



Full wwPDB EM Validation Report ⓘ

Jun 21, 2023 – 11:52 pm BST

PDB ID : 8AZW
EMDB ID : EMD-15773
Title : Cryo-EM structure of the plant 60S subunit
Authors : Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.; Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.
Deposited on : 2022-09-06
Resolution : 2.14 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:

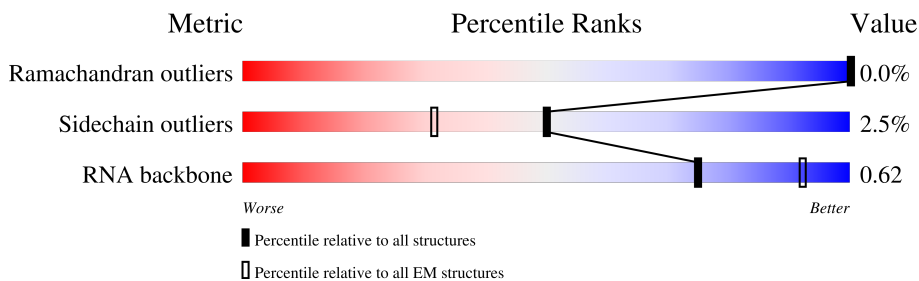
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

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 2.14 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.



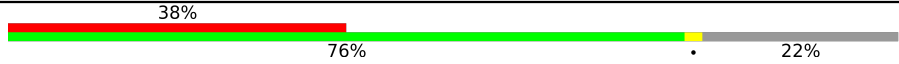

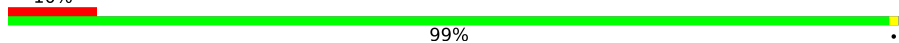
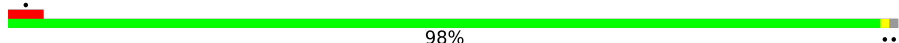




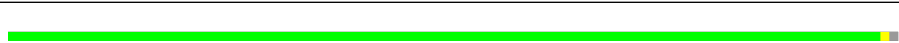

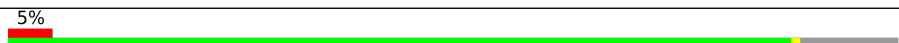


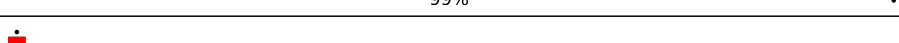
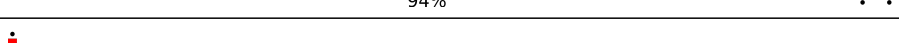
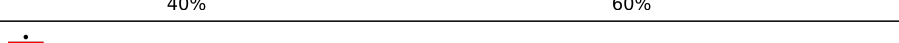
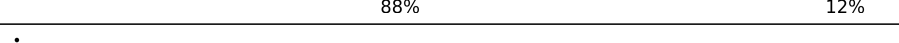
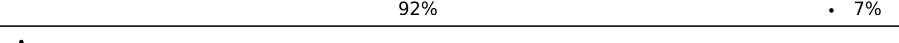
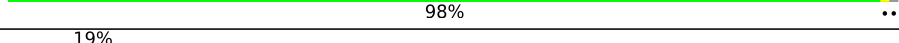


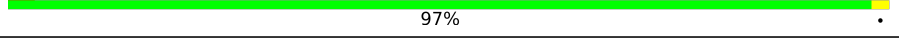
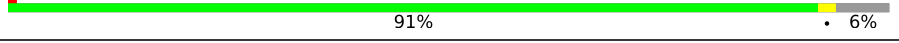
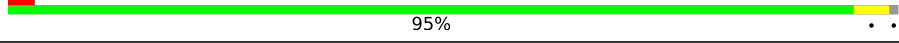
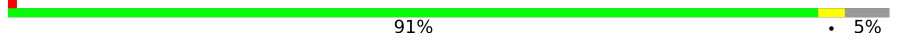
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C	119	
2	D	206	
3	E	134	
4	F	204	
5	G	187	
6	H	214	
7	I	178	
8	J	164	




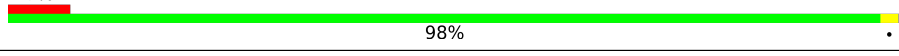
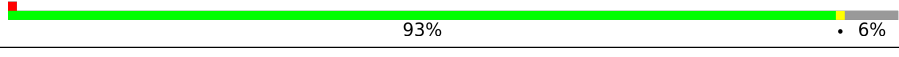
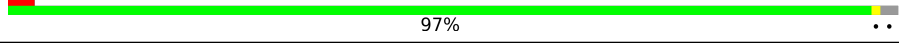
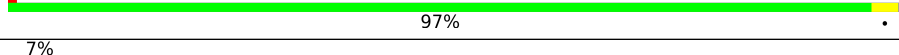
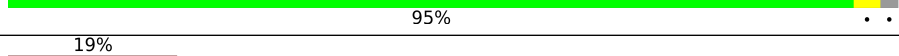
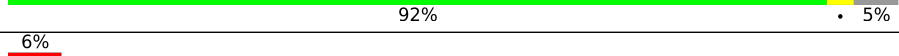
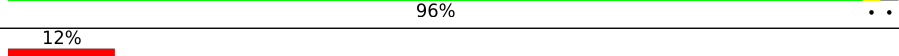

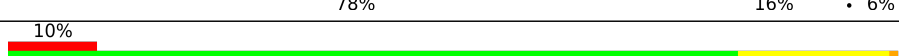
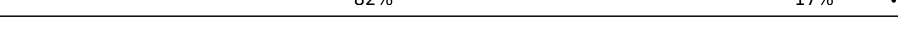
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Mol	Chain	Length	Quality of chain
9	K	127	
10	L	164	
11	M	135	
12	N	143	
13	O	61	
14	P	113	
15	Q	120	
16	R	133	
17	S	112	
18	T	120	
19	U	110	
20	V	95	
21	W	69	
22	X	51	
23	Y	128	
24	p	25	
25	Z	105	
26	a	92	
27	b	230	
28	c	258	
29	d	206	
30	e	140	
31	f	148	
32	g	221	
33	h	301	

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Mol	Chain	Length	Quality of chain
34	j	175	 87% 12%
35	k	154	 74% 24%
36	m	146	 84% 14%
37	n	123	 7% 98%
38	o	260	 93% 6%
39	q	242	 97%
40	r	389	 97%
41	s	405	 7% 95%
42	t	181	 19% 92% 5%
43	u	194	 6% 96%
44	l	24	 12% 17% 83%
45	A	3390	 8% 78% 16% 6%
46	B	163	 10% 82% 17%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 223261 atoms, of which 92404 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 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	C	119	3823	1133	1285	457	829	119	0	0

- Molecule 2 is a protein called eL13 (60S ribosomal protein L13).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	200	3296	1007	1691	324	270	4	0	0

- Molecule 3 is a protein called eL14 (60S ribosomal protein L14).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	130	2206	678	1150	196	179	3	0	0

- Molecule 4 is a protein called eL15 (60S ribosomal protein L15).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	F	203	3469	1071	1768	350	277	3	0	0

- Molecule 5 is a protein called eL18 (60S ribosomal protein L18).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	G	186	3042	931	1580	283	245	3	0	0

- Molecule 6 is a protein called eL19 (60S ribosomal protein L19).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	H	182	3181	946	1652	327	247	9	0	0

- Molecule 7 is a protein called eL20 (60S ribosomal protein L18a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	I	177	3061	969	1556	277	251	8	0	0

- Molecule 8 is a protein called eL21 (60S ribosomal protein L21).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	J	163	2672	823	1366	255	224	4	0	0

- Molecule 9 is a protein called eL22 (60S ribosomal protein L22).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	K	99	1653	515	845	141	150	2	0	0

- Molecule 10 is a protein called eL24 (60S ribosomal protein L24).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	L	62	1079	341	553	101	81	3	0	0

- Molecule 11 is a protein called eL27 (60S ribosomal protein L27).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	M	134	2283	708	1184	206	183	2	0	0

- Molecule 12 is a protein called eL28 (60S ribosomal protein L28).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	N	142	2298	701	1187	207	201	2	0	0

- Molecule 13 is a protein called eL29 (60S ribosomal protein L29).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	O	49	831	250	419	95	66	1	0	0

- Molecule 14 is a protein called eL30 (60S ribosomal protein L30).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	P	97	1526	475	781	130	135	5	0	0

- Molecule 15 is a protein called eL31 (60S ribosomal protein L31).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	Q	108	1809	549	934	168	156	2	0	0

- Molecule 16 is a protein called eL32 (60S ribosomal protein L32).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	R	126	2151	655	1115	207	169	5	0	0

- Molecule 17 is a protein called eL33 (60S ribosomal protein L35a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	S	111	1832	571	932	171	153	5	0	0

- Molecule 18 is a protein called eL34 (60S ribosomal protein L34).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	T	114	1939	579	1013	193	153	1	0	0

- Molecule 19 is a protein called eL36 (60S ribosomal protein L36).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	U	98	1650	489	868	162	129	2	0	0

- Molecule 20 is a protein called eL37 (60S ribosomal protein L37).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	V	86	1427	429	726	155	112	5	0	0

- Molecule 21 is a protein called eL38 (60S ribosomal protein L38).

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	W	68	Total	C	H	N	O	S	0	0
			1160	358	602	99	98	3		

- Molecule 22 is a protein called eL39 (60S ribosomal protein L39).

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	X	50	Total	C	H	N	O	S	0	0
			928	286	480	96	64	2		

- Molecule 23 is a protein called eL40 (60S ribosomal protein L40).

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	Y	51	Total	C	H	N	O	S	0	0
			881	262	460	88	65	6		

- Molecule 24 is a protein called eL41 (60S ribosomal protein L41).

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	p	25	Total	C	H	N	O	S	0	0
			527	145	289	62	28	3		

- Molecule 25 is a protein called eL42 (60S ribosomal protein L42).

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	Z	98	Total	C	H	N	O	S	0	0
			1629	494	842	157	131	5		

- Molecule 26 is a protein called eL43 (60S ribosomal protein L37a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	a	91	Total	C	H	N	O	S	0	0
			1453	443	745	136	124	5		

- Molecule 27 is a protein called eL6 (60S ribosomal protein L6).

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	b	208	Total	C	H	N	O	S	0	0
			3360	1046	1749	290	271	4		

- Molecule 28 is a protein called eL8 (60S ribosomal protein L7a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	c	233	3907	1206	2028	347	319	7	0	0

- Molecule 29 is a protein called uL13 (60S ribosomal protein L13a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	d	205	3414	1046	1774	318	268	8	0	0

- Molecule 30 is a protein called uL14 (60S ribosomal protein L23).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	e	131	2029	623	1044	183	170	9	0	0

- Molecule 31 is a protein called uL15 (60S ribosomal protein L27a).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	f	147	2361	740	1200	228	190	3	0	0

- Molecule 32 is a protein called uL16 (60S ribosomal protein L10).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	g	209	3397	1058	1726	329	273	11	0	0

- Molecule 33 is a protein called uL18 (60S ribosomal protein L5).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	h	288	4715	1481	2374	426	429	5	0	0

- Molecule 34 is a protein called uL22 (60S ribosomal protein L17).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	j	154	2515	775	1270	246	219	5	0	0

- Molecule 35 is a protein called uL23 (60S ribosomal protein L23a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	k	117	1980	609	1030	170	169	2	0	0

- Molecule 36 is a protein called uL24 (60S ribosomal protein L26).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	m	126	2124	634	1103	209	175	3	0	0

- Molecule 37 is a protein called uL29 (60S ribosomal protein L35).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	n	122	2140	642	1141	191	165	1	0	0

- Molecule 38 is a protein called uL2 (60S ribosomal protein L8).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	o	245	3791	1174	1911	381	315	10	0	0

- Molecule 39 is a protein called uL30 (60S ribosomal protein L7).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	q	238	4016	1256	2058	359	339	4	0	0

- Molecule 40 is a protein called uL3 (60S ribosomal protein L3).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	r	386	6327	1981	3223	578	530	15	0	0

- Molecule 41 is a protein called uL4 (60S ribosomal protein L4).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	s	398	6324	1956	3227	583	548	10	0	0

- Molecule 42 is a protein called uL5 (60S ribosomal protein L11).

Mol	Chain	Residues	Atoms					AltConf	Trace	
42	t	172	Total	C	H	N	O	S	0	0
			2836	882	1444	259	244	7		

- Molecule 43 is a protein called uL6 (60S ribosomal protein L9).

Mol	Chain	Residues	Atoms					AltConf	Trace	
43	u	191	Total	C	H	N	O	S	0	0
			3124	963	1604	276	276	5		

- Molecule 44 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
44	l	4	Total	C	H	N	O		0	0
			29	12	9	4	4			

- Molecule 45 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
45	A	3196	Total	C	H	N	O	P	0	0
			103169	30602	34651	12456	22264	3196		

- Molecule 46 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
46	B	163	Total	C	H	N	O	P	0	0
			5243	1555	1763	627	1135	163		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	U	C	conflict	GB 1782605526

- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	C	4	Total	Mg	0
			4	4	
47	V	1	Total	Mg	0
			1	1	
47	e	1	Total	Mg	0
			1	1	
47	j	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
47	q	1	Total 1	Mg 1	0
47	r	2	Total 2	Mg 2	0
47	A	50	Total 50	Mg 50	0

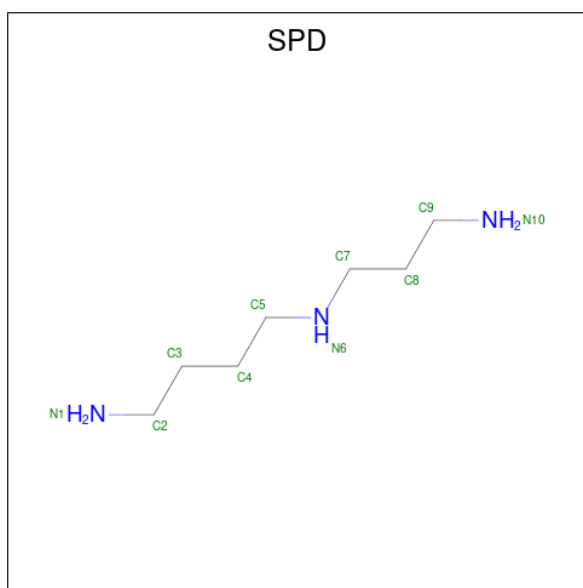
- Molecule 48 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
48	D	1	Total 1	K 1	0
48	R	1	Total 1	K 1	0
48	T	1	Total 1	K 1	0
48	Z	1	Total 1	K 1	0
48	f	1	Total 1	K 1	0
48	g	1	Total 1	K 1	0
48	o	2	Total 2	K 2	0
48	r	1	Total 1	K 1	0
48	A	83	Total 83	K 83	0
48	B	2	Total 2	K 2	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

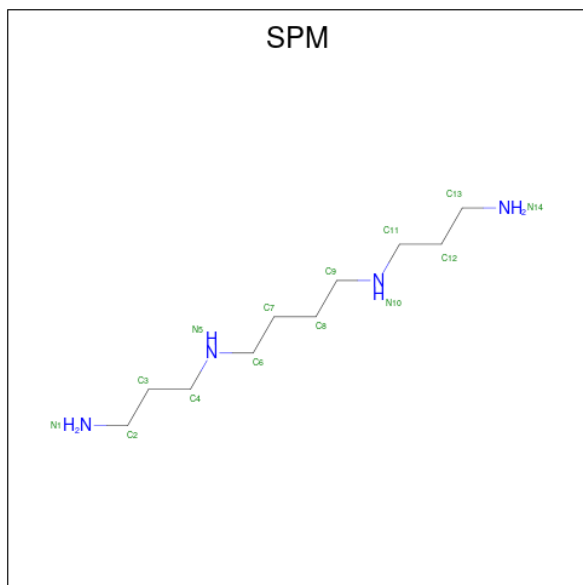
Mol	Chain	Residues	Atoms		AltConf
49	V	1	Total 1	Zn 1	0
49	Y	1	Total 1	Zn 1	0
49	Z	1	Total 1	Zn 1	0
49	a	1	Total 1	Zn 1	0

- Molecule 50 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
50	A	1	Total	C	N	0
			10	7	3	

- Molecule 51 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	H	N	0
			40	10	26	4	
51	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	C	88	Total 88	O 88	0
52	D	47	Total 47	O 47	0
52	F	105	Total 105	O 105	0
52	G	53	Total 53	O 53	0
52	H	11	Total 11	O 11	0
52	I	13	Total 13	O 13	0
52	J	27	Total 27	O 27	0
52	M	2	Total 2	O 2	0
52	N	8	Total 8	O 8	0
52	O	26	Total 26	O 26	0
52	Q	3	Total 3	O 3	0
52	R	42	Total 42	O 42	0
52	S	5	Total 5	O 5	0
52	T	12	Total 12	O 12	0
52	U	3	Total 3	O 3	0
52	V	30	Total 30	O 30	0
52	W	1	Total 1	O 1	0
52	X	6	Total 6	O 6	0
52	Y	2	Total 2	O 2	0
52	Z	25	Total 25	O 25	0
52	a	6	Total 6	O 6	0

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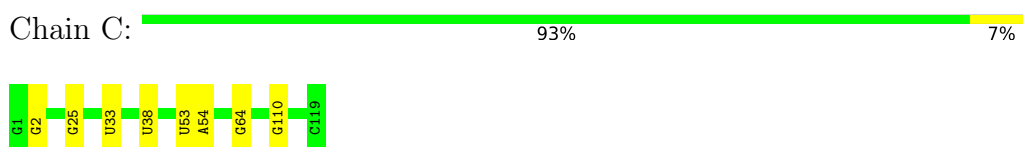
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	b	1	Total 1	O 1	0
52	c	10	Total 10	O 10	0
52	d	12	Total 12	O 12	0
52	e	13	Total 13	O 13	0
52	f	41	Total 41	O 41	0
52	g	16	Total 16	O 16	0
52	h	19	Total 19	O 19	0
52	j	15	Total 15	O 15	0
52	k	16	Total 16	O 16	0
52	m	8	Total 8	O 8	0
52	n	17	Total 17	O 17	0
52	o	56	Total 56	O 56	0
52	q	27	Total 27	O 27	0
52	r	27	Total 27	O 27	0
52	s	66	Total 66	O 66	0
52	t	1	Total 1	O 1	0
52	u	2	Total 2	O 2	0
52	A	3376	Total 3376	O 3376	0
52	B	168	Total 168	O 168	0

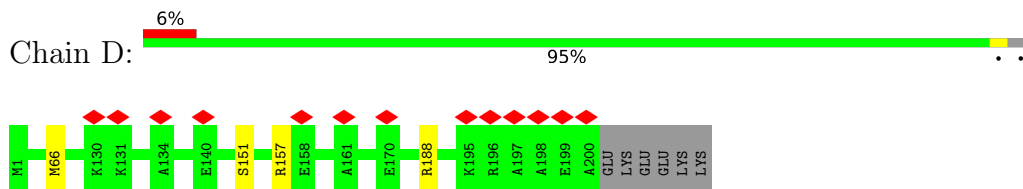
3 Residue-property plots [i](#)

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

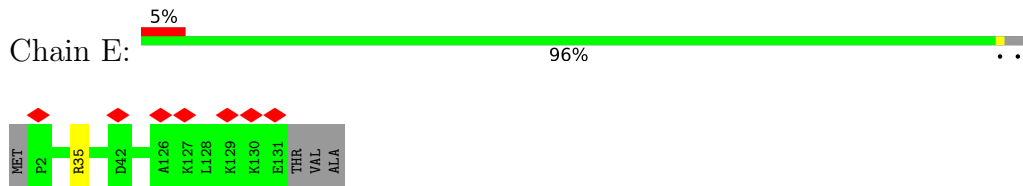
- Molecule 1: 5S rRNA



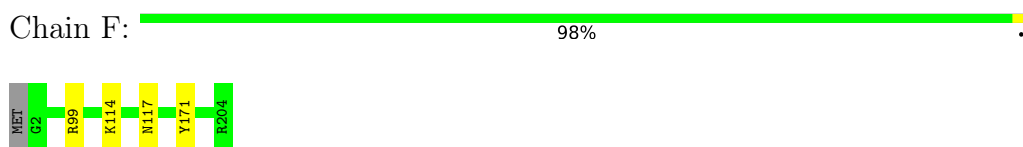
- Molecule 2: eL13 (60S ribosomal protein L13)



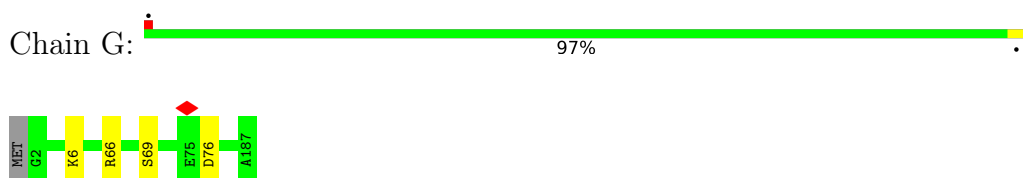
- Molecule 3: eL14 (60S ribosomal protein L14)



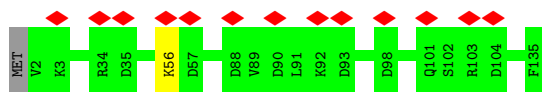
- Molecule 4: eL15 (60S ribosomal protein L15)



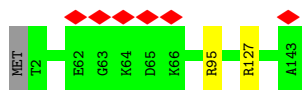
- Molecule 5: eL18 (60S ribosomal protein L18)



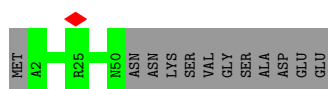
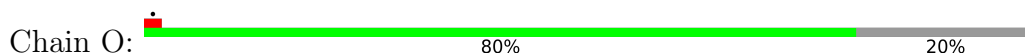
- Molecule 6: eL19 (60S ribosomal protein L19)



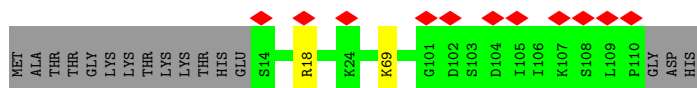
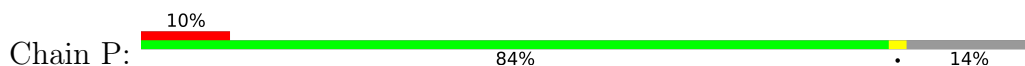
- Molecule 12: eL28 (60S ribosomal protein L28)



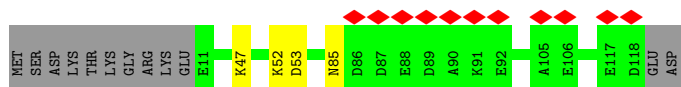
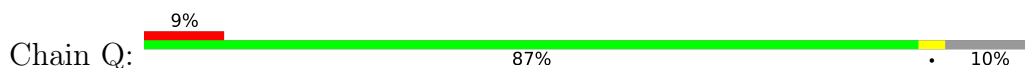
- Molecule 13: eL29 (60S ribosomal protein L29)



- Molecule 14: eL30 (60S ribosomal protein L30)



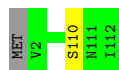
- Molecule 15: eL31 (60S ribosomal protein L31)



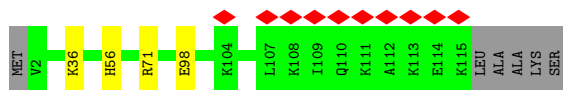
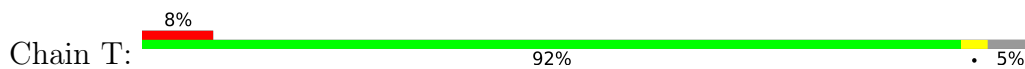
- Molecule 16: eL32 (60S ribosomal protein L32)



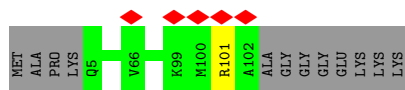
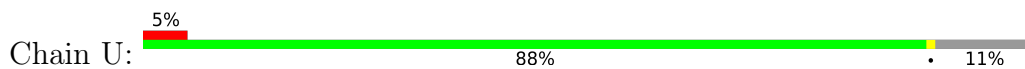
- Molecule 17: eL33 (60S ribosomal protein L35a)



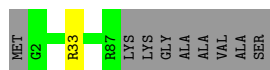
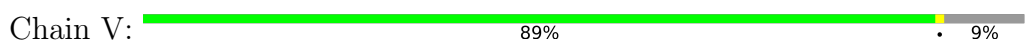
- Molecule 18: eL34 (60S ribosomal protein L34)



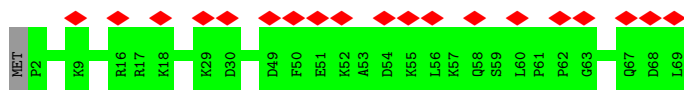
• Molecule 19: eL36 (60S ribosomal protein L36)



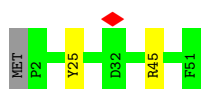
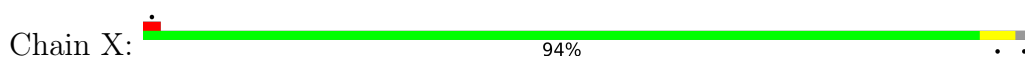
• Molecule 20: eL37 (60S ribosomal protein L37)



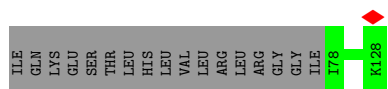
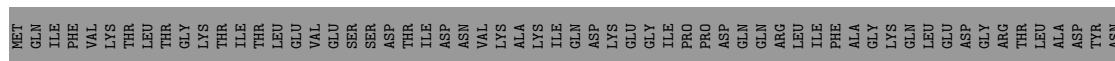
• Molecule 21: eL38 (60S ribosomal protein L38)



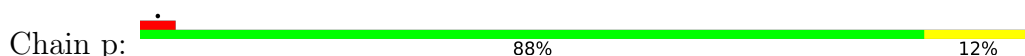
• Molecule 22: eL39 (60S ribosomal protein L39)

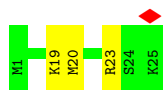


• Molecule 23: eL40 (60S ribosomal protein L40)

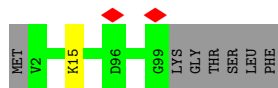
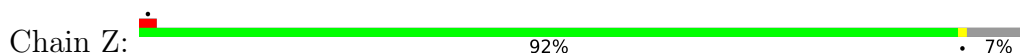


• Molecule 24: eL41 (60S ribosomal protein L41)





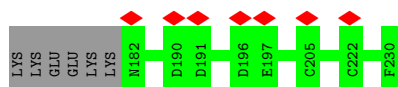
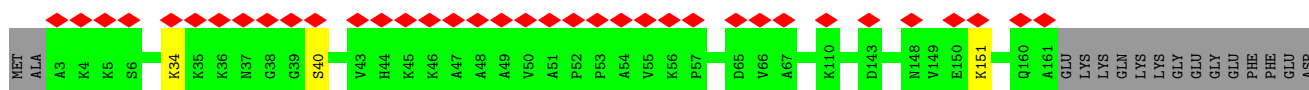
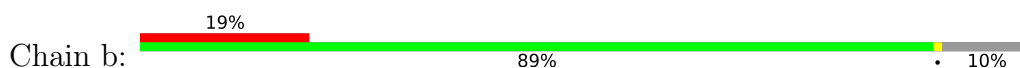
- Molecule 25: eL42 (60S ribosomal protein L42)



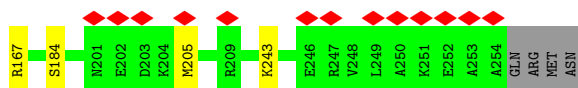
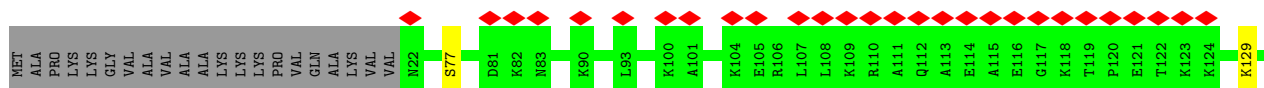
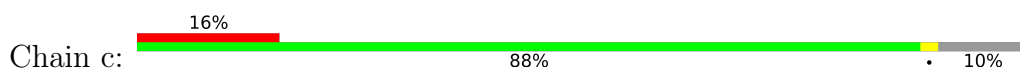
- Molecule 26: eL43 (60S ribosomal protein L37a)



- Molecule 27: eL6 (60S ribosomal protein L6)



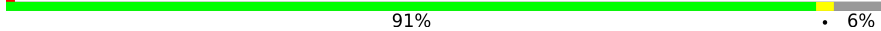
- Molecule 28: eL8 (60S ribosomal protein L7a)

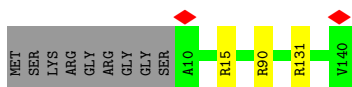


- Molecule 29: uL13 (60S ribosomal protein L13a)



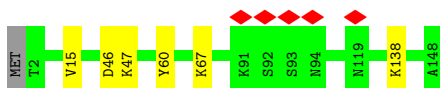
- Molecule 30: uL14 (60S ribosomal protein L23)

Chain e:  91% • 6%



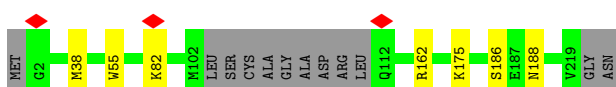
- Molecule 31: uL15 (60S ribosomal protein L27a)

Chain f:  95% ••



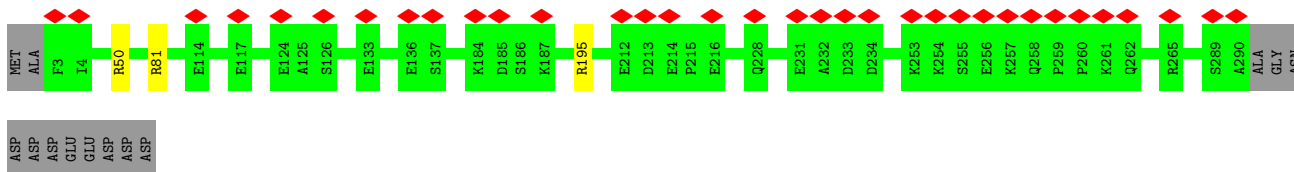
- Molecule 32: uL16 (60S ribosomal protein L10)

Chain g:  91% • 5%




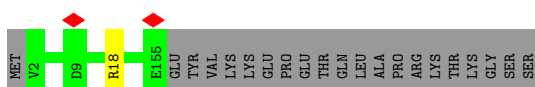
- Molecule 33: uL18 (60S ribosomal protein L5)

Chain h:  11% 95% ••




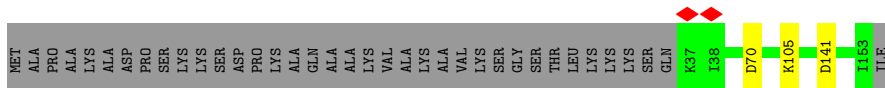
- Molecule 34: uL22 (60S ribosomal protein L17)

Chain j:  87% • 12%




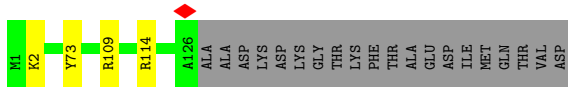
- Molecule 35: uL23 (60S ribosomal protein L23a)

Chain k:  74% • 24%

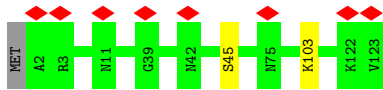


- Molecule 36: uL24 (60S ribosomal protein L26)

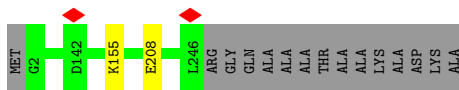
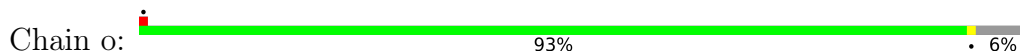
Chain m:  84% • 14%



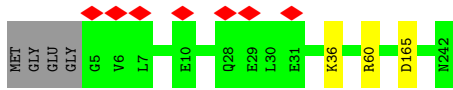
- Molecule 37: uL29 (60S ribosomal protein L35)



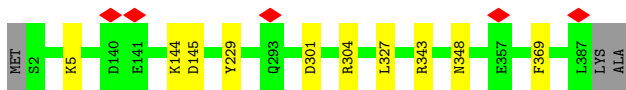
- Molecule 38: uL2 (60S ribosomal protein L8)



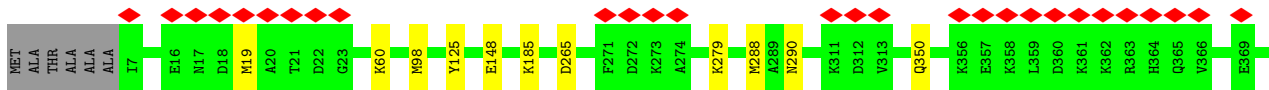
- Molecule 39: uL30 (60S ribosomal protein L7)



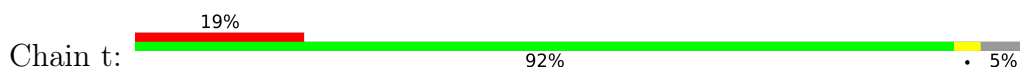
- Molecule 40: uL3 (60S ribosomal protein L3)

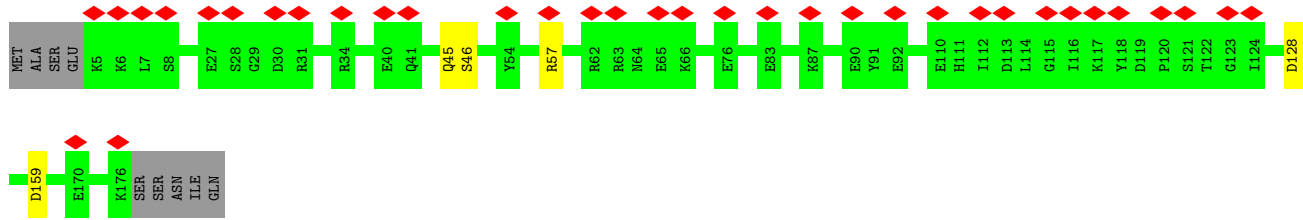


- Molecule 41: uL4 (60S ribosomal protein L4)

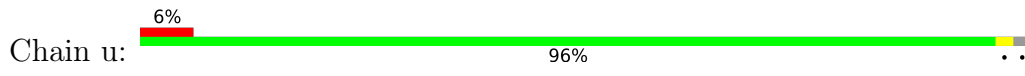


- Molecule 42: uL5 (60S ribosomal protein L11)





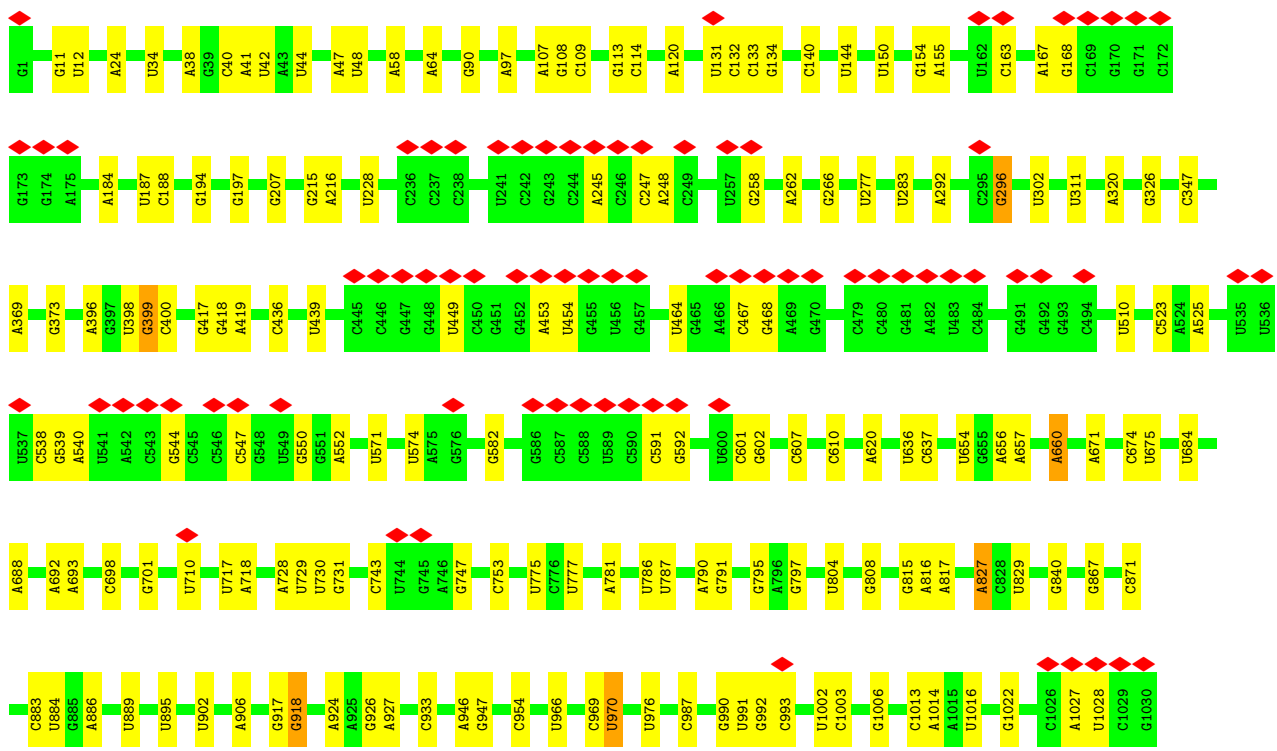
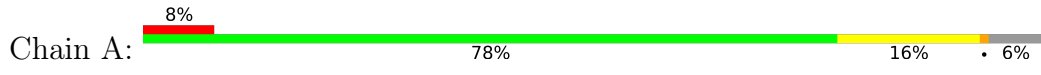
• Molecule 43: uL6 (60S ribosomal protein L9)



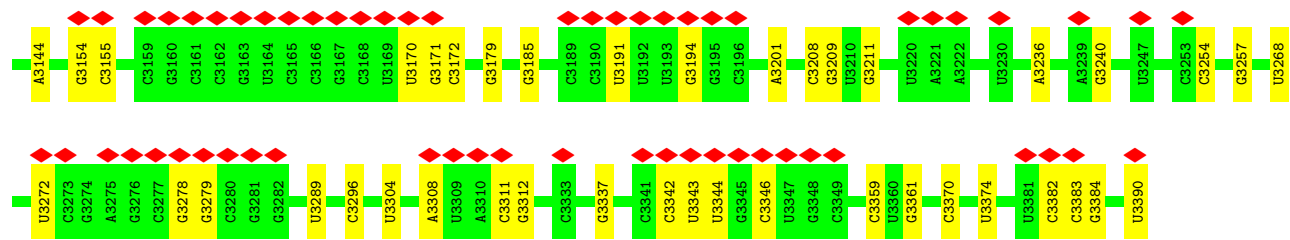
• Molecule 44: nascent chain



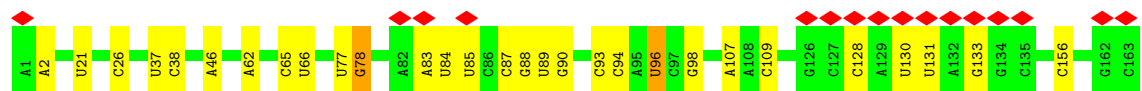
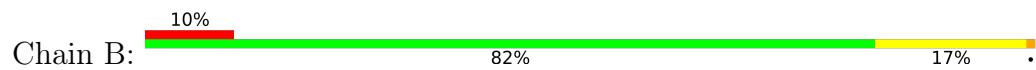
• Molecule 45: 25S rRNA



U2924	G2486	C2576	G2486	U2487	A2405	U2263	G1748	G1491	U1202	G1031
G2925	U2487	A2577	G2487	G2406	G2405	G2264	A1755	A1492	C1202	G1032
U2926	G2488	G2578	G2488	C2265	C2407	A2265	G1756	G1493	A1205	G1033
U2938	A2489	G2588	A2489	U2267	G2412	G2268	U1505	G1494	C1213	G1034
A2939	A2490	A2596	A2490	U2269	U2413	G2269	C1764	G1505	G1218	G1035
U2947	A2491	A2596	A2491	A2273	U2414	G2270	A1765	G1513	U1211	C1037
G2948	U2492	G2601	U2492	G2276	G2415	U2276	C1766	C1525	G1221	A1038
A2949	A2493	G2610	A2493	A2273	U2419	U2277	U1767	U1537	A1232	A1039
G2950	C2494	G2611	C2494	G2276	U2424	A2282	U1768	C1538	G1041	A1040
C2951	C2495	G2617	C2495	G2276	U2435	A2282	C1769	C1538	A1233	G1042
G2954	A2496	G2622	A2496	U2283	U2448	A2283	G1770	G1547	G1234	C1043
G2955	C2497	A2629	C2497	A2284	U2449	A2284	U1771	G1547	A1235	A1043
A2956	U2498	A2629	U2498	U2285	G2448	U2285	G1772	A1566	C1236	C1044
A2957	A2499	A2640	A2499	G2286	U2448	G2286	U1773	G1571	A1237	U1045
U2958	C2500	A2640	C2500	G2291	U2449	G2291	G1774	A1298	G1238	U1046
C2962	U2501	A2643	U2501	C2296	G2445	C2296	G1775	A1299	A1047	G1047
A2972	U2502	A2643	U2502	C2296	G2445	C2296	G1802	U1321	A	A1048
C2973	U2503	U12653	U2503	G2309	G2446	G2309	A1803	U1328	G	U1056
A2974	U2504	G2654	U2504	G2310	C2447	G2310	G1820	A1329	G	U1059
U2978	A2505	U2655	A2505	U2313	U2448	U2313	U1821	G1335	G	U1064
U2983	A2506	U2655	A2506	U2313	G2450	U2313	G1822	G1343	G	U1068
C2986	C2507	U2655	C2507	U2316	G2451	U2316	C1827	A1360	C	A1076
G2993	G2508	U2655	G2508	U2317	G2452	U2317	C1828	A1361	C	C1077
A3000	U2509	U2655	U2509	G2318	A2453	G2318	U1849	U1362	A	U1093
A3014	U2510	U2655	U2510	U2321	G2454	U2321	C1852	U1363	G	U1094
G3030	U2511	U2655	U2511	U2324	G2455	U2324	C1855	C1365	A	C1106
A3014	U2512	U2655	U2512	A2324	U	A2324	A1856	C1366	G	G1107
G3030	U2519	G2692	U2519	A2329	G2457	A2329	A1857	A1378	G	G1108
A3031	A2520	G2693	A2520	A2329	U2458	A2329	G1862	U1410	C	A1109
G3032	A2520	A2694	A2520	A2329	U2458	A2329	C1862	G1430	A	A1114
C3060	A2529	A2699	A2529	U2337	G2460	U2337	C1872	G1430	A	G1115
G3080	C2537	A2706	C2537	U2338	U2461	U2338	A1873	G1445	A	G1128
U3081	G2538	A2707	G2538	U2339	U2461	U2339	G1884	C1448	C	U1133
C3094	G2539	A2717	G2539	C2340	U2467	C2340	A1886	A1457	C	U1134
G3103	G2540	U2720	G2540	U2350	G2467	U2350	U1894	A1461	C	U1135
U3113	C2542	U2722	C2542	C2368	G2468	C2368	G1912	G1462	A	G1142
G3118	A2543	U2731	A2543	A2376	G2469	A2376	C1949	A1463	G	A1144
U3123	U2544	U2732	U2544	G2377	G2469	G2377	U1957	A1474	G	A1170
A3124	G2546	U2738	G2546	G2378	G2470	G2378	G1958	U1480	G	G1185
A3132	C2547	U2747	C2547	G2388	A2471	G2388	U1959	U1481	U	C1191
U3133	G2548	U2757	G2548	G2394	G2472	G2394	G	U1482	U	U1192
U3133	C2550	C2758	C2550	G2395	C2473	G2395	C		U	C1193
	U2551		U2551	G2396	G	G2396			U	G1195
	C2552		C2552	G2397	A	G2397			U	
	U2556		U2556	G2398	A	G2398			U	
	G2559		G2559	A2400	A	A2400			U	
	U2570		U2570						U	
	G2571		G2571						U	
	C2572		C2572						U	
	U2573		U2573						U	
	U2574		U2574						U	
	G2575		G2575						U	



• Molecule 46: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.519	Depositor
Minimum map value	-7.827	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.314	Depositor
Recommended contour level	1.05	Depositor
Map size (\AA)	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.848, 0.848, 0.848	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: ZN, 1MA, MG, UY1, K, OMU, OMC, 5MC, A2M, SPM, OMG, UR3, SPD, PSU

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	C	0.18	0/2837	0.71	0/4420
2	D	0.25	0/1635	0.55	0/2194
3	E	0.24	0/1069	0.52	0/1427
4	F	0.24	0/1740	0.59	0/2333
5	G	0.25	0/1487	0.55	0/1989
6	H	0.24	0/1548	0.57	0/2042
7	I	0.25	0/1544	0.51	0/2071
8	J	0.24	0/1331	0.54	0/1784
9	K	0.24	0/819	0.51	0/1098
10	L	0.26	0/539	0.52	0/716
11	M	0.25	0/1118	0.52	0/1492
12	N	0.24	0/1126	0.47	0/1508
13	O	0.26	0/422	0.54	0/558
14	P	0.25	0/757	0.47	0/1018
15	Q	0.25	0/885	0.55	0/1184
16	R	0.24	0/1053	0.56	0/1408
17	S	0.26	0/920	0.52	0/1232
18	T	0.25	0/939	0.58	0/1251
19	U	0.25	0/791	0.56	0/1047
20	V	0.27	0/714	0.64	0/949
21	W	0.25	0/566	0.49	0/752
22	X	0.22	0/460	0.58	0/611
23	Y	0.25	0/427	0.54	0/562
24	p	0.25	0/239	0.68	0/302
25	Z	0.25	0/801	0.48	0/1058
26	a	0.24	0/717	0.55	0/952
27	b	0.26	0/1645	0.45	0/2210
28	c	0.25	0/1912	0.49	0/2562
29	d	0.25	0/1669	0.52	0/2235
30	e	0.25	0/1001	0.54	0/1345
31	f	0.25	0/1190	0.49	0/1591
32	g	0.25	0/1707	0.54	0/2283

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.25	0/2386	0.51	0/3200
34	j	0.25	0/1270	0.56	0/1704
35	k	0.25	0/965	0.48	0/1295
36	m	0.24	0/1035	0.57	0/1383
37	n	0.24	0/1009	0.50	0/1343
38	o	0.25	0/1924	0.56	0/2585
39	q	0.27	0/1992	0.49	0/2670
40	r	0.24	0/3172	0.51	0/4249
41	s	0.24	0/3159	0.51	0/4259
42	t	0.25	0/1414	0.54	0/1890
43	u	0.25	0/1539	0.50	0/2059
45	A	0.21	5/73586 (0.0%)	0.74	9/114785 (0.0%)
46	B	0.20	0/3772	0.74	0/5878
All	All	0.23	5/132831 (0.0%)	0.67	9/195484 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2972	A	O3'-P	9.05	1.72	1.61
45	A	654	U	O3'-P	7.35	1.70	1.61
45	A	1491	G	O3'-P	5.98	1.68	1.61
45	A	2973	C	O3'-P	5.31	1.67	1.61
45	A	2116	U	O3'-P	5.02	1.67	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	654	U	P-O3'-C3'	10.41	132.19	119.70
45	A	2972	A	P-O3'-C3'	10.05	131.76	119.70
45	A	657	A	O5'-P-OP1	-9.56	97.09	105.70
45	A	808	G	P-O3'-C3'	8.50	129.90	119.70
45	A	1491	G	P-O3'-C3'	7.67	128.91	119.70
45	A	113	G	O4'-C1'-N9	5.82	112.86	108.20
45	A	710	U	C2-N1-C1'	5.36	124.14	117.70
45	A	2116	U	P-O3'-C3'	5.26	126.02	119.70
45	A	1505	U	P-O3'-C3'	5.22	125.96	119.70

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
3	E	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
4	F	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
5	G	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
6	H	180/214 (84%)	180 (100%)	0	0	100	100
7	I	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
8	J	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
9	K	97/127 (76%)	96 (99%)	1 (1%)	0	100	100
10	L	60/164 (37%)	60 (100%)	0	0	100	100
11	M	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
12	N	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
13	O	47/61 (77%)	44 (94%)	3 (6%)	0	100	100
14	P	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
15	Q	106/120 (88%)	106 (100%)	0	0	100	100
16	R	124/133 (93%)	124 (100%)	0	0	100	100
17	S	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
18	T	112/120 (93%)	112 (100%)	0	0	100	100
19	U	96/110 (87%)	96 (100%)	0	0	100	100
20	V	84/95 (88%)	83 (99%)	1 (1%)	0	100	100
21	W	66/69 (96%)	66 (100%)	0	0	100	100
22	X	48/51 (94%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y	49/128 (38%)	49 (100%)	0	0	100	100
24	p	23/25 (92%)	23 (100%)	0	0	100	100
25	Z	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
26	a	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
27	b	204/230 (89%)	200 (98%)	4 (2%)	0	100	100
28	c	231/258 (90%)	229 (99%)	2 (1%)	0	100	100
29	d	203/206 (98%)	203 (100%)	0	0	100	100
30	e	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
31	f	145/148 (98%)	138 (95%)	6 (4%)	1 (1%)	22	14
32	g	205/221 (93%)	202 (98%)	3 (2%)	0	100	100
33	h	286/301 (95%)	281 (98%)	5 (2%)	0	100	100
34	j	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
35	k	115/154 (75%)	115 (100%)	0	0	100	100
36	m	124/146 (85%)	122 (98%)	2 (2%)	0	100	100
37	n	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	o	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
39	q	236/242 (98%)	231 (98%)	5 (2%)	0	100	100
40	r	384/389 (99%)	379 (99%)	5 (1%)	0	100	100
41	s	396/405 (98%)	391 (99%)	5 (1%)	0	100	100
42	t	170/181 (94%)	168 (99%)	2 (1%)	0	100	100
43	u	189/194 (97%)	188 (100%)	1 (0%)	0	100	100
All	All	6332/6963 (91%)	6244 (99%)	87 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	f	15	VAL

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	165/171 (96%)	161 (98%)	4 (2%)	49	49
3	E	114/117 (97%)	113 (99%)	1 (1%)	78	81
4	F	176/177 (99%)	172 (98%)	4 (2%)	50	51
5	G	154/155 (99%)	150 (97%)	4 (3%)	46	45
6	H	160/182 (88%)	152 (95%)	8 (5%)	24	20
7	I	163/164 (99%)	161 (99%)	2 (1%)	71	74
8	J	140/141 (99%)	137 (98%)	3 (2%)	53	54
9	K	91/109 (84%)	89 (98%)	2 (2%)	52	53
10	L	57/133 (43%)	53 (93%)	4 (7%)	15	9
11	M	117/118 (99%)	116 (99%)	1 (1%)	78	81
12	N	123/124 (99%)	121 (98%)	2 (2%)	62	65
13	O	43/53 (81%)	43 (100%)	0	100	100
14	P	85/98 (87%)	83 (98%)	2 (2%)	49	49
15	Q	95/106 (90%)	91 (96%)	4 (4%)	30	26
16	R	114/121 (94%)	111 (97%)	3 (3%)	46	45
17	S	98/99 (99%)	97 (99%)	1 (1%)	76	79
18	T	100/104 (96%)	96 (96%)	4 (4%)	31	28
19	U	83/90 (92%)	82 (99%)	1 (1%)	71	74
20	V	72/77 (94%)	71 (99%)	1 (1%)	67	70
21	W	64/65 (98%)	64 (100%)	0	100	100
22	X	47/48 (98%)	45 (96%)	2 (4%)	29	25
23	Y	46/114 (40%)	46 (100%)	0	100	100
24	p	24/24 (100%)	21 (88%)	3 (12%)	4	1
25	Z	86/92 (94%)	85 (99%)	1 (1%)	71	74
26	a	73/74 (99%)	72 (99%)	1 (1%)	67	70
27	b	175/194 (90%)	172 (98%)	3 (2%)	60	63
28	c	202/221 (91%)	196 (97%)	6 (3%)	41	39
29	d	173/174 (99%)	168 (97%)	5 (3%)	42	40
30	e	103/109 (94%)	100 (97%)	3 (3%)	42	40
31	f	119/120 (99%)	114 (96%)	5 (4%)	30	26
32	g	173/181 (96%)	166 (96%)	7 (4%)	31	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	244/254 (96%)	241 (99%)	3 (1%)	71	74
34	j	135/154 (88%)	134 (99%)	1 (1%)	84	87
35	k	106/134 (79%)	103 (97%)	3 (3%)	43	42
36	m	115/131 (88%)	111 (96%)	4 (4%)	36	33
37	n	109/110 (99%)	107 (98%)	2 (2%)	59	60
38	o	190/197 (96%)	188 (99%)	2 (1%)	73	76
39	q	207/209 (99%)	204 (99%)	3 (1%)	67	70
40	r	330/332 (99%)	320 (97%)	10 (3%)	41	39
41	s	326/329 (99%)	314 (96%)	12 (4%)	34	31
42	t	149/157 (95%)	144 (97%)	5 (3%)	37	34
43	u	167/170 (98%)	163 (98%)	4 (2%)	49	49
All	All	5513/5932 (93%)	5377 (98%)	136 (2%)	50	47

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	66	MET
2	D	151	SER
2	D	157	ARG
2	D	188	ARG
3	E	35	ARG
4	F	99	ARG
4	F	114	LYS
4	F	117	ASN
4	F	171	TYR
5	G	6	LYS
5	G	66	ARG
5	G	69	SER
5	G	76	ASP
6	H	3	SER
6	H	62	ARG
6	H	68	GLU
6	H	111	GLU
6	H	114	LYS
6	H	117	ARG
6	H	122	ASP
6	H	160	GLU
7	I	10	GLN

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Mol	Chain	Res	Type
7	I	59	GLN
8	J	96	VAL
8	J	111	LYS
8	J	130	ARG
9	K	66	LYS
9	K	77	PHE
10	L	9	ARG
10	L	36	SER
10	L	39	LYS
10	L	59	LYS
11	M	56	LYS
12	N	95	ARG
12	N	127	ARG
14	P	18	ARG
14	P	69	LYS
15	Q	47	LYS
15	Q	52	LYS
15	Q	53	ASP
15	Q	85	ASN
16	R	31	GLU
16	R	42	ARG
16	R	108	GLU
17	S	110	SER
18	T	36	LYS
18	T	56	HIS
18	T	71	ARG
18	T	98	GLU
19	U	101	ARG
20	V	33	ARG
22	X	25	TYR
22	X	45	ARG
24	p	19	LYS
24	p	20	MET
24	p	23	ARG
25	Z	15	LYS
26	a	80	ARG
27	b	34	LYS
27	b	40	SER
27	b	151	LYS
28	c	77	SER
28	c	129	LYS
28	c	167	ARG

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Mol	Chain	Res	Type
28	c	184	SER
28	c	205	MET
28	c	243	LYS
29	d	114	PRO
29	d	127	ASP
29	d	155	TYR
29	d	174	GLU
29	d	194	LEU
30	e	15	ARG
30	e	90	ARG
30	e	131	ARG
31	f	46	ASP
31	f	47	LYS
31	f	60	TYR
31	f	67	LYS
31	f	138	LYS
32	g	38	MET
32	g	55	TRP
32	g	82	LYS
32	g	162	ARG
32	g	175	LYS
32	g	186	SER
32	g	188	ASN
33	h	50	ARG
33	h	81	ARG
33	h	195	ARG
34	j	18	ARG
35	k	70	ASP
35	k	105	LYS
35	k	141	ASP
36	m	2	LYS
36	m	73	TYR
36	m	109	ARG
36	m	114	ARG
37	n	45	SER
37	n	103	LYS
38	o	155	LYS
38	o	208	GLU
39	q	36	LYS
39	q	60	ARG
39	q	165	ASP
40	r	5	LYS

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Mol	Chain	Res	Type
40	r	144	LYS
40	r	145	ASP
40	r	229	TYR
40	r	301	ASP
40	r	304	ARG
40	r	327	LEU
40	r	343	ARG
40	r	348	ASN
40	r	369	PHE
41	s	19	MET
41	s	60	LYS
41	s	98	MET
41	s	125	TYR
41	s	148	GLU
41	s	185	LYS
41	s	265	ASP
41	s	279	LYS
41	s	288	MET
41	s	290	ASN
41	s	350	GLN
41	s	390	ASP
42	t	45	GLN
42	t	46	SER
42	t	57	ARG
42	t	128	ASP
42	t	159	ASP
43	u	1	MET
43	u	33	LYS
43	u	142	LYS
43	u	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
15	Q	85	ASN
33	h	122	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	118/119 (99%)	8 (6%)	0
45	A	3191/3390 (94%)	415 (13%)	16 (0%)
46	B	162/163 (99%)	26 (16%)	0
All	All	3471/3672 (94%)	449 (12%)	16 (0%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	25	G
1	C	33	U
1	C	38	U
1	C	53	U
1	C	54	A
1	C	64	G
1	C	110	G
45	A	11	G
45	A	12	U
45	A	24	A
45	A	38	A
45	A	41	A
45	A	47	A
45	A	58	A
45	A	64	A
45	A	90	G
45	A	97	A
45	A	107	A
45	A	108	G
45	A	109	C
45	A	114	C
45	A	120	A
45	A	131	U
45	A	132	C
45	A	133	C
45	A	134	G
45	A	140	C
45	A	154	G
45	A	155	A
45	A	163	C
45	A	167	A
45	A	168	G
45	A	184	A
45	A	187	U

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Mol	Chain	Res	Type
45	A	188	C
45	A	194	G
45	A	197	G
45	A	207	G
45	A	215	G
45	A	216	A
45	A	245	A
45	A	247	C
45	A	248	A
45	A	258	G
45	A	262	A
45	A	266	G
45	A	283	U
45	A	292	A
45	A	296	OMG
45	A	302	U
45	A	320	A
45	A	326	G
45	A	347	C
45	A	373	G
45	A	396	A
45	A	398	U
45	A	399	OMG
45	A	400	C
45	A	417	G
45	A	418	G
45	A	419	A
45	A	436	C
45	A	439	U
45	A	449	U
45	A	453	A
45	A	454	U
45	A	467	C
45	A	468	G
45	A	523	C
45	A	525	A
45	A	538	C
45	A	539	G
45	A	540	A
45	A	544	G
45	A	547	C
45	A	550	G

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Mol	Chain	Res	Type
45	A	552	A
45	A	571	U
45	A	574	U
45	A	582	G
45	A	591	C
45	A	592	G
45	A	602	G
45	A	607	C
45	A	610	C
45	A	620	A
45	A	636	U
45	A	637	C
45	A	660	A2M
45	A	671	A
45	A	688	A
45	A	693	A
45	A	698	C
45	A	701	G
45	A	718	A
45	A	728	A
45	A	729	U
45	A	730	U
45	A	731	G
45	A	743	C
45	A	747	G
45	A	753	C
45	A	775	U
45	A	777	U
45	A	781	A
45	A	790	A
45	A	791	G
45	A	795	G
45	A	797	G
45	A	816	A
45	A	827	A2M
45	A	840	G
45	A	867	G
45	A	871	C
45	A	884	U
45	A	889	U
45	A	906	A
45	A	917	G

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Mol	Chain	Res	Type
45	A	918	OMG
45	A	924	A
45	A	926	G
45	A	927	A
45	A	933	C
45	A	947	G
45	A	954	C
45	A	969	C
45	A	970	PSU
45	A	987	C
45	A	991	U
45	A	992	G
45	A	993	C
45	A	1003	C
45	A	1006	G
45	A	1013	C
45	A	1014	A
45	A	1022	G
45	A	1028	U
45	A	1036	G
45	A	1041	G
45	A	1048	A
45	A	1059	A
45	A	1076	A
45	A	1077	C
45	A	1093	U
45	A	1094	U
45	A	1106	C
45	A	1107	G
45	A	1108	G
45	A	1109	A
45	A	1114	A
45	A	1115	G
45	A	1128	G
45	A	1142	G
45	A	1170	A
45	A	1185	G
45	A	1191	C
45	A	1192	U
45	A	1193	G
45	A	1195	G
45	A	1202	C

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Mol	Chain	Res	Type
45	A	1205	A
45	A	1213	C
45	A	1218	G
45	A	1221	G
45	A	1295	C
45	A	1297	G
45	A	1299	A
45	A	1321	U
45	A	1328	U
45	A	1329	A
45	A	1335	G
45	A	1343	C
45	A	1344	A
45	A	1360	A
45	A	1361	A
45	A	1362	G
45	A	1363	U
45	A	1364	G
45	A	1365	C
45	A	1366	C
45	A	1410	U
45	A	1430	G
45	A	1445	G
45	A	1448	OMC
45	A	1457	A
45	A	1463	A
45	A	1492	A
45	A	1494	G
45	A	1513	G
45	A	1525	C
45	A	1538	C
45	A	1547	G
45	A	1566	A
45	A	1571	G
45	A	1577	U
45	A	1578	U
45	A	1585	U
45	A	1587	C
45	A	1588	U
45	A	1592	A
45	A	1593	A
45	A	1594	A

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Mol	Chain	Res	Type
45	A	1598	A
45	A	1602	G
45	A	1609	A
45	A	1625	C
45	A	1633	U
45	A	1635	G
45	A	1636	A
45	A	1643	C
45	A	1649	G
45	A	1661	C
45	A	1698	U
45	A	1729	G
45	A	1748	G
45	A	1755	A
45	A	1756	G
45	A	1763	G
45	A	1764	C
45	A	1770	G
45	A	1771	C
45	A	1772	G
45	A	1774	G
45	A	1775	G
45	A	1802	G
45	A	1803	A
45	A	1821	U
45	A	1827	C
45	A	1828	C
45	A	1855	C
45	A	1856	A
45	A	1872	C
45	A	1873	A
45	A	1884	G
45	A	1885	A
45	A	1886	U
45	A	1912	G
45	A	1949	C
45	A	2096	A
45	A	2100	G
45	A	2116	U
45	A	2118	C
45	A	2126	OMG
45	A	2135	A

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Mol	Chain	Res	Type
45	A	2144	U
45	A	2162	A
45	A	2208	U
45	A	2213	G
45	A	2244	U
45	A	2245	A
45	A	2259	A2M
45	A	2265	A
45	A	2273	A
45	A	2276	G
45	A	2283	A
45	A	2285	U
45	A	2286	G
45	A	2291	OMG
45	A	2310	G
45	A	2313	U
45	A	2316	A
45	A	2317	PSU
45	A	2318	G
45	A	2337	U
45	A	2339	U
45	A	2368	OMC
45	A	2376	A
45	A	2377	C
45	A	2378	G
45	A	2388	G
45	A	2396	G
45	A	2397	G
45	A	2400	A
45	A	2405	A
45	A	2406	G
45	A	2407	A
45	A	2414	U
45	A	2415	G
45	A	2438	G
45	A	2448	U
45	A	2457	G
45	A	2459	A
45	A	2462	A
45	A	2463	U
45	A	2464	A
45	A	2465	A

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Mol	Chain	Res	Type
45	A	2466	G
45	A	2468	G
45	A	2469	G
45	A	2470	G
45	A	2471	A
45	A	2483	A
45	A	2486	G
45	A	2488	G
45	A	2492	U
45	A	2495	C
45	A	2496	A
45	A	2497	C
45	A	2499	A
45	A	2503	U
45	A	2504	U
45	A	2505	A
45	A	2506	A
45	A	2519	U
45	A	2520	A
45	A	2529	A
45	A	2544	C
45	A	2545	U
45	A	2546	G
45	A	2556	U
45	A	2559	G
45	A	2573	U
45	A	2574	U
45	A	2575	G
45	A	2576	C
45	A	2588	G
45	A	2596	A
45	A	2609	G
45	A	2610	G
45	A	2617	G
45	A	2629	A
45	A	2640	A
45	A	2655	U
45	A	2659	A
45	A	2660	A
45	A	2677	A
45	A	2680	G
45	A	2692	G

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Mol	Chain	Res	Type
45	A	2694	A
45	A	2699	A
45	A	2706	A
45	A	2707	A
45	A	2717	G
45	A	2722	U
45	A	2731	G
45	A	2732	OMU
45	A	2756	G
45	A	2758	C
45	A	2780	G
45	A	2781	G
45	A	2799	G
45	A	2802	A
45	A	2803	G
45	A	2804	A2M
45	A	2806	A
45	A	2813	C
45	A	2817	G
45	A	2820	A
45	A	2845	U
45	A	2846	U
45	A	2847	C
45	A	2848	A
45	A	2870	C
45	A	2874	G
45	A	2875	A
45	A	2890	A
45	A	2892	C
45	A	2902	C
45	A	2914	A2M
45	A	2938	U
45	A	2939	A
45	A	2948	G
45	A	2950	G
45	A	2954	G
45	A	2956	UR3
45	A	2974	A
45	A	2983	U
45	A	2986	C
45	A	2993	G
45	A	3000	G

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Mol	Chain	Res	Type
45	A	3014	A
45	A	3030	G
45	A	3032	G
45	A	3060	C
45	A	3061	G
45	A	3080	G
45	A	3081	U
45	A	3094	C
45	A	3103	G
45	A	3118	G
45	A	3124	A
45	A	3132	A
45	A	3133	U
45	A	3144	A
45	A	3154	G
45	A	3155	C
45	A	3170	U
45	A	3171	G
45	A	3172	C
45	A	3179	G
45	A	3185	G
45	A	3191	U
45	A	3194	G
45	A	3201	A
45	A	3208	C
45	A	3209	G
45	A	3211	G
45	A	3236	A
45	A	3240	G
45	A	3254	C
45	A	3257	G
45	A	3268	U
45	A	3272	U
45	A	3278	G
45	A	3279	G
45	A	3296	C
45	A	3308	A
45	A	3311	C
45	A	3312	G
45	A	3337	G
45	A	3342	C
45	A	3343	U

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Mol	Chain	Res	Type
45	A	3344	U
45	A	3346	C
45	A	3359	C
45	A	3361	G
45	A	3370	C
45	A	3374	U
45	A	3382	C
45	A	3383	C
45	A	3384	G
45	A	3390	U
46	B	2	A
46	B	26	C
46	B	37	U
46	B	38	C
46	B	62	A
46	B	65	C
46	B	66	U
46	B	78	OMG
46	B	83	A
46	B	84	U
46	B	85	U
46	B	87	C
46	B	88	G
46	B	89	U
46	B	90	G
46	B	93	C
46	B	94	C
46	B	96	PSU
46	B	98	G
46	B	107	A
46	B	109	C
46	B	128	C
46	B	130	U
46	B	131	U
46	B	133	G
46	B	156	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	A	11	G
45	A	398	U

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Mol	Chain	Res	Type
45	A	399	OMG
45	A	601	C
45	A	692	A
45	A	883	C
45	A	926	G
45	A	990	G
45	A	1027	A
45	A	1852	OMC
45	A	2468	G
45	A	2482	G
45	A	2496	A
45	A	2503	U
45	A	2543	A
45	A	3123	U

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

135 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
45	OMU	A	2738	45	19,22,23	3.21	8 (42%)	26,31,34	1.69	5 (19%)
45	OMC	A	2951	45	19,22,23	3.24	8 (42%)	26,31,34	0.77	0
46	A2M	B	46	46	18,25,26	4.14	7 (38%)	18,36,39	3.84	4 (22%)
45	OMC	A	1849	45	19,22,23	3.26	8 (42%)	26,31,34	0.72	0
45	PSU	A	1482	45	18,21,22	4.65	8 (44%)	22,30,33	1.81	5 (22%)
45	OMG	A	296	45	18,26,27	2.84	8 (44%)	19,38,41	1.55	5 (26%)
45	A2M	A	2329	45	18,25,26	4.13	7 (38%)	18,36,39	3.78	5 (27%)
45	PSU	A	1134	45	18,21,22	4.61	8 (44%)	22,30,33	1.86	5 (22%)
45	5MC	A	2281	45	18,22,23	4.00	7 (38%)	26,32,35	1.00	2 (7%)
45	OMG	A	918	48,45	18,26,27	2.81	8 (44%)	19,38,41	1.49	4 (21%)
45	1MA	A	656	45	16,25,26	1.51	2 (12%)	18,37,40	1.09	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	A	786	45	18,21,22	4.65	8 (44%)	22,30,33	1.75	5 (22%)
45	OMU	A	1537	45	19,22,23	3.21	8 (42%)	26,31,34	1.61	4 (15%)
45	OMU	A	1894	45	19,22,23	3.21	8 (42%)	26,31,34	1.72	5 (19%)
45	PSU	A	829	45	18,21,22	4.63	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	34	45	18,21,22	4.63	8 (44%)	22,30,33	1.91	5 (22%)
45	PSU	A	2857	45	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
45	PSU	A	2978	45	18,21,22	4.64	8 (44%)	22,30,33	1.78	5 (22%)
45	OMU	A	787	45	19,22,23	3.21	8 (42%)	26,31,34	1.64	5 (19%)
45	PSU	A	277	45	18,21,22	4.61	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2321	45,47	18,21,22	4.63	8 (44%)	22,30,33	1.87	5 (22%)
45	OMC	A	1852	45	19,22,23	3.30	8 (42%)	26,31,34	0.75	0
45	PSU	A	2267	45	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
45	OMG	A	2291	45	18,26,27	2.83	8 (44%)	19,38,41	1.52	4 (21%)
45	A2M	A	817	45	18,25,26	4.13	7 (38%)	18,36,39	3.79	5 (27%)
45	A2M	A	2914	45	18,25,26	4.15	7 (38%)	18,36,39	3.90	4 (22%)
45	OMU	A	2424	45	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
45	PSU	A	2137	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.93	5 (22%)
45	OMC	A	2685	45	19,22,23	3.29	8 (42%)	26,31,34	0.71	0
45	OMC	A	2962	45	19,22,23	3.26	8 (42%)	26,31,34	0.74	0
45	OMU	A	3289	45	19,22,23	3.21	8 (42%)	26,31,34	1.68	4 (15%)
45	PSU	A	2435	45	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
45	OMG	A	399	45	18,26,27	2.87	8 (44%)	19,38,41	1.53	4 (21%)
45	PSU	A	1064	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
45	OMC	A	2296	45	19,22,23	3.29	8 (42%)	26,31,34	0.74	0
45	OMU	A	44	48,45	19,22,23	3.23	8 (42%)	26,31,34	1.63	4 (15%)
45	OMU	A	675	45	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
45	A2M	A	1460	45	18,25,26	4.13	7 (38%)	18,36,39	3.81	5 (27%)
45	A2M	A	827	48,45,47	18,25,26	4.18	7 (38%)	18,36,39	3.86	4 (22%)
45	PSU	A	2747	45	18,21,22	4.63	8 (44%)	22,30,33	1.78	5 (22%)
45	PSU	A	970	45	18,21,22	4.66	8 (44%)	22,30,33	1.87	6 (27%)
45	OMU	A	2413	48,45	19,22,23	3.19	8 (42%)	26,31,34	1.58	4 (15%)
45	UR3	A	2956	45	19,22,23	2.80	8 (42%)	26,32,35	1.31	2 (7%)
45	PSU	A	2257	45	18,21,22	4.66	8 (44%)	22,30,33	1.85	5 (22%)
45	A2M	A	1144	45	18,25,26	4.11	7 (38%)	18,36,39	3.87	4 (22%)
45	PSU	A	2269	45	18,21,22	4.69	8 (44%)	22,30,33	1.77	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	A	2350	45	19,22,23	3.23	8 (42%)	26,31,34	1.66	5 (19%)
45	OMC	A	40	45	19,22,23	3.26	8 (42%)	26,31,34	0.88	1 (3%)
45	PSU	A	966	45	18,21,22	4.61	8 (44%)	22,30,33	1.73	5 (22%)
45	PSU	A	510	45	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
45	OMU	A	48	45	19,22,23	3.18	8 (42%)	26,31,34	1.61	4 (15%)
45	OMG	A	2394	45	18,26,27	2.83	8 (44%)	19,38,41	1.58	5 (26%)
45	PSU	A	2883	45	18,21,22	4.64	8 (44%)	22,30,33	1.85	6 (27%)
45	PSU	A	1056	45	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
45	OMU	A	1068	45	19,22,23	3.22	8 (42%)	26,31,34	1.71	5 (19%)
45	OMC	A	1448	45	19,22,23	3.29	8 (42%)	26,31,34	0.73	0
45	OMG	A	2398	45	18,26,27	2.80	8 (44%)	19,38,41	1.60	5 (26%)
45	OMU	A	144	45	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
45	A2M	A	2129	45	18,25,26	4.16	7 (38%)	18,36,39	3.83	4 (22%)
45	UY1	A	2653	45	19,22,23	4.18	7 (36%)	22,31,34	1.84	5 (22%)
46	PSU	B	96	48,46	18,21,22	4.66	8 (44%)	22,30,33	1.76	5 (22%)
45	A2M	A	2284	45	18,25,26	4.05	7 (38%)	18,36,39	4.00	4 (22%)
45	PSU	A	2139	45	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)
45	PSU	A	2947	48,45	18,21,22	4.63	9 (50%)	22,30,33	1.86	6 (27%)
45	OMC	A	674	45	19,22,23	3.24	8 (42%)	26,31,34	0.68	0
45	PSU	A	1016	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.85	5 (22%)
45	OMU	A	3304	45	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
45	PSU	A	902	48,45,47	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
46	PSU	B	77	46	18,21,22	4.64	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	464	45	18,21,22	4.66	8 (44%)	22,30,33	1.80	6 (27%)
45	5MC	A	2873	48,45	18,22,23	4.02	7 (38%)	26,32,35	1.11	1 (3%)
45	OMG	A	2796	45	18,26,27	2.80	8 (44%)	19,38,41	1.53	5 (26%)
45	A2M	A	2804	45	18,25,26	4.10	7 (38%)	18,36,39	4.13	6 (33%)
45	OMG	A	2127	45	18,26,27	2.82	8 (44%)	19,38,41	1.64	5 (26%)
45	OMG	A	1857	45	18,26,27	2.80	8 (44%)	19,38,41	1.50	5 (26%)
45	PSU	A	2419	45	18,21,22	4.63	8 (44%)	22,30,33	1.79	5 (22%)
45	OMC	A	1862	45	19,22,23	3.25	8 (42%)	26,31,34	0.66	0
45	OMC	A	2368	45	19,22,23	3.26	8 (42%)	26,31,34	0.69	0
45	PSU	A	2868	45	18,21,22	4.64	8 (44%)	22,30,33	1.87	6 (27%)
45	PSU	A	2194	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
45	PSU	A	42	48,45	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A2M	A	2643	45	18,25,26	4.12	7 (38%)	18,36,39	3.74	4 (22%)
45	PSU	A	150	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
45	PSU	A	895	45	18,21,22	4.61	8 (44%)	22,30,33	1.79	5 (22%)
45	OMG	A	1461	45	18,26,27	2.80	8 (44%)	19,38,41	1.53	4 (21%)
45	PSU	A	2261	45	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
45	OMU	A	2886	45	19,22,23	3.22	8 (42%)	26,31,34	1.64	4 (15%)
45	PSU	A	2958	45	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2926	48,45	18,21,22	4.64	8 (44%)	22,30,33	1.88	5 (22%)
45	A2M	A	2324	45	18,25,26	4.09	7 (38%)	18,36,39	3.82	4 (22%)
45	PSU	A	228	45	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
45	PSU	A	684	45	18,21,22	4.63	8 (44%)	22,30,33	1.80	5 (22%)
45	PSU	A	1135	45	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
45	PSU	A	976	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
46	PSU	B	21	45,46	18,21,22	4.60	8 (44%)	22,30,33	1.83	5 (22%)
45	A2M	A	2259	45	18,25,26	4.17	7 (38%)	18,36,39	3.89	4 (22%)
45	OMG	A	2920	45	18,26,27	2.81	8 (44%)	19,38,41	1.54	5 (26%)
45	OMC	A	1480	45	19,22,23	3.30	8 (42%)	26,31,34	0.71	0
45	PSU	A	3113	45	18,21,22	4.62	8 (44%)	22,30,33	1.75	5 (22%)
45	PSU	A	1685	45	18,21,22	4.66	8 (44%)	22,30,33	1.88	6 (27%)
45	PSU	A	2829	45	18,21,22	4.62	8 (44%)	22,30,33	1.86	6 (27%)
45	OMG	A	2794	45	18,26,27	2.79	8 (44%)	19,38,41	1.47	4 (21%)
45	A2M	A	886	45	18,25,26	4.14	7 (38%)	18,36,39	3.75	6 (33%)
45	OMG	A	2126	45	18,26,27	2.81	8 (44%)	19,38,41	1.56	5 (26%)
45	PSU	A	1133	45	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
45	PSU	A	717	45	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
45	PSU	A	2317	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.90	5 (22%)
45	OMC	A	2200	48,45	19,22,23	3.29	8 (42%)	26,31,34	0.79	0
45	PSU	A	2214	45	18,21,22	4.64	8 (44%)	22,30,33	1.84	6 (27%)
45	A2M	A	946	45	18,25,26	4.12	8 (44%)	18,36,39	4.01	7 (38%)
45	OMU	A	2720	45	19,22,23	3.21	8 (42%)	26,31,34	1.67	5 (19%)
45	A2M	A	660	45	18,25,26	4.13	7 (38%)	18,36,39	3.99	6 (33%)
45	A2M	A	1378	45	18,25,26	4.13	7 (38%)	18,36,39	3.72	4 (22%)
45	OMG	A	2239	45	18,26,27	2.84	8 (44%)	19,38,41	1.52	4 (21%)
45	OMG	A	815	45	18,26,27	2.83	8 (44%)	19,38,41	1.54	5 (26%)
45	PSU	A	1002	45	18,21,22	4.67	8 (44%)	22,30,33	1.85	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A2M	A	2949	45	18,25,26	4.14	7 (38%)	18,36,39	3.78	4 (22%)
45	A2M	A	369	45	18,25,26	4.12	7 (38%)	18,36,39	3.84	5 (27%)
45	OMU	A	2732	45	19,22,23	3.19	8 (42%)	26,31,34	1.62	4 (15%)
45	OMG	A	2412	48,45	18,26,27	2.83	8 (44%)	19,38,41	1.58	5 (26%)
45	PSU	A	2263	45	18,21,22	4.66	8 (44%)	22,30,33	1.84	6 (27%)
45	OMG	A	2622	45	18,26,27	2.83	8 (44%)	19,38,41	1.52	4 (21%)
46	OMG	B	78	46	18,26,27	2.81	8 (44%)	19,38,41	1.52	5 (26%)
45	OMC	A	2340	45	19,22,23	3.26	8 (42%)	26,31,34	0.68	0
45	OMG	A	2925	45	18,26,27	2.81	8 (44%)	19,38,41	1.51	4 (21%)
45	OMG	A	2654	45	18,26,27	2.79	8 (44%)	19,38,41	1.67	6 (31%)
45	OMC	A	2882	45	19,22,23	3.27	8 (42%)	26,31,34	0.75	0
45	OMU	A	2924	48,45	19,22,23	3.21	8 (42%)	26,31,34	1.68	5 (19%)
45	A2M	A	2223	45	18,25,26	4.16	7 (38%)	18,36,39	3.78	4 (22%)
45	PSU	A	2897	45	18,21,22	4.65	8 (44%)	22,30,33	1.79	5 (22%)
45	PSU	A	311	48,45	18,21,22	4.66	8 (44%)	22,30,33	1.76	5 (22%)
45	OMG	A	2818	45	18,26,27	2.79	8 (44%)	19,38,41	1.57	5 (26%)
45	OMU	A	804	45	19,22,23	3.20	8 (42%)	26,31,34	1.67	5 (19%)
45	OMC	A	2839	45	19,22,23	3.29	8 (42%)	26,31,34	0.76	0
45	PSU	A	1474	45	18,21,22	4.63	8 (44%)	22,30,33	1.81	6 (27%)

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
45	OMU	A	2738	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2951	45	-	0/9/27/28	0/2/2/2
46	A2M	B	46	46	-	0/5/27/28	0/3/3/3
45	OMC	A	1849	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1482	45	-	0/7/25/26	0/2/2/2
45	OMG	A	296	45	-	2/5/27/28	0/3/3/3
45	A2M	A	2329	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1134	45	-	0/7/25/26	0/2/2/2
45	5MC	A	2281	45	-	0/7/25/26	0/2/2/2
45	OMG	A	918	48,45	-	2/5/27/28	0/3/3/3
45	1MA	A	656	45	-	0/3/25/26	0/3/3/3
45	PSU	A	786	45	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMU	A	1537	45	-	0/9/27/28	0/2/2/2
45	OMU	A	1894	45	-	0/9/27/28	0/2/2/2
45	PSU	A	829	45	-	0/7/25/26	0/2/2/2
45	PSU	A	34	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2857	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2978	45	-	0/7/25/26	0/2/2/2
45	OMU	A	787	45	-	0/9/27/28	0/2/2/2
45	PSU	A	277	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2321	45,47	-	2/7/25/26	0/2/2/2
45	OMC	A	1852	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2267	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2291	45	-	2/5/27/28	0/3/3/3
45	A2M	A	817	45	-	0/5/27/28	0/3/3/3
45	A2M	A	2914	45	-	2/5/27/28	0/3/3/3
45	OMU	A	2424	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2137	48,45	-	0/7/25/26	0/2/2/2
45	OMC	A	2685	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2962	45	-	0/9/27/28	0/2/2/2
45	OMU	A	3289	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2435	45	-	0/7/25/26	0/2/2/2
45	OMG	A	399	45	-	2/5/27/28	0/3/3/3
45	PSU	A	1064	48,45	-	0/7/25/26	0/2/2/2
45	OMC	A	2296	45	-	0/9/27/28	0/2/2/2
45	OMU	A	44	48,45	-	0/9/27/28	0/2/2/2
45	OMU	A	675	45	-	0/9/27/28	0/2/2/2
45	A2M	A	1460	45	-	0/5/27/28	0/3/3/3
45	A2M	A	827	48,45,47	-	3/5/27/28	0/3/3/3
45	PSU	A	2747	45	-	0/7/25/26	0/2/2/2
45	PSU	A	970	45	-	1/7/25/26	0/2/2/2
45	OMU	A	2413	48,45	-	2/9/27/28	0/2/2/2
45	UR3	A	2956	45	-	2/7/25/26	0/2/2/2
45	PSU	A	2257	45	-	0/7/25/26	0/2/2/2
45	A2M	A	1144	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2269	45	-	2/7/25/26	0/2/2/2
45	OMU	A	2350	45	-	0/9/27/28	0/2/2/2
45	OMC	A	40	45	-	1/9/27/28	0/2/2/2
45	PSU	A	966	45	-	0/7/25/26	0/2/2/2
45	PSU	A	510	45	-	0/7/25/26	0/2/2/2
45	OMU	A	48	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2394	45	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	2883	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1056	45	-	0/7/25/26	0/2/2/2
45	OMU	A	1068	45	-	0/9/27/28	0/2/2/2
45	OMC	A	1448	45	-	3/9/27/28	0/2/2/2
45	OMG	A	2398	45	-	0/5/27/28	0/3/3/3
45	OMU	A	144	45	-	1/9/27/28	0/2/2/2
45	A2M	A	2129	45	-	0/5/27/28	0/3/3/3
45	UY1	A	2653	45	-	0/9/27/28	0/2/2/2
46	PSU	B	96	48,46	-	2/7/25/26	0/2/2/2
45	A2M	A	2284	45	-	2/5/27/28	0/3/3/3
45	PSU	A	2139	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2947	48,45	-	2/7/25/26	0/2/2/2
45	OMC	A	674	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1016	48,45	-	0/7/25/26	0/2/2/2
45	OMU	A	3304	45	-	0/9/27/28	0/2/2/2
45	PSU	A	902	48,45,47	-	0/7/25/26	0/2/2/2
46	PSU	B	77	46	-	0/7/25/26	0/2/2/2
45	PSU	A	464	45	-	0/7/25/26	0/2/2/2
45	5MC	A	2873	48,45	-	4/7/25/26	0/2/2/2
45	OMG	A	2796	45	-	0/5/27/28	0/3/3/3
45	A2M	A	2804	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2127	45	-	0/5/27/28	0/3/3/3
45	OMG	A	1857	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2419	45	-	0/7/25/26	0/2/2/2
45	OMC	A	1862	45	-	0/9/27/28	0/2/2/2
45	OMC	A	2368	45	-	2/9/27/28	0/2/2/2
45	PSU	A	2868	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2194	48,45	-	0/7/25/26	0/2/2/2
45	PSU	A	42	48,45	-	0/7/25/26	0/2/2/2
45	A2M	A	2643	45	-	0/5/27/28	0/3/3/3
45	PSU	A	150	48,45	-	0/7/25/26	0/2/2/2
45	PSU	A	895	45	-	0/7/25/26	0/2/2/2
45	OMG	A	1461	45	-	1/5/27/28	0/3/3/3
45	PSU	A	2261	45	-	1/7/25/26	0/2/2/2
45	OMU	A	2886	45	-	0/9/27/28	0/2/2/2
45	PSU	A	2958	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2926	48,45	-	3/7/25/26	0/2/2/2
45	A2M	A	2324	45	-	0/5/27/28	0/3/3/3
45	PSU	A	228	45	-	2/7/25/26	0/2/2/2
45	PSU	A	684	45	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	A	1135	45	-	0/7/25/26	0/2/2/2
45	PSU	A	976	48,45	-	0/7/25/26	0/2/2/2
46	PSU	B	21	45,46	-	0/7/25/26	0/2/2/2
45	A2M	A	2259	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2920	45	-	0/5/27/28	0/3/3/3
45	OMC	A	1480	45	-	0/9/27/28	0/2/2/2
45	PSU	A	3113	45	-	0/7/25/26	0/2/2/2
45	PSU	A	1685	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2829	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2794	45	-	0/5/27/28	0/3/3/3
45	A2M	A	886	45	-	0/5/27/28	0/3/3/3
45	OMG	A	2126	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1133	45	-	0/7/25/26	0/2/2/2
45	PSU	A	717	45	-	0/7/25/26	0/2/2/2
45	PSU	A	2317	48,45	-	3/7/25/26	0/2/2/2
45	OMC	A	2200	48,45	-	4/9/27/28	0/2/2/2
45	PSU	A	2214	45	-	0/7/25/26	0/2/2/2
45	A2M	A	946	45	-	0/5/27/28	0/3/3/3
45	OMU	A	2720	45	-	0/9/27/28	0/2/2/2
45	A2M	A	660	45	-	2/5/27/28	0/3/3/3
45	A2M	A	1378	45	-	2/5/27/28	0/3/3/3
45	OMG	A	2239	45	-	0/5/27/28	0/3/3/3
45	OMG	A	815	45	-	0/5/27/28	0/3/3/3
45	PSU	A	1002	45	-	2/7/25/26	0/2/2/2
45	A2M	A	2949	45	-	0/5/27/28	0/3/3/3
45	A2M	A	369	45	-	1/5/27/28	0/3/3/3
45	OMU	A	2732	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2412	48,45	-	1/5/27/28	0/3/3/3
45	PSU	A	2263	45	-	0/7/25/26	0/2/2/2
45	OMG	A	2622	45	-	0/5/27/28	0/3/3/3
46	OMG	B	78	46	-	2/5/27/28	0/3/3/3
45	OMC	A	2340	45	-	0/9/27/28	0/2/2/2
45	OMG	A	2925	45	-	0/5/27/28	0/3/3/3
45	OMG	A	2654	45	-	0/5/27/28	0/3/3/3
45	OMC	A	2882	45	-	0/9/27/28	0/2/2/2
45	OMU	A	2924	48,45	-	0/9/27/28	0/2/2/2
45	A2M	A	2223	45	-	0/5/27/28	0/3/3/3
45	PSU	A	2897	45	-	0/7/25/26	0/2/2/2
45	PSU	A	311	48,45	-	0/7/25/26	0/2/2/2
45	OMG	A	2818	45	-	0/5/27/28	0/3/3/3
45	OMU	A	804	45	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OMC	A	2839	45	-	0/9/27/28	0/2/2/2
45	PSU	A	1474	45	-	0/7/25/26	0/2/2/2

All (1053) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2269	PSU	C6-C5	12.27	1.49	1.35
45	A	1002	PSU	C6-C5	12.24	1.49	1.35
45	A	2317	PSU	C6-C5	12.23	1.49	1.35
45	A	311	PSU	C6-C5	12.21	1.49	1.35
45	A	2137	PSU	C6-C5	12.21	1.49	1.35
45	A	1133	PSU	C6-C5	12.20	1.49	1.35
45	A	1685	PSU	C6-C5	12.19	1.49	1.35
45	A	970	PSU	C6-C5	12.19	1.49	1.35
45	A	2139	PSU	C6-C5	12.19	1.49	1.35
45	A	464	PSU	C6-C5	12.19	1.49	1.35
45	A	1482	PSU	C6-C5	12.19	1.49	1.35
45	A	786	PSU	C6-C5	12.18	1.49	1.35
45	A	2978	PSU	C6-C5	12.18	1.49	1.35
45	A	829	PSU	C6-C5	12.18	1.49	1.35
45	A	717	PSU	C6-C5	12.17	1.49	1.35
45	A	2926	PSU	C6-C5	12.17	1.49	1.35
45	A	2897	PSU	C6-C5	12.17	1.49	1.35
45	A	1056	PSU	C6-C5	12.16	1.49	1.35
45	A	2261	PSU	C6-C5	12.16	1.49	1.35
45	A	2958	PSU	C6-C5	12.16	1.49	1.35
45	A	3113	PSU	C6-C5	12.15	1.49	1.35
45	A	510	PSU	C6-C5	12.15	1.49	1.35
46	B	96	PSU	C6-C5	12.15	1.49	1.35
45	A	2257	PSU	C6-C5	12.14	1.49	1.35
45	A	902	PSU	C6-C5	12.14	1.49	1.35
45	A	2194	PSU	C6-C5	12.14	1.49	1.35
45	A	1135	PSU	C6-C5	12.14	1.49	1.35
45	A	976	PSU	C6-C5	12.13	1.49	1.35
45	A	2883	PSU	C6-C5	12.13	1.49	1.35
45	A	2263	PSU	C6-C5	12.12	1.49	1.35
45	A	228	PSU	C6-C5	12.12	1.49	1.35
45	A	150	PSU	C6-C5	12.11	1.49	1.35
45	A	2214	PSU	C6-C5	12.11	1.49	1.35
45	A	2947	PSU	C6-C5	12.11	1.49	1.35
45	A	34	PSU	C6-C5	12.10	1.49	1.35
45	A	2435	PSU	C6-C5	12.10	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	1064	PSU	C6-C5	12.09	1.49	1.35
46	B	77	PSU	C6-C5	12.09	1.49	1.35
45	A	2419	PSU	C6-C5	12.09	1.49	1.35
45	A	1016	PSU	C6-C5	12.08	1.49	1.35
45	A	2267	PSU	C6-C5	12.08	1.49	1.35
45	A	2868	PSU	C6-C5	12.08	1.49	1.35
45	A	2857	PSU	C6-C5	12.08	1.49	1.35
45	A	1474	PSU	C6-C5	12.06	1.49	1.35
45	A	2321	PSU	C6-C5	12.06	1.49	1.35
45	A	42	PSU	C6-C5	12.05	1.49	1.35
45	A	277	PSU	C6-C5	12.05	1.49	1.35
45	A	966	PSU	C6-C5	12.02	1.49	1.35
45	A	1134	PSU	C6-C5	12.01	1.49	1.35
45	A	2747	PSU	C6-C5	12.01	1.49	1.35
45	A	2829	PSU	C6-C5	12.01	1.49	1.35
45	A	895	PSU	C6-C5	12.01	1.49	1.35
46	B	21	PSU	C6-C5	12.00	1.49	1.35
45	A	684	PSU	C6-C5	11.98	1.49	1.35
45	A	2653	UY1	C6-C5	11.16	1.48	1.35
45	A	827	A2M	O4'-C1'	10.88	1.56	1.41
45	A	2259	A2M	O4'-C1'	10.84	1.56	1.41
45	A	2223	A2M	O4'-C1'	10.80	1.56	1.41
45	A	2129	A2M	O4'-C1'	10.78	1.56	1.41
45	A	2914	A2M	O4'-C1'	10.77	1.56	1.41
45	A	886	A2M	O4'-C1'	10.76	1.56	1.41
45	A	2949	A2M	O4'-C1'	10.73	1.56	1.41
46	B	46	A2M	O4'-C1'	10.72	1.56	1.41
45	A	2329	A2M	O4'-C1'	10.72	1.56	1.41
45	A	2643	A2M	O4'-C1'	10.69	1.56	1.41
45	A	1378	A2M	O4'-C1'	10.66	1.55	1.41
45	A	1460	A2M	O4'-C1'	10.63	1.55	1.41
45	A	660	A2M	O4'-C1'	10.63	1.55	1.41
45	A	369	A2M	O4'-C1'	10.63	1.55	1.41
45	A	1144	A2M	O4'-C1'	10.59	1.55	1.41
45	A	817	A2M	O4'-C1'	10.57	1.55	1.41
45	A	2324	A2M	O4'-C1'	10.54	1.55	1.41
45	A	946	A2M	O4'-C1'	10.48	1.55	1.41
45	A	2804	A2M	O4'-C1'	10.35	1.55	1.41
45	A	2284	A2M	O4'-C1'	10.27	1.55	1.41
45	A	946	A2M	C3'-C4'	-9.84	1.27	1.53
45	A	817	A2M	C3'-C4'	-9.83	1.27	1.53
45	A	2259	A2M	C3'-C4'	-9.83	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	827	A2M	C3'-C4'	-9.83	1.27	1.53
45	A	2914	A2M	C3'-C4'	-9.81	1.27	1.53
45	A	1378	A2M	C3'-C4'	-9.77	1.28	1.53
45	A	2223	A2M	C3'-C4'	-9.75	1.28	1.53
45	A	2129	A2M	C3'-C4'	-9.75	1.28	1.53
45	A	2873	5MC	C6-C5	9.74	1.50	1.34
45	A	660	A2M	C3'-C4'	-9.70	1.28	1.53
45	A	2804	A2M	C3'-C4'	-9.69	1.28	1.53
45	A	2949	A2M	C3'-C4'	-9.69	1.28	1.53
45	A	1460	A2M	C3'-C4'	-9.68	1.28	1.53
45	A	42	PSU	C2-N1	9.67	1.49	1.36
45	A	886	A2M	C3'-C4'	-9.67	1.28	1.53
45	A	2329	A2M	C3'-C4'	-9.66	1.28	1.53
45	A	2281	5MC	C6-C5	9.65	1.50	1.34
46	B	46	A2M	C3'-C4'	-9.65	1.28	1.53
45	A	510	PSU	C2-N1	9.62	1.49	1.36
45	A	1144	A2M	C3'-C4'	-9.62	1.28	1.53
45	A	2653	UY1	C2-N1	9.62	1.49	1.36
45	A	2643	A2M	C3'-C4'	-9.61	1.28	1.53
45	A	2958	PSU	C2-N1	9.60	1.49	1.36
45	A	1016	PSU	C2-N1	9.60	1.49	1.36
45	A	34	PSU	C2-N1	9.59	1.49	1.36
45	A	2137	PSU	C2-N1	9.59	1.49	1.36
45	A	2267	PSU	C2-N1	9.59	1.49	1.36
45	A	2317	PSU	C2-N1	9.57	1.49	1.36
45	A	369	A2M	C3'-C4'	-9.57	1.28	1.53
45	A	1056	PSU	C2-N1	9.57	1.49	1.36
45	A	970	PSU	C2-N1	9.56	1.49	1.36
45	A	1133	PSU	C2-N1	9.56	1.49	1.36
45	A	2257	PSU	C2-N1	9.56	1.49	1.36
45	A	976	PSU	C2-N1	9.56	1.49	1.36
45	A	2435	PSU	C2-N1	9.55	1.49	1.36
45	A	1064	PSU	C2-N1	9.55	1.49	1.36
45	A	464	PSU	C2-N1	9.55	1.49	1.36
45	A	2269	PSU	C2-N1	9.55	1.49	1.36
45	A	684	PSU	C2-N1	9.55	1.49	1.36
45	A	2321	PSU	C2-N1	9.54	1.49	1.36
46	B	96	PSU	C2-N1	9.54	1.49	1.36
45	A	1685	PSU	C2-N1	9.54	1.49	1.36
45	A	1002	PSU	C2-N1	9.53	1.49	1.36
46	B	77	PSU	C2-N1	9.53	1.49	1.36
45	A	2263	PSU	C2-N1	9.53	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2978	PSU	C2-N1	9.53	1.49	1.36
45	A	1134	PSU	C2-N1	9.52	1.49	1.36
45	A	2261	PSU	C2-N1	9.52	1.49	1.36
45	A	228	PSU	C2-N1	9.52	1.49	1.36
45	A	717	PSU	C2-N1	9.52	1.49	1.36
45	A	2324	A2M	C3'-C4'	-9.52	1.28	1.53
45	A	2214	PSU	C2-N1	9.51	1.49	1.36
45	A	895	PSU	C2-N1	9.50	1.49	1.36
45	A	2284	A2M	C3'-C4'	-9.50	1.28	1.53
45	A	2194	PSU	C2-N1	9.49	1.49	1.36
45	A	2926	PSU	C2-N1	9.49	1.49	1.36
45	A	1135	PSU	C2-N1	9.48	1.49	1.36
45	A	2868	PSU	C2-N1	9.48	1.49	1.36
45	A	2897	PSU	C2-N1	9.48	1.49	1.36
45	A	2419	PSU	C2-N1	9.48	1.49	1.36
45	A	2857	PSU	C2-N1	9.47	1.49	1.36
45	A	829	PSU	C2-N1	9.47	1.49	1.36
45	A	1482	PSU	C2-N1	9.47	1.49	1.36
45	A	1474	PSU	C2-N1	9.47	1.49	1.36
45	A	2747	PSU	C2-N1	9.47	1.49	1.36
45	A	2883	PSU	C2-N1	9.45	1.49	1.36
45	A	150	PSU	C2-N1	9.44	1.49	1.36
45	A	2947	PSU	C2-N1	9.43	1.49	1.36
45	A	311	PSU	C2-N1	9.43	1.49	1.36
45	A	2829	PSU	C2-N1	9.42	1.49	1.36
45	A	3113	PSU	C2-N1	9.41	1.49	1.36
45	A	277	PSU	C2-N1	9.41	1.49	1.36
46	B	21	PSU	C2-N1	9.41	1.49	1.36
45	A	902	PSU	C2-N1	9.37	1.49	1.36
45	A	966	PSU	C2-N1	9.37	1.49	1.36
45	A	786	PSU	C2-N1	9.35	1.49	1.36
45	A	2139	PSU	C2-N1	9.34	1.49	1.36
45	A	2747	PSU	C2-N3	8.31	1.51	1.37
45	A	2926	PSU	C2-N3	8.31	1.51	1.37
45	A	228	PSU	C2-N3	8.28	1.51	1.37
45	A	2263	PSU	C2-N3	8.28	1.51	1.37
45	A	2269	PSU	C2-N3	8.28	1.51	1.37
45	A	1016	PSU	C2-N3	8.27	1.51	1.37
46	B	77	PSU	C2-N3	8.26	1.51	1.37
45	A	2257	PSU	C2-N3	8.26	1.51	1.37
45	A	150	PSU	C2-N3	8.25	1.51	1.37
45	A	717	PSU	C2-N3	8.25	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	902	PSU	C2-N3	8.24	1.51	1.37
45	A	1135	PSU	C2-N3	8.24	1.51	1.37
45	A	2317	PSU	C2-N3	8.24	1.51	1.37
45	A	1482	PSU	C2-N3	8.23	1.51	1.37
45	A	464	PSU	C2-N3	8.23	1.51	1.37
45	A	1685	PSU	C2-N3	8.22	1.51	1.37
45	A	2261	PSU	C2-N3	8.22	1.51	1.37
45	A	786	PSU	C2-N3	8.22	1.51	1.37
45	A	2829	PSU	C2-N3	8.22	1.51	1.37
45	A	1064	PSU	C2-N3	8.21	1.51	1.37
45	A	1474	PSU	C2-N3	8.21	1.51	1.37
45	A	2214	PSU	C2-N3	8.21	1.51	1.37
45	A	1002	PSU	C2-N3	8.21	1.51	1.37
45	A	311	PSU	C2-N3	8.20	1.51	1.37
45	A	2958	PSU	C2-N3	8.20	1.51	1.37
45	A	976	PSU	C2-N3	8.20	1.51	1.37
45	A	2267	PSU	C2-N3	8.20	1.51	1.37
45	A	970	PSU	C2-N3	8.20	1.51	1.37
46	B	96	PSU	C2-N3	8.20	1.51	1.37
45	A	2139	PSU	C2-N3	8.20	1.51	1.37
45	A	2857	PSU	C2-N3	8.19	1.51	1.37
45	A	2868	PSU	C2-N3	8.19	1.51	1.37
46	B	21	PSU	C2-N3	8.19	1.51	1.37
45	A	2883	PSU	C2-N3	8.19	1.51	1.37
45	A	2321	PSU	C2-N3	8.19	1.51	1.37
45	A	2435	PSU	C2-N3	8.18	1.51	1.37
45	A	684	PSU	C2-N3	8.17	1.51	1.37
45	A	2419	PSU	C2-N3	8.17	1.51	1.37
45	A	2947	PSU	C2-N3	8.16	1.51	1.37
45	A	277	PSU	C2-N3	8.16	1.51	1.37
45	A	1056	PSU	C2-N3	8.16	1.51	1.37
45	A	895	PSU	C2-N3	8.15	1.51	1.37
45	A	2897	PSU	C2-N3	8.15	1.51	1.37
45	A	966	PSU	C2-N3	8.14	1.51	1.37
45	A	510	PSU	C2-N3	8.14	1.51	1.37
45	A	34	PSU	C2-N3	8.14	1.51	1.37
45	A	1133	PSU	C2-N3	8.14	1.51	1.37
45	A	3113	PSU	C2-N3	8.13	1.51	1.37
45	A	2194	PSU	C2-N3	8.12	1.51	1.37
45	A	1134	PSU	C2-N3	8.10	1.51	1.37
45	A	829	PSU	C2-N3	8.10	1.51	1.37
45	A	2137	PSU	C2-N3	8.08	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	42	PSU	C2-N3	8.07	1.51	1.37
45	A	2978	PSU	C2-N3	8.07	1.51	1.37
45	A	2653	UY1	C2-N3	7.34	1.50	1.37
45	A	2956	UR3	C2-N1	7.25	1.49	1.38
45	A	2281	5MC	C4-N3	7.18	1.46	1.34
45	A	2873	5MC	C4-N3	7.10	1.46	1.34
45	A	2886	OMU	C2-N3	7.05	1.50	1.38
45	A	2350	OMU	C2-N3	7.01	1.50	1.38
45	A	3289	OMU	C2-N3	6.99	1.50	1.38
45	A	144	OMU	C2-N3	6.99	1.50	1.38
45	A	1480	OMC	C2-N3	6.98	1.50	1.36
45	A	2685	OMC	C2-N3	6.97	1.50	1.36
45	A	2296	OMC	C2-N3	6.97	1.50	1.36
45	A	675	OMU	C2-N3	6.97	1.50	1.38
45	A	2839	OMC	C2-N3	6.96	1.50	1.36
45	A	44	OMU	C2-N3	6.96	1.50	1.38
45	A	2738	OMU	C2-N3	6.95	1.50	1.38
45	A	2424	OMU	C2-N3	6.95	1.50	1.38
45	A	1448	OMC	C2-N3	6.94	1.50	1.36
45	A	2720	OMU	C2-N3	6.94	1.50	1.38
45	A	1852	OMC	C2-N3	6.94	1.50	1.36
45	A	804	OMU	C2-N3	6.94	1.50	1.38
45	A	2882	OMC	C2-N3	6.92	1.50	1.36
45	A	2924	OMU	C2-N3	6.92	1.50	1.38
45	A	2962	OMC	C2-N3	6.91	1.50	1.36
45	A	2200	OMC	C2-N3	6.91	1.50	1.36
45	A	2951	OMC	C2-N3	6.89	1.50	1.36
45	A	1068	OMU	C2-N3	6.89	1.50	1.38
45	A	2368	OMC	C2-N3	6.88	1.50	1.36
45	A	787	OMU	C2-N3	6.87	1.50	1.38
45	A	1894	OMU	C2-N3	6.87	1.50	1.38
45	A	2281	5MC	C2-N3	6.85	1.50	1.36
45	A	3304	OMU	C2-N3	6.85	1.50	1.38
45	A	1537	OMU	C2-N3	6.85	1.50	1.38
45	A	2413	OMU	C2-N3	6.85	1.50	1.38
45	A	2873	5MC	C2-N3	6.85	1.50	1.36
45	A	40	OMC	C2-N3	6.84	1.50	1.36
45	A	674	OMC	C2-N3	6.83	1.50	1.36
45	A	2340	OMC	C2-N3	6.83	1.50	1.36
45	A	2732	OMU	C2-N3	6.81	1.50	1.38
45	A	1862	OMC	C2-N3	6.79	1.50	1.36
45	A	1849	OMC	C2-N3	6.79	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	48	OMU	C2-N3	6.76	1.50	1.38
45	A	1537	OMU	C2-N1	6.63	1.49	1.38
45	A	2413	OMU	C2-N1	6.58	1.49	1.38
45	A	1894	OMU	C2-N1	6.58	1.49	1.38
45	A	2886	OMU	C2-N1	6.57	1.49	1.38
45	A	675	OMU	C2-N1	6.57	1.49	1.38
45	A	3304	OMU	C2-N1	6.57	1.49	1.38
45	A	44	OMU	C2-N1	6.57	1.49	1.38
45	A	144	OMU	C2-N1	6.56	1.49	1.38
45	A	2738	OMU	C2-N1	6.54	1.48	1.38
45	A	2424	OMU	C2-N1	6.54	1.48	1.38
45	A	1068	OMU	C2-N1	6.53	1.48	1.38
45	A	804	OMU	C2-N1	6.52	1.48	1.38
45	A	2924	OMU	C2-N1	6.52	1.48	1.38
45	A	48	OMU	C2-N1	6.50	1.48	1.38
45	A	3289	OMU	C2-N1	6.50	1.48	1.38
45	A	2350	OMU	C2-N1	6.50	1.48	1.38
45	A	787	OMU	C2-N1	6.49	1.48	1.38
45	A	2720	OMU	C2-N1	6.48	1.48	1.38
45	A	2732	OMU	C2-N1	6.47	1.48	1.38
45	A	2804	A2M	C3'-C2'	6.39	1.67	1.52
45	A	2956	UR3	C6-C5	6.18	1.49	1.35
45	A	817	A2M	C3'-C2'	6.18	1.66	1.52
45	A	1849	OMC	C6-C5	6.17	1.49	1.35
45	A	2340	OMC	C6-C5	6.17	1.49	1.35
45	A	1448	OMC	C6-C5	6.16	1.49	1.35
45	A	2200	OMC	C6-C5	6.15	1.49	1.35
45	A	674	OMC	C6-C5	6.14	1.49	1.35
45	A	1480	OMC	C6-C5	6.14	1.49	1.35
45	A	1862	OMC	C6-C5	6.14	1.49	1.35
45	A	2296	OMC	C6-C5	6.12	1.49	1.35
45	A	1852	OMC	C6-C5	6.12	1.49	1.35
45	A	2685	OMC	C6-C5	6.12	1.49	1.35
45	A	2882	OMC	C6-C5	6.12	1.49	1.35
45	A	2962	OMC	C6-C5	6.10	1.49	1.35
45	A	2368	OMC	C6-C5	6.09	1.49	1.35
45	A	2839	OMC	C6-C5	6.09	1.49	1.35
45	A	40	OMC	C6-C5	6.03	1.49	1.35
45	A	369	A2M	C3'-C2'	5.99	1.66	1.52
45	A	2873	5MC	C6-N1	5.99	1.48	1.38
45	A	2951	OMC	C6-C5	5.99	1.49	1.35
45	A	660	A2M	C3'-C2'	5.99	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	1460	A2M	C3'-C2'	5.99	1.66	1.52
45	A	827	A2M	C3'-C2'	5.99	1.66	1.52
45	A	2223	A2M	C3'-C2'	5.96	1.66	1.52
45	A	946	A2M	C3'-C2'	5.95	1.66	1.52
45	A	2129	A2M	C3'-C2'	5.91	1.66	1.52
45	A	399	OMG	C2-N3	5.91	1.47	1.33
45	A	2259	A2M	C3'-C2'	5.90	1.66	1.52
45	A	2914	A2M	C3'-C2'	5.89	1.66	1.52
45	A	886	A2M	C3'-C2'	5.88	1.66	1.52
45	A	2281	5MC	C6-N1	5.88	1.48	1.38
45	A	1144	A2M	C3'-C2'	5.88	1.66	1.52
45	A	2284	A2M	C3'-C2'	5.86	1.66	1.52
45	A	2949	A2M	C3'-C2'	5.86	1.66	1.52
45	A	42	PSU	C6-N1	5.85	1.45	1.36
45	A	2261	PSU	C6-N1	5.85	1.45	1.36
45	A	976	PSU	C6-N1	5.84	1.45	1.36
45	A	2257	PSU	C6-N1	5.84	1.45	1.36
45	A	2239	OMG	C2-N3	5.84	1.47	1.33
45	A	1056	PSU	C6-N1	5.83	1.45	1.36
45	A	2194	PSU	C6-N1	5.83	1.45	1.36
45	A	2643	A2M	C3'-C2'	5.82	1.65	1.52
45	A	1064	PSU	C6-N1	5.82	1.45	1.36
45	A	1482	PSU	C6-N1	5.81	1.45	1.36
45	A	1133	PSU	C6-N1	5.81	1.45	1.36
45	A	684	PSU	C6-N1	5.80	1.45	1.36
46	B	46	A2M	C3'-C2'	5.80	1.65	1.52
45	A	2137	PSU	C6-N1	5.80	1.45	1.36
46	B	96	PSU	C6-N1	5.79	1.45	1.36
45	A	2324	A2M	C3'-C2'	5.79	1.65	1.52
45	A	2269	PSU	C6-N1	5.79	1.45	1.36
45	A	1002	PSU	C6-N1	5.78	1.45	1.36
45	A	2622	OMG	C2-N3	5.78	1.47	1.33
45	A	918	OMG	C2-N3	5.78	1.47	1.33
45	A	717	PSU	C6-N1	5.78	1.45	1.36
45	A	150	PSU	C6-N1	5.77	1.45	1.36
45	A	2329	A2M	C3'-C2'	5.77	1.65	1.52
45	A	1378	A2M	C3'-C2'	5.77	1.65	1.52
45	A	902	PSU	C6-N1	5.77	1.45	1.36
45	A	2925	OMG	C2-N3	5.76	1.47	1.33
45	A	464	PSU	C6-N1	5.76	1.45	1.36
45	A	510	PSU	C6-N1	5.76	1.45	1.36
45	A	2868	PSU	C6-N1	5.76	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2958	PSU	C6-N1	5.76	1.45	1.36
45	A	2419	PSU	C6-N1	5.75	1.45	1.36
45	A	1016	PSU	C6-N1	5.75	1.45	1.36
45	A	3113	PSU	C6-N1	5.75	1.45	1.36
45	A	2267	PSU	C6-N1	5.75	1.45	1.36
45	A	786	PSU	C6-N1	5.75	1.45	1.36
45	A	1685	PSU	C6-N1	5.75	1.45	1.36
45	A	1134	PSU	C6-N1	5.74	1.45	1.36
45	A	2897	PSU	C6-N1	5.74	1.45	1.36
45	A	2978	PSU	C6-N1	5.74	1.45	1.36
46	B	77	PSU	C6-N1	5.74	1.45	1.36
45	A	2263	PSU	C6-N1	5.74	1.45	1.36
45	A	2214	PSU	C6-N1	5.73	1.45	1.36
46	B	78	OMG	C2-N3	5.73	1.47	1.33
45	A	228	PSU	C6-N1	5.73	1.45	1.36
45	A	311	PSU	C6-N1	5.73	1.45	1.36
45	A	34	PSU	C6-N1	5.73	1.45	1.36
45	A	2435	PSU	C6-N1	5.72	1.45	1.36
45	A	895	PSU	C6-N1	5.72	1.45	1.36
45	A	2321	PSU	C6-N1	5.71	1.45	1.36
45	A	2317	PSU	C6-N1	5.71	1.45	1.36
45	A	296	OMG	C2-N3	5.71	1.47	1.33
45	A	2281	5MC	C4-N4	5.71	1.49	1.34
45	A	970	PSU	C6-N1	5.71	1.45	1.36
45	A	1135	PSU	C6-N1	5.71	1.45	1.36
45	A	2829	PSU	C6-N1	5.71	1.45	1.36
45	A	815	OMG	C2-N3	5.70	1.47	1.33
45	A	277	PSU	C6-N1	5.69	1.45	1.36
45	A	2926	PSU	C6-N1	5.69	1.45	1.36
45	A	2291	OMG	C2-N3	5.69	1.47	1.33
45	A	1474	PSU	C6-N1	5.69	1.45	1.36
45	A	2947	PSU	C6-N1	5.68	1.45	1.36
45	A	2139	PSU	C6-N1	5.68	1.45	1.36
45	A	2883	PSU	C6-N1	5.66	1.45	1.36
45	A	2873	5MC	C4-N4	5.66	1.48	1.34
45	A	2857	PSU	C6-N1	5.66	1.45	1.36
45	A	966	PSU	C6-N1	5.65	1.45	1.36
45	A	2747	PSU	C6-N1	5.65	1.45	1.36
45	A	1857	OMG	C2-N3	5.65	1.46	1.33
45	A	1461	OMG	C2-N3	5.63	1.46	1.33
45	A	2796	OMG	C2-N3	5.63	1.46	1.33
45	A	2794	OMG	C2-N3	5.62	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	21	PSU	C6-N1	5.62	1.45	1.36
45	A	2920	OMG	C2-N3	5.61	1.46	1.33
45	A	2126	OMG	C2-N3	5.61	1.46	1.33
45	A	829	PSU	C6-N1	5.61	1.45	1.36
45	A	2412	OMG	C2-N3	5.60	1.46	1.33
45	A	1894	OMU	C6-C5	5.57	1.48	1.35
45	A	2350	OMU	C6-C5	5.55	1.47	1.35
45	A	3304	OMU	C6-C5	5.54	1.47	1.35
45	A	1068	OMU	C6-C5	5.54	1.47	1.35
45	A	48	OMU	C6-C5	5.52	1.47	1.35
45	A	1448	OMC	C4-N3	5.52	1.45	1.34
45	A	675	OMU	C6-C5	5.52	1.47	1.35
45	A	2394	OMG	C2-N3	5.51	1.46	1.33
45	A	674	OMC	C4-N3	5.51	1.45	1.34
45	A	2924	OMU	C6-C5	5.51	1.47	1.35
45	A	1852	OMC	C4-N3	5.51	1.45	1.34
45	A	2839	OMC	C4-N3	5.51	1.45	1.34
45	A	2685	OMC	C4-N3	5.50	1.45	1.34
45	A	2818	OMG	C2-N3	5.49	1.46	1.33
45	A	2424	OMU	C6-C5	5.49	1.47	1.35
45	A	2413	OMU	C6-C5	5.49	1.47	1.35
45	A	2738	OMU	C6-C5	5.49	1.47	1.35
45	A	787	OMU	C6-C5	5.49	1.47	1.35
45	A	2127	OMG	C2-N3	5.49	1.46	1.33
45	A	1537	OMU	C6-C5	5.49	1.47	1.35
45	A	2368	OMC	C4-N3	5.49	1.45	1.34
45	A	2720	OMU	C6-C5	5.49	1.47	1.35
45	A	804	OMU	C6-C5	5.48	1.47	1.35
45	A	44	OMU	C6-C5	5.48	1.47	1.35
45	A	2732	OMU	C6-C5	5.48	1.47	1.35
45	A	1480	OMC	C4-N3	5.47	1.45	1.34
45	A	2200	OMC	C4-N3	5.47	1.45	1.34
45	A	2296	OMC	C4-N3	5.47	1.45	1.34
45	A	2239	OMG	C2-N2	5.47	1.47	1.34
45	A	2962	OMC	C4-N3	5.46	1.45	1.34
45	A	40	OMC	C4-N3	5.46	1.45	1.34
45	A	3289	OMU	C6-C5	5.46	1.47	1.35
45	A	2398	OMG	C2-N3	5.46	1.46	1.33
45	A	1862	OMC	C4-N3	5.45	1.45	1.34
45	A	2882	OMC	C4-N3	5.43	1.45	1.34
45	A	399	OMG	C2-N2	5.43	1.47	1.34
45	A	296	OMG	C2-N2	5.42	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2886	OMU	C6-C5	5.42	1.47	1.35
45	A	2340	OMC	C4-N3	5.41	1.45	1.34
45	A	2394	OMG	C2-N2	5.40	1.47	1.34
45	A	144	OMU	C6-C5	5.40	1.47	1.35
45	A	2925	OMG	C2-N2	5.39	1.47	1.34
45	A	2794	OMG	C2-N2	5.39	1.47	1.34
45	A	2951	OMC	C4-N3	5.39	1.45	1.34
45	A	2291	OMG	C2-N2	5.39	1.47	1.34
45	A	2622	OMG	C2-N2	5.39	1.47	1.34
45	A	2412	OMG	C2-N2	5.38	1.47	1.34
45	A	918	OMG	C2-N2	5.38	1.47	1.34
45	A	2920	OMG	C2-N2	5.37	1.47	1.34
45	A	815	OMG	C2-N2	5.35	1.46	1.34
45	A	2654	OMG	C2-N2	5.35	1.46	1.34
45	A	1849	OMC	C4-N3	5.35	1.45	1.34
46	B	78	OMG	C2-N2	5.34	1.46	1.34
45	A	2796	OMG	C2-N2	5.33	1.46	1.34
45	A	1461	OMG	C2-N2	5.32	1.46	1.34
45	A	1857	OMG	C2-N2	5.31	1.46	1.34
45	A	2818	OMG	C2-N2	5.31	1.46	1.34
45	A	2126	OMG	C2-N2	5.31	1.46	1.34
45	A	2654	OMG	C2-N3	5.28	1.46	1.33
45	A	2956	UR3	C2-N3	5.27	1.49	1.39
45	A	2398	OMG	C2-N2	5.27	1.46	1.34
45	A	2127	OMG	C2-N2	5.25	1.46	1.34
45	A	2653	UY1	C6-N1	5.25	1.44	1.36
45	A	399	OMG	C4-N3	5.23	1.50	1.37
45	A	2685	OMC	C4-N4	5.22	1.46	1.33
45	A	1480	OMC	C4-N4	5.21	1.46	1.33
45	A	2368	OMC	C4-N4	5.20	1.46	1.33
45	A	1852	OMC	C4-N4	5.20	1.46	1.33
45	A	2329	A2M	O4'-C4'	5.19	1.56	1.45
45	A	2839	OMC	C4-N4	5.18	1.46	1.33
45	A	2951	OMC	C4-N4	5.17	1.46	1.33
45	A	2962	OMC	C4-N4	5.17	1.46	1.33
45	A	2296	OMC	C4-N4	5.16	1.46	1.33
45	A	2239	OMG	C4-N3	5.16	1.49	1.37
45	A	2324	A2M	O4'-C4'	5.16	1.56	1.45
45	A	2622	OMG	C4-N3	5.15	1.49	1.37
45	A	918	OMG	C4-N3	5.15	1.49	1.37
45	A	674	OMC	C4-N4	5.15	1.46	1.33
45	A	2882	OMC	C4-N4	5.14	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	46	A2M	O4'-C4'	5.14	1.56	1.45
45	A	2200	OMC	C4-N4	5.14	1.46	1.33
45	A	1862	OMC	C4-N4	5.13	1.46	1.33
45	A	40	OMC	C4-N4	5.13	1.46	1.33
45	A	2340	OMC	C4-N4	5.13	1.46	1.33
45	A	1849	OMC	C4-N4	5.12	1.46	1.33
45	A	1448	OMC	C4-N4	5.11	1.46	1.33
45	A	2291	OMG	C4-N3	5.11	1.49	1.37
45	A	296	OMG	C4-N3	5.10	1.49	1.37
45	A	1144	A2M	O4'-C4'	5.09	1.56	1.45
45	A	2259	A2M	O4'-C4'	5.09	1.56	1.45
45	A	2925	OMG	C4-N3	5.08	1.49	1.37
45	A	2949	A2M	O4'-C4'	5.08	1.56	1.45
45	A	2129	A2M	O4'-C4'	5.07	1.56	1.45
45	A	2284	A2M	O4'-C4'	5.07	1.56	1.45
46	B	78	OMG	C4-N3	5.07	1.49	1.37
45	A	2794	OMG	C4-N3	5.06	1.49	1.37
45	A	886	A2M	O4'-C4'	5.06	1.56	1.45
45	A	1378	A2M	O4'-C4'	5.05	1.56	1.45
45	A	815	OMG	C4-N3	5.05	1.49	1.37
45	A	2796	OMG	C4-N3	5.05	1.49	1.37
45	A	2223	A2M	O4'-C4'	5.01	1.56	1.45
45	A	2643	A2M	O4'-C4'	5.00	1.56	1.45
45	A	660	A2M	O4'-C4'	5.00	1.56	1.45
45	A	2412	OMG	C4-N3	4.98	1.49	1.37
45	A	1460	A2M	O4'-C4'	4.98	1.56	1.45
45	A	1461	OMG	C4-N3	4.98	1.49	1.37
45	A	369	A2M	O4'-C4'	4.97	1.56	1.45
45	A	2126	OMG	C4-N3	4.97	1.49	1.37
45	A	827	A2M	O4'-C4'	4.96	1.56	1.45
45	A	1857	OMG	C4-N3	4.96	1.49	1.37
45	A	2920	OMG	C4-N3	4.95	1.49	1.37
45	A	2914	A2M	O4'-C4'	4.95	1.56	1.45
45	A	946	A2M	O4'-C4'	4.94	1.56	1.45
45	A	2127	OMG	C4-N3	4.94	1.49	1.37
45	A	2398	OMG	C4-N3	4.90	1.49	1.37
45	A	2394	OMG	C4-N3	4.89	1.49	1.37
45	A	2818	OMG	C4-N3	4.83	1.49	1.37
45	A	817	A2M	O4'-C4'	4.77	1.55	1.45
45	A	2654	OMG	C4-N3	4.74	1.48	1.37
45	A	2804	A2M	O4'-C4'	4.68	1.55	1.45
45	A	2873	5MC	C2-N1	4.68	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	44	OMU	C4-N3	4.66	1.46	1.38
45	A	2281	5MC	C2-N1	4.66	1.50	1.40
45	A	144	OMU	C4-N3	4.62	1.46	1.38
45	A	2924	OMU	C4-N3	4.60	1.46	1.38
45	A	2738	OMU	C4-N3	4.60	1.46	1.38
45	A	2350	OMU	C4-N3	4.58	1.46	1.38
45	A	2720	OMU	C4-N3	4.58	1.46	1.38
45	A	3289	OMU	C4-N3	4.58	1.46	1.38
45	A	1894	OMU	O4-C4	-4.57	1.15	1.24
45	A	2732	OMU	O4-C4	-4.57	1.15	1.24
45	A	3304	OMU	C4-N3	4.57	1.46	1.38
45	A	1537	OMU	O4-C4	-4.57	1.15	1.24
45	A	1068	OMU	C4-N3	4.56	1.46	1.38
45	A	2886	OMU	C4-N3	4.56	1.46	1.38
45	A	1480	OMC	C2-N1	4.56	1.49	1.40
45	A	2424	OMU	C4-N3	4.55	1.46	1.38
45	A	787	OMU	O4-C4	-4.55	1.15	1.24
45	A	2413	OMU	O4-C4	-4.55	1.15	1.24
45	A	1537	OMU	C4-N3	4.54	1.46	1.38
45	A	48	OMU	O4-C4	-4.54	1.15	1.24
45	A	787	OMU	C4-N3	4.54	1.46	1.38
45	A	3289	OMU	O4-C4	-4.54	1.15	1.24
45	A	675	OMU	C4-N3	4.53	1.46	1.38
45	A	2424	OMU	O4-C4	-4.53	1.15	1.24
45	A	804	OMU	C4-N3	4.53	1.46	1.38
45	A	2720	OMU	O4-C4	-4.53	1.15	1.24
45	A	1068	OMU	O4-C4	-4.52	1.15	1.24
45	A	1852	OMC	C2-N1	4.52	1.49	1.40
45	A	3304	OMU	O4-C4	-4.50	1.15	1.24
45	A	144	OMU	O4-C4	-4.50	1.15	1.24
45	A	804	OMU	O4-C4	-4.50	1.15	1.24
45	A	2296	OMC	C2-N1	4.50	1.49	1.40
45	A	675	OMU	O4-C4	-4.50	1.15	1.24
45	A	1894	OMU	C4-N3	4.49	1.46	1.38
45	A	44	OMU	O4-C4	-4.49	1.15	1.24
45	A	2886	OMU	O4-C4	-4.49	1.15	1.24
45	A	2200	OMC	C2-N1	4.48	1.49	1.40
45	A	2839	OMC	C2-N1	4.48	1.49	1.40
45	A	2350	OMU	O4-C4	-4.48	1.15	1.24
45	A	2738	OMU	O4-C4	-4.47	1.15	1.24
45	A	2685	OMC	C2-N1	4.45	1.49	1.40
45	A	2924	OMU	O4-C4	-4.43	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2732	OMU	C4-N3	4.43	1.46	1.38
45	A	2951	OMC	C2-N1	4.42	1.49	1.40
45	A	2882	OMC	C2-N1	4.42	1.49	1.40
45	A	150	PSU	C4-N3	4.41	1.47	1.38
45	A	311	PSU	C4-N3	4.40	1.47	1.38
45	A	228	PSU	C4-N3	4.39	1.47	1.38
45	A	464	PSU	C4-N3	4.39	1.47	1.38
45	A	48	OMU	C4-N3	4.39	1.46	1.38
45	A	2269	PSU	C4-N3	4.39	1.47	1.38
45	A	2261	PSU	C4-N3	4.38	1.47	1.38
45	A	1448	OMC	C2-N1	4.38	1.49	1.40
45	A	2829	PSU	C4-N3	4.38	1.47	1.38
45	A	40	OMC	C2-N1	4.38	1.49	1.40
45	A	902	PSU	C4-N3	4.38	1.47	1.38
45	A	2747	PSU	C4-N3	4.38	1.47	1.38
45	A	1016	PSU	C4-N3	4.38	1.47	1.38
45	A	2214	PSU	C4-N3	4.37	1.47	1.38
46	B	77	PSU	C4-N3	4.37	1.47	1.38
45	A	1135	PSU	C4-N3	4.37	1.46	1.38
45	A	2413	OMU	C4-N3	4.37	1.46	1.38
45	A	1849	OMC	O2-C2	-4.36	1.15	1.23
45	A	1685	PSU	C4-N3	4.36	1.46	1.38
45	A	786	PSU	C4-N3	4.36	1.46	1.38
45	A	2857	PSU	C4-N3	4.36	1.46	1.38
45	A	966	PSU	C4-N3	4.36	1.46	1.38
45	A	1133	PSU	C4-N3	4.36	1.46	1.38
45	A	1474	PSU	C4-N3	4.35	1.46	1.38
45	A	2263	PSU	C4-N3	4.35	1.46	1.38
45	A	2267	PSU	C4-N3	4.35	1.46	1.38
45	A	2317	PSU	C4-N3	4.35	1.46	1.38
45	A	2435	PSU	C4-N3	4.35	1.46	1.38
45	A	829	PSU	C4-N3	4.35	1.46	1.38
45	A	2194	PSU	C4-N3	4.35	1.46	1.38
45	A	2257	PSU	C4-N3	4.34	1.46	1.38
45	A	2654	OMG	C6-N1	4.34	1.44	1.37
45	A	1482	PSU	C4-N3	4.33	1.46	1.38
45	A	2883	PSU	C4-N3	4.33	1.46	1.38
45	A	2340	OMC	C2-N1	4.33	1.49	1.40
45	A	2368	OMC	C2-N1	4.33	1.49	1.40
46	B	96	PSU	C4-N3	4.33	1.46	1.38
45	A	2127	OMG	C6-N1	4.32	1.44	1.37
45	A	976	PSU	C4-N3	4.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2139	PSU	C4-N3	4.32	1.46	1.38
45	A	1849	OMC	C2-N1	4.32	1.49	1.40
45	A	656	1MA	C2-N3	4.32	1.34	1.29
45	A	2882	OMC	O2-C2	-4.32	1.15	1.23
45	A	2897	PSU	C4-N3	4.32	1.46	1.38
45	A	2926	PSU	C4-N3	4.31	1.46	1.38
45	A	2962	OMC	C2-N1	4.31	1.49	1.40
45	A	277	PSU	C4-N3	4.31	1.46	1.38
45	A	2419	PSU	C4-N3	4.31	1.46	1.38
45	A	2200	OMC	O2-C2	-4.31	1.15	1.23
45	A	2978	PSU	C4-N3	4.30	1.46	1.38
45	A	2412	OMG	C6-N1	4.30	1.44	1.37
45	A	2868	PSU	C4-N3	4.30	1.46	1.38
45	A	1002	PSU	C4-N3	4.30	1.46	1.38
45	A	717	PSU	C4-N3	4.30	1.46	1.38
45	A	2340	OMC	O2-C2	-4.29	1.15	1.23
45	A	2951	OMC	O2-C2	-4.29	1.15	1.23
46	B	21	PSU	C4-N3	4.28	1.46	1.38
45	A	2394	OMG	C6-N1	4.28	1.44	1.37
45	A	2321	PSU	C4-N3	4.28	1.46	1.38
45	A	2839	OMC	O2-C2	-4.27	1.15	1.23
45	A	1056	PSU	C4-N3	4.27	1.46	1.38
45	A	970	PSU	C4-N3	4.27	1.46	1.38
45	A	684	PSU	C4-N3	4.27	1.46	1.38
45	A	674	OMC	O2-C2	-4.27	1.15	1.23
45	A	2368	OMC	O2-C2	-4.26	1.15	1.23
45	A	2947	PSU	C4-N3	4.26	1.46	1.38
45	A	1852	OMC	O2-C2	-4.25	1.15	1.23
45	A	40	OMC	O2-C2	-4.25	1.15	1.23
45	A	1064	PSU	C4-N3	4.25	1.46	1.38
45	A	2296	OMC	O2-C2	-4.25	1.15	1.23
45	A	1862	OMC	O2-C2	-4.25	1.15	1.23
45	A	34	PSU	C4-N3	4.25	1.46	1.38
45	A	1480	OMC	O2-C2	-4.24	1.15	1.23
45	A	2958	PSU	C4-N3	4.24	1.46	1.38
45	A	1134	PSU	C4-N3	4.24	1.46	1.38
45	A	1862	OMC	C2-N1	4.24	1.49	1.40
45	A	510	PSU	C4-N3	4.23	1.46	1.38
45	A	2962	OMC	O2-C2	-4.22	1.15	1.23
45	A	895	PSU	C4-N3	4.22	1.46	1.38
45	A	2685	OMC	O2-C2	-4.21	1.15	1.23
45	A	2818	OMG	C6-N1	4.21	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	1448	OMC	O2-C2	-4.20	1.15	1.23
45	A	3113	PSU	C4-N3	4.19	1.46	1.38
45	A	2398	OMG	C6-N1	4.18	1.44	1.37
45	A	815	OMG	C6-N1	4.18	1.44	1.37
45	A	42	PSU	C4-N3	4.17	1.46	1.38
45	A	674	OMC	C2-N1	4.16	1.49	1.40
45	A	2920	OMG	C6-N1	4.15	1.44	1.37
45	A	2126	OMG	C6-N1	4.15	1.44	1.37
46	B	78	OMG	C6-N1	4.14	1.44	1.37
45	A	399	OMG	C6-N1	4.14	1.44	1.37
45	A	296	OMG	C6-N1	4.14	1.44	1.37
45	A	1857	OMG	C6-N1	4.12	1.44	1.37
45	A	2137	PSU	C4-N3	4.12	1.46	1.38
45	A	2291	OMG	C6-N1	4.10	1.44	1.37
45	A	2925	OMG	C6-N1	4.04	1.43	1.37
45	A	2239	OMG	C6-N1	4.02	1.43	1.37
45	A	2796	OMG	C6-N1	4.02	1.43	1.37
45	A	2622	OMG	C6-N1	4.02	1.43	1.37
45	A	2398	OMG	C5-C6	4.01	1.55	1.47
45	A	1461	OMG	C6-N1	4.01	1.43	1.37
45	A	2394	OMG	C5-C6	4.01	1.55	1.47
45	A	1461	OMG	C5-C6	4.01	1.55	1.47
45	A	2127	OMG	C5-C6	3.99	1.55	1.47
45	A	2654	OMG	C5-C6	3.98	1.55	1.47
45	A	2200	OMC	C6-N1	3.97	1.47	1.38
45	A	2794	OMG	C6-N1	3.95	1.43	1.37
45	A	1448	OMC	C6-N1	3.94	1.47	1.38
45	A	2412	OMG	C5-C6	3.94	1.55	1.47
45	A	2818	OMG	C5-C6	3.94	1.55	1.47
45	A	296	OMG	C5-C6	3.93	1.55	1.47
45	A	2291	OMG	C5-C6	3.90	1.55	1.47
45	A	815	OMG	C5-C6	3.90	1.55	1.47
45	A	1480	OMC	C6-N1	3.89	1.47	1.38
45	A	1852	OMC	C6-N1	3.89	1.47	1.38
45	A	2340	OMC	C6-N1	3.89	1.47	1.38
45	A	918	OMG	C6-N1	3.88	1.43	1.37
45	A	399	OMG	C5-C6	3.88	1.55	1.47
45	A	1849	OMC	C6-N1	3.86	1.47	1.38
45	A	2920	OMG	C5-C6	3.85	1.55	1.47
45	A	2126	OMG	C5-C6	3.85	1.55	1.47
45	A	2685	OMC	C6-N1	3.84	1.47	1.38
45	A	2296	OMC	C6-N1	3.84	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	40	OMC	C6-N1	3.84	1.47	1.38
45	A	1857	OMG	C5-C6	3.83	1.55	1.47
45	A	1862	OMC	C6-N1	3.83	1.47	1.38
45	A	2239	OMG	C5-C6	3.83	1.55	1.47
45	A	2839	OMC	C6-N1	3.82	1.47	1.38
45	A	2962	OMC	C6-N1	3.81	1.47	1.38
45	A	44	OMU	C6-N1	3.81	1.47	1.38
45	A	918	OMG	C5-C6	3.81	1.55	1.47
45	A	2796	OMG	C5-C6	3.81	1.55	1.47
45	A	2622	OMG	C5-C6	3.80	1.55	1.47
45	A	2794	OMG	C5-C6	3.80	1.55	1.47
45	A	2882	OMC	C6-N1	3.79	1.47	1.38
45	A	2368	OMC	C6-N1	3.78	1.47	1.38
46	B	78	OMG	C5-C6	3.77	1.55	1.47
45	A	2653	UY1	C4-N3	3.77	1.45	1.38
45	A	2925	OMG	C5-C6	3.77	1.55	1.47
45	A	674	OMC	C6-N1	3.74	1.47	1.38
45	A	2886	OMU	C6-N1	3.74	1.47	1.38
45	A	2951	OMC	C6-N1	3.73	1.47	1.38
45	A	48	OMU	C6-N1	3.72	1.47	1.38
45	A	1068	OMU	C6-N1	3.72	1.47	1.38
45	A	3289	OMU	C6-N1	3.72	1.47	1.38
45	A	2732	OMU	O2-C2	-3.71	1.16	1.23
45	A	2350	OMU	C6-N1	3.71	1.46	1.38
45	A	2732	OMU	C6-N1	3.71	1.46	1.38
45	A	2924	OMU	C6-N1	3.70	1.46	1.38
45	A	2424	OMU	C6-N1	3.70	1.46	1.38
45	A	2720	OMU	C6-N1	3.70	1.46	1.38
45	A	1537	OMU	C6-N1	3.70	1.46	1.38
45	A	2738	OMU	C6-N1	3.69	1.46	1.38
45	A	3304	OMU	C6-N1	3.68	1.46	1.38
45	A	804	OMU	C6-N1	3.68	1.46	1.38
45	A	44	OMU	O2-C2	-3.67	1.16	1.23
45	A	675	OMU	C6-N1	3.67	1.46	1.38
45	A	787	OMU	O2-C2	-3.67	1.16	1.23
45	A	144	OMU	C6-N1	3.66	1.46	1.38
45	A	787	OMU	C6-N1	3.66	1.46	1.38
45	A	144	OMU	O2-C2	-3.65	1.16	1.23
45	A	1894	OMU	C6-N1	3.64	1.46	1.38
45	A	48	OMU	O2-C2	-3.64	1.16	1.23
45	A	1068	OMU	O2-C2	-3.64	1.16	1.23
45	A	2350	OMU	O2-C2	-3.64	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	675	OMU	O2-C2	-3.64	1.16	1.23
45	A	2886	OMU	O2-C2	-3.63	1.16	1.23
45	A	2424	OMU	O2-C2	-3.61	1.16	1.23
45	A	2413	OMU	O2-C2	-3.60	1.16	1.23
45	A	804	OMU	O2-C2	-3.60	1.16	1.23
45	A	2924	OMU	O2-C2	-3.59	1.16	1.23
45	A	2738	OMU	O2-C2	-3.59	1.16	1.23
45	A	2413	OMU	C6-N1	3.58	1.46	1.38
45	A	1537	OMU	O2-C2	-3.58	1.16	1.23
45	A	2720	OMU	O2-C2	-3.58	1.16	1.23
45	A	1894	OMU	O2-C2	-3.58	1.16	1.23
45	A	3289	OMU	O2-C2	-3.57	1.16	1.23
45	A	3304	OMU	O2-C2	-3.57	1.16	1.23
45	A	829	PSU	O4-C4	-3.33	1.17	1.23
45	A	684	PSU	O4-C4	-3.30	1.17	1.23
45	A	1135	PSU	O4-C4	-3.29	1.17	1.23
46	B	21	PSU	O4-C4	-3.29	1.17	1.23
45	A	966	PSU	O4-C4	-3.28	1.17	1.23
45	A	2883	PSU	O4-C4	-3.27	1.17	1.23
45	A	2978	PSU	O4-C4	-3.27	1.17	1.23
45	A	42	PSU	O4-C4	-3.26	1.17	1.23
45	A	2139	PSU	O4-C4	-3.26	1.17	1.23
45	A	902	PSU	O4-C4	-3.25	1.17	1.23
45	A	786	PSU	O4-C4	-3.25	1.17	1.23
45	A	1002	PSU	O4-C4	-3.25	1.17	1.23
45	A	277	PSU	O4-C4	-3.25	1.17	1.23
45	A	1134	PSU	O4-C4	-3.25	1.17	1.23
45	A	976	PSU	O4-C4	-3.24	1.17	1.23
45	A	2897	PSU	O4-C4	-3.24	1.17	1.23
45	A	717	PSU	O4-C4	-3.23	1.17	1.23
45	A	2947	PSU	O4-C4	-3.23	1.17	1.23
45	A	2214	PSU	O4-C4	-3.22	1.17	1.23
45	A	2958	PSU	O4-C4	-3.22	1.17	1.23
45	A	1482	PSU	O4-C4	-3.22	1.17	1.23
45	A	311	PSU	O4-C4	-3.22	1.17	1.23
46	B	77	PSU	O4-C4	-3.22	1.17	1.23
46	B	96	PSU	O4-C4	-3.22	1.17	1.23
45	A	2435	PSU	O4-C4	-3.22	1.17	1.23
45	A	2419	PSU	O4-C4	-3.22	1.17	1.23
45	A	2857	PSU	O4-C4	-3.21	1.17	1.23
45	A	2194	PSU	O4-C4	-3.21	1.17	1.23
45	A	510	PSU	O4-C4	-3.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	895	PSU	O4-C4	-3.21	1.17	1.23
45	A	1016	PSU	O4-C4	-3.21	1.17	1.23
45	A	2747	PSU	O4-C4	-3.20	1.17	1.23
45	A	2868	PSU	O4-C4	-3.20	1.17	1.23
45	A	1064	PSU	O4-C4	-3.20	1.17	1.23
45	A	3113	PSU	O4-C4	-3.19	1.17	1.23
45	A	228	PSU	O4-C4	-3.19	1.17	1.23
45	A	464	PSU	O4-C4	-3.19	1.17	1.23
45	A	2269	PSU	O4-C4	-3.19	1.17	1.23
45	A	2137	PSU	O4-C4	-3.19	1.17	1.23
45	A	2263	PSU	O4-C4	-3.19	1.17	1.23
45	A	2829	PSU	O4-C4	-3.19	1.17	1.23
45	A	34	PSU	O4-C4	-3.19	1.17	1.23
45	A	150	PSU	O4-C4	-3.18	1.17	1.23
45	A	2267	PSU	O4-C4	-3.18	1.17	1.23
45	A	970	PSU	O4-C4	-3.18	1.17	1.23
45	A	1474	PSU	O4-C4	-3.17	1.17	1.23
45	A	1685	PSU	O4-C4	-3.17	1.17	1.23
45	A	2259	A2M	C6-N6	3.17	1.45	1.34
45	A	1056	PSU	O4-C4	-3.17	1.17	1.23
45	A	2643	A2M	C6-N6	3.17	1.45	1.34
45	A	2257	PSU	O4-C4	-3.17	1.17	1.23
45	A	1460	A2M	C6-N6	3.16	1.45	1.34
45	A	2321	PSU	O4-C4	-3.16	1.17	1.23
45	A	1133	PSU	O4-C4	-3.16	1.17	1.23
45	A	2654	OMG	C2-N1	3.15	1.45	1.37
45	A	2329	A2M	C6-N6	3.15	1.45	1.34
45	A	2926	PSU	O4-C4	-3.15	1.17	1.23
45	A	946	A2M	C6-N6	3.14	1.45	1.34
45	A	2261	PSU	O4-C4	-3.14	1.17	1.23
45	A	2317	PSU	O4-C4	-3.14	1.17	1.23
45	A	1144	A2M	C6-N6	3.13	1.45	1.34
45	A	2949	A2M	C6-N6	3.13	1.45	1.34
46	B	46	A2M	C6-N6	3.13	1.45	1.34
45	A	827	A2M	C6-N6	3.13	1.45	1.34
45	A	2129	A2M	C6-N6	3.12	1.45	1.34
45	A	2804	A2M	C6-N6	3.12	1.45	1.34
45	A	2956	UR3	C6-N1	3.12	1.45	1.38
45	A	369	A2M	C6-N6	3.12	1.45	1.34
45	A	2223	A2M	C6-N6	3.12	1.45	1.34
45	A	886	A2M	C6-N6	3.12	1.45	1.34
45	A	2394	OMG	C2-N1	3.11	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	1378	A2M	C6-N6	3.10	1.45	1.34
45	A	817	A2M	C6-N6	3.10	1.45	1.34
45	A	2914	A2M	C6-N6	3.10	1.45	1.34
45	A	2324	A2M	C6-N6	3.09	1.45	1.34
45	A	2920	OMG	C2-N1	3.09	1.45	1.37
45	A	2127	OMG	C2-N1	3.08	1.45	1.37
45	A	656	1MA	C6-N6	3.07	1.35	1.27
45	A	2818	OMG	C2-N1	3.06	1.45	1.37
45	A	660	A2M	C6-N6	3.06	1.45	1.34
45	A	2412	OMG	C2-N1	3.05	1.45	1.37
45	A	2398	OMG	C2-N1	3.04	1.45	1.37
45	A	399	OMG	C2-N1	3.03	1.45	1.37
45	A	2796	OMG	C2-N1	3.02	1.45	1.37
45	A	2291	OMG	C2-N1	3.02	1.45	1.37
45	A	1857	OMG	C2-N1	3.02	1.45	1.37
45	A	2126	OMG	C2-N1	3.02	1.45	1.37
45	A	296	OMG	C2-N1	3.02	1.45	1.37
45	A	918	OMG	C2-N1	3.01	1.45	1.37
45	A	1461	OMG	C2-N1	3.01	1.45	1.37
45	A	2622	OMG	C2-N1	3.01	1.45	1.37
46	B	78	OMG	C2-N1	2.99	1.45	1.37
45	A	786	PSU	C1'-C5	2.99	1.57	1.50
45	A	2284	A2M	C6-N6	2.97	1.44	1.34
45	A	2925	OMG	C2-N1	2.97	1.45	1.37
45	A	815	OMG	C2-N1	2.97	1.45	1.37
45	A	2239	OMG	C2-N1	2.96	1.45	1.37
45	A	311	PSU	C1'-C5	2.94	1.56	1.50
46	B	96	PSU	C1'-C5	2.91	1.56	1.50
45	A	2747	PSU	C1'-C5	2.91	1.56	1.50
45	A	1474	PSU	C1'-C5	2.89	1.56	1.50
45	A	1448	OMC	C5-C4	2.88	1.49	1.42
45	A	40	OMC	C5-C4	2.88	1.49	1.42
45	A	2194	PSU	C1'-C5	2.87	1.56	1.50
45	A	2794	OMG	C2-N1	2.86	1.44	1.37
45	A	1852	OMC	C5-C4	2.86	1.49	1.42
45	A	2419	PSU	C1'-C5	2.85	1.56	1.50
45	A	2269	PSU	C1'-C5	2.85	1.56	1.50
45	A	2263	PSU	C1'-C5	2.84	1.56	1.50
45	A	2137	PSU	O2-C2	-2.84	1.17	1.23
45	A	2296	OMC	C5-C4	2.83	1.49	1.42
45	A	2340	OMC	C5-C4	2.83	1.49	1.42
45	A	464	PSU	C1'-C5	2.83	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	1480	OMC	C5-C4	2.83	1.49	1.42
45	A	2200	OMC	C5-C4	2.81	1.49	1.42
45	A	1862	OMC	C5-C4	2.81	1.49	1.42
45	A	1849	OMC	C5-C4	2.81	1.49	1.42
45	A	2829	PSU	C1'-C5	2.81	1.56	1.50
45	A	2883	PSU	C1'-C5	2.80	1.56	1.50
45	A	2214	PSU	C1'-C5	2.80	1.56	1.50
45	A	2368	OMC	C5-C4	2.80	1.49	1.42
45	A	2962	OMC	C5-C4	2.80	1.49	1.42
45	A	2321	PSU	C1'-C5	2.80	1.56	1.50
45	A	976	PSU	C1'-C5	2.79	1.56	1.50
45	A	966	PSU	C1'-C5	2.79	1.56	1.50
45	A	902	PSU	C1'-C5	2.79	1.56	1.50
45	A	2654	OMG	C5-C4	-2.79	1.36	1.43
45	A	2261	PSU	C1'-C5	2.79	1.56	1.50
45	A	2882	OMC	C5-C4	2.78	1.49	1.42
45	A	2685	OMC	C5-C4	2.78	1.49	1.42
45	A	2868	PSU	C1'-C5	2.78	1.56	1.50
45	A	2958	PSU	C1'-C5	2.77	1.56	1.50
45	A	150	PSU	C1'-C5	2.77	1.56	1.50
45	A	2804	A2M	C5-C4	-2.77	1.33	1.40
45	A	2897	PSU	C1'-C5	2.77	1.56	1.50
45	A	2839	OMC	C5-C4	2.76	1.49	1.42
45	A	2127	OMG	C5-C4	-2.76	1.36	1.43
45	A	2324	A2M	C5-C4	-2.76	1.33	1.40
45	A	2284	A2M	C5-C4	-2.75	1.33	1.40
45	A	1133	PSU	C1'-C5	2.75	1.56	1.50
45	A	2139	PSU	C1'-C5	2.75	1.56	1.50
45	A	277	PSU	C1'-C5	2.75	1.56	1.50
45	A	2949	A2M	C5-C4	-2.74	1.33	1.40
45	A	1002	PSU	C1'-C5	2.74	1.56	1.50
45	A	2978	PSU	C1'-C5	2.74	1.56	1.50
45	A	2139	PSU	O2-C2	-2.74	1.17	1.23
45	A	1064	PSU	C1'-C5	2.74	1.56	1.50
45	A	1056	PSU	C1'-C5	2.74	1.56	1.50
45	A	684	PSU	C1'-C5	2.73	1.56	1.50
46	B	21	PSU	C1'-C5	2.73	1.56	1.50
45	A	3113	PSU	C1'-C5	2.73	1.56	1.50
45	A	2267	PSU	C1'-C5	2.72	1.56	1.50
45	A	1016	PSU	C1'-C5	2.72	1.56	1.50
45	A	2257	PSU	C1'-C5	2.72	1.56	1.50
45	A	660	A2M	C5-C4	-2.72	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2435	PSU	C1'-C5	2.71	1.56	1.50
45	A	2883	PSU	O2-C2	-2.71	1.17	1.23
45	A	1016	PSU	O2-C2	-2.71	1.17	1.23
45	A	1134	PSU	O2-C2	-2.71	1.17	1.23
45	A	1685	PSU	C1'-C5	2.71	1.56	1.50
45	A	970	PSU	C1'-C5	2.71	1.56	1.50
46	B	77	PSU	C1'-C5	2.70	1.56	1.50
45	A	829	PSU	O2-C2	-2.70	1.17	1.23
45	A	2897	PSU	O2-C2	-2.70	1.17	1.23
45	A	228	PSU	C1'-C5	2.70	1.56	1.50
46	B	46	A2M	C5-C4	-2.70	1.33	1.40
45	A	369	A2M	C5-C4	-2.70	1.33	1.40
45	A	2398	OMG	C5-C4	-2.69	1.36	1.43
45	A	1482	PSU	C1'-C5	2.69	1.56	1.50
45	A	2926	PSU	C1'-C5	2.69	1.56	1.50
45	A	2914	A2M	C5-C4	-2.69	1.33	1.40
45	A	827	A2M	C5-C4	-2.68	1.33	1.40
45	A	2129	A2M	C5-C4	-2.68	1.33	1.40
45	A	2868	PSU	O2-C2	-2.68	1.17	1.23
45	A	674	OMC	C5-C4	2.68	1.49	1.42
45	A	966	PSU	O2-C2	-2.68	1.17	1.23
45	A	2857	PSU	C1'-C5	2.68	1.56	1.50
45	A	1460	A2M	C5-C4	-2.68	1.33	1.40
45	A	2394	OMG	C5-C4	-2.68	1.36	1.43
45	A	1144	A2M	C5-C4	-2.68	1.33	1.40
45	A	1133	PSU	O2-C2	-2.68	1.17	1.23
45	A	2978	PSU	O2-C2	-2.68	1.17	1.23
45	A	1135	PSU	O2-C2	-2.67	1.17	1.23
45	A	1135	PSU	C1'-C5	2.67	1.56	1.50
45	A	2126	OMG	C5-C4	-2.67	1.36	1.43
46	B	96	PSU	O2-C2	-2.67	1.17	1.23
45	A	1134	PSU	C1'-C5	2.67	1.56	1.50
45	A	2947	PSU	C1'-C5	2.66	1.56	1.50
45	A	277	PSU	O2-C2	-2.66	1.17	1.23
45	A	2435	PSU	O2-C2	-2.66	1.17	1.23
45	A	1378	A2M	C5-C4	-2.66	1.33	1.40
45	A	817	A2M	C5-C4	-2.66	1.33	1.40
45	A	976	PSU	O2-C2	-2.66	1.17	1.23
45	A	2321	PSU	O2-C2	-2.66	1.17	1.23
45	A	2958	PSU	O2-C2	-2.66	1.17	1.23
45	A	2259	A2M	C5-C4	-2.66	1.33	1.40
45	A	2818	OMG	C5-C4	-2.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2419	PSU	O2-C2	-2.66	1.17	1.23
45	A	717	PSU	C1'-C5	2.66	1.56	1.50
45	A	311	PSU	O2-C2	-2.66	1.17	1.23
45	A	34	PSU	O2-C2	-2.65	1.17	1.23
45	A	684	PSU	O2-C2	-2.65	1.17	1.23
45	A	2829	PSU	O2-C2	-2.65	1.17	1.23
45	A	34	PSU	C1'-C5	2.65	1.56	1.50
45	A	886	A2M	C5-C4	-2.65	1.33	1.40
45	A	2329	A2M	C5-C4	-2.65	1.33	1.40
45	A	510	PSU	C1'-C5	2.65	1.56	1.50
45	A	42	PSU	C1'-C5	2.65	1.56	1.50
45	A	2857	PSU	O2-C2	-2.65	1.17	1.23
45	A	2794	OMG	C5-C4	-2.65	1.36	1.43
45	A	1056	PSU	O2-C2	-2.64	1.17	1.23
45	A	1002	PSU	O2-C2	-2.64	1.17	1.23
45	A	2257	PSU	O2-C2	-2.64	1.17	1.23
45	A	510	PSU	O2-C2	-2.64	1.17	1.23
45	A	786	PSU	O2-C2	-2.64	1.17	1.23
45	A	895	PSU	O2-C2	-2.64	1.17	1.23
45	A	1064	PSU	O2-C2	-2.64	1.17	1.23
46	B	21	PSU	O2-C2	-2.64	1.17	1.23
45	A	2194	PSU	O2-C2	-2.64	1.17	1.23
45	A	2920	OMG	C5-C4	-2.64	1.36	1.43
45	A	42	PSU	O2-C2	-2.64	1.17	1.23
45	A	2747	PSU	O2-C2	-2.63	1.17	1.23
45	A	2223	A2M	C5-C4	-2.63	1.34	1.40
45	A	2412	OMG	C5-C4	-2.63	1.36	1.43
45	A	2643	A2M	C5-C4	-2.63	1.34	1.40
45	A	815	OMG	C5-C4	-2.63	1.36	1.43
45	A	228	PSU	O2-C2	-2.62	1.17	1.23
45	A	902	PSU	O2-C2	-2.62	1.17	1.23
45	A	2947	PSU	O2-C2	-2.62	1.17	1.23
45	A	1857	OMG	C5-C4	-2.62	1.36	1.43
45	A	2796	OMG	C5-C4	-2.62	1.36	1.43
45	A	296	OMG	C5-C4	-2.62	1.36	1.43
45	A	2137	PSU	C1'-C5	2.62	1.56	1.50
45	A	970	PSU	O2-C2	-2.62	1.17	1.23
45	A	3113	PSU	O2-C2	-2.62	1.17	1.23
45	A	1685	PSU	O2-C2	-2.61	1.17	1.23
45	A	2267	PSU	O2-C2	-2.61	1.17	1.23
45	A	946	A2M	C5-C4	-2.61	1.34	1.40
45	A	1474	PSU	O2-C2	-2.61	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	150	PSU	O2-C2	-2.61	1.17	1.23
45	A	2269	PSU	O2-C2	-2.60	1.17	1.23
45	A	2951	OMC	C5-C4	2.60	1.48	1.42
45	A	1482	PSU	O2-C2	-2.60	1.17	1.23
46	B	77	PSU	O2-C2	-2.60	1.17	1.23
45	A	2291	OMG	C5-C4	-2.60	1.36	1.43
45	A	2214	PSU	O2-C2	-2.59	1.18	1.23
45	A	2622	OMG	C5-C4	-2.59	1.36	1.43
45	A	2263	PSU	O2-C2	-2.58	1.18	1.23
45	A	2261	PSU	O2-C2	-2.58	1.18	1.23
45	A	2926	PSU	O2-C2	-2.58	1.18	1.23
45	A	2925	OMG	C5-C4	-2.58	1.36	1.43
45	A	2239	OMG	C5-C4	-2.57	1.36	1.43
45	A	2317	PSU	O2-C2	-2.57	1.18	1.23
45	A	829	PSU	C1'-C5	2.57	1.56	1.50
46	B	78	OMG	C5-C4	-2.56	1.36	1.43
45	A	1461	OMG	C5-C4	-2.56	1.36	1.43
45	A	1857	OMG	O6-C6	-2.56	1.18	1.23
45	A	815	OMG	O6-C6	-2.56	1.18	1.23
45	A	717	PSU	O2-C2	-2.56	1.18	1.23
45	A	2818	OMG	O6-C6	-2.55	1.18	1.23
45	A	2291	OMG	O6-C6	-2.55	1.18	1.23
45	A	2317	PSU	C1'-C5	2.54	1.56	1.50
45	A	464	PSU	O2-C2	-2.54	1.18	1.23
45	A	2794	OMG	O6-C6	-2.53	1.18	1.23
45	A	2653	UY1	O4-C4	-2.53	1.18	1.23
45	A	918	OMG	C5-C4	-2.52	1.36	1.43
45	A	2796	OMG	O6-C6	-2.52	1.18	1.23
45	A	895	PSU	C1'-C5	2.52	1.56	1.50
45	A	2127	OMG	O6-C6	-2.52	1.18	1.23
45	A	399	OMG	C5-C4	-2.51	1.36	1.43
45	A	2126	OMG	O6-C6	-2.50	1.18	1.23
45	A	918	OMG	O6-C6	-2.49	1.18	1.23
46	B	78	OMG	O6-C6	-2.48	1.18	1.23
45	A	2622	OMG	O6-C6	-2.48	1.18	1.23
45	A	2412	OMG	O6-C6	-2.48	1.18	1.23
45	A	2398	OMG	O6-C6	-2.48	1.18	1.23
45	A	2239	OMG	O6-C6	-2.47	1.18	1.23
45	A	2654	OMG	O6-C6	-2.47	1.18	1.23
45	A	296	OMG	O6-C6	-2.46	1.18	1.23
45	A	1461	OMG	O6-C6	-2.45	1.18	1.23
45	A	2394	OMG	O6-C6	-2.45	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	2920	OMG	O6-C6	-2.45	1.18	1.23
45	A	2281	5MC	O2-C2	-2.44	1.19	1.23
45	A	2925	OMG	O6-C6	-2.44	1.18	1.23
45	A	787	OMU	C5-C4	2.42	1.49	1.43
45	A	399	OMG	O6-C6	-2.41	1.18	1.23
45	A	1068	OMU	C5-C4	2.40	1.48	1.43
45	A	3304	OMU	C5-C4	2.39	1.48	1.43
45	A	2738	OMU	C5-C4	2.38	1.48	1.43
45	A	44	OMU	C5-C4	2.37	1.48	1.43
45	A	2350	OMU	C5-C4	2.37	1.48	1.43
45	A	2720	OMU	C5-C4	2.37	1.48	1.43
45	A	1894	OMU	C5-C4	2.37	1.48	1.43
45	A	946	A2M	O5'-C5'	-2.37	1.39	1.44
45	A	2873	5MC	O2-C2	-2.37	1.19	1.23
45	A	48	OMU	C5-C4	2.37	1.48	1.43
45	A	2424	OMU	C5-C4	2.37	1.48	1.43
45	A	2732	OMU	C5-C4	2.35	1.48	1.43
45	A	2924	OMU	C5-C4	2.35	1.48	1.43
45	A	675	OMU	C5-C4	2.32	1.48	1.43
45	A	2947	PSU	O4'-C1'	-2.31	1.40	1.43
45	A	1537	OMU	C5-C4	2.31	1.48	1.43
45	A	2643	A2M	C2-N3	2.30	1.35	1.32
45	A	3289	OMU	C5-C4	2.28	1.48	1.43
45	A	2413	OMU	C5-C4	2.28	1.48	1.43
45	A	804	OMU	C5-C4	2.28	1.48	1.43
45	A	144	OMU	C5-C4	2.27	1.48	1.43
45	A	660	A2M	C2-N3	2.25	1.35	1.32
45	A	2956	UR3	C5-C4	2.24	1.49	1.43
45	A	2223	A2M	C2-N3	2.22	1.35	1.32
45	A	2653	UY1	O2-C2	-2.21	1.18	1.23
45	A	2914	A2M	C2-N3	2.21	1.35	1.32
45	A	2886	OMU	C5-C4	2.20	1.48	1.43
45	A	2259	A2M	C2-N3	2.20	1.35	1.32
45	A	2949	A2M	C2-N3	2.20	1.35	1.32
45	A	1378	A2M	C2-N3	2.18	1.35	1.32
45	A	369	A2M	C2-N3	2.17	1.35	1.32
45	A	2956	UR3	C4-N3	2.17	1.45	1.40
45	A	2129	A2M	C2-N3	2.17	1.35	1.32
45	A	2284	A2M	C2-N3	2.17	1.35	1.32
46	B	46	A2M	C2-N3	2.16	1.35	1.32
45	A	2956	UR3	O4-C4	-2.16	1.18	1.23
45	A	2329	A2M	C2-N3	2.14	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	827	A2M	C2-N3	2.14	1.35	1.32
45	A	1460	A2M	C2-N3	2.13	1.35	1.32
45	A	946	A2M	C2-N3	2.12	1.35	1.32
45	A	817	A2M	C2-N3	2.11	1.35	1.32
45	A	2324	A2M	C2-N3	2.08	1.35	1.32
45	A	2956	UR3	O2-C2	-2.08	1.18	1.22
45	A	1144	A2M	C2-N3	2.07	1.35	1.32
45	A	886	A2M	C2-N3	2.07	1.35	1.32
45	A	2804	A2M	C2-N3	2.02	1.35	1.32

All (572) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	946	A2M	C5-C6-N6	10.90	136.92	120.35
45	A	2284	A2M	C5-C6-N6	10.82	136.80	120.35
45	A	2804	A2M	C5-C6-N6	10.80	136.77	120.35
45	A	817	A2M	C5-C6-N6	10.72	136.65	120.35
45	A	2914	A2M	C5-C6-N6	10.71	136.62	120.35
45	A	2259	A2M	C5-C6-N6	10.69	136.59	120.35
45	A	660	A2M	C5-C6-N6	10.68	136.57	120.35
46	B	46	A2M	C5-C6-N6	10.66	136.55	120.35
45	A	827	A2M	C5-C6-N6	10.63	136.50	120.35
45	A	1144	A2M	C5-C6-N6	10.63	136.50	120.35
45	A	2129	A2M	C5-C6-N6	10.62	136.49	120.35
45	A	1460	A2M	C5-C6-N6	10.57	136.42	120.35
45	A	886	A2M	C5-C6-N6	10.53	136.35	120.35
45	A	2329	A2M	C5-C6-N6	10.50	136.32	120.35
45	A	369	A2M	C5-C6-N6	10.46	136.25	120.35
45	A	1378	A2M	C5-C6-N6	10.46	136.25	120.35
45	A	2223	A2M	C5-C6-N6	10.44	136.22	120.35
45	A	2324	A2M	C5-C6-N6	10.41	136.17	120.35
45	A	2949	A2M	C5-C6-N6	10.39	136.13	120.35
45	A	2643	A2M	C5-C6-N6	10.38	136.12	120.35
45	A	2804	A2M	C1'-N9-C4	-9.02	110.78	126.64
45	A	2284	A2M	C1'-N9-C4	-8.38	111.92	126.64
45	A	1144	A2M	C1'-N9-C4	-8.34	111.99	126.64
45	A	2914	A2M	C1'-N9-C4	-8.21	112.22	126.64
45	A	2324	A2M	C1'-N9-C4	-8.18	112.28	126.64
45	A	660	A2M	C1'-N9-C4	-8.10	112.42	126.64
45	A	827	A2M	C1'-N9-C4	-8.09	112.42	126.64
45	A	2259	A2M	C1'-N9-C4	-8.04	112.52	126.64
45	A	946	A2M	C1'-N9-C4	-7.95	112.67	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	369	A2M	C1'-N9-C4	-7.89	112.79	126.64
45	A	2949	A2M	C1'-N9-C4	-7.87	112.81	126.64
45	A	2129	A2M	C1'-N9-C4	-7.85	112.85	126.64
46	B	46	A2M	C1'-N9-C4	-7.78	112.96	126.64
45	A	2223	A2M	C1'-N9-C4	-7.67	113.16	126.64
45	A	2284	A2M	N6-C6-N1	-7.62	102.76	118.57
45	A	1460	A2M	C1'-N9-C4	-7.55	113.38	126.64
45	A	946	A2M	N6-C6-N1	-7.51	102.99	118.57
45	A	2329	A2M	C1'-N9-C4	-7.50	113.47	126.64
45	A	817	A2M	N6-C6-N1	-7.36	103.29	118.57
45	A	2643	A2M	C1'-N9-C4	-7.36	113.70	126.64
45	A	660	A2M	N6-C6-N1	-7.33	103.36	118.57
45	A	2259	A2M	N6-C6-N1	-7.32	103.38	118.57
45	A	2914	A2M	N6-C6-N1	-7.31	103.40	118.57
45	A	2804	A2M	N6-C6-N1	-7.30	103.41	118.57
46	B	46	A2M	N6-C6-N1	-7.25	103.53	118.57
45	A	827	A2M	N6-C6-N1	-7.24	103.55	118.57
45	A	2129	A2M	N6-C6-N1	-7.20	103.62	118.57
45	A	1378	A2M	N6-C6-N1	-7.16	103.72	118.57
45	A	2329	A2M	N6-C6-N1	-7.14	103.75	118.57
45	A	1460	A2M	N6-C6-N1	-7.13	103.76	118.57
45	A	2324	A2M	N6-C6-N1	-7.09	103.86	118.57
45	A	369	A2M	N6-C6-N1	-7.08	103.87	118.57
45	A	2643	A2M	N6-C6-N1	-7.08	103.89	118.57
45	A	886	A2M	N6-C6-N1	-7.06	103.92	118.57
45	A	2949	A2M	N6-C6-N1	-7.06	103.92	118.57
45	A	1144	A2M	N6-C6-N1	-7.06	103.92	118.57
45	A	2223	A2M	N6-C6-N1	-7.04	103.95	118.57
45	A	1378	A2M	C1'-N9-C4	-6.95	114.44	126.64
45	A	886	A2M	C1'-N9-C4	-6.92	114.48	126.64
45	A	817	A2M	C1'-N9-C4	-6.86	114.60	126.64
45	A	2804	A2M	N3-C2-N1	-5.70	119.77	128.68
45	A	1144	A2M	N3-C2-N1	-5.61	119.91	128.68
46	B	46	A2M	N3-C2-N1	-5.61	119.92	128.68
45	A	2329	A2M	N3-C2-N1	-5.56	120.00	128.68
45	A	2284	A2M	N3-C2-N1	-5.54	120.01	128.68
45	A	886	A2M	N3-C2-N1	-5.53	120.03	128.68
45	A	660	A2M	N3-C2-N1	-5.53	120.03	128.68
45	A	2259	A2M	N3-C2-N1	-5.52	120.05	128.68
45	A	2129	A2M	N3-C2-N1	-5.50	120.08	128.68
45	A	2914	A2M	N3-C2-N1	-5.50	120.08	128.68
45	A	2949	A2M	N3-C2-N1	-5.48	120.12	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	946	A2M	N3-C2-N1	-5.48	120.12	128.68
45	A	827	A2M	N3-C2-N1	-5.47	120.13	128.68
45	A	369	A2M	N3-C2-N1	-5.45	120.16	128.68
45	A	2223	A2M	N3-C2-N1	-5.40	120.24	128.68
45	A	817	A2M	N3-C2-N1	-5.35	120.31	128.68
45	A	2643	A2M	N3-C2-N1	-5.35	120.31	128.68
45	A	1460	A2M	N3-C2-N1	-5.33	120.34	128.68
45	A	2324	A2M	N3-C2-N1	-5.30	120.39	128.68
45	A	1378	A2M	N3-C2-N1	-5.28	120.43	128.68
45	A	1894	OMU	C4-N3-C2	-5.27	119.63	126.58
45	A	1068	OMU	C4-N3-C2	-5.23	119.68	126.58
45	A	2424	OMU	C4-N3-C2	-5.17	119.76	126.58
45	A	2738	OMU	C4-N3-C2	-5.17	119.76	126.58
45	A	2924	OMU	C4-N3-C2	-5.16	119.78	126.58
45	A	2350	OMU	C4-N3-C2	-5.13	119.81	126.58
45	A	2720	OMU	C4-N3-C2	-5.10	119.86	126.58
45	A	3289	OMU	C4-N3-C2	-5.09	119.87	126.58
45	A	3304	OMU	C4-N3-C2	-5.05	119.92	126.58
45	A	144	OMU	C4-N3-C2	-5.05	119.92	126.58
45	A	675	OMU	C4-N3-C2	-5.00	119.98	126.58
45	A	787	OMU	C4-N3-C2	-4.99	120.00	126.58
45	A	44	OMU	C4-N3-C2	-4.98	120.02	126.58
45	A	2732	OMU	C4-N3-C2	-4.98	120.02	126.58
45	A	804	OMU	C4-N3-C2	-4.96	120.03	126.58
45	A	48	OMU	C4-N3-C2	-4.93	120.07	126.58
45	A	1537	OMU	C4-N3-C2	-4.92	120.09	126.58
45	A	2413	OMU	C4-N3-C2	-4.83	120.22	126.58
45	A	2956	UR3	C4-N3-C2	-4.81	120.03	124.56
45	A	2137	PSU	C4-N3-C2	-4.79	119.44	126.34
45	A	2857	PSU	C4-N3-C2	-4.72	119.54	126.34
45	A	2886	OMU	C4-N3-C2	-4.71	120.37	126.58
45	A	970	PSU	C4-N3-C2	-4.70	119.57	126.34
45	A	1135	PSU	C4-N3-C2	-4.68	119.59	126.34
45	A	2321	PSU	C4-N3-C2	-4.67	119.61	126.34
45	A	2958	PSU	C4-N3-C2	-4.67	119.61	126.34
45	A	2926	PSU	C4-N3-C2	-4.67	119.61	126.34
45	A	2257	PSU	C4-N3-C2	-4.65	119.64	126.34
46	B	77	PSU	C4-N3-C2	-4.65	119.64	126.34
45	A	1064	PSU	C4-N3-C2	-4.63	119.66	126.34
45	A	1685	PSU	C4-N3-C2	-4.63	119.67	126.34
45	A	34	PSU	C4-N3-C2	-4.62	119.68	126.34
45	A	1056	PSU	C4-N3-C2	-4.62	119.69	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	1016	PSU	C4-N3-C2	-4.61	119.70	126.34
46	B	21	PSU	C4-N3-C2	-4.59	119.72	126.34
45	A	2435	PSU	C4-N3-C2	-4.59	119.72	126.34
45	A	2868	PSU	C4-N3-C2	-4.59	119.72	126.34
45	A	150	PSU	C4-N3-C2	-4.59	119.72	126.34
45	A	976	PSU	C4-N3-C2	-4.58	119.74	126.34
45	A	2317	PSU	C4-N3-C2	-4.58	119.74	126.34
45	A	717	PSU	C4-N3-C2	-4.58	119.74	126.34
45	A	2214	PSU	C4-N3-C2	-4.57	119.75	126.34
45	A	228	PSU	C4-N3-C2	-4.57	119.75	126.34
45	A	2194	PSU	C4-N3-C2	-4.56	119.77	126.34
45	A	42	PSU	C4-N3-C2	-4.56	119.77	126.34
45	A	2261	PSU	C4-N3-C2	-4.56	119.77	126.34
45	A	2829	PSU	C4-N3-C2	-4.55	119.78	126.34
45	A	2263	PSU	C4-N3-C2	-4.55	119.79	126.34
45	A	2883	PSU	C4-N3-C2	-4.54	119.80	126.34
45	A	902	PSU	C4-N3-C2	-4.54	119.80	126.34
45	A	786	PSU	C4-N3-C2	-4.54	119.80	126.34
45	A	1134	PSU	C4-N3-C2	-4.54	119.80	126.34
45	A	464	PSU	C4-N3-C2	-4.53	119.81	126.34
45	A	1002	PSU	C4-N3-C2	-4.53	119.81	126.34
45	A	829	PSU	C4-N3-C2	-4.52	119.83	126.34
45	A	2267	PSU	C4-N3-C2	-4.52	119.83	126.34
45	A	2897	PSU	C4-N3-C2	-4.51	119.84	126.34
45	A	2747	PSU	C4-N3-C2	-4.50	119.86	126.34
45	A	2137	PSU	N1-C2-N3	4.49	120.22	115.13
45	A	510	PSU	C4-N3-C2	-4.49	119.86	126.34
45	A	2947	PSU	C4-N3-C2	-4.48	119.88	126.34
45	A	1474	PSU	C4-N3-C2	-4.48	119.88	126.34
45	A	684	PSU	C4-N3-C2	-4.48	119.88	126.34
45	A	2419	PSU	C4-N3-C2	-4.48	119.89	126.34
45	A	2269	PSU	C4-N3-C2	-4.48	119.89	126.34
45	A	2653	UY1	C4-N3-C2	-4.47	119.89	126.34
45	A	1482	PSU	C4-N3-C2	-4.47	119.89	126.34
45	A	1133	PSU	C4-N3-C2	-4.46	119.92	126.34
45	A	2978	PSU	C4-N3-C2	-4.45	119.93	126.34
46	B	96	PSU	C4-N3-C2	-4.45	119.93	126.34
45	A	277	PSU	C4-N3-C2	-4.44	119.94	126.34
45	A	311	PSU	C4-N3-C2	-4.44	119.95	126.34
45	A	2139	PSU	C4-N3-C2	-4.37	120.05	126.34
45	A	34	PSU	N1-C2-N3	4.32	120.03	115.13
45	A	2926	PSU	N1-C2-N3	4.28	119.98	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	895	PSU	C4-N3-C2	-4.26	120.20	126.34
45	A	2435	PSU	N1-C2-N3	4.25	119.95	115.13
45	A	2321	PSU	N1-C2-N3	4.25	119.94	115.13
45	A	829	PSU	N1-C2-N3	4.25	119.94	115.13
45	A	2857	PSU	N1-C2-N3	4.24	119.93	115.13
45	A	966	PSU	C4-N3-C2	-4.23	120.25	126.34
45	A	1685	PSU	N1-C2-N3	4.23	119.92	115.13
45	A	3113	PSU	C4-N3-C2	-4.22	120.25	126.34
45	A	2317	PSU	N1-C2-N3	4.22	119.91	115.13
45	A	150	PSU	N1-C2-N3	4.21	119.90	115.13
45	A	277	PSU	N1-C2-N3	4.21	119.90	115.13
45	A	2958	PSU	N1-C2-N3	4.20	119.89	115.13
45	A	1056	PSU	N1-C2-N3	4.20	119.89	115.13
45	A	1002	PSU	N1-C2-N3	4.20	119.89	115.13
45	A	1134	PSU	N1-C2-N3	4.20	119.88	115.13
45	A	228	PSU	N1-C2-N3	4.19	119.88	115.13
45	A	1135	PSU	N1-C2-N3	4.18	119.87	115.13
45	A	1016	PSU	N1-C2-N3	4.18	119.87	115.13
45	A	2868	PSU	N1-C2-N3	4.18	119.87	115.13
45	A	2214	PSU	N1-C2-N3	4.18	119.86	115.13
46	B	77	PSU	N1-C2-N3	4.18	119.86	115.13
45	A	2883	PSU	N1-C2-N3	4.17	119.85	115.13
45	A	2257	PSU	N1-C2-N3	4.16	119.85	115.13
46	B	21	PSU	N1-C2-N3	4.15	119.84	115.13
45	A	970	PSU	N1-C2-N3	4.15	119.83	115.13
45	A	976	PSU	N1-C2-N3	4.15	119.83	115.13
45	A	1064	PSU	N1-C2-N3	4.15	119.83	115.13
45	A	2829	PSU	N1-C2-N3	4.13	119.81	115.13
45	A	510	PSU	N1-C2-N3	4.13	119.81	115.13
45	A	2653	UY1	N1-C2-N3	4.13	119.80	115.13
45	A	2194	PSU	N1-C2-N3	4.12	119.80	115.13
45	A	2261	PSU	N1-C2-N3	4.12	119.80	115.13
45	A	2947	PSU	N1-C2-N3	4.12	119.80	115.13
45	A	717	PSU	N1-C2-N3	4.12	119.79	115.13
45	A	1133	PSU	N1-C2-N3	4.11	119.79	115.13
45	A	2263	PSU	N1-C2-N3	4.11	119.78	115.13
45	A	2267	PSU	N1-C2-N3	4.11	119.78	115.13
45	A	902	PSU	N1-C2-N3	4.10	119.78	115.13
45	A	2139	PSU	N1-C2-N3	4.10	119.77	115.13
45	A	2897	PSU	N1-C2-N3	4.09	119.76	115.13
45	A	2419	PSU	N1-C2-N3	4.09	119.76	115.13
45	A	1482	PSU	N1-C2-N3	4.07	119.74	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	42	PSU	N1-C2-N3	4.07	119.74	115.13
45	A	1474	PSU	N1-C2-N3	4.05	119.72	115.13
45	A	2978	PSU	N1-C2-N3	4.05	119.72	115.13
45	A	464	PSU	N1-C2-N3	4.05	119.72	115.13
45	A	2269	PSU	N1-C2-N3	4.03	119.70	115.13
45	A	895	PSU	N1-C2-N3	4.01	119.68	115.13
45	A	684	PSU	N1-C2-N3	4.01	119.67	115.13
45	A	311	PSU	N1-C2-N3	3.99	119.65	115.13
45	A	2747	PSU	N1-C2-N3	3.98	119.64	115.13
46	B	96	PSU	N1-C2-N3	3.96	119.61	115.13
45	A	3113	PSU	N1-C2-N3	3.94	119.59	115.13
45	A	786	PSU	N1-C2-N3	3.91	119.56	115.13
45	A	966	PSU	N1-C2-N3	3.89	119.54	115.13
45	A	675	OMU	N3-C2-N1	3.87	120.02	114.89
45	A	1894	OMU	N3-C2-N1	3.86	120.02	114.89
45	A	1068	OMU	N3-C2-N1	3.84	119.98	114.89
45	A	2350	OMU	N3-C2-N1	3.83	119.97	114.89
45	A	2738	OMU	N3-C2-N1	3.82	119.96	114.89
45	A	3304	OMU	N3-C2-N1	3.81	119.95	114.89
45	A	2924	OMU	N3-C2-N1	3.80	119.93	114.89
45	A	2886	OMU	N3-C2-N1	3.79	119.92	114.89
45	A	804	OMU	N3-C2-N1	3.74	119.86	114.89
45	A	2424	OMU	N3-C2-N1	3.74	119.86	114.89
45	A	2720	OMU	N3-C2-N1	3.72	119.83	114.89
45	A	48	OMU	N3-C2-N1	3.71	119.82	114.89
45	A	2732	OMU	N3-C2-N1	3.70	119.80	114.89
45	A	3289	OMU	N3-C2-N1	3.69	119.78	114.89
45	A	787	OMU	N3-C2-N1	3.68	119.78	114.89
45	A	144	OMU	N3-C2-N1	3.68	119.77	114.89
45	A	44	OMU	N3-C2-N1	3.68	119.77	114.89
45	A	2317	PSU	C6-C5-C4	3.65	120.75	118.20
45	A	1537	OMU	N3-C2-N1	3.63	119.70	114.89
45	A	815	OMG	C5-C6-N1	3.46	120.06	113.95
45	A	2413	OMU	N3-C2-N1	3.45	119.48	114.89
45	A	2281	5MC	C5-C6-N1	-3.45	119.79	123.34
45	A	2127	OMG	C5-C6-N1	3.44	120.02	113.95
45	A	2622	OMG	C5-C6-N1	3.43	120.01	113.95
45	A	2291	OMG	C5-C6-N1	3.42	120.00	113.95
45	A	2925	OMG	C5-C6-N1	3.42	119.99	113.95
45	A	2412	OMG	C5-C6-N1	3.41	119.97	113.95
45	A	2239	OMG	C5-C6-N1	3.40	119.96	113.95
45	A	34	PSU	C6-C5-C4	3.40	120.57	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	296	OMG	C5-C6-N1	3.40	119.95	113.95
45	A	2818	OMG	C5-C6-N1	3.39	119.94	113.95
45	A	1134	PSU	C6-C5-C4	3.39	120.57	118.20
46	B	78	OMG	C5-C6-N1	3.39	119.93	113.95
45	A	2796	OMG	C5-C6-N1	3.39	119.93	113.95
45	A	1461	OMG	C5-C6-N1	3.38	119.92	113.95
45	A	399	OMG	C5-C6-N1	3.38	119.92	113.95
45	A	1894	OMU	C5-C4-N3	3.38	119.90	114.84
45	A	2424	OMU	C5-C4-N3	3.38	119.89	114.84
45	A	510	PSU	C6-C5-C4	3.38	120.56	118.20
45	A	918	OMG	C5-C6-N1	3.36	119.89	113.95
45	A	2398	OMG	C5-C6-N1	3.36	119.89	113.95
45	A	1068	OMU	C5-C4-N3	3.36	119.86	114.84
45	A	3289	OMU	C5-C4-N3	3.36	119.86	114.84
45	A	2738	OMU	C5-C4-N3	3.33	119.82	114.84
45	A	2920	OMG	C5-C6-N1	3.33	119.83	113.95
45	A	2924	OMU	C5-C4-N3	3.32	119.81	114.84
45	A	2394	OMG	C5-C6-N1	3.32	119.82	113.95
45	A	2126	OMG	C5-C6-N1	3.32	119.81	113.95
45	A	1857	OMG	C5-C6-N1	3.31	119.80	113.95
45	A	2137	PSU	C6-C5-C4	3.31	120.51	118.20
45	A	2720	OMU	C5-C4-N3	3.31	119.79	114.84
45	A	48	OMU	C5-C4-N3	3.30	119.78	114.84
45	A	2653	UY1	C6-C5-C4	3.30	120.50	118.20
45	A	829	PSU	C6-C5-C4	3.29	120.50	118.20
45	A	2413	OMU	C5-C4-N3	3.29	119.76	114.84
45	A	1537	OMU	C5-C4-N3	3.29	119.76	114.84
45	A	1685	PSU	C6-C5-C4	3.29	120.50	118.20
45	A	2794	OMG	C5-C6-N1	3.29	119.75	113.95
45	A	2435	PSU	C6-C5-C4	3.27	120.48	118.20
45	A	44	OMU	C5-C4-N3	3.27	119.72	114.84
45	A	144	OMU	C5-C4-N3	3.26	119.72	114.84
45	A	3304	OMU	C5-C4-N3	3.26	119.71	114.84
45	A	895	PSU	C6-C5-C4	3.25	120.47	118.20
45	A	2350	OMU	C5-C4-N3	3.25	119.70	114.84
45	A	2732	OMU	C5-C4-N3	3.25	119.70	114.84
45	A	804	OMU	C5-C4-N3	3.24	119.69	114.84
45	A	2654	OMG	C5-C6-N1	3.24	119.68	113.95
45	A	787	OMU	C5-C4-N3	3.24	119.69	114.84
45	A	2857	PSU	C6-C5-C4	3.21	120.44	118.20
46	B	77	PSU	C6-C5-C4	3.20	120.43	118.20
45	A	2139	PSU	C6-C5-C4	3.18	120.42	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	228	PSU	C6-C5-C4	3.17	120.41	118.20
45	A	2257	PSU	C6-C5-C4	3.17	120.41	118.20
45	A	2926	PSU	C6-C5-C4	3.17	120.41	118.20
45	A	675	OMU	C5-C4-N3	3.16	119.58	114.84
45	A	1135	PSU	C6-C5-C4	3.15	120.40	118.20
45	A	2873	5MC	C5-C6-N1	-3.15	120.10	123.34
45	A	1064	PSU	C6-C5-C4	3.15	120.40	118.20
45	A	2829	PSU	C6-C5-C4	3.15	120.40	118.20
45	A	2868	PSU	C6-C5-C4	3.14	120.39	118.20
45	A	2654	OMG	N2-C2-N1	3.14	123.39	116.71
45	A	1002	PSU	C6-C5-C4	3.14	120.39	118.20
45	A	2947	PSU	C6-C5-C4	3.13	120.39	118.20
45	A	2267	PSU	C6-C5-C4	3.13	120.39	118.20
45	A	717	PSU	C6-C5-C4	3.13	120.39	118.20
45	A	150	PSU	C6-C5-C4	3.12	120.38	118.20
45	A	1016	PSU	C6-C5-C4	3.11	120.37	118.20
45	A	277	PSU	C6-N1-C2	-3.11	119.51	122.68
45	A	966	PSU	C6-N1-C2	-3.07	119.55	122.68
45	A	895	PSU	C6-N1-C2	-3.06	119.55	122.68
45	A	2883	PSU	C6-C5-C4	3.06	120.34	118.20
45	A	970	PSU	C6-C5-C4	3.06	120.34	118.20
45	A	277	PSU	C6-C5-C4	3.06	120.34	118.20
45	A	1482	PSU	C6-C5-C4	3.06	120.33	118.20
45	A	1133	PSU	C6-C5-C4	3.05	120.33	118.20
45	A	42	PSU	C6-C5-C4	3.02	120.31	118.20
45	A	2398	OMG	C8-N7-C5	3.02	108.73	102.99
45	A	3113	PSU	C6-N1-C2	-3.01	119.61	122.68
45	A	2886	OMU	C5-C4-N3	3.00	119.33	114.84
45	A	2263	PSU	C6-C5-C4	3.00	120.29	118.20
45	A	1056	PSU	C6-C5-C4	2.99	120.29	118.20
45	A	2897	PSU	C6-C5-C4	2.99	120.29	118.20
46	B	21	PSU	C6-C5-C4	2.98	120.28	118.20
45	A	976	PSU	C6-C5-C4	2.98	120.28	118.20
45	A	684	PSU	C6-C5-C4	2.97	120.28	118.20
45	A	1002	PSU	C6-N1-C2	-2.97	119.64	122.68
45	A	2139	PSU	C6-N1-C2	-2.97	119.65	122.68
45	A	2321	PSU	C6-C5-C4	2.97	120.27	118.20
45	A	2214	PSU	C6-N1-C2	-2.97	119.65	122.68
45	A	2978	PSU	C6-N1-C2	-2.97	119.65	122.68
45	A	3113	PSU	C6-C5-C4	2.97	120.27	118.20
45	A	296	OMG	C8-N7-C5	2.96	108.64	102.99
45	A	1461	OMG	C8-N7-C5	2.96	108.62	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	829	PSU	C6-N1-C2	-2.95	119.66	122.68
45	A	1474	PSU	C6-N1-C2	-2.95	119.66	122.68
45	A	902	PSU	C6-C5-C4	2.95	120.26	118.20
45	A	2239	OMG	C8-N7-C5	2.95	108.61	102.99
45	A	2622	OMG	C8-N7-C5	2.95	108.61	102.99
45	A	150	PSU	C6-N1-C2	-2.95	119.67	122.68
45	A	34	PSU	C6-N1-C2	-2.95	119.67	122.68
45	A	2435	PSU	C6-N1-C2	-2.95	119.67	122.68
45	A	2127	OMG	C8-N7-C5	2.94	108.60	102.99
45	A	1016	PSU	C6-N1-C2	-2.94	119.67	122.68
45	A	1133	PSU	C6-N1-C2	-2.94	119.67	122.68
45	A	2394	OMG	C8-N7-C5	2.94	108.59	102.99
45	A	2926	PSU	C6-N1-C2	-2.94	119.68	122.68
45	A	228	PSU	C6-N1-C2	-2.93	119.69	122.68
45	A	1461	OMG	C2-N1-C6	-2.93	119.70	125.10
45	A	1857	OMG	C8-N7-C5	2.93	108.56	102.99
45	A	2137	PSU	C6-N1-C2	-2.92	119.69	122.68
45	A	2214	PSU	C6-C5-C4	2.92	120.24	118.20
45	A	399	OMG	C2-N1-C6	-2.92	119.72	125.10
45	A	2291	OMG	C8-N7-C5	2.92	108.55	102.99
45	A	2925	OMG	C2-N1-C6	-2.91	119.74	125.10
45	A	510	PSU	C6-N1-C2	-2.91	119.71	122.68
45	A	2291	OMG	C2-N1-C6	-2.91	119.74	125.10
45	A	1056	PSU	C6-N1-C2	-2.91	119.71	122.68
46	B	78	OMG	C8-N7-C5	2.91	108.53	102.99
45	A	2653	UY1	C6-N1-C2	-2.91	119.71	122.68
45	A	2947	PSU	C6-N1-C2	-2.90	119.71	122.68
45	A	2126	OMG	C8-N7-C5	2.90	108.52	102.99
45	A	902	PSU	C6-N1-C2	-2.90	119.72	122.68
45	A	2261	PSU	C6-N1-C2	-2.90	119.72	122.68
45	A	2920	OMG	C2-N1-C6	-2.90	119.76	125.10
45	A	918	OMG	C2-N1-C6	-2.89	119.77	125.10
45	A	2239	OMG	C2-N1-C6	-2.89	119.77	125.10
45	A	2419	PSU	C6-N1-C2	-2.89	119.72	122.68
45	A	2794	OMG	C8-N7-C5	2.89	108.50	102.99
45	A	2267	PSU	C6-N1-C2	-2.89	119.72	122.68
45	A	2925	OMG	C8-N7-C5	2.89	108.50	102.99
45	A	2622	OMG	C2-N1-C6	-2.89	119.77	125.10
45	A	2920	OMG	C8-N7-C5	2.89	108.50	102.99
45	A	311	PSU	C6-N1-C2	-2.89	119.73	122.68
46	B	96	PSU	C6-N1-C2	-2.89	119.73	122.68
45	A	2317	PSU	C6-N1-C2	-2.89	119.73	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	2263	PSU	C6-N1-C2	-2.89	119.73	122.68
45	A	2269	PSU	C6-N1-C2	-2.89	119.73	122.68
45	A	2412	OMG	C8-N7-C5	2.88	108.48	102.99
45	A	976	PSU	C6-N1-C2	-2.88	119.74	122.68
45	A	2654	OMG	C8-N7-C5	2.88	108.48	102.99
45	A	684	PSU	C6-N1-C2	-2.88	119.74	122.68
45	A	2321	PSU	C6-N1-C2	-2.88	119.74	122.68
45	A	1685	PSU	C6-N1-C2	-2.88	119.74	122.68
46	B	78	OMG	C2-N1-C6	-2.88	119.80	125.10
45	A	1482	PSU	C6-N1-C2	-2.87	119.74	122.68
45	A	1134	PSU	C6-N1-C2	-2.87	119.75	122.68
45	A	2958	PSU	C6-N1-C2	-2.87	119.75	122.68
45	A	2958	PSU	C6-C5-C4	2.87	120.21	118.20
45	A	2747	PSU	C6-N1-C2	-2.87	119.75	122.68
45	A	3289	OMU	O4-C4-C5	-2.87	120.12	125.16
45	A	2412	OMG	C2-N1-C6	-2.86	119.83	125.10
45	A	804	OMU	O4-C4-C5	-2.86	120.13	125.16
45	A	2883	PSU	C6-N1-C2	-2.86	119.76	122.68
45	A	42	PSU	C6-N1-C2	-2.86	119.76	122.68
45	A	2818	OMG	C2-N1-C6	-2.86	119.84	125.10
45	A	2829	PSU	C6-N1-C2	-2.86	119.76	122.68
45	A	2796	OMG	C8-N7-C5	2.85	108.42	102.99
45	A	464	PSU	C6-N1-C2	-2.85	119.77	122.68
45	A	2127	OMG	C2-N1-C6	-2.85	119.84	125.10
46	B	21	PSU	C6-N1-C2	-2.85	119.77	122.68
46	B	77	PSU	C6-N1-C2	-2.85	119.77	122.68
45	A	918	OMG	C8-N7-C5	2.85	108.41	102.99
45	A	815	OMG	C2-N1-C6	-2.84	119.86	125.10
45	A	2897	PSU	C6-N1-C2	-2.84	119.78	122.68
45	A	1857	OMG	C2-N1-C6	-2.84	119.87	125.10
45	A	2818	OMG	C8-N7-C5	2.84	108.40	102.99
45	A	144	OMU	O4-C4-C5	-2.83	120.18	125.16
45	A	2738	OMU	O4-C4-C5	-2.83	120.18	125.16
45	A	296	OMG	C2-N1-C6	-2.82	119.90	125.10
45	A	2868	PSU	C6-N1-C2	-2.82	119.80	122.68
45	A	2194	PSU	C6-N1-C2	-2.82	119.80	122.68
45	A	2261	PSU	C6-C5-C4	2.81	120.16	118.20
45	A	815	OMG	C8-N7-C5	2.81	108.34	102.99
45	A	2886	OMU	O4-C4-C5	-2.81	120.22	125.16
45	A	2194	PSU	C6-C5-C4	2.81	120.16	118.20
45	A	2796	OMG	C2-N1-C6	-2.80	119.94	125.10
45	A	2257	PSU	C6-N1-C2	-2.80	119.82	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	1537	OMU	O4-C4-C5	-2.80	120.24	125.16
45	A	399	OMG	C8-N7-C5	2.80	108.32	102.99
45	A	717	PSU	C6-N1-C2	-2.79	119.83	122.68
45	A	2419	PSU	C6-C5-C4	2.78	120.14	118.20
45	A	2804	A2M	C3'-C2'-C1'	2.78	108.12	102.89
45	A	2394	OMG	C2-N1-C6	-2.78	119.99	125.10
45	A	2398	OMG	C2-N1-C6	-2.78	119.99	125.10
45	A	2924	OMU	O4-C4-C5	-2.78	120.28	125.16
45	A	1474	PSU	C6-C5-C4	2.77	120.14	118.20
45	A	2350	OMU	O4-C4-C5	-2.77	120.29	125.16
45	A	1064	PSU	C6-N1-C2	-2.77	119.86	122.68
45	A	2857	PSU	C6-N1-C2	-2.75	119.87	122.68
45	A	2720	OMU	O4-C4-C5	-2.75	120.32	125.16
45	A	464	PSU	C6-C5-C4	2.75	120.12	118.20
45	A	2269	PSU	C6-C5-C4	2.74	120.12	118.20
45	A	2126	OMG	C2-N1-C6	-2.74	120.05	125.10
45	A	3304	OMU	O4-C4-C5	-2.74	120.34	125.16
45	A	2424	OMU	O4-C4-C5	-2.73	120.36	125.16
45	A	660	A2M	C2'-C3'-C4'	2.72	107.90	101.99
45	A	1068	OMU	O4-C4-C5	-2.72	120.38	125.16
45	A	2978	PSU	C6-C5-C4	2.71	120.09	118.20
45	A	1135	PSU	C6-N1-C2	-2.71	119.91	122.68
45	A	2747	PSU	C6-C5-C4	2.70	120.09	118.20
45	A	44	OMU	O4-C4-C5	-2.70	120.42	125.16
45	A	2435	PSU	O2-C2-N1	-2.69	119.83	122.79
45	A	2394	OMG	N2-C2-N1	2.68	122.43	116.71
45	A	675	OMU	O4-C4-C5	-2.68	120.45	125.16
45	A	1894	OMU	O4-C4-C5	-2.67	120.47	125.16
45	A	970	PSU	C6-N1-C2	-2.67	119.96	122.68
45	A	2413	OMU	O4-C4-C5	-2.64	120.51	125.16
45	A	2654	OMG	C2-N1-C6	-2.64	120.24	125.10
45	A	786	PSU	O2-C2-N1	-2.63	119.90	122.79
45	A	2732	OMU	O4-C4-C5	-2.63	120.54	125.16
45	A	787	OMU	O4-C4-C5	-2.62	120.56	125.16
46	B	21	PSU	O2-C2-N1	-2.61	119.92	122.79
45	A	2829	PSU	O2-C2-N1	-2.61	119.92	122.79
45	A	150	PSU	O2-C2-N1	-2.60	119.92	122.79
45	A	2127	OMG	N2-C2-N1	2.60	122.25	116.71
45	A	2883	PSU	O2-C2-N1	-2.60	119.93	122.79
45	A	1135	PSU	O2-C2-N1	-2.59	119.94	122.79
45	A	786	PSU	C6-N1-C2	-2.59	120.03	122.68
45	A	2857	PSU	O2-C2-N1	-2.58	119.95	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	2747	PSU	O2-C2-N1	-2.58	119.95	122.79
45	A	656	1MA	C8-N7-C5	2.58	107.90	102.99
45	A	1474	PSU	O2-C2-N1	-2.57	119.96	122.79
45	A	48	OMU	O4-C4-C5	-2.57	120.64	125.16
45	A	2926	PSU	O2-C2-N1	-2.57	119.97	122.79
45	A	2398	OMG	N2-C2-N1	2.56	122.16	116.71
45	A	1685	PSU	O2-C2-N1	-2.52	120.01	122.79
45	A	2804	A2M	C2'-C3'-C4'	2.52	107.47	101.99
45	A	2321	PSU	O2-C2-N1	-2.52	120.02	122.79
45	A	2818	OMG	N2-C2-N1	2.51	122.06	116.71
45	A	829	PSU	O2-C2-N1	-2.50	120.03	122.79
46	B	77	PSU	O2-C2-N1	-2.50	120.04	122.79
46	B	96	PSU	C6-C5-C4	2.50	119.94	118.20
45	A	966	PSU	C6-C5-C4	2.50	119.94	118.20
45	A	311	PSU	O2-C2-N1	-2.50	120.04	122.79
45	A	2794	OMG	C2-N1-C6	-2.49	120.51	125.10
45	A	2263	PSU	O2-C2-N1	-2.49	120.05	122.79
45	A	311	PSU	C6-C5-C4	2.49	119.94	118.20
45	A	2868	PSU	O2-C2-N1	-2.49	120.05	122.79
45	A	277	PSU	O2-C2-N1	-2.48	120.06	122.79
45	A	2214	PSU	O2-C2-N1	-2.47	120.07	122.79
45	A	2126	OMG	N2-C2-N1	2.46	121.96	116.71
45	A	34	PSU	O2-C2-N1	-2.46	120.08	122.79
45	A	2139	PSU	O2-C2-N1	-2.45	120.09	122.79
45	A	1016	PSU	O2-C2-N1	-2.44	120.10	122.79
45	A	2267	PSU	O2-C2-N1	-2.44	120.10	122.79
45	A	2947	PSU	O2-C2-N1	-2.44	120.11	122.79
45	A	1002	PSU	O2-C2-N1	-2.44	120.11	122.79
45	A	228	PSU	O2-C2-N1	-2.44	120.11	122.79
45	A	966	PSU	O2-C2-N1	-2.44	120.11	122.79
45	A	2261	PSU	O2-C2-N1	-2.44	120.11	122.79
45	A	970	PSU	O2-C2-N1	-2.43	120.11	122.79
45	A	1482	PSU	O2-C2-N1	-2.43	120.11	122.79
45	A	1133	PSU	O2-C2-N1	-2.43	120.12	122.79
45	A	2419	PSU	O2-C2-N1	-2.42	120.13	122.79
45	A	2958	PSU	O2-C2-N1	-2.42	120.13	122.79
45	A	464	PSU	O2-C2-N1	-2.40	120.15	122.79
45	A	1056	PSU	O2-C2-N1	-2.38	120.17	122.79
45	A	1134	PSU	O2-C2-N1	-2.38	120.17	122.79
46	B	96	PSU	O2-C2-N1	-2.38	120.17	122.79
45	A	2194	PSU	O2-C2-N1	-2.38	120.17	122.79
45	A	902	PSU	O2-C2-N1	-2.37	120.18	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	2269	PSU	O2-C2-N1	-2.36	120.20	122.79
45	A	2317	PSU	O2-C2-N1	-2.35	120.20	122.79
45	A	2257	PSU	O2-C2-N1	-2.34	120.21	122.79
45	A	817	A2M	C3'-C2'-C1'	2.33	107.27	102.89
45	A	946	A2M	C3'-C2'-C1'	2.32	107.25	102.89
45	A	2653	UY1	O2-C2-N1	-2.32	120.24	122.79
45	A	895	PSU	O2-C2-N1	-2.31	120.25	122.79
45	A	717	PSU	O2-C2-N1	-2.31	120.25	122.79
45	A	1064	PSU	O2-C2-N1	-2.31	120.25	122.79
45	A	2897	PSU	O2-C2-N1	-2.29	120.27	122.79
45	A	976	PSU	O2-C2-N1	-2.26	120.30	122.79
45	A	40	OMC	CM2-O2'-C2'	2.25	120.42	114.52
45	A	2920	OMG	O6-C6-C5	-2.25	119.99	124.37
45	A	684	PSU	O2-C2-N1	-2.24	120.33	122.79
45	A	2239	OMG	O6-C6-C5	-2.24	120.00	124.37
45	A	2920	OMG	N2-C2-N1	2.23	121.47	116.71
45	A	2956	UR3	C6-N1-C2	-2.23	119.79	121.79
46	B	78	OMG	O6-C6-C5	-2.23	120.01	124.37
45	A	656	1MA	C5-C6-N1	2.22	117.20	113.90
45	A	2622	OMG	O6-C6-C5	-2.22	120.04	124.37
45	A	399	OMG	O6-C6-C5	-2.22	120.04	124.37
45	A	2947	PSU	O4'-C1'-C2'	2.21	108.26	105.14
45	A	2818	OMG	O6-C6-C5	-2.21	120.06	124.37
45	A	2796	OMG	O6-C6-C5	-2.19	120.09	124.37
45	A	369	A2M	C2'-C3'-C4'	2.19	106.75	101.99
45	A	3113	PSU	O2-C2-N1	-2.19	120.38	122.79
45	A	2978	PSU	O2-C2-N1	-2.19	120.38	122.79
45	A	2925	OMG	O6-C6-C5	-2.18	120.11	124.37
45	A	815	OMG	O6-C6-C5	-2.18	120.12	124.37
45	A	510	PSU	O2-C2-N1	-2.18	120.39	122.79
45	A	2883	PSU	O4'-C1'-C2'	2.17	108.21	105.14
45	A	2412	OMG	N2-C2-N1	2.17	121.33	116.71
45	A	2394	OMG	O6-C6-C5	-2.16	120.15	124.37
45	A	918	OMG	O6-C6-C5	-2.16	120.15	124.37
45	A	2291	OMG	O6-C6-C5	-2.16	120.16	124.37
45	A	946	A2M	C2'-C3'-C4'	2.15	106.67	101.99
45	A	786	PSU	C6-C5-C4	2.15	119.70	118.20
45	A	2720	OMU	O2-C2-N1	-2.15	119.93	122.79
45	A	1857	OMG	O6-C6-C5	-2.14	120.19	124.37
45	A	296	OMG	O6-C6-C5	-2.14	120.19	124.37
45	A	2329	A2M	O4'-C1'-C2'	-2.13	102.89	106.59
45	A	2127	OMG	O6-C6-C5	-2.13	120.22	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	2829	PSU	O4'-C1'-C2'	2.11	108.12	105.14
45	A	946	A2M	C5'-C4'-C3'	-2.11	107.28	115.18
45	A	2412	OMG	O6-C6-C5	-2.10	120.27	124.37
45	A	2796	OMG	N2-C2-N1	2.09	121.17	116.71
45	A	2281	5MC	CM5-C5-C6	-2.09	120.06	122.85
45	A	2435	PSU	O4'-C1'-C2'	2.08	108.08	105.14
45	A	2424	OMU	O2-C2-N1	-2.08	120.02	122.79
45	A	2794	OMG	N1-C2-N3	-2.08	119.43	123.32
45	A	1460	A2M	C2'-C3'-C4'	2.08	106.51	101.99
45	A	1461	OMG	N2-C2-N1	2.08	121.13	116.71
45	A	2654	OMG	O6-C6-C5	-2.08	120.32	124.37
45	A	1894	OMU	O2-C2-N1	-2.07	120.03	122.79
45	A	787	OMU	O2-C2-N1	-2.07	120.03	122.79
45	A	2924	OMU	O2-C2-N1	-2.07	120.03	122.79
45	A	42	PSU	O2-C2-N1	-2.07	120.51	122.79
45	A	2654	OMG	N1-C2-N3	-2.07	119.45	123.32
45	A	2137	PSU	O2-C2-N1	-2.07	120.52	122.79
45	A	1002	PSU	O4'-C1'-C2'	2.07	108.06	105.14
45	A	886	A2M	C3'-C2'-C1'	2.07	106.77	102.89
45	A	2126	OMG	O6-C6-C5	-2.06	120.34	124.37
45	A	970	PSU	O4'-C1'-C2'	2.06	108.04	105.14
45	A	2738	OMU	O2-C2-N1	-2.06	120.05	122.79
45	A	660	A2M	C3'-C2'-C1'	2.05	106.75	102.89
45	A	2868	PSU	O4'-C1'-C2'	2.05	108.04	105.14
45	A	2350	OMU	O2-C2-N1	-2.05	120.06	122.79
45	A	1068	OMU	O2-C2-N1	-2.04	120.07	122.79
45	A	464	PSU	O4'-C1'-C2'	2.04	108.02	105.14
45	A	1857	OMG	N2-C2-N1	2.03	121.04	116.71
45	A	1685	PSU	O4'-C1'-C2'	2.03	108.01	105.14
45	A	1474	PSU	O4'-C1'-C2'	2.03	108.01	105.14
45	A	2398	OMG	O6-C6-C5	-2.03	120.41	124.37
45	A	804	OMU	O2-C2-N1	-2.03	120.09	122.79
45	A	2263	PSU	O4'-C1'-C2'	2.03	108.00	105.14
45	A	2214	PSU	O4'-C1'-C2'	2.02	108.00	105.14
45	A	815	OMG	N2-C2-N1	2.02	121.01	116.71
45	A	886	A2M	C2'-C3'-C4'	2.02	106.38	101.99
45	A	296	OMG	N2-C2-N1	2.02	121.00	116.71
45	A	675	OMU	O2-C2-N1	-2.01	120.11	122.79
46	B	78	OMG	N2-C2-N1	2.01	120.99	116.71

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	78	OMG	O4'-C4'-C5'-O5'
46	B	78	OMG	C3'-C4'-C5'-O5'
46	B	96	PSU	C3'-C4'-C5'-O5'
46	B	96	PSU	O4'-C4'-C5'-O5'
45	A	40	OMC	C3'-C2'-O2'-CM2
45	A	296	OMG	O4'-C4'-C5'-O5'
45	A	296	OMG	C3'-C4'-C5'-O5'
45	A	660	A2M	C1'-C2'-O2'-CM'
45	A	786	PSU	C2'-C1'-C5-C4
45	A	918	OMG	O4'-C4'-C5'-O5'
45	A	918	OMG	C3'-C4'-C5'-O5'
45	A	2200	OMC	C2'-C1'-N1-C6
45	A	2259	A2M	O4'-C4'-C5'-O5'
45	A	2259	A2M	C3'-C4'-C5'-O5'
45	A	2284	A2M	O4'-C4'-C5'-O5'
45	A	2291	OMG	O4'-C4'-C5'-O5'
45	A	2291	OMG	C3'-C4'-C5'-O5'
45	A	2368	OMC	C3'-C4'-C5'-O5'
45	A	2368	OMC	O4'-C4'-C5'-O5'
45	A	2804	A2M	C1'-C2'-O2'-CM'
45	A	2956	UR3	O4'-C4'-C5'-O5'
45	A	2956	UR3	C3'-C4'-C5'-O5'
45	A	2200	OMC	C2'-C1'-N1-C2
45	A	399	OMG	O4'-C4'-C5'-O5'
45	A	1002	PSU	C3'-C4'-C5'-O5'
45	A	2317	PSU	C3'-C4'-C5'-O5'
45	A	2317	PSU	O4'-C4'-C5'-O5'
45	A	2321	PSU	O4'-C4'-C5'-O5'
45	A	2914	A2M	C3'-C4'-C5'-O5'
45	A	399	OMG	C3'-C4'-C5'-O5'
45	A	1002	PSU	O4'-C4'-C5'-O5'
45	A	2284	A2M	C3'-C4'-C5'-O5'
45	A	2914	A2M	O4'-C4'-C5'-O5'
45	A	827	A2M	C3'-C2'-O2'-CM'
45	A	228	PSU	C3'-C4'-C5'-O5'
45	A	2321	PSU	C3'-C4'-C5'-O5'
45	A	2873	5MC	C2'-C1'-N1-C6
45	A	1378	A2M	O4'-C4'-C5'-O5'
45	A	228	PSU	O4'-C4'-C5'-O5'
45	A	2873	5MC	O4'-C1'-N1-C6
45	A	2269	PSU	C3'-C4'-C5'-O5'
45	A	2926	PSU	C3'-C4'-C5'-O5'
45	A	2413	OMU	C3'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	A	2926	PSU	C4'-C5'-O5'-P
45	A	2200	OMC	O4'-C1'-N1-C2
45	A	2200	OMC	O4'-C1'-N1-C6
45	A	2317	PSU	C4'-C5'-O5'-P
45	A	1461	OMG	C4'-C5'-O5'-P
45	A	2804	A2M	C4'-C5'-O5'-P
45	A	2261	PSU	O4'-C4'-C5'-O5'
45	A	144	OMU	O4'-C4'-C5'-O5'
45	A	827	A2M	C4'-C5'-O5'-P
45	A	2873	5MC	C2'-C1'-N1-C2
45	A	2873	5MC	O4'-C1'-N1-C2
45	A	2947	PSU	O4'-C1'-C5-C4
45	A	1378	A2M	C3'-C4'-C5'-O5'
45	A	2269	PSU	O4'-C4'-C5'-O5'
45	A	2926	PSU	O4'-C4'-C5'-O5'
45	A	369	A2M	C1'-C2'-O2'-CM'
45	A	1448	OMC	C3'-C2'-O2'-CM2
45	A	660	A2M	C4'-C5'-O5'-P
45	A	970	PSU	O4'-C1'-C5-C6
45	A	2947	PSU	O4'-C1'-C5-C6
45	A	827	A2M	O4'-C4'-C5'-O5'
45	A	1448	OMC	C2'-C1'-N1-C2
45	A	2413	OMU	C4'-C5'-O5'-P
45	A	2412	OMG	C3'-C2'-O2'-CM2
45	A	1448	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 161 ligands modelled in this entry, 158 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	SPM	A	3453	-	13,13,13	0.38	0	12,12,12	1.01	0
51	SPM	A	3452	-	13,13,13	0.37	0	12,12,12	1.02	0
50	SPD	A	3451	-	9,9,9	0.32	0	8,8,8	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SPM	A	3453	-	-	7/11/11/11	-
51	SPM	A	3452	-	-	5/11/11/11	-
50	SPD	A	3451	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3453	SPM	N10-C11-C12-C13
51	A	3453	SPM	C7-C8-C9-N10
51	A	3453	SPM	C2-C3-C4-N5
51	A	3453	SPM	N5-C6-C7-C8
50	A	3451	SPD	C2-C3-C4-C5
51	A	3452	SPM	C3-C4-N5-C6
51	A	3453	SPM	C7-C6-N5-C4
51	A	3452	SPM	C7-C8-C9-N10
51	A	3452	SPM	C11-C12-C13-N14
50	A	3451	SPD	C3-C4-C5-N6
51	A	3452	SPM	N10-C11-C12-C13
51	A	3453	SPM	C11-C12-C13-N14
51	A	3452	SPM	C8-C9-N10-C11
51	A	3453	SPM	C8-C9-N10-C11

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

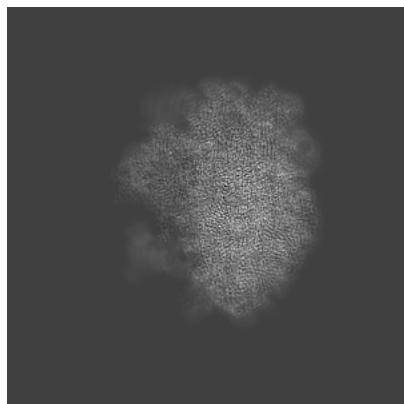
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15773. These allow visual inspection of the internal detail of the map and identification of artifacts.

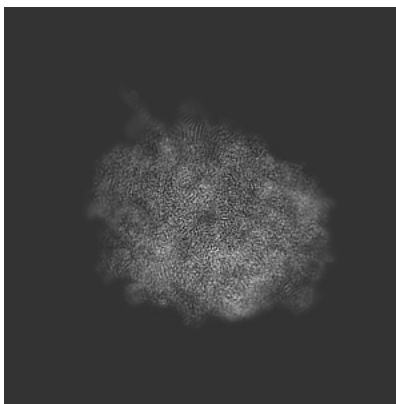
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

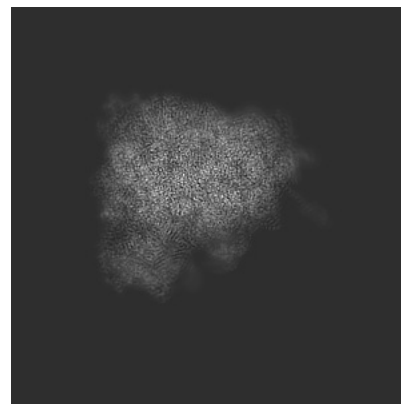
6.1.1 Primary map



X

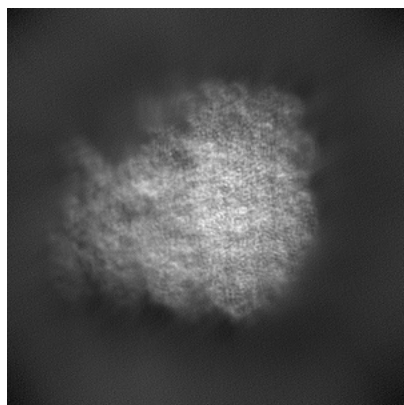


Y

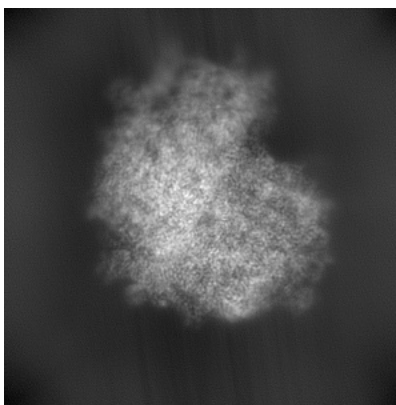


Z

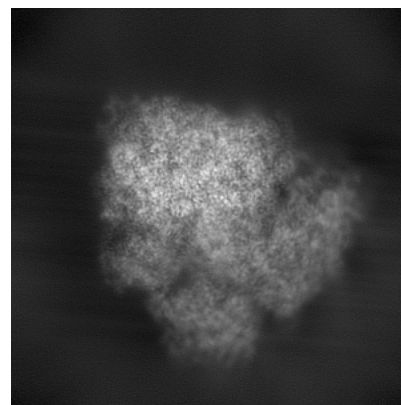
6.1.2 Raw map



X



Y

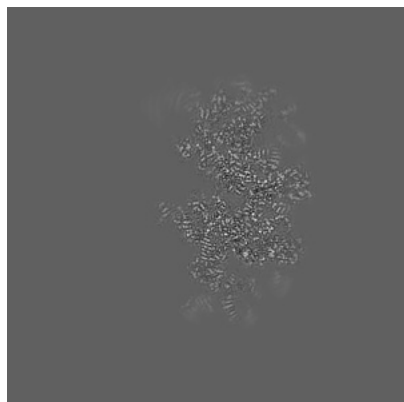


Z

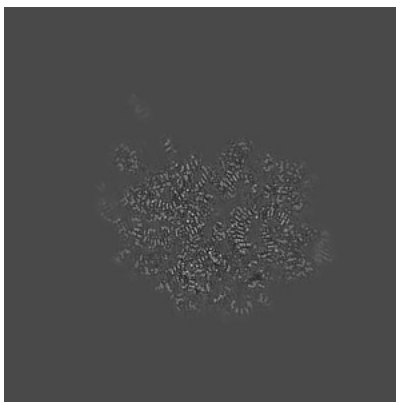
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

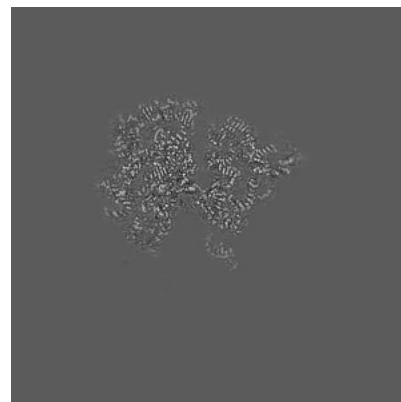
6.2.1 Primary map



X Index: 225

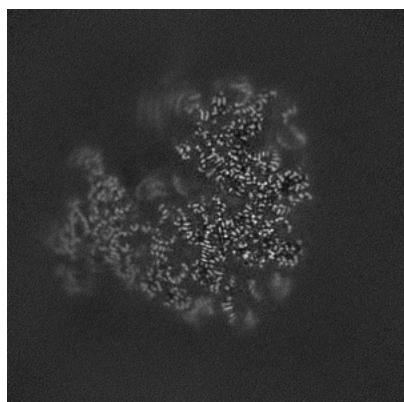


Y Index: 225

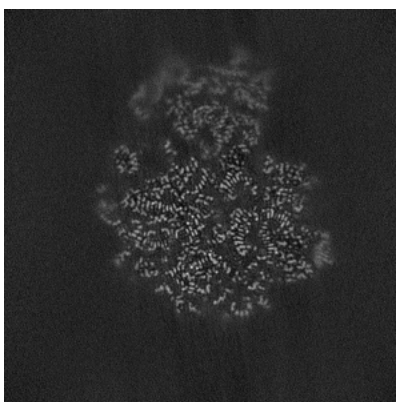


Z Index: 225

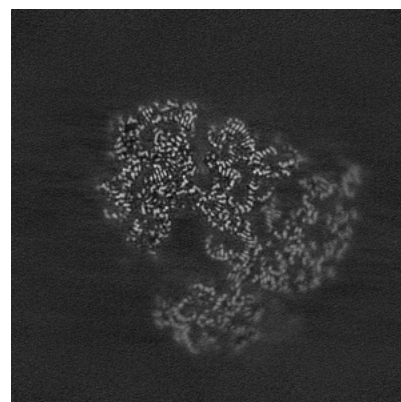
6.2.2 Raw map



X Index: 225



Y Index: 225

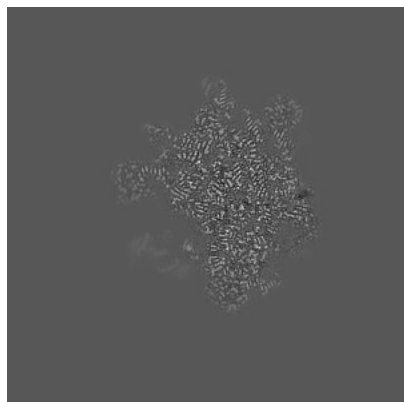


Z Index: 225

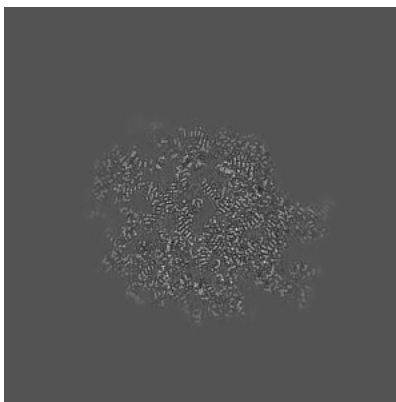
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

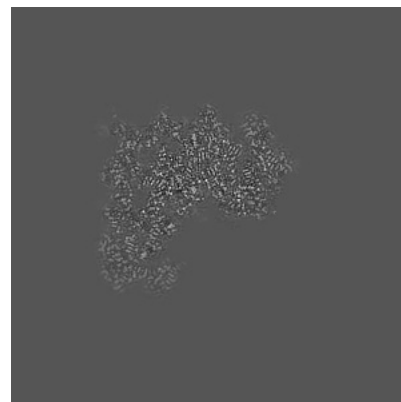
6.3.1 Primary map



X Index: 169

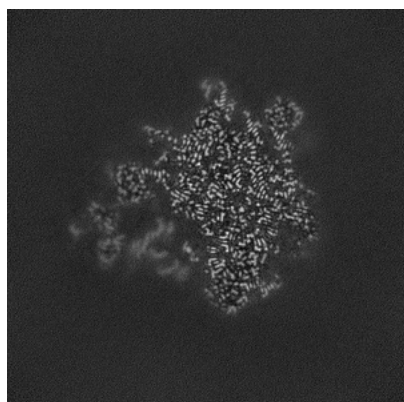


Y Index: 262

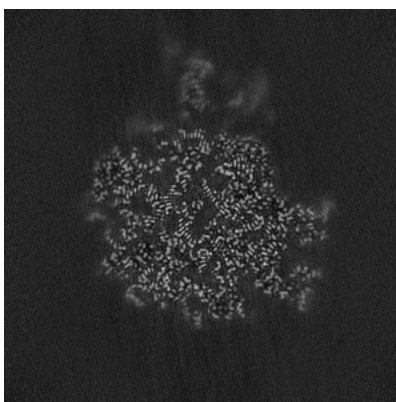


Z Index: 250

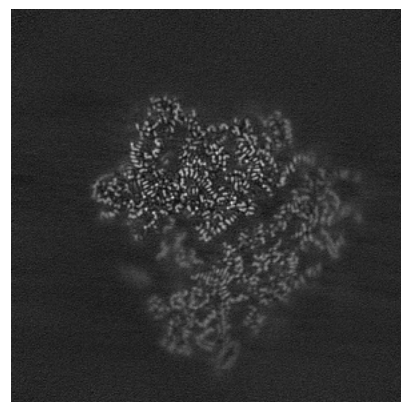
6.3.2 Raw map



X Index: 169



Y Index: 262

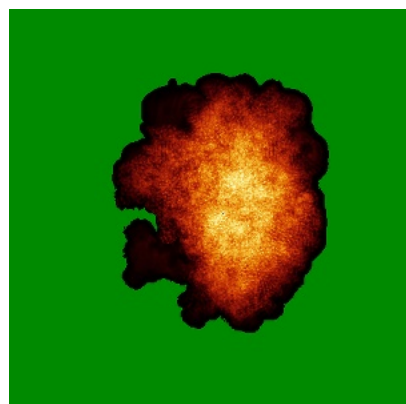


Z Index: 206

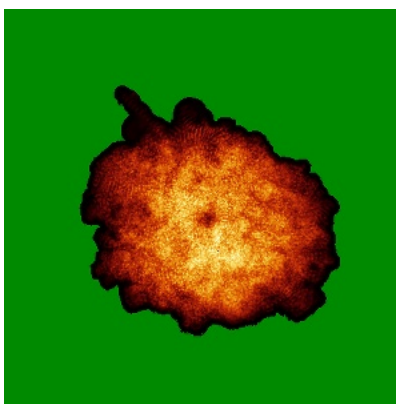
The images above show the largest variance slices of the map in three orthogonal directions.

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

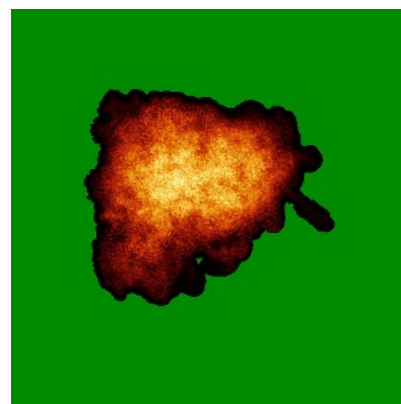
6.4.1 Primary map



X

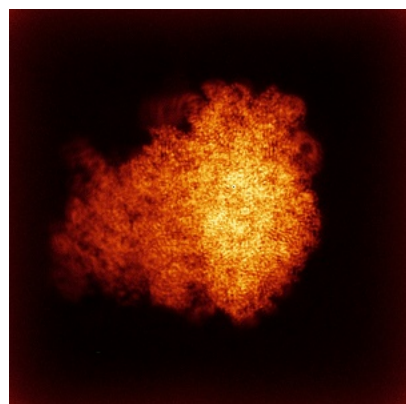


Y

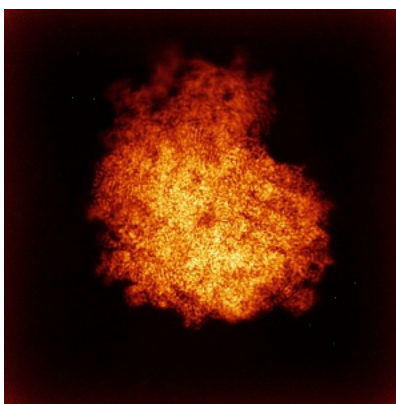


Z

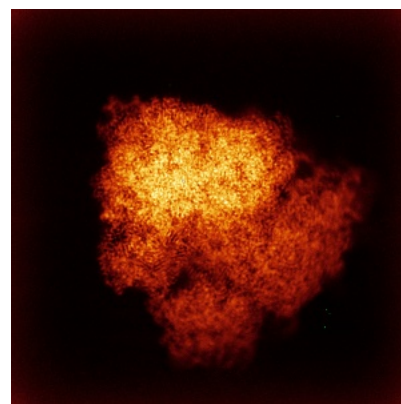
6.4.2 Raw map



X



Y

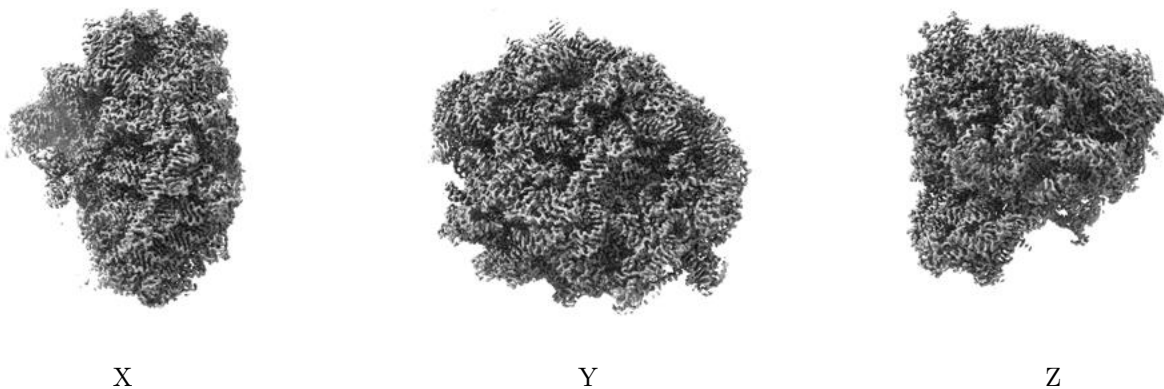


Z

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.

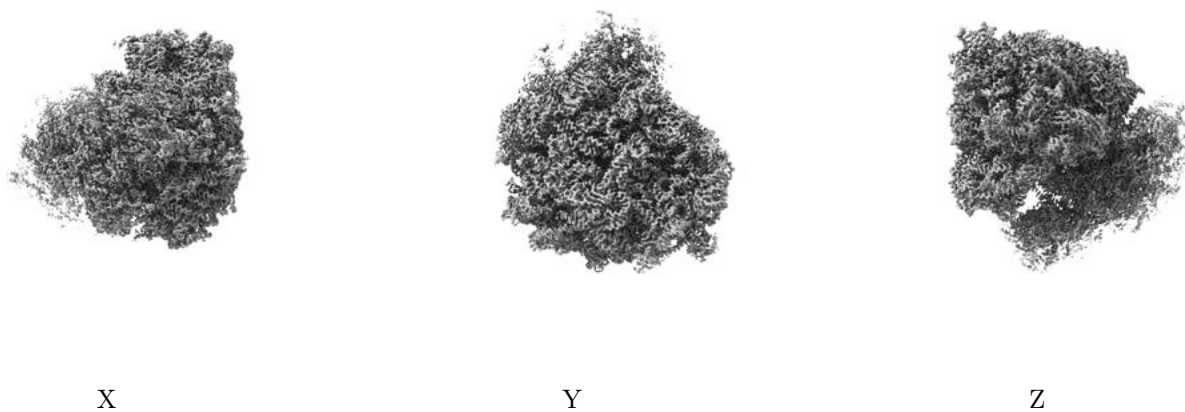
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.05. 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.

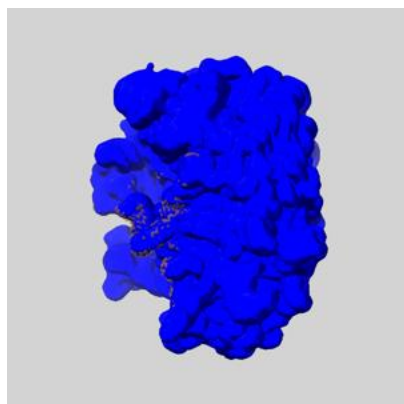
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

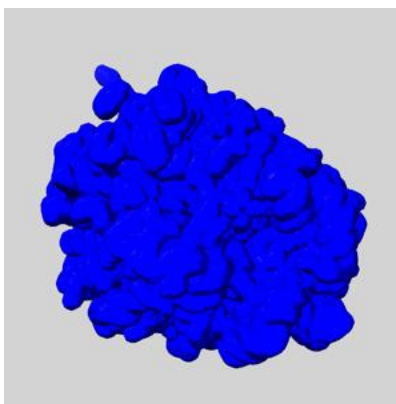
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

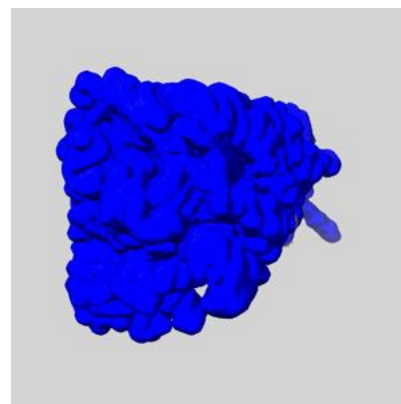
6.6.1 emd_15773_msk_1.map [i](#)



X



Y

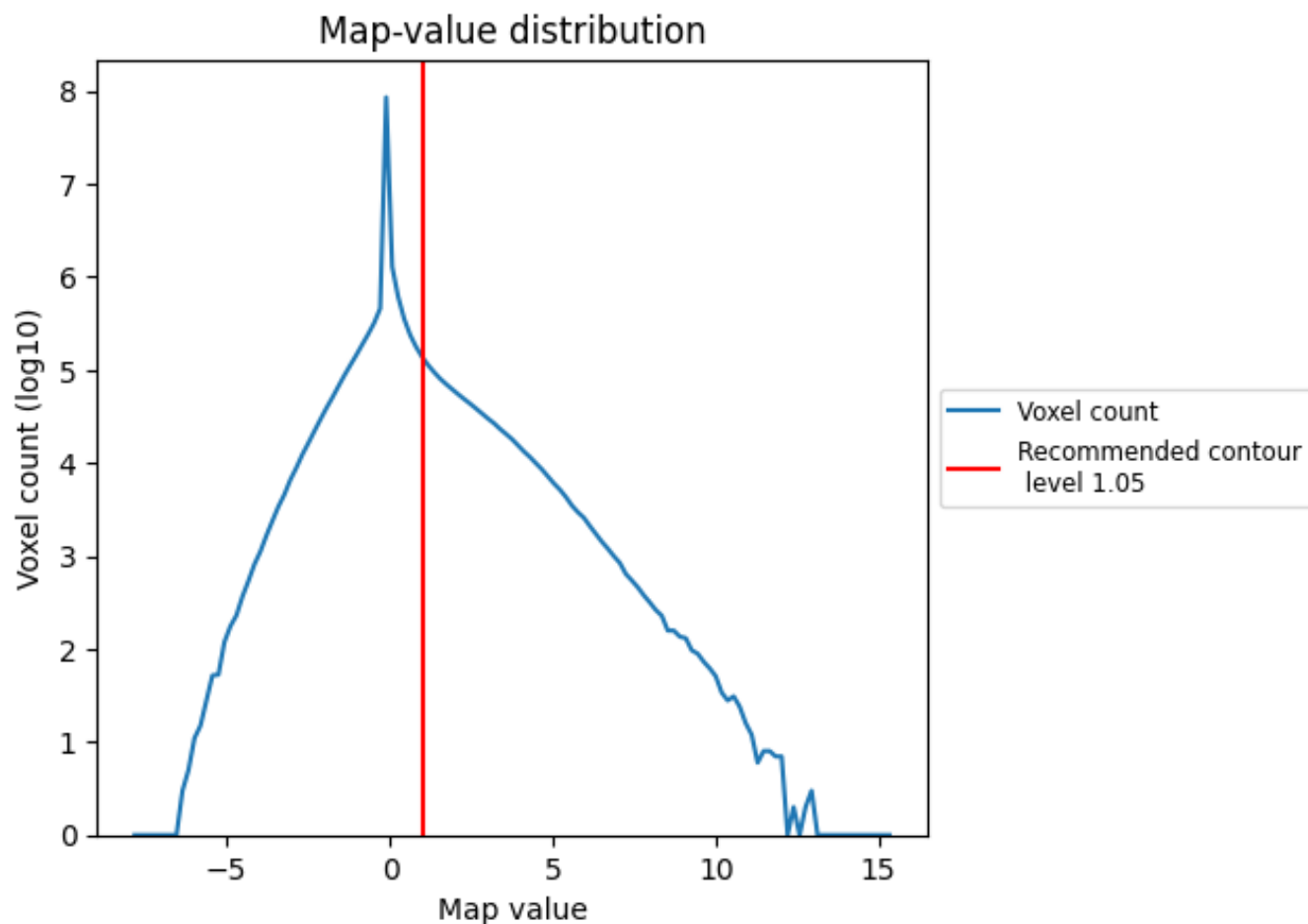


Z

7 Map analysis [i](#)

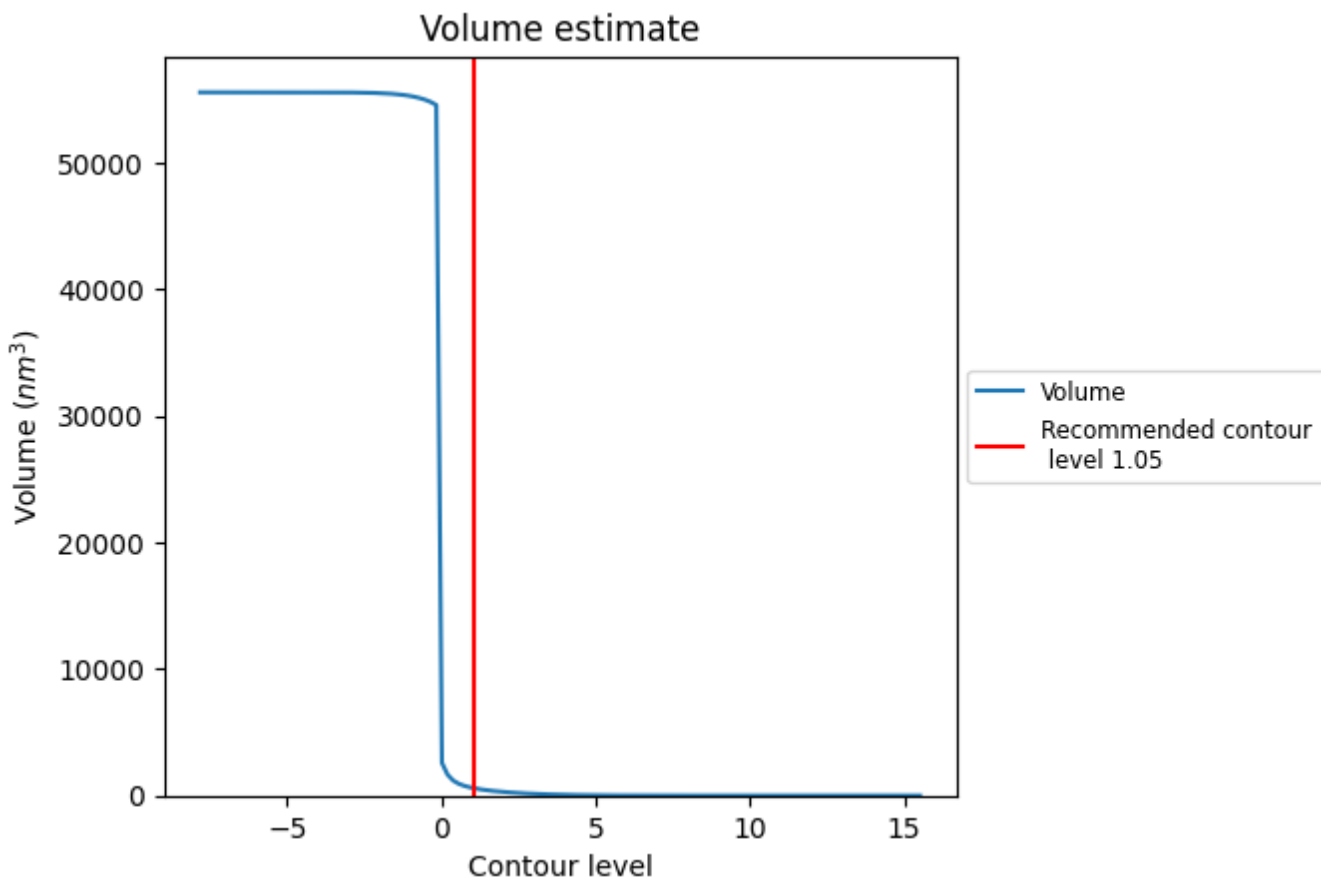
This section contains the results of statistical analysis of the map.

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.

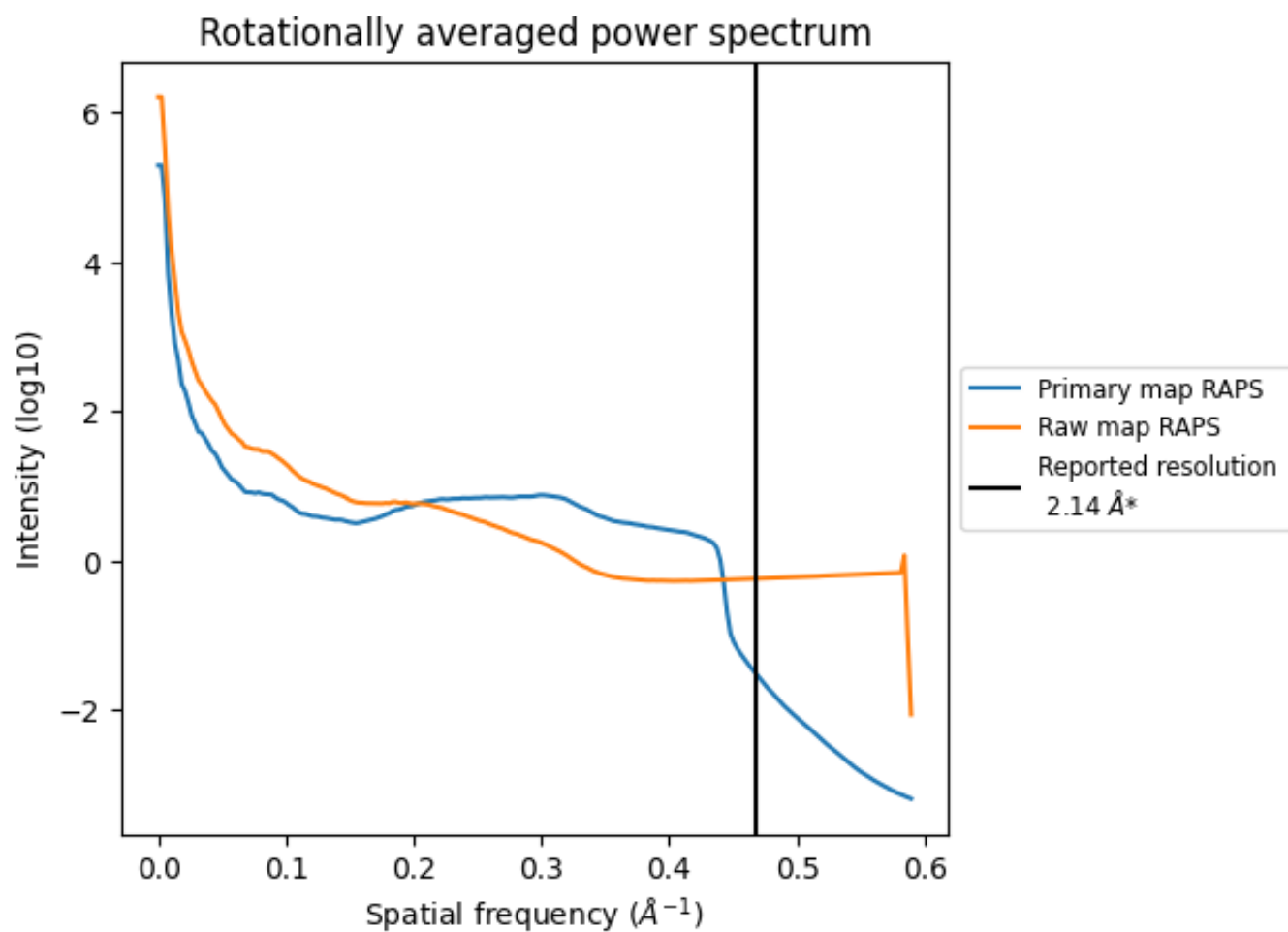
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 586 nm^3 ; this corresponds to an approximate mass of 530 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

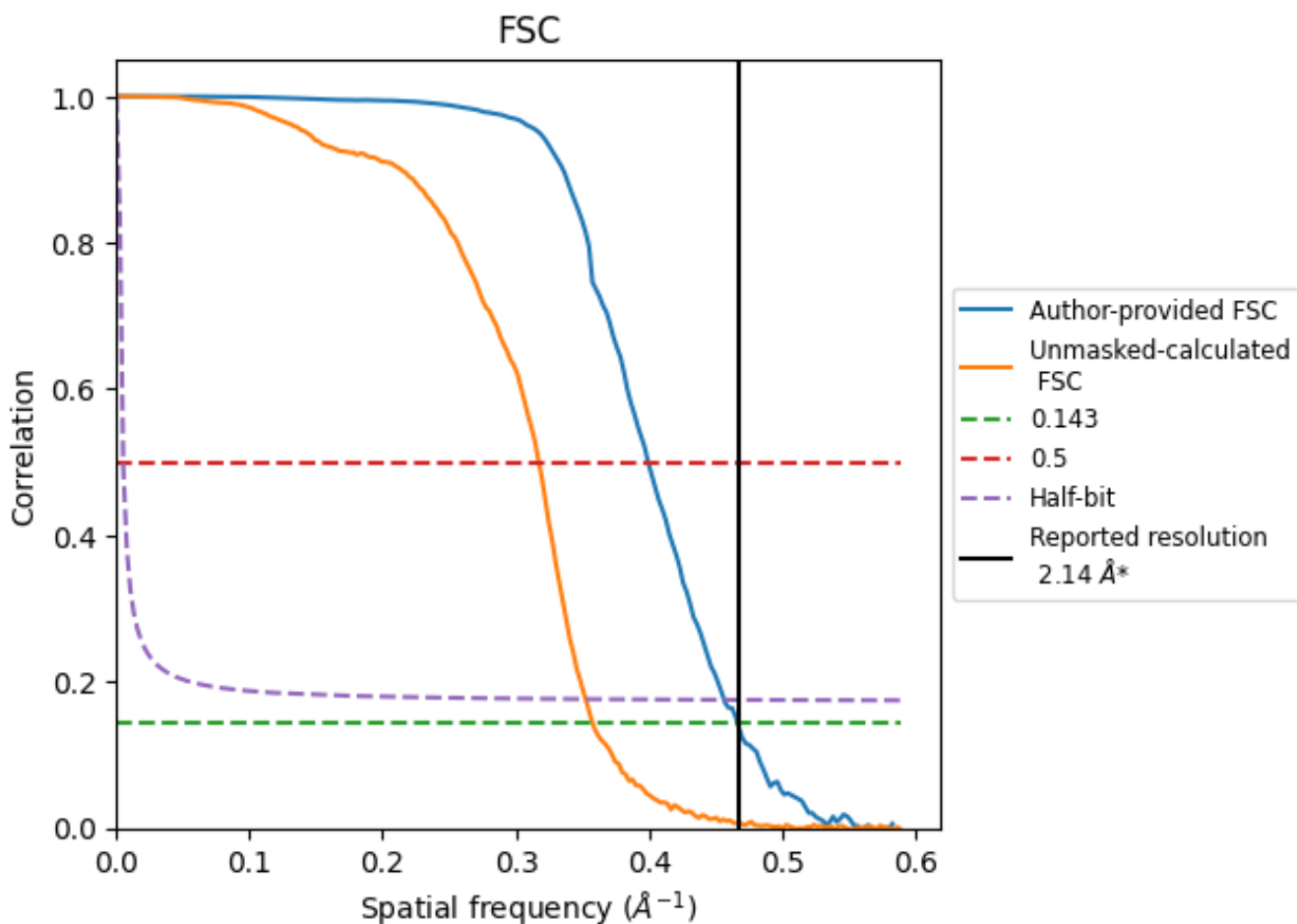


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

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 0.467 Å⁻¹

8.2 Resolution estimates [i](#)

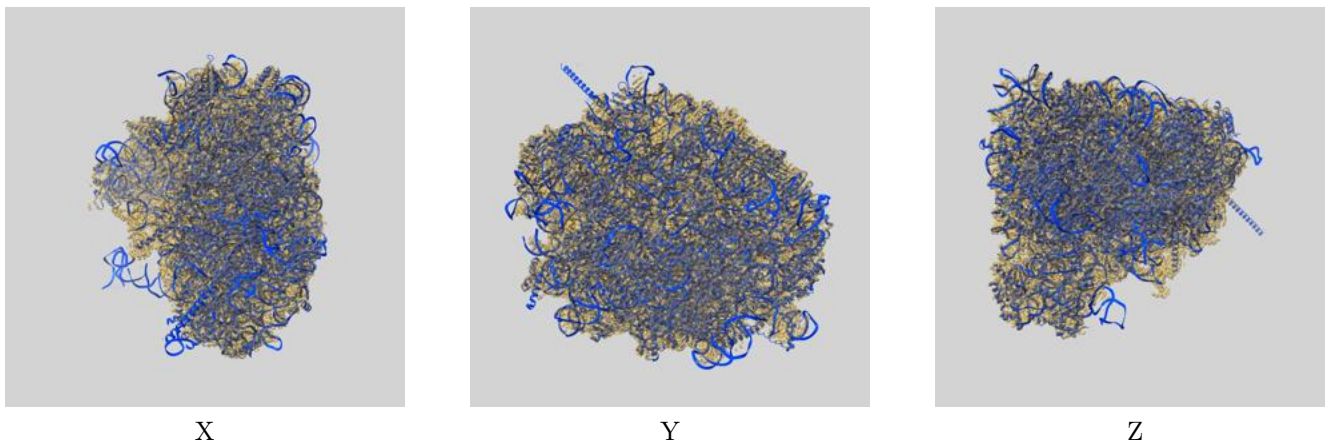
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.50	2.19
Unmasked-calculated*	2.79	3.15	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

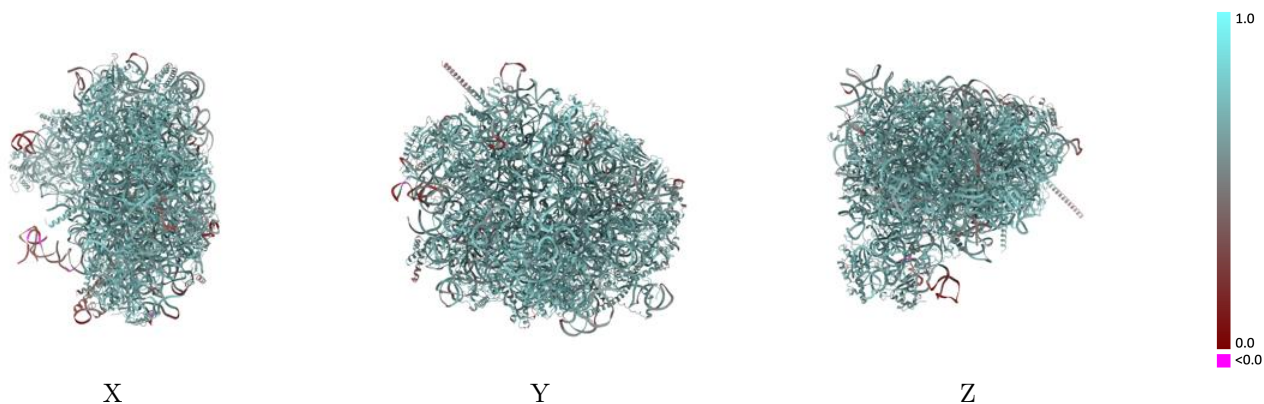
This section contains information regarding the fit between EMDB map EMD-15773 and PDB model 8AZW. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



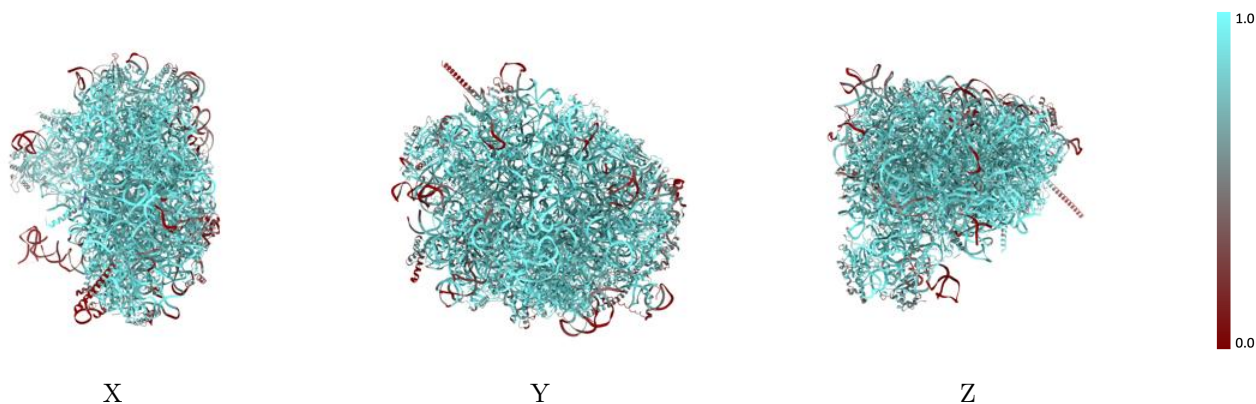
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



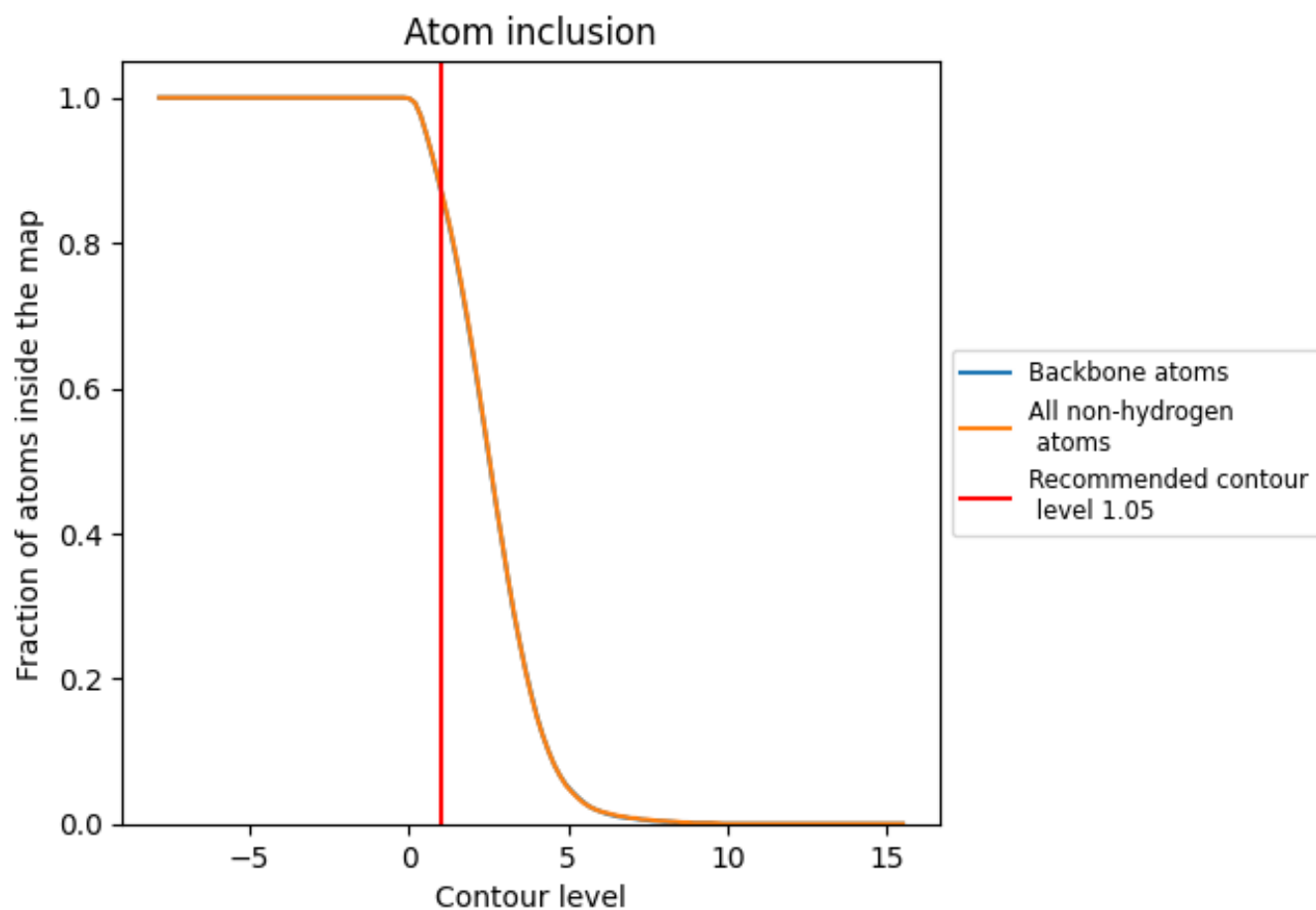
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.6750
A	 0.8750	 0.6650
B	 0.8640	 0.6600
C	 0.9510	 0.6770
D	 0.8720	 0.6980
E	 0.8390	 0.6830
F	 0.9900	 0.7400
G	 0.9570	 0.7290
H	 0.7360	 0.6410
I	 0.9230	 0.7090
J	 0.9000	 0.7040
K	 0.4530	 0.5630
L	 0.9020	 0.7060
M	 0.8090	 0.6660
N	 0.8800	 0.6960
O	 0.9370	 0.7180
P	 0.8020	 0.6560
Q	 0.8100	 0.6730
R	 0.9530	 0.7270
S	 0.9520	 0.7200
T	 0.8750	 0.6860
U	 0.8550	 0.6790
V	 0.9760	 0.7370
W	 0.6570	 0.6140
X	 0.9530	 0.7270
Y	 0.9170	 0.7030
Z	 0.9240	 0.7210
a	 0.8980	 0.7110
b	 0.6980	 0.6420
c	 0.7390	 0.6490
d	 0.9140	 0.7150
e	 0.9160	 0.7120
f	 0.9170	 0.7130
g	 0.8950	 0.6980
h	 0.7670	 0.6560



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Chain	Atom inclusion	Q-score
j	 0.9210	 0.7100
k	 0.8620	 0.6920
l	 0.3000	 0.3230
m	 0.9060	 0.6940
n	 0.8290	 0.6700
o	 0.9710	 0.7300
p	 0.7670	 0.6500
q	 0.8870	 0.7030
r	 0.9320	 0.7210
s	 0.8690	 0.6930
t	 0.6530	 0.6230
u	 0.8140	 0.6700