



## Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 05:46 pm BST

PDB ID : 6ZXH  
EMDB ID : EMD-11521  
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State H2  
Authors : Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.;  
Kutay, U.; Beckmann, R.  
Deposited on : 2020-07-29  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

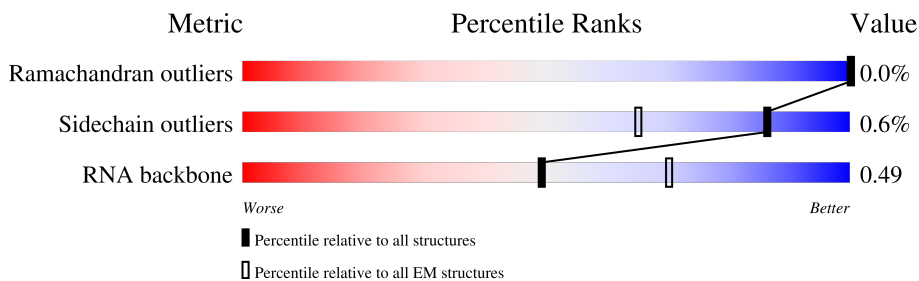
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1869	
2	A	295	
3	B	264	
4	C	293	
5	h	115	
6	E	263	
7	D	243	
8	G	249	

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Mol	Chain	Length	Quality of chain
9	H	194	24% 92% 8%
10	I	208	16% 94% .
11	J	194	12% 90% .
12	F	204	5% 89% .
13	L	158	. 85% .
14	K	165	7% 57% .
15	N	151	5% 98% ..
16	O	151	. 81% .
17	M	132	75% 81% .
18	P	145	10% 91% 9%
19	R	135	16% 96% ..
20	Q	146	. 95% .
21	S	152	9% 91% .
22	T	145	6% 97% .
23	V	83	. 100% .
24	W	130	. 99% .
25	X	143	. 96% ..
26	Y	133	7% 92% 8%
27	U	119	18% 82% 18%
28	Z	125	18% 66% 34%
29	b	84	7% 92% 8%
30	c	69	30% 86% .
31	d	56	. 96% .
32	e	59	7% 85% 15%
33	f	156	25% 37% 63%

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Mol	Chain	Length	Quality of chain
34	g	317	
35	j	165	
36	z	568	

## 2 Entry composition i

There are 40 unique types of molecules in this entry. The entry contains 76979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1651	35310	15787	6344	11528	1651	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	216	1705	1083	299	315	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	211	1715	1088	307	306	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	216	1674	1085	287	292	10	0	0

- Molecule 5 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	h	99	792	492	165	130	5	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	255	2031	1299	377	347	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	224	1745	1112	314	312	7	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	223	1802	1128	358	309	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	179	1446	927	264	254	1	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	199	1638	1027	322	284	5	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	176	1465	934	295	234	2	0	0

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	184	1461	914	276	264	7	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	136	1127	719	212	190	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	126	Total	C	N	O	S	0	0
			947	580	188	173	6		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 18 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	132	Total	C	N	O	S	0	0
			1077	685	202	183	7		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 21 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	141	1162	731	232	198	1	0	0

- Molecule 22 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	T	141	1094	685	210	196	3	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21.

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

- Molecule 24 is a protein called 40S ribosomal protein S15a.

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

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	139	1080	682	214	181	3	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	122	987	624	193	165	5	0	0

- Molecule 27 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	98	774	486	145	139	4	0	0

- Molecule 28 is a protein called 40S ribosomal protein S25.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	82	Total	C	N	O	S	0	0
			638	410	117	110	1		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	77	Total	C	N	O	S	0	0
			611	386	113	107	5		

- Molecule 30 is a protein called 40S ribosomal protein S28.

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

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	54	Total	C	N	O	S	0	0
			450	282	93	70	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	50	Total	C	N	O	S	0	0
			398	244	90	63	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	295	Total	C	N	O	S	0	0
			2306	1460	403	431	12		

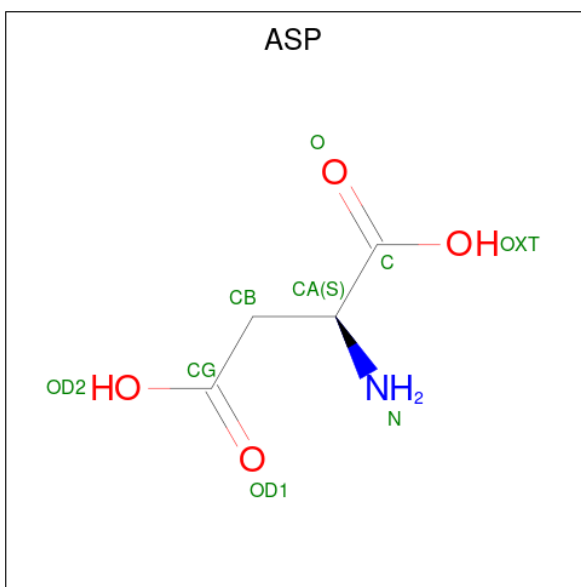
- Molecule 35 is a protein called Probable RNA-binding protein EIF1AD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	116	Total	C	N	O	S	0	0
			934	593	167	172	2		

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	349	Total	C	N	O	S	0	0
			2803	1757	515	511	20		

- Molecule 37 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
37	2	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	124	Total	Mg	0
			124	124	
38	h	1	Total	Mg	0
			1	1	
38	G	1	Total	Mg	0
			1	1	
38	F	1	Total	Mg	0
			1	1	

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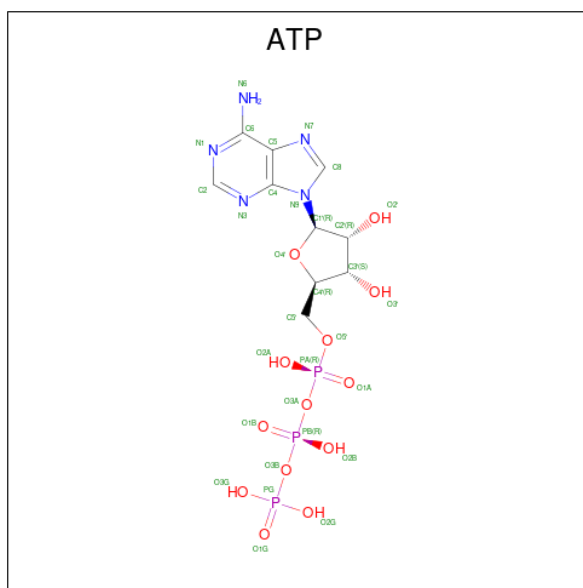
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Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Mg	0
			1	1	
38	d	1	Total	Mg	0
			1	1	
38	z	2	Total	Mg	0
			2	2	

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	h	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

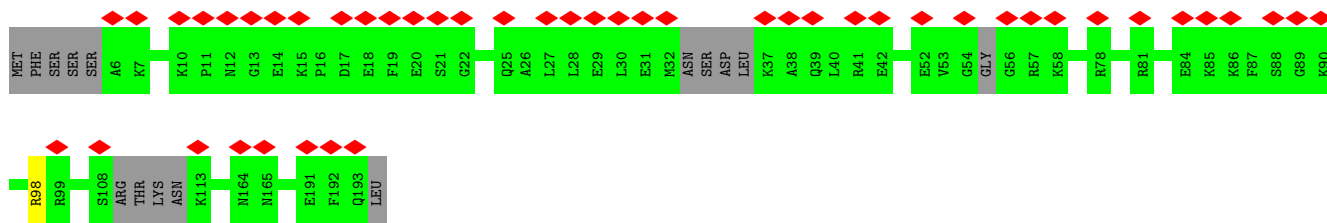


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	z	1	31	10	5	13	3	0

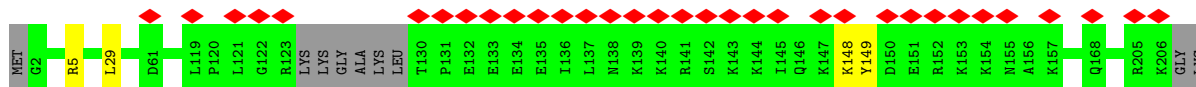
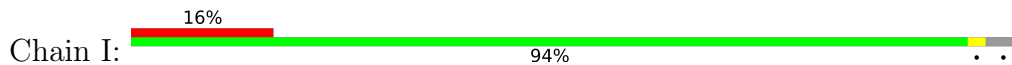




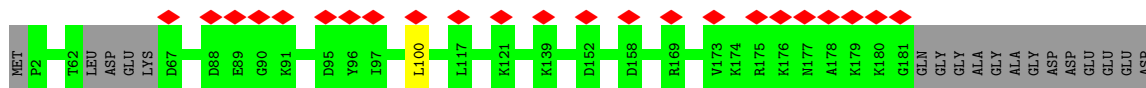
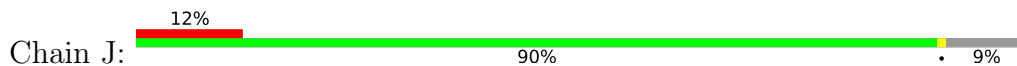




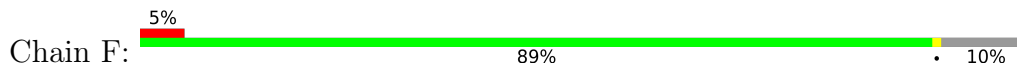
• Molecule 10: 40S ribosomal protein S8



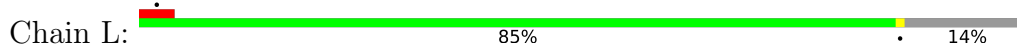
• Molecule 11: 40S ribosomal protein S9



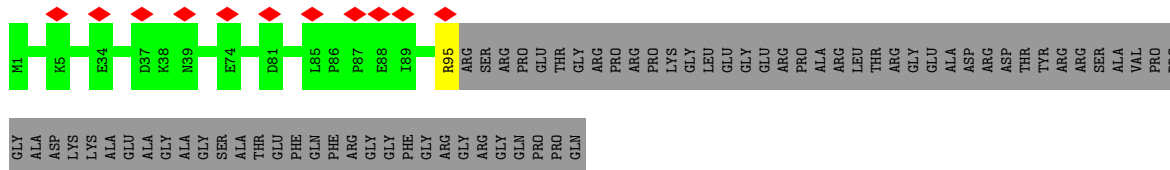
• Molecule 12: 40S ribosomal protein S5



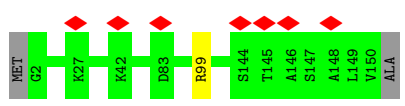
• Molecule 13: 40S ribosomal protein S11



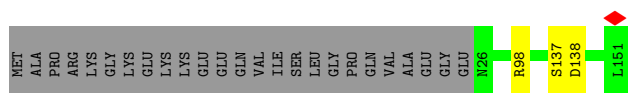
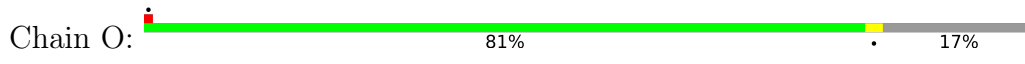
• Molecule 14: 40S ribosomal protein S10



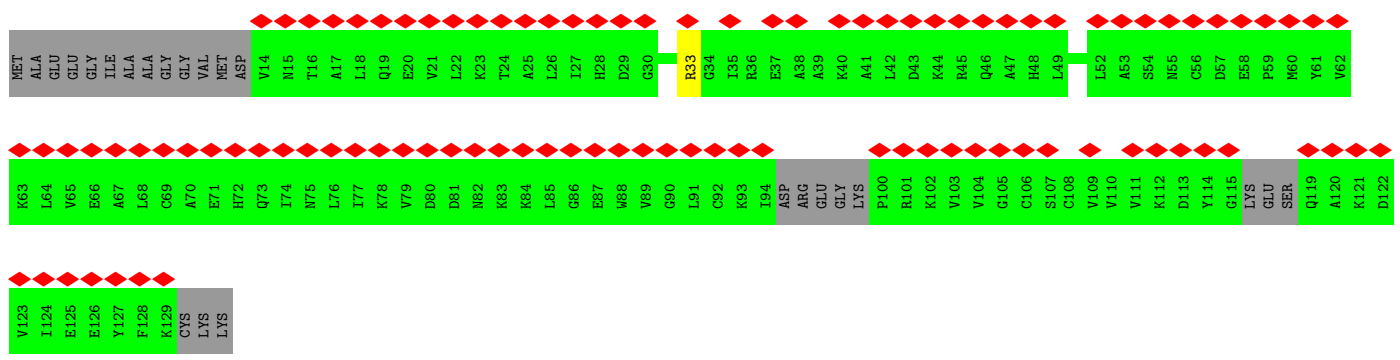
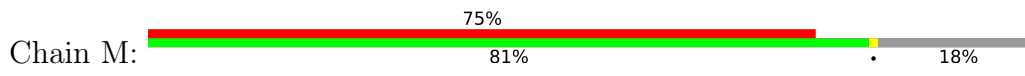
• Molecule 15: 40S ribosomal protein S13



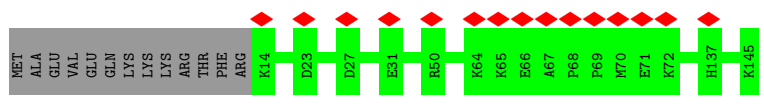
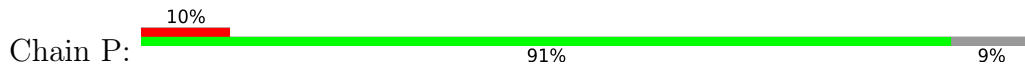
• Molecule 16: 40S ribosomal protein S14



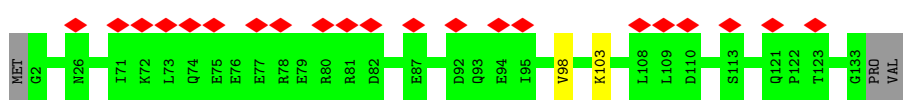
• Molecule 17: 40S ribosomal protein S12



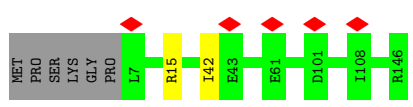
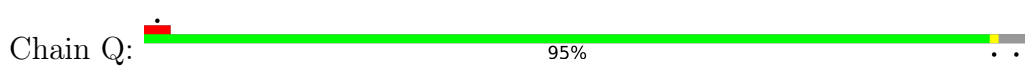
• Molecule 18: 40S ribosomal protein S15



• Molecule 19: 40S ribosomal protein S17

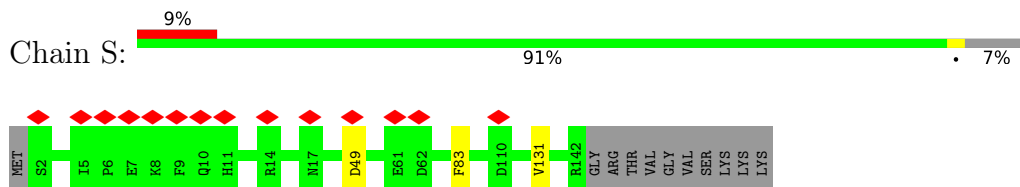


• Molecule 20: 40S ribosomal protein S16

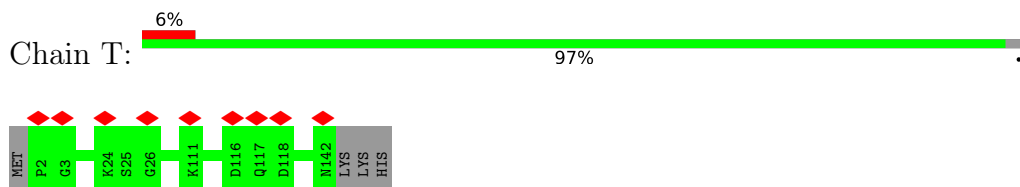




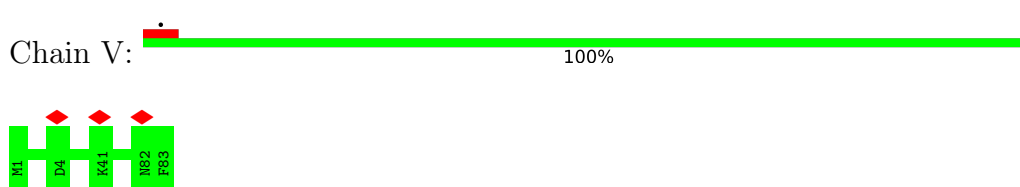
- Molecule 21: 40S ribosomal protein S18



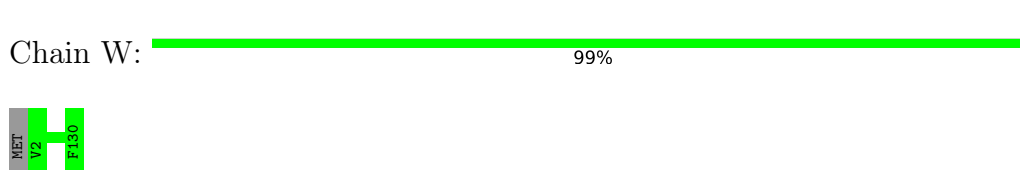
- Molecule 22: 40S ribosomal protein S19



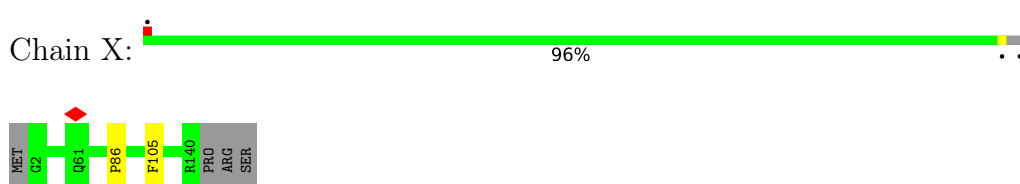
- Molecule 23: 40S ribosomal protein S21



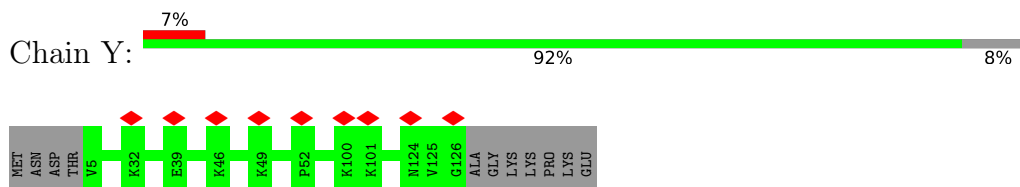
- Molecule 24: 40S ribosomal protein S15a



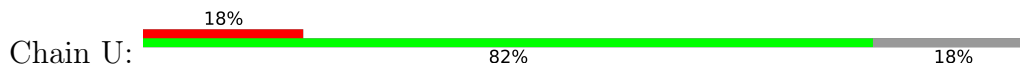
- Molecule 25: 40S ribosomal protein S23

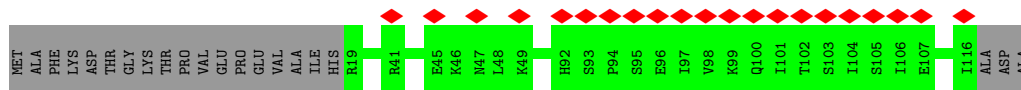


- Molecule 26: 40S ribosomal protein S24

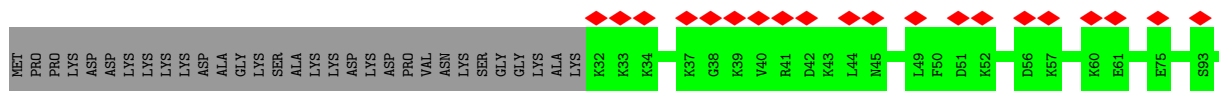


- Molecule 27: 40S ribosomal protein S20

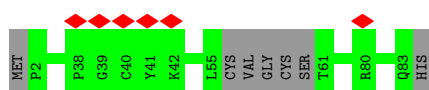
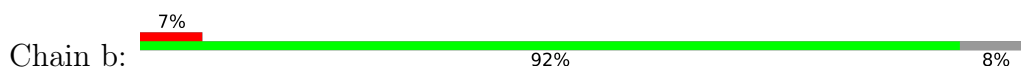




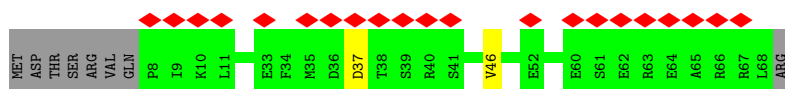
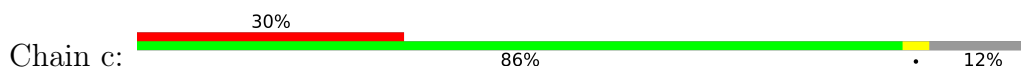
• Molecule 28: 40S ribosomal protein S25



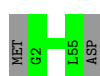
• Molecule 29: 40S ribosomal protein S27



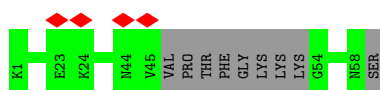
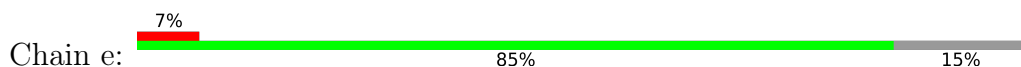
• Molecule 30: 40S ribosomal protein S28



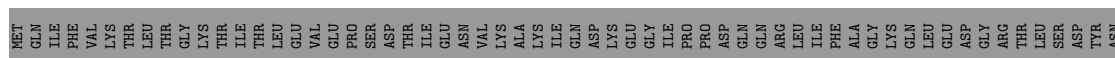
• Molecule 31: 40S ribosomal protein S29



• Molecule 32: 40S ribosomal protein S30



• Molecule 33: Ubiquitin-40S ribosomal protein S27a







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.868	Depositor
Minimum map value	-0.424	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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, OMU, MG, OMG, A2M, OMC, MA6, ATP, 4AC, 6MZ, B8N, 7MG, 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	2	1.02	1/37709 (0.0%)	1.18	220/58755 (0.4%)
2	A	0.44	0/1742	0.54	0/2367
3	B	0.39	0/1742	0.56	0/2330
4	C	0.47	0/1710	0.58	0/2310
5	h	0.49	0/805	0.55	0/1079
6	E	0.41	0/2073	0.56	1/2791 (0.0%)
7	D	0.41	0/1773	0.56	0/2387
8	G	0.36	0/1825	0.53	0/2431
9	H	0.36	0/1466	0.55	0/1959
10	I	0.41	0/1666	0.55	1/2223 (0.0%)
11	J	0.40	0/1489	0.59	1/1987 (0.1%)
12	F	0.38	0/1481	0.55	0/1988
13	L	0.49	0/1147	0.55	0/1535
14	K	0.37	0/823	0.52	0/1111
15	N	0.43	0/1226	0.54	0/1649
16	O	0.42	0/959	0.60	0/1286
17	M	0.31	0/845	0.57	0/1134
18	P	0.38	0/1099	0.55	0/1471
19	R	0.38	0/1080	0.58	0/1449
20	Q	0.43	0/1133	0.57	0/1517
21	S	0.38	0/1180	0.58	1/1582 (0.1%)
22	T	0.44	0/1113	0.56	0/1493
23	V	0.42	0/643	0.52	0/860
24	W	0.46	0/1051	0.57	0/1406
25	X	0.47	0/1097	0.57	0/1464
26	Y	0.39	0/1004	0.53	0/1337
27	U	0.39	0/783	0.58	0/1052
28	Z	0.33	0/646	0.54	0/869
29	b	0.41	0/623	0.55	0/834
30	c	0.33	0/481	0.61	1/643 (0.2%)
31	d	0.47	0/461	0.66	0/612
32	e	0.37	0/401	0.56	0/526

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.36	0/474	0.56	0/626
34	g	0.34	0/2360	0.62	3/3207 (0.1%)
35	j	0.36	0/952	0.57	1/1282 (0.1%)
36	z	0.40	0/2848	0.57	1/3816 (0.0%)
All	All	0.76	1/79910 (0.0%)	0.93	230/115368 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	O	0	2
20	Q	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1139	C	N3-C4	-5.05	1.30	1.33

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	668	A2M	P-O3'-C3'	33.01	159.31	119.70
1	2	166	A2M	P-O3'-C3'	28.31	153.67	119.70
1	2	166	A2M	OP1-P-O3'	25.32	160.89	105.20
1	2	99	A2M	OP1-P-O3'	-24.29	51.77	105.20
1	2	1031	A2M	P-O3'-C3'	23.05	147.35	119.70
1	2	159	A2M	P-O3'-C3'	22.60	146.82	119.70
1	2	99	A2M	P-O3'-C3'	-20.91	94.60	119.70
1	2	1678	A2M	O3'-P-O5'	19.92	141.84	104.00
1	2	27	A2M	P-O3'-C3'	19.87	143.54	119.70
1	2	576	A2M	OP1-P-O3'	-19.52	62.26	105.20
1	2	1031	A2M	OP1-P-O3'	18.79	146.53	105.20
1	2	576	A2M	OP2-P-O3'	18.48	145.85	105.20
1	2	512	A2M	OP1-P-O3'	-18.09	65.41	105.20
1	2	166	A2M	OP2-P-O3'	-17.75	66.16	105.20
1	2	668	A2M	OP1-P-O3'	17.33	143.32	105.20
1	2	1031	A2M	OP2-P-O3'	-15.51	71.08	105.20
1	2	501	C	N1-C2-O2	13.51	127.01	118.90
1	2	501	C	C2-N1-C1'	13.01	133.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	576	A2M	P-O3'-C3'	-12.56	104.62	119.70
1	2	668	A2M	OP2-P-O3'	-12.24	78.26	105.20
1	2	1678	A2M	OP1-P-O3'	-11.86	79.11	105.20
1	2	99	A2M	OP2-P-O3'	11.80	131.16	105.20
1	2	1383	A2M	P-O3'-C3'	11.24	133.18	119.70
1	2	1139	C	N3-C2-O2	-11.20	114.06	121.90
1	2	512	A2M	OP2-P-O3'	11.06	129.53	105.20
1	2	501	C	N3-C2-O2	-10.98	114.22	121.90
1	2	27	A2M	OP1-P-O3'	10.89	129.16	105.20
1	2	1864	U	N3-C2-O2	-10.40	114.92	122.20
1	2	293	C	N1-C2-O2	10.32	125.09	118.90
1	2	1618	C	N3-C2-O2	-10.19	114.77	121.90
1	2	501	C	C6-N1-C1'	-10.09	108.69	120.80
1	2	1618	C	N1-C2-O2	10.06	124.94	118.90
1	2	166	A2M	O3'-P-O5'	-9.56	85.83	104.00
1	2	72	C	N1-C2-O2	9.56	124.64	118.90
1	2	120	U	N3-C2-O2	-9.52	115.53	122.20
1	2	422	U	N3-C2-O2	-9.51	115.54	122.20
1	2	1139	C	C6-N1-C2	-9.48	116.51	120.30
1	2	1016	U	N1-C2-O2	9.46	129.42	122.80
1	2	853	C	C6-N1-C2	-9.34	116.56	120.30
1	2	853	C	N3-C2-O2	-9.34	115.36	121.90
1	2	1016	U	N3-C2-O2	-9.32	115.67	122.20
1	2	1453	C	N1-C2-O2	9.22	124.43	118.90
1	2	1683	C	N3-C2-O2	-9.16	115.48	121.90
1	2	1485	U	N3-C2-O2	-9.02	115.89	122.20
1	2	1683	C	C6-N1-C2	-9.01	116.70	120.30
1	2	99	A2M	O3'-P-O5'	8.88	120.87	104.00
1	2	1453	C	C2-N1-C1'	8.60	128.25	118.80
1	2	1864	U	N1-C2-O2	8.57	128.80	122.80
1	2	27	A2M	OP2-P-O3'	-8.56	86.36	105.20
1	2	293	C	C2-N1-C1'	8.51	128.16	118.80
1	2	853	C	C2-N1-C1'	8.46	128.10	118.80
1	2	293	C	N3-C2-O2	-8.31	116.08	121.90
1	2	1073	U	N3-C2-O2	-8.29	116.39	122.20
36	z	284	ASP	CB-CG-OD1	8.23	125.71	118.30
1	2	72	C	C2-N1-C1'	8.11	127.72	118.80
1	2	851	C	C2-N1-C1'	8.11	127.72	118.80
1	2	1551	U	N3-C2-O2	-8.08	116.54	122.20
1	2	427	U	N3-C2-O2	-8.04	116.57	122.20
1	2	1683	C	N1-C2-O2	8.02	123.72	118.90
1	2	72	C	N3-C2-O2	-7.79	116.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	746	C	C2-N1-C1'	7.75	127.32	118.80
1	2	1315	U	N3-C2-O2	-7.69	116.82	122.20
1	2	1016	U	C2-N1-C1'	7.68	126.92	117.70
1	2	1864	U	C2-N1-C1'	7.65	126.88	117.70
1	2	1139	C	C2-N1-C1'	7.64	127.21	118.80
34	g	249	CYS	CA-CB-SG	7.64	127.75	114.00
1	2	309	G	O4'-C1'-N9	7.59	114.27	108.20
1	2	422	U	C2-N1-C1'	7.59	126.80	117.70
1	2	851	C	N1-C2-O2	7.55	123.43	118.90
1	2	1683	C	C2-N1-C1'	7.50	127.05	118.80
1	2	1139	C	N1-C2-O2	7.50	123.40	118.90
1	2	1073	U	C2-N1-C1'	7.46	126.65	117.70
1	2	512	A2M	O3'-P-O5'	7.44	118.14	104.00
1	2	1261	C	N3-C2-O2	-7.44	116.69	121.90
1	2	851	C	N3-C2-O2	-7.37	116.74	121.90
1	2	1315	U	N1-C2-O2	7.36	127.95	122.80
1	2	1618	C	C2-N1-C1'	7.32	126.85	118.80
1	2	427	U	C2-N1-C1'	7.30	126.46	117.70
1	2	823	U	N3-C2-O2	-7.27	117.11	122.20
1	2	1663	A	O4'-C1'-N9	7.26	114.01	108.20
1	2	120	U	C2-N1-C1'	7.23	126.37	117.70
1	2	1453	C	N3-C2-O2	-7.16	116.89	121.90
1	2	1618	C	C6-N1-C2	-7.14	117.44	120.30
1	2	1261	C	C6-N1-C2	-7.12	117.45	120.30
1	2	1520	G	C4-N9-C1'	7.10	135.73	126.50
1	2	1022	U	C2-N1-C1'	7.08	126.19	117.70
1	2	148	U	C2-N1-C1'	7.07	126.19	117.70
1	2	1520	G	C8-N9-C1'	-6.93	117.98	127.00
1	2	1283	C	C2-N1-C1'	6.92	126.42	118.80
1	2	381	C	C6-N1-C2	-6.92	117.53	120.30
1	2	1261	C	N1-C2-O2	6.89	123.03	118.90
1	2	194	C	N1-C2-O2	6.88	123.03	118.90
1	2	1485	U	N1-C2-O2	6.84	127.59	122.80
1	2	853	C	N1-C2-O2	6.79	122.97	118.90
1	2	685	A	O4'-C1'-N9	6.78	113.63	108.20
1	2	579	C	N1-C2-O2	6.74	122.94	118.90
1	2	1551	U	C2-N1-C1'	6.74	125.79	117.70
1	2	148	U	N3-C2-O2	-6.73	117.49	122.20
1	2	579	C	C2-N1-C1'	6.73	126.20	118.80
1	2	1073	U	N1-C2-O2	6.70	127.49	122.80
1	2	1485	U	C2-N1-C1'	6.70	125.74	117.70
1	2	1520	G	N3-C4-N9	6.69	130.01	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1551	U	N1-C2-O2	6.65	127.45	122.80
1	2	1389	C	C2-N1-C1'	6.64	126.10	118.80
1	2	1315	U	C2-N1-C1'	6.63	125.65	117.70
1	2	823	U	C2-N1-C1'	6.59	125.61	117.70
1	2	120	U	N1-C2-O2	6.52	127.36	122.80
1	2	1632	G	O4'-C1'-N9	6.52	113.41	108.20
1	2	1060	A	P-O3'-C3'	6.51	127.51	119.70
1	2	1123	C	N1-C2-O2	6.51	122.81	118.90
1	2	427	U	N1-C2-O2	6.50	127.35	122.80
1	2	1283	C	N1-C2-O2	6.37	122.72	118.90
1	2	1123	C	N3-C2-O2	-6.36	117.45	121.90
1	2	1149	A	N1-C6-N6	-6.33	114.80	118.60
1	2	72	C	C6-N1-C2	-6.33	117.77	120.30
1	2	666	U	C2-N1-C1'	6.28	125.23	117.70
1	2	484	A2M	P-O3'-C3'	6.27	127.22	119.70
1	2	1271	C	N1-C2-O2	6.24	122.65	118.90
34	g	240	CYS	CA-CB-SG	6.24	125.24	114.00
1	2	422	U	N1-C2-O2	6.23	127.16	122.80
1	2	666	U	N3-C2-O2	-6.22	117.85	122.20
1	2	179	C	N1-C2-O2	6.21	122.62	118.90
1	2	666	U	N1-C2-O2	6.18	127.13	122.80
1	2	1022	U	N1-C2-O2	6.16	127.11	122.80
1	2	1242	U	C2-N1-C1'	6.13	125.06	117.70
1	2	493	A	O4'-C1'-N9	6.07	113.06	108.20
1	2	551	U	N3-C2-O2	-6.04	117.97	122.20
1	2	1271	C	N3-C2-O2	-6.03	117.68	121.90
1	2	579	C	N3-C2-O2	-6.01	117.70	121.90
1	2	1453	C	C6-N1-C1'	-6.00	113.60	120.80
1	2	484	A2M	OP1-P-O3'	5.99	118.38	105.20
1	2	293	C	C6-N1-C1'	-5.97	113.63	120.80
1	2	1865	C	N3-C2-O2	-5.97	117.72	121.90
1	2	1002	U	N1-C2-O2	5.95	126.96	122.80
1	2	953	C	C2-N1-C1'	5.93	125.32	118.80
1	2	194	C	N3-C2-O2	-5.93	117.75	121.90
1	2	402	C	C6-N1-C2	-5.90	117.94	120.30
1	2	659	G	C4-N9-C1'	5.90	134.16	126.50
1	2	1623	A	O4'-C1'-N9	5.87	112.90	108.20
1	2	747	U	C5-C6-N1	5.87	125.63	122.70
1	2	49	C	C6-N1-C2	-5.86	117.96	120.30
1	2	665	G	N1-C6-O6	-5.86	116.39	119.90
1	2	407	G	C4-N9-C1'	5.85	134.10	126.50
1	2	1111	U	N3-C2-O2	-5.84	118.11	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1696	C	C6-N1-C2	-5.84	117.96	120.30
1	2	1149	A	C2-N3-C4	5.83	113.52	110.60
6	E	139	LEU	CA-CB-CG	5.81	128.67	115.30
1	2	1396	A	O4'-C1'-N9	5.81	112.85	108.20
1	2	159	A2M	OP2-P-O3'	5.79	117.94	105.20
1	2	748	C	C5-C6-N1	5.78	123.89	121.00
1	2	953	C	N3-C2-O2	-5.77	117.86	121.90
1	2	823	U	N1-C2-O2	5.76	126.83	122.80
1	2	1552	G	C5-C6-O6	-5.76	125.14	128.60
1	2	1022	U	N3-C2-O2	-5.75	118.17	122.20
1	2	746	C	C5-C6-N1	5.75	123.87	121.00
1	2	179	C	C2-N1-C1'	5.71	125.08	118.80
1	2	851	C	C6-N1-C2	-5.70	118.02	120.30
1	2	494	C	N1-C2-O2	5.68	122.31	118.90
1	2	570	C	N3-C2-O2	-5.68	117.92	121.90
1	2	746	C	N1-C2-O2	5.67	122.30	118.90
1	2	1277	C	C2-N1-C1'	5.66	125.02	118.80
1	2	20	G	N1-C6-O6	-5.65	116.51	119.90
1	2	195	C	N1-C2-O2	5.65	122.29	118.90
21	S	49	ASP	CB-CG-OD1	5.64	123.38	118.30
1	2	664	A	N1-C2-N3	-5.62	126.49	129.30
1	2	1002	U	N3-C2-O2	-5.61	118.27	122.20
1	2	570	C	C6-N1-C2	-5.60	118.06	120.30
1	2	1591	C	N1-C2-O2	5.60	122.26	118.90
1	2	685	A	C5-N7-C8	-5.58	101.11	103.90
1	2	1522	A	C5-N7-C8	-5.51	101.14	103.90
1	2	1552	G	N9-C4-C5	-5.51	103.20	105.40
1	2	493	A	C5-N7-C8	-5.50	101.15	103.90
1	2	746	C	C6-N1-C1'	-5.49	114.22	120.80
1	2	747	U	C2-N1-C1'	5.48	124.27	117.70
1	2	1522	A	N7-C8-N9	5.47	116.54	113.80
1	2	1123	C	C6-N1-C2	-5.46	118.12	120.30
1	2	1243	U	N3-C2-O2	-5.46	118.38	122.20
1	2	851	C	C6-N1-C1'	-5.45	114.26	120.80
1	2	493	A	N7-C8-N9	5.45	116.52	113.80
1	2	1453	C	C6-N1-C2	-5.42	118.13	120.30
1	2	749	U	C2-N1-C1'	5.40	124.18	117.70
1	2	468	A2M	P-O3'-C3'	5.39	126.17	119.70
10	I	29	LEU	CA-CB-CG	5.39	127.69	115.30
1	2	919	A	O4'-C1'-N9	5.38	112.50	108.20
34	g	227	LEU	CA-CB-CG	5.38	127.67	115.30
1	2	1271	C	C6-N1-C2	-5.37	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	579	C	C6-N1-C2	-5.36	118.16	120.30
1	2	1606	G	O4'-C1'-N9	5.36	112.49	108.20
1	2	381	C	C5-C6-N1	5.34	123.67	121.00
1	2	1346	U	N3-C2-O2	-5.34	118.46	122.20
1	2	1389	C	C6-N1-C2	-5.34	118.17	120.30
1	2	488	U	C5-C6-N1	5.33	125.36	122.70
1	2	659	G	C8-N9-C1'	-5.32	120.09	127.00
1	2	293	C	C6-N1-C2	-5.31	118.18	120.30
30	c	37	ASP	CB-CG-OD1	5.30	123.07	118.30
1	2	1534	C	N1-C2-O2	5.30	122.08	118.90
1	2	31	U	N3-C2-O2	-5.29	118.50	122.20
1	2	1283	C	N3-C2-O2	-5.29	118.20	121.90
1	2	1283	C	C6-N1-C1'	-5.29	114.46	120.80
1	2	493	A	C2-N3-C4	-5.28	107.96	110.60
1	2	1534	C	C2-N1-C1'	5.28	124.61	118.80
1	2	1864	U	C6-N1-C1'	-5.27	113.82	121.20
11	J	100	LEU	CA-CB-CG	5.25	127.39	115.30
1	2	192	C	C2-N1-C1'	5.25	124.58	118.80
1	2	1130	G	O4'-C1'-N9	5.25	112.40	108.20
1	2	501	C	C6-N1-C2	-5.25	118.20	120.30
1	2	72	C	C6-N1-C1'	-5.24	114.51	120.80
1	2	21	U	N3-C2-O2	-5.24	118.54	122.20
1	2	1696	C	C2-N1-C1'	5.23	124.55	118.80
1	2	1552	G	C4-C5-N7	5.23	112.89	110.80
1	2	381	C	P-O3'-C3'	5.19	125.93	119.70
1	2	1591	C	N3-C2-O2	-5.19	118.27	121.90
1	2	1218	C	C5-C6-N1	5.19	123.59	121.00
1	2	1060	A	OP2-P-O3'	5.17	116.58	105.20
35	j	23	ASP	CB-CG-OD2	5.17	122.95	118.30
1	2	409	C	C6-N1-C2	-5.14	118.24	120.30
1	2	685	A	N7-C8-N9	5.14	116.37	113.80
1	2	1066	U	O5'-P-OP1	-5.13	101.08	105.70
1	2	72	C	C5-C6-N1	5.13	123.57	121.00
1	2	1161	U	N3-C2-O2	-5.13	118.61	122.20
1	2	1649	U	N3-C2-O2	-5.12	118.61	122.20
1	2	615	C	C6-N1-C2	-5.11	118.26	120.30
1	2	687	C	N3-C2-O2	-5.10	118.33	121.90
1	2	1836	G	O5'-P-OP1	-5.09	101.11	105.70
1	2	140	U	N3-C2-O2	-5.09	118.64	122.20
1	2	31	U	N1-C2-O2	5.06	126.34	122.80
1	2	616	A	N1-C6-N6	-5.05	115.57	118.60
1	2	953	C	C6-N1-C2	-5.04	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	796	G	N3-C4-N9	5.00	129.00	126.00
1	2	1590	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	O	137	SER	Peptide
16	O	138	ASP	Peptide
20	Q	15	ARG	Peptide
20	Q	42	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	214/295 (72%)	207 (97%)	6 (3%)	1 (0%)	29	54
3	B	209/264 (79%)	207 (99%)	2 (1%)	0	100	100
4	C	214/293 (73%)	207 (97%)	7 (3%)	0	100	100
5	h	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
6	E	253/263 (96%)	245 (97%)	8 (3%)	0	100	100
7	D	222/243 (91%)	219 (99%)	3 (1%)	0	100	100
8	G	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
9	H	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
10	I	195/208 (94%)	187 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	172/194 (89%)	165 (96%)	7 (4%)	0	100	100
12	F	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
13	L	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
14	K	93/165 (56%)	88 (95%)	5 (5%)	0	100	100
15	N	147/151 (97%)	147 (100%)	0	0	100	100
16	O	124/151 (82%)	120 (97%)	4 (3%)	0	100	100
17	M	102/132 (77%)	98 (96%)	4 (4%)	0	100	100
18	P	130/145 (90%)	122 (94%)	8 (6%)	0	100	100
19	R	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
20	Q	138/146 (94%)	129 (94%)	9 (6%)	0	100	100
21	S	139/152 (91%)	132 (95%)	7 (5%)	0	100	100
22	T	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
23	V	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
24	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
25	X	137/143 (96%)	132 (96%)	4 (3%)	1 (1%)	22	46
26	Y	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
27	U	96/119 (81%)	91 (95%)	5 (5%)	0	100	100
28	Z	80/125 (64%)	75 (94%)	5 (6%)	0	100	100
29	b	73/84 (87%)	68 (93%)	5 (7%)	0	100	100
30	c	59/69 (86%)	57 (97%)	2 (3%)	0	100	100
31	d	52/56 (93%)	48 (92%)	4 (8%)	0	100	100
32	e	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
33	f	53/156 (34%)	49 (92%)	4 (8%)	0	100	100
34	g	287/317 (90%)	266 (93%)	21 (7%)	0	100	100
35	j	112/165 (68%)	108 (96%)	4 (4%)	0	100	100
36	z	343/568 (60%)	319 (93%)	24 (7%)	0	100	100
All	All	5088/6209 (82%)	4877 (96%)	209 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	6	ASP
25	X	86	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/243 (74%)	179 (99%)	1 (1%)	86	95
3	B	192/231 (83%)	191 (100%)	1 (0%)	88	96
4	C	182/225 (81%)	181 (100%)	1 (0%)	88	96
5	h	86/98 (88%)	85 (99%)	1 (1%)	71	88
6	E	220/225 (98%)	220 (100%)	0	100	100
7	D	188/202 (93%)	186 (99%)	2 (1%)	73	90
8	G	194/218 (89%)	192 (99%)	2 (1%)	76	91
9	H	160/174 (92%)	159 (99%)	1 (1%)	86	95
10	I	174/180 (97%)	171 (98%)	3 (2%)	60	84
11	J	156/168 (93%)	156 (100%)	0	100	100
12	F	156/170 (92%)	154 (99%)	2 (1%)	69	87
13	L	126/142 (89%)	124 (98%)	2 (2%)	62	85
14	K	86/136 (63%)	85 (99%)	1 (1%)	71	88
15	N	130/131 (99%)	129 (99%)	1 (1%)	81	93
16	O	99/119 (83%)	98 (99%)	1 (1%)	76	91
17	M	91/108 (84%)	90 (99%)	1 (1%)	73	90
18	P	117/130 (90%)	117 (100%)	0	100	100
19	R	118/122 (97%)	116 (98%)	2 (2%)	60	84
20	Q	116/121 (96%)	116 (100%)	0	100	100
21	S	122/132 (92%)	120 (98%)	2 (2%)	62	85
22	T	111/115 (96%)	111 (100%)	0	100	100
23	V	67/67 (100%)	67 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	110 (99%)	1 (1%)	78	92
26	Y	103/115 (90%)	103 (100%)	0	100	100
27	U	90/107 (84%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Z	67/103 (65%)	67 (100%)	0	100	100
29	b	70/76 (92%)	70 (100%)	0	100	100
30	c	54/62 (87%)	53 (98%)	1 (2%)	57	82
31	d	47/49 (96%)	47 (100%)	0	100	100
32	e	40/48 (83%)	40 (100%)	0	100	100
33	f	51/140 (36%)	51 (100%)	0	100	100
34	g	255/275 (93%)	253 (99%)	2 (1%)	81	93
35	j	103/150 (69%)	103 (100%)	0	100	100
36	z	299/512 (58%)	298 (100%)	1 (0%)	92	98
All	All	4473/5322 (84%)	4444 (99%)	29 (1%)	86	95

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	124	VAL
3	B	48	LEU
4	C	248	TYR
5	h	84	VAL
7	D	76	ARG
7	D	143	ARG
8	G	13	GLN
8	G	98	ARG
9	H	98	ARG
10	I	5	ARG
10	I	148	LYS
10	I	149	TYR
12	F	122	ARG
12	F	201	LYS
13	L	48	LYS
13	L	69	ARG
14	K	95	ARG
15	N	99	ARG
16	O	98	ARG
17	M	33	ARG
19	R	98	VAL
19	R	103	LYS
21	S	83	PHE
21	S	131	VAL
25	X	105	PHE

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Mol	Chain	Res	Type
30	c	46	VAL
34	g	5	MET
34	g	291	TRP
36	z	346	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	84	GLN
2	A	132	GLN
3	B	101	HIS
3	B	186	ASN
4	C	113	GLN
6	E	8	HIS
6	E	50	ASN
6	E	161	GLN
6	E	216	ASN
7	D	101	GLN
8	G	56	ASN
8	G	155	GLN
9	H	73	GLN
9	H	91	HIS
9	H	165	ASN
9	H	193	GLN
10	I	84	ASN
10	I	116	HIS
10	I	165	GLN
10	I	167	GLN
11	J	113	GLN
11	J	132	GLN
12	F	79	HIS
12	F	83	ASN
12	F	95	HIS
13	L	108	ASN
14	K	32	HIS
14	K	50	GLN
15	N	105	ASN
16	O	38	ASN
17	M	15	ASN
17	M	46	GLN
18	P	41	GLN
18	P	53	GLN

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Mol	Chain	Res	Type
18	P	79	HIS
19	R	74	GLN
19	R	93	GLN
20	Q	35	ASN
20	Q	80	GLN
21	S	120	HIS
22	T	91	HIS
23	V	29	HIS
24	W	15	ASN
24	W	16	ASN
24	W	113	HIS
25	X	73	GLN
26	Y	22	GLN
28	Z	103	HIS
29	b	26	GLN
31	d	45	GLN
32	e	15	GLN
33	f	135	HIS
34	g	64	HIS
34	g	117	ASN
34	g	222	ASN
34	g	237	ASN
35	j	18	HIS
36	z	133	ASN
36	z	306	GLN
36	z	316	GLN
36	z	322	HIS
36	z	363	ASN
36	z	365	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1633/1869 (87%)	361 (22%)	14 (0%)

All (361) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	17	C
1	2	33	G
1	2	41	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	44	U
1	2	46	A
1	2	49	C
1	2	56	G
1	2	58	C
1	2	59	U
1	2	64	A
1	2	67	C
1	2	68	A
1	2	72	C
1	2	99	A2M
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	127	C
1	2	129	C
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	155	G
1	2	159	A2M
1	2	160	U
1	2	161	U
1	2	168	C
1	2	171	A
1	2	172	OMU
1	2	177	G
1	2	178	C
1	2	182	C
1	2	184	G
1	2	192	C
1	2	195	C
1	2	198	U
1	2	199	C
1	2	201	C
1	2	202	G
1	2	203	G
1	2	204	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	205	G
1	2	214	U
1	2	291	G
1	2	292	A
1	2	302	A
1	2	305	U
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	320	G
1	2	331	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	351	G
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	381	C
1	2	382	C
1	2	385	G
1	2	386	C
1	2	388	U
1	2	407	G
1	2	408	A
1	2	409	C
1	2	428	OMU
1	2	436	OMG
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	455	A
1	2	465	A
1	2	467	G
1	2	470	G
1	2	471	G
1	2	472	C
1	2	474	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	482	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	508	A
1	2	509	OMG
1	2	512	A2M
1	2	516	A
1	2	525	A
1	2	529	A
1	2	539	C
1	2	540	U
1	2	541	U
1	2	542	U
1	2	544	G
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	561	A
1	2	563	G
1	2	568	C
1	2	574	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	623	G
1	2	626	G
1	2	629	A
1	2	632	C
1	2	639	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	640	A
1	2	643	A
1	2	644	OMG
1	2	655	A
1	2	663	C
1	2	664	A
1	2	666	U
1	2	668	A2M
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	684	G
1	2	687	C
1	2	749	U
1	2	750	C
1	2	792	C
1	2	793	G
1	2	795	A
1	2	797	C
1	2	798	G
1	2	799	U
1	2	810	A
1	2	811	A
1	2	821	G
1	2	822	PSU
1	2	823	U
1	2	824	C
1	2	830	A
1	2	831	G
1	2	847	A
1	2	862	A
1	2	869	A
1	2	870	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	879	C
1	2	880	G
1	2	884	C
1	2	901	G
1	2	902	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	913	A
1	2	914	U
1	2	916	A
1	2	917	U
1	2	919	A
1	2	920	A
1	2	921	G
1	2	922	A
1	2	933	G
1	2	943	U
1	2	970	G
1	2	971	G
1	2	972	A
1	2	982	G
1	2	983	A
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1031	A2M
1	2	1034	A
1	2	1036	A
1	2	1045	PSU
1	2	1048	G
1	2	1049	A
1	2	1055	A
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1066	U
1	2	1067	C
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1096	G
1	2	1100	A
1	2	1109	C
1	2	1120	U
1	2	1121	G
1	2	1123	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1126	G
1	2	1133	A
1	2	1144	A
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1168	G
1	2	1171	G
1	2	1188	A
1	2	1195	A
1	2	1207	G
1	2	1215	C
1	2	1221	G
1	2	1242	U
1	2	1243	U
1	2	1249	C
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1271	C
1	2	1274	G
1	2	1275	G
1	2	1286	G
1	2	1300	U
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1306	U
1	2	1308	U
1	2	1313	A
1	2	1315	U
1	2	1341	C
1	2	1342	U
1	2	1343	U
1	2	1348	G
1	2	1371	U
1	2	1372	U
1	2	1378	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1402	A
1	2	1405	A
1	2	1418	C
1	2	1429	G
1	2	1430	C
1	2	1440	C
1	2	1441	U
1	2	1447	G
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1484	A
1	2	1487	A
1	2	1488	C
1	2	1489	A
1	2	1490	OMG
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1508	A
1	2	1509	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1544	C
1	2	1553	C
1	2	1558	C
1	2	1559	C
1	2	1560	U
1	2	1569	A
1	2	1570	G
1	2	1573	G
1	2	1576	G
1	2	1580	A
1	2	1585	U
1	2	1588	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1594	A
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1639	7MG
1	2	1648	G
1	2	1654	G
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1679	A
1	2	1680	G
1	2	1695	A
1	2	1706	G
1	2	1707	U
1	2	1709	G
1	2	1712	A
1	2	1715	A
1	2	1719	A
1	2	1721	U
1	2	1722	G
1	2	1724	A
1	2	1725	U
1	2	1726	G
1	2	1744	G
1	2	1755	C
1	2	1757	G
1	2	1759	G
1	2	1761	U
1	2	1774	C
1	2	1775	U
1	2	1780	G
1	2	1781	A
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1809	A

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Mol	Chain	Res	Type
1	2	1813	A
1	2	1814	G
1	2	1815	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1834	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1848	U
1	2	1849	A
1	2	1852	C
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	291	G
1	2	381	C
1	2	435	A
1	2	683	OMG
1	2	791	C
1	2	809	A
1	2	912	C
1	2	1060	A
1	2	1065	G
1	2	1119	A
1	2	1165	G
1	2	1440	C
1	2	1605	G
1	2	1814	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	2	34	1	18,21,22	1.01	1 (5%)	22,30,33	1.97	4 (18%)
1	A2M	2	159	1	18,25,26	4.13	5 (27%)	18,36,39	1.32	2 (11%)
1	PSU	2	1174	38,1	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	2	1045	1	18,21,22	1.06	1 (5%)	22,30,33	1.62	4 (18%)
1	A2M	2	1031	1	18,25,26	4.15	7 (38%)	18,36,39	1.40	2 (11%)
1	PSU	2	1004	1	18,21,22	1.08	1 (5%)	22,30,33	1.90	4 (18%)
1	OMG	2	509	38,1	18,26,27	2.73	7 (38%)	19,38,41	1.46	4 (21%)
1	4AC	2	1842	38,1	21,24,25	1.92	6 (28%)	29,34,37	1.61	5 (17%)
1	PSU	2	1367	1	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
1	PSU	2	1692	1	18,21,22	1.19	1 (5%)	22,30,33	1.98	5 (22%)
1	PSU	2	814	1	18,21,22	0.95	1 (5%)	22,30,33	1.73	3 (13%)
1	A2M	2	166	1	18,25,26	4.17	5 (27%)	18,36,39	1.38	2 (11%)
1	4AC	2	1337	1	21,24,25	1.90	6 (28%)	29,34,37	1.12	1 (3%)
1	OMG	2	1490	38,1	18,26,27	2.74	7 (38%)	19,38,41	1.23	3 (15%)
1	OMU	2	1326	38,1	19,22,23	2.90	7 (36%)	26,31,34	1.90	4 (15%)
1	PSU	2	1643	38,1	18,21,22	1.04	1 (5%)	22,30,33	1.62	4 (18%)
1	OMU	2	121	1	19,22,23	3.02	7 (36%)	26,31,34	1.76	5 (19%)
1	MA6	2	1851	1	18,26,27	1.19	2 (11%)	19,38,41	1.33	2 (10%)
1	OMU	2	116	1	19,22,23	3.00	8 (42%)	26,31,34	1.76	7 (26%)
1	PSU	2	1625	1	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	2	966	1	18,21,22	0.94	1 (5%)	22,30,33	1.65	3 (13%)
1	PSU	2	1244	1	18,21,22	1.06	1 (5%)	22,30,33	1.91	5 (22%)
1	PSU	2	36	1	18,21,22	1.09	2 (11%)	22,30,33	1.80	3 (13%)
1	OMG	2	601	1	18,26,27	2.74	7 (38%)	19,38,41	1.45	4 (21%)
1	PSU	2	1445	1	18,21,22	1.11	1 (5%)	22,30,33	1.98	5 (22%)
1	OMC	2	174	1	19,22,23	2.31	7 (36%)	26,31,34	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	2	1272	1	19,22,23	2.28	6 (31%)	26,31,34	0.91	1 (3%)
1	OMG	2	644	1	18,26,27	2.69	6 (33%)	19,38,41	1.34	3 (15%)
1	PSU	2	1232	1	18,21,22	1.09	1 (5%)	22,30,33	1.76	3 (13%)
1	PSU	2	93	1	18,21,22	1.21	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	2	1238	1	18,21,22	1.07	1 (5%)	22,30,33	1.77	3 (13%)
1	PSU	2	1177	1	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
1	B8N	2	1248	1	24,29,30	2.30	10 (41%)	29,42,45	1.64	5 (17%)
1	OMU	2	428	1	19,22,23	2.93	7 (36%)	26,31,34	2.06	8 (30%)
1	MA6	2	1850	1	18,26,27	0.93	1 (5%)	19,38,41	1.44	2 (10%)
1	A2M	2	512	1	18,25,26	4.17	6 (33%)	18,36,39	1.52	3 (16%)
1	A2M	2	484	1	18,25,26	4.10	7 (38%)	18,36,39	1.50	2 (11%)
1	PSU	2	651	1	18,21,22	1.15	2 (11%)	22,30,33	1.68	3 (13%)
1	OMG	2	1328	1	18,26,27	2.75	6 (33%)	19,38,41	1.39	4 (21%)
1	PSU	2	681	1	18,21,22	1.13	1 (5%)	22,30,33	1.83	4 (18%)
1	PSU	2	815	1	18,21,22	0.95	1 (5%)	22,30,33	1.80	3 (13%)
1	OMG	2	683	1	18,26,27	2.72	6 (33%)	19,38,41	1.78	6 (31%)
1	A2M	2	668	38,1	18,25,26	4.02	7 (38%)	18,36,39	1.52	2 (11%)
1	OMU	2	1288	1	19,22,23	2.89	7 (36%)	26,31,34	1.76	5 (19%)
1	PSU	2	105	1	18,21,22	1.11	1 (5%)	22,30,33	1.69	4 (18%)
1	PSU	2	119	1	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
1	OMG	2	867	1	18,26,27	2.69	6 (33%)	19,38,41	1.42	4 (21%)
1	A2M	2	468	1	18,25,26	4.19	5 (27%)	18,36,39	1.46	2 (11%)
1	A2M	2	1383	1	18,25,26	4.19	5 (27%)	18,36,39	1.45	2 (11%)
1	OMU	2	354	1	19,22,23	2.94	8 (42%)	26,31,34	1.92	5 (19%)
1	PSU	2	218	1	18,21,22	0.94	1 (5%)	22,30,33	1.75	4 (18%)
1	OMU	2	1442	38,1	19,22,23	3.00	7 (36%)	26,31,34	1.73	6 (23%)
1	OMC	2	517	1	19,22,23	2.35	7 (36%)	26,31,34	0.75	1 (3%)
1	PSU	2	1046	1	18,21,22	1.02	1 (5%)	22,30,33	1.77	3 (13%)
1	OMU	2	172	1	19,22,23	2.97	7 (36%)	26,31,34	1.78	5 (19%)
1	PSU	2	649	1	18,21,22	1.25	1 (5%)	22,30,33	1.79	4 (18%)
1	OMG	2	436	1	18,26,27	2.74	6 (33%)	19,38,41	1.38	4 (21%)
1	OMC	2	1391	1	19,22,23	2.28	6 (31%)	26,31,34	0.83	1 (3%)
1	A2M	2	1678	1	18,25,26	4.08	6 (33%)	18,36,39	1.48	2 (11%)
1	OMC	2	1703	1	19,22,23	2.33	7 (36%)	26,31,34	0.87	1 (3%)
1	PSU	2	1081	1	18,21,22	1.10	2 (11%)	22,30,33	1.86	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	2	1347	1	18,21,22	1.04	1 (5%)	22,30,33	1.76	3 (13%)
1	7MG	2	1639	1	22,26,27	5.49	6 (27%)	29,39,42	2.41	9 (31%)
1	OMC	2	462	1	19,22,23	2.29	5 (26%)	26,31,34	0.82	1 (3%)
1	PSU	2	109	1	18,21,22	1.09	1 (5%)	22,30,33	1.89	4 (18%)
1	PSU	2	406	1	18,21,22	1.01	1 (5%)	22,30,33	2.00	3 (13%)
1	PSU	2	572	1	18,21,22	1.04	3 (16%)	22,30,33	1.77	4 (18%)
1	PSU	2	686	1	18,21,22	1.00	1 (5%)	22,30,33	1.76	4 (18%)
1	A2M	2	27	38,1	18,25,26	4.20	6 (33%)	18,36,39	1.44	2 (11%)
1	6MZ	2	1832	38,1	18,25,26	2.26	1 (5%)	16,36,39	1.82	3 (18%)
1	A2M	2	576	1	18,25,26	4.05	5 (27%)	18,36,39	1.32	2 (11%)
1	PSU	2	822	1	18,21,22	1.02	1 (5%)	22,30,33	1.90	5 (22%)
1	PSU	2	1056	1	18,21,22	1.05	1 (5%)	22,30,33	1.73	3 (13%)
1	A2M	2	99	38,1	18,25,26	4.23	6 (33%)	18,36,39	1.21	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	34	1	-	0/7/25/26	0/2/2/2
1	A2M	2	159	1	-	0/5/27/28	0/3/3/3
1	PSU	2	1174	38,1	-	0/7/25/26	0/2/2/2
1	PSU	2	1045	1	-	0/7/25/26	0/2/2/2
1	A2M	2	1031	1	-	1/5/27/28	0/3/3/3
1	PSU	2	1004	1	-	0/7/25/26	0/2/2/2
1	OMG	2	509	38,1	-	3/5/27/28	0/3/3/3
1	4AC	2	1842	38,1	-	2/11/29/30	0/2/2/2
1	PSU	2	1367	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1692	1	-	2/7/25/26	0/2/2/2
1	PSU	2	814	1	-	0/7/25/26	0/2/2/2
1	A2M	2	166	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1337	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1490	38,1	-	2/5/27/28	0/3/3/3
1	OMU	2	1326	38,1	-	0/9/27/28	0/2/2/2
1	PSU	2	1643	38,1	-	0/7/25/26	0/2/2/2
1	OMU	2	121	1	-	0/9/27/28	0/2/2/2
1	MA6	2	1851	1	-	1/7/29/30	0/3/3/3
1	OMU	2	116	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	1625	1	-	0/7/25/26	0/2/2/2
1	PSU	2	966	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	2	36	1	-	0/7/25/26	0/2/2/2
1	OMG	2	601	1	-	0/5/27/28	0/3/3/3
1	PSU	2	1445	1	-	0/7/25/26	0/2/2/2
1	OMC	2	174	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1272	1	-	1/9/27/28	0/2/2/2
1	OMG	2	644	1	-	3/5/27/28	0/3/3/3
1	PSU	2	1232	1	-	0/7/25/26	0/2/2/2
1	PSU	2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1177	1	-	0/7/25/26	0/2/2/2
1	B8N	2	1248	1	-	7/16/34/35	0/2/2/2
1	OMU	2	428	1	-	5/9/27/28	0/2/2/2
1	MA6	2	1850	1	-	2/7/29/30	0/3/3/3
1	A2M	2	512	1	-	0/5/27/28	0/3/3/3
1	A2M	2	484	1	-	0/5/27/28	0/3/3/3
1	PSU	2	651	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1328	1	-	0/5/27/28	0/3/3/3
1	PSU	2	681	1	-	0/7/25/26	0/2/2/2
1	PSU	2	815	1	-	0/7/25/26	0/2/2/2
1	OMG	2	683	1	-	2/5/27/28	0/3/3/3
1	A2M	2	668	38,1	-	2/5/27/28	0/3/3/3
1	OMU	2	1288	1	-	0/9/27/28	0/2/2/2
1	PSU	2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	2	119	1	-	2/7/25/26	0/2/2/2
1	OMG	2	867	1	-	3/5/27/28	0/3/3/3
1	A2M	2	468	1	-	1/5/27/28	0/3/3/3
1	A2M	2	1383	1	-	0/5/27/28	0/3/3/3
1	OMU	2	354	1	-	0/9/27/28	0/2/2/2
1	PSU	2	218	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1442	38,1	-	0/9/27/28	0/2/2/2
1	OMC	2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1046	1	-	0/7/25/26	0/2/2/2
1	OMU	2	172	1	-	2/9/27/28	0/2/2/2
1	PSU	2	649	1	-	2/7/25/26	0/2/2/2
1	OMG	2	436	1	-	0/5/27/28	0/3/3/3
1	OMC	2	1391	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1678	1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2	1703	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1081	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1347	1	-	0/7/25/26	0/2/2/2
1	7MG	2	1639	1	-	0/7/37/38	0/3/3/3
1	OMC	2	462	1	-	1/9/27/28	0/2/2/2
1	PSU	2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	2	572	1	-	0/7/25/26	0/2/2/2
1	PSU	2	686	1	-	0/7/25/26	0/2/2/2
1	A2M	2	27	38,1	-	0/5/27/28	0/3/3/3
1	6MZ	2	1832	38,1	-	0/5/27/28	0/3/3/3
1	A2M	2	576	1	-	0/5/27/28	0/3/3/3
1	PSU	2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1056	1	-	0/7/25/26	0/2/2/2
1	A2M	2	99	38,1	-	2/5/27/28	0/3/3/3

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	7MG	C8-N9	-22.93	1.33	1.46
1	2	468	A2M	O4'-C1'	15.34	1.62	1.41
1	2	1383	A2M	O4'-C1'	15.32	1.62	1.41
1	2	99	A2M	O4'-C1'	15.30	1.62	1.41
1	2	166	A2M	O4'-C1'	15.16	1.62	1.41
1	2	27	A2M	O4'-C1'	15.09	1.62	1.41
1	2	159	A2M	O4'-C1'	14.99	1.62	1.41
1	2	512	A2M	O4'-C1'	14.99	1.62	1.41
1	2	1031	A2M	O4'-C1'	14.95	1.61	1.41
1	2	1678	A2M	O4'-C1'	14.58	1.61	1.41
1	2	484	A2M	O4'-C1'	14.53	1.61	1.41
1	2	576	A2M	O4'-C1'	14.51	1.61	1.41
1	2	668	A2M	O4'-C1'	13.74	1.60	1.41
1	2	1639	7MG	O6-C6	9.04	1.40	1.23
1	2	1832	6MZ	C6-N6	9.03	1.49	1.35
1	2	1288	OMU	O4-C4	8.59	1.41	1.24
1	2	1442	OMU	O4-C4	8.42	1.40	1.24
1	2	172	OMU	O4-C4	8.34	1.40	1.24
1	2	116	OMU	O4-C4	8.26	1.40	1.24
1	2	1326	OMU	O4-C4	8.23	1.40	1.24
1	2	121	OMU	O4-C4	8.18	1.40	1.24
1	2	428	OMU	O4-C4	8.11	1.40	1.24
1	2	867	OMG	O6-C6	8.10	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	436	OMG	O6-C6	8.08	1.39	1.23
1	2	683	OMG	O6-C6	8.02	1.39	1.23
1	2	354	OMU	O4-C4	8.00	1.40	1.24
1	2	644	OMG	O6-C6	7.91	1.39	1.23
1	2	1328	OMG	O6-C6	7.88	1.39	1.23
1	2	1490	OMG	O6-C6	7.65	1.38	1.23
1	2	509	OMG	O6-C6	7.55	1.38	1.23
1	2	601	OMG	O6-C6	7.53	1.38	1.23
1	2	668	A2M	O4'-C4'	-7.48	1.28	1.45
1	2	484	A2M	O4'-C4'	-6.89	1.29	1.45
1	2	1678	A2M	O4'-C4'	-6.67	1.30	1.45
1	2	576	A2M	O4'-C4'	-6.50	1.30	1.45
1	2	27	A2M	O4'-C4'	-6.48	1.30	1.45
1	2	1031	A2M	O4'-C4'	-6.47	1.30	1.45
1	2	99	A2M	O4'-C4'	-6.43	1.30	1.45
1	2	166	A2M	O4'-C4'	-6.43	1.30	1.45
1	2	159	A2M	O4'-C4'	-6.37	1.30	1.45
1	2	512	A2M	O4'-C4'	-6.34	1.30	1.45
1	2	468	A2M	O4'-C4'	-6.27	1.31	1.45
1	2	1383	A2M	O4'-C4'	-6.23	1.31	1.45
1	2	462	OMC	C4-N4	6.15	1.48	1.33
1	2	1272	OMC	C4-N4	6.08	1.48	1.33
1	2	354	OMU	C4-N3	-6.02	1.27	1.38
1	2	428	OMU	C4-N3	-5.92	1.28	1.38
1	2	121	OMU	C4-N3	-5.91	1.28	1.38
1	2	1391	OMC	C4-N4	5.91	1.47	1.33
1	2	174	OMC	C4-N4	5.88	1.47	1.33
1	2	1248	B8N	O4-C4	5.87	1.35	1.23
1	2	172	OMU	C4-N3	-5.85	1.28	1.38
1	2	116	OMU	C4-N3	-5.83	1.28	1.38
1	2	1703	OMC	C4-N4	5.81	1.47	1.33
1	2	517	OMC	C4-N4	5.72	1.47	1.33
1	2	1442	OMU	C4-N3	-5.66	1.28	1.38
1	2	1703	OMC	O2-C2	-5.64	1.13	1.23
1	2	517	OMC	O2-C2	-5.61	1.13	1.23
1	2	1326	OMU	C4-N3	-5.45	1.28	1.38
1	2	1288	OMU	C4-N3	-5.35	1.29	1.38
1	2	1272	OMC	O2-C2	-5.25	1.14	1.23
1	2	1391	OMC	O2-C2	-5.18	1.14	1.23
1	2	174	OMC	O2-C2	-5.11	1.14	1.23
1	2	462	OMC	O2-C2	-5.05	1.14	1.23
1	2	121	OMU	C2-N1	-5.04	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1248	B8N	C4-N3	-4.97	1.31	1.40
1	2	1842	4AC	C4-N4	4.83	1.46	1.39
1	2	1337	4AC	C4-N4	4.81	1.46	1.39
1	2	116	OMU	C2-N1	-4.74	1.30	1.38
1	2	1639	7MG	C2-N2	4.71	1.45	1.34
1	2	601	OMG	C6-N1	-4.69	1.30	1.37
1	2	1442	OMU	C2-N1	-4.63	1.31	1.38
1	2	867	OMG	C2-N2	4.57	1.45	1.34
1	2	509	OMG	C6-N1	-4.49	1.31	1.37
1	2	1490	OMG	C6-N1	-4.48	1.31	1.37
1	2	1328	OMG	C6-N1	-4.47	1.31	1.37
1	2	172	OMU	C2-N1	-4.46	1.31	1.38
1	2	1248	B8N	C2-N3	-4.40	1.31	1.38
1	2	354	OMU	C2-N3	-4.38	1.30	1.38
1	2	172	OMU	C2-N3	-4.31	1.30	1.38
1	2	1326	OMU	C2-N1	-4.31	1.31	1.38
1	2	428	OMU	C2-N3	-4.27	1.30	1.38
1	2	121	OMU	C2-N3	-4.26	1.30	1.38
1	2	436	OMG	C2-N2	4.25	1.44	1.34
1	2	1442	OMU	C2-N3	-4.21	1.30	1.38
1	2	683	OMG	C2-N2	4.18	1.44	1.34
1	2	116	OMU	C2-N3	-4.18	1.30	1.38
1	2	683	OMG	C6-N1	-4.17	1.31	1.37
1	2	1328	OMG	C2-N2	4.16	1.44	1.34
1	2	1326	OMU	C2-N3	-4.14	1.30	1.38
1	2	644	OMG	C6-N1	-4.14	1.31	1.37
1	2	644	OMG	C2-N2	4.12	1.44	1.34
1	2	1288	OMU	C2-N3	-4.11	1.30	1.38
1	2	428	OMU	C2-N1	-4.08	1.31	1.38
1	2	1288	OMU	C2-N1	-4.06	1.31	1.38
1	2	509	OMG	C5-C6	-4.05	1.39	1.47
1	2	601	OMG	C2-N2	4.03	1.43	1.34
1	2	354	OMU	C2-N1	-4.03	1.32	1.38
1	2	436	OMG	C6-N1	-3.96	1.32	1.37
1	2	601	OMG	C5-C6	-3.96	1.39	1.47
1	2	1490	OMG	C2-N2	3.90	1.43	1.34
1	2	509	OMG	C2-N2	3.90	1.43	1.34
1	2	867	OMG	C6-N1	-3.87	1.32	1.37
1	2	1490	OMG	C5-C6	-3.86	1.39	1.47
1	2	436	OMG	C5-C6	-3.83	1.39	1.47
1	2	1337	4AC	O2-C2	-3.77	1.16	1.23
1	2	93	PSU	C6-C5	3.73	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1328	OMG	C5-C6	-3.71	1.39	1.47
1	2	1639	7MG	C6-N1	-3.70	1.32	1.38
1	2	1842	4AC	C2-N1	-3.59	1.32	1.40
1	2	644	OMG	C5-C6	-3.54	1.40	1.47
1	2	867	OMG	C5-C6	-3.54	1.40	1.47
1	2	1842	4AC	O2-C2	-3.52	1.17	1.23
1	2	683	OMG	C5-C6	-3.45	1.40	1.47
1	2	517	OMC	C2-N1	-3.44	1.32	1.40
1	2	174	OMC	C2-N1	-3.41	1.32	1.40
1	2	105	PSU	C6-C5	3.33	1.39	1.35
1	2	1842	4AC	C7-N4	3.27	1.43	1.37
1	2	1326	OMU	C6-N1	-3.24	1.30	1.38
1	2	1625	PSU	C6-C5	3.23	1.39	1.35
1	2	1337	4AC	C2-N1	-3.23	1.33	1.40
1	2	27	A2M	O3'-C3'	-3.23	1.35	1.43
1	2	1391	OMC	C2-N1	-3.20	1.33	1.40
1	2	649	PSU	C6-C5	3.19	1.39	1.35
1	2	468	A2M	O3'-C3'	-3.15	1.35	1.43
1	2	1004	PSU	C6-C5	3.14	1.39	1.35
1	2	1445	PSU	C6-C5	3.13	1.39	1.35
1	2	354	OMU	C6-N1	-3.12	1.30	1.38
1	2	1045	PSU	C6-C5	3.10	1.38	1.35
1	2	121	OMU	C6-N1	-3.10	1.30	1.38
1	2	116	OMU	C6-N1	-3.09	1.30	1.38
1	2	1639	7MG	C4-N9	-3.08	1.34	1.37
1	2	576	A2M	O3'-C3'	-3.06	1.35	1.43
1	2	512	A2M	O3'-C3'	-3.04	1.35	1.43
1	2	462	OMC	C2-N1	-3.04	1.33	1.40
1	2	172	OMU	C6-N1	-3.03	1.30	1.38
1	2	1272	OMC	C2-N1	-3.02	1.33	1.40
1	2	119	PSU	C6-C5	3.02	1.38	1.35
1	2	159	A2M	C6-N6	3.00	1.45	1.34
1	2	1442	OMU	C6-N1	-3.00	1.30	1.38
1	2	159	A2M	O3'-C3'	-3.00	1.35	1.43
1	2	462	OMC	C6-C5	2.99	1.42	1.35
1	2	484	A2M	O3'-C3'	-2.97	1.36	1.43
1	2	1703	OMC	C6-N1	-2.96	1.30	1.38
1	2	166	A2M	C6-N6	2.94	1.44	1.34
1	2	1678	A2M	C6-N6	2.94	1.44	1.34
1	2	1851	MA6	C4-N3	-2.93	1.31	1.35
1	2	576	A2M	C6-N6	2.92	1.44	1.34
1	2	668	A2M	O2'-C2'	2.92	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	174	OMC	C6-N1	-2.91	1.30	1.38
1	2	1337	4AC	C7-N4	2.90	1.42	1.37
1	2	1238	PSU	C6-C5	2.89	1.38	1.35
1	2	1174	PSU	C6-C5	2.88	1.38	1.35
1	2	1703	OMC	C2-N1	-2.88	1.33	1.40
1	2	822	PSU	C6-C5	2.88	1.38	1.35
1	2	166	A2M	O3'-C3'	-2.86	1.36	1.43
1	2	468	A2M	C6-N6	2.86	1.44	1.34
1	2	1490	OMG	C2-N1	-2.86	1.30	1.37
1	2	512	A2M	C6-N6	2.85	1.44	1.34
1	2	1391	OMC	C6-C5	2.85	1.41	1.35
1	2	1232	PSU	C6-C5	2.84	1.38	1.35
1	2	509	OMG	C2-N1	-2.84	1.30	1.37
1	2	462	OMC	C6-N1	-2.84	1.31	1.38
1	2	1383	A2M	C6-N6	2.83	1.44	1.34
1	2	681	PSU	C6-C5	2.83	1.38	1.35
1	2	815	PSU	C6-C5	2.82	1.38	1.35
1	2	1031	A2M	C6-N6	2.82	1.44	1.34
1	2	99	A2M	O3'-C3'	-2.82	1.36	1.43
1	2	484	A2M	O2'-C2'	2.82	1.49	1.42
1	2	484	A2M	C6-N6	2.82	1.44	1.34
1	2	99	A2M	C6-N6	2.79	1.44	1.34
1	2	34	PSU	C6-C5	2.79	1.38	1.35
1	2	1031	A2M	O2'-C2'	2.79	1.49	1.42
1	2	27	A2M	C6-N6	2.79	1.44	1.34
1	2	428	OMU	C6-N1	-2.78	1.31	1.38
1	2	1272	OMC	C6-N1	-2.78	1.31	1.38
1	2	668	A2M	C6-N6	2.78	1.44	1.34
1	2	1678	A2M	O3'-C3'	-2.77	1.36	1.43
1	2	1347	PSU	C6-C5	2.77	1.38	1.35
1	2	116	OMU	O2-C2	-2.76	1.18	1.23
1	2	1692	PSU	C6-C5	2.76	1.38	1.35
1	2	428	OMU	O2-C2	-2.76	1.18	1.23
1	2	1442	OMU	O2-C2	-2.75	1.18	1.23
1	2	572	PSU	C6-C5	2.75	1.38	1.35
1	2	1031	A2M	O3'-C3'	-2.75	1.36	1.43
1	2	99	A2M	O2'-C2'	2.75	1.49	1.42
1	2	1244	PSU	C6-C5	2.75	1.38	1.35
1	2	1383	A2M	O3'-C3'	-2.73	1.36	1.43
1	2	354	OMU	O2-C2	-2.73	1.18	1.23
1	2	172	OMU	O2-C2	-2.72	1.18	1.23
1	2	159	A2M	O2'-C2'	2.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1703	OMC	C6-C5	2.70	1.41	1.35
1	2	121	OMU	O2-C2	-2.69	1.18	1.23
1	2	517	OMC	C6-N1	-2.68	1.31	1.38
1	2	1288	OMU	C6-N1	-2.68	1.31	1.38
1	2	517	OMC	C6-C5	2.68	1.41	1.35
1	2	1328	OMG	C2-N1	-2.68	1.31	1.37
1	2	166	A2M	O2'-C2'	2.67	1.49	1.42
1	2	966	PSU	C6-C5	2.67	1.38	1.35
1	2	644	OMG	C2-N1	-2.66	1.31	1.37
1	2	1056	PSU	C6-C5	2.65	1.38	1.35
1	2	1248	B8N	C6-C5	2.65	1.38	1.34
1	2	27	A2M	O2'-C2'	2.64	1.49	1.42
1	2	1383	A2M	O2'-C2'	2.64	1.49	1.42
1	2	174	OMC	C6-C5	2.63	1.41	1.35
1	2	512	A2M	O2'-C2'	2.63	1.49	1.42
1	2	601	OMG	C5-C4	-2.61	1.36	1.43
1	2	1678	A2M	O2'-C2'	2.60	1.49	1.42
1	2	1272	OMC	C6-C5	2.59	1.41	1.35
1	2	683	OMG	C5-C4	-2.59	1.36	1.43
1	2	686	PSU	C6-C5	2.58	1.38	1.35
1	2	36	PSU	C6-C5	2.58	1.38	1.35
1	2	109	PSU	C6-C5	2.56	1.38	1.35
1	2	1391	OMC	C6-N1	-2.56	1.31	1.38
1	2	406	PSU	C6-C5	2.55	1.38	1.35
1	2	1177	PSU	C6-C5	2.55	1.38	1.35
1	2	576	A2M	O2'-C2'	2.53	1.49	1.42
1	2	651	PSU	C6-C5	2.53	1.38	1.35
1	2	1337	4AC	C2-N3	-2.53	1.31	1.36
1	2	668	A2M	O3'-C3'	-2.52	1.37	1.43
1	2	436	OMG	C2-N1	-2.50	1.31	1.37
1	2	601	OMG	C2-N1	-2.49	1.31	1.37
1	2	1643	PSU	C6-C5	2.49	1.38	1.35
1	2	683	OMG	C2-N1	-2.48	1.31	1.37
1	2	1288	OMU	O2-C2	-2.48	1.18	1.23
1	2	1248	B8N	C1'-C5	2.46	1.55	1.50
1	2	1367	PSU	C6-C5	2.46	1.38	1.35
1	2	218	PSU	C6-C5	2.46	1.38	1.35
1	2	1337	4AC	C6-C5	2.45	1.40	1.35
1	2	517	OMC	C5-C4	-2.45	1.37	1.42
1	2	509	OMG	C8-N7	-2.44	1.30	1.35
1	2	1328	OMG	C5-C4	-2.43	1.36	1.43
1	2	174	OMC	C5-C4	-2.43	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1081	PSU	O4'-C1'	-2.41	1.40	1.43
1	2	436	OMG	C5-C4	-2.39	1.37	1.43
1	2	1851	MA6	C10-N6	2.38	1.51	1.45
1	2	1850	MA6	C10-N6	2.37	1.51	1.45
1	2	1326	OMU	O2'-CM2	-2.36	1.34	1.42
1	2	1490	OMG	C5-C4	-2.35	1.37	1.43
1	2	1442	OMU	O2'-CM2	-2.34	1.34	1.42
1	2	668	A2M	O5'-C5'	-2.34	1.39	1.44
1	2	1490	OMG	C8-N7	-2.33	1.31	1.35
1	2	1326	OMU	O2-C2	-2.32	1.18	1.23
1	2	468	A2M	O2'-C2'	2.30	1.48	1.42
1	2	1081	PSU	C6-C5	2.30	1.38	1.35
1	2	354	OMU	O2'-CM2	-2.29	1.34	1.42
1	2	121	OMU	O2'-CM2	-2.28	1.34	1.42
1	2	1842	4AC	C6-C5	2.28	1.40	1.35
1	2	867	OMG	C2-N1	-2.28	1.32	1.37
1	2	644	OMG	C5-C4	-2.27	1.37	1.43
1	2	428	OMU	O2'-CM2	-2.27	1.34	1.42
1	2	601	OMG	C8-N7	-2.26	1.31	1.35
1	2	512	A2M	O5'-C5'	-2.24	1.39	1.44
1	2	509	OMG	C5-C4	-2.24	1.37	1.43
1	2	1046	PSU	C6-C5	2.24	1.37	1.35
1	2	867	OMG	C5-C4	-2.23	1.37	1.43
1	2	116	OMU	O2'-CM2	-2.21	1.34	1.42
1	2	668	A2M	C8-N7	-2.21	1.30	1.34
1	2	116	OMU	C5-C4	-2.17	1.38	1.43
1	2	172	OMU	O2'-CM2	-2.16	1.34	1.42
1	2	1288	OMU	O2'-CM2	-2.16	1.34	1.42
1	2	1703	OMC	C2-N3	-2.16	1.32	1.36
1	2	1703	OMC	C5-C4	-2.15	1.38	1.42
1	2	1248	B8N	O4'-C1'	-2.14	1.40	1.43
1	2	99	A2M	C8-N7	-2.13	1.30	1.34
1	2	354	OMU	C5-C4	-2.13	1.38	1.43
1	2	174	OMC	C2-N3	-2.13	1.32	1.36
1	2	1639	7MG	C2-N1	-2.13	1.32	1.37
1	2	517	OMC	C2-N3	-2.12	1.32	1.36
1	2	814	PSU	C6-C5	2.11	1.37	1.35
1	2	1842	4AC	C2-N3	-2.11	1.32	1.36
1	2	1272	OMC	C5-C4	-2.11	1.38	1.42
1	2	36	PSU	C4-C5	-2.10	1.38	1.44
1	2	1391	OMC	C5-C4	-2.10	1.38	1.42
1	2	1031	A2M	C8-N7	-2.09	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1031	A2M	O5'-C5'	-2.07	1.39	1.44
1	2	651	PSU	O4'-C1'	-2.06	1.41	1.43
1	2	27	A2M	O5'-C5'	-2.06	1.39	1.44
1	2	484	A2M	O5'-C5'	-2.05	1.39	1.44
1	2	572	PSU	O4'-C1'	-2.05	1.41	1.43
1	2	1678	A2M	O5'-C5'	-2.04	1.39	1.44
1	2	1248	B8N	C32-C31	2.03	1.56	1.52
1	2	1248	B8N	O2-C2	-2.03	1.18	1.22
1	2	572	PSU	C4-C5	-2.03	1.38	1.44
1	2	1248	B8N	C6-N1	-2.02	1.32	1.36
1	2	1248	B8N	C2-N1	-2.02	1.32	1.39
1	2	484	A2M	C8-N7	-2.01	1.31	1.34

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	7MG	C5-C6-N1	5.64	120.93	110.99
1	2	1842	4AC	CM7-C7-N4	5.57	124.92	115.29
1	2	34	PSU	N1-C2-N3	5.45	121.30	115.13
1	2	1692	PSU	C4-N3-C2	-5.38	118.58	126.34
1	2	1639	7MG	N9-C4-N3	5.22	133.28	125.47
1	2	406	PSU	C4-N3-C2	-5.21	118.84	126.34
1	2	1445	PSU	N1-C2-N3	5.20	121.02	115.13
1	2	1004	PSU	N1-C2-N3	5.12	120.93	115.13
1	2	1850	MA6	N3-C2-N1	-5.12	120.67	128.68
1	2	109	PSU	N1-C2-N3	5.10	120.91	115.13
1	2	1639	7MG	C2-N3-C4	5.07	121.34	112.30
1	2	1244	PSU	N1-C2-N3	5.05	120.86	115.13
1	2	406	PSU	N1-C2-N3	5.04	120.83	115.13
1	2	172	OMU	N3-C2-N1	5.02	121.56	114.89
1	2	34	PSU	C4-N3-C2	-5.02	119.11	126.34
1	2	1445	PSU	C4-N3-C2	-5.01	119.11	126.34
1	2	681	PSU	N1-C2-N3	5.01	120.81	115.13
1	2	1177	PSU	N1-C2-N3	5.00	120.79	115.13
1	2	1367	PSU	N1-C2-N3	4.97	120.76	115.13
1	2	1081	PSU	N1-C2-N3	4.96	120.75	115.13
1	2	1692	PSU	N1-C2-N3	4.94	120.73	115.13
1	2	93	PSU	N1-C2-N3	4.92	120.70	115.13
1	2	815	PSU	C4-N3-C2	-4.89	119.29	126.34
1	2	36	PSU	N1-C2-N3	4.89	120.67	115.13
1	2	27	A2M	N3-C2-N1	-4.88	121.05	128.68
1	2	1367	PSU	C4-N3-C2	-4.86	119.34	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	822	PSU	N1-C2-N3	4.84	120.61	115.13
1	2	428	OMU	N3-C2-N1	4.83	121.30	114.89
1	2	512	A2M	N3-C2-N1	-4.83	121.13	128.68
1	2	354	OMU	N3-C2-N1	4.82	121.29	114.89
1	2	1625	PSU	N1-C2-N3	4.81	120.58	115.13
1	2	1056	PSU	C4-N3-C2	-4.75	119.49	126.34
1	2	1174	PSU	N1-C2-N3	4.75	120.51	115.13
1	2	1347	PSU	N1-C2-N3	4.75	120.51	115.13
1	2	1046	PSU	C4-N3-C2	-4.75	119.50	126.34
1	2	572	PSU	C4-N3-C2	-4.72	119.54	126.34
1	2	1232	PSU	C4-N3-C2	-4.71	119.55	126.34
1	2	1238	PSU	C4-N3-C2	-4.70	119.56	126.34
1	2	1639	7MG	C5-C4-N3	-4.69	119.20	128.13
1	2	1177	PSU	C4-N3-C2	-4.68	119.60	126.34
1	2	1639	7MG	N9-C8-N7	4.68	110.07	103.38
1	2	1326	OMU	C4-N3-C2	-4.67	120.41	126.58
1	2	1326	OMU	N3-C2-N1	4.66	121.08	114.89
1	2	681	PSU	C4-N3-C2	-4.65	119.63	126.34
1	2	649	PSU	C4-N3-C2	-4.65	119.64	126.34
1	2	815	PSU	N1-C2-N3	4.64	120.39	115.13
1	2	1442	OMU	N3-C2-N1	4.63	121.04	114.89
1	2	1244	PSU	C4-N3-C2	-4.63	119.67	126.34
1	2	109	PSU	C4-N3-C2	-4.63	119.67	126.34
1	2	686	PSU	N1-C2-N3	4.62	120.37	115.13
1	2	1248	B8N	C4-N3-C2	-4.62	119.62	125.46
1	2	116	OMU	N3-C2-N1	4.62	121.02	114.89
1	2	651	PSU	C4-N3-C2	-4.62	119.69	126.34
1	2	814	PSU	C4-N3-C2	-4.61	119.69	126.34
1	2	966	PSU	C4-N3-C2	-4.59	119.73	126.34
1	2	572	PSU	N1-C2-N3	4.58	120.32	115.13
1	2	822	PSU	C4-N3-C2	-4.57	119.75	126.34
1	2	121	OMU	N3-C2-N1	4.57	120.95	114.89
1	2	218	PSU	C4-N3-C2	-4.55	119.78	126.34
1	2	1056	PSU	N1-C2-N3	4.55	120.29	115.13
1	2	354	OMU	C4-N3-C2	-4.54	120.59	126.58
1	2	1174	PSU	C4-N3-C2	-4.54	119.80	126.34
1	2	1832	6MZ	C2-N1-C6	4.54	120.48	116.59
1	2	1232	PSU	N1-C2-N3	4.54	120.27	115.13
1	2	218	PSU	N1-C2-N3	4.53	120.27	115.13
1	2	166	A2M	N3-C2-N1	-4.52	121.62	128.68
1	2	1031	A2M	N3-C2-N1	-4.51	121.63	128.68
1	2	814	PSU	N1-C2-N3	4.51	120.24	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	105	PSU	N1-C2-N3	4.50	120.23	115.13
1	2	1851	MA6	N3-C2-N1	-4.50	121.65	128.68
1	2	1288	OMU	N3-C2-N1	4.48	120.84	114.89
1	2	1081	PSU	C4-N3-C2	-4.47	119.90	126.34
1	2	1046	PSU	N1-C2-N3	4.46	120.19	115.13
1	2	1347	PSU	C4-N3-C2	-4.44	119.94	126.34
1	2	1625	PSU	C4-N3-C2	-4.44	119.94	126.34
1	2	1383	A2M	N3-C2-N1	-4.43	121.75	128.68
1	2	1678	A2M	N3-C2-N1	-4.43	121.76	128.68
1	2	686	PSU	C4-N3-C2	-4.42	119.98	126.34
1	2	1238	PSU	N1-C2-N3	4.41	120.13	115.13
1	2	1004	PSU	C4-N3-C2	-4.41	119.99	126.34
1	2	428	OMU	C4-N3-C2	-4.38	120.80	126.58
1	2	668	A2M	N3-C2-N1	-4.38	121.84	128.68
1	2	1248	B8N	N3-C2-N1	4.37	122.94	116.76
1	2	93	PSU	C4-N3-C2	-4.36	120.05	126.34
1	2	172	OMU	C4-N3-C2	-4.33	120.87	126.58
1	2	468	A2M	N3-C2-N1	-4.32	121.93	128.68
1	2	1643	PSU	C4-N3-C2	-4.28	120.17	126.34
1	2	651	PSU	N1-C2-N3	4.28	119.98	115.13
1	2	484	A2M	N3-C2-N1	-4.27	122.01	128.68
1	2	576	A2M	N3-C2-N1	-4.26	122.02	128.68
1	2	119	PSU	N1-C2-N3	4.26	119.96	115.13
1	2	105	PSU	C4-N3-C2	-4.25	120.22	126.34
1	2	159	A2M	N3-C2-N1	-4.22	122.09	128.68
1	2	1832	6MZ	N3-C2-N1	-4.21	122.10	128.68
1	2	1045	PSU	C4-N3-C2	-4.20	120.29	126.34
1	2	36	PSU	C4-N3-C2	-4.18	120.31	126.34
1	2	649	PSU	N1-C2-N3	4.16	119.84	115.13
1	2	966	PSU	N1-C2-N3	4.16	119.84	115.13
1	2	121	OMU	C4-N3-C2	-4.15	121.11	126.58
1	2	1643	PSU	N1-C2-N3	4.14	119.82	115.13
1	2	1045	PSU	N1-C2-N3	4.11	119.79	115.13
1	2	1288	OMU	C4-N3-C2	-4.05	121.24	126.58
1	2	119	PSU	C4-N3-C2	-3.99	120.58	126.34
1	2	1442	OMU	C4-N3-C2	-3.95	121.36	126.58
1	2	354	OMU	C5-C4-N3	3.82	120.56	114.84
1	2	116	OMU	C4-N3-C2	-3.81	121.56	126.58
1	2	99	A2M	N3-C2-N1	-3.77	122.78	128.68
1	2	509	OMG	C5-C6-N1	3.75	120.57	113.95
1	2	428	OMU	C5-C4-N3	3.69	120.37	114.84
1	2	601	OMG	C5-C6-N1	3.68	120.46	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1326	OMU	C5-C4-N3	3.67	120.34	114.84
1	2	406	PSU	O2-C2-N1	-3.65	118.78	122.79
1	2	822	PSU	O2-C2-N1	-3.60	118.83	122.79
1	2	484	A2M	C4-C5-N7	-3.56	105.68	109.40
1	2	428	OMU	C1'-N1-C2	3.53	123.95	117.57
1	2	1288	OMU	C5-C4-N3	3.50	120.07	114.84
1	2	109	PSU	O2-C2-N1	-3.49	118.94	122.79
1	2	121	OMU	C5-C4-N3	3.44	119.98	114.84
1	2	172	OMU	C5-C4-N3	3.44	119.98	114.84
1	2	1337	4AC	O2-C2-N3	-3.43	116.75	122.33
1	2	683	OMG	C5-C6-N1	3.40	119.95	113.95
1	2	1326	OMU	O4-C4-C5	-3.38	119.22	125.16
1	2	1328	OMG	C5-C6-N1	3.36	119.89	113.95
1	2	116	OMU	C5-C4-N3	3.36	119.87	114.84
1	2	1832	6MZ	C4-C5-N7	-3.36	105.90	109.40
1	2	683	OMG	O3'-C3'-C4'	3.32	120.65	111.05
1	2	1046	PSU	O2-C2-N1	-3.29	119.17	122.79
1	2	867	OMG	C5-C6-N1	3.25	119.70	113.95
1	2	1442	OMU	C5-C4-N3	3.20	119.64	114.84
1	2	36	PSU	C6-N1-C2	-3.19	119.42	122.68
1	2	1004	PSU	C6-N1-C2	-3.11	119.50	122.68
1	2	668	A2M	C4-C5-N7	-3.09	106.17	109.40
1	2	1639	7MG	C2-N1-C6	-3.08	119.48	125.10
1	2	683	OMG	C8-N7-C5	3.07	108.84	102.99
1	2	686	PSU	O2-C2-N1	-3.07	119.41	122.79
1	2	1004	PSU	O2-C2-N1	-3.06	119.43	122.79
1	2	1692	PSU	O4-C4-N3	-3.05	114.26	120.12
1	2	116	OMU	O4-C4-C5	-3.05	119.79	125.16
1	2	121	OMU	O4-C4-C5	-3.04	119.81	125.16
1	2	1442	OMU	O4-C4-C5	-3.03	119.83	125.16
1	2	436	OMG	C5-C6-N1	3.00	119.26	113.95
1	2	159	A2M	C4-C5-N7	-2.99	106.28	109.40
1	2	1842	4AC	O2-C2-N3	-2.99	117.47	122.33
1	2	644	OMG	C8-N7-C5	2.98	108.68	102.99
1	2	1490	OMG	C5-C6-N1	2.98	119.21	113.95
1	2	354	OMU	O4-C4-C5	-2.95	119.97	125.16
1	2	644	OMG	C5-C6-N1	2.94	119.15	113.95
1	2	1445	PSU	O2-C2-N1	-2.93	119.56	122.79
1	2	436	OMG	C8-N7-C5	2.93	108.57	102.99
1	2	1288	OMU	O4-C4-C5	-2.93	120.01	125.16
1	2	649	PSU	O4-C4-N3	-2.89	114.57	120.12
1	2	1383	A2M	C4-C5-N7	-2.89	106.38	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	7MG	O6-C6-C5	-2.88	120.48	127.54
1	2	815	PSU	O2-C2-N1	-2.87	119.63	122.79
1	2	93	PSU	C6-N1-C2	-2.86	119.76	122.68
1	2	867	OMG	C8-N7-C5	2.86	108.43	102.99
1	2	1678	A2M	C4-C5-N7	-2.85	106.42	109.40
1	2	1851	MA6	C4-C5-N7	-2.84	106.44	109.40
1	2	1842	4AC	O7-C7-N4	-2.83	117.23	121.82
1	2	1850	MA6	C4-C5-N7	-2.83	106.45	109.40
1	2	1328	OMG	C8-N7-C5	2.82	108.37	102.99
1	2	1238	PSU	O2-C2-N1	-2.79	119.72	122.79
1	2	468	A2M	O4'-C4'-C3'	-2.77	99.64	105.11
1	2	1232	PSU	O2-C2-N1	-2.76	119.75	122.79
1	2	109	PSU	C6-N1-C2	-2.76	119.86	122.68
1	2	1639	7MG	C6-C5-C4	-2.74	116.98	122.62
1	2	1244	PSU	O2-C2-N1	-2.72	119.80	122.79
1	2	34	PSU	O2-C2-N1	-2.71	119.81	122.79
1	2	166	A2M	C4-C5-N7	-2.69	106.59	109.40
1	2	1625	PSU	O2-C2-N1	-2.69	119.83	122.79
1	2	601	OMG	C2-N1-C6	-2.68	120.17	125.10
1	2	428	OMU	O2-C2-N3	-2.67	116.53	121.50
1	2	651	PSU	O2-C2-N1	-2.65	119.88	122.79
1	2	1174	PSU	O2-C2-N1	-2.63	119.89	122.79
1	2	218	PSU	O2-C2-N1	-2.63	119.90	122.79
1	2	1703	OMC	O2-C2-N3	-2.61	118.08	122.33
1	2	172	OMU	O4-C4-C5	-2.60	120.59	125.16
1	2	1639	7MG	C6-C5-N7	2.60	136.00	131.91
1	2	1391	OMC	O2-C2-N3	-2.60	118.11	122.33
1	2	1367	PSU	O2-C2-N1	-2.59	119.94	122.79
1	2	1288	OMU	C1'-N1-C2	2.58	122.25	117.57
1	2	681	PSU	C6-N1-C2	-2.58	120.04	122.68
1	2	428	OMU	C1'-N1-C6	-2.58	115.22	120.84
1	2	119	PSU	O4-C4-N3	-2.57	115.20	120.12
1	2	1625	PSU	C6-N1-C2	-2.56	120.06	122.68
1	2	1842	4AC	C5-C4-N3	-2.56	118.48	122.59
1	2	1174	PSU	C6-N1-C2	-2.55	120.07	122.68
1	2	822	PSU	C6-N1-C2	-2.54	120.08	122.68
1	2	576	A2M	C4-C5-N7	-2.54	106.75	109.40
1	2	1347	PSU	C6-N1-C2	-2.53	120.10	122.68
1	2	509	OMG	C2-N1-C6	-2.52	120.46	125.10
1	2	105	PSU	C6-N1-C2	-2.50	120.13	122.68
1	2	601	OMG	C8-N7-C5	2.49	107.74	102.99
1	2	1328	OMG	C2-N1-C6	-2.48	120.53	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	34	PSU	C6-N1-C2	-2.47	120.15	122.68
1	2	428	OMU	O4-C4-C5	-2.47	120.82	125.16
1	2	1045	PSU	C6-N1-C2	-2.46	120.17	122.68
1	2	1244	PSU	C6-N1-C2	-2.46	120.17	122.68
1	2	105	PSU	O2-C2-N1	-2.45	120.09	122.79
1	2	814	PSU	O2-C2-N1	-2.45	120.10	122.79
1	2	1177	PSU	C6-N1-C2	-2.45	120.18	122.68
1	2	1490	OMG	C8-N7-C5	2.45	107.65	102.99
1	2	1177	PSU	O2-C2-N1	-2.42	120.12	122.79
1	2	512	A2M	C5'-C4'-C3'	-2.39	106.23	115.18
1	2	1045	PSU	O2-C2-N1	-2.39	120.16	122.79
1	2	867	OMG	O6-C6-C5	-2.39	119.71	124.37
1	2	572	PSU	O2-C2-N1	-2.38	120.17	122.79
1	2	1248	B8N	C31-N3-C2	2.37	121.23	117.67
1	2	683	OMG	C2-N1-C6	-2.37	120.74	125.10
1	2	509	OMG	C8-N7-C5	2.36	107.49	102.99
1	2	116	OMU	O2-C2-N1	-2.35	119.66	122.79
1	2	867	OMG	C2-N1-C6	-2.35	120.77	125.10
1	2	93	PSU	O2-C2-N1	-2.35	120.21	122.79
1	2	1692	PSU	C5-C4-N3	2.34	121.87	116.58
1	2	99	A2M	C4-C5-N7	-2.33	106.97	109.40
1	2	686	PSU	C6-N1-C2	-2.33	120.31	122.68
1	2	1490	OMG	C2-N1-C6	-2.32	120.82	125.10
1	2	1272	OMC	O2-C2-N3	-2.32	118.56	122.33
1	2	649	PSU	C5-C4-N3	2.32	121.83	116.58
1	2	1031	A2M	C4-C5-N7	-2.30	107.00	109.40
1	2	1081	PSU	C6-N1-C2	-2.30	120.33	122.68
1	2	121	OMU	O2-C2-N1	-2.28	119.76	122.79
1	2	428	OMU	O2'-C2'-C1'	2.27	113.51	109.08
1	2	1248	B8N	O2-C2-N3	-2.27	118.83	121.99
1	2	1445	PSU	C6-N1-C2	-2.27	120.36	122.68
1	2	1842	4AC	O7-C7-CM7	-2.27	117.84	122.06
1	2	683	OMG	O3'-C3'-C2'	2.27	117.61	111.17
1	2	822	PSU	O4'-C1'-C2'	2.27	108.34	105.14
1	2	512	A2M	C4-C5-N7	-2.27	107.03	109.40
1	2	1643	PSU	C6-N1-C2	-2.25	120.39	122.68
1	2	644	OMG	C2-N1-C6	-2.25	120.96	125.10
1	2	462	OMC	O2-C2-N3	-2.24	118.69	122.33
1	2	601	OMG	O6-C6-C5	-2.24	120.00	124.37
1	2	1367	PSU	C6-N1-C2	-2.23	120.40	122.68
1	2	116	OMU	C1'-N1-C2	2.22	121.60	117.57
1	2	116	OMU	C6-C5-C4	-2.20	116.51	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	509	OMG	O6-C6-C5	-2.20	120.08	124.37
1	2	119	PSU	C6-N1-C2	-2.19	120.44	122.68
1	2	517	OMC	O2-C2-N3	-2.19	118.77	122.33
1	2	1445	PSU	C6-C5-C4	2.18	119.72	118.20
1	2	572	PSU	C6-N1-C2	-2.17	120.46	122.68
1	2	966	PSU	O2-C2-N1	-2.17	120.40	122.79
1	2	683	OMG	C3'-C2'-C1'	-2.16	98.83	102.89
1	2	172	OMU	O2-C2-N1	-2.15	119.92	122.79
1	2	1692	PSU	O2-C2-N3	-2.15	117.76	121.82
1	2	27	A2M	C4-C5-N7	-2.15	107.16	109.40
1	2	1248	B8N	C5-C4-N3	2.14	120.13	116.17
1	2	681	PSU	O2-C2-N1	-2.13	120.44	122.79
1	2	354	OMU	C1'-N1-C2	2.13	121.43	117.57
1	2	1244	PSU	C6-C5-C4	2.12	119.68	118.20
1	2	1081	PSU	O4'-C1'-C2'	2.12	108.13	105.14
1	2	1442	OMU	O2-C2-N1	-2.12	119.97	122.79
1	2	1328	OMG	O6-C6-N1	-2.12	118.15	120.65
1	2	1056	PSU	C6-N1-C2	-2.08	120.55	122.68
1	2	436	OMG	O6-C6-C5	-2.07	120.32	124.37
1	2	436	OMG	C2-N1-C6	-2.07	121.28	125.10
1	2	1643	PSU	O2-C2-N1	-2.05	120.54	122.79
1	2	1442	OMU	C1'-N1-C2	2.03	121.24	117.57
1	2	218	PSU	C6-N1-C2	-2.03	120.61	122.68

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	428	OMU	C3'-C4'-C5'-O5'
1	2	428	OMU	O4'-C4'-C5'-O5'
1	2	509	OMG	O4'-C4'-C5'-O5'
1	2	509	OMG	C3'-C4'-C5'-O5'
1	2	644	OMG	O4'-C4'-C5'-O5'
1	2	644	OMG	C3'-C4'-C5'-O5'
1	2	649	PSU	O4'-C1'-C5-C4
1	2	649	PSU	O4'-C1'-C5-C6
1	2	668	A2M	C3'-C4'-C5'-O5'
1	2	867	OMG	C1'-C2'-O2'-CM2
1	2	1248	B8N	O4'-C4'-C5'-O5'
1	2	1248	B8N	C3'-C4'-C5'-O5'
1	2	1248	B8N	N34-C33-C34-O35
1	2	1248	B8N	N3-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
1	2	1248	B8N	C31-C32-C33-N34
1	2	1272	OMC	C1'-C2'-O2'-CM2
1	2	1678	A2M	C1'-C2'-O2'-CM'
1	2	1692	PSU	O4'-C1'-C5-C4
1	2	1692	PSU	O4'-C1'-C5-C6
1	2	99	A2M	O4'-C4'-C5'-O5'
1	2	172	OMU	O4'-C4'-C5'-O5'
1	2	668	A2M	O4'-C4'-C5'-O5'
1	2	172	OMU	C3'-C4'-C5'-O5'
1	2	683	OMG	C3'-C4'-C5'-O5'
1	2	1248	B8N	N34-C33-C34-O36
1	2	99	A2M	C3'-C4'-C5'-O5'
1	2	119	PSU	C3'-C4'-C5'-O5'
1	2	683	OMG	O4'-C4'-C5'-O5'
1	2	1850	MA6	O4'-C4'-C5'-O5'
1	2	468	A2M	O4'-C4'-C5'-O5'
1	2	1842	4AC	O7-C7-N4-C4
1	2	1842	4AC	CM7-C7-N4-C4
1	2	428	OMU	O4'-C1'-N1-C6
1	2	867	OMG	O4'-C4'-C5'-O5'
1	2	1248	B8N	C31-C32-C33-C34
1	2	509	OMG	C4'-C5'-O5'-P
1	2	1490	OMG	C4'-C5'-O5'-P
1	2	119	PSU	O4'-C4'-C5'-O5'
1	2	1490	OMG	O4'-C4'-C5'-O5'
1	2	644	OMG	C4'-C5'-O5'-P
1	2	1850	MA6	C3'-C4'-C5'-O5'
1	2	428	OMU	O4'-C1'-N1-C2
1	2	1031	A2M	O4'-C4'-C5'-O5'
1	2	462	OMC	C1'-C2'-O2'-CM2
1	2	428	OMU	C2'-C1'-N1-C2
1	2	867	OMG	C3'-C4'-C5'-O5'
1	2	1851	MA6	C3'-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

Of 136 ligands modelled in this entry, 134 are monoatomic - leaving 2 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
40	ATP	z	602	38	26,33,33	1.02	1 (3%)	31,52,52	1.29	4 (12%)
37	ASP	2	1901	-	6,7,8	0.86	0	5,8,10	1.07	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
40	ATP	z	602	38	-	1/18/38/38	0/3/3/3
37	ASP	2	1901	-	-	2/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	z	602	ATP	C5-C4	2.22	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	z	602	ATP	N3-C2-N1	-3.00	123.98	128.68
40	z	602	ATP	C3'-C2'-C1'	2.55	104.82	100.98
40	z	602	ATP	PA-O3A-PB	-2.54	124.10	132.83
40	z	602	ATP	C4-C5-N7	-2.37	106.93	109.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1901	ASP	C-CA-CB-CG

*Continued on next page...*



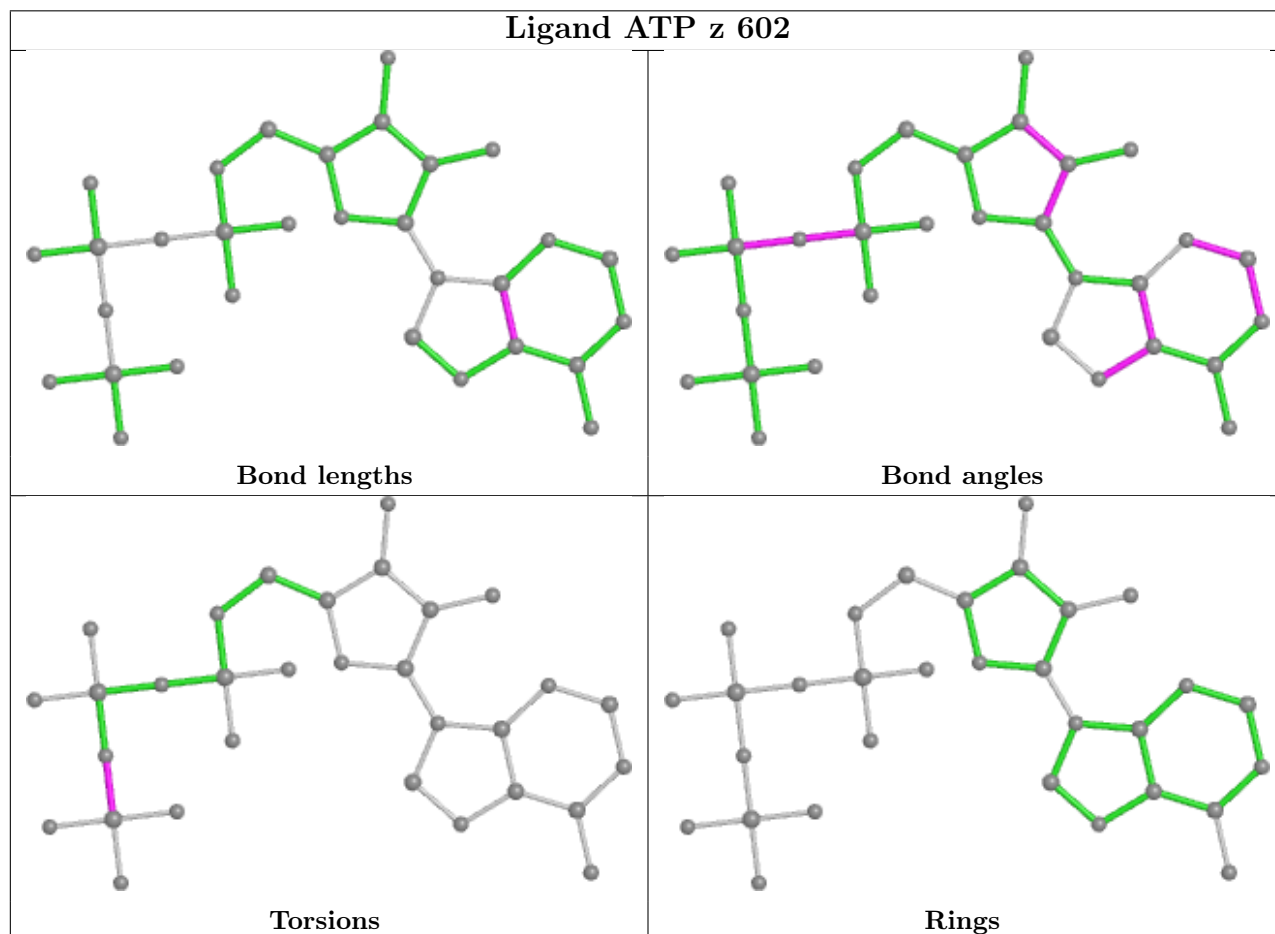
Continued from previous page...

Mol	Chain	Res	Type	Atoms
40	z	602	ATP	PB-O3B-PG-O3G
37	2	1901	ASP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	563:G	O3'	564:A	P	3.12

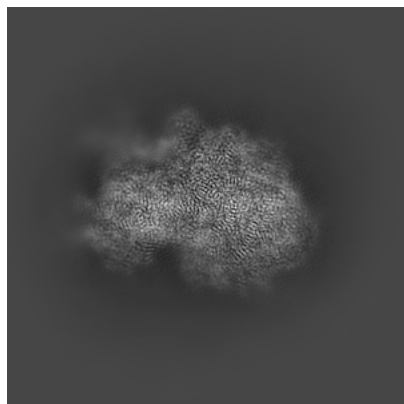
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11521. These allow visual inspection of the internal detail of the map and identification of artifacts.

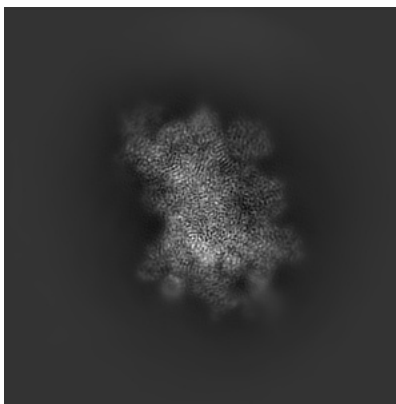
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

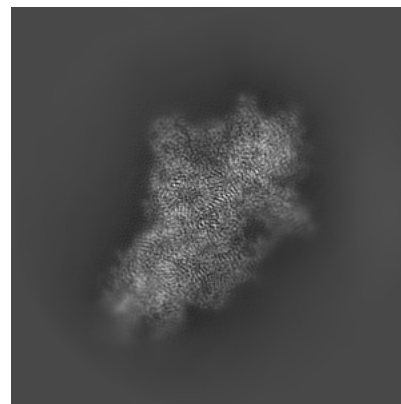
#### 6.1.1 Primary map



X

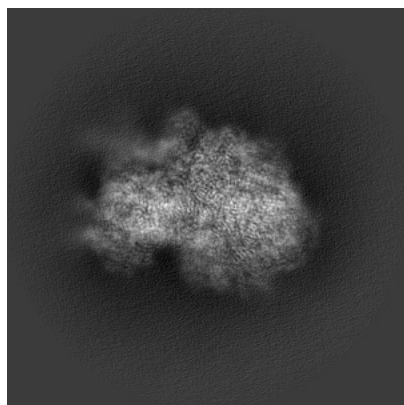


Y

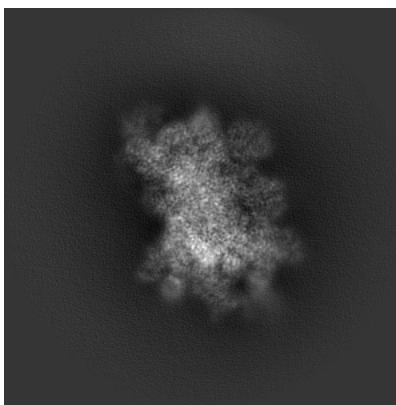


Z

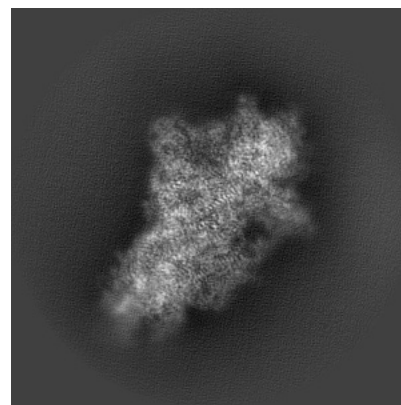
#### 6.1.2 Raw map



X



Y

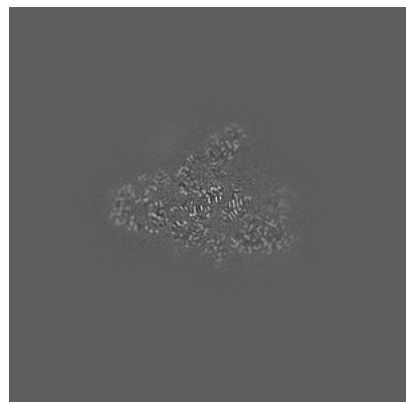


Z

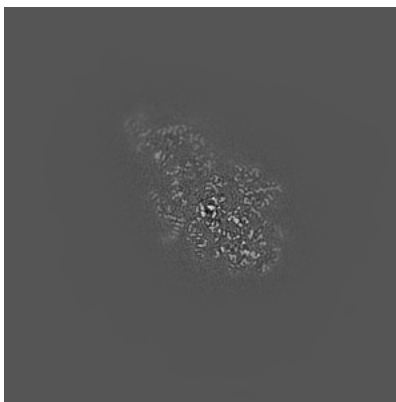
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

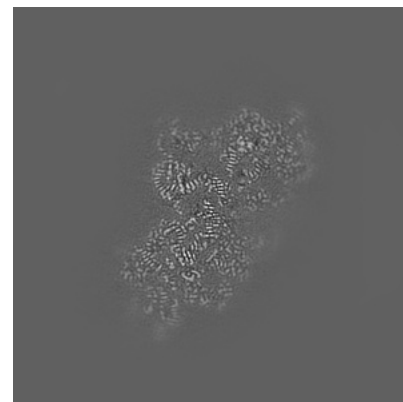
### 6.2.1 Primary map



X Index: 180

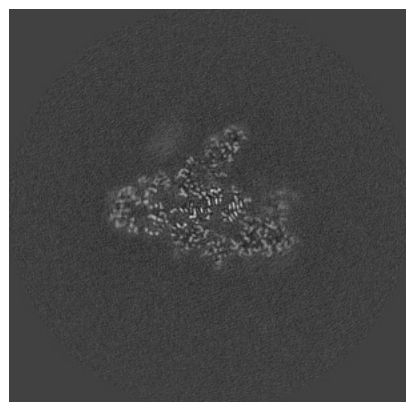


Y Index: 180

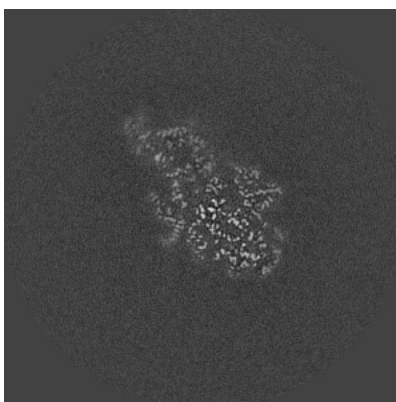


Z Index: 180

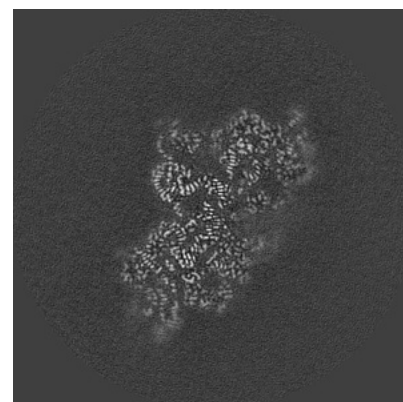
### 6.2.2 Raw map



X Index: 180



Y Index: 180

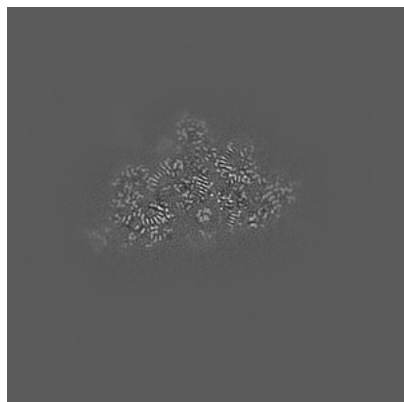


Z Index: 180

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

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

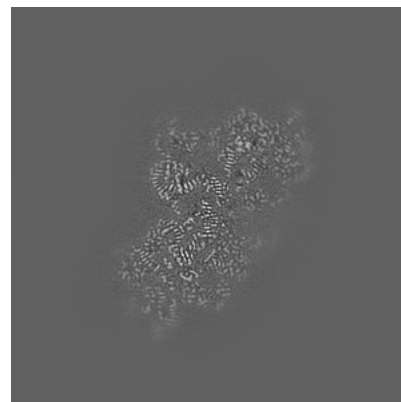
### 6.3.1 Primary map



X Index: 155

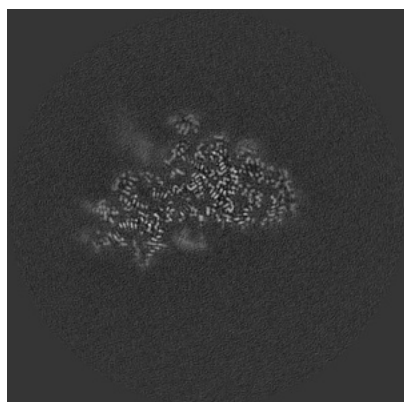


Y Index: 199

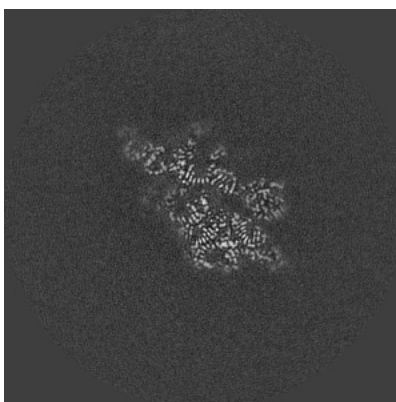


Z Index: 180

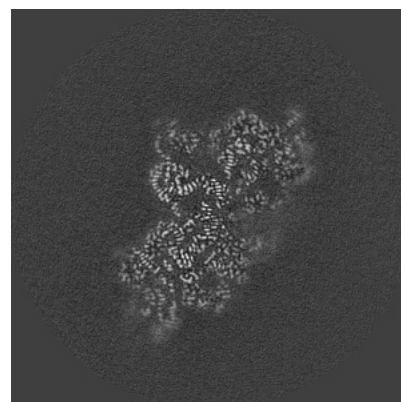
### 6.3.2 Raw map



X Index: 145



Y Index: 199

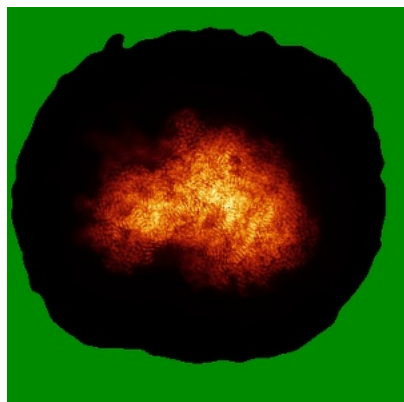


Z Index: 180

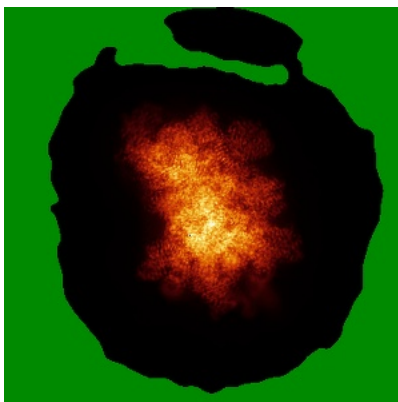
The images above show the largest variance slices of the map in three orthogonal directions.

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

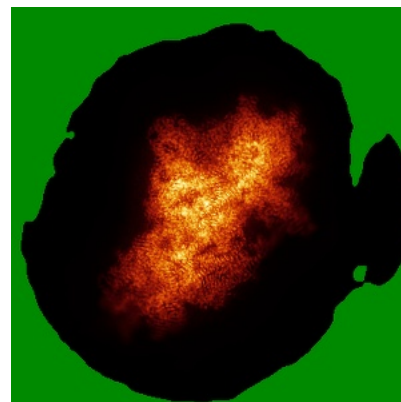
### 6.4.1 Primary map



X

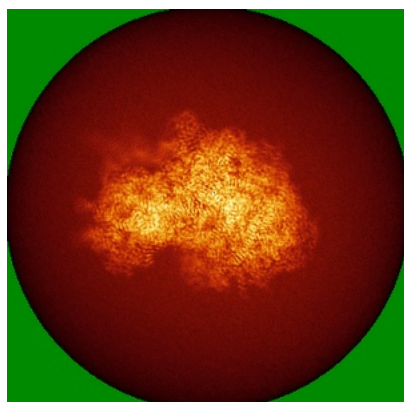


Y

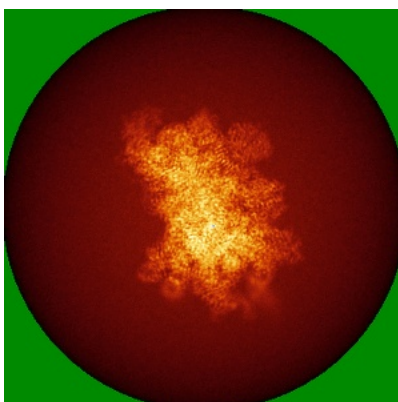


Z

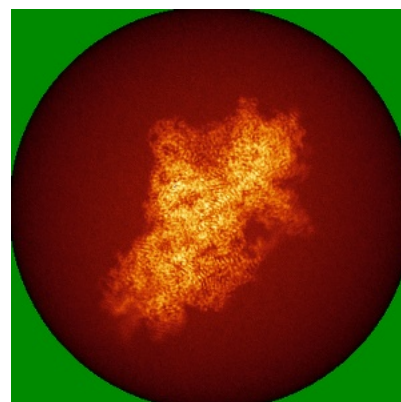
### 6.4.2 Raw map



X



Y

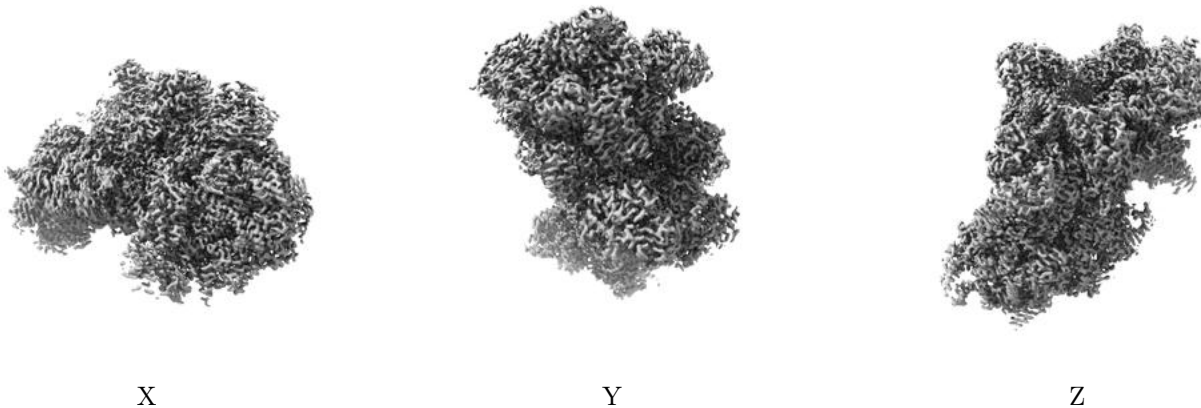


Z

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

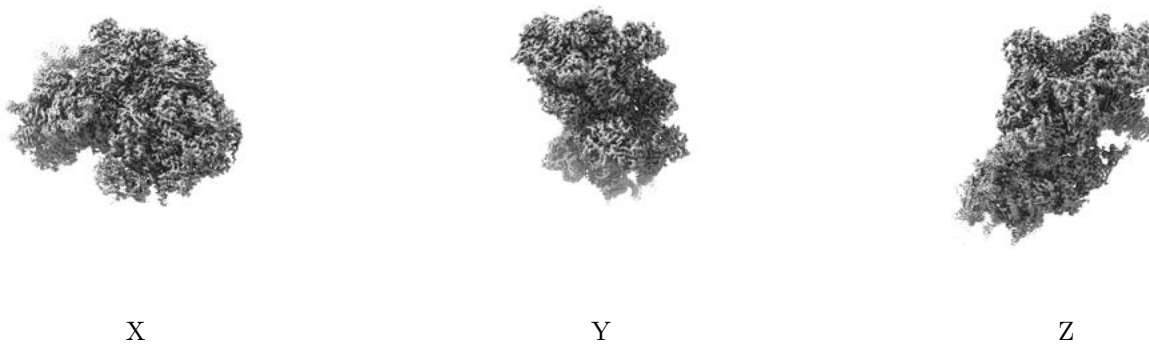
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.



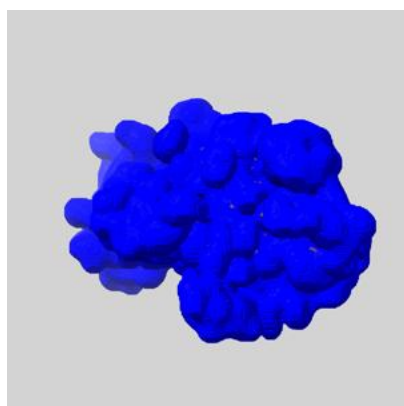
## 6.6 Mask visualisation [i](#)

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

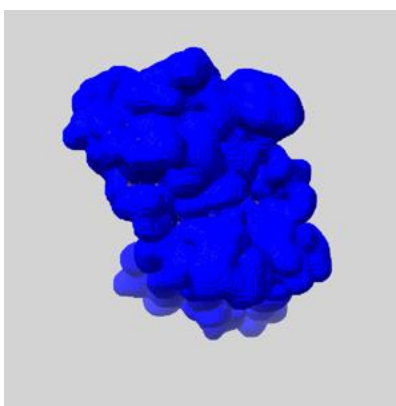
A mask typically either:

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

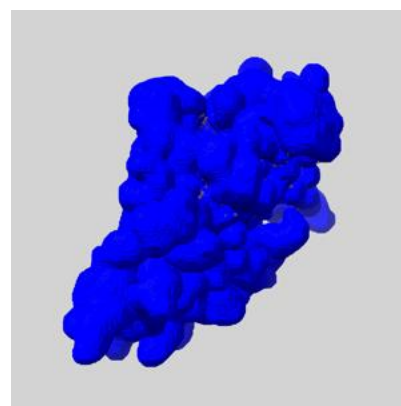
### 6.6.1 emd\_11521\_msk\_1.map [i](#)



X



Y

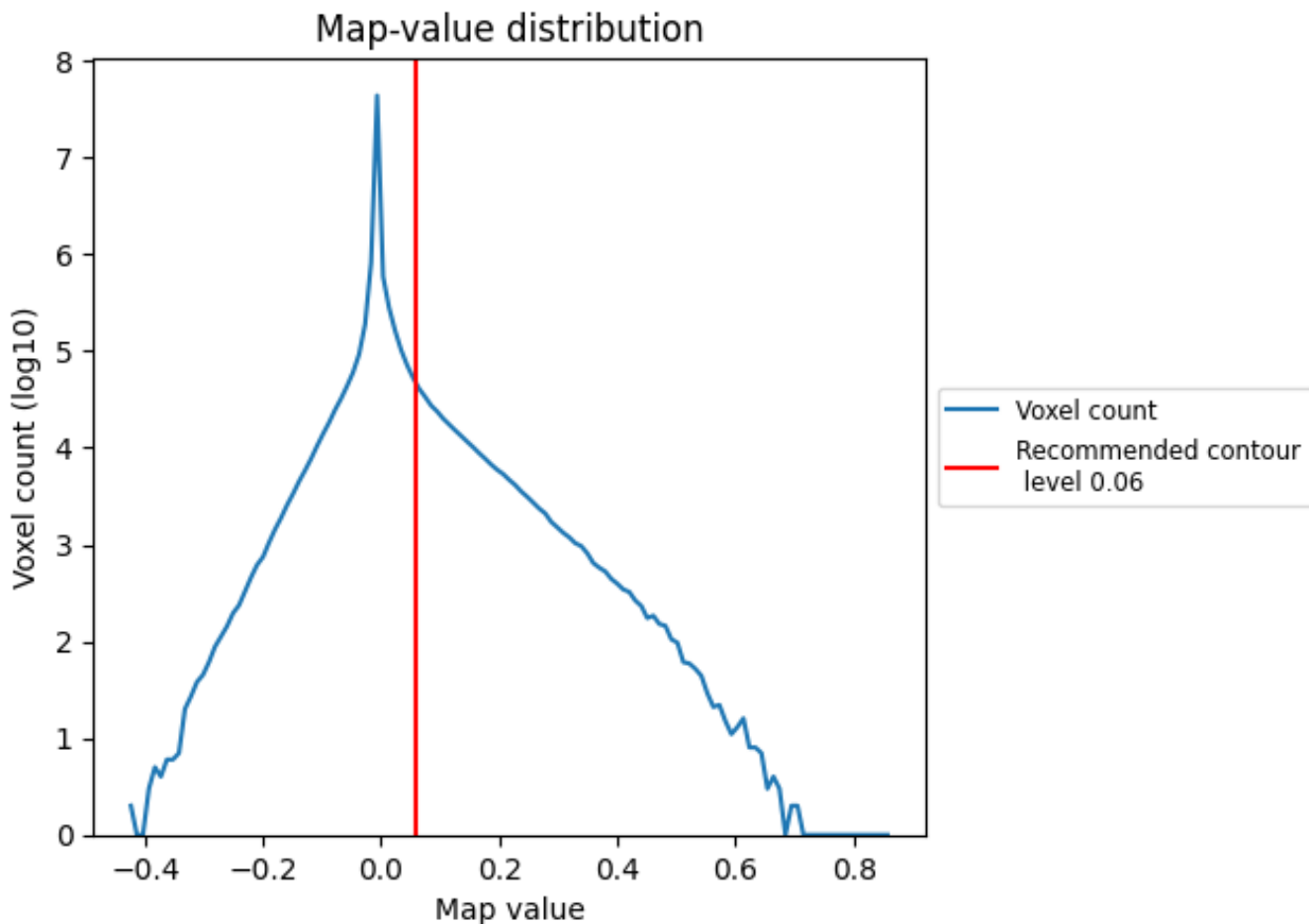


Z

## 7 Map analysis [i](#)

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

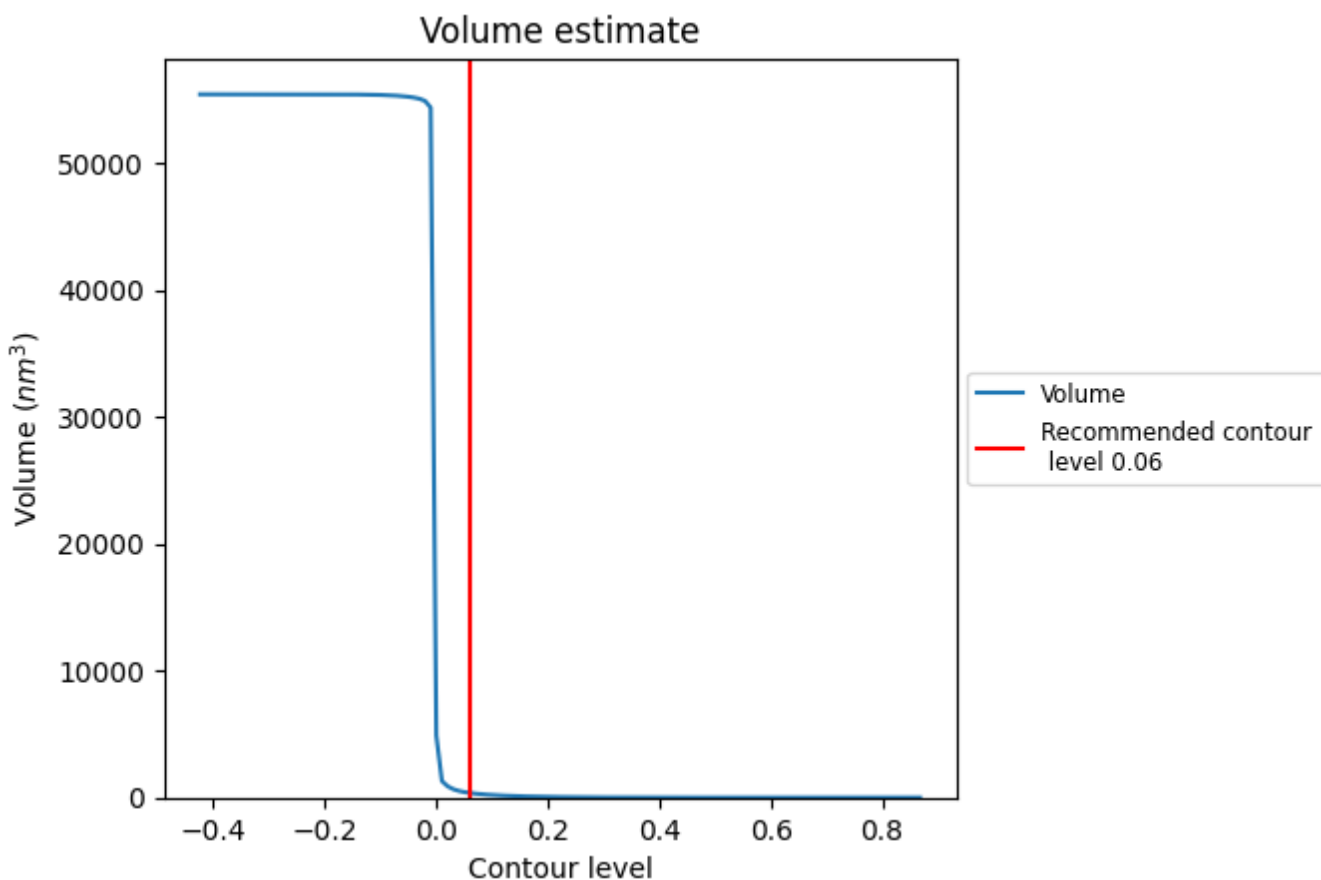
### 7.1 Map-value distribution [i](#)



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.



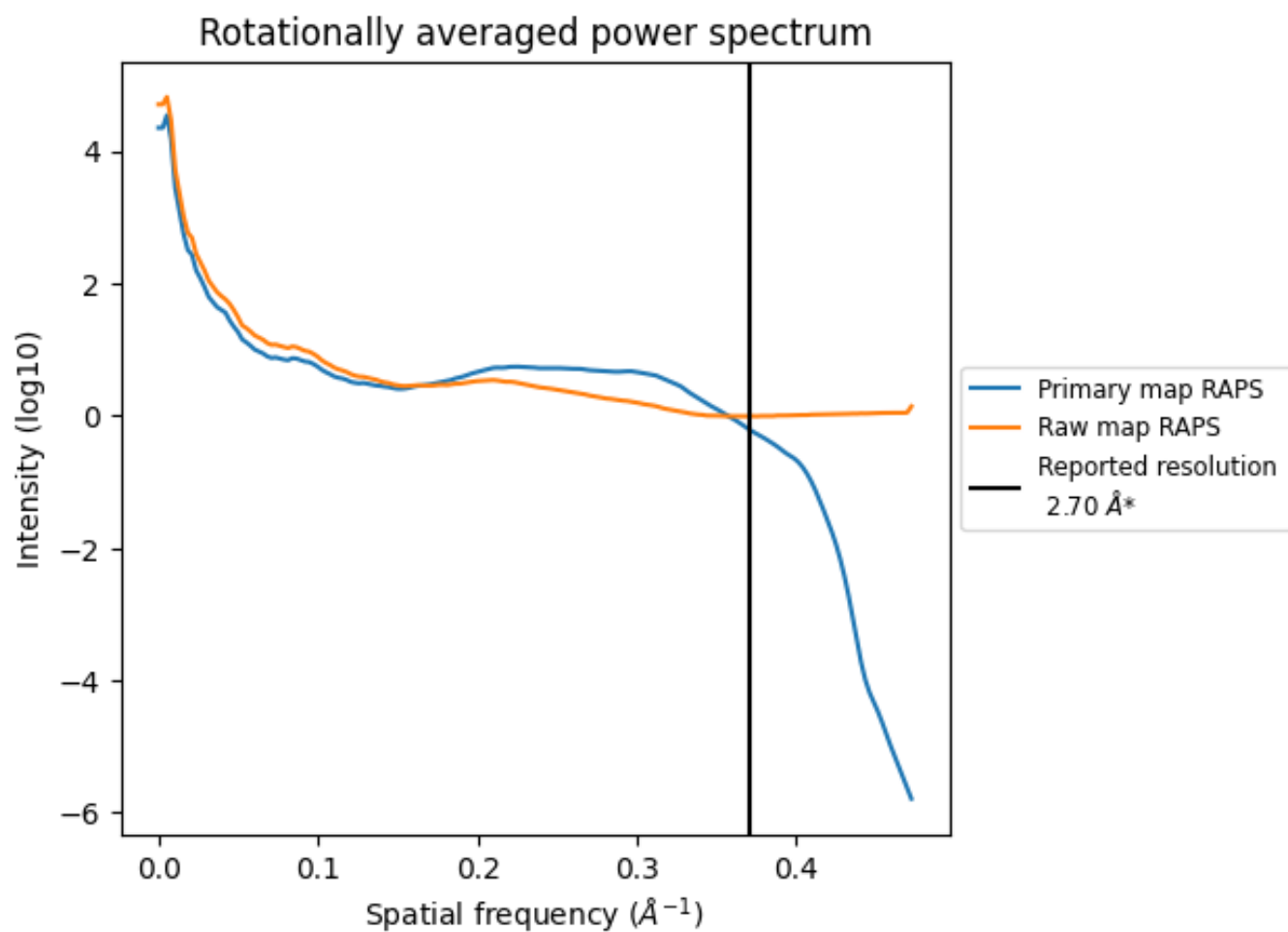
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 363  $\text{nm}^3$ ; this corresponds to an approximate mass of 328 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

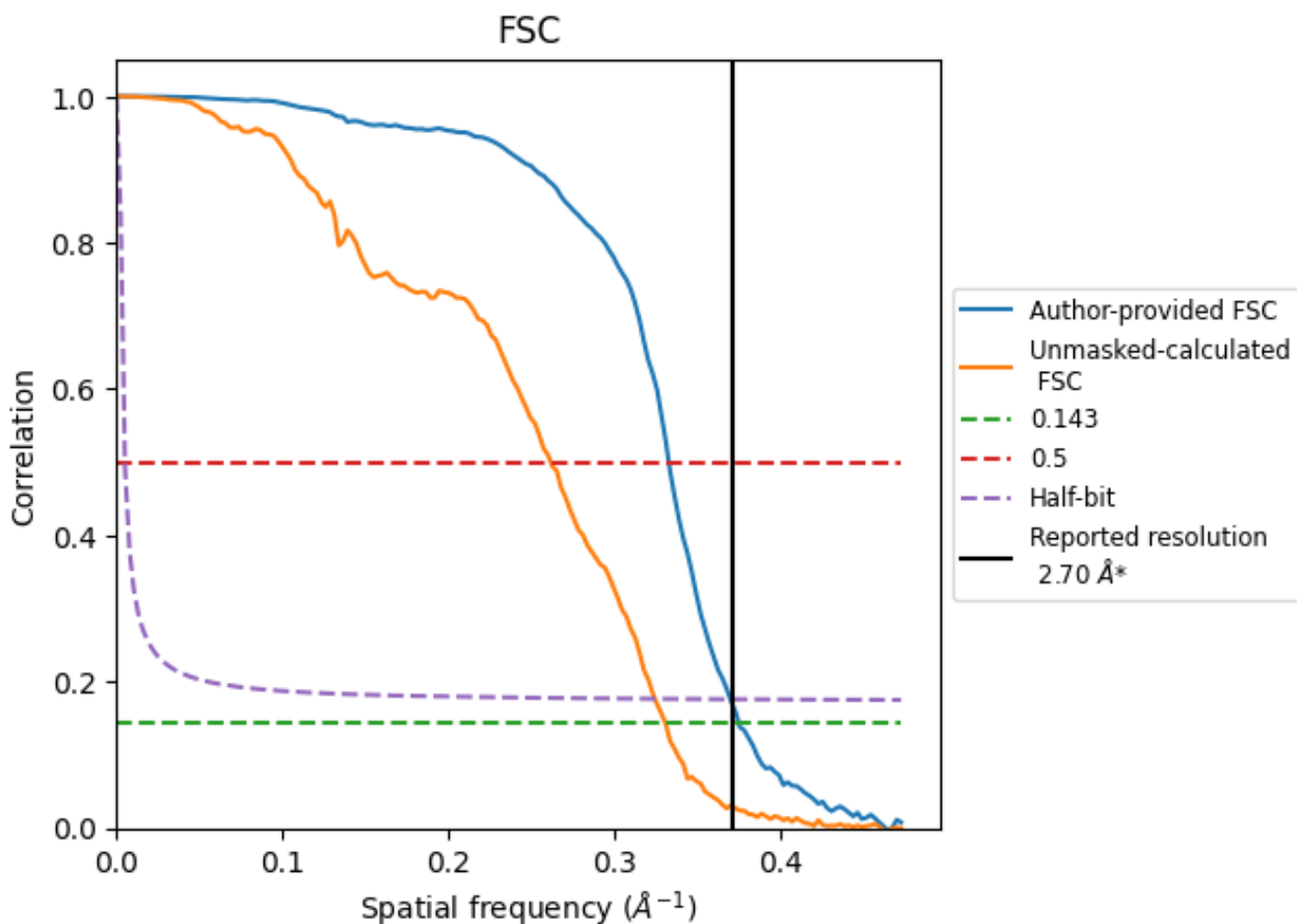


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

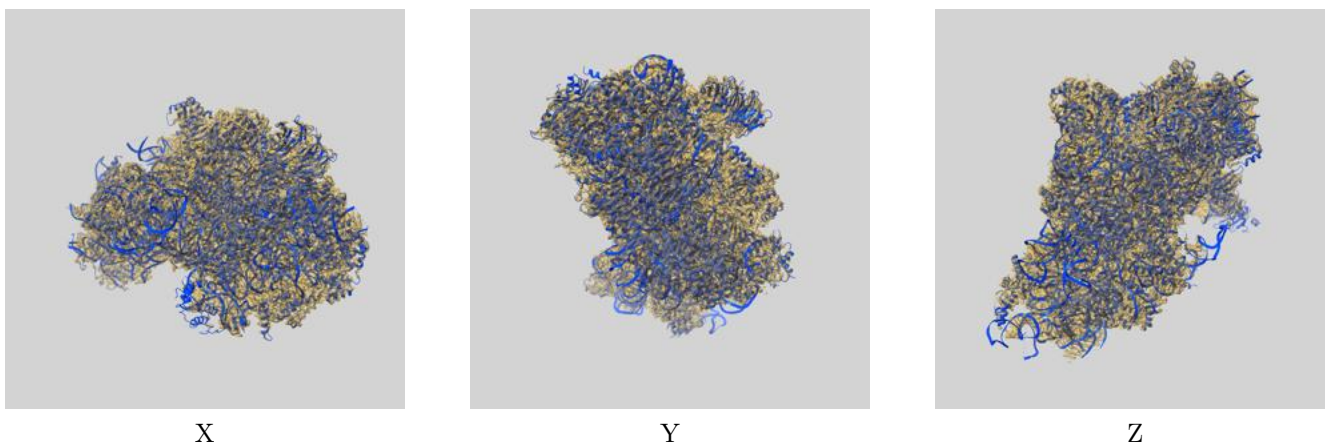
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.01	2.71
Unmasked-calculated*	3.03	3.83	3.09

\*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 3.03 differs from the reported value 2.7 by more than 10 %

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

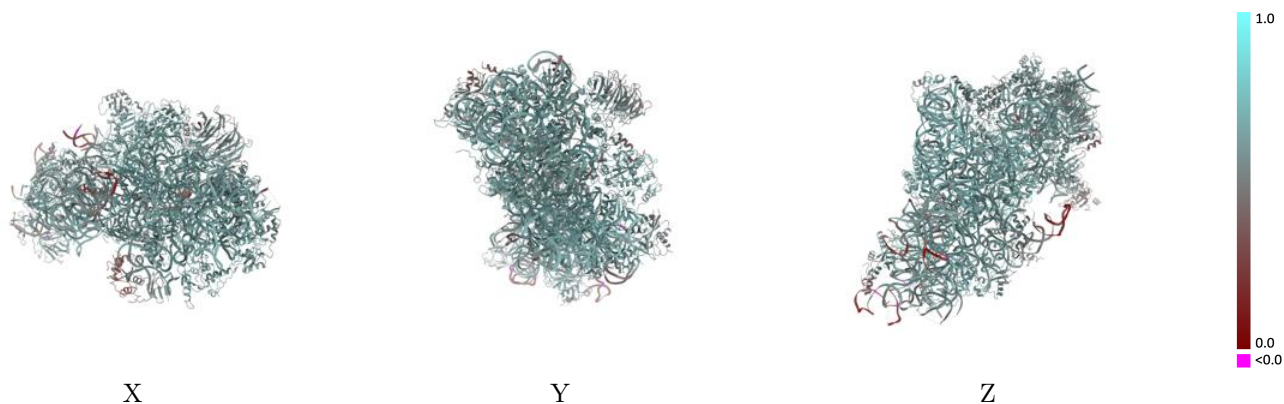
This section contains information regarding the fit between EMDB map EMD-11521 and PDB model 6ZXH. Per-residue inclusion information can be found in section 3 on page 12.

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



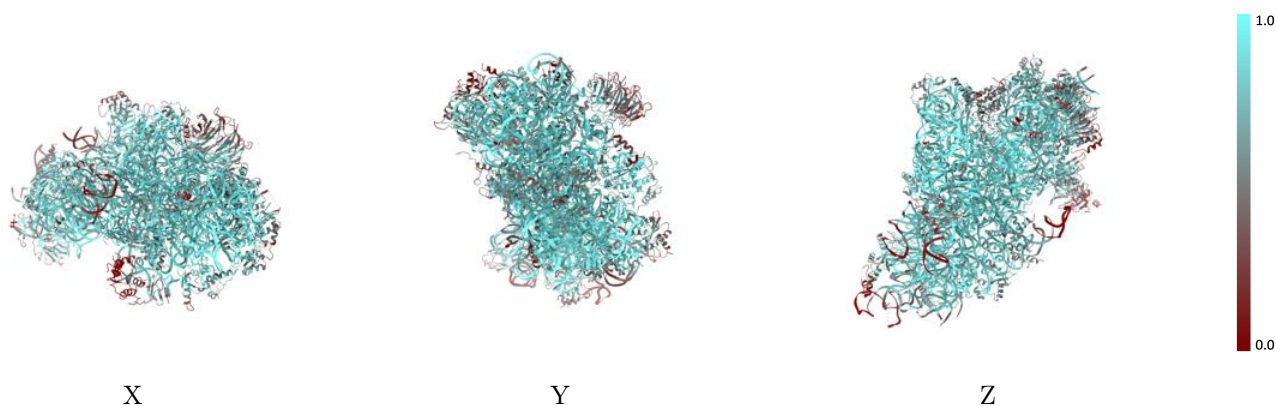
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



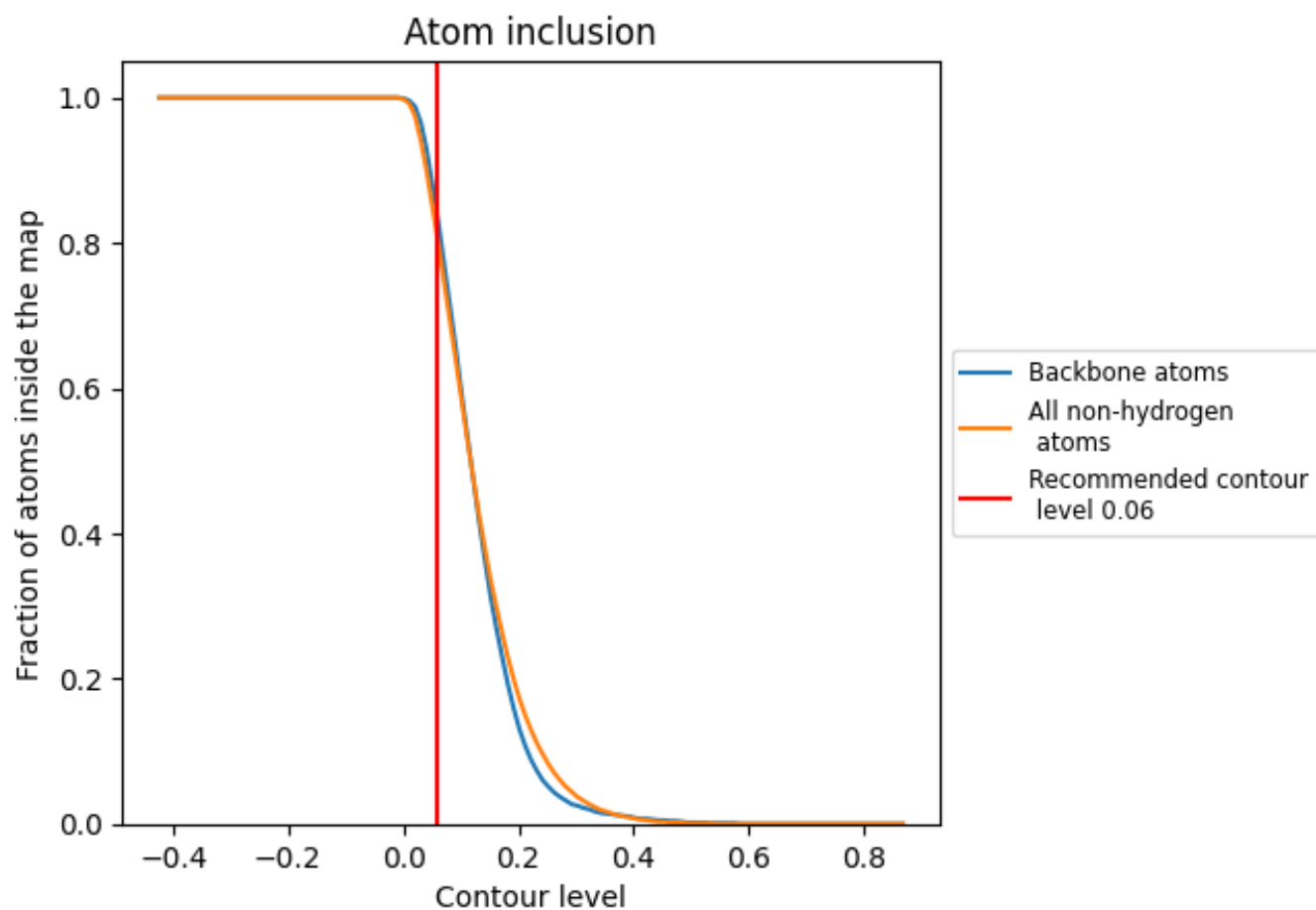
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.





Chain	Atom inclusion	Q-score
All	 0.8030	 0.6090
2	 0.8820	 0.6210
A	 0.8600	 0.6310
B	 0.7690	 0.6170
C	 0.9050	 0.6580
D	 0.7270	 0.5980
E	 0.8400	 0.6310
F	 0.7690	 0.5910
G	 0.6090	 0.5490
H	 0.6080	 0.5590
I	 0.7190	 0.5920
J	 0.7050	 0.5460
K	 0.7170	 0.5920
L	 0.8760	 0.6380
M	 0.1140	 0.3940
N	 0.8640	 0.6400
O	 0.8560	 0.6310
P	 0.7420	 0.6070
Q	 0.8300	 0.6250
R	 0.7060	 0.5890
S	 0.7150	 0.6060
T	 0.8100	 0.6280
U	 0.6640	 0.5790
V	 0.8540	 0.6410
W	 0.9450	 0.6720
X	 0.9170	 0.6610
Y	 0.7700	 0.5940
Z	 0.5660	 0.5690
b	 0.7750	 0.6250
c	 0.5360	 0.5460
d	 0.9330	 0.6640
e	 0.7650	 0.5970
f	 0.3050	 0.4810
g	 0.5090	 0.5380
h	 0.8560	 0.6530



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Chain	Atom inclusion	Q-score
j	 0.6660	 0.5890
z	 0.7110	 0.5990