC	C2-N1	4.97	1.50	1.40
1	Aa	2189	PSU	C6-N1	4.95	1.44	1.36
1	Aa	2134	PSU	C6-N1	4.94	1.44	1.36
1	Aa	1473	OMC	C4-N3	4.91	1.44	1.34
5	CB	246	HIC	CD2-NE2	-4.90	1.30	1.38
1	Aa	2829	PSU	C6-N1	4.89	1.44	1.36
1	Aa	1475	PSU	C6-N1	4.88	1.44	1.36
1	Aa	378	PSU	C6-N1	4.87	1.44	1.36
1	Aa	650	1MA	C2-N1	4.86	1.44	1.35
1	Aa	2316	PSU	C6-N1	4.86	1.44	1.36
1	Aa	1047	PSU	C6-N1	4.86	1.44	1.36
1	Aa	2685	OMC	C4-N3	4.84	1.44	1.34
1	Aa	1126	PSU	C6-N1	4.84	1.44	1.36
1	Aa	35	PSU	C6-N1	4.83	1.44	1.36
1	Aa	2223	PSU	C6-N1	4.83	1.44	1.36
1	Aa	1473	OMC	C4-N4	4.81	1.45	1.33
1	Aa	2685	OMC	C4-N4	4.81	1.45	1.33
1	Aa	1530	OMC	C4-N3	4.80	1.44	1.34
1	Aa	2951	OMC	C4-N3	4.79	1.44	1.34
1	Aa	2995	PSU	C6-N1	4.79	1.44	1.36
1	Aa	1127	PSU	C6-N1	4.78	1.44	1.36
1	Aa	2132	PSU	C6-N1	4.78	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1847	OMC	C4-N3	4.78	1.44	1.34
1	Aa	1857	OMC	C4-N3	4.78	1.44	1.34
1	Aa	2947	PSU	C6-N1	4.77	1.44	1.36
1	Aa	2962	OMC	C4-N3	4.77	1.44	1.34
1	Aa	2839	OMC	C2-N1	4.77	1.50	1.40
1	Aa	2121	OMG	C4-N3	4.76	1.48	1.37
1	Aa	995	PSU	C6-N1	4.75	1.44	1.36
1	Aa	1847	OMC	C4-N4	4.75	1.45	1.33
1	Aa	2839	OMC	C4-N4	4.75	1.45	1.33
1	Aa	2883	PSU	C6-N1	4.74	1.44	1.36
1	Aa	2286	OMG	C4-N3	4.74	1.48	1.37
3	Ac	18	PSU	C6-N1	4.72	1.44	1.36
1	Aa	2234	OMG	C4-N3	4.71	1.48	1.37
3	Ac	75	OMG	C4-N3	4.71	1.48	1.37
1	Aa	2335	OMC	C4-N3	4.70	1.44	1.34
1	Aa	2195	OMC	C4-N4	4.70	1.45	1.33
1	Aa	2978	PSU	C6-N1	4.70	1.44	1.36
1	Aa	1128	PSU	C6-N1	4.70	1.44	1.36
1	Aa	668	OMC	C4-N4	4.69	1.45	1.33
1	Aa	2794	OMG	C4-N3	4.69	1.48	1.37
1	Aa	2291	OMC	C4-N4	4.69	1.45	1.33
1	Aa	1847	OMC	C2-N1	4.69	1.50	1.40
1	Aa	2430	PSU	C6-N1	4.69	1.44	1.36
1	Aa	2363	OMC	C2-N1	4.69	1.50	1.40
1	Aa	2882	OMC	C4-N4	4.68	1.44	1.33
1	Aa	2291	OMC	C4-N3	4.67	1.43	1.34
1	Aa	809	OMG	C4-N3	4.66	1.48	1.37
1	Aa	2291	OMC	C2-N1	4.66	1.50	1.40
1	Aa	912	OMG	C4-N3	4.66	1.48	1.37
1	Aa	2393	OMG	C4-N3	4.65	1.48	1.37
1	Aa	668	OMC	C4-N3	4.65	1.43	1.34
1	Aa	1852	OMG	C4-N3	4.64	1.48	1.37
1	Aa	1844	OMC	C4-N4	4.64	1.44	1.33
1	Aa	823	PSU	C6-N1	4.63	1.43	1.36
1	Aa	2335	OMC	C4-N4	4.63	1.44	1.33
1	Aa	2276	5MC	C6-N1	4.63	1.45	1.38
1	Aa	2389	OMG	C4-N3	4.62	1.48	1.37
1	Aa	2962	OMC	C4-N4	4.61	1.44	1.33
1	Aa	2882	OMC	C4-N3	4.61	1.43	1.34
1	Aa	2951	OMC	C4-N4	4.61	1.44	1.33
1	Aa	2796	OMG	C4-N3	4.61	1.48	1.37
1	Aa	1441	OMC	C4-N4	4.60	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2195	OMC	C4-N3	4.59	1.43	1.34
1	Aa	1857	OMC	C4-N4	4.59	1.44	1.33
1	Aa	2920	OMG	C4-N3	4.58	1.48	1.37
1	Aa	2122	OMG	C4-N3	4.58	1.48	1.37
1	Aa	1454	OMG	C4-N3	4.58	1.48	1.37
1	Aa	2654	OMG	C4-N3	4.58	1.48	1.37
1	Aa	2818	OMG	C4-N3	4.57	1.48	1.37
1	Aa	2925	OMG	C4-N3	4.57	1.48	1.37
1	Aa	2407	OMG	C4-N3	4.57	1.48	1.37
1	Aa	2951	OMC	C2-N1	4.57	1.49	1.40
1	Aa	1530	OMC	C4-N4	4.57	1.44	1.33
1	Aa	68	PSU	C6-N1	4.56	1.43	1.36
1	Aa	2622	OMG	C4-N3	4.56	1.48	1.37
1	Aa	1512	OMC	C4-N3	4.56	1.43	1.34
1	Aa	1512	OMC	C4-N4	4.55	1.44	1.33
1	Aa	2363	OMC	C4-N4	4.55	1.44	1.33
1	Aa	2414	PSU	C6-N1	4.54	1.43	1.36
1	Aa	3296	OMG	C4-N3	4.53	1.48	1.37
1	Aa	2839	OMC	C4-N3	4.52	1.43	1.34
1	Aa	2882	OMC	C2-N1	4.42	1.49	1.40
1	Aa	2873	5MC	C6-N1	4.41	1.45	1.38
1	Aa	2685	OMC	C2-N1	4.41	1.49	1.40
1	Aa	1844	OMC	C4-N3	4.40	1.43	1.34
1	Aa	1512	OMC	C2-N1	4.36	1.49	1.40
1	Aa	1441	OMC	C4-N3	4.34	1.43	1.34
1	Aa	1473	OMC	C2-N1	4.30	1.49	1.40
1	Aa	2962	OMC	C2-N1	4.28	1.49	1.40
1	Aa	1857	OMC	C2-N1	4.24	1.49	1.40
1	Aa	1904	PSU	C6-N1	4.24	1.43	1.36
1	Aa	2276	5MC	C2-N1	4.16	1.49	1.40
1	Aa	668	OMC	C2-N1	4.15	1.49	1.40
1	Aa	2873	5MC	C4-N4	4.12	1.44	1.34
1	Aa	2738	OMU	C4-N3	4.12	1.45	1.38
1	Aa	2363	OMC	C4-N3	4.09	1.42	1.34
1	Aa	1530	OMC	C2-N1	4.09	1.48	1.40
1	Aa	2335	OMC	C2-N1	4.07	1.48	1.40
1	Aa	2276	5MC	C4-N4	4.05	1.44	1.34
1	Aa	2111	OMU	C4-N3	3.99	1.45	1.38
1	Aa	2195	OMC	C2-N1	3.98	1.48	1.40
1	Aa	2732	OMU	C4-N3	3.97	1.45	1.38
1	Aa	2886	OMU	C4-N3	3.93	1.45	1.38
1	Aa	2234	OMG	C2-N2	3.93	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	144	OMU	C4-N3	3.90	1.45	1.38
1	Aa	2925	OMG	C2-N2	3.87	1.43	1.34
1	Aa	2873	5MC	C2-N1	3.85	1.48	1.40
1	Aa	2363	OMC	O2-C2	-3.84	1.16	1.23
1	Aa	2286	OMG	C2-N2	3.83	1.43	1.34
1	Aa	2407	OMG	C2-N2	3.83	1.43	1.34
1	Aa	3296	OMG	C2-N2	3.83	1.43	1.34
1	Aa	2794	OMG	C2-N2	3.81	1.43	1.34
1	Aa	2389	OMG	C2-N2	3.81	1.43	1.34
1	Aa	2796	OMG	C2-N2	3.80	1.43	1.34
1	Aa	2818	OMG	C2-N2	3.78	1.43	1.34
1	Aa	1454	OMG	C2-N2	3.78	1.43	1.34
1	Aa	809	OMG	C2-N2	3.78	1.43	1.34
3	Ac	75	OMG	C2-N2	3.77	1.43	1.34
1	Aa	650	1MA	C4-N3	3.77	1.49	1.37
1	Aa	2622	OMG	C2-N2	3.76	1.43	1.34
1	Aa	798	OMU	C4-N3	3.75	1.45	1.38
1	Aa	2121	OMG	C2-N2	3.74	1.43	1.34
1	Aa	2122	OMG	C2-N2	3.73	1.43	1.34
1	Aa	2883	PSU	C4-N3	3.71	1.45	1.38
1	Aa	912	OMG	C2-N2	3.71	1.43	1.34
1	Aa	2653	OMU	C4-N3	3.70	1.45	1.38
1	Aa	2312	PSU	C4-N3	3.70	1.45	1.38
1	Aa	2654	OMG	C2-N2	3.69	1.43	1.34
1	Aa	889	PSU	O4-C4	-3.68	1.16	1.23
1	Aa	2926	PSU	C4-N3	3.68	1.45	1.38
1	Aa	2408	OMU	O2-C2	-3.68	1.16	1.23
1	Aa	68	PSU	C4-N3	3.67	1.45	1.38
1	Aa	2920	OMG	C2-N2	3.66	1.42	1.34
1	Aa	2393	OMG	C2-N2	3.66	1.42	1.34
1	Aa	1889	OMU	C4-N3	3.66	1.45	1.38
1	Aa	1047	PSU	C4-N3	3.65	1.45	1.38
1	Aa	3305	OMU	C4-N3	3.64	1.45	1.38
1	Aa	48	OMU	C4-N3	3.64	1.45	1.38
1	Aa	2189	PSU	C4-N3	3.63	1.45	1.38
1	Aa	1128	PSU	C4-N3	3.60	1.45	1.38
1	Aa	1852	OMG	C2-N2	3.60	1.42	1.34
1	Aa	2654	OMG	C6-N1	3.59	1.43	1.37
1	Aa	964	PSU	C4-N3	3.59	1.45	1.38
1	Aa	2223	PSU	C4-N3	3.56	1.45	1.38
1	Aa	2234	OMG	C6-N1	3.56	1.43	1.37
1	Aa	2518	PSU	O4-C4	-3.55	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1057	PSU	C4-N3	3.55	1.45	1.38
1	Aa	2995	PSU	C4-N3	3.55	1.45	1.38
1	Aa	3113	PSU	O4-C4	-3.54	1.16	1.23
1	Aa	2345	OMU	C4-N3	3.54	1.44	1.38
1	Aa	2209	PSU	C4-N3	3.54	1.45	1.38
1	Aa	2715	PSU	C4-N3	3.53	1.45	1.38
1	Aa	2419	OMU	C4-N3	3.53	1.44	1.38
1	Aa	1889	OMU	O4-C4	-3.51	1.17	1.24
1	Aa	2924	OMU	C4-N3	3.50	1.44	1.38
3	Ac	75	OMG	C6-N1	3.50	1.43	1.37
1	Aa	3296	OMG	C6-N1	3.49	1.43	1.37
1	Aa	2286	OMG	C6-N1	3.48	1.43	1.37
1	Aa	1127	PSU	C4-N3	3.48	1.45	1.38
1	Aa	2132	PSU	C4-N3	3.48	1.45	1.38
1	Aa	2868	PSU	C4-N3	3.47	1.45	1.38
1	Aa	1904	PSU	C4-N3	3.47	1.45	1.38
1	Aa	2925	OMG	C6-N1	3.46	1.43	1.37
1	Aa	2978	PSU	C4-N3	3.46	1.45	1.38
1	Aa	995	PSU	C4-N3	3.44	1.45	1.38
1	Aa	2962	OMC	C6-N1	3.44	1.46	1.38
1	Aa	1061	OMU	C4-N3	3.43	1.44	1.38
1	Aa	2616	PSU	C4-N3	3.42	1.45	1.38
1	Aa	48	OMU	O4-C4	-3.42	1.17	1.24
1	Aa	2873	5MC	O2-C2	-3.42	1.17	1.23
1	Aa	2958	PSU	C4-N3	3.41	1.45	1.38
1	Aa	1126	PSU	C4-N3	3.40	1.45	1.38
1	Aa	912	OMG	C6-N1	3.40	1.42	1.37
1	Aa	2134	PSU	O4-C4	-3.39	1.17	1.23
1	Aa	378	PSU	C4-N3	3.39	1.45	1.38
1	Aa	2857	PSU	C4-N3	3.39	1.45	1.38
1	Aa	2347	PSU	C4-N3	3.39	1.45	1.38
1	Aa	2857	PSU	O4-C4	-3.38	1.17	1.23
1	Aa	2345	OMU	O4-C4	-3.37	1.17	1.24
1	Aa	2794	OMG	C6-N1	3.37	1.42	1.37
1	Aa	2732	OMU	O4-C4	-3.37	1.18	1.24
1	Aa	2430	PSU	C4-N3	3.36	1.45	1.38
1	Aa	2616	PSU	O4-C4	-3.36	1.17	1.23
3	Ac	74	PSU	C4-N3	3.35	1.45	1.38
1	Aa	1009	PSU	C4-N3	3.35	1.45	1.38
1	Aa	2414	PSU	O4-C4	-3.34	1.17	1.23
1	Aa	1475	PSU	C4-N3	3.34	1.45	1.38
3	Ac	18	PSU	C4-N3	3.32	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	798	OMU	O4-C4	-3.32	1.18	1.24
1	Aa	1467	PSU	C4-N3	3.32	1.45	1.38
1	Aa	669	OMU	C4-N3	3.31	1.44	1.38
1	Aa	2393	OMG	C6-N1	3.31	1.42	1.37
1	Aa	2121	OMG	C6-N1	3.30	1.42	1.37
1	Aa	2796	OMG	C6-N1	3.30	1.42	1.37
1	Aa	1126	PSU	O4-C4	-3.30	1.17	1.23
1	Aa	2408	OMU	O4-C4	-3.29	1.18	1.24
1	Aa	2747	PSU	C4-N3	3.29	1.44	1.38
1	Aa	2622	OMG	C6-N1	3.29	1.42	1.37
1	Aa	2924	OMU	O4-C4	-3.28	1.18	1.24
1	Aa	2839	OMC	O2-C2	-3.28	1.17	1.23
1	Aa	2720	OMU	O4-C4	-3.28	1.18	1.24
1	Aa	3305	OMU	O4-C4	-3.27	1.18	1.24
1	Aa	2920	OMG	C6-N1	3.27	1.42	1.37
1	Aa	2291	OMC	O2-C2	-3.27	1.17	1.23
1	Aa	1454	OMG	C6-N1	3.26	1.42	1.37
1	Aa	2316	PSU	C4-N3	3.26	1.44	1.38
1	Aa	2720	OMU	O2-C2	-3.24	1.17	1.23
1	Aa	889	PSU	C4-N3	3.23	1.44	1.38
1	Aa	378	PSU	O4-C4	-3.23	1.17	1.23
1	Aa	1061	OMU	O4-C4	-3.22	1.18	1.24
1	Aa	2886	OMU	O4-C4	-3.22	1.18	1.24
1	Aa	144	OMU	O4-C4	-3.21	1.18	1.24
1	Aa	2407	OMG	C6-N1	3.21	1.42	1.37
1	Aa	2951	OMC	C6-N1	3.20	1.45	1.38
1	Aa	1844	OMC	O2-C2	-3.20	1.17	1.23
1	Aa	2122	OMG	C6-N1	3.20	1.42	1.37
1	Aa	669	OMU	O2-C2	-3.20	1.17	1.23
1	Aa	2956	UR3	C6-N1	3.19	1.45	1.38
1	Aa	2829	PSU	C4-N3	3.19	1.44	1.38
1	Aa	809	OMG	C6-N1	3.19	1.42	1.37
1	Aa	3113	PSU	C4-N3	3.19	1.44	1.38
1	Aa	35	PSU	C4-N3	3.17	1.44	1.38
1	Aa	2747	PSU	O4-C4	-3.17	1.17	1.23
1	Aa	2720	OMU	C4-N3	3.17	1.44	1.38
1	Aa	669	OMU	O4-C4	-3.16	1.18	1.24
1	Aa	2947	PSU	C4-N3	3.16	1.44	1.38
1	Aa	2347	PSU	O4-C4	-3.15	1.17	1.23
1	Aa	668	OMC	C6-N1	3.15	1.45	1.38
1	Aa	2685	OMC	C6-N1	3.15	1.45	1.38
1	Aa	2518	PSU	C4-N3	3.14	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1530	OMC	C6-N1	3.13	1.45	1.38
1	Aa	2818	OMG	C6-N1	3.13	1.42	1.37
1	Aa	2738	OMU	O4-C4	-3.13	1.18	1.24
1	Aa	823	PSU	O4-C4	-3.13	1.17	1.23
1	Aa	2195	OMC	O2-C2	-3.13	1.17	1.23
1	Aa	823	PSU	C4-N3	3.12	1.44	1.38
1	Aa	2335	OMC	O2-C2	-3.12	1.17	1.23
1	Aa	2653	OMU	O4-C4	-3.12	1.18	1.24
1	Aa	2419	OMU	O4-C4	-3.11	1.18	1.24
1	Aa	2882	OMC	C6-N1	3.11	1.45	1.38
1	Aa	2947	PSU	O4-C4	-3.10	1.17	1.23
1	Aa	2653	OMU	O2-C2	-3.09	1.17	1.23
1	Aa	2122	OMG	C5-C6	3.09	1.53	1.47
1	Aa	369	A2M	C6-N6	3.08	1.45	1.34
1	Aa	2134	PSU	C4-N3	3.08	1.44	1.38
1	Aa	2829	PSU	O4-C4	-3.08	1.17	1.23
1	Aa	2276	5MC	O2-C2	-3.07	1.18	1.23
1	Aa	821	A2M	C6-N6	3.07	1.45	1.34
1	Aa	2951	OMC	O2-C2	-3.07	1.18	1.23
1	Aa	1061	OMU	O2-C2	-3.07	1.17	1.23
1	Aa	1512	OMC	O2-C2	-3.07	1.18	1.23
1	Aa	1857	OMC	C6-N1	3.07	1.45	1.38
1	Aa	35	PSU	O4-C4	-3.06	1.17	1.23
1	Aa	1473	OMC	C6-N1	3.06	1.45	1.38
1	Aa	1868	A2M	C6-N6	3.05	1.45	1.34
1	Aa	2408	OMU	C4-N3	3.05	1.44	1.38
1	Aa	2195	OMC	C6-N1	3.05	1.45	1.38
1	Aa	1371	A2M	C6-N6	3.04	1.45	1.34
1	Aa	668	OMC	O2-C2	-3.04	1.18	1.23
3	Ac	43	A2M	C5-C4	-3.04	1.32	1.40
1	Aa	811	A2M	C6-N6	3.04	1.45	1.34
1	Aa	2335	OMC	C6-N1	3.03	1.45	1.38
1	Aa	2218	A2M	C6-N6	3.03	1.45	1.34
3	Ac	74	PSU	O4-C4	-3.03	1.17	1.23
1	Aa	2279	A2M	O3'-C3'	3.03	1.50	1.43
1	Aa	1467	PSU	O4-C4	-3.03	1.17	1.23
1	Aa	2111	OMU	O4-C4	-3.03	1.18	1.24
1	Aa	995	PSU	O4-C4	-3.03	1.17	1.23
1	Aa	2132	PSU	O4-C4	-3.02	1.17	1.23
1	Aa	2291	OMC	C6-N1	3.02	1.45	1.38
1	Aa	2839	OMC	C6-N1	3.02	1.45	1.38
1	Aa	1009	PSU	O4-C4	-3.02	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2818	OMG	O6-C6	-3.01	1.17	1.23
1	Aa	1857	OMC	O2-C2	-3.01	1.18	1.23
1	Aa	1847	OMC	C6-N1	3.01	1.45	1.38
1	Aa	2868	PSU	O4-C4	-3.01	1.17	1.23
1	Aa	940	A2M	C6-N6	3.00	1.45	1.34
1	Aa	1852	OMG	C6-N1	3.00	1.42	1.37
1	Aa	880	A2M	C6-N6	3.00	1.45	1.34
1	Aa	2882	OMC	O2-C2	-2.99	1.18	1.23
1	Aa	2937	A2M	C6-N6	2.99	1.45	1.34
1	Aa	3108	A2M	C6-N6	2.98	1.44	1.34
1	Aa	3296	OMG	C5-C4	-2.98	1.35	1.43
1	Aa	2124	A2M	C6-N6	2.98	1.44	1.34
1	Aa	1137	A2M	C5-C4	-2.98	1.33	1.40
1	Aa	1512	OMC	C6-N1	2.98	1.45	1.38
1	Aa	2389	OMG	C5-C6	2.97	1.53	1.47
1	Aa	880	A2M	C5-C4	-2.97	1.33	1.40
1	Aa	3305	OMU	O2-C2	-2.97	1.17	1.23
1	Aa	2279	A2M	C5-C4	-2.96	1.33	1.40
1	Aa	2949	A2M	C6-N6	2.96	1.44	1.34
1	Aa	1441	OMC	O2-C2	-2.96	1.18	1.23
1	Aa	2389	OMG	C6-N1	2.96	1.42	1.37
1	Aa	2643	A2M	O3'-C3'	2.96	1.49	1.43
1	Aa	2914	A2M	C5-C4	-2.96	1.33	1.40
1	Aa	2643	A2M	C6-N6	2.95	1.44	1.34
1	Aa	2124	A2M	O3'-C3'	2.95	1.49	1.43
1	Aa	654	A2M	C5-C4	-2.95	1.33	1.40
3	Ac	75	OMG	C5-C6	2.95	1.53	1.47
1	Aa	1473	OMC	O2-C2	-2.95	1.18	1.23
1	Aa	2926	PSU	O4-C4	-2.94	1.18	1.23
1	Aa	2924	OMU	O2-C2	-2.94	1.17	1.23
1	Aa	1453	A2M	C6-N6	2.94	1.44	1.34
1	Aa	2886	OMU	O2-C2	-2.94	1.17	1.23
1	Aa	1852	OMG	O6-C6	-2.94	1.17	1.23
1	Aa	1371	A2M	O3'-C3'	2.94	1.49	1.43
3	Ac	43	A2M	C6-N6	2.94	1.44	1.34
1	Aa	1127	PSU	O4-C4	-2.93	1.18	1.23
1	Aa	1454	OMG	C5-C4	-2.93	1.35	1.43
1	Aa	654	A2M	O3'-C3'	2.92	1.49	1.43
1	Aa	2883	PSU	O4-C4	-2.92	1.18	1.23
3	Ac	18	PSU	O4-C4	-2.92	1.18	1.23
1	Aa	2914	A2M	C6-N6	2.91	1.44	1.34
1	Aa	2622	OMG	C5-C6	2.90	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2914	A2M	O3'-C3'	2.90	1.49	1.43
1	Aa	2949	A2M	C5-C4	-2.90	1.33	1.40
1	Aa	2393	OMG	C5-C4	-2.90	1.35	1.43
1	Aa	1530	OMC	O2-C2	-2.89	1.18	1.23
1	Aa	3108	A2M	C5-C4	-2.89	1.33	1.40
1	Aa	2937	A2M	O3'-C3'	2.89	1.49	1.43
1	Aa	2414	PSU	C4-N3	2.89	1.44	1.38
1	Aa	1137	A2M	C6-N6	2.89	1.44	1.34
1	Aa	2925	OMG	C5-C6	2.89	1.53	1.47
1	Aa	1453	A2M	C5-C4	-2.88	1.33	1.40
1	Aa	1847	OMC	O2-C2	-2.88	1.18	1.23
1	Aa	1844	OMC	C6-N1	2.88	1.44	1.38
1	Aa	2124	A2M	C5-C4	-2.88	1.33	1.40
1	Aa	2319	A2M	C6-N6	2.88	1.44	1.34
1	Aa	48	OMU	C6-N1	2.88	1.44	1.38
1	Aa	2363	OMC	C6-N1	2.88	1.44	1.38
1	Aa	2738	OMU	C6-N1	2.88	1.44	1.38
1	Aa	2316	PSU	O4-C4	-2.87	1.18	1.23
1	Aa	1904	PSU	O4-C4	-2.86	1.18	1.23
1	Aa	880	A2M	O3'-C3'	2.86	1.49	1.43
1	Aa	654	A2M	C6-N6	2.86	1.44	1.34
1	Aa	2920	OMG	C5-C4	-2.86	1.35	1.43
1	Aa	369	A2M	C5-C4	-2.85	1.33	1.40
1	Aa	2738	OMU	O2-C2	-2.85	1.17	1.23
1	Aa	2962	OMC	O2-C2	-2.85	1.18	1.23
1	Aa	1128	PSU	O4-C4	-2.85	1.18	1.23
1	Aa	1868	A2M	C5-C4	-2.85	1.33	1.40
1	Aa	2818	OMG	C5-C4	-2.85	1.35	1.43
1	Aa	2622	OMG	C5-C4	-2.85	1.35	1.43
1	Aa	2924	OMU	C6-N1	2.85	1.44	1.38
1	Aa	2189	PSU	O4-C4	-2.85	1.18	1.23
1	Aa	809	OMG	O6-C6	-2.85	1.17	1.23
1	Aa	2319	A2M	C5-C4	-2.85	1.33	1.40
1	Aa	811	A2M	C5-C4	-2.84	1.33	1.40
1	Aa	2949	A2M	O3'-C3'	2.84	1.49	1.43
1	Aa	2995	PSU	O4-C4	-2.84	1.18	1.23
1	Aa	2715	PSU	O4-C4	-2.84	1.18	1.23
1	Aa	2279	A2M	C6-N6	2.84	1.44	1.34
1	Aa	1061	OMU	C6-N1	2.84	1.44	1.38
1	Aa	1057	PSU	O4-C4	-2.84	1.18	1.23
1	Aa	2430	PSU	O4-C4	-2.83	1.18	1.23
1	Aa	2407	OMG	O6-C6	-2.83	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1371	A2M	C5-C4	-2.83	1.33	1.40
1	Aa	2407	OMG	C5-C6	2.83	1.53	1.47
1	Aa	2111	OMU	O2-C2	-2.83	1.17	1.23
1	Aa	2886	OMU	C6-N1	2.83	1.44	1.38
1	Aa	2794	OMG	C5-C4	-2.83	1.35	1.43
1	Aa	2393	OMG	O6-C6	-2.83	1.17	1.23
1	Aa	1475	PSU	O4-C4	-2.83	1.18	1.23
1	Aa	809	OMG	C5-C4	-2.82	1.35	1.43
1	Aa	2122	OMG	C5-C4	-2.82	1.35	1.43
1	Aa	650	1MA	CM1-N1	-2.82	1.41	1.46
1	Aa	144	OMU	C6-N1	2.82	1.44	1.38
1	Aa	2218	A2M	C5-C4	-2.82	1.33	1.40
1	Aa	2654	OMG	C5-C6	2.82	1.53	1.47
1	Aa	2654	OMG	C5-C4	-2.81	1.35	1.43
1	Aa	821	A2M	C5-C4	-2.81	1.33	1.40
1	Aa	2419	OMU	C6-N1	2.81	1.44	1.38
1	Aa	2978	PSU	O4-C4	-2.81	1.18	1.23
1	Aa	3296	OMG	O6-C6	-2.81	1.17	1.23
1	Aa	2209	PSU	O4-C4	-2.81	1.18	1.23
1	Aa	2122	OMG	O6-C6	-2.81	1.17	1.23
1	Aa	2796	OMG	C5-C6	2.80	1.53	1.47
1	Aa	1047	PSU	O4-C4	-2.80	1.18	1.23
1	Aa	1454	OMG	O6-C6	-2.80	1.17	1.23
1	Aa	2794	OMG	O6-C6	-2.80	1.17	1.23
1	Aa	2223	PSU	O4-C4	-2.80	1.18	1.23
1	Aa	2643	A2M	C5-C4	-2.79	1.33	1.40
1	Aa	2622	OMG	O6-C6	-2.79	1.17	1.23
1	Aa	3108	A2M	O2'-C2'	-2.78	1.35	1.42
1	Aa	3108	A2M	O3'-C3'	2.78	1.49	1.43
1	Aa	809	OMG	C5-C6	2.78	1.53	1.47
1	Aa	2389	OMG	C5-C4	-2.78	1.36	1.43
1	Aa	2920	OMG	C5-C6	2.78	1.53	1.47
1	Aa	912	OMG	C5-C4	-2.78	1.36	1.43
1	Aa	811	A2M	O3'-C3'	2.78	1.49	1.43
1	Aa	821	A2M	O3'-C3'	2.78	1.49	1.43
1	Aa	2937	A2M	C5-C4	-2.77	1.33	1.40
1	Aa	1889	OMU	O2-C2	-2.77	1.18	1.23
1	Aa	2389	OMG	O6-C6	-2.76	1.17	1.23
1	Aa	2286	OMG	C5-C4	-2.76	1.36	1.43
1	Aa	2958	PSU	O4-C4	-2.76	1.18	1.23
3	Ac	43	A2M	O3'-C3'	2.76	1.49	1.43
1	Aa	1441	OMC	C6-N1	2.76	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2111	OMU	C6-N1	2.76	1.44	1.38
1	Aa	940	A2M	O3'-C3'	2.76	1.49	1.43
1	Aa	68	PSU	O4-C4	-2.76	1.18	1.23
1	Aa	2653	OMU	C6-N1	2.75	1.44	1.38
1	Aa	1852	OMG	C5-C4	-2.75	1.36	1.43
1	Aa	940	A2M	C5-C4	-2.75	1.33	1.40
1	Aa	2920	OMG	O6-C6	-2.74	1.17	1.23
1	Aa	2121	OMG	C5-C6	2.74	1.53	1.47
1	Aa	2218	A2M	O3'-C3'	2.73	1.49	1.43
1	Aa	669	OMU	C6-N1	2.73	1.44	1.38
1	Aa	1454	OMG	C5-C6	2.72	1.52	1.47
1	Aa	2286	OMG	O6-C6	-2.72	1.17	1.23
1	Aa	2796	OMG	C5-C4	-2.72	1.36	1.43
1	Aa	1868	A2M	O3'-C3'	2.72	1.49	1.43
1	Aa	2393	OMG	C5-C6	2.71	1.52	1.47
1	Aa	2732	OMU	O2-C2	-2.71	1.18	1.23
1	Aa	1137	A2M	O3'-C3'	2.71	1.49	1.43
1	Aa	2319	A2M	O2'-C2'	-2.70	1.35	1.42
1	Aa	912	OMG	O6-C6	-2.70	1.17	1.23
1	Aa	2794	OMG	C5-C6	2.70	1.52	1.47
1	Aa	798	OMU	O2-C2	-2.70	1.18	1.23
1	Aa	2407	OMG	C5-C4	-2.70	1.36	1.43
1	Aa	2121	OMG	C5-C4	-2.69	1.36	1.43
1	Aa	2732	OMU	C6-N1	2.69	1.44	1.38
1	Aa	2234	OMG	C5-C4	-2.69	1.36	1.43
1	Aa	3296	OMG	C5-C6	2.69	1.52	1.47
1	Aa	2925	OMG	C5-C4	-2.68	1.36	1.43
1	Aa	821	A2M	O2'-C2'	-2.68	1.35	1.42
1	Aa	2121	OMG	O6-C6	-2.68	1.17	1.23
1	Aa	2796	OMG	O6-C6	-2.67	1.17	1.23
1	Aa	48	OMU	O2-C2	-2.67	1.18	1.23
1	Aa	2720	OMU	C6-N1	2.67	1.44	1.38
1	Aa	1889	OMU	C6-N1	2.67	1.44	1.38
1	Aa	2685	OMC	O2-C2	-2.67	1.18	1.23
1	Aa	2654	OMG	O6-C6	-2.66	1.17	1.23
1	Aa	1371	A2M	O2'-C2'	-2.66	1.35	1.42
1	Aa	798	OMU	C6-N1	2.66	1.44	1.38
1	Aa	369	A2M	O3'-C3'	2.66	1.49	1.43
3	Ac	75	OMG	C5-C4	-2.66	1.36	1.43
1	Aa	3113	PSU	O2-C2	-2.65	1.17	1.23
1	Aa	654	A2M	O2'-C2'	-2.65	1.35	1.42
1	Aa	2947	PSU	O2-C2	-2.65	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2414	PSU	O2-C2	-2.65	1.17	1.23
1	Aa	144	OMU	O2-C2	-2.65	1.18	1.23
1	Aa	2914	A2M	O2'-C2'	-2.64	1.35	1.42
1	Aa	1137	A2M	O2'-C2'	-2.64	1.35	1.42
1	Aa	912	OMG	C5-C6	2.64	1.52	1.47
1	Aa	1453	A2M	O2'-C2'	-2.64	1.35	1.42
1	Aa	35	PSU	O2-C2	-2.63	1.17	1.23
3	Ac	74	PSU	O2-C2	-2.63	1.17	1.23
1	Aa	2937	A2M	O2'-C2'	-2.63	1.35	1.42
1	Aa	2312	PSU	O4-C4	-2.63	1.18	1.23
1	Aa	2643	A2M	O2'-C2'	-2.63	1.35	1.42
1	Aa	2345	OMU	O2-C2	-2.62	1.18	1.23
1	Aa	2218	A2M	O2'-C2'	-2.62	1.35	1.42
1	Aa	1453	A2M	O3'-C3'	2.62	1.49	1.43
1	Aa	2345	OMU	C6-N1	2.61	1.44	1.38
1	Aa	2286	OMG	C5-C6	2.61	1.52	1.47
1	Aa	964	PSU	O4'-C1'	-2.61	1.40	1.43
1	Aa	2319	A2M	O3'-C3'	2.61	1.49	1.43
1	Aa	2347	PSU	O2-C2	-2.60	1.17	1.23
1	Aa	1904	PSU	O2-C2	-2.60	1.17	1.23
1	Aa	964	PSU	O4-C4	-2.59	1.18	1.23
1	Aa	2925	OMG	O6-C6	-2.59	1.18	1.23
1	Aa	2430	PSU	O2-C2	-2.59	1.18	1.23
1	Aa	2949	A2M	O2'-C2'	-2.58	1.36	1.42
1	Aa	2234	OMG	C5-C6	2.58	1.52	1.47
1	Aa	2134	PSU	O2-C2	-2.57	1.18	1.23
1	Aa	2279	A2M	O2'-C2'	-2.57	1.36	1.42
1	Aa	2124	A2M	O2'-C2'	-2.57	1.36	1.42
3	Ac	18	PSU	O2-C2	-2.57	1.18	1.23
3	Ac	75	OMG	O6-C6	-2.56	1.18	1.23
1	Aa	889	PSU	O2-C2	-2.55	1.18	1.23
1	Aa	940	A2M	O2'-C2'	-2.55	1.36	1.42
1	Aa	2419	OMU	O2-C2	-2.55	1.18	1.23
1	Aa	2234	OMG	O6-C6	-2.55	1.18	1.23
1	Aa	823	PSU	O2-C2	-2.53	1.18	1.23
1	Aa	2195	OMC	C5-C4	2.53	1.48	1.42
1	Aa	811	A2M	O2'-C2'	-2.52	1.36	1.42
1	Aa	2829	PSU	O2-C2	-2.52	1.18	1.23
1	Aa	2312	PSU	O2-C2	-2.51	1.18	1.23
1	Aa	2818	OMG	C5-C6	2.50	1.52	1.47
1	Aa	995	PSU	O2-C2	-2.49	1.18	1.23
1	Aa	2132	PSU	O2-C2	-2.49	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ac	43	A2M	O2'-C2'	-2.48	1.36	1.42
1	Aa	2747	PSU	O2-C2	-2.46	1.18	1.23
1	Aa	1128	PSU	O2-C2	-2.46	1.18	1.23
1	Aa	3305	OMU	C6-N1	2.46	1.43	1.38
1	Aa	2868	PSU	O2-C2	-2.46	1.18	1.23
1	Aa	2286	OMG	C2-N1	2.46	1.43	1.37
1	Aa	880	A2M	O2'-C2'	-2.45	1.36	1.42
1	Aa	2958	PSU	O2-C2	-2.45	1.18	1.23
1	Aa	1852	OMG	C5-C6	2.44	1.52	1.47
1	Aa	2883	PSU	O2-C2	-2.44	1.18	1.23
1	Aa	1009	PSU	O2-C2	-2.43	1.18	1.23
1	Aa	1057	PSU	O2-C2	-2.43	1.18	1.23
1	Aa	1530	OMC	C5-C4	2.43	1.48	1.42
1	Aa	1847	OMC	C5-C4	2.42	1.48	1.42
1	Aa	1475	PSU	O2-C2	-2.41	1.18	1.23
1	Aa	2316	PSU	O2-C2	-2.41	1.18	1.23
1	Aa	2715	PSU	O2-C2	-2.41	1.18	1.23
1	Aa	2995	PSU	O2-C2	-2.41	1.18	1.23
1	Aa	2111	OMU	C5-C4	2.41	1.49	1.43
1	Aa	369	A2M	O2'-C2'	-2.41	1.36	1.42
1	Aa	1868	A2M	O2'-C2'	-2.40	1.36	1.42
1	Aa	2616	PSU	O2-C2	-2.39	1.18	1.23
1	Aa	2223	PSU	O2-C2	-2.39	1.18	1.23
1	Aa	2654	OMG	C2-N1	2.39	1.43	1.37
1	Aa	2839	OMC	C5-C4	2.38	1.48	1.42
1	Aa	2857	PSU	O2-C2	-2.38	1.18	1.23
1	Aa	2518	PSU	O2-C2	-2.38	1.18	1.23
1	Aa	2962	OMC	C5-C4	2.38	1.48	1.42
1	Aa	2925	OMG	C2-N1	2.38	1.43	1.37
1	Aa	2978	PSU	O2-C2	-2.38	1.18	1.23
1	Aa	1467	PSU	O2-C2	-2.38	1.18	1.23
1	Aa	2393	OMG	C2-N1	2.37	1.43	1.37
1	Aa	2794	OMG	C2-N1	2.37	1.43	1.37
1	Aa	2408	OMU	C6-N1	2.37	1.43	1.38
1	Aa	2951	OMC	C5-C4	2.36	1.48	1.42
1	Aa	1512	OMC	C5-C4	2.35	1.48	1.42
1	Aa	1047	PSU	O2-C2	-2.34	1.18	1.23
1	Aa	2189	PSU	O2-C2	-2.34	1.18	1.23
1	Aa	809	OMG	C2-N1	2.34	1.43	1.37
1	Aa	964	PSU	O2-C2	-2.34	1.18	1.23
1	Aa	1126	PSU	O2-C2	-2.33	1.18	1.23
1	Aa	378	PSU	O2-C2	-2.33	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1127	PSU	O2-C2	-2.32	1.18	1.23
1	Aa	2924	OMU	C5-C4	2.32	1.48	1.43
1	Aa	650	1MA	C5-C4	-2.31	1.37	1.43
1	Aa	2882	OMC	C5-C4	2.31	1.48	1.42
1	Aa	68	PSU	O2-C2	-2.31	1.18	1.23
1	Aa	2319	A2M	O5'-C5'	-2.30	1.39	1.44
1	Aa	2920	OMG	C2-N1	2.30	1.43	1.37
1	Aa	2121	OMG	C2-N1	2.30	1.43	1.37
1	Aa	2685	OMC	C5-C4	2.29	1.48	1.42
1	Aa	68	PSU	O4'-C1'	-2.29	1.40	1.43
1	Aa	2738	OMU	C5-C4	2.28	1.48	1.43
1	Aa	2234	OMG	C2-N1	2.28	1.43	1.37
1	Aa	1852	OMG	C2-N1	2.28	1.43	1.37
1	Aa	1889	OMU	C5-C4	2.28	1.48	1.43
1	Aa	2419	OMU	C5-C4	2.26	1.48	1.43
3	Ac	75	OMG	C2-N1	2.25	1.43	1.37
1	Aa	48	OMU	C5-C4	2.25	1.48	1.43
1	Aa	1061	OMU	C5-C4	2.25	1.48	1.43
1	Aa	2335	OMC	C5-C4	2.25	1.48	1.42
1	Aa	1473	OMC	C5-C4	2.24	1.48	1.42
1	Aa	2363	OMC	C5-C4	2.24	1.48	1.42
1	Aa	2407	OMG	C2-N1	2.24	1.43	1.37
1	Aa	2218	A2M	O5'-C5'	-2.22	1.39	1.44
1	Aa	1454	OMG	C2-N1	2.21	1.43	1.37
1	Aa	2796	OMG	C2-N1	2.21	1.43	1.37
1	Aa	144	OMU	C5-C4	2.20	1.48	1.43
1	Aa	2122	OMG	C2-N1	2.20	1.43	1.37
1	Aa	2291	OMC	C5-C4	2.20	1.48	1.42
1	Aa	1844	OMC	C5-C4	2.20	1.48	1.42
1	Aa	1868	A2M	O5'-C5'	-2.19	1.39	1.44
1	Aa	2209	PSU	O2-C2	-2.19	1.18	1.23
1	Aa	3296	OMG	C2-N1	2.18	1.43	1.37
1	Aa	2622	OMG	C2-N1	2.18	1.43	1.37
1	Aa	2124	A2M	C2-N3	2.17	1.35	1.32
1	Aa	1857	OMC	C5-C4	2.17	1.47	1.42
1	Aa	798	OMU	C5-C4	2.16	1.48	1.43
1	Aa	2345	OMU	C5-C4	2.16	1.48	1.43
1	Aa	912	OMG	C2-N1	2.14	1.43	1.37
1	Aa	1441	OMC	C5-C4	2.13	1.47	1.42
1	Aa	2732	OMU	C5-C4	2.13	1.48	1.43
1	Aa	2926	PSU	O2-C2	-2.12	1.18	1.23
1	Aa	2818	OMG	C2-N1	2.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	2715	PSU	O4'-C1'	-2.11	1.40	1.43
1	Aa	2389	OMG	C2-N1	2.09	1.42	1.37
1	Aa	940	A2M	O5'-C5'	-2.09	1.39	1.44
1	Aa	2886	OMU	C5-C4	2.09	1.48	1.43
1	Aa	2653	OMU	C5-C4	2.08	1.48	1.43
1	Aa	2720	OMU	C5-C4	2.07	1.48	1.43
1	Aa	668	OMC	C5-C4	2.05	1.47	1.42
1	Aa	1137	A2M	O5'-C5'	-2.04	1.39	1.44
1	Aa	2956	UR3	C5-C4	2.04	1.49	1.43
1	Aa	2956	UR3	C4-N3	2.03	1.45	1.40
1	Aa	2408	OMU	C5-C4	2.02	1.48	1.43
1	Aa	2279	A2M	O5'-C5'	-2.01	1.39	1.44

All (457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1453	A2M	C5-C6-N6	11.21	137.39	120.35
1	Aa	2643	A2M	C5-C6-N6	11.18	137.34	120.35
1	Aa	2937	A2M	C5-C6-N6	11.15	137.29	120.35
1	Aa	2914	A2M	C5-C6-N6	11.06	137.16	120.35
1	Aa	3108	A2M	C5-C6-N6	10.91	136.93	120.35
1	Aa	940	A2M	C5-C6-N6	10.90	136.91	120.35
1	Aa	2218	A2M	C5-C6-N6	10.83	136.82	120.35
1	Aa	880	A2M	C5-C6-N6	10.78	136.73	120.35
1	Aa	2949	A2M	C5-C6-N6	10.75	136.69	120.35
1	Aa	1371	A2M	C5-C6-N6	10.74	136.67	120.35
3	Ac	43	A2M	C5-C6-N6	10.69	136.60	120.35
1	Aa	1137	A2M	C5-C6-N6	10.62	136.49	120.35
1	Aa	821	A2M	C5-C6-N6	10.61	136.47	120.35
1	Aa	1868	A2M	C5-C6-N6	10.55	136.38	120.35
1	Aa	2319	A2M	C5-C6-N6	10.43	136.20	120.35
1	Aa	811	A2M	C5-C6-N6	10.40	136.16	120.35
1	Aa	2124	A2M	C5-C6-N6	10.40	136.16	120.35
1	Aa	654	A2M	C5-C6-N6	10.38	136.12	120.35
1	Aa	2279	A2M	C5-C6-N6	10.26	135.95	120.35
1	Aa	369	A2M	C5-C6-N6	10.18	135.82	120.35
1	Aa	1453	A2M	N6-C6-N1	-7.76	102.47	118.57
1	Aa	2914	A2M	N6-C6-N1	-7.62	102.75	118.57
1	Aa	2643	A2M	N6-C6-N1	-7.61	102.78	118.57
3	Ac	43	A2M	N6-C6-N1	-7.49	103.02	118.57
1	Aa	940	A2M	N6-C6-N1	-7.49	103.03	118.57
1	Aa	2124	A2M	N6-C6-N1	-7.47	103.07	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	3108	A2M	N6-C6-N1	-7.43	103.16	118.57
1	Aa	1371	A2M	N6-C6-N1	-7.38	103.25	118.57
1	Aa	2279	A2M	N6-C6-N1	-7.34	103.33	118.57
1	Aa	2937	A2M	N6-C6-N1	-7.34	103.35	118.57
1	Aa	2218	A2M	N6-C6-N1	-7.33	103.36	118.57
1	Aa	2949	A2M	N6-C6-N1	-7.32	103.38	118.57
1	Aa	1137	A2M	N6-C6-N1	-7.31	103.41	118.57
1	Aa	2319	A2M	N6-C6-N1	-7.29	103.44	118.57
1	Aa	880	A2M	N6-C6-N1	-7.28	103.46	118.57
1	Aa	654	A2M	N6-C6-N1	-7.26	103.51	118.57
1	Aa	811	A2M	N6-C6-N1	-7.21	103.60	118.57
1	Aa	821	A2M	N6-C6-N1	-7.14	103.76	118.57
1	Aa	1868	A2M	N6-C6-N1	-7.02	103.99	118.57
1	Aa	369	A2M	N6-C6-N1	-6.94	104.16	118.57
1	Aa	2408	OMU	C4-N3-C2	-6.42	118.11	126.58
1	Aa	2408	OMU	N3-C2-N1	6.07	122.95	114.89
1	Aa	3305	OMU	C4-N3-C2	-5.97	118.70	126.58
1	Aa	1889	OMU	C4-N3-C2	-5.88	118.83	126.58
1	Aa	1453	A2M	N3-C2-N1	-5.87	119.50	128.68
1	Aa	654	A2M	N3-C2-N1	-5.84	119.55	128.68
1	Aa	2279	A2M	N3-C2-N1	-5.81	119.59	128.68
1	Aa	798	OMU	C4-N3-C2	-5.78	118.96	126.58
1	Aa	2949	A2M	N3-C2-N1	-5.77	119.66	128.68
3	Ac	43	A2M	N3-C2-N1	-5.77	119.66	128.68
1	Aa	2218	A2M	N3-C2-N1	-5.76	119.67	128.68
1	Aa	3108	A2M	N3-C2-N1	-5.72	119.74	128.68
1	Aa	880	A2M	N3-C2-N1	-5.69	119.79	128.68
1	Aa	1137	A2M	N3-C2-N1	-5.68	119.80	128.68
1	Aa	940	A2M	N3-C2-N1	-5.67	119.81	128.68
1	Aa	369	A2M	N3-C2-N1	-5.67	119.81	128.68
1	Aa	2914	A2M	N3-C2-N1	-5.66	119.83	128.68
1	Aa	2732	OMU	C4-N3-C2	-5.65	119.12	126.58
1	Aa	2643	A2M	N3-C2-N1	-5.64	119.86	128.68
1	Aa	669	OMU	C4-N3-C2	-5.62	119.17	126.58
1	Aa	1868	A2M	N3-C2-N1	-5.60	119.92	128.68
1	Aa	2720	OMU	C4-N3-C2	-5.60	119.19	126.58
1	Aa	2111	OMU	C4-N3-C2	-5.58	119.22	126.58
1	Aa	650	1MA	N1-C2-N3	-5.51	119.60	126.02
1	Aa	2653	OMU	C4-N3-C2	-5.50	119.33	126.58
1	Aa	821	A2M	N3-C2-N1	-5.49	120.10	128.68
1	Aa	2345	OMU	C4-N3-C2	-5.45	119.39	126.58
1	Aa	2414	PSU	C4-N3-C2	-5.44	118.50	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2937	A2M	N3-C2-N1	-5.43	120.19	128.68
1	Aa	2124	A2M	N3-C2-N1	-5.40	120.24	128.68
1	Aa	1371	A2M	N3-C2-N1	-5.37	120.29	128.68
1	Aa	68	PSU	C4-N3-C2	-5.29	118.72	126.34
1	Aa	2419	OMU	C4-N3-C2	-5.28	119.62	126.58
1	Aa	2924	OMU	C4-N3-C2	-5.26	119.64	126.58
1	Aa	2319	A2M	N3-C2-N1	-5.25	120.47	128.68
1	Aa	2747	PSU	C4-N3-C2	-5.23	118.81	126.34
1	Aa	1061	OMU	C4-N3-C2	-5.19	119.73	126.58
1	Aa	48	OMU	C4-N3-C2	-5.19	119.74	126.58
1	Aa	889	PSU	C4-N3-C2	-5.14	118.93	126.34
1	Aa	144	OMU	C4-N3-C2	-5.14	119.80	126.58
1	Aa	2886	OMU	C4-N3-C2	-5.13	119.81	126.58
1	Aa	2518	PSU	C4-N3-C2	-5.13	118.95	126.34
1	Aa	811	A2M	N3-C2-N1	-5.10	120.71	128.68
1	Aa	1126	PSU	C4-N3-C2	-5.08	119.02	126.34
1	Aa	3113	PSU	C4-N3-C2	-5.05	119.06	126.34
1	Aa	2616	PSU	C4-N3-C2	-5.05	119.07	126.34
1	Aa	35	PSU	C4-N3-C2	-5.00	119.13	126.34
1	Aa	2738	OMU	C4-N3-C2	-4.98	120.01	126.58
3	Ac	18	PSU	C4-N3-C2	-4.96	119.19	126.34
1	Aa	995	PSU	C4-N3-C2	-4.96	119.20	126.34
1	Aa	2720	OMU	N3-C2-N1	4.95	121.47	114.89
1	Aa	1904	PSU	C4-N3-C2	-4.93	119.24	126.34
1	Aa	2995	PSU	C4-N3-C2	-4.93	119.24	126.34
1	Aa	378	PSU	C4-N3-C2	-4.92	119.25	126.34
1	Aa	2947	PSU	C4-N3-C2	-4.88	119.30	126.34
1	Aa	2430	PSU	N1-C2-N3	4.88	120.66	115.13
1	Aa	2134	PSU	C4-N3-C2	-4.87	119.32	126.34
1	Aa	1467	PSU	C4-N3-C2	-4.87	119.33	126.34
1	Aa	2829	PSU	C4-N3-C2	-4.85	119.34	126.34
1	Aa	3305	OMU	N3-C2-N1	4.85	121.32	114.89
1	Aa	1128	PSU	C4-N3-C2	-4.84	119.36	126.34
1	Aa	2430	PSU	C4-N3-C2	-4.83	119.38	126.34
1	Aa	823	PSU	C4-N3-C2	-4.81	119.41	126.34
1	Aa	669	OMU	N3-C2-N1	4.80	121.26	114.89
1	Aa	2868	PSU	C4-N3-C2	-4.79	119.43	126.34
1	Aa	2857	PSU	C4-N3-C2	-4.78	119.45	126.34
1	Aa	2715	PSU	C4-N3-C2	-4.78	119.45	126.34
1	Aa	2312	PSU	C4-N3-C2	-4.76	119.48	126.34
1	Aa	1128	PSU	N1-C2-N3	4.76	120.52	115.13
1	Aa	2189	PSU	C4-N3-C2	-4.74	119.51	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ac	74	PSU	C4-N3-C2	-4.73	119.52	126.34
1	Aa	68	PSU	N1-C2-N3	4.73	120.49	115.13
1	Aa	1127	PSU	C4-N3-C2	-4.73	119.53	126.34
1	Aa	2414	PSU	N1-C2-N3	4.69	120.44	115.13
3	Ac	18	PSU	N1-C2-N3	4.69	120.44	115.13
1	Aa	2978	PSU	C4-N3-C2	-4.69	119.58	126.34
1	Aa	2132	PSU	C4-N3-C2	-4.67	119.61	126.34
1	Aa	1009	PSU	C4-N3-C2	-4.67	119.61	126.34
1	Aa	1475	PSU	C4-N3-C2	-4.65	119.64	126.34
1	Aa	35	PSU	N1-C2-N3	4.62	120.37	115.13
1	Aa	1057	PSU	C4-N3-C2	-4.62	119.68	126.34
1	Aa	2316	PSU	N1-C2-N3	4.60	120.34	115.13
1	Aa	2747	PSU	N1-C2-N3	4.58	120.32	115.13
1	Aa	2926	PSU	C4-N3-C2	-4.57	119.75	126.34
1	Aa	2312	PSU	N1-C2-N3	4.57	120.31	115.13
1	Aa	2947	PSU	N1-C2-N3	4.55	120.28	115.13
1	Aa	964	PSU	C4-N3-C2	-4.52	119.82	126.34
1	Aa	1904	PSU	N1-C2-N3	4.51	120.24	115.13
1	Aa	2316	PSU	C4-N3-C2	-4.49	119.86	126.34
1	Aa	2347	PSU	C4-N3-C2	-4.49	119.88	126.34
1	Aa	3305	OMU	C1'-N1-C2	4.48	125.68	117.57
1	Aa	1475	PSU	N1-C2-N3	4.46	120.18	115.13
1	Aa	1047	PSU	C4-N3-C2	-4.46	119.92	126.34
1	Aa	2883	PSU	C4-N3-C2	-4.45	119.93	126.34
1	Aa	1061	OMU	N3-C2-N1	4.44	120.79	114.89
1	Aa	2924	OMU	N3-C2-N1	4.43	120.77	114.89
1	Aa	2956	UR3	C4-N3-C2	-4.41	120.41	124.56
1	Aa	2653	OMU	N3-C2-N1	4.39	120.72	114.89
1	Aa	2209	PSU	C4-N3-C2	-4.38	120.02	126.34
1	Aa	2873	5MC	C5-C6-N1	-4.35	118.86	123.34
1	Aa	2829	PSU	N1-C2-N3	4.34	120.05	115.13
1	Aa	964	PSU	N1-C2-N3	4.34	120.04	115.13
1	Aa	2958	PSU	C4-N3-C2	-4.33	120.10	126.34
1	Aa	2995	PSU	N1-C2-N3	4.31	120.01	115.13
1	Aa	2223	PSU	N1-C2-N3	4.30	120.01	115.13
1	Aa	2223	PSU	C4-N3-C2	-4.30	120.15	126.34
1	Aa	823	PSU	N1-C2-N3	4.29	119.99	115.13
1	Aa	995	PSU	N1-C2-N3	4.26	119.96	115.13
1	Aa	2978	PSU	N1-C2-N3	4.26	119.96	115.13
1	Aa	1047	PSU	N1-C2-N3	4.24	119.94	115.13
1	Aa	3113	PSU	N1-C2-N3	4.23	119.93	115.13
1	Aa	1127	PSU	N1-C2-N3	4.18	119.86	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2868	PSU	N1-C2-N3	4.17	119.86	115.13
1	Aa	1467	PSU	N1-C2-N3	4.17	119.85	115.13
1	Aa	2419	OMU	N3-C2-N1	4.17	120.42	114.89
1	Aa	1009	PSU	N1-C2-N3	4.17	119.85	115.13
1	Aa	798	OMU	N3-C2-N1	4.16	120.42	114.89
3	Ac	74	PSU	N1-C2-N3	4.16	119.84	115.13
1	Aa	2616	PSU	N1-C2-N3	4.14	119.82	115.13
1	Aa	2132	PSU	N1-C2-N3	4.13	119.81	115.13
1	Aa	2926	PSU	N1-C2-N3	4.11	119.78	115.13
1	Aa	2345	OMU	N3-C2-N1	4.09	120.32	114.89
1	Aa	2209	PSU	N1-C2-N3	4.09	119.76	115.13
1	Aa	2715	PSU	N1-C2-N3	4.08	119.75	115.13
1	Aa	2111	OMU	N3-C2-N1	4.07	120.30	114.89
1	Aa	1889	OMU	N3-C2-N1	4.06	120.28	114.89
1	Aa	1057	PSU	N1-C2-N3	4.06	119.73	115.13
1	Aa	2958	PSU	N1-C2-N3	3.98	119.63	115.13
1	Aa	669	OMU	C1'-N1-C2	3.95	124.72	117.57
1	Aa	1844	OMC	O2-C2-N3	-3.94	115.92	122.33
1	Aa	1126	PSU	N1-C2-N3	3.91	119.56	115.13
1	Aa	2886	OMU	N3-C2-N1	3.86	120.02	114.89
1	Aa	2134	PSU	N1-C2-N3	3.86	119.50	115.13
1	Aa	2189	PSU	N1-C2-N3	3.86	119.50	115.13
1	Aa	378	PSU	N1-C2-N3	3.84	119.49	115.13
1	Aa	2857	PSU	N1-C2-N3	3.84	119.48	115.13
1	Aa	2407	OMG	C5-C6-N1	3.84	120.73	113.95
1	Aa	1061	OMU	C1'-N1-C2	3.81	124.47	117.57
1	Aa	2518	PSU	N1-C2-N3	3.81	119.45	115.13
1	Aa	2794	OMG	C5-C6-N1	3.80	120.67	113.95
1	Aa	1889	OMU	C5-C4-N3	3.79	120.50	114.84
1	Aa	2883	PSU	N1-C2-N3	3.78	119.42	115.13
1	Aa	2732	OMU	N3-C2-N1	3.76	119.88	114.89
1	Aa	48	OMU	N3-C2-N1	3.73	119.84	114.89
1	Aa	2122	OMG	C5-C6-N1	3.71	120.50	113.95
1	Aa	2732	OMU	C5-C4-N3	3.67	120.33	114.84
1	Aa	2818	OMG	C5-C6-N1	3.67	120.43	113.95
1	Aa	48	OMU	C5-C4-N3	3.67	120.33	114.84
1	Aa	2738	OMU	N3-C2-N1	3.66	119.75	114.89
1	Aa	144	OMU	N3-C2-N1	3.66	119.75	114.89
1	Aa	2363	OMC	O2-C2-N3	-3.65	116.39	122.33
1	Aa	2653	OMU	C1'-N1-C2	3.65	124.17	117.57
1	Aa	2920	OMG	C5-C6-N1	3.64	120.38	113.95
1	Aa	2347	PSU	N1-C2-N3	3.63	119.24	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2345	OMU	C1'-N1-C2	3.63	124.14	117.57
1	Aa	3296	OMG	C5-C6-N1	3.62	120.34	113.95
1	Aa	798	OMU	C5-C4-N3	3.61	120.24	114.84
1	Aa	2622	OMG	C5-C6-N1	3.60	120.31	113.95
1	Aa	2720	OMU	C1'-N1-C2	3.60	124.08	117.57
1	Aa	144	OMU	C5-C4-N3	3.57	120.18	114.84
1	Aa	68	PSU	O2-C2-N1	-3.56	118.87	122.79
1	Aa	650	1MA	C5-C6-N1	3.55	119.20	113.90
1	Aa	2796	OMG	C5-C6-N1	3.53	120.18	113.95
1	Aa	2393	OMG	C5-C6-N1	3.52	120.16	113.95
1	Aa	2234	OMG	C5-C6-N1	3.50	120.13	113.95
1	Aa	912	OMG	C5-C6-N1	3.48	120.10	113.95
1	Aa	2111	OMU	C5-C4-N3	3.48	120.04	114.84
1	Aa	1454	OMG	C5-C6-N1	3.47	120.08	113.95
1	Aa	2121	OMG	C5-C6-N1	3.45	120.04	113.95
3	Ac	75	OMG	C5-C6-N1	3.45	120.04	113.95
1	Aa	889	PSU	N1-C2-N3	3.44	119.03	115.13
1	Aa	2316	PSU	C6-N1-C2	-3.44	119.17	122.68
1	Aa	2345	OMU	C5-C4-N3	3.44	119.99	114.84
1	Aa	1852	OMG	C5-C6-N1	3.42	119.99	113.95
1	Aa	2223	PSU	C6-N1-C2	-3.41	119.19	122.68
1	Aa	2286	OMG	C5-C6-N1	3.41	119.97	113.95
1	Aa	2886	OMU	C5-C4-N3	3.40	119.93	114.84
1	Aa	1128	PSU	C6-N1-C2	-3.39	119.21	122.68
1	Aa	2738	OMU	C5-C4-N3	3.39	119.91	114.84
1	Aa	2924	OMU	C1'-N1-C2	3.38	123.69	117.57
1	Aa	809	OMG	C5-C6-N1	3.37	119.91	113.95
1	Aa	2389	OMG	C5-C6-N1	3.37	119.91	113.95
1	Aa	1904	PSU	O2-C2-N1	-3.34	119.11	122.79
1	Aa	2925	OMG	C5-C6-N1	3.34	119.85	113.95
1	Aa	2419	OMU	C5-C4-N3	3.32	119.80	114.84
1	Aa	2924	OMU	C5-C4-N3	3.31	119.79	114.84
1	Aa	2732	OMU	O4-C4-C5	-3.30	119.36	125.16
1	Aa	2654	OMG	C5-C6-N1	3.30	119.78	113.95
1	Aa	2279	A2M	O4'-C1'-C2'	-3.26	100.93	106.59
1	Aa	2414	PSU	C6-C5-C4	3.23	120.45	118.20
1	Aa	2430	PSU	C6-N1-C2	-3.23	119.38	122.68
1	Aa	2312	PSU	C6-C5-C4	3.22	120.45	118.20
1	Aa	2794	OMG	C2-N1-C6	-3.21	119.19	125.10
1	Aa	2312	PSU	C6-N1-C2	-3.19	119.42	122.68
1	Aa	2839	OMC	O2-C2-N3	-3.19	117.14	122.33
1	Aa	2407	OMG	C2-N1-C6	-3.18	119.25	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1047	PSU	C6-N1-C2	-3.17	119.44	122.68
1	Aa	2653	OMU	C5-C4-N3	3.17	119.59	114.84
1	Aa	1061	OMU	C5-C4-N3	3.15	119.56	114.84
3	Ac	18	PSU	C6-N1-C2	-3.14	119.47	122.68
1	Aa	964	PSU	C6-N1-C2	-3.13	119.48	122.68
1	Aa	1475	PSU	C6-C5-C4	3.13	120.39	118.20
1	Aa	48	OMU	O4-C4-C5	-3.13	119.66	125.16
1	Aa	35	PSU	C6-C5-C4	3.12	120.38	118.20
1	Aa	2223	PSU	C6-C5-C4	3.12	120.38	118.20
1	Aa	798	OMU	O4-C4-C5	-3.11	119.69	125.16
1	Aa	2122	OMG	C2-N1-C6	-3.11	119.37	125.10
1	Aa	2393	OMG	C2-N1-C6	-3.10	119.39	125.10
1	Aa	669	OMU	C5-C4-N3	3.09	119.46	114.84
1	Aa	2920	OMG	C2-N1-C6	-3.08	119.42	125.10
1	Aa	2886	OMU	O4-C4-C5	-3.07	119.76	125.16
1	Aa	912	OMG	C2-N1-C6	-3.07	119.44	125.10
1	Aa	2926	PSU	C6-N1-C2	-3.06	119.55	122.68
1	Aa	1441	OMC	O2-C2-N3	-3.05	117.36	122.33
3	Ac	18	PSU	C6-C5-C4	3.05	120.33	118.20
1	Aa	1475	PSU	C6-N1-C2	-3.04	119.57	122.68
1	Aa	2622	OMG	C2-N1-C6	-3.04	119.51	125.10
1	Aa	1852	OMG	C2-N1-C6	-3.03	119.52	125.10
3	Ac	75	OMG	C2-N1-C6	-3.03	119.53	125.10
1	Aa	2291	OMC	O2-C2-N3	-3.01	117.44	122.33
1	Aa	2234	OMG	C2-N1-C6	-3.00	119.58	125.10
1	Aa	2430	PSU	C6-C5-C4	2.99	120.29	118.20
3	Ac	18	PSU	O2-C2-N1	-2.99	119.50	122.79
1	Aa	2978	PSU	C6-N1-C2	-2.98	119.64	122.68
1	Aa	3305	OMU	C5-C4-N3	2.97	119.29	114.84
1	Aa	2393	OMG	C8-N7-C5	2.96	108.62	102.99
1	Aa	2209	PSU	C6-N1-C2	-2.95	119.66	122.68
1	Aa	1904	PSU	C6-C5-C4	2.95	120.26	118.20
1	Aa	2408	OMU	C1'-N1-C2	2.93	122.88	117.57
1	Aa	2796	OMG	C2-N1-C6	-2.93	119.70	125.10
1	Aa	2978	PSU	O2-C2-N1	-2.93	119.57	122.79
1	Aa	2818	OMG	C2-N1-C6	-2.92	119.72	125.10
1	Aa	2883	PSU	C6-N1-C2	-2.92	119.70	122.68
1	Aa	68	PSU	C6-N1-C2	-2.91	119.70	122.68
1	Aa	2121	OMG	C2-N1-C6	-2.91	119.74	125.10
1	Aa	2720	OMU	C5-C4-N3	2.91	119.19	114.84
1	Aa	1454	OMG	C8-N7-C5	2.87	108.46	102.99
1	Aa	2363	OMC	C6-C5-C4	2.86	122.12	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2738	OMU	O4-C4-C5	-2.86	120.13	125.16
1	Aa	1889	OMU	O4-C4-C5	-2.86	120.14	125.16
1	Aa	3296	OMG	C8-N7-C5	2.84	108.41	102.99
1	Aa	2122	OMG	C8-N7-C5	2.83	108.38	102.99
1	Aa	2947	PSU	C6-N1-C2	-2.83	119.79	122.68
1	Aa	1009	PSU	C6-N1-C2	-2.83	119.79	122.68
1	Aa	650	1MA	C8-N7-C5	2.82	108.37	102.99
1	Aa	2223	PSU	O2-C2-N1	-2.82	119.69	122.79
1	Aa	2389	OMG	C2-N1-C6	-2.82	119.91	125.10
1	Aa	2276	5MC	C5-C6-N1	-2.82	120.44	123.34
1	Aa	2654	OMG	C2-N1-C6	-2.82	119.91	125.10
1	Aa	2363	OMC	C1'-N1-C2	2.81	124.70	118.42
1	Aa	2925	OMG	C2-N1-C6	-2.81	119.92	125.10
1	Aa	1868	A2M	C1'-N9-C4	2.80	131.57	126.64
1	Aa	144	OMU	O4-C4-C5	-2.80	120.23	125.16
1	Aa	964	PSU	C6-C5-C4	2.80	120.16	118.20
1	Aa	1454	OMG	C2-N1-C6	-2.79	119.95	125.10
1	Aa	2286	OMG	C2-N1-C6	-2.78	119.98	125.10
1	Aa	3296	OMG	C2-N1-C6	-2.77	120.00	125.10
1	Aa	1844	OMC	C6-C5-C4	2.76	121.95	117.50
1	Aa	1844	OMC	C1'-N1-C2	2.75	124.55	118.42
1	Aa	2430	PSU	O2-C2-N1	-2.74	119.77	122.79
1	Aa	2286	OMG	C8-N7-C5	2.74	108.20	102.99
1	Aa	2794	OMG	C8-N7-C5	2.73	108.20	102.99
3	Ac	74	PSU	C6-N1-C2	-2.73	119.89	122.68
1	Aa	2653	OMU	O4-C4-C5	-2.72	120.38	125.16
1	Aa	2622	OMG	C8-N7-C5	2.72	108.17	102.99
3	Ac	75	OMG	C8-N7-C5	2.71	108.15	102.99
1	Aa	2111	OMU	O4-C4-C5	-2.71	120.40	125.16
1	Aa	2958	PSU	C6-N1-C2	-2.70	119.92	122.68
1	Aa	2925	OMG	C8-N7-C5	2.70	108.14	102.99
1	Aa	809	OMG	C8-N7-C5	2.70	108.13	102.99
1	Aa	2408	OMU	C5-C4-N3	2.70	118.88	114.84
1	Aa	1127	PSU	C6-N1-C2	-2.69	119.93	122.68
1	Aa	2654	OMG	C8-N7-C5	2.69	108.11	102.99
1	Aa	3305	OMU	O4-C4-C5	-2.69	120.44	125.16
1	Aa	823	PSU	C6-N1-C2	-2.68	119.94	122.68
1	Aa	2234	OMG	C8-N7-C5	2.68	108.09	102.99
1	Aa	35	PSU	O2-C2-N1	-2.67	119.85	122.79
1	Aa	1852	OMG	C8-N7-C5	2.66	108.06	102.99
1	Aa	1475	PSU	O2-C2-N1	-2.65	119.88	122.79
1	Aa	798	OMU	O2-C2-N1	-2.65	119.27	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1128	PSU	C6-C5-C4	2.64	120.04	118.20
1	Aa	2345	OMU	O4-C4-C5	-2.64	120.53	125.16
1	Aa	2389	OMG	C8-N7-C5	2.63	108.00	102.99
1	Aa	2407	OMG	C8-N7-C5	2.63	108.00	102.99
1	Aa	1467	PSU	C6-N1-C2	-2.63	120.00	122.68
1	Aa	2121	OMG	C8-N7-C5	2.62	107.98	102.99
1	Aa	1441	OMC	C6-C5-C4	2.61	121.72	117.50
1	Aa	2920	OMG	C8-N7-C5	2.61	107.97	102.99
1	Aa	35	PSU	C6-N1-C2	-2.59	120.03	122.68
1	Aa	669	OMU	O2-C2-N3	-2.59	116.68	121.50
1	Aa	654	A2M	C1'-N9-C4	2.59	131.19	126.64
1	Aa	2408	OMU	C6-C5-C4	2.58	123.05	119.52
1	Aa	3113	PSU	C6-N1-C2	-2.58	120.04	122.68
1	Aa	669	OMU	O4-C4-C5	-2.58	120.63	125.16
1	Aa	2818	OMG	O6-C6-C5	-2.57	119.36	124.37
1	Aa	809	OMG	C2-N1-C6	-2.56	120.38	125.10
1	Aa	2408	OMU	O2-C2-N3	-2.55	116.75	121.50
1	Aa	3305	OMU	O2-C2-N3	-2.55	116.75	121.50
1	Aa	2720	OMU	O2-C2-N3	-2.54	116.76	121.50
1	Aa	2419	OMU	O4-C4-C5	-2.54	120.70	125.16
1	Aa	68	PSU	C6-C5-C4	2.54	119.97	118.20
1	Aa	889	PSU	C5-C4-N3	2.53	122.31	116.58
1	Aa	1904	PSU	C6-N1-C2	-2.53	120.10	122.68
1	Aa	2132	PSU	C6-C5-C4	2.52	119.96	118.20
1	Aa	912	OMG	C8-N7-C5	2.52	107.79	102.99
1	Aa	1847	OMC	O2-C2-N3	-2.52	118.24	122.33
1	Aa	2796	OMG	C8-N7-C5	2.52	107.78	102.99
1	Aa	2926	PSU	O2-C2-N1	-2.50	120.04	122.79
1	Aa	2747	PSU	C6-N1-C2	-2.50	120.13	122.68
1	Aa	2829	PSU	C6-N1-C2	-2.50	120.13	122.68
1	Aa	2995	PSU	O2-C2-N1	-2.50	120.04	122.79
1	Aa	1852	OMG	O6-C6-C5	-2.50	119.50	124.37
1	Aa	1057	PSU	C6-N1-C2	-2.49	120.13	122.68
1	Aa	2868	PSU	C6-N1-C2	-2.49	120.14	122.68
1	Aa	2518	PSU	C5-C4-N3	2.48	122.20	116.58
1	Aa	2924	OMU	O4-C4-C5	-2.48	120.80	125.16
1	Aa	2995	PSU	C6-C5-C4	2.48	119.93	118.20
1	Aa	2720	OMU	O4-C4-C5	-2.47	120.82	125.16
1	Aa	2883	PSU	O2-C2-N1	-2.45	120.09	122.79
1	Aa	1061	OMU	O4-C4-C5	-2.44	120.86	125.16
1	Aa	912	OMG	O6-C6-C5	-2.42	119.65	124.37
1	Aa	2347	PSU	C6-N1-C2	-2.42	120.21	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2857	PSU	C6-N1-C2	-2.41	120.22	122.68
1	Aa	1047	PSU	O2-C2-N1	-2.41	120.14	122.79
1	Aa	2886	OMU	C1'-N1-C2	2.41	121.93	117.57
1	Aa	2312	PSU	O2-C2-N1	-2.41	120.14	122.79
1	Aa	2715	PSU	C6-N1-C2	-2.41	120.22	122.68
1	Aa	1127	PSU	O2-C2-N1	-2.40	120.15	122.79
1	Aa	811	A2M	C1'-N9-C4	2.40	130.86	126.64
1	Aa	2286	OMG	O6-C6-C5	-2.39	119.70	124.37
1	Aa	2291	OMC	C6-C5-C4	2.39	121.37	117.50
1	Aa	2653	OMU	O2-C2-N3	-2.39	117.05	121.50
1	Aa	2616	PSU	C6-N1-C2	-2.38	120.25	122.68
1	Aa	369	A2M	C1'-N9-C4	2.38	130.82	126.64
1	Aa	1128	PSU	O2-C2-N1	-2.38	120.17	122.79
1	Aa	2234	OMG	O6-C6-C5	-2.38	119.73	124.37
1	Aa	2218	A2M	C1'-N9-C4	2.37	130.81	126.64
1	Aa	1371	A2M	C1'-N9-C4	2.37	130.80	126.64
1	Aa	2920	OMG	O6-C6-C5	-2.36	119.76	124.37
1	Aa	1061	OMU	O2-C2-N3	-2.36	117.11	121.50
1	Aa	2189	PSU	C6-N1-C2	-2.35	120.28	122.68
1	Aa	2882	OMC	O2-C2-N3	-2.34	118.52	122.33
1	Aa	2132	PSU	C6-N1-C2	-2.34	120.29	122.68
1	Aa	2407	OMG	O6-C6-C5	-2.34	119.80	124.37
1	Aa	2839	OMC	C1'-N1-C2	2.34	123.63	118.42
1	Aa	2978	PSU	C6-C5-C4	2.33	119.83	118.20
1	Aa	2829	PSU	O4'-C1'-C2'	2.32	108.42	105.14
1	Aa	2316	PSU	C6-C5-C4	2.32	119.82	118.20
1	Aa	823	PSU	C6-C5-C4	2.31	119.81	118.20
1	Aa	2956	UR3	C1'-N1-C2	2.31	120.89	116.99
1	Aa	2408	OMU	C6-N1-C2	-2.30	118.05	120.99
1	Aa	2732	OMU	O2-C2-N1	-2.29	119.74	122.79
1	Aa	2839	OMC	C6-C5-C4	2.28	121.19	117.50
1	Aa	2209	PSU	C6-C5-C4	2.28	119.79	118.20
1	Aa	2715	PSU	O4'-C1'-C2'	2.27	108.35	105.14
1	Aa	995	PSU	C6-N1-C2	-2.27	120.36	122.68
1	Aa	2829	PSU	C6-C5-C4	2.27	119.79	118.20
1	Aa	2218	A2M	C5'-C4'-C3'	-2.27	106.68	115.18
1	Aa	1441	OMC	C1'-N1-C2	2.25	123.44	118.42
1	Aa	995	PSU	O2-C2-N1	-2.25	120.31	122.79
1	Aa	2995	PSU	C6-N1-C2	-2.25	120.39	122.68
1	Aa	3305	OMU	C1'-N1-C6	-2.24	115.95	120.84
1	Aa	2654	OMG	O6-C6-C5	-2.23	120.02	124.37
1	Aa	2794	OMG	O6-C6-C5	-2.21	120.05	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	823	PSU	O2-C2-N1	-2.20	120.37	122.79
1	Aa	2868	PSU	O4'-C1'-C2'	2.20	108.24	105.14
1	Aa	1047	PSU	C6-C5-C4	2.20	119.73	118.20
1	Aa	2924	OMU	O2-C2-N3	-2.19	117.41	121.50
1	Aa	2345	OMU	O2-C2-N3	-2.19	117.42	121.50
1	Aa	2947	PSU	C6-C5-C4	2.18	119.72	118.20
1	Aa	68	PSU	O4'-C1'-C2'	2.18	108.22	105.14
1	Aa	3296	OMG	O6-C6-C5	-2.18	120.12	124.37
1	Aa	2132	PSU	O2-C2-N1	-2.17	120.40	122.79
1	Aa	2414	PSU	C5-C6-N1	-2.17	118.85	122.11
1	Aa	2121	OMG	O6-C6-C5	-2.17	120.14	124.37
1	Aa	3113	PSU	C5-C4-N3	2.16	121.47	116.58
1	Aa	669	OMU	C6-N1-C2	-2.16	118.23	120.99
1	Aa	2111	OMU	O2-C2-N1	-2.14	119.94	122.79
1	Aa	2189	PSU	O2-C2-N1	-2.14	120.44	122.79
1	Aa	1061	OMU	C6-N1-C2	-2.14	118.26	120.99
1	Aa	144	OMU	O2-C2-N1	-2.13	119.95	122.79
1	Aa	2134	PSU	C5-C4-N3	2.13	121.39	116.58
1	Aa	880	A2M	C1'-N9-C4	2.13	130.38	126.64
1	Aa	2720	OMU	C6-N1-C2	-2.13	118.27	120.99
1	Aa	2715	PSU	O2-C2-N1	-2.12	120.46	122.79
1	Aa	2518	PSU	C6-N1-C2	-2.12	120.52	122.68
1	Aa	1126	PSU	C5-C4-N3	2.11	121.36	116.58
1	Aa	2291	OMC	C1'-N1-C2	2.11	123.13	118.42
1	Aa	2347	PSU	O4'-C1'-C2'	2.10	108.10	105.14
1	Aa	2958	PSU	O2-C2-N1	-2.09	120.49	122.79
1	Aa	2209	PSU	O4'-C1'-C2'	2.07	108.07	105.14
1	Aa	2276	5MC	CM5-C5-C6	-2.07	120.09	122.85
3	Ac	75	OMG	O6-C6-C5	-2.06	120.34	124.37
1	Aa	2857	PSU	C5-C4-N3	2.06	121.24	116.58
1	Aa	2408	OMU	O4-C4-C5	-2.06	121.54	125.16
1	Aa	2818	OMG	C8-N7-C5	2.06	106.91	102.99
1	Aa	3305	OMU	C6-N1-C2	-2.05	118.36	120.99
1	Aa	3296	OMG	N1-C2-N3	-2.05	119.48	123.32
1	Aa	1127	PSU	C6-C5-C4	2.05	119.63	118.20
1	Aa	2956	UR3	C6-N1-C2	-2.04	119.96	121.79
1	Aa	2654	OMG	N2-C2-N1	2.04	121.06	116.71
1	Aa	1467	PSU	O4'-C1'-C2'	2.04	108.02	105.14
1	Aa	809	OMG	N1-C2-N3	-2.04	119.51	123.32
1	Aa	2622	OMG	O6-C6-C5	-2.04	120.40	124.37
1	Aa	1126	PSU	O2-C2-N1	-2.03	120.56	122.79
1	Aa	2616	PSU	C5-C4-N3	2.03	121.17	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	2873	5MC	CM5-C5-C6	-2.03	120.14	122.85
1	Aa	2414	PSU	O4'-C1'-C2'	2.02	107.99	105.14
1	Aa	2949	A2M	C1'-N9-C4	2.01	130.18	126.64
1	Aa	940	A2M	C1'-N9-C4	2.01	130.18	126.64
1	Aa	2276	5MC	O2-C2-N3	-2.01	119.06	122.33
1	Aa	2124	A2M	C1'-N9-C4	2.01	130.17	126.64
1	Aa	2873	5MC	O2-C2-N3	-2.01	119.07	122.33
1	Aa	2616	PSU	O2-C2-N1	-2.01	120.58	122.79
1	Aa	2947	PSU	O4'-C1'-C2'	2.01	107.97	105.14
1	Aa	2747	PSU	C5-C4-N3	2.01	121.12	116.58
1	Aa	2747	PSU	O2-C2-N1	-2.00	120.58	122.79

There are no chirality outliers.

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	48	OMU	C3'-C4'-C5'-O5'
1	Aa	48	OMU	O4'-C4'-C5'-O5'
1	Aa	68	PSU	O4'-C1'-C5-C4
1	Aa	68	PSU	O4'-C1'-C5-C6
1	Aa	369	A2M	C1'-C2'-O2'-CM'
1	Aa	378	PSU	O4'-C1'-C5-C4
1	Aa	378	PSU	O4'-C1'-C5-C6
1	Aa	669	OMU	O4'-C1'-N1-C2
1	Aa	669	OMU	O4'-C1'-N1-C6
1	Aa	889	PSU	C2'-C1'-C5-C4
1	Aa	889	PSU	O4'-C1'-C5-C4
1	Aa	889	PSU	O4'-C1'-C5-C6
1	Aa	889	PSU	C3'-C4'-C5'-O5'
1	Aa	889	PSU	O4'-C4'-C5'-O5'
1	Aa	912	OMG	O4'-C4'-C5'-O5'
1	Aa	912	OMG	C3'-C4'-C5'-O5'
1	Aa	964	PSU	O4'-C1'-C5-C6
1	Aa	995	PSU	O4'-C1'-C5-C4
1	Aa	995	PSU	O4'-C1'-C5-C6
1	Aa	1009	PSU	O4'-C1'-C5-C4
1	Aa	1009	PSU	O4'-C1'-C5-C6
1	Aa	1047	PSU	O4'-C1'-C5-C4
1	Aa	1047	PSU	O4'-C1'-C5-C6
1	Aa	1057	PSU	O4'-C1'-C5-C4
1	Aa	1057	PSU	O4'-C1'-C5-C6
1	Aa	1057	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Aa	1057	PSU	O4'-C4'-C5'-O5'
1	Aa	1061	OMU	O4'-C1'-N1-C2
1	Aa	1061	OMU	O4'-C1'-N1-C6
1	Aa	1126	PSU	C2'-C1'-C5-C4
1	Aa	1126	PSU	O4'-C1'-C5-C4
1	Aa	1126	PSU	O4'-C1'-C5-C6
1	Aa	1127	PSU	C2'-C1'-C5-C4
1	Aa	1127	PSU	O4'-C1'-C5-C4
1	Aa	1127	PSU	O4'-C1'-C5-C6
1	Aa	1128	PSU	C2'-C1'-C5-C4
1	Aa	1128	PSU	O4'-C1'-C5-C4
1	Aa	1128	PSU	O4'-C1'-C5-C6
1	Aa	1441	OMC	O4'-C1'-N1-C2
1	Aa	1441	OMC	O4'-C1'-N1-C6
1	Aa	1454	OMG	C1'-C2'-O2'-CM2
1	Aa	1467	PSU	O4'-C1'-C5-C4
1	Aa	1467	PSU	O4'-C1'-C5-C6
1	Aa	1844	OMC	O4'-C1'-N1-C2
1	Aa	1844	OMC	O4'-C1'-N1-C6
1	Aa	1844	OMC	O4'-C4'-C5'-O5'
1	Aa	1847	OMC	C3'-C4'-C5'-O5'
1	Aa	1847	OMC	O4'-C4'-C5'-O5'
1	Aa	1868	A2M	O4'-C4'-C5'-O5'
1	Aa	1868	A2M	C3'-C4'-C5'-O5'
1	Aa	2121	OMG	C3'-C4'-C5'-O5'
1	Aa	2122	OMG	C3'-C4'-C5'-O5'
1	Aa	2132	PSU	C2'-C1'-C5-C4
1	Aa	2132	PSU	O4'-C1'-C5-C4
1	Aa	2132	PSU	O4'-C1'-C5-C6
1	Aa	2134	PSU	C2'-C1'-C5-C4
1	Aa	2134	PSU	O4'-C1'-C5-C4
1	Aa	2134	PSU	O4'-C1'-C5-C6
1	Aa	2189	PSU	O4'-C1'-C5-C4
1	Aa	2189	PSU	O4'-C1'-C5-C6
1	Aa	2195	OMC	C2'-C1'-N1-C2
1	Aa	2195	OMC	C2'-C1'-N1-C6
1	Aa	2209	PSU	O4'-C1'-C5-C4
1	Aa	2209	PSU	C2'-C1'-C5-C6
1	Aa	2209	PSU	O4'-C1'-C5-C6
1	Aa	2276	5MC	C3'-C4'-C5'-O5'
1	Aa	2291	OMC	O4'-C1'-N1-C2
1	Aa	2291	OMC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	Aa	2316	PSU	O4'-C1'-C5-C4
1	Aa	2316	PSU	O4'-C1'-C5-C6
1	Aa	2319	A2M	O4'-C4'-C5'-O5'
1	Aa	2319	A2M	C3'-C4'-C5'-O5'
1	Aa	2345	OMU	O4'-C1'-N1-C2
1	Aa	2345	OMU	O4'-C1'-N1-C6
1	Aa	2347	PSU	O4'-C1'-C5-C4
1	Aa	2347	PSU	O4'-C1'-C5-C6
1	Aa	2363	OMC	O4'-C1'-N1-C2
1	Aa	2363	OMC	O4'-C1'-N1-C6
1	Aa	2363	OMC	C3'-C4'-C5'-O5'
1	Aa	2363	OMC	O4'-C4'-C5'-O5'
1	Aa	2389	OMG	O4'-C4'-C5'-O5'
1	Aa	2389	OMG	C3'-C4'-C5'-O5'
1	Aa	2408	OMU	O4'-C1'-N1-C2
1	Aa	2408	OMU	O4'-C1'-N1-C6
1	Aa	2408	OMU	O4'-C4'-C5'-O5'
1	Aa	2414	PSU	C2'-C1'-C5-C4
1	Aa	2414	PSU	O4'-C1'-C5-C4
1	Aa	2414	PSU	O4'-C1'-C5-C6
1	Aa	2518	PSU	C2'-C1'-C5-C4
1	Aa	2518	PSU	O4'-C1'-C5-C4
1	Aa	2518	PSU	O4'-C1'-C5-C6
1	Aa	2616	PSU	O4'-C1'-C5-C4
1	Aa	2616	PSU	O4'-C1'-C5-C6
1	Aa	2622	OMG	O4'-C4'-C5'-O5'
1	Aa	2622	OMG	C1'-C2'-O2'-CM2
1	Aa	2643	A2M	C1'-C2'-O2'-CM'
1	Aa	2653	OMU	O4'-C1'-N1-C2
1	Aa	2653	OMU	O4'-C1'-N1-C6
1	Aa	2715	PSU	O4'-C1'-C5-C4
1	Aa	2715	PSU	C2'-C1'-C5-C6
1	Aa	2715	PSU	O4'-C1'-C5-C6
1	Aa	2715	PSU	C3'-C4'-C5'-O5'
1	Aa	2715	PSU	O4'-C4'-C5'-O5'
1	Aa	2720	OMU	O4'-C1'-N1-C2
1	Aa	2720	OMU	O4'-C1'-N1-C6
1	Aa	2747	PSU	O4'-C1'-C5-C4
1	Aa	2747	PSU	O4'-C1'-C5-C6
1	Aa	2794	OMG	C3'-C4'-C5'-O5'
1	Aa	2818	OMG	C3'-C4'-C5'-O5'
1	Aa	2829	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	Aa	2829	PSU	O4'-C1'-C5-C4
1	Aa	2829	PSU	O4'-C1'-C5-C6
1	Aa	2839	OMC	O4'-C1'-N1-C2
1	Aa	2839	OMC	O4'-C1'-N1-C6
1	Aa	2839	OMC	C1'-C2'-O2'-CM2
1	Aa	2857	PSU	O4'-C1'-C5-C4
1	Aa	2857	PSU	O4'-C1'-C5-C6
1	Aa	2868	PSU	O4'-C1'-C5-C4
1	Aa	2868	PSU	C2'-C1'-C5-C6
1	Aa	2868	PSU	O4'-C1'-C5-C6
1	Aa	2886	OMU	C1'-C2'-O2'-CM2
1	Aa	2886	OMU	C3'-C4'-C5'-O5'
1	Aa	2924	OMU	O4'-C1'-N1-C2
1	Aa	2924	OMU	O4'-C1'-N1-C6
1	Aa	2926	PSU	O4'-C1'-C5-C4
1	Aa	2926	PSU	O4'-C1'-C5-C6
1	Aa	2947	PSU	O4'-C1'-C5-C4
1	Aa	2947	PSU	O4'-C1'-C5-C6
1	Aa	2949	A2M	C1'-C2'-O2'-CM2
1	Aa	2958	PSU	C3'-C4'-C5'-O5'
1	Aa	2958	PSU	O4'-C4'-C5'-O5'
1	Aa	2995	PSU	O4'-C1'-C5-C4
1	Aa	2995	PSU	C2'-C1'-C5-C6
1	Aa	2995	PSU	O4'-C1'-C5-C6
1	Aa	2995	PSU	C3'-C4'-C5'-O5'
1	Aa	2995	PSU	O4'-C4'-C5'-O5'
1	Aa	3113	PSU	O4'-C1'-C5-C4
1	Aa	3113	PSU	O4'-C1'-C5-C6
1	Aa	3305	OMU	O4'-C1'-N1-C2
1	Aa	3305	OMU	O4'-C1'-N1-C6
3	Ac	74	PSU	O4'-C1'-C5-C4
3	Ac	74	PSU	C2'-C1'-C5-C6
3	Ac	74	PSU	O4'-C1'-C5-C6
3	Ac	74	PSU	C3'-C4'-C5'-O5'
3	Ac	74	PSU	O4'-C4'-C5'-O5'
3	Ac	75	OMG	O4'-C4'-C5'-O5'
3	Ac	75	OMG	C3'-C4'-C5'-O5'
5	CB	246	HIC	CA-CB-CG-ND1
1	Aa	1454	OMG	O4'-C4'-C5'-O5'
1	Aa	2122	OMG	O4'-C4'-C5'-O5'
1	Aa	2195	OMC	O4'-C4'-C5'-O5'
1	Aa	2223	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Aa	2622	OMG	C3'-C4'-C5'-O5'
1	Aa	2794	OMG	O4'-C4'-C5'-O5'
1	Aa	2886	OMU	O4'-C4'-C5'-O5'
1	Aa	2914	A2M	O4'-C4'-C5'-O5'
1	Aa	2111	OMU	O4'-C1'-N1-C2
1	Aa	1371	A2M	O4'-C4'-C5'-O5'
1	Aa	1371	A2M	C3'-C4'-C5'-O5'
1	Aa	1454	OMG	C3'-C4'-C5'-O5'
1	Aa	1844	OMC	C3'-C4'-C5'-O5'
1	Aa	2195	OMC	C3'-C4'-C5'-O5'
1	Aa	2223	PSU	C3'-C4'-C5'-O5'
1	Aa	2408	OMU	C3'-C4'-C5'-O5'
1	Aa	2732	OMU	C3'-C4'-C5'-O5'
1	Aa	2818	OMG	O4'-C4'-C5'-O5'
1	Aa	2914	A2M	C3'-C4'-C5'-O5'
1	Aa	2962	OMC	C3'-C4'-C5'-O5'
1	Aa	2111	OMU	O4'-C1'-N1-C6
42	Co	55	MLZ	CG-CD-CE-NZ
1	Aa	1473	OMC	C3'-C4'-C5'-O5'
1	Aa	2654	OMG	C3'-C4'-C5'-O5'
1	Aa	1473	OMC	O4'-C4'-C5'-O5'
1	Aa	1512	OMC	O4'-C4'-C5'-O5'
1	Aa	2121	OMG	O4'-C4'-C5'-O5'
1	Aa	2276	5MC	O4'-C4'-C5'-O5'
1	Aa	2654	OMG	O4'-C4'-C5'-O5'
1	Aa	3296	OMG	O4'-C4'-C5'-O5'
1	Aa	2732	OMU	O4'-C4'-C5'-O5'
1	Aa	2962	OMC	O4'-C4'-C5'-O5'
1	Aa	3296	OMG	C3'-C4'-C5'-O5'
1	Aa	2873	5MC	C2'-C1'-N1-C6
1	Aa	1852	OMG	O4'-C4'-C5'-O5'
1	Aa	1512	OMC	C3'-C4'-C5'-O5'
1	Aa	2794	OMG	C1'-C2'-O2'-CM2
1	Aa	1847	OMC	O4'-C1'-N1-C6
1	Aa	2926	PSU	C4'-C5'-O5'-P
1	Aa	912	OMG	C3'-C2'-O2'-CM2
1	Aa	2312	PSU	C4'-C5'-O5'-P
1	Aa	2873	5MC	O4'-C1'-N1-C6
1	Aa	2195	OMC	O4'-C1'-N1-C6
1	Aa	2408	OMU	C4'-C5'-O5'-P
1	Aa	1847	OMC	O4'-C1'-N1-C2
1	Aa	2873	5MC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	Aa	1847	OMC	C3'-C2'-O2'-CM2
1	Aa	2279	A2M	C3'-C2'-O2'-CM'
1	Aa	2407	OMG	C3'-C2'-O2'-CM2
1	Aa	2796	OMG	C3'-C2'-O2'-CM2
1	Aa	2195	OMC	O4'-C1'-N1-C2
1	Aa	2956	UR3	O4'-C4'-C5'-O5'
1	Aa	1847	OMC	C2'-C1'-N1-C2
1	Aa	1852	OMG	C3'-C4'-C5'-O5'
1	Aa	68	PSU	C4'-C5'-O5'-P
1	Aa	2873	5MC	C2'-C1'-N1-C2
1	Aa	144	OMU	O4'-C4'-C5'-O5'
1	Aa	48	OMU	C2'-C1'-N1-C2
1	Aa	821	A2M	C4'-C5'-O5'-P
1	Aa	821	A2M	O4'-C4'-C5'-O5'
1	Aa	1441	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 317 ligands modelled in this entry, 317 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

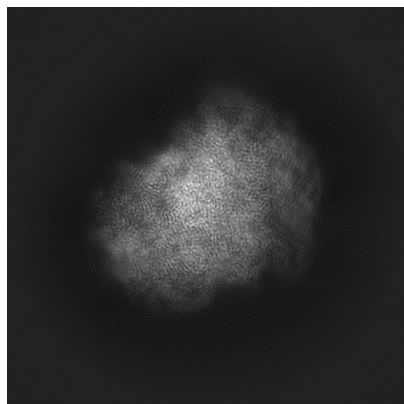
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36331. These allow visual inspection of the internal detail of the map and identification of artifacts.

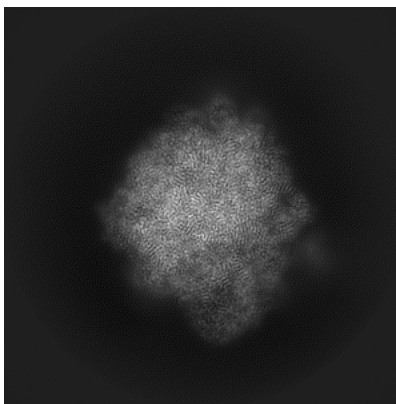
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

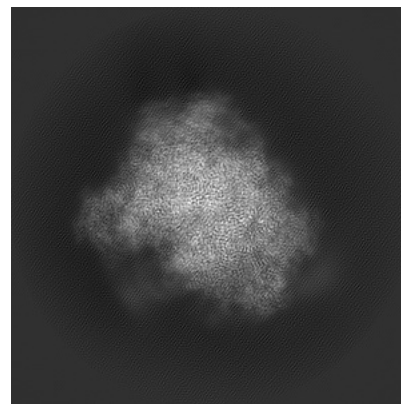
6.1.1 Primary map



X

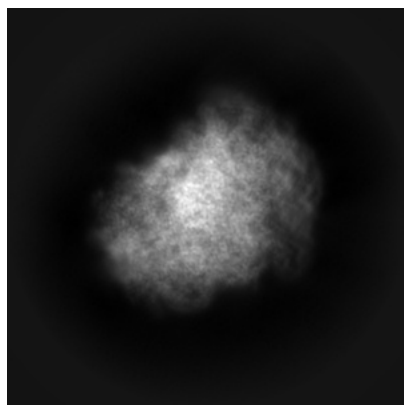


Y

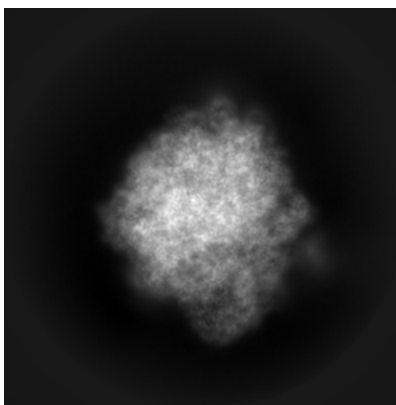


Z

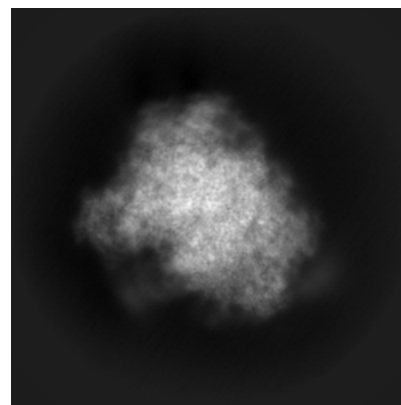
6.1.2 Raw map



X



Y

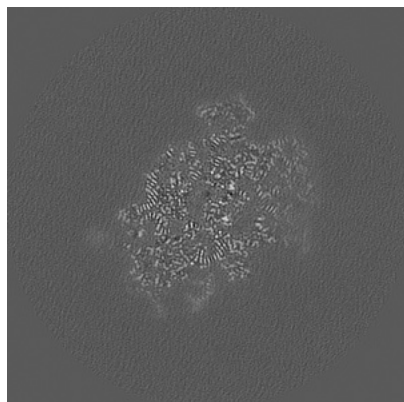


Z

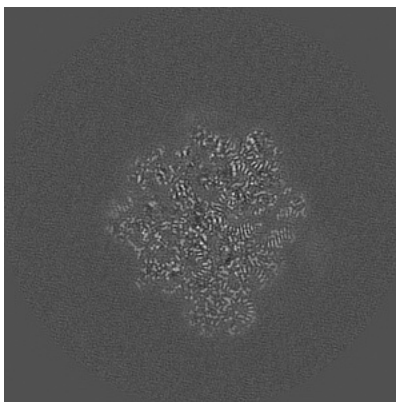
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

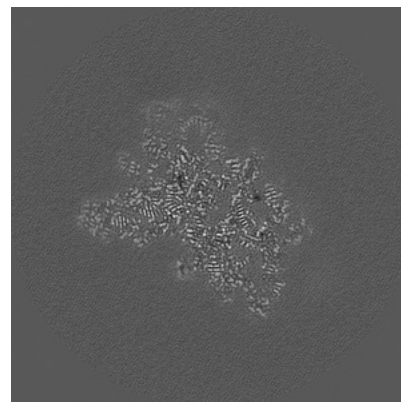
6.2.1 Primary map



X Index: 180

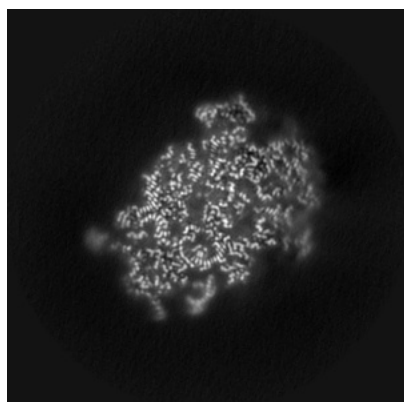


Y Index: 180

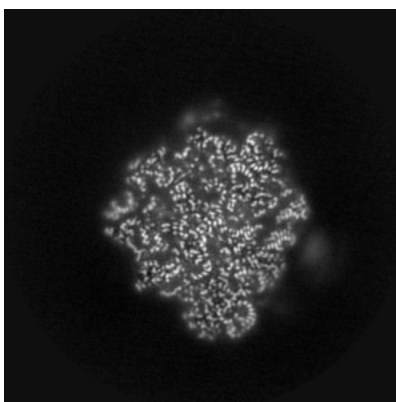


Z Index: 180

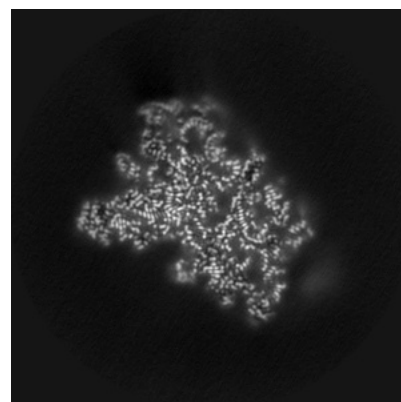
6.2.2 Raw map



X Index: 180



Y Index: 180

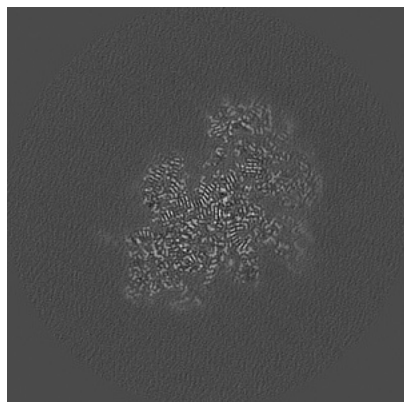


Z Index: 180

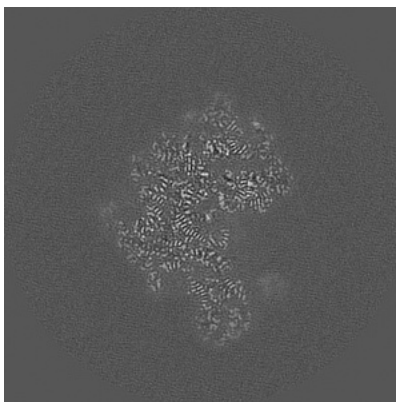
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

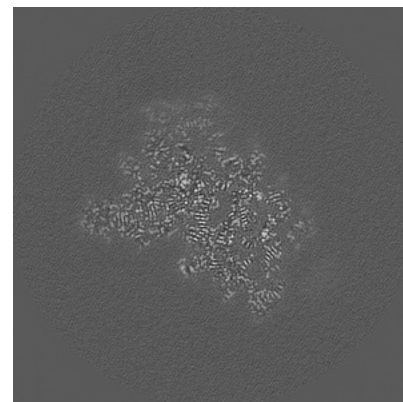
6.3.1 Primary map



X Index: 168

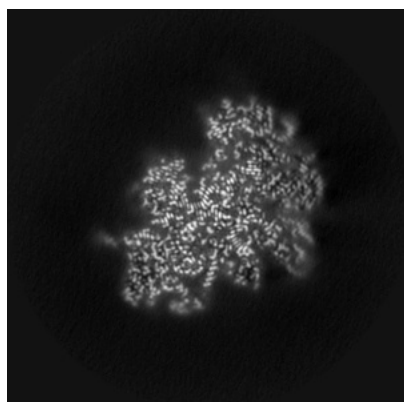


Y Index: 165

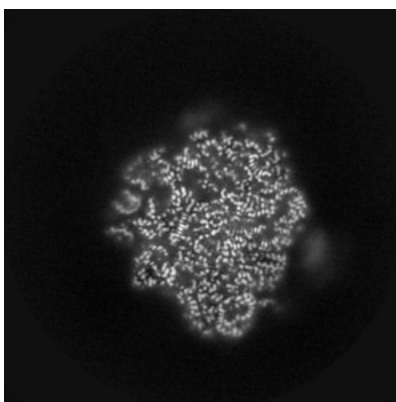


Z Index: 182

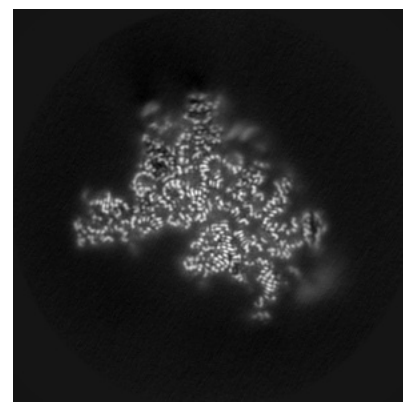
6.3.2 Raw map



X Index: 168



Y Index: 184

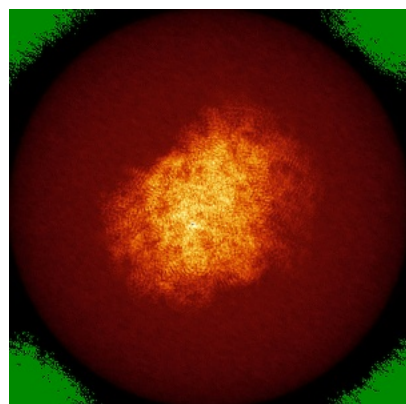


Z Index: 195

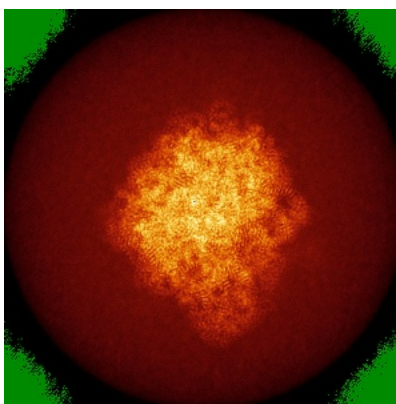
The images above show the largest variance slices of the map in three orthogonal directions.

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

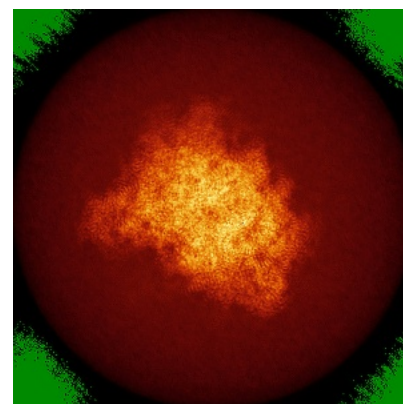
6.4.1 Primary map



X

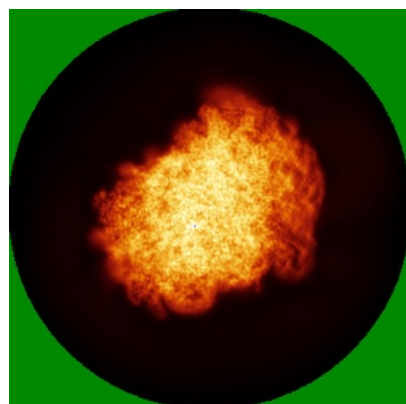


Y

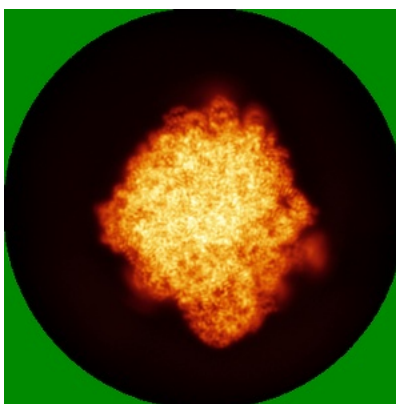


Z

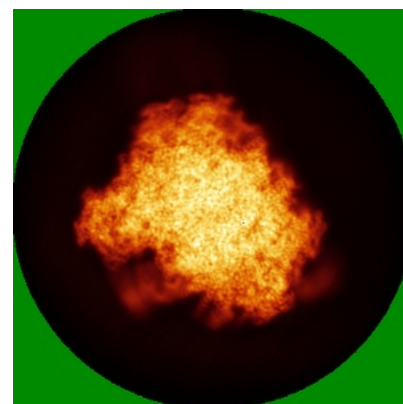
6.4.2 Raw map



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.

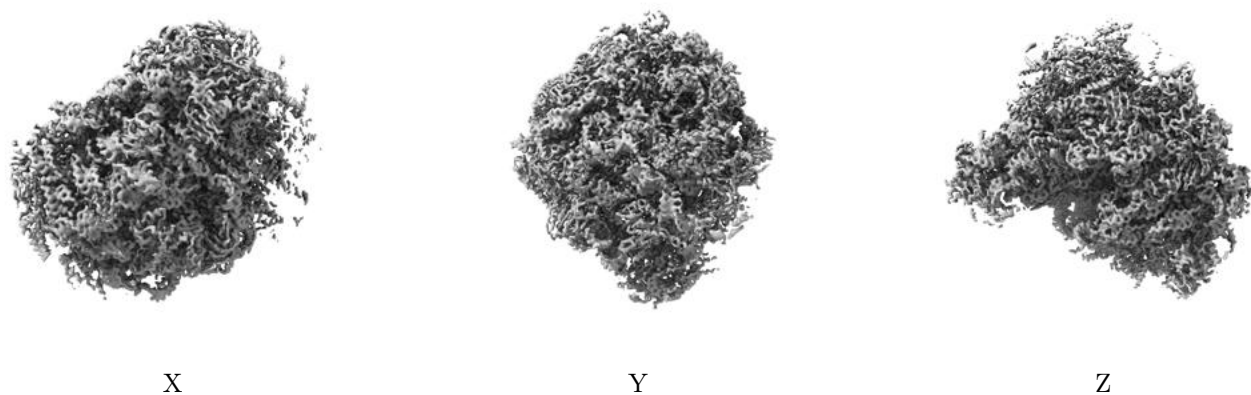
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

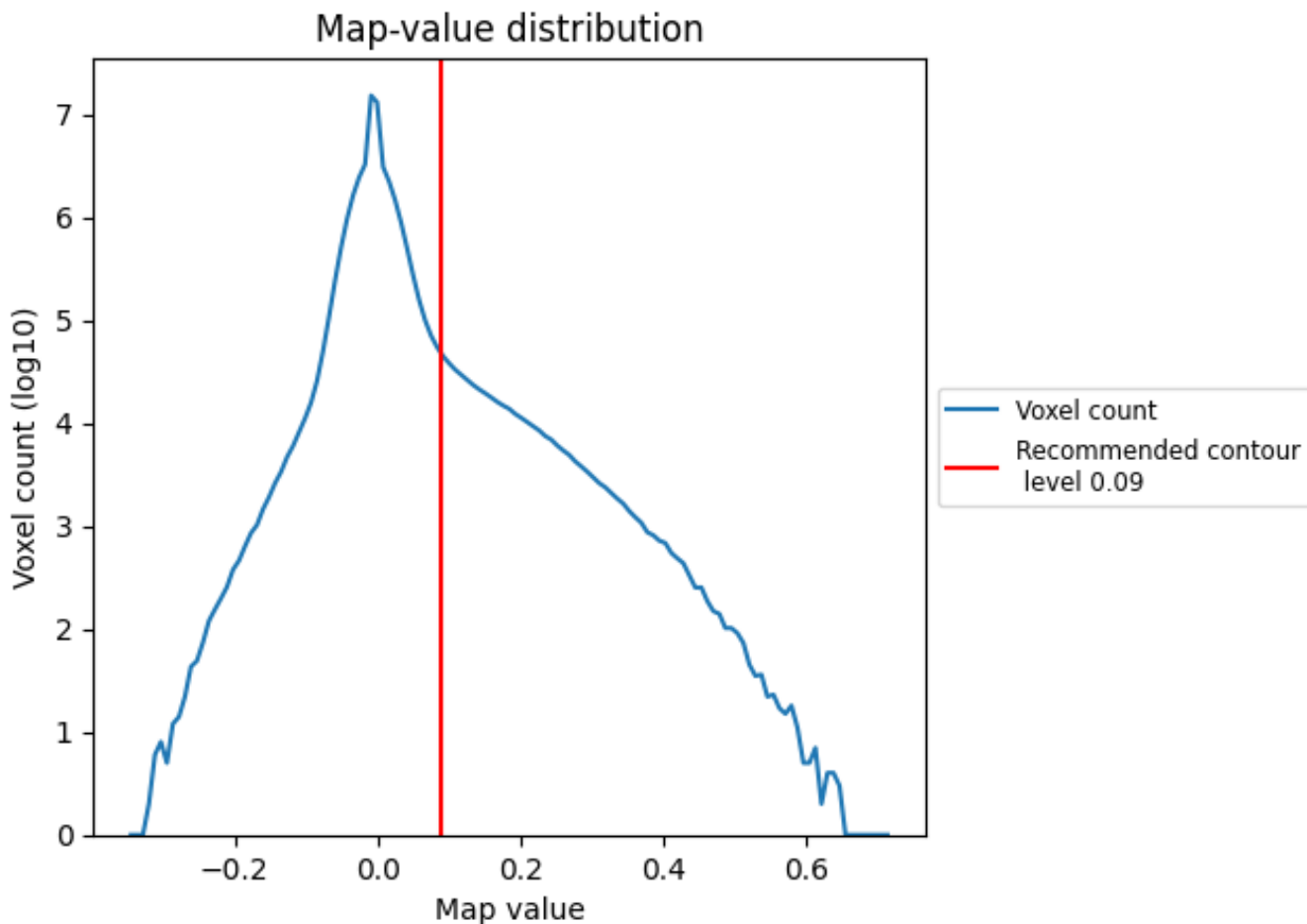
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

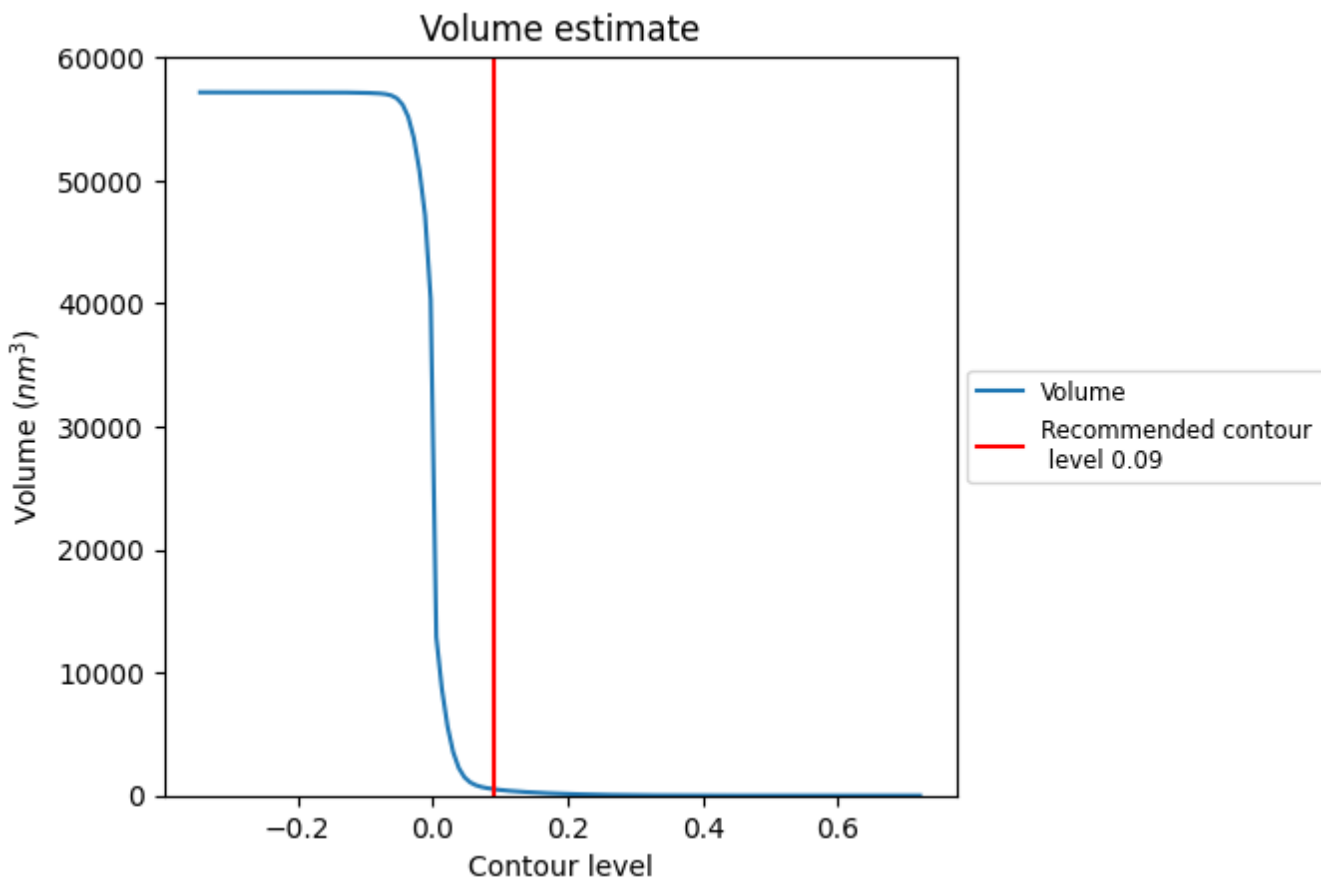
This section contains the results of statistical analysis of the map.

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.

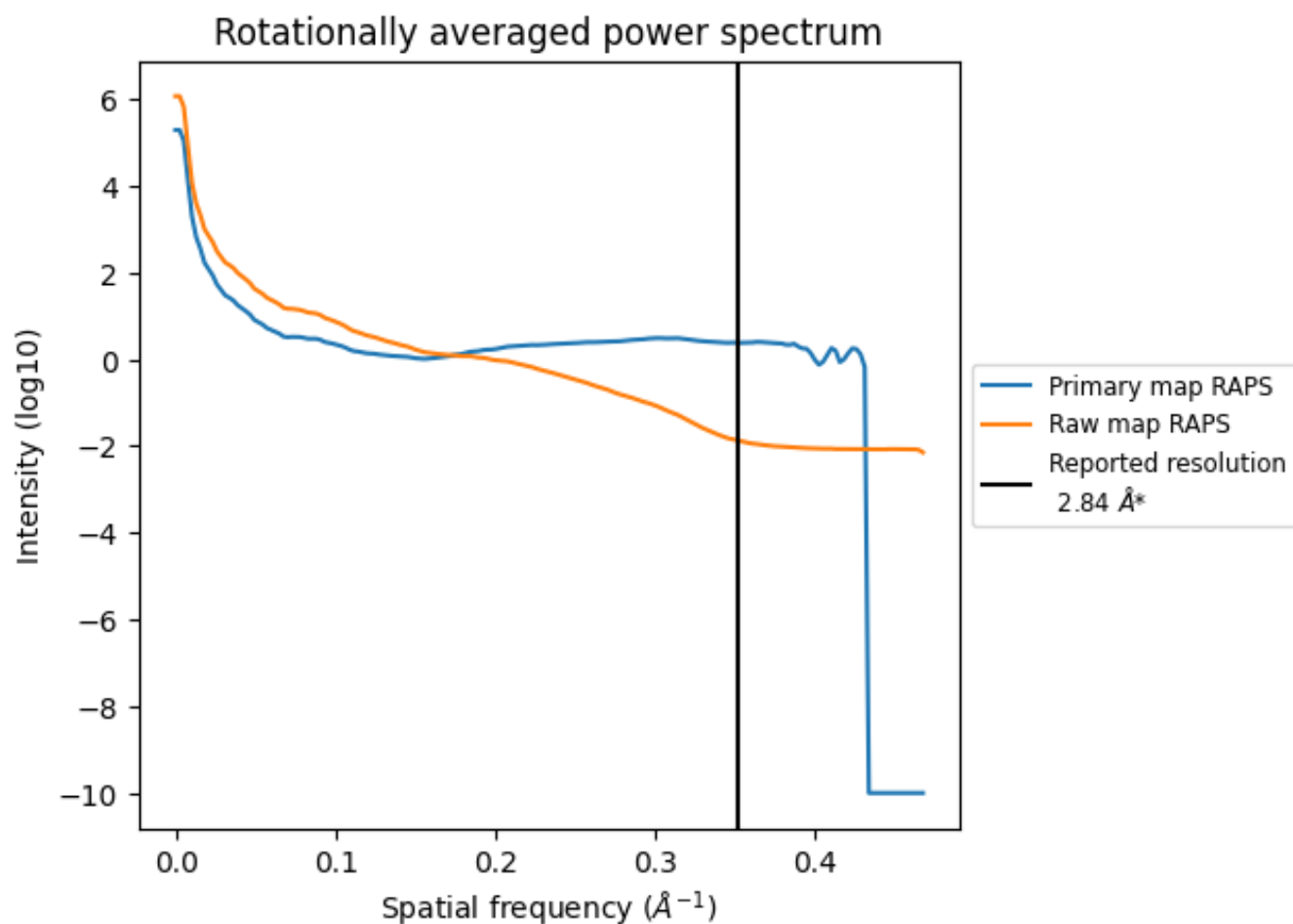
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522 nm³; this corresponds to an approximate mass of 472 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 i

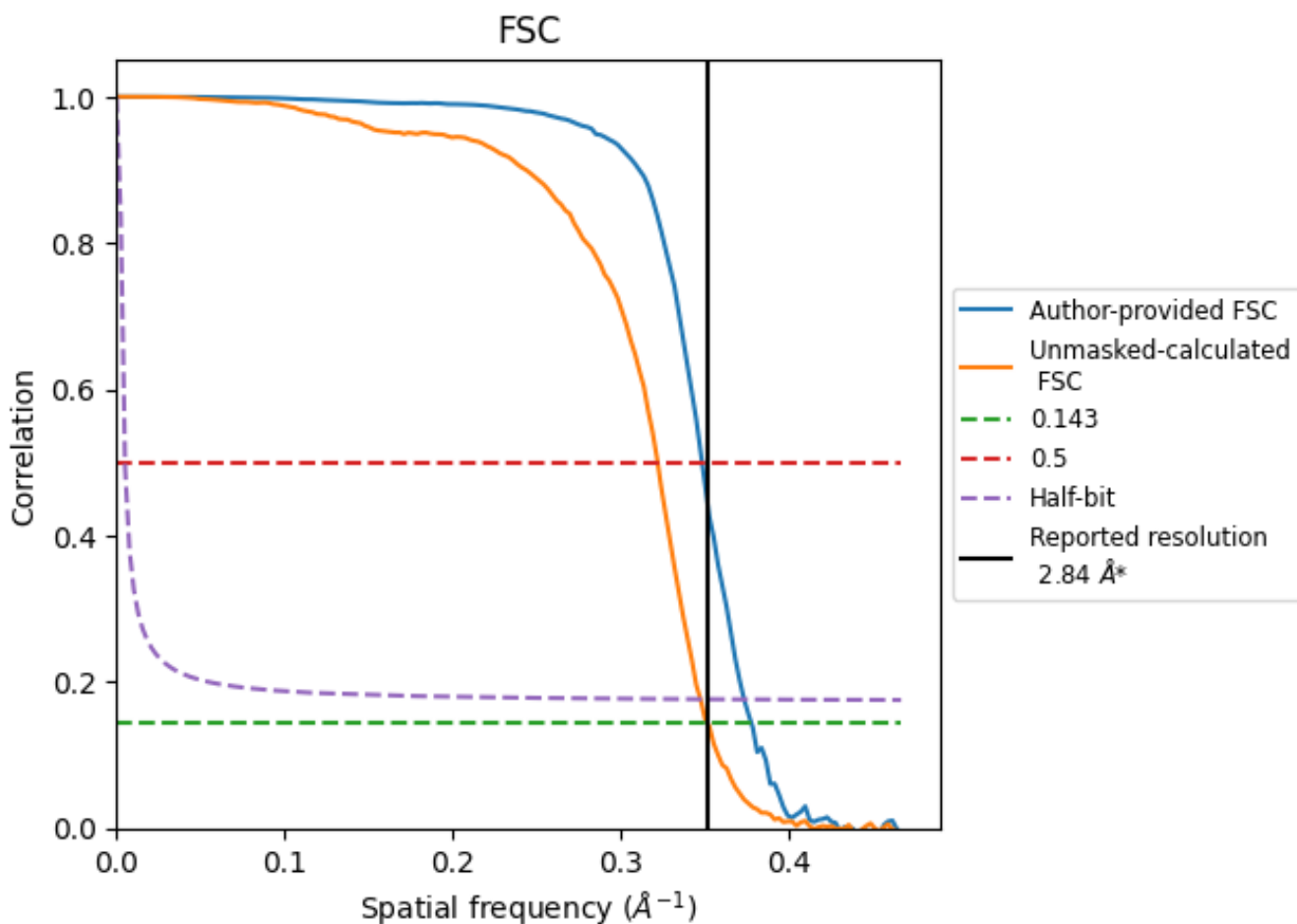


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 \AA^{-1}

8.2 Resolution estimates [i](#)

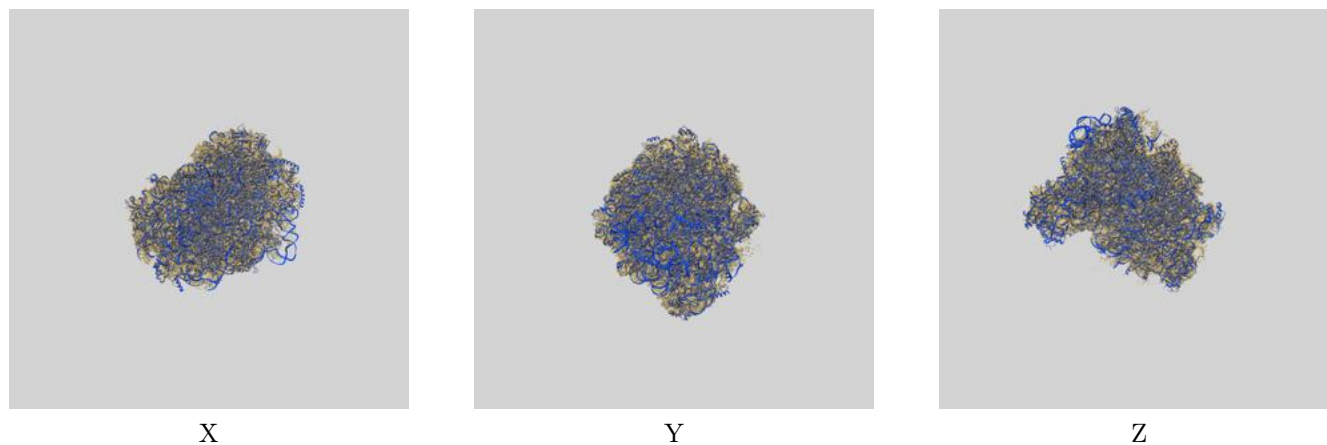
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.64	2.87	2.68
Unmasked-calculated*	2.84	3.10	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

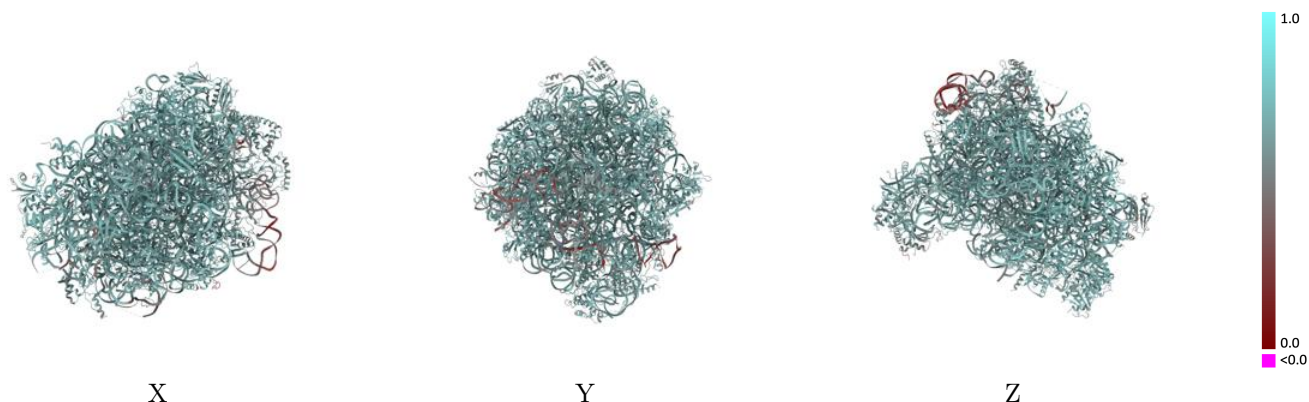
This section contains information regarding the fit between EMDB map EMD-36331 and PDB model 8JIV. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



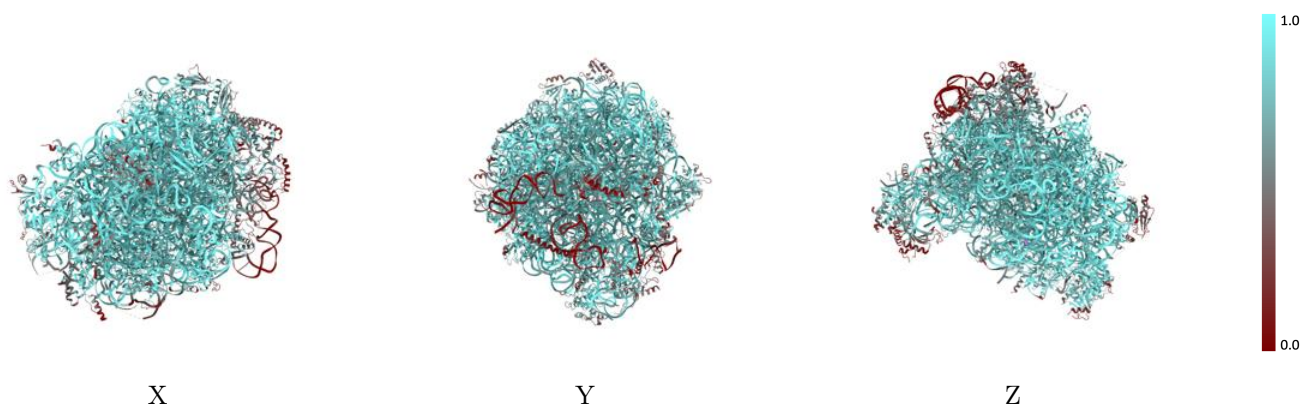
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



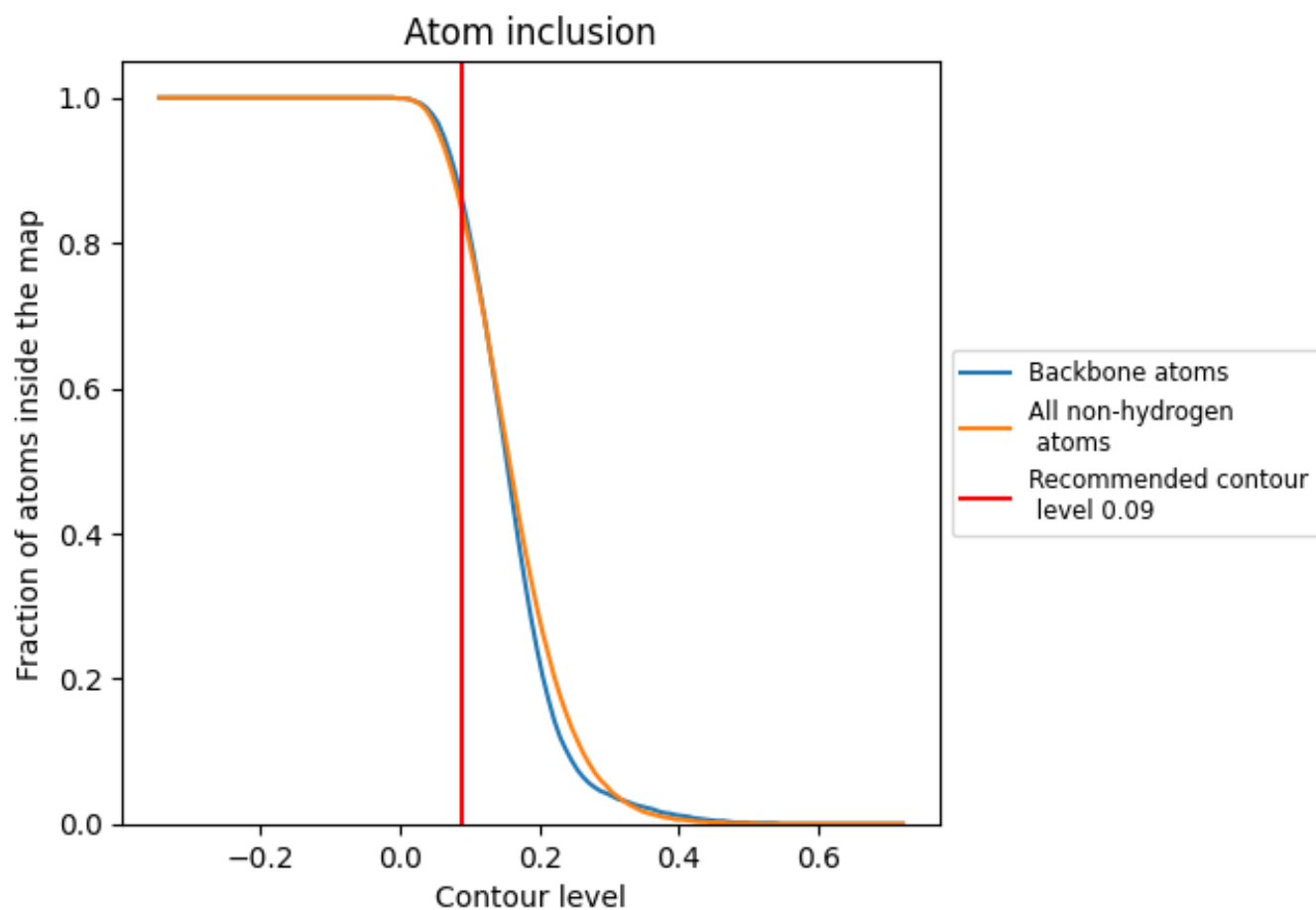
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.6490
Aa	 0.8840	 0.6450
Ab	 0.8810	 0.6430
Ac	 0.8980	 0.6540
CA	 0.9470	 0.6940
CB	 0.8880	 0.6830
CC	 0.7450	 0.6390
CD	 0.6780	 0.6380
CE	 0.3820	 0.5590
CF	 0.7290	 0.6430
CG	 0.7120	 0.6400
CH	 0.6780	 0.6380
CI	 0.7060	 0.6400
CJ	 0.3640	 0.5770
CL	 0.8410	 0.6660
CM	 0.6430	 0.6290
CN	 0.9740	 0.6950
CO	 0.7780	 0.6540
CP	 0.8840	 0.6670
CQ	 0.8940	 0.6690
CR	 0.8610	 0.6800
CS	 0.8050	 0.6570
CT	 0.7940	 0.6590
CU	 0.4120	 0.5750
CV	 0.8980	 0.6820
CW	 0.8430	 0.6690
CX	 0.8290	 0.6670
CY	 0.8630	 0.6680
CZ	 0.7500	 0.6540
Ca	 0.9170	 0.6850
Cb	 0.8760	 0.6590
Cc	 0.6950	 0.6400
Cd	 0.8520	 0.6770
Ce	 0.8940	 0.6720
Cf	 0.8200	 0.6480



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Chain	Atom inclusion	Q-score
Cg	 0.9090	 0.6920
Ch	 0.8070	 0.6450
Ci	 0.7450	 0.6420
Cj	 0.9190	 0.6730
Ck	 0.5820	 0.6180
Cl	 0.9180	 0.6730
Cm	 0.8350	 0.6700
Co	 0.8570	 0.6800
Cp	 0.8440	 0.6780
Cr	 0.6780	 0.6300