Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 01:32 pm GMT

PDB ID	:	7R4X
EMDB ID	:	EMD-14317
Title	:	Cryo-EM reconstruction of the human 40S ribosomal subunit - Full map
Authors	:	Pellegrino, S.; Dent, K.C.; Spikes, T.; Warren, A.J.
Deposited on	:	2022-02-09
Resolution	:	2.15 Å(reported)

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

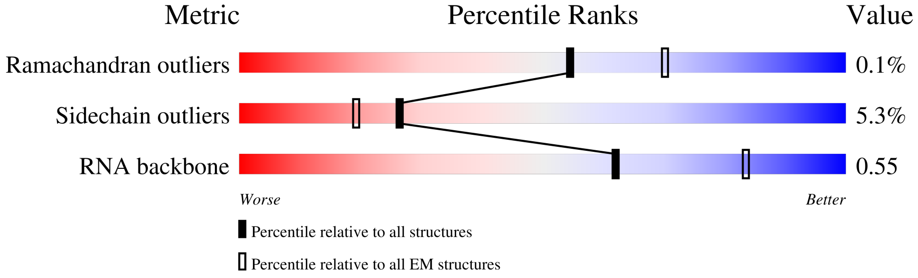
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

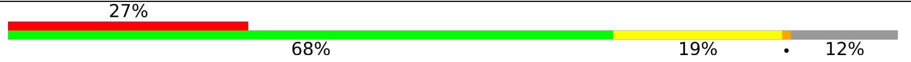
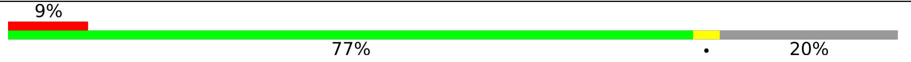
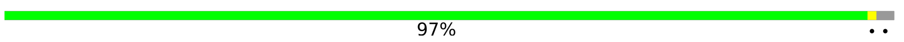
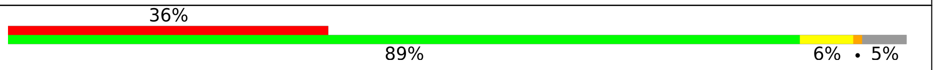
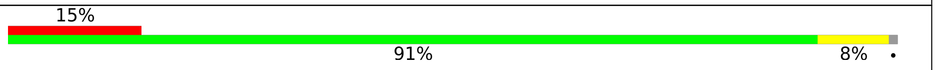
The reported resolution of this entry is 2.15 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	n	25	
2	2	1868	
3	B	264	
4	D	243	
5	E	263	
6	F	204	
7	H	194	
8	I	208	

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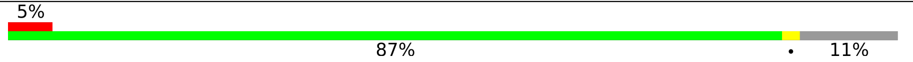
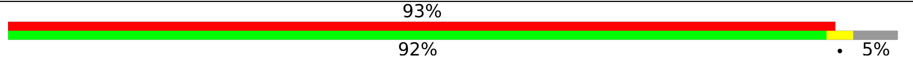
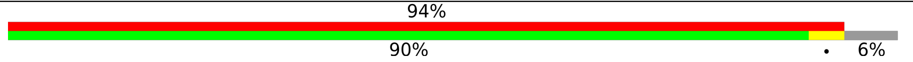
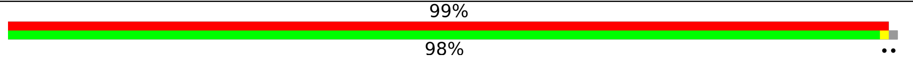
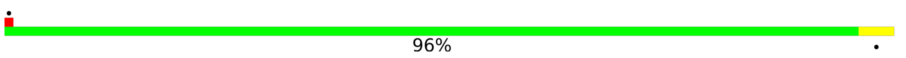
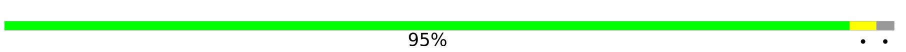
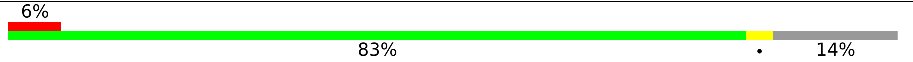
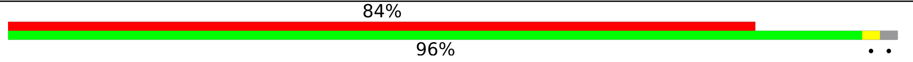
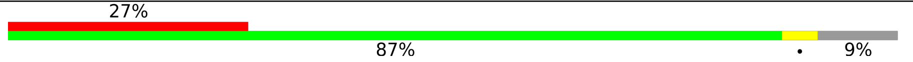
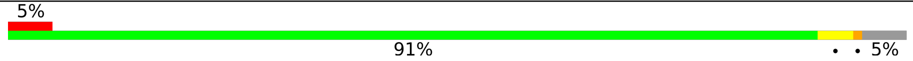
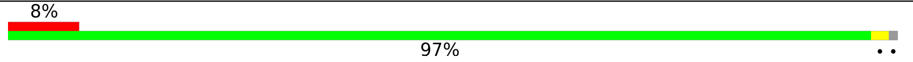
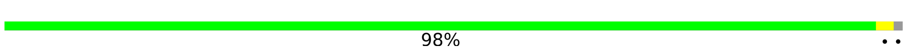
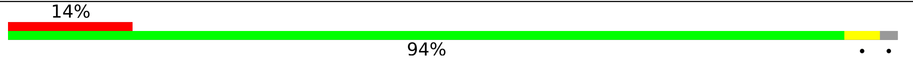
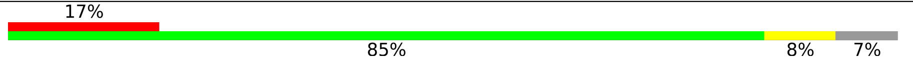
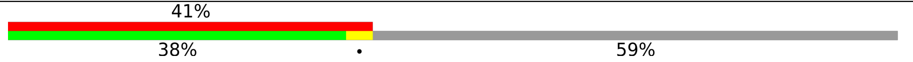
Mol	Chain	Length	Quality of chain
9	K	165	
10	L	158	
11	P	145	
12	Q	146	
13	R	135	
14	S	152	
15	T	145	
16	U	119	
17	V	83	
18	X	143	
19	a	115	
20	c	69	
21	d	56	
22	C	293	
23	G	249	
24	J	194	
25	M	132	
26	N	151	
27	O	151	
28	W	130	
29	Y	133	
30	Z	125	
31	b	84	
32	e	59	
33	f	156	

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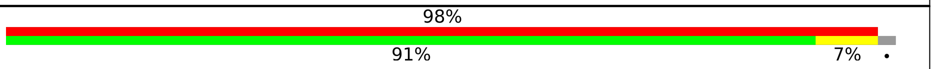
Mol	Chain	Length	Quality of chain
34	g	317	
35	A	295	

2 Entry composition ⓘ

There are 39 unique types of molecules in this entry. The entry contains 77936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	n	20	193	119	51	20	3	0	0

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1646	35347	15805	6355	11535	1652	7	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	210	1711	1086	306	305	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

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

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	257	2041	1305	379	349	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	182	1445	906	271	261	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	184	1477	942	271	263	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	205	1682	1056	331	290	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	97	816	533	144	133	6	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	141	1157	737	217	197	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	123	1005	638	188	172	7	0	0

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Q	139	1105	704	207	191	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	131	1064	668	198	194	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	143	1192	751	240	200	1	1	0

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	T	143	1112	697	214	198	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	104	821	514	155	148	4	0	0

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	V	83	639	395	117	122	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	140	1088	687	215	183	3	0	0

- Molecule 19 is a protein called 40S ribosomal protein S26.

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

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	c	59	464	281	93	88	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	C	219	1708	1105	295	298	10	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	G	227	1840	1149	367	317	7	0	0

- Molecule 24 is a protein called 40S ribosomal protein S9.

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

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	M	104	790	494	138	151	7	0	0

- Molecule 26 is a protein called 40S ribosomal protein S13.

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

- Molecule 27 is a protein called 40S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	conflict	UNP P62263

- Molecule 28 is a protein called 40S ribosomal protein S15a.

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

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	122	1002	635	196	166	5	0	0

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	72	570	366	104	99	1	0	0

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	b	82	640	402	118	113	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	55	438	271	95	71	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	64	522	329	99	87	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	312	Total 2429	C 1531	N 423	O 463	S 12	0	0

- Molecule 35 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	206	Total 1628	C 1042	N 287	O 291	S 8	1	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	2	76	Total 76	K 76	0
36	E	1	Total 1	K 1	0
36	L	1	Total 1	K 1	0
36	S	1	Total 1	K 1	0
36	U	1	Total 1	K 1	0
36	d	1	Total 1	K 1	0
36	O	1	Total 1	K 1	0

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	88	Total 88	Mg 88	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	a	1	Total 1	Zn 1	0
38	d	1	Total 1	Zn 1	0
38	f	1	Total 1	Zn 1	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	AltConf
39	n	10	Total O 10 10	0
39	2	3102	Total O 3102 3102	0
39	B	30	Total O 30 30	0
39	D	24	Total O 24 24	0
39	E	79	Total O 79 79	0
39	F	34	Total O 34 34	0
39	H	8	Total O 8 8	0
39	I	45	Total O 45 45	0
39	K	20	Total O 20 20	0
39	L	62	Total O 62 62	0
39	P	32	Total O 32 32	0
39	Q	46	Total O 46 46	0
39	R	13	Total O 13 13	0
39	S	30	Total O 30 30	0
39	T	51	Total O 51 51	0
39	U	25	Total O 25 25	0
39	V	19	Total O 19 19	0
39	X	47	Total O 47 47	0
39	a	30	Total O 30 30	0
39	c	6	Total O 6 6	0
39	d	26	Total O 26 26	0

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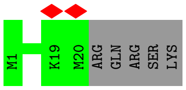
Mol	Chain	Residues	Atoms	AltConf
39	C	56	Total O 56 56	0
39	G	18	Total O 18 18	0
39	J	85	Total O 85 85	0
39	N	30	Total O 30 30	0
39	O	28	Total O 28 28	0
39	W	63	Total O 63 63	0
39	Y	25	Total O 25 25	0
39	Z	2	Total O 2 2	0
39	b	12	Total O 12 12	0
39	e	13	Total O 13 13	0
39	g	16	Total O 16 16	0
39	A	30	Total O 30 30	0

3 Residue-property plots ⓘ

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

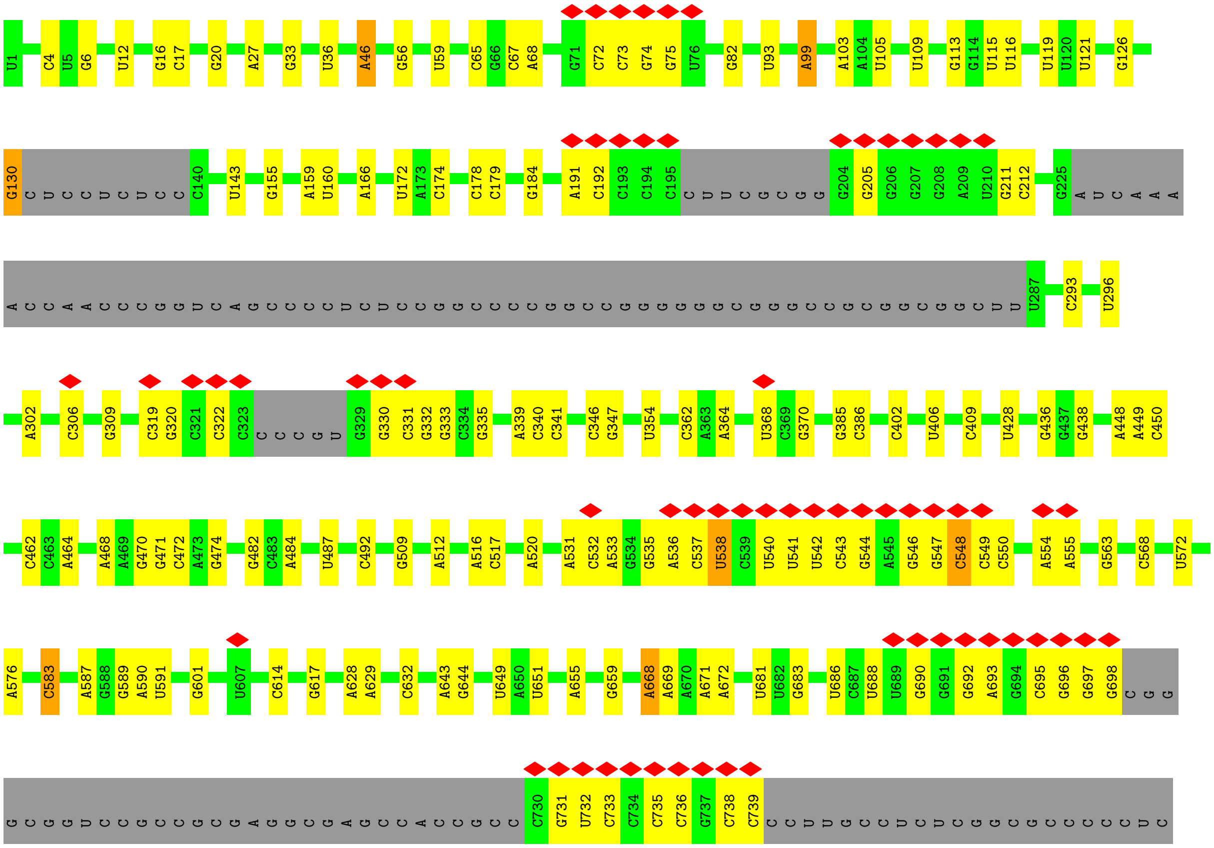
- Molecule 1: 60S ribosomal protein L41

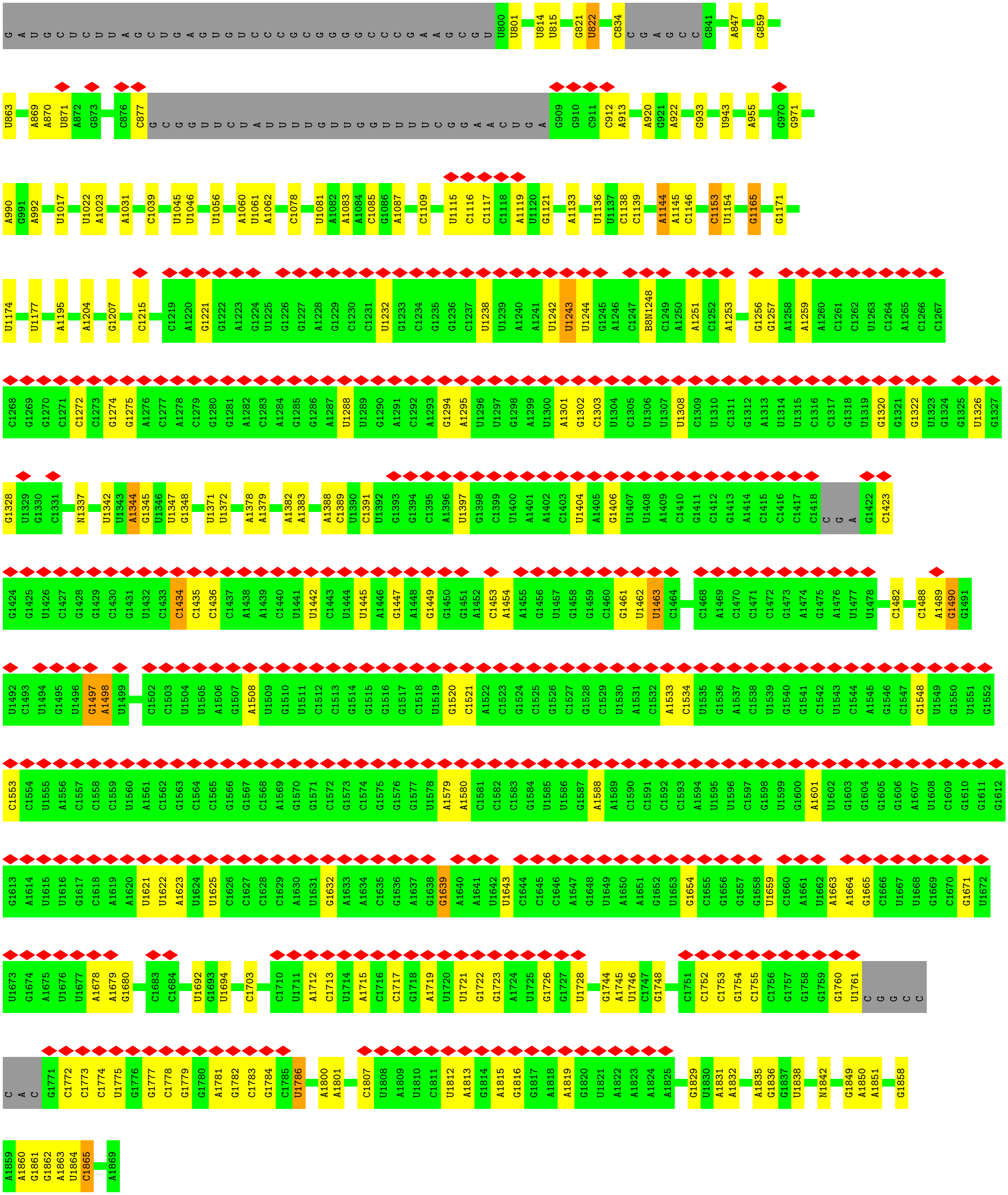
Chain n:



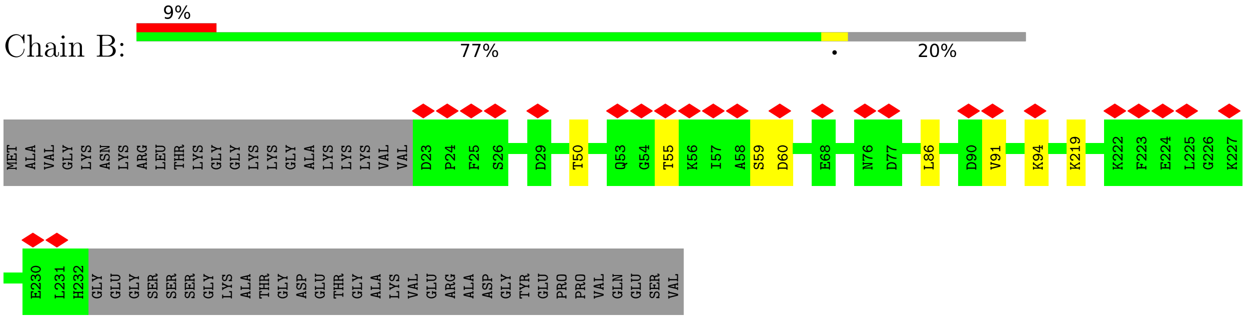
- Molecule 2: 18S ribosomal RNA

Chain 2:

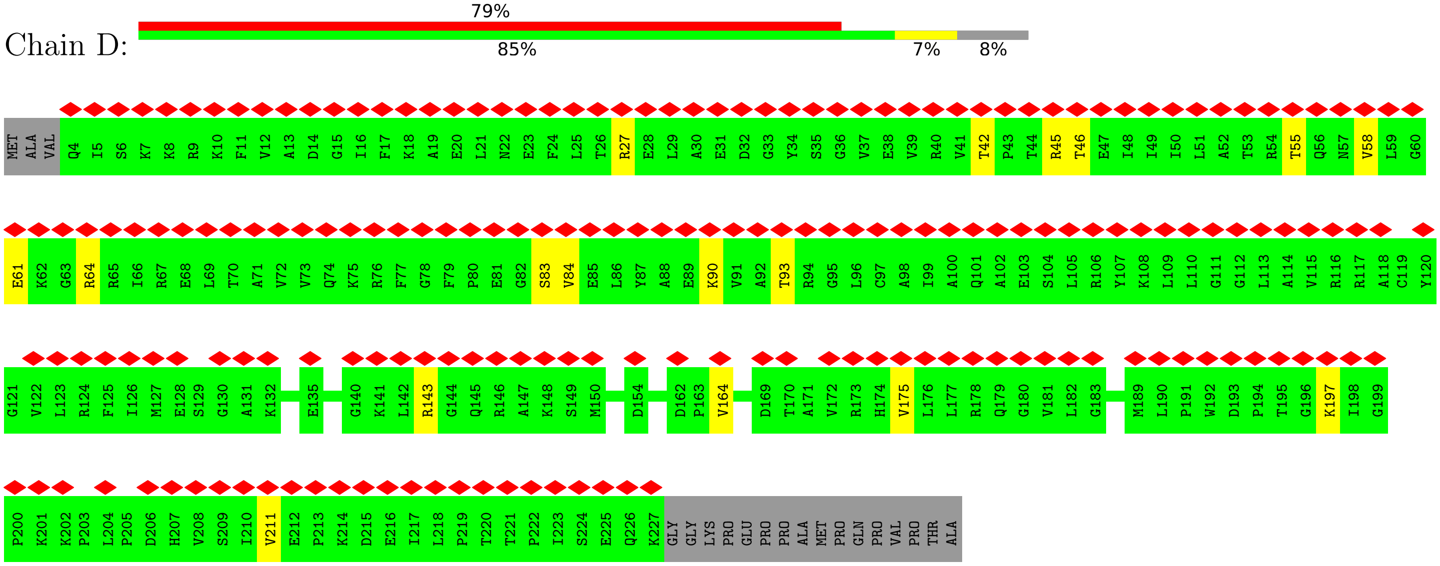




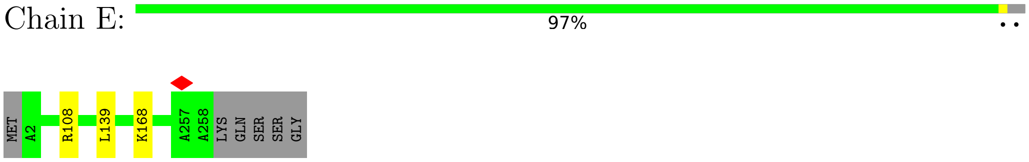
- Molecule 3: 40S ribosomal protein S3a



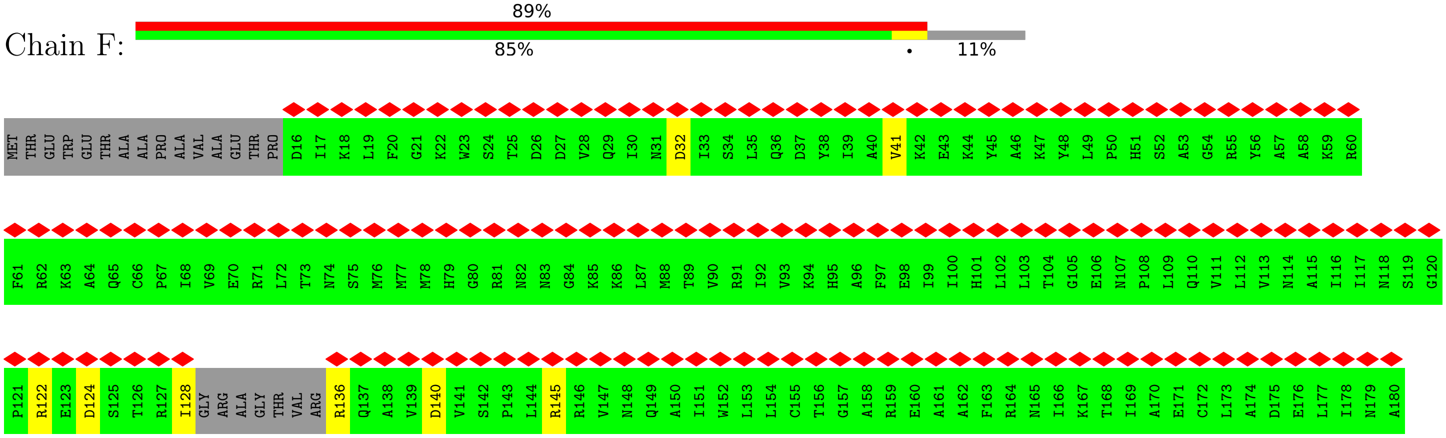
- Molecule 4: 40S ribosomal protein S3

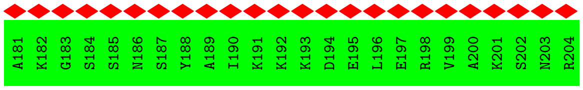


- Molecule 5: 40S ribosomal protein S4, X isoform



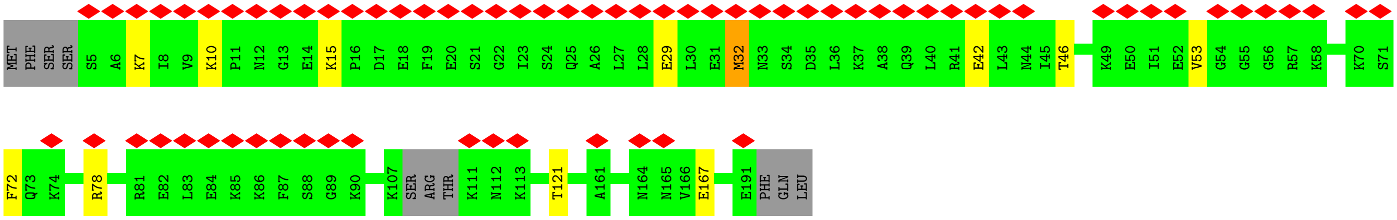
- Molecule 6: 40S ribosomal protein S5





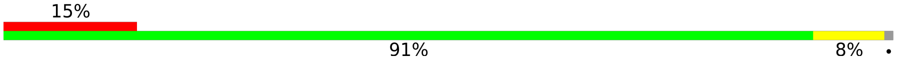
- Molecule 7: 40S ribosomal protein S7

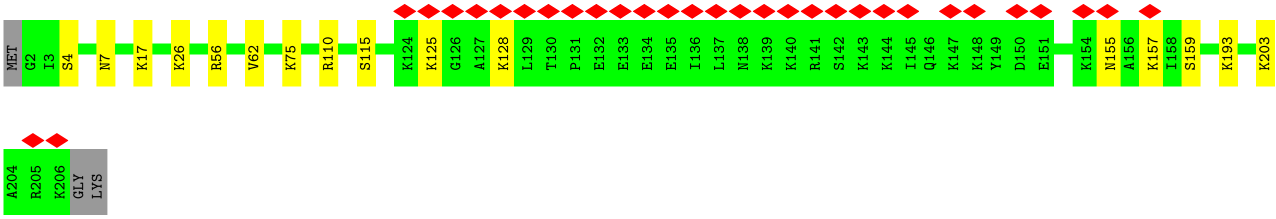
Chain H:



- Molecule 8: 40S ribosomal protein S8

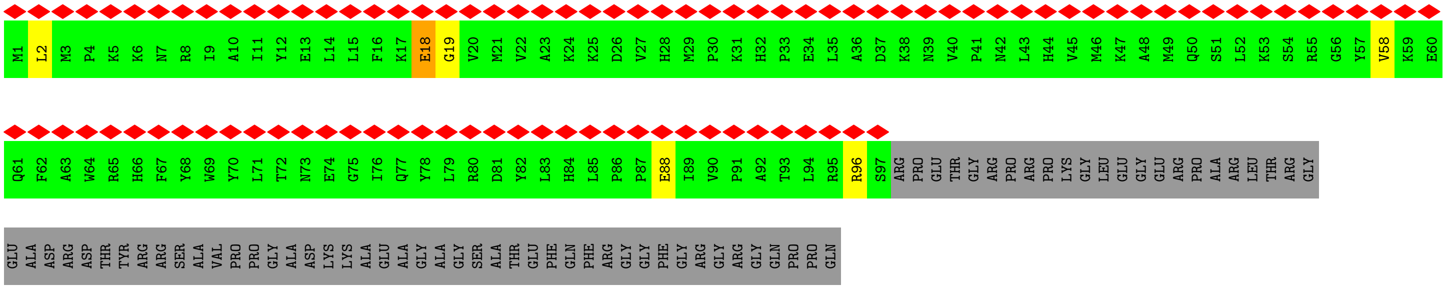
Chain I:





- Molecule 9: 40S ribosomal protein S10

Chain K:

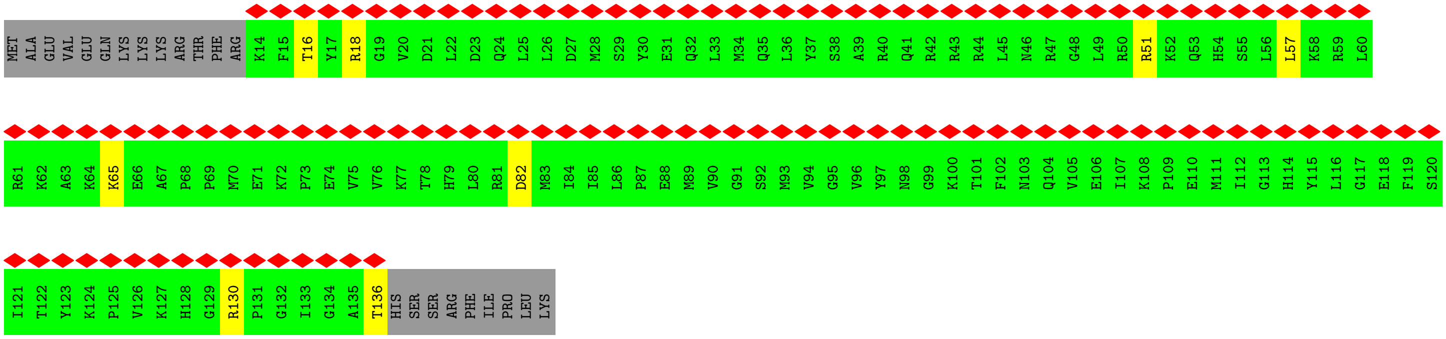


- Molecule 10: 40S ribosomal protein S11

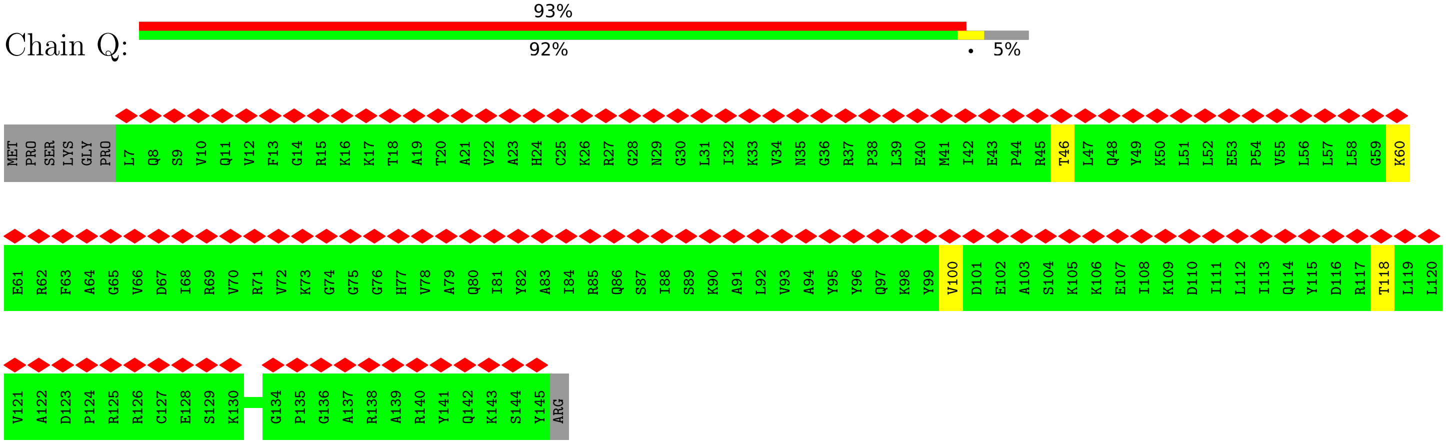
Chain L:

- Molecule 11: 40S ribosomal protein S15

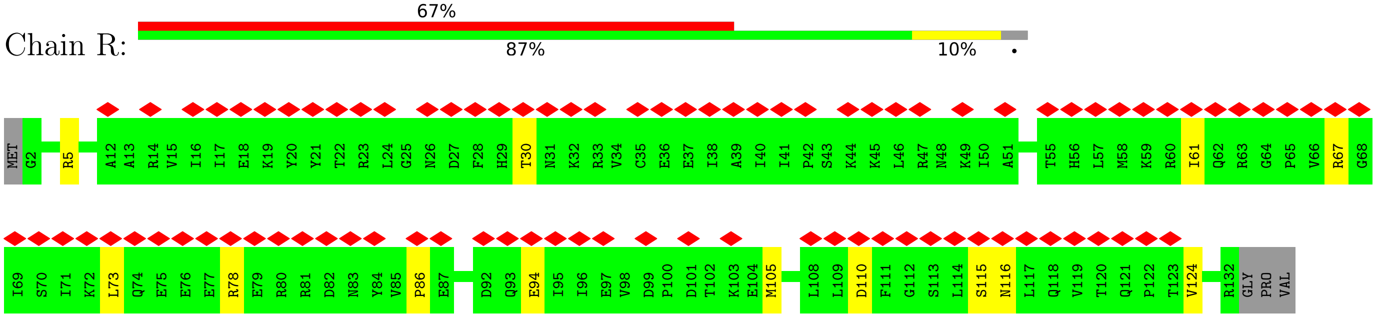
Chain P:



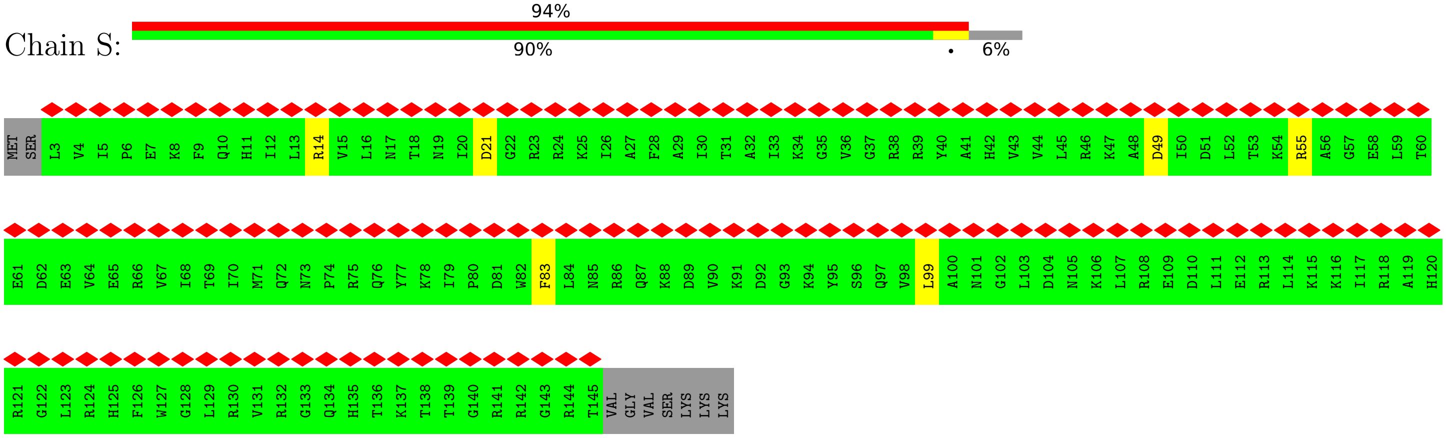
- Molecule 12: 40S ribosomal protein S16



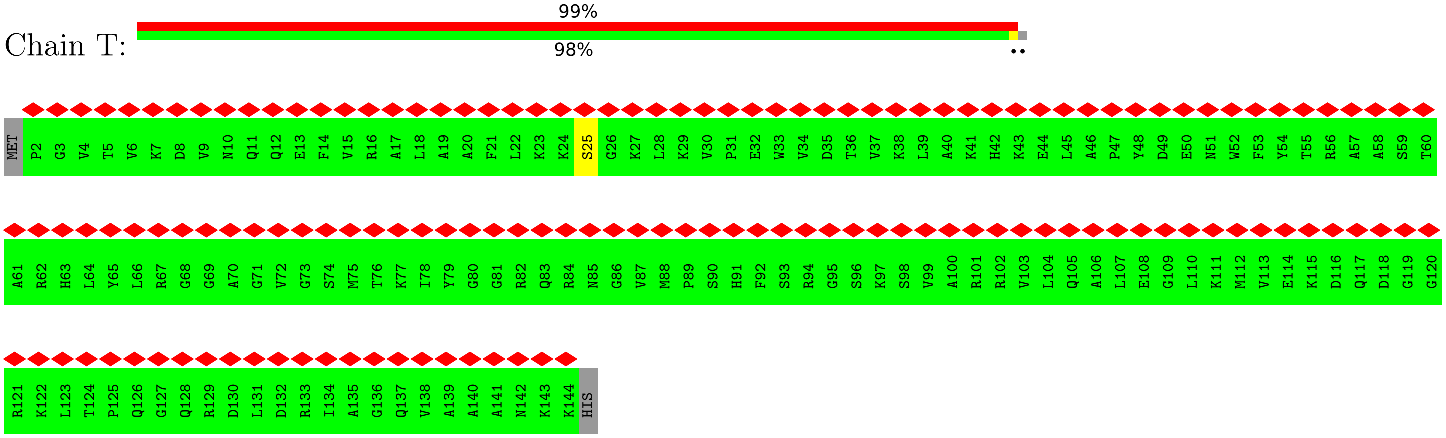
- Molecule 13: 40S ribosomal protein S17



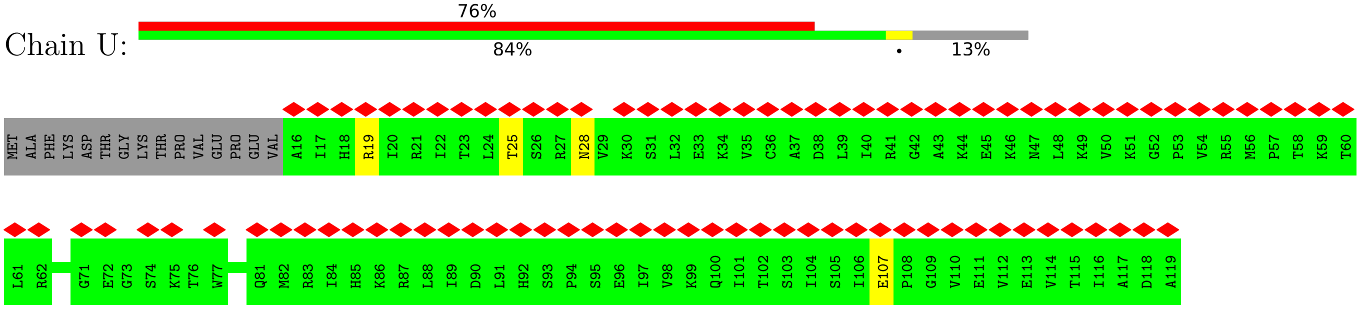
- Molecule 14: 40S ribosomal protein S18



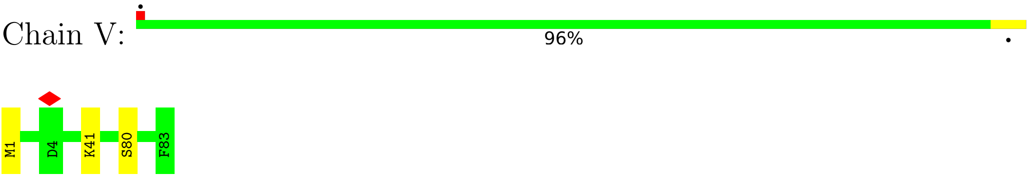
- Molecule 15: 40S ribosomal protein S19



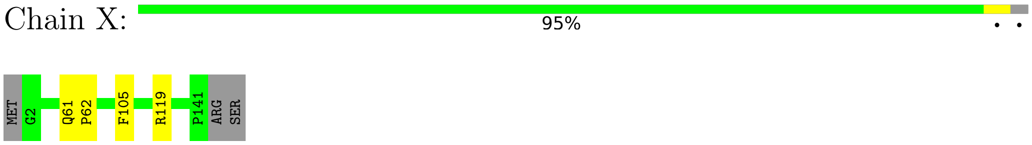
- Molecule 16: 40S ribosomal protein S20



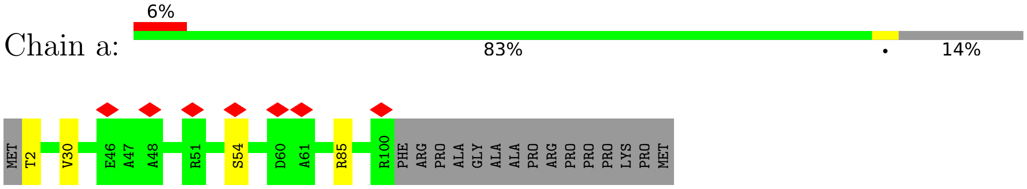
- Molecule 17: 40S ribosomal protein S21



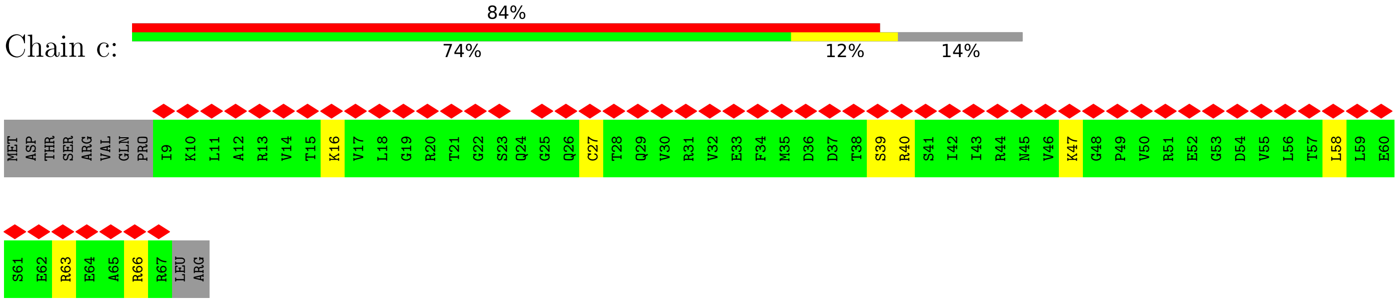
- Molecule 18: 40S ribosomal protein S23



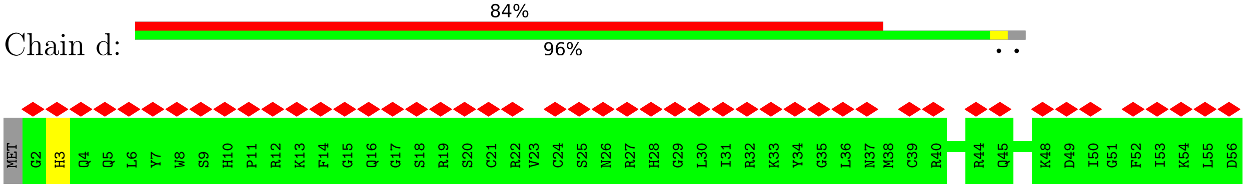
- Molecule 19: 40S ribosomal protein S26



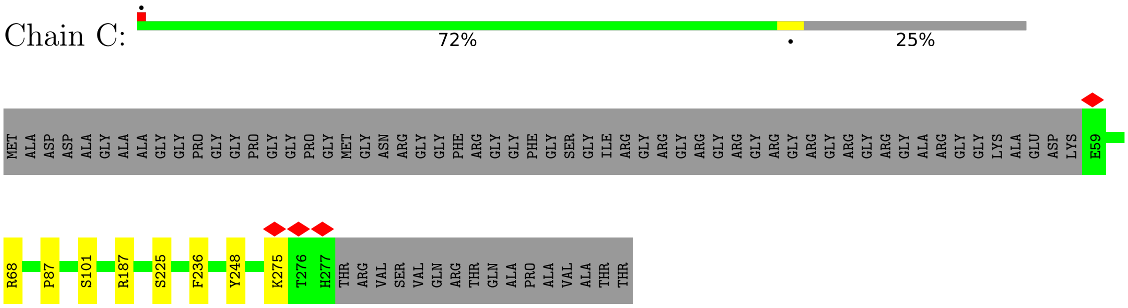
- Molecule 20: 40S ribosomal protein S28



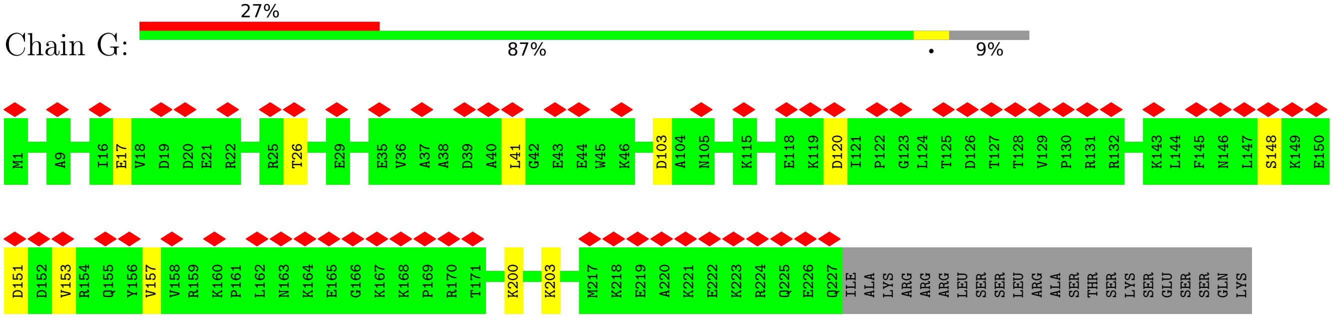
- Molecule 21: 40S ribosomal protein S29



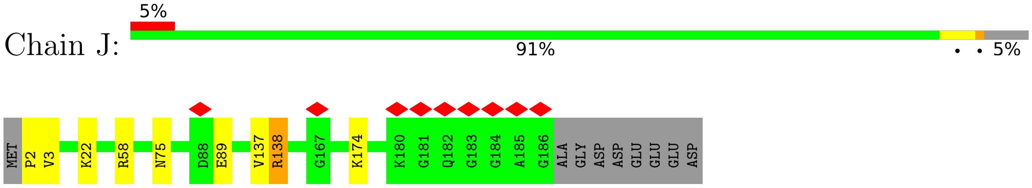
- Molecule 22: 40S ribosomal protein S2



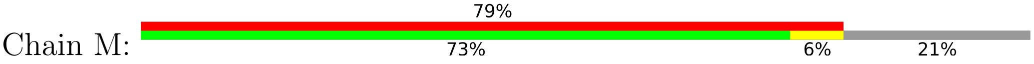
- Molecule 23: 40S ribosomal protein S6

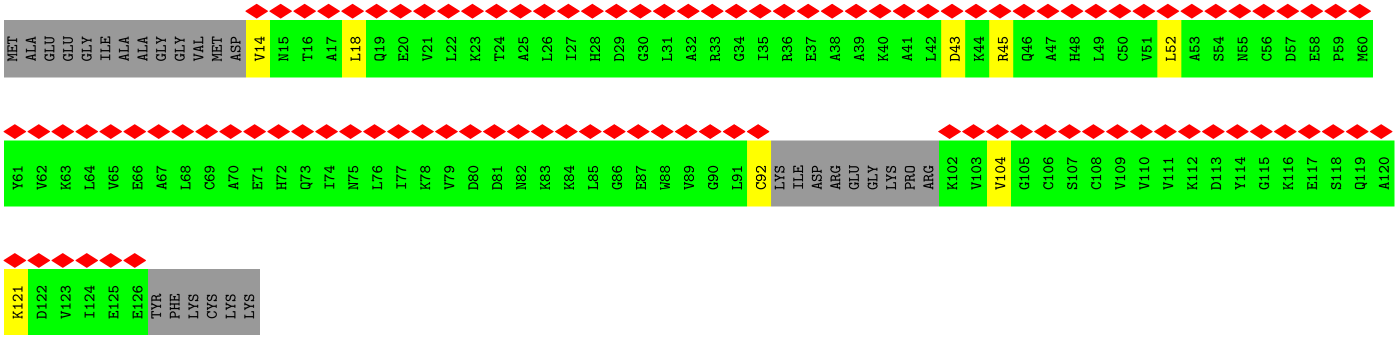


- Molecule 24: 40S ribosomal protein S9



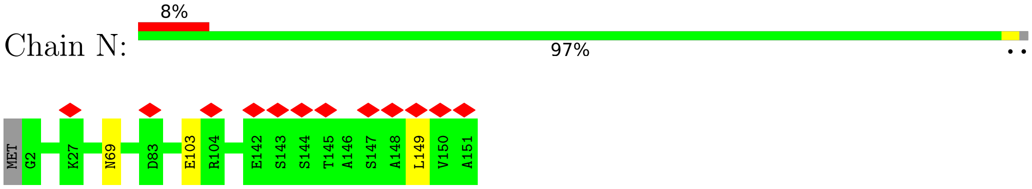
- Molecule 25: 40S ribosomal protein S12





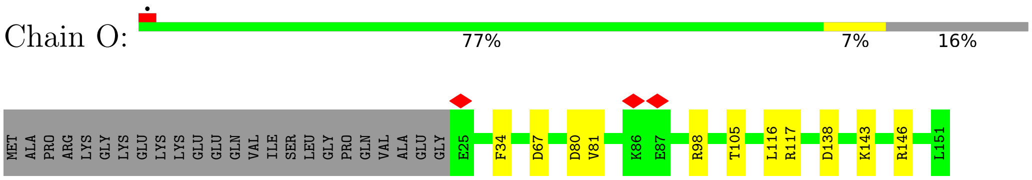
- Molecule 26: 40S ribosomal protein S13

Chain N:



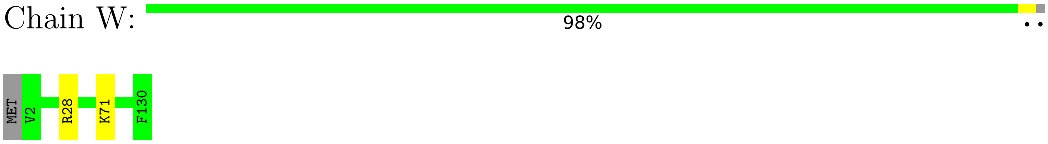
- Molecule 27: 40S ribosomal protein S14

Chain O:



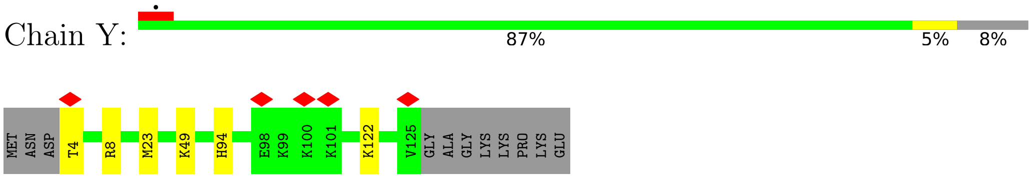
- Molecule 28: 40S ribosomal protein S15a

Chain W:



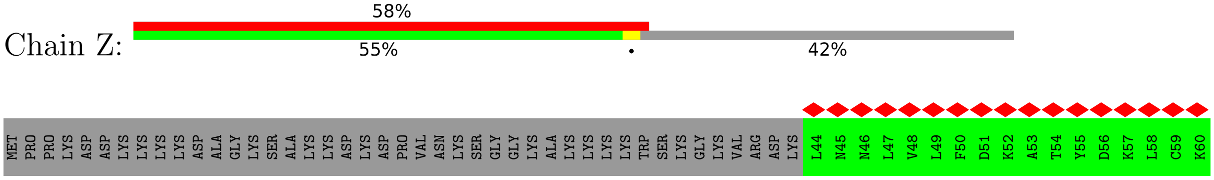
- Molecule 29: 40S ribosomal protein S24

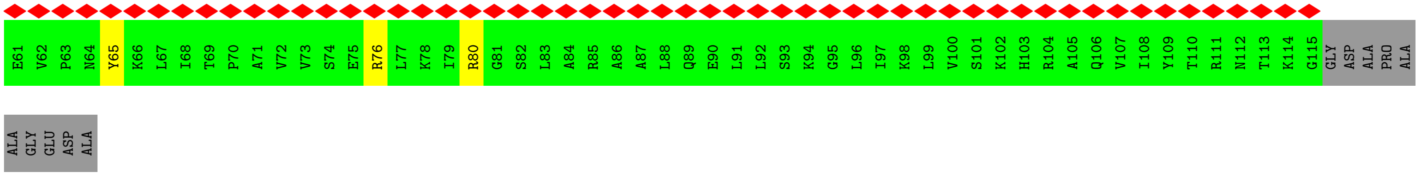
Chain Y:



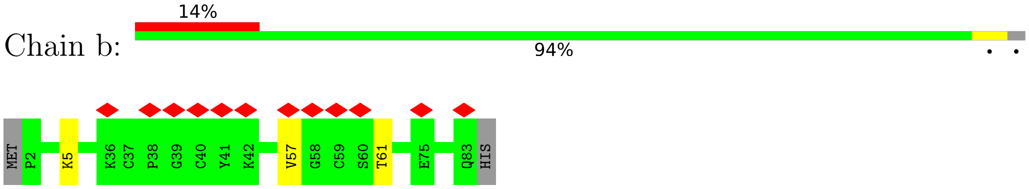
- Molecule 30: 40S ribosomal protein S25

Chain Z:

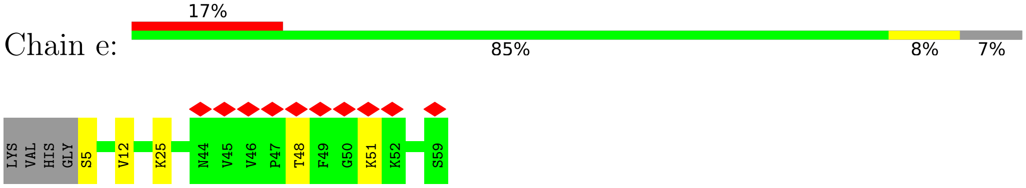




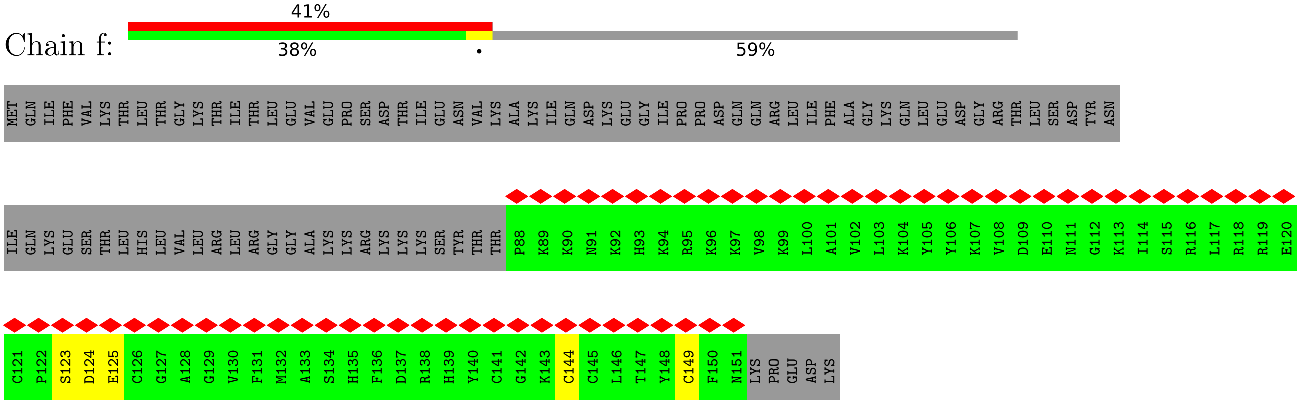
- Molecule 31: 40S ribosomal protein S27



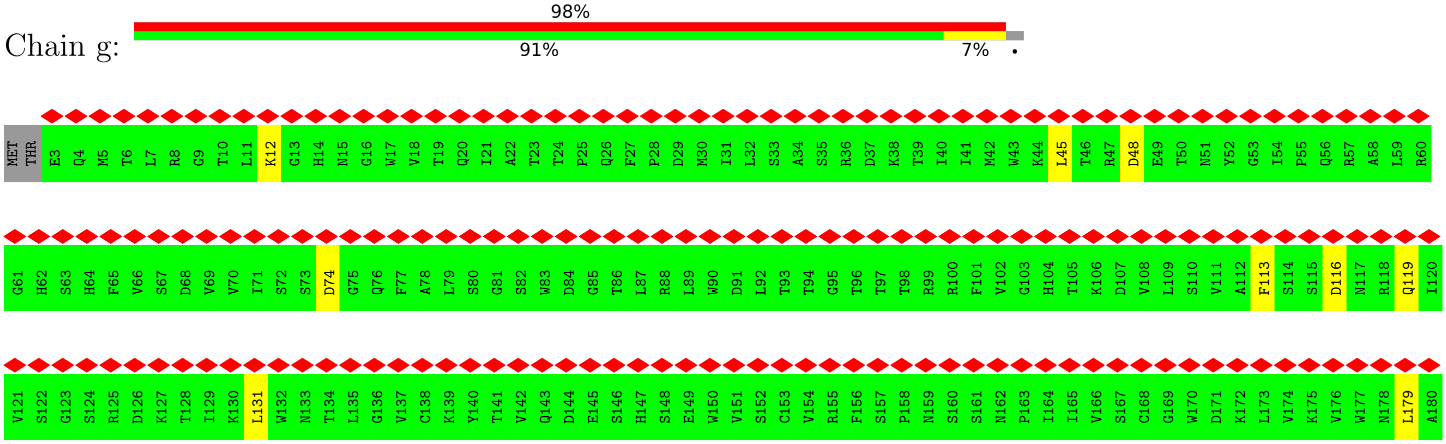
- Molecule 32: 40S ribosomal protein S30



- Molecule 33: Ubiquitin-40S ribosomal protein S27a

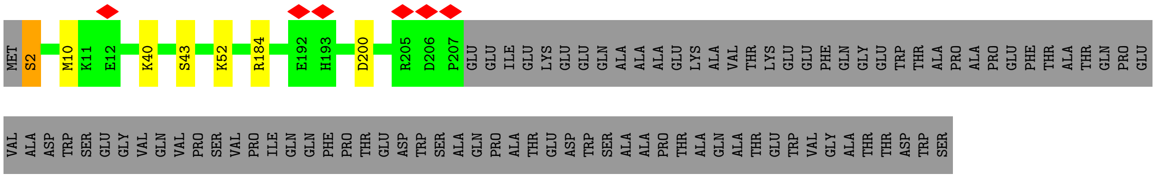


- Molecule 34: Receptor of activated protein C kinase 1



- Molecule 35: 40S ribosomal protein SA

Chain A:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474276	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 $(e^-/\text{Å}^2)$	40.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	423.2704, 423.2704, 423.2704	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8267, 0.8267, 0.8267	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: IAS, 6MZ, SAC, MA6, OMG, OMC, PSU, AME, MG, 4AC, B8N, 7MG, HY3, K, A2M, OMU, ZN

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	n	0.47	0/194	0.61	0/246
2	2	1.06	18/37770 (0.0%)	1.06	72/58857 (0.1%)
3	B	0.41	0/1738	0.53	0/2325
4	D	0.48	0/1773	0.58	0/2387
5	E	0.45	0/2083	0.58	1/2805 (0.0%)
6	F	0.44	0/1465	0.55	0/1969
7	H	0.35	0/1498	0.56	1/2005 (0.0%)
8	I	0.44	0/1711	0.60	0/2282
9	K	0.48	0/840	0.58	1/1133 (0.1%)
10	L	0.48	0/1177	0.58	0/1574
11	P	0.40	0/1024	0.53	0/1369
12	Q	0.44	0/1122	0.56	0/1503
13	R	0.45	0/1078	0.62	2/1447 (0.1%)
14	S	0.39	0/1214	0.55	0/1626
15	T	0.41	0/1131	0.54	0/1515
16	U	0.41	0/831	0.57	0/1115
17	V	0.47	0/635	0.58	0/850
18	X	0.48	0/1096	0.61	0/1461
19	a	0.57	0/805	0.62	0/1079
20	c	0.47	0/465	0.62	0/621
21	d	0.43	0/470	0.57	0/623
22	C	0.53	0/1748	0.60	0/2361
23	G	0.39	0/1863	0.56	0/2481
24	J	0.47	0/1550	0.57	0/2069
25	M	0.34	0/796	0.51	0/1072
26	N	0.41	0/1232	0.53	0/1656
27	O	0.53	1/960 (0.1%)	0.68	0/1284
28	W	0.50	0/1051	0.58	0/1406
29	Y	0.46	0/1019	0.54	0/1354
30	Z	0.33	0/576	0.59	0/774
31	b	0.42	0/653	0.52	0/876
32	e	0.43	0/443	0.54	0/582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.43	0/533	0.59	0/706
34	g	0.41	0/2486	0.59	0/3384
35	A	0.50	0/1659	0.56	0/2254
All	All	0.81	19/76689 (0.0%)	0.86	77/111051 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	2
14	S	0	1
16	U	0	1
24	J	0	1
35	A	0	1
All	All	0	6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1622	U	O3'-P	-16.84	1.41	1.61
2	2	1145	A	N9-C4	-7.04	1.33	1.37
2	2	1345	G	N7-C5	-6.10	1.35	1.39
2	2	1498	A	N9-C4	-6.07	1.34	1.37
2	2	1860	A	N7-C5	-5.68	1.35	1.39
2	2	1345	G	C6-N1	-5.60	1.35	1.39
2	2	6	G	C8-N7	-5.58	1.27	1.30
27	O	146	ARG	CB-CG	-5.55	1.37	1.52
2	2	1694	U	C4-O4	-5.53	1.19	1.23
2	2	1389	C	N3-C4	-5.41	1.30	1.33
2	2	1204	A	C8-N7	-5.34	1.27	1.31
2	2	1344	A	N9-C4	-5.24	1.34	1.37
2	2	1388	A	N9-C4	-5.17	1.34	1.37
2	2	1145	A	C5-C4	-5.12	1.35	1.38
2	2	46	A	N9-C4	-5.12	1.34	1.37
2	2	1858	G	C8-N7	-5.11	1.27	1.30
2	2	1865	C	N3-C4	-5.11	1.30	1.33
2	2	1482	C	N3-C4	-5.09	1.30	1.33
2	2	12	U	C2-N3	-5.06	1.34	1.37

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	293	C	N1-C2-O2	9.81	124.78	118.90
2	2	1865	C	C4-C5-C6	9.72	122.26	117.40
2	2	1622	U	P-O3'-C3'	9.08	130.59	119.70
2	2	293	C	N3-C2-O2	-8.72	115.80	121.90
2	2	1453	C	N1-C2-O2	8.69	124.12	118.90
2	2	568[A]	C	C2-N1-C1'	8.31	127.94	118.80
2	2	568[B]	C	C2-N1-C1'	8.31	127.94	118.80
2	2	1865	C	C5-C6-N1	-8.27	116.87	121.00
2	2	583	C	N1-C2-O2	7.68	123.51	118.90
2	2	73	C	N1-C2-O2	7.61	123.46	118.90
2	2	1632	G	O4'-C1'-N9	7.56	114.25	108.20
2	2	1453	C	C2-N1-C1'	7.52	127.07	118.80
2	2	1146	C	O5'-P-OP1	-7.37	99.07	105.70
2	2	293	C	C2-N1-C1'	7.31	126.84	118.80
2	2	583	C	C2-N1-C1'	7.25	126.78	118.80
13	R	86	PRO	N-CD-CG	-7.13	92.51	103.20
2	2	1453	C	N3-C2-O2	-7.11	116.92	121.90
2	2	1243	U	O5'-P-OP2	-7.10	99.31	105.70
2	2	179	C	N1-C2-O2	7.10	123.16	118.90
2	2	1144	A	O5'-P-OP2	-7.06	99.34	105.70
2	2	1865	C	N3-C2-O2	-6.96	117.03	121.90
2	2	73	C	N3-C2-O2	-6.91	117.06	121.90
2	2	583	C	N3-C2-O2	-6.60	117.28	121.90
2	2	1865	C	N1-C2-N3	6.51	123.76	119.20
2	2	1243	U	N1-C2-O2	6.37	127.26	122.80
2	2	73	C	C6-N1-C2	-6.16	117.84	120.30
2	2	568[A]	C	C6-N1-C1'	-6.02	113.57	120.80
2	2	568[B]	C	C6-N1-C1'	-6.02	113.57	120.80
2	2	568[A]	C	N1-C2-O2	5.85	122.41	118.90
2	2	568[B]	C	N1-C2-O2	5.85	122.41	118.90
2	2	293	C	C6-N1-C2	-5.82	117.97	120.30
2	2	1165	G	O4'-C1'-N9	5.81	112.84	108.20
2	2	1463	U	C2-N1-C1'	5.80	124.66	117.70
2	2	1434	C	P-O3'-C3'	5.77	126.62	119.70
2	2	346	C	C6-N1-C2	-5.76	117.99	120.30
2	2	1146	C	C6-N1-C2	-5.75	118.00	120.30
2	2	1453	C	C6-N1-C2	-5.68	118.03	120.30
2	2	1786	U	N3-C2-O2	-5.66	118.24	122.20
2	2	520	A	C6-N1-C2	5.66	122.00	118.60
2	2	341	C	C6-N1-C2	-5.63	118.05	120.30
2	2	583	C	C6-N1-C2	-5.62	118.05	120.30
2	2	1022	U	C2-N1-C1'	5.61	124.43	117.70
2	2	1865	C	C2-N3-C4	-5.60	117.10	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1534	C	C2-N1-C1'	5.60	124.96	118.80
2	2	322	C	C5-C6-N1	5.54	123.77	121.00
2	2	1623[A]	A	O4'-C1'-N9	5.52	112.61	108.20
2	2	1623[B]	A	O4'-C1'-N9	5.52	112.61	108.20
2	2	402	C	C2-N3-C4	5.47	122.64	119.90
2	2	1243	U	N3-C2-O2	-5.46	118.38	122.20
13	R	86	PRO	CA-N-CD	-5.41	103.92	111.50
2	2	1434	C	OP2-P-O3'	5.40	117.07	105.20
2	2	834	C	N3-C2-O2	-5.36	118.14	121.90
2	2	1659	U	O4'-C1'-N1	5.35	112.48	108.20
2	2	538	U	N3-C2-O2	-5.28	118.51	122.20
2	2	130	G	N3-C4-N9	5.27	129.16	126.00
2	2	1663	A	O4'-C1'-N9	5.26	112.41	108.20
2	2	179	C	N3-C2-O2	-5.26	118.22	121.90
2	2	73	C	C2-N1-C1'	5.25	124.58	118.80
5	E	139	LEU	CA-CB-CG	5.24	127.35	115.30
2	2	46	A	C8-N9-C4	5.24	107.89	105.80
2	2	1497	G	N3-C4-N9	-5.21	122.87	126.00
2	2	1165	G	C2-N3-C4	5.18	114.49	111.90
7	H	32	MET	CA-CB-CG	5.18	122.11	113.30
2	2	548	C	C2-N1-C1'	5.15	124.47	118.80
2	2	1039	C	C6-N1-C2	-5.13	118.25	120.30
2	2	16	G	C5-C6-O6	-5.10	125.54	128.60
2	2	568[A]	C	N3-C2-O2	-5.09	118.33	121.90
2	2	568[B]	C	N3-C2-O2	-5.09	118.33	121.90
2	2	1139	C	C5-C4-N4	5.09	123.76	120.20
2	2	1453	C	C5-C6-N1	5.08	123.54	121.00
2	2	20	G	N1-C6-O6	-5.08	116.85	119.90
2	2	1379	A	N9-C4-C5	-5.07	103.77	105.80
2	2	1153	C	C6-N1-C2	5.06	122.32	120.30
9	K	18	GLU	N-CA-C	-5.04	97.38	111.00
2	2	1022	U	N3-C2-O2	-5.04	118.67	122.20
2	2	659	G	C8-N9-C1'	-5.02	120.47	127.00
2	2	659	G	C4-N9-C1'	5.01	133.01	126.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	A	2	SAC	Mainchain
7	H	15	LYS	Peptide
7	H	42	GLU	Peptide

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Mol	Chain	Res	Type	Group
24	J	137	VAL	Peptide
14	S	99	LEU	Peptide
16	U	107	GLU	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	18/25 (72%)	17 (94%)	1 (6%)	0	100	100
3	B	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
4	D	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
5	E	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
6	F	178/204 (87%)	171 (96%)	7 (4%)	0	100	100
7	H	180/194 (93%)	156 (87%)	24 (13%)	0	100	100
8	I	203/208 (98%)	199 (98%)	4 (2%)	0	100	100
9	K	95/165 (58%)	86 (90%)	8 (8%)	1 (1%)	14	8
10	L	137/158 (87%)	131 (96%)	6 (4%)	0	100	100
11	P	121/145 (83%)	118 (98%)	2 (2%)	1 (1%)	19	12
12	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
13	R	129/135 (96%)	121 (94%)	8 (6%)	0	100	100
14	S	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
15	T	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
16	U	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
17	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
19	a	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
20	c	57/69 (83%)	53 (93%)	4 (7%)	0	100	100
21	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
22	C	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
23	G	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
24	J	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	29	22
25	M	100/132 (76%)	92 (92%)	8 (8%)	0	100	100
26	N	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
27	O	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
28	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
29	Y	120/133 (90%)	118 (98%)	2 (2%)	0	100	100
30	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
31	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
32	e	53/59 (90%)	48 (91%)	5 (9%)	0	100	100
33	f	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
34	g	310/317 (98%)	286 (92%)	24 (8%)	0	100	100
35	A	205/295 (70%)	200 (98%)	5 (2%)	0	100	100
All	All	4717/5501 (86%)	4535 (96%)	179 (4%)	3 (0%)	54	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	K	19	GLY
24	J	138	ARG
11	P	18	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	19/24 (79%)	19 (100%)	0	100	100
3	B	192/231 (83%)	184 (96%)	8 (4%)	30	28
4	D	188/202 (93%)	171 (91%)	17 (9%)	9	5
5	E	220/225 (98%)	218 (99%)	2 (1%)	78	83
6	F	155/170 (91%)	147 (95%)	8 (5%)	23	19
7	H	164/174 (94%)	154 (94%)	10 (6%)	18	14
8	I	178/180 (99%)	162 (91%)	16 (9%)	9	5
9	K	88/136 (65%)	83 (94%)	5 (6%)	20	16
10	L	128/142 (90%)	125 (98%)	3 (2%)	50	53
11	P	109/130 (84%)	102 (94%)	7 (6%)	17	12
12	Q	115/121 (95%)	111 (96%)	4 (4%)	36	34
13	R	119/122 (98%)	107 (90%)	12 (10%)	7	4
14	S	125/132 (95%)	120 (96%)	5 (4%)	31	29
15	T	113/115 (98%)	112 (99%)	1 (1%)	78	83
16	U	94/107 (88%)	91 (97%)	3 (3%)	39	38
17	V	66/66 (100%)	64 (97%)	2 (3%)	41	40
18	X	111/114 (97%)	108 (97%)	3 (3%)	44	46
19	a	86/98 (88%)	82 (95%)	4 (5%)	26	23
20	c	52/62 (84%)	44 (85%)	8 (15%)	2	1
21	d	48/49 (98%)	47 (98%)	1 (2%)	53	57
22	C	186/225 (83%)	178 (96%)	8 (4%)	29	27
23	G	198/218 (91%)	187 (94%)	11 (6%)	21	16
24	J	161/168 (96%)	153 (95%)	8 (5%)	24	21
25	M	86/108 (80%)	78 (91%)	8 (9%)	9	5
26	N	130/131 (99%)	127 (98%)	3 (2%)	50	53
27	O	99/118 (84%)	90 (91%)	9 (9%)	9	5
28	W	112/113 (99%)	110 (98%)	2 (2%)	59	63
29	Y	107/115 (93%)	101 (94%)	6 (6%)	21	16
30	Z	63/103 (61%)	60 (95%)	3 (5%)	25	22
31	b	74/76 (97%)	71 (96%)	3 (4%)	30	29
32	e	45/48 (94%)	40 (89%)	5 (11%)	6	2
33	f	57/140 (41%)	52 (91%)	5 (9%)	10	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	g	271/275 (98%)	249 (92%)	22 (8%)	11	7
35	A	172/242 (71%)	166 (96%)	6 (4%)	36	34
All	All	4131/4680 (88%)	3913 (95%)	218 (5%)	26	19

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	50	THR
3	B	55	THR
3	B	59	SER
3	B	60	ASP
3	B	86	LEU
3	B	91	VAL
3	B	94	LYS
3	B	219	LYS
4	D	27	ARG
4	D	42	THR
4	D	45	ARG
4	D	46	THR
4	D	55	THR
4	D	58	VAL
4	D	61	GLU
4	D	64	ARG
4	D	83	SER
4	D	84	VAL
4	D	90	LYS
4	D	93	THR
4	D	143	ARG
4	D	164	VAL
4	D	175	VAL
4	D	197	LYS
4	D	211	VAL
5	E	108	ARG
5	E	168	LYS
6	F	32	ASP
6	F	41	VAL
6	F	122	ARG
6	F	124	ASP
6	F	128	ILE
6	F	136	ARG
6	F	140	ASP

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Mol	Chain	Res	Type
6	F	145	ARG
7	H	7	LYS
7	H	10	LYS
7	H	29	GLU
7	H	32	MET
7	H	46	THR
7	H	53	VAL
7	H	72	PHE
7	H	78	ARG
7	H	121	THR
7	H	167	GLU
8	I	4	SER
8	I	7	ASN
8	I	17	LYS
8	I	26	LYS
8	I	56	ARG
8	I	62	VAL
8	I	75	LYS
8	I	110	ARG
8	I	115	SER
8	I	125	LYS
8	I	128	LYS
8	I	155	ASN
8	I	157	LYS
8	I	159	SER
8	I	193	LYS
8	I	203	LYS
9	K	2	LEU
9	K	18	GLU
9	K	58	VAL
9	K	88	GLU
9	K	96	ARG
10	L	69	ARG
10	L	74	SER
10	L	141	ASN
11	P	16	THR
11	P	51	ARG
11	P	57	LEU
11	P	65	LYS
11	P	82	ASP
11	P	130	ARG
11	P	136	THR

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Mol	Chain	Res	Type
12	Q	46	THR
12	Q	60	LYS
12	Q	100	VAL
12	Q	118	THR
13	R	5	ARG
13	R	30	THR
13	R	61	ILE
13	R	67	ARG
13	R	73	LEU
13	R	78	ARG
13	R	94	GLU
13	R	105	MET
13	R	110	ASP
13	R	115	SER
13	R	116	ASN
13	R	124	VAL
14	S	14	ARG
14	S	21	ASP
14	S	49	ASP
14	S	55	ARG
14	S	83	PHE
15	T	25	SER
16	U	19	ARG
16	U	25	THR
16	U	28	ASN
17	V	41	LYS
17	V	80	SER
18	X	61	GLN
18	X	105	PHE
18	X	119	ARG
19	a	2	THR
19	a	30	VAL
19	a	54	SER
19	a	85	ARG
20	c	16	LYS
20	c	27	CYS
20	c	39	SER
20	c	40	ARG
20	c	47	LYS
20	c	58	LEU
20	c	63	ARG
20	c	66	ARG

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Mol	Chain	Res	Type
21	d	3	HIS
22	C	68	ARG
22	C	87	PRO
22	C	101	SER
22	C	187	ARG
22	C	225	SER
22	C	236	PHE
22	C	248	TYR
22	C	275	LYS
23	G	17	GLU
23	G	26	THR
23	G	41	LEU
23	G	103	ASP
23	G	120	ASP
23	G	148	SER
23	G	151	ASP
23	G	153	VAL
23	G	157	VAL
23	G	200	LYS
23	G	203	LYS
24	J	2	PRO
24	J	3	VAL
24	J	22	LYS
24	J	58	ARG
24	J	75	ASN
24	J	89	GLU
24	J	138	ARG
24	J	174	LYS
25	M	14	VAL
25	M	18	LEU
25	M	43	ASP
25	M	45	ARG
25	M	52	LEU
25	M	92	CYS
25	M	104	VAL
25	M	121	LYS
26	N	69	ASN
26	N	103	GLU
26	N	149	LEU
27	O	34	PHE
27	O	67	ASP
27	O	80	ASP

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Mol	Chain	Res	Type
27	O	81	VAL
27	O	98	ARG
27	O	105	THR
27	O	116	LEU
27	O	117	ARG
27	O	143	LYS
28	W	28	ARG
28	W	71	LYS
29	Y	4	THR
29	Y	8	ARG
29	Y	23	MET
29	Y	49	LYS
29	Y	94	HIS
29	Y	122	LYS
30	Z	65	TYR
30	Z	76	ARG
30	Z	80	ARG
31	b	5	LYS
31	b	57	VAL
31	b	61	THR
32	e	5	SER
32	e	12	VAL
32	e	25	LYS
32	e	48	THR
32	e	51	LYS
33	f	123	SER
33	f	124	ASP
33	f	125	GLU
33	f	144	CYS
33	f	149	CYS
34	g	12	LYS
34	g	45	LEU
34	g	48	ASP
34	g	74	ASP
34	g	113	PHE
34	g	116	ASP
34	g	119	GLN
34	g	131	LEU
34	g	179	LEU
34	g	201	SER
34	g	205	SER
34	g	213	ASP

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Mol	Chain	Res	Type
34	g	231	ASP
34	g	268	ASP
34	g	272	GLN
34	g	276	SER
34	g	277	THR
34	g	280	LYS
34	g	294	ASP
34	g	297	THR
34	g	304	ASP
34	g	313	THR
35	A	10	MET
35	A	40	LYS
35	A	43	SER
35	A	52	LYS
35	A	184	ARG
35	A	200	ASP

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

Mol	Chain	Res	Type
16	U	92	HIS
18	X	26	GLN
21	d	10	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1622/1868 (86%)	261 (16%)	7 (0%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	4	C
2	2	17	C
2	2	33	G
2	2	46	A
2	2	56	G
2	2	59	U
2	2	65	C
2	2	67	C

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Mol	Chain	Res	Type
2	2	68	A
2	2	72	C
2	2	74	G
2	2	75	G
2	2	82	G
2	2	99	A2M
2	2	103	A
2	2	113	G
2	2	115	U
2	2	126	G
2	2	130	G
2	2	143	U
2	2	155	G
2	2	160	U
2	2	178	C
2	2	184	G
2	2	191	A
2	2	192	C
2	2	205	G
2	2	211	G
2	2	212	C
2	2	302	A
2	2	306	C
2	2	309	G
2	2	319	C
2	2	320	G
2	2	330	G
2	2	332	G
2	2	333	G
2	2	335	G
2	2	339	A
2	2	340	C
2	2	347	G
2	2	362	C
2	2	364	A
2	2	368	U
2	2	370	G
2	2	385	G
2	2	386	C
2	2	409	C
2	2	438	G
2	2	448	A

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Mol	Chain	Res	Type
2	2	449	A
2	2	450	C
2	2	464	A
2	2	470	G
2	2	471	G
2	2	472	C
2	2	474	G
2	2	482	G
2	2	487	U
2	2	492	C
2	2	516	A
2	2	532	C
2	2	533	A
2	2	535	G
2	2	536	A
2	2	537	C
2	2	538	U
2	2	540	U
2	2	541	U
2	2	542	U
2	2	543	C
2	2	544	G
2	2	546	G
2	2	547	G
2	2	548	C
2	2	549	C
2	2	550	C
2	2	554	A
2	2	555	A
2	2	563	G
2	2	583	C
2	2	587	A
2	2	589	G
2	2	591	U
2	2	614	C
2	2	617	G
2	2	628	A
2	2	629	A
2	2	632	C
2	2	643	A
2	2	655	A
2	2	668	A2M

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Mol	Chain	Res	Type
2	2	669	A
2	2	671	A
2	2	672	A
2	2	688	U
2	2	690	G
2	2	692	G
2	2	693	A
2	2	695	C
2	2	696	G
2	2	697	G
2	2	698	G
2	2	731	G
2	2	732	U
2	2	733	C
2	2	735	C
2	2	736	C
2	2	738	C
2	2	739	C
2	2	801	U
2	2	821	G
2	2	822	PSU
2	2	847	A
2	2	859	G
2	2	869	A
2	2	870	A
2	2	871	U
2	2	877	C
2	2	913	A
2	2	920	A
2	2	922	A
2	2	933	G
2	2	943	U
2	2	955	A
2	2	971	G
2	2	990	A
2	2	992	A
2	2	1017	U
2	2	1023	A
2	2	1060	A
2	2	1061	U
2	2	1062	A
2	2	1078	C

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Mol	Chain	Res	Type
2	2	1083	A
2	2	1085	C
2	2	1087	A
2	2	1109	C
2	2	1115	U
2	2	1116	C
2	2	1117	C
2	2	1119	A
2	2	1121	G
2	2	1133	A
2	2	1138	C
2	2	1144	A
2	2	1153	C
2	2	1154	U
2	2	1171	G
2	2	1195	A
2	2	1207	G
2	2	1215	C
2	2	1221	G
2	2	1242	U
2	2	1243	U
2	2	1251	A
2	2	1253	A
2	2	1256	G
2	2	1257	G
2	2	1259	A
2	2	1274	G
2	2	1275	G
2	2	1294	G
2	2	1295	A
2	2	1301	A
2	2	1302	G
2	2	1303	C
2	2	1308	U
2	2	1320	G
2	2	1322	G
2	2	1342	U
2	2	1344	A
2	2	1348	G
2	2	1371	U
2	2	1372	U
2	2	1378	A

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Mol	Chain	Res	Type
2	2	1382	A
2	2	1397	U
2	2	1404	U
2	2	1406	G
2	2	1423	C
2	2	1435	C
2	2	1436	C
2	2	1449	G
2	2	1454	A
2	2	1461	G
2	2	1462	U
2	2	1463	U
2	2	1488	C
2	2	1489	A
2	2	1490	OMG
2	2	1497	G
2	2	1498	A
2	2	1508	A
2	2	1520	G
2	2	1521	C
2	2	1533	A
2	2	1548	G
2	2	1553	C
2	2	1579	A
2	2	1580	A
2	2	1588	A
2	2	1601	A
2	2	1621	U
2	2	1639	7MG
2	2	1654	G
2	2	1664	A
2	2	1665	G
2	2	1671	G
2	2	1680	G
2	2	1712	A
2	2	1713	C
2	2	1715	A
2	2	1717	C
2	2	1719	A
2	2	1721	U
2	2	1722	G
2	2	1723	G

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Mol	Chain	Res	Type
2	2	1726	G
2	2	1728	U
2	2	1744	G
2	2	1745	A
2	2	1746	U
2	2	1748	G
2	2	1752	C
2	2	1753	C
2	2	1754	G
2	2	1755	C
2	2	1760	G
2	2	1761	U
2	2	1772	C
2	2	1773	C
2	2	1774	C
2	2	1775	U
2	2	1777	G
2	2	1778	C
2	2	1779	G
2	2	1781	A
2	2	1782	G
2	2	1783	C
2	2	1784	G
2	2	1786	U
2	2	1800	A
2	2	1801	A
2	2	1807	C
2	2	1812	U
2	2	1813	A
2	2	1815	A
2	2	1816	G
2	2	1819	A
2	2	1829	G
2	2	1831	A
2	2	1835	A
2	2	1836	G
2	2	1838	U
2	2	1849	G
2	2	1861	G
2	2	1862	G
2	2	1863	A
2	2	1864	U

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Mol	Chain	Res	Type
2	2	1865	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	331	C
2	2	531	A
2	2	912	C
2	2	1165	G
2	2	1434	C
2	2	1520	G
2	2	1679	A

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

77 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	$\#\|Z\| > 2$
2	PSU	2	815	2	18,21,22	4.01	7 (38%)	22,30,33	1.85	4 (18%)
2	PSU	2	1081	2	18,21,22	3.99	8 (44%)	22,30,33	1.87	6 (27%)
2	A2M	2	1678	2	18,25,26	0.95	1 (5%)	18,36,39	1.21	2 (11%)
17	AME	V	1	17	9,10,11	1.36	1 (11%)	9,11,13	2.01	2 (22%)
2	PSU	2	1238	2	18,21,22	3.92	7 (38%)	22,30,33	1.79	4 (18%)
18	HY3	X	62	36,18	6,8,9	8.45	4 (66%)	5,10,12	1.18	0
2	PSU	2	1244	2	18,21,22	3.98	7 (38%)	22,30,33	2.12	5 (22%)
2	PSU	2	1177	2	18,21,22	1.36	4 (22%)	22,30,33	1.89	4 (18%)
2	A2M	2	590	2	18,25,26	3.63	7 (38%)	18,36,39	3.47	5 (27%)
2	PSU	2	1136	2	18,21,22	3.86	8 (44%)	22,30,33	1.96	4 (18%)
2	PSU	2	1347	2	18,21,22	1.44	3 (16%)	22,30,33	1.90	4 (18%)
2	PSU	2	863	2	18,21,22	3.72	7 (38%)	22,30,33	2.05	5 (22%)
2	OMU	2	1288	2	19,22,23	2.86	7 (36%)	26,31,34	1.75	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	OMC	2	174	2,37	19,22,23	2.75	8 (42%)	26,31,34	0.93	0
2	OMU	2	1442	2,37	19,22,23	2.87	8 (42%)	26,31,34	1.81	5 (19%)
2	A2M	2	99	2,37	18,25,26	3.59	7 (38%)	18,36,39	3.41	4 (22%)
2	A2M	2	576	2,36	18,25,26	3.76	8 (44%)	18,36,39	3.60	5 (27%)
2	A2M	2	668	2,37	18,25,26	0.92	1 (5%)	18,36,39	1.57	4 (22%)
2	PSU	2	296	2	18,21,22	3.97	7 (38%)	22,30,33	1.81	5 (22%)
2	6MZ	2	1832	2,37,36	18,25,26	2.61	5 (27%)	16,36,39	2.49	4 (25%)
2	OMC	2	462	2	19,22,23	2.73	8 (42%)	26,31,34	0.77	0
2	PSU	2	109	2,36	18,21,22	4.06	7 (38%)	22,30,33	1.82	4 (18%)
2	PSU	2	119	2	18,21,22	3.99	7 (38%)	22,30,33	1.80	5 (22%)
2	PSU	2	1643	2,37	18,21,22	1.48	4 (22%)	22,30,33	1.89	4 (18%)
2	A2M	2	1031	2	18,25,26	3.66	8 (44%)	18,36,39	3.77	4 (22%)
2	PSU	2	681	2	18,21,22	3.93	8 (44%)	22,30,33	1.83	4 (18%)
2	OMC	2	1703	2	19,22,23	2.67	8 (42%)	26,31,34	0.86	0
2	PSU	2	1625	2	18,21,22	3.95	7 (38%)	22,30,33	1.92	5 (22%)
2	PSU	2	1056	2	18,21,22	3.82	7 (38%)	22,30,33	2.08	5 (22%)
2	PSU	2	105	2,36	18,21,22	3.91	7 (38%)	22,30,33	2.12	5 (22%)
2	B8N	2	1248	2	24,29,30	2.86	7 (29%)	29,42,45	1.91	7 (24%)
2	PSU	2	649	2	18,21,22	4.06	7 (38%)	22,30,33	1.93	5 (22%)
2	OMG	2	1328	2,36	18,26,27	2.42	8 (44%)	19,38,41	1.80	5 (26%)
2	OMU	2	354	2	19,22,23	2.88	8 (42%)	26,31,34	1.91	6 (23%)
2	OMG	2	436	2	18,26,27	2.37	8 (44%)	19,38,41	1.51	5 (26%)
2	PSU	2	686	2	18,21,22	4.08	7 (38%)	22,30,33	1.98	5 (22%)
2	PSU	2	1046	2,36	18,21,22	4.00	7 (38%)	22,30,33	1.78	3 (13%)
2	PSU	2	36	2	18,21,22	1.45	4 (22%)	22,30,33	1.80	4 (18%)
2	A2M	2	484	2	18,25,26	0.93	1 (5%)	18,36,39	1.36	3 (16%)
2	OMG	2	601	2	18,26,27	2.27	8 (44%)	19,38,41	1.70	5 (26%)
2	PSU	2	1045	2	18,21,22	4.14	7 (38%)	22,30,33	1.94	5 (22%)
2	A2M	2	468	2	18,25,26	3.67	8 (44%)	18,36,39	3.85	4 (22%)
2	OMG	2	1490	2,37	18,26,27	0.97	1 (5%)	19,38,41	1.10	2 (10%)
2	MA6	2	1851	2	19,26,27	0.97	1 (5%)	18,38,41	1.91	5 (27%)
2	PSU	2	572	2,36	18,21,22	4.06	7 (38%)	22,30,33	1.88	4 (18%)
2	7MG	2	1639	2	22,26,27	1.38	3 (13%)	29,39,42	2.53	7 (24%)
35	SAC	A	2	35	7,8,9	1.57	2 (28%)	8,9,11	1.45	2 (25%)
2	OMU	2	1326	2,37	19,22,23	2.86	8 (42%)	26,31,34	2.02	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	OMC	2	517	2	19,22,23	2.68	8 (42%)	26,31,34	0.79	0
2	OMG	2	509	2,37	18,26,27	2.26	8 (44%)	19,38,41	1.58	4 (21%)
2	OMG	2	644	2	18,26,27	2.30	8 (44%)	19,38,41	1.60	5 (26%)
2	A2M	2	27	2,37	18,25,26	0.99	1 (5%)	18,36,39	1.35	3 (16%)
2	OMU	2	121	2	19,22,23	2.73	8 (42%)	26,31,34	1.75	5 (19%)
2	A2M	2	512	2	18,25,26	3.72	9 (50%)	18,36,39	3.38	5 (27%)
2	4AC	2	1337	2	21,24,25	3.37	10 (47%)	29,34,37	1.63	6 (20%)
2	PSU	2	1174	2,36	18,21,22	1.41	3 (16%)	22,30,33	1.83	3 (13%)
2	PSU	2	1445	2	18,21,22	3.99	7 (38%)	22,30,33	1.78	4 (18%)
2	OMG	2	1447	2	18,26,27	2.33	8 (44%)	19,38,41	1.57	4 (21%)
2	A2M	2	1383	2	18,25,26	3.83	9 (50%)	18,36,39	3.55	6 (33%)
2	PSU	2	822	2	18,21,22	3.94	8 (44%)	22,30,33	1.77	4 (18%)
2	OMC	2	1391	2	19,22,23	2.70	8 (42%)	26,31,34	0.91	0
2	OMC	2	1272	2	19,22,23	2.71	8 (42%)	26,31,34	0.68	0
2	A2M	2	159	2	18,25,26	3.61	7 (38%)	18,36,39	3.73	4 (22%)
2	OMU	2	116	2	19,22,23	2.78	7 (36%)	26,31,34	1.56	5 (19%)
2	OMG	2	683	2	18,26,27	2.39	8 (44%)	19,38,41	1.70	6 (31%)
2	PSU	2	651	2	18,21,22	3.93	8 (44%)	22,30,33	2.29	5 (22%)
2	PSU	2	1692	2,36	18,21,22	3.74	7 (38%)	22,30,33	1.79	4 (18%)
27	IAS	O	138	27	6,7,8	0.99	0	6,8,10	1.97	3 (50%)
2	PSU	2	93	2	18,21,22	4.01	7 (38%)	22,30,33	1.66	4 (18%)
2	OMU	2	172	2	19,22,23	2.86	7 (36%)	26,31,34	1.85	6 (23%)
2	PSU	2	814	2	18,21,22	3.86	7 (38%)	22,30,33	1.66	3 (13%)
2	PSU	2	406	2	18,21,22	3.94	7 (38%)	22,30,33	1.78	4 (18%)
2	4AC	2	1842	2	21,24,25	3.02	10 (47%)	29,34,37	1.51	4 (13%)
2	PSU	2	1232	2	18,21,22	3.98	7 (38%)	22,30,33	1.74	4 (18%)
2	OMU	2	428	2,37	19,22,23	2.86	8 (42%)	26,31,34	1.59	5 (19%)
2	A2M	2	166	2	18,25,26	3.68	8 (44%)	18,36,39	3.63	5 (27%)
2	MA6	2	1850	2	19,26,27	1.18	2 (10%)	18,38,41	2.05	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	815	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1081	2	-	1/7/25/26	0/2/2/2
2	A2M	2	1678	2	-	1/5/27/28	0/3/3/3
17	AME	V	1	17	-	3/9/10/12	-
2	PSU	2	1238	2	-	0/7/25/26	0/2/2/2
18	HY3	X	62	36,18	-	1/1/12/14	0/1/1/1
2	PSU	2	1244	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1177	2	-	0/7/25/26	0/2/2/2
2	A2M	2	590	2	-	0/5/27/28	0/3/3/3
2	PSU	2	1136	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1347	2	-	1/7/25/26	0/2/2/2
2	PSU	2	863	2	-	0/7/25/26	0/2/2/2
2	OMU	2	1288	2	-	0/9/27/28	0/2/2/2
2	OMC	2	174	2,37	-	1/9/27/28	0/2/2/2
2	OMU	2	1442	2,37	-	0/9/27/28	0/2/2/2
2	A2M	2	99	2,37	-	2/5/27/28	0/3/3/3
2	A2M	2	576	2,36	-	2/5/27/28	0/3/3/3
2	A2M	2	668	2,37	-	2/5/27/28	0/3/3/3
2	PSU	2	296	2	-	0/7/25/26	0/2/2/2
2	6MZ	2	1832	2,37,36	-	0/5/27/28	0/3/3/3
2	OMC	2	462	2	-	0/9/27/28	0/2/2/2
2	PSU	2	109	2,36	-	0/7/25/26	0/2/2/2
2	PSU	2	119	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1643	2,37	-	0/7/25/26	0/2/2/2
2	A2M	2	1031	2	-	0/5/27/28	0/3/3/3
2	PSU	2	681	2	-	0/7/25/26	0/2/2/2
2	OMC	2	1703	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1625	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1056	2	-	0/7/25/26	0/2/2/2
2	PSU	2	105	2,36	-	0/7/25/26	0/2/2/2
2	B8N	2	1248	2	-	2/16/34/35	0/2/2/2
2	PSU	2	649	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1328	2,36	-	0/5/27/28	0/3/3/3
2	OMU	2	354	2	-	0/9/27/28	0/2/2/2
2	OMG	2	436	2	-	0/5/27/28	0/3/3/3
2	PSU	2	686	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1046	2,36	-	0/7/25/26	0/2/2/2
2	PSU	2	36	2	-	0/7/25/26	0/2/2/2
2	A2M	2	484	2	-	1/5/27/28	0/3/3/3
2	OMG	2	601	2	-	0/5/27/28	0/3/3/3
2	PSU	2	1045	2	-	0/7/25/26	0/2/2/2
2	A2M	2	468	2	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	1490	2,37	-	1/5/27/28	0/3/3/3
2	MA6	2	1851	2	-	6/7/29/30	0/3/3/3
2	PSU	2	572	2,36	-	0/7/25/26	0/2/2/2
2	7MG	2	1639	2	-	0/7/37/38	0/3/3/3
35	SAC	A	2	35	-	0/7/8/10	-
2	OMU	2	1326	2,37	-	0/9/27/28	0/2/2/2
2	OMC	2	517	2	-	0/9/27/28	0/2/2/2
2	OMG	2	509	2,37	-	0/5/27/28	0/3/3/3
2	OMG	2	644	2	-	1/5/27/28	0/3/3/3
2	A2M	2	27	2,37	-	1/5/27/28	0/3/3/3
2	OMU	2	121	2	-	0/9/27/28	0/2/2/2
2	A2M	2	512	2	-	0/5/27/28	0/3/3/3
2	4AC	2	1337	2	-	2/11/29/30	0/2/2/2
2	PSU	2	1174	2,36	-	0/7/25/26	0/2/2/2
2	PSU	2	1445	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1447	2	-	2/5/27/28	0/3/3/3
2	A2M	2	1383	2	-	0/5/27/28	0/3/3/3
2	PSU	2	822	2	-	0/7/25/26	0/2/2/2
2	OMC	2	1391	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1272	2	-	0/9/27/28	0/2/2/2
2	A2M	2	159	2	-	0/5/27/28	0/3/3/3
2	OMU	2	116	2	-	1/9/27/28	0/2/2/2
2	OMG	2	683	2	-	0/5/27/28	0/3/3/3
2	PSU	2	651	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1692	2,36	-	0/7/25/26	0/2/2/2
27	IAS	O	138	27	-	2/7/7/8	-
2	PSU	2	93	2	-	0/7/25/26	0/2/2/2
2	OMU	2	172	2	-	1/9/27/28	0/2/2/2
2	PSU	2	814	2	-	0/7/25/26	0/2/2/2
2	PSU	2	406	2	-	0/7/25/26	0/2/2/2
2	4AC	2	1842	2	-	2/11/29/30	0/2/2/2
2	PSU	2	1232	2	-	0/7/25/26	0/2/2/2
2	OMU	2	428	2,37	-	4/9/27/28	0/2/2/2
2	A2M	2	166	2	-	0/5/27/28	0/3/3/3
2	MA6	2	1850	2	-	2/7/29/30	0/3/3/3

All (491) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	62	HY3	C3-CA	-19.76	1.35	1.55
2	2	686	PSU	C6-C5	10.90	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	93	PSU	C6-C5	10.88	1.48	1.35
2	2	815	PSU	C6-C5	10.84	1.47	1.35
2	2	1232	PSU	C6-C5	10.77	1.47	1.35
2	2	109	PSU	C6-C5	10.76	1.47	1.35
2	2	649	PSU	C6-C5	10.73	1.47	1.35
2	2	572	PSU	C6-C5	10.71	1.47	1.35
2	2	651	PSU	C6-C5	10.53	1.47	1.35
2	2	1045	PSU	C6-C5	10.51	1.47	1.35
2	2	1445	PSU	C6-C5	10.50	1.47	1.35
2	2	296	PSU	C6-C5	10.46	1.47	1.35
2	2	1046	PSU	C6-C5	10.46	1.47	1.35
2	2	1136	PSU	C6-C5	10.42	1.47	1.35
2	2	406	PSU	C6-C5	10.39	1.47	1.35
2	2	1625	PSU	C6-C5	10.33	1.47	1.35
2	2	105	PSU	C6-C5	10.24	1.47	1.35
2	2	1081	PSU	C6-C5	10.21	1.47	1.35
2	2	1238	PSU	C6-C5	10.11	1.47	1.35
2	2	119	PSU	C6-C5	10.00	1.47	1.35
2	2	814	PSU	C6-C5	9.96	1.46	1.35
2	2	1692	PSU	C6-C5	9.87	1.46	1.35
2	2	681	PSU	C6-C5	9.81	1.46	1.35
2	2	1244	PSU	C6-C5	9.80	1.46	1.35
2	2	822	PSU	C6-C5	9.76	1.46	1.35
2	2	1056	PSU	C6-C5	9.66	1.46	1.35
2	2	1832	6MZ	C6-N6	9.37	1.50	1.35
2	2	1045	PSU	C2-N1	9.34	1.49	1.36
2	2	863	PSU	C6-C5	9.26	1.46	1.35
2	2	1244	PSU	C2-N1	9.23	1.49	1.36
2	2	166	A2M	C3'-C4'	-9.22	1.29	1.53
2	2	119	PSU	C2-N1	8.99	1.48	1.36
2	2	686	PSU	C2-N1	8.98	1.48	1.36
2	2	109	PSU	C2-N1	8.98	1.48	1.36
2	2	572	PSU	C2-N1	8.98	1.48	1.36
2	2	649	PSU	C2-N1	8.96	1.48	1.36
2	2	822	PSU	C2-N1	8.93	1.48	1.36
2	2	590	A2M	C3'-C4'	-8.91	1.30	1.53
2	2	576	A2M	C3'-C4'	-8.87	1.30	1.53
2	2	468	A2M	C3'-C4'	-8.86	1.30	1.53
2	2	1046	PSU	C2-N1	8.86	1.48	1.36
2	2	681	PSU	C2-N1	8.86	1.48	1.36
2	2	815	PSU	C2-N1	8.84	1.48	1.36
2	2	1238	PSU	C2-N1	8.83	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	406	PSU	C2-N1	8.82	1.48	1.36
2	2	1081	PSU	C2-N1	8.80	1.48	1.36
2	2	1383	A2M	C3’-C4’	-8.75	1.30	1.53
2	2	159	A2M	C3’-C4’	-8.74	1.30	1.53
2	2	512	A2M	C3’-C4’	-8.74	1.30	1.53
2	2	1445	PSU	C2-N1	8.71	1.48	1.36
2	2	1056	PSU	C2-N1	8.69	1.48	1.36
2	2	1248	B8N	C4-N3	-8.69	1.24	1.40
2	2	99	A2M	C3’-C4’	-8.64	1.30	1.53
2	2	1031	A2M	C3’-C4’	-8.64	1.30	1.53
2	2	1232	PSU	C2-N1	8.60	1.48	1.36
2	2	1136	PSU	C2-N1	8.59	1.48	1.36
2	2	814	PSU	C2-N1	8.53	1.48	1.36
2	2	296	PSU	C2-N1	8.48	1.48	1.36
2	2	1625	PSU	C2-N1	8.45	1.48	1.36
2	2	651	PSU	C2-N1	8.40	1.48	1.36
2	2	93	PSU	C2-N1	8.36	1.48	1.36
2	2	105	PSU	C2-N1	8.16	1.47	1.36
2	2	1383	A2M	O4’-C1’	-8.09	1.29	1.41
2	2	590	A2M	O4’-C1’	-8.02	1.29	1.41
2	2	1383	A2M	O4’-C4’	7.96	1.62	1.45
2	2	863	PSU	C2-N1	7.93	1.47	1.36
2	2	576	A2M	O4’-C1’	-7.85	1.30	1.41
2	2	468	A2M	O4’-C1’	-7.85	1.30	1.41
2	2	512	A2M	O4’-C4’	7.84	1.62	1.45
2	2	1031	A2M	O4’-C1’	-7.83	1.30	1.41
2	2	576	A2M	O4’-C4’	7.78	1.62	1.45
2	2	1692	PSU	C2-N1	7.77	1.47	1.36
2	2	159	A2M	O4’-C4’	7.75	1.62	1.45
2	2	166	A2M	O4’-C4’	7.74	1.62	1.45
2	2	512	A2M	O4’-C1’	-7.64	1.30	1.41
2	2	99	A2M	O4’-C4’	7.60	1.62	1.45
2	2	1031	A2M	O4’-C4’	7.53	1.61	1.45
2	2	468	A2M	O4’-C4’	7.35	1.61	1.45
2	2	166	A2M	O4’-C1’	-7.17	1.31	1.41
2	2	159	A2M	O4’-C1’	-7.10	1.31	1.41
2	2	99	A2M	O4’-C1’	-7.09	1.31	1.41
2	2	1045	PSU	C2-N3	7.07	1.49	1.37
2	2	1248	B8N	C6-N1	7.05	1.54	1.36
2	2	1625	PSU	C2-N3	6.93	1.49	1.37
2	2	1244	PSU	C2-N3	6.86	1.49	1.37
2	2	590	A2M	O4’-C4’	6.79	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	105	PSU	C2-N3	6.71	1.49	1.37
2	2	296	PSU	C2-N3	6.71	1.49	1.37
2	2	572	PSU	C2-N3	6.70	1.49	1.37
2	2	686	PSU	C2-N3	6.69	1.49	1.37
2	2	119	PSU	C2-N3	6.63	1.48	1.37
2	2	93	PSU	C2-N3	6.62	1.48	1.37
2	2	681	PSU	C2-N3	6.59	1.48	1.37
2	2	649	PSU	C2-N3	6.59	1.48	1.37
2	2	172	OMU	C2-N3	6.56	1.49	1.38
2	2	863	PSU	C2-N3	6.56	1.48	1.37
2	2	651	PSU	C2-N3	6.52	1.48	1.37
2	2	1445	PSU	C2-N3	6.51	1.48	1.37
2	2	1046	PSU	C2-N3	6.51	1.48	1.37
2	2	172	OMU	C2-N1	6.48	1.48	1.38
2	2	1288	OMU	C2-N1	6.47	1.48	1.38
2	2	354	OMU	C2-N1	6.43	1.48	1.38
2	2	1442	OMU	C2-N1	6.42	1.48	1.38
2	2	1056	PSU	C2-N3	6.34	1.48	1.37
2	2	822	PSU	C2-N3	6.28	1.48	1.37
2	2	1232	PSU	C2-N3	6.28	1.48	1.37
2	2	1326	OMU	C2-N1	6.28	1.48	1.38
2	2	1288	OMU	C2-N3	6.28	1.49	1.38
2	2	1337	4AC	C7-N4	6.22	1.48	1.37
2	2	116	OMU	C2-N3	6.22	1.49	1.38
2	2	406	PSU	C2-N3	6.19	1.48	1.37
2	2	1081	PSU	C2-N3	6.19	1.48	1.37
2	2	428	OMU	C2-N1	6.18	1.48	1.38
2	2	814	PSU	C2-N3	6.17	1.48	1.37
2	2	1326	OMU	C2-N3	6.15	1.48	1.38
2	2	109	PSU	C2-N3	6.14	1.48	1.37
2	2	116	OMU	C2-N1	6.14	1.48	1.38
2	2	1238	PSU	C2-N3	6.11	1.48	1.37
2	2	815	PSU	C2-N3	6.10	1.48	1.37
2	2	428	OMU	C2-N3	6.10	1.48	1.38
2	2	1337	4AC	C6-C5	6.07	1.49	1.35
2	2	174	OMC	C6-C5	6.05	1.49	1.35
2	2	1442	OMU	C2-N3	6.03	1.48	1.38
2	2	1337	4AC	C4-N3	5.97	1.43	1.32
2	2	1692	PSU	C2-N3	5.82	1.47	1.37
2	2	121	OMU	C2-N3	5.78	1.48	1.38
2	2	462	OMC	C6-C5	5.77	1.48	1.35
2	2	1136	PSU	C2-N3	5.73	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	354	OMU	C2-N3	5.73	1.48	1.38
2	2	121	OMU	C2-N1	5.70	1.47	1.38
2	2	517	OMC	C6-C5	5.67	1.48	1.35
2	2	354	OMU	C6-C5	5.59	1.48	1.35
2	2	1842	4AC	C6-C5	5.58	1.48	1.35
2	2	1391	OMC	C6-C5	5.54	1.47	1.35
2	2	428	OMU	C6-C5	5.52	1.47	1.35
2	2	121	OMU	C6-C5	5.50	1.47	1.35
2	2	1272	OMC	C6-C5	5.46	1.47	1.35
2	2	1272	OMC	C2-N3	5.43	1.47	1.36
2	2	174	OMC	C2-N3	5.37	1.47	1.36
2	2	1391	OMC	C2-N3	5.34	1.47	1.36
2	2	1442	OMU	C6-C5	5.28	1.47	1.35
2	2	462	OMC	C2-N3	5.27	1.47	1.36
2	2	1703	OMC	C6-C5	5.27	1.47	1.35
2	2	1248	B8N	C2-N1	5.23	1.54	1.39
2	2	1288	OMU	C6-C5	5.23	1.47	1.35
2	2	1842	4AC	C4-N3	5.20	1.41	1.32
2	2	517	OMC	C2-N3	5.13	1.46	1.36
2	2	116	OMU	C6-C5	5.12	1.46	1.35
2	2	1337	4AC	C4-N4	5.11	1.47	1.39
2	2	172	OMU	C6-C5	5.08	1.46	1.35
2	2	1703	OMC	C2-N3	5.07	1.46	1.36
2	2	1045	PSU	C6-N1	5.05	1.44	1.36
2	2	1326	OMU	C6-C5	5.01	1.46	1.35
2	2	119	PSU	C6-N1	4.94	1.44	1.36
2	2	1842	4AC	C7-N4	4.94	1.46	1.37
2	2	1337	4AC	C5-C4	4.92	1.51	1.40
2	2	1337	4AC	C2-N3	4.86	1.46	1.36
2	2	822	PSU	C6-N1	4.68	1.44	1.36
2	2	109	PSU	C6-N1	4.66	1.44	1.36
2	2	1337	4AC	C2-N1	4.66	1.50	1.40
2	2	1842	4AC	C5-C4	4.61	1.50	1.40
2	2	815	PSU	C6-N1	4.58	1.43	1.36
2	2	1081	PSU	C6-N1	4.58	1.43	1.36
2	2	1391	OMC	C4-N4	4.57	1.44	1.33
2	2	644	OMG	C2-N3	4.50	1.44	1.33
2	2	1046	PSU	C6-N1	4.49	1.43	1.36
2	2	572	PSU	C6-N1	4.49	1.43	1.36
2	2	406	PSU	C6-N1	4.48	1.43	1.36
2	2	296	PSU	C6-N1	4.48	1.43	1.36
2	2	93	PSU	C6-N1	4.47	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	649	PSU	C6-N1	4.46	1.43	1.36
2	2	1445	PSU	C6-N1	4.45	1.43	1.36
2	2	1328	OMG	C2-N3	4.44	1.44	1.33
2	2	174	OMC	C4-N4	4.43	1.44	1.33
2	2	1703	OMC	O2-C2	-4.43	1.15	1.23
2	2	1842	4AC	O2-C2	-4.43	1.15	1.23
2	2	1447	OMG	C2-N3	4.41	1.43	1.33
18	X	62	HY3	C5-N	-4.40	1.33	1.49
2	2	436	OMG	C4-N3	4.39	1.48	1.37
2	2	686	PSU	C6-N1	4.39	1.43	1.36
2	2	814	PSU	C6-N1	4.37	1.43	1.36
2	2	1232	PSU	C6-N1	4.37	1.43	1.36
2	2	462	OMC	C4-N4	4.37	1.44	1.33
2	2	1625	PSU	C6-N1	4.36	1.43	1.36
2	2	436	OMG	C2-N3	4.34	1.43	1.33
2	2	1272	OMC	C4-N4	4.34	1.44	1.33
2	2	1447	OMG	C2-N2	4.31	1.44	1.34
2	2	1136	PSU	C6-N1	4.29	1.43	1.36
2	2	517	OMC	C4-N4	4.29	1.44	1.33
2	2	683	OMG	C2-N3	4.28	1.43	1.33
2	2	1328	OMG	C2-N2	4.26	1.44	1.34
2	2	436	OMG	C2-N2	4.22	1.44	1.34
2	2	683	OMG	C2-N2	4.19	1.44	1.34
2	2	1842	4AC	C4-N4	4.19	1.45	1.39
2	2	683	OMG	C4-N3	4.19	1.47	1.37
2	2	1238	PSU	C6-N1	4.19	1.43	1.36
2	2	1328	OMG	C4-N3	4.18	1.47	1.37
2	2	174	OMC	C4-N3	4.18	1.42	1.34
2	2	105	PSU	C6-N1	4.17	1.43	1.36
2	2	462	OMC	C4-N3	4.17	1.42	1.34
2	2	1272	OMC	C4-N3	4.16	1.42	1.34
2	2	1842	4AC	C2-N1	4.14	1.49	1.40
2	2	1703	OMC	C4-N3	4.14	1.42	1.34
2	2	1248	B8N	C6-C5	4.13	1.40	1.34
2	2	509	OMG	C2-N3	4.12	1.43	1.33
2	2	354	OMU	O4-C4	-4.09	1.16	1.24
2	2	601	OMG	C2-N3	4.09	1.43	1.33
2	2	1391	OMC	C4-N3	4.08	1.42	1.34
2	2	1703	OMC	C4-N4	4.06	1.43	1.33
2	2	863	PSU	C6-N1	4.05	1.42	1.36
2	2	1447	OMG	C4-N3	4.02	1.47	1.37
2	2	681	PSU	C6-N1	4.00	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1244	PSU	C6-N1	3.95	1.42	1.36
2	2	517	OMC	C4-N3	3.91	1.42	1.34
2	2	462	OMC	C2-N1	3.90	1.48	1.40
2	2	1692	PSU	C6-N1	3.89	1.42	1.36
2	2	1288	OMU	C4-N3	3.88	1.45	1.38
2	2	1272	OMC	C2-N1	3.88	1.48	1.40
2	2	1326	OMU	C4-N3	3.86	1.45	1.38
2	2	651	PSU	C6-N1	3.86	1.42	1.36
2	2	1326	OMU	O4-C4	-3.85	1.17	1.24
2	2	174	OMC	C2-N1	3.85	1.48	1.40
2	2	1056	PSU	C6-N1	3.84	1.42	1.36
2	2	1692	PSU	O4-C4	-3.84	1.16	1.23
2	2	601	OMG	C2-N2	3.82	1.43	1.34
2	2	296	PSU	C4-N3	3.79	1.45	1.38
2	2	644	OMG	C4-N3	3.77	1.46	1.37
2	2	509	OMG	C4-N3	3.77	1.46	1.37
2	2	172	OMU	C4-N3	3.76	1.45	1.38
2	2	601	OMG	C4-N3	3.74	1.46	1.37
2	2	681	PSU	O4-C4	-3.74	1.16	1.23
2	2	109	PSU	O4-C4	-3.72	1.16	1.23
2	2	1238	PSU	O4-C4	-3.72	1.16	1.23
2	2	1391	OMC	C2-N1	3.71	1.48	1.40
2	2	517	OMC	C2-N1	3.70	1.48	1.40
2	2	509	OMG	C2-N2	3.69	1.43	1.34
2	2	1442	OMU	O4-C4	-3.69	1.17	1.24
2	2	683	OMG	C5-C4	-3.68	1.33	1.43
2	2	601	OMG	O6-C6	-3.67	1.15	1.23
2	2	1045	PSU	C4-N3	3.64	1.45	1.38
2	2	863	PSU	O4-C4	-3.64	1.16	1.23
2	2	644	OMG	C2-N2	3.63	1.42	1.34
2	2	822	PSU	O4-C4	-3.60	1.16	1.23
2	2	116	OMU	O4-C4	-3.59	1.17	1.24
2	2	509	OMG	O6-C6	-3.59	1.16	1.23
2	2	1442	OMU	C4-N3	3.57	1.45	1.38
2	2	428	OMU	O4-C4	-3.55	1.17	1.24
2	2	644	OMG	C5-C4	-3.53	1.34	1.43
2	2	121	OMU	O4-C4	-3.53	1.17	1.24
2	2	1703	OMC	C2-N1	3.52	1.47	1.40
2	2	1842	4AC	C2-N3	3.49	1.43	1.36
2	2	1244	PSU	C4-N3	3.48	1.45	1.38
2	2	428	OMU	C4-N3	3.47	1.44	1.38
2	2	1328	OMG	C5-C4	-3.46	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	814	PSU	C4-N3	3.46	1.45	1.38
2	2	462	OMC	O2-C2	-3.44	1.17	1.23
2	2	105	PSU	O2-C2	-3.43	1.16	1.23
2	2	517	OMC	O2-C2	-3.43	1.17	1.23
2	2	1383	A2M	C5-C4	-3.42	1.31	1.40
2	2	1328	OMG	C6-N1	3.41	1.43	1.37
2	2	172	OMU	O4-C4	-3.40	1.17	1.24
2	2	1288	OMU	O4-C4	-3.40	1.17	1.24
2	2	1244	PSU	O4-C4	-3.40	1.17	1.23
2	2	509	OMG	C5-C4	-3.40	1.34	1.43
2	2	815	PSU	O4-C4	-3.38	1.17	1.23
2	2	406	PSU	O4-C4	-3.37	1.17	1.23
2	2	651	PSU	O4-C4	-3.37	1.17	1.23
2	2	1056	PSU	O4-C4	-3.36	1.17	1.23
2	2	1383	A2M	O3'-C3'	3.36	1.50	1.43
2	2	1445	PSU	O4-C4	-3.34	1.17	1.23
2	2	1447	OMG	C6-N1	3.34	1.42	1.37
2	2	1081	PSU	O4-C4	-3.32	1.17	1.23
2	2	1692	PSU	O2-C2	-3.32	1.16	1.23
2	2	1842	4AC	O7-C7	-3.31	1.15	1.23
2	2	601	OMG	C5-C4	-3.31	1.34	1.43
2	2	93	PSU	O4-C4	-3.30	1.17	1.23
2	2	1046	PSU	O4-C4	-3.29	1.17	1.23
2	2	105	PSU	O4-C4	-3.28	1.17	1.23
2	2	1328	OMG	O6-C6	-3.28	1.16	1.23
2	2	119	PSU	C4-N3	3.28	1.44	1.38
2	2	1046	PSU	O2-C2	-3.27	1.16	1.23
2	2	1337	4AC	C6-N1	3.26	1.45	1.38
2	2	1272	OMC	O2-C2	-3.26	1.17	1.23
2	2	863	PSU	C4-N3	3.26	1.44	1.38
2	2	116	OMU	C4-N3	3.25	1.44	1.38
2	2	174	OMC	O2-C2	-3.24	1.17	1.23
2	2	1136	PSU	O4-C4	-3.24	1.17	1.23
2	2	1625	PSU	C4-N3	3.24	1.44	1.38
2	2	36	PSU	C4-N3	-3.23	1.32	1.38
2	2	105	PSU	C4-N3	3.23	1.44	1.38
18	X	62	HY3	C4-C5	3.21	1.58	1.53
2	2	686	PSU	O4-C4	-3.21	1.17	1.23
2	2	121	OMU	O2-C2	-3.21	1.17	1.23
2	2	1391	OMC	O2-C2	-3.20	1.17	1.23
2	2	1445	PSU	C4-N3	3.19	1.44	1.38
2	2	1081	PSU	O2-C2	-3.19	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1337	4AC	O2-C2	-3.18	1.17	1.23
2	2	572	PSU	C4-N3	3.18	1.44	1.38
2	2	1136	PSU	O2-C2	-3.18	1.16	1.23
2	2	436	OMG	C5-C4	-3.17	1.35	1.43
2	2	644	OMG	C6-N1	3.16	1.42	1.37
2	2	649	PSU	O4-C4	-3.16	1.17	1.23
2	2	1272	OMC	C6-N1	3.16	1.45	1.38
2	2	649	PSU	C4-N3	3.16	1.44	1.38
2	2	822	PSU	C4-N3	3.15	1.44	1.38
2	2	354	OMU	O2-C2	-3.13	1.17	1.23
2	2	649	PSU	O2-C2	-3.13	1.16	1.23
2	2	683	OMG	C6-N1	3.12	1.42	1.37
2	2	681	PSU	O2-C2	-3.12	1.16	1.23
2	2	354	OMU	C4-N3	3.12	1.44	1.38
2	2	436	OMG	C6-N1	3.12	1.42	1.37
17	V	1	AME	CT1-N	3.12	1.45	1.34
2	2	1347	PSU	C4-N3	-3.11	1.33	1.38
2	2	1639	7MG	C4-N9	-3.11	1.34	1.37
2	2	1031	A2M	C5-C4	-3.11	1.32	1.40
2	2	681	PSU	C4-N3	3.10	1.44	1.38
2	2	1391	OMC	C6-N1	3.10	1.45	1.38
2	2	512	A2M	C5-C4	-3.10	1.32	1.40
2	2	1238	PSU	C4-N3	3.10	1.44	1.38
2	2	436	OMG	O6-C6	-3.10	1.17	1.23
2	2	462	OMC	C6-N1	3.10	1.45	1.38
2	2	1232	PSU	O4-C4	-3.09	1.17	1.23
2	2	166	A2M	C6-N6	3.09	1.45	1.34
2	2	1643	PSU	C4-N3	-3.08	1.33	1.38
2	2	572	PSU	O4-C4	-3.08	1.17	1.23
2	2	468	A2M	C5-C4	-3.08	1.32	1.40
2	2	119	PSU	O4-C4	-3.07	1.17	1.23
2	2	517	OMC	C6-N1	3.07	1.45	1.38
2	2	814	PSU	O4-C4	-3.06	1.17	1.23
2	2	1442	OMU	O2-C2	-3.06	1.17	1.23
2	2	109	PSU	O2-C2	-3.06	1.17	1.23
2	2	1692	PSU	C4-N3	3.05	1.44	1.38
2	2	686	PSU	C4-N3	3.05	1.44	1.38
2	2	683	OMG	O6-C6	-3.05	1.17	1.23
35	A	2	SAC	C1A-N	3.05	1.44	1.34
2	2	1447	OMG	C5-C4	-3.04	1.35	1.43
2	2	863	PSU	O2-C2	-3.04	1.17	1.23
2	2	1232	PSU	C4-N3	3.03	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1347	PSU	C6-C5	3.02	1.38	1.35
2	2	1056	PSU	C4-N3	3.01	1.44	1.38
2	2	651	PSU	O2-C2	-3.01	1.17	1.23
2	2	1625	PSU	O4-C4	-3.01	1.17	1.23
2	2	121	OMU	C4-N3	3.01	1.43	1.38
2	2	814	PSU	O2-C2	-3.00	1.17	1.23
2	2	576	A2M	C6-N6	3.00	1.45	1.34
2	2	166	A2M	C5-C4	-3.00	1.33	1.40
2	2	296	PSU	O4-C4	-3.00	1.17	1.23
2	2	1244	PSU	O2-C2	-3.00	1.17	1.23
2	2	159	A2M	C6-N6	3.00	1.45	1.34
2	2	822	PSU	O2-C2	-2.99	1.17	1.23
2	2	815	PSU	C4-N3	2.99	1.44	1.38
2	2	116	OMU	O2-C2	-2.99	1.17	1.23
2	2	590	A2M	C5-C4	-2.99	1.33	1.40
2	2	1326	OMU	O2-C2	-2.98	1.17	1.23
2	2	1232	PSU	O2-C2	-2.98	1.17	1.23
2	2	93	PSU	O2-C2	-2.97	1.17	1.23
2	2	93	PSU	C4-N3	2.97	1.44	1.38
2	2	1081	PSU	C4-N3	2.97	1.44	1.38
2	2	1056	PSU	O2-C2	-2.97	1.17	1.23
2	2	651	PSU	C4-N3	2.97	1.44	1.38
2	2	1625	PSU	O2-C2	-2.96	1.17	1.23
2	2	1238	PSU	O2-C2	-2.96	1.17	1.23
2	2	686	PSU	O2-C2	-2.96	1.17	1.23
2	2	1177	PSU	C4-N3	-2.96	1.33	1.38
2	2	174	OMC	C6-N1	2.96	1.45	1.38
2	2	119	PSU	O2-C2	-2.95	1.17	1.23
2	2	576	A2M	O2'-C2'	-2.95	1.35	1.42
2	2	1832	6MZ	C5-C4	-2.93	1.33	1.40
2	2	1383	A2M	O2'-C2'	-2.92	1.35	1.42
2	2	406	PSU	O2-C2	-2.91	1.17	1.23
2	2	1445	PSU	O2-C2	-2.91	1.17	1.23
2	2	1174	PSU	C6-C5	2.90	1.38	1.35
2	2	576	A2M	C5-C4	-2.89	1.33	1.40
2	2	644	OMG	C5-C6	2.88	1.53	1.47
2	2	1639	7MG	C5-C4	2.87	1.47	1.38
2	2	1643	PSU	C6-C5	2.87	1.38	1.35
2	2	406	PSU	C4-N3	2.86	1.44	1.38
2	2	468	A2M	C6-N6	2.86	1.44	1.34
2	2	99	A2M	C5-C4	-2.85	1.33	1.40
2	2	428	OMU	C6-N1	2.84	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	172	OMU	O2-C2	-2.84	1.17	1.23
2	2	109	PSU	C4-N3	2.83	1.44	1.38
2	2	1174	PSU	C4-N3	-2.83	1.33	1.38
2	2	1046	PSU	C4-N3	2.82	1.44	1.38
2	2	159	A2M	O2'-C2'	-2.80	1.35	1.42
2	2	436	OMG	C5-C6	2.80	1.53	1.47
2	2	572	PSU	O2-C2	-2.80	1.17	1.23
2	2	159	A2M	C5-C4	-2.79	1.33	1.40
2	2	509	OMG	C5-C6	2.79	1.53	1.47
2	2	644	OMG	O6-C6	-2.78	1.17	1.23
2	2	99	A2M	C6-N6	2.78	1.44	1.34
2	2	815	PSU	O2-C2	-2.78	1.17	1.23
2	2	512	A2M	O3'-C3'	2.77	1.49	1.43
2	2	1031	A2M	C6-N6	2.76	1.44	1.34
2	2	1703	OMC	C6-N1	2.76	1.44	1.38
2	2	428	OMU	O2-C2	-2.76	1.18	1.23
2	2	99	A2M	O2'-C2'	-2.74	1.35	1.42
2	2	590	A2M	C6-N6	2.74	1.44	1.34
2	2	512	A2M	C6-N6	2.74	1.44	1.34
2	2	601	OMG	C5-C6	2.74	1.53	1.47
2	2	354	OMU	C6-N1	2.74	1.44	1.38
2	2	1045	PSU	O4-C4	-2.73	1.18	1.23
2	2	1447	OMG	C5-C6	2.73	1.52	1.47
2	2	1326	OMU	C6-N1	2.73	1.44	1.38
2	2	512	A2M	O2'-C2'	-2.72	1.35	1.42
2	2	1288	OMU	O2-C2	-2.72	1.18	1.23
2	2	1832	6MZ	C6-N1	-2.70	1.30	1.34
2	2	1031	A2M	O2'-C2'	-2.69	1.35	1.42
2	2	1842	4AC	C6-N1	2.69	1.44	1.38
2	2	590	A2M	O2'-C2'	-2.68	1.35	1.42
2	2	509	OMG	C6-N1	2.67	1.41	1.37
2	2	1337	4AC	O7-C7	-2.67	1.17	1.23
2	2	36	PSU	C6-C5	2.64	1.38	1.35
2	2	1383	A2M	C6-N6	2.64	1.43	1.34
2	2	468	A2M	O3'-C3'	2.63	1.49	1.43
2	2	121	OMU	C6-N1	2.62	1.44	1.38
2	2	601	OMG	C6-N1	2.62	1.41	1.37
2	2	1328	OMG	C5-C6	2.61	1.52	1.47
2	2	1288	OMU	C6-N1	2.60	1.44	1.38
2	2	166	A2M	O2'-C2'	-2.56	1.36	1.42
2	2	1177	PSU	C6-C5	2.56	1.38	1.35
2	2	1639	7MG	C6-N1	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	576	A2M	O3’-C3’	2.54	1.49	1.43
2	2	296	PSU	O2-C2	-2.54	1.18	1.23
2	2	468	A2M	O2’-C2’	-2.53	1.36	1.42
2	2	1447	OMG	O6-C6	-2.52	1.18	1.23
2	2	1045	PSU	O2-C2	-2.52	1.18	1.23
2	2	166	A2M	O3’-C3’	2.51	1.48	1.43
2	2	1490	OMG	C6-N1	-2.50	1.34	1.37
2	2	683	OMG	C5-C6	2.46	1.52	1.47
2	2	159	A2M	O3’-C3’	2.44	1.48	1.43
2	2	1248	B8N	O2-C2	-2.44	1.18	1.22
2	2	1447	OMG	C2-N1	2.43	1.43	1.37
2	2	1850	MA6	C2’-C1’	-2.43	1.50	1.53
2	2	1328	OMG	C2-N1	2.41	1.43	1.37
2	2	1081	PSU	O4’-C1’	-2.41	1.40	1.43
2	2	517	OMC	C5-C4	2.41	1.48	1.42
2	2	1248	B8N	O4-C4	-2.41	1.18	1.23
2	2	428	OMU	C5-C4	2.40	1.48	1.43
2	2	1442	OMU	C6-N1	2.40	1.43	1.38
2	2	354	OMU	C5-C4	2.40	1.48	1.43
2	2	116	OMU	C6-N1	2.38	1.43	1.38
2	2	512	A2M	O5’-C5’	-2.37	1.38	1.44
2	2	1850	MA6	C5-C4	2.36	1.47	1.40
2	2	1031	A2M	O3’-C3’	2.34	1.48	1.43
2	2	683	OMG	C2-N1	2.34	1.43	1.37
2	2	484	A2M	C5-C4	2.33	1.47	1.40
2	2	590	A2M	O3’-C3’	2.33	1.48	1.43
2	2	27	A2M	C5-C4	2.32	1.47	1.40
2	2	36	PSU	C2-N3	-2.32	1.33	1.37
2	2	1851	MA6	C5-C4	2.31	1.47	1.40
2	2	1272	OMC	C5-C4	2.30	1.48	1.42
2	2	601	OMG	C2-N1	2.27	1.43	1.37
2	2	1031	A2M	O5’-C5’	-2.26	1.39	1.44
2	2	99	A2M	O3’-C3’	2.26	1.48	1.43
2	2	462	OMC	C5-C4	2.24	1.48	1.42
2	2	1703	OMC	C5-C4	2.24	1.48	1.42
2	2	822	PSU	O4’-C1’	-2.23	1.40	1.43
2	2	1347	PSU	C2-N3	-2.23	1.33	1.37
2	2	166	A2M	O5’-C5’	-2.21	1.39	1.44
2	2	436	OMG	C2-N1	2.20	1.43	1.37
2	2	509	OMG	C2-N1	2.19	1.43	1.37
2	2	668	A2M	C5-C4	2.18	1.46	1.40
2	2	651	PSU	O4’-C1’	-2.18	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	62	HY3	C4-C3	2.16	1.56	1.52
2	2	1643	PSU	C2-N3	-2.16	1.33	1.37
2	2	172	OMU	C6-N1	2.16	1.43	1.38
35	A	2	SAC	OAC-C1A	-2.16	1.18	1.23
2	2	1136	PSU	C4-N3	2.15	1.42	1.38
2	2	1442	OMU	C5-C4	2.14	1.48	1.43
2	2	1678	A2M	C5-C4	2.13	1.46	1.40
2	2	1174	PSU	C2-N3	-2.13	1.33	1.37
2	2	1248	B8N	O4'-C1'	-2.12	1.40	1.43
2	2	1643	PSU	C2'-C1'	-2.12	1.51	1.53
2	2	36	PSU	C2-N1	-2.12	1.33	1.36
2	2	576	A2M	O5'-C5'	-2.10	1.39	1.44
2	2	174	OMC	C5-C4	2.09	1.47	1.42
2	2	1383	A2M	O5'-C5'	-2.07	1.39	1.44
2	2	1832	6MZ	C5-N7	-2.07	1.32	1.39
2	2	1832	6MZ	C4-N3	-2.06	1.32	1.35
2	2	1326	OMU	C5-C4	2.06	1.48	1.43
2	2	1177	PSU	C2-N3	-2.06	1.34	1.37
2	2	1383	A2M	C6-C5	-2.05	1.35	1.43
2	2	468	A2M	O5'-C5'	-2.05	1.39	1.44
2	2	1391	OMC	C5-C4	2.04	1.47	1.42
2	2	512	A2M	C2-N3	2.03	1.35	1.32
2	2	644	OMG	C2-N1	2.03	1.42	1.37
2	2	681	PSU	O4'-C1'	-2.02	1.41	1.43
2	2	1177	PSU	C2-N1	-2.01	1.34	1.36
2	2	121	OMU	C5-C4	2.01	1.48	1.43
2	2	1136	PSU	O4'-C1'	-2.01	1.41	1.43

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	468	A2M	C5-C6-N6	10.92	136.94	120.35
2	2	159	A2M	C5-C6-N6	10.76	136.71	120.35
2	2	1031	A2M	C5-C6-N6	10.22	135.89	120.35
2	2	576	A2M	C5-C6-N6	10.17	135.80	120.35
2	2	590	A2M	C5-C6-N6	10.08	135.67	120.35
2	2	166	A2M	C5-C6-N6	9.92	135.43	120.35
2	2	1383	A2M	C5-C6-N6	9.56	134.88	120.35
2	2	99	A2M	C5-C6-N6	9.55	134.87	120.35
2	2	512	A2M	C5-C6-N6	9.07	134.13	120.35
2	2	1639	7MG	N9-C4-N3	8.72	138.51	125.47
2	2	1031	A2M	C1'-N9-C4	-7.66	113.18	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	468	A2M	N6-C6-N1	-7.43	103.14	118.57
2	2	590	A2M	N6-C6-N1	-7.26	103.51	118.57
2	2	468	A2M	C1'-N9-C4	-7.22	113.95	126.64
2	2	166	A2M	C1'-N9-C4	-7.14	114.09	126.64
2	2	159	A2M	N6-C6-N1	-7.09	103.85	118.57
2	2	159	A2M	C1'-N9-C4	-7.07	114.22	126.64
2	2	576	A2M	C1'-N9-C4	-6.99	114.35	126.64
2	2	1383	A2M	C1'-N9-C4	-6.99	114.37	126.64
2	2	166	A2M	N6-C6-N1	-6.62	104.83	118.57
2	2	1031	A2M	N6-C6-N1	-6.60	104.88	118.57
2	2	576	A2M	N6-C6-N1	-6.55	104.98	118.57
2	2	1326	OMU	C4-N3-C2	-6.52	117.98	126.58
2	2	1031	A2M	N3-C2-N1	-6.37	118.72	128.68
2	2	1832	6MZ	N3-C2-N1	-6.22	118.96	128.68
2	2	99	A2M	N3-C2-N1	-6.19	119.01	128.68
2	2	1832	6MZ	C2-N1-C6	6.13	121.85	116.59
2	2	1383	A2M	N6-C6-N1	-6.13	105.84	118.57
2	2	512	A2M	N6-C6-N1	-6.13	105.84	118.57
2	2	512	A2M	C1'-N9-C4	-6.10	115.93	126.64
2	2	99	A2M	N6-C6-N1	-6.10	105.92	118.57
2	2	512	A2M	N3-C2-N1	-6.05	119.23	128.68
2	2	1347	PSU	N1-C2-N3	6.04	121.97	115.13
2	2	1850	MA6	N1-C6-N6	5.95	123.32	117.06
2	2	590	A2M	N3-C2-N1	-5.91	119.44	128.68
2	2	166	A2M	N3-C2-N1	-5.85	119.54	128.68
2	2	1643	PSU	N1-C2-N3	5.80	121.70	115.13
2	2	1442	OMU	C4-N3-C2	-5.80	118.93	126.58
2	2	1174	PSU	N1-C2-N3	5.66	121.54	115.13
2	2	354	OMU	C4-N3-C2	-5.65	119.13	126.58
2	2	36	PSU	N1-C2-N3	5.62	121.50	115.13
2	2	1177	PSU	N1-C2-N3	5.54	121.41	115.13
2	2	468	A2M	N3-C2-N1	-5.54	120.02	128.68
2	2	651	PSU	N1-C2-N3	5.53	121.39	115.13
2	2	1383	A2M	N3-C2-N1	-5.51	120.06	128.68
2	2	99	A2M	C1'-N9-C4	-5.49	117.00	126.64
2	2	1244	PSU	C4-N3-C2	-5.48	118.44	126.34
2	2	576	A2M	N3-C2-N1	-5.47	120.13	128.68
2	2	1288	OMU	C4-N3-C2	-5.40	119.46	126.58
2	2	172	OMU	C4-N3-C2	-5.38	119.48	126.58
2	2	1639	7MG	N9-C8-N7	-5.33	95.75	103.38
2	2	1639	7MG	C5-C4-N3	-5.32	118.00	128.13
2	2	863	PSU	C4-N3-C2	-5.28	118.73	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	105	PSU	C4-N3-C2	-5.25	118.77	126.34
2	2	121	OMU	C4-N3-C2	-5.23	119.69	126.58
2	2	105	PSU	N1-C2-N3	5.22	121.05	115.13
2	2	109	PSU	C4-N3-C2	-5.19	118.86	126.34
2	2	1337	4AC	CM7-C7-N4	5.19	124.26	115.29
2	2	159	A2M	N3-C2-N1	-5.18	120.59	128.68
2	2	1056	PSU	C4-N3-C2	-5.16	118.90	126.34
2	2	681	PSU	C4-N3-C2	-5.12	118.97	126.34
2	2	651	PSU	C4-N3-C2	-5.07	119.04	126.34
2	2	1248	B8N	C5-C4-N3	5.07	125.55	116.17
2	2	649	PSU	C4-N3-C2	-5.05	119.06	126.34
2	2	1244	PSU	N1-C2-N3	5.01	120.81	115.13
2	2	1056	PSU	N1-C2-N3	4.98	120.77	115.13
2	2	686	PSU	C4-N3-C2	-4.98	119.17	126.34
2	2	815	PSU	C4-N3-C2	-4.89	119.29	126.34
2	2	1238	PSU	C4-N3-C2	-4.84	119.37	126.34
2	2	686	PSU	N1-C2-N3	4.83	120.61	115.13
2	2	428	OMU	C4-N3-C2	-4.82	120.22	126.58
2	2	814	PSU	C4-N3-C2	-4.81	119.41	126.34
2	2	119	PSU	C4-N3-C2	-4.79	119.44	126.34
2	2	1625	PSU	C4-N3-C2	-4.74	119.51	126.34
2	2	1136	PSU	N1-C2-N3	4.72	120.48	115.13
2	2	1081	PSU	C4-N3-C2	-4.72	119.54	126.34
2	2	863	PSU	N1-C2-N3	4.68	120.44	115.13
2	2	1046	PSU	C4-N3-C2	-4.66	119.62	126.34
2	2	572	PSU	N1-C2-N3	4.66	120.41	115.13
2	2	296	PSU	C4-N3-C2	-4.66	119.63	126.34
2	2	1045	PSU	C4-N3-C2	-4.65	119.63	126.34
2	2	1248	B8N	C4-N3-C2	-4.64	119.59	125.46
2	2	649	PSU	N1-C2-N3	4.64	120.39	115.13
2	2	572	PSU	C4-N3-C2	-4.59	119.73	126.34
2	2	1625	PSU	N1-C2-N3	4.54	120.27	115.13
2	2	93	PSU	C4-N3-C2	-4.51	119.83	126.34
2	2	822	PSU	C4-N3-C2	-4.50	119.85	126.34
2	2	815	PSU	N1-C2-N3	4.48	120.21	115.13
2	2	1692	PSU	C4-N3-C2	-4.48	119.89	126.34
2	2	1045	PSU	N1-C2-N3	4.43	120.15	115.13
2	2	1326	OMU	C5-C4-N3	4.41	121.44	114.84
2	2	1445	PSU	C4-N3-C2	-4.39	120.02	126.34
2	2	681	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	1232	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	651	PSU	C6-C5-C4	4.36	121.25	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1842	4AC	CM7-C7-N4	4.34	122.79	115.29
2	2	354	OMU	N3-C2-N1	4.33	120.64	114.89
2	2	1177	PSU	C4-N3-C2	-4.32	120.11	126.34
2	2	1136	PSU	C4-N3-C2	-4.32	120.11	126.34
2	2	406	PSU	N1-C2-N3	4.31	120.02	115.13
2	2	590	A2M	C1'-N9-C4	-4.31	119.07	126.64
2	2	1692	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	116	OMU	C4-N3-C2	-4.29	120.92	126.58
2	2	1238	PSU	N1-C2-N3	4.29	119.99	115.13
2	2	296	PSU	N1-C2-N3	4.29	119.99	115.13
2	2	1046	PSU	N1-C2-N3	4.27	119.97	115.13
2	2	822	PSU	N1-C2-N3	4.22	119.91	115.13
2	2	109	PSU	N1-C2-N3	4.20	119.89	115.13
2	2	651	PSU	O2-C2-N1	-4.20	118.17	122.79
2	2	119	PSU	N1-C2-N3	4.18	119.86	115.13
2	2	1639	7MG	C2-N3-C4	4.18	119.74	112.30
2	2	1445	PSU	N1-C2-N3	4.17	119.86	115.13
2	2	1248	B8N	C32-C31-N3	-4.15	104.22	112.00
2	2	1232	PSU	C4-N3-C2	-4.13	120.39	126.34
2	2	93	PSU	N1-C2-N3	4.03	119.70	115.13
2	2	121	OMU	N3-C2-N1	4.01	120.22	114.89
2	2	1136	PSU	C6-C5-C4	3.98	120.98	118.20
2	2	863	PSU	O2-C2-N1	-3.97	118.42	122.79
2	2	406	PSU	C4-N3-C2	-3.97	120.62	126.34
2	2	354	OMU	C5-C4-N3	3.96	120.76	114.84
2	2	601	OMG	C5-C6-N1	3.92	120.87	113.95
2	2	1328	OMG	C5-C6-N1	3.91	120.85	113.95
2	2	1442	OMU	N3-C2-N1	3.91	120.08	114.89
2	2	1081	PSU	N1-C2-N3	3.88	119.53	115.13
2	2	1288	OMU	C5-C4-N3	3.88	120.64	114.84
2	2	1842	4AC	C5-C4-N4	3.87	129.63	122.92
2	2	1326	OMU	N3-C2-N1	3.85	120.00	114.89
2	2	105	PSU	O2-C2-N1	-3.81	118.60	122.79
2	2	1851	MA6	C10-N6-C6	-3.79	108.04	119.51
2	2	406	PSU	C6-N1-C2	-3.78	118.82	122.68
2	2	1442	OMU	C5-C4-N3	3.77	120.48	114.84
2	2	1174	PSU	C4-N3-C2	-3.75	120.94	126.34
2	2	1347	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	1643	PSU	C4-N3-C2	-3.72	120.98	126.34
2	2	428	OMU	C5-C4-N3	3.70	120.37	114.84
2	2	814	PSU	N1-C2-N3	3.69	119.32	115.13
2	2	683	OMG	C5-C6-N1	3.66	120.42	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1056	PSU	C6-C5-C4	3.64	120.75	118.20
2	2	172	OMU	N3-C2-N1	3.56	119.62	114.89
2	2	36	PSU	C4-N3-C2	-3.55	121.23	126.34
2	2	509	OMG	C5-C6-N1	3.54	120.21	113.95
17	V	1	AME	CT2-CT1-N	3.53	122.08	116.10
2	2	27	A2M	N3-C2-N1	-3.52	123.17	128.68
2	2	121	OMU	C5-C4-N3	3.52	120.10	114.84
2	2	1328	OMG	C2-N1-C6	-3.50	118.65	125.10
2	2	116	OMU	C5-C4-N3	3.50	120.08	114.84
2	2	484	A2M	N3-C2-N1	-3.48	123.24	128.68
2	2	1244	PSU	O2-C2-N1	-3.48	118.96	122.79
2	2	172	OMU	C5-C4-N3	3.47	120.04	114.84
2	2	1347	PSU	O2-C2-N1	-3.44	119.01	122.79
2	2	1832	6MZ	C9-N6-C6	3.42	125.82	122.87
2	2	644	OMG	C5-C6-N1	3.42	119.98	113.95
2	2	1232	PSU	C6-N1-C2	-3.41	119.20	122.68
2	2	1678	A2M	N3-C2-N1	-3.40	123.37	128.68
2	2	1337	4AC	C5-C4-N4	3.40	128.81	122.92
2	2	1288	OMU	O4-C4-C5	-3.38	119.22	125.16
2	2	1625	PSU	O2-C2-N1	-3.38	119.07	122.79
2	2	1288	OMU	N3-C2-N1	3.36	119.35	114.89
2	2	1851	MA6	C9-N6-C6	-3.33	109.42	119.51
2	2	1851	MA6	C4-C5-N7	-3.32	105.94	109.40
2	2	1692	PSU	O2-C2-N1	-3.31	119.14	122.79
2	2	651	PSU	C6-N1-C2	-3.31	119.30	122.68
2	2	1326	OMU	O4-C4-C5	-3.28	119.39	125.16
2	2	172	OMU	O4-C4-C5	-3.28	119.39	125.16
2	2	572	PSU	C6-N1-C2	-3.28	119.33	122.68
2	2	1045	PSU	C6-N1-C2	-3.28	119.33	122.68
2	2	1625	PSU	C6-N1-C2	-3.24	119.36	122.68
2	2	1447	OMG	C5-C6-N1	3.24	119.68	113.95
2	2	436	OMG	C5-C6-N1	3.24	119.67	113.95
2	2	1445	PSU	C6-N1-C2	-3.24	119.37	122.68
2	2	1174	PSU	O2-C2-N1	-3.24	119.23	122.79
2	2	105	PSU	C6-N1-C2	-3.23	119.38	122.68
2	2	644	OMG	C8-N7-C5	3.22	109.13	102.99
17	V	1	AME	CE-SD-CG	3.22	111.46	100.40
2	2	1136	PSU	C6-N1-C2	-3.20	119.41	122.68
2	2	1248	B8N	N3-C2-N1	3.19	121.26	116.76
2	2	1851	MA6	N3-C2-N1	-3.18	123.71	128.68
2	2	1046	PSU	C6-N1-C2	-3.18	119.43	122.68
2	2	686	PSU	C6-N1-C2	-3.18	119.44	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	822	PSU	C6-N1-C2	-3.18	119.44	122.68
2	2	121	OMU	O2-C2-N1	-3.16	118.58	122.79
2	2	668	A2M	N3-C2-N1	-3.16	123.74	128.68
2	2	1643	PSU	O2-C2-N1	-3.15	119.32	122.79
2	2	1056	PSU	C6-N1-C2	-3.15	119.46	122.68
2	2	1850	MA6	N3-C2-N1	-3.14	123.78	128.68
2	2	1383	A2M	O4'-C1'-C2'	-3.12	101.17	106.59
2	2	428	OMU	N3-C2-N1	3.11	119.02	114.89
2	2	1244	PSU	C6-N1-C2	-3.10	119.52	122.68
2	2	683	OMG	C8-N7-C5	3.06	108.81	102.99
2	2	116	OMU	N3-C2-N1	3.02	118.90	114.89
27	O	138	IAS	OXT-C-O	-3.00	117.27	124.09
2	2	1045	PSU	C6-C5-C4	2.98	120.28	118.20
2	2	1177	PSU	O2-C2-N1	-2.96	119.54	122.79
2	2	509	OMG	C2-N1-C6	-2.94	119.68	125.10
2	2	428	OMU	O4-C4-C5	-2.93	120.01	125.16
2	2	1850	MA6	C10-N6-C6	-2.93	110.65	119.51
2	2	436	OMG	C8-N7-C5	2.91	108.53	102.99
2	2	668	A2M	C4-C5-N7	-2.89	106.39	109.40
2	2	1328	OMG	N2-C2-N1	2.89	122.86	116.71
2	2	1850	MA6	C9-N6-C6	-2.88	110.80	119.51
2	2	296	PSU	O2-C2-N1	-2.88	119.62	122.79
2	2	1447	OMG	C8-N7-C5	2.87	108.47	102.99
2	2	1337	4AC	O7-C7-N4	-2.87	117.17	121.82
2	2	601	OMG	C2-N1-C6	-2.87	119.81	125.10
2	2	1442	OMU	O4-C4-C5	-2.86	120.13	125.16
2	2	1244	PSU	C6-C5-C4	2.85	120.19	118.20
2	2	601	OMG	C8-N7-C5	2.85	108.42	102.99
2	2	105	PSU	C6-C5-C4	2.81	120.16	118.20
2	2	1328	OMG	O6-C6-C5	-2.78	118.93	124.37
2	2	27	A2M	C4-C5-N7	-2.78	106.50	109.40
2	2	572	PSU	C6-C5-C4	2.77	120.14	118.20
2	2	1328	OMG	C8-N7-C5	2.76	108.24	102.99
2	2	296	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	172	OMU	O2-C2-N1	-2.75	119.13	122.79
2	2	36	PSU	O2-C2-N1	-2.73	119.78	122.79
2	2	484	A2M	C4-C5-N7	-2.73	106.56	109.40
2	2	686	PSU	O2-C2-N1	-2.72	119.79	122.79
2	2	649	PSU	C6-N1-C2	-2.67	119.95	122.68
2	2	1851	MA6	C10-N6-C9	-2.64	107.61	116.12
2	2	863	PSU	C6-N1-C2	-2.64	119.98	122.68
2	2	644	OMG	O6-C6-N1	-2.63	117.54	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1447	OMG	N2-C2-N1	2.62	122.29	116.71
2	2	1238	PSU	C6-N1-C2	-2.60	120.02	122.68
2	2	1639	7MG	C5-C6-N1	2.59	115.56	110.99
2	2	1447	OMG	C2-N1-C6	-2.59	120.33	125.10
2	2	1248	B8N	C31-N3-C4	2.57	121.10	117.31
2	2	644	OMG	C2-N1-C6	-2.56	120.38	125.10
2	2	1445	PSU	O2-C2-N1	-2.56	119.97	122.79
2	2	509	OMG	C8-N7-C5	2.56	107.86	102.99
2	2	1326	OMU	O2-C2-N1	-2.55	119.40	122.79
2	2	116	OMU	O4-C4-C5	-2.54	120.69	125.16
2	2	1045	PSU	O2-C2-N1	-2.54	119.99	122.79
2	2	1678	A2M	C4-C5-N7	-2.52	106.77	109.40
2	2	863	PSU	C6-C5-C4	2.52	119.96	118.20
2	2	1081	PSU	O4'-C1'-C2'	2.52	108.70	105.14
2	2	681	PSU	C6-N1-C2	-2.50	120.12	122.68
2	2	686	PSU	C6-C5-C4	2.50	119.94	118.20
2	2	1639	7MG	O4'-C1'-N9	2.49	112.69	109.30
2	2	683	OMG	C2-N1-C6	-2.48	120.53	125.10
2	2	119	PSU	C6-N1-C2	-2.48	120.15	122.68
2	2	1692	PSU	C6-N1-C2	-2.48	120.15	122.68
2	2	119	PSU	C6-C5-C4	2.47	119.93	118.20
27	O	138	IAS	OXT-C-CA	2.46	121.77	113.38
2	2	683	OMG	N2-C2-N1	2.46	121.95	116.71
2	2	601	OMG	N2-C2-N1	2.46	121.95	116.71
2	2	1643	PSU	C3'-C2'-C1'	2.46	104.50	101.64
2	2	436	OMG	N2-C2-N1	2.44	121.91	116.71
2	2	815	PSU	C6-N1-C2	-2.44	120.19	122.68
2	2	1842	4AC	O2-C2-N3	-2.43	118.38	122.33
2	2	406	PSU	C6-C5-C4	2.43	119.90	118.20
2	2	590	A2M	O4'-C4'-C3'	-2.39	100.38	105.11
2	2	1832	6MZ	C4-C5-N7	-2.37	106.93	109.40
2	2	121	OMU	O4-C4-C5	-2.36	121.00	125.16
2	2	683	OMG	N1-C2-N3	-2.36	118.91	123.32
2	2	649	PSU	O2-C2-N1	-2.34	120.22	122.79
2	2	116	OMU	O2-C2-N1	-2.34	119.68	122.79
2	2	93	PSU	C6-N1-C2	-2.33	120.30	122.68
2	2	815	PSU	C6-C5-C4	2.32	119.82	118.20
2	2	1081	PSU	C6-N1-C2	-2.31	120.32	122.68
2	2	668	A2M	C2-N1-C6	2.31	122.71	118.75
2	2	814	PSU	O2-C2-N1	-2.31	120.25	122.79
2	2	683	OMG	O6-C6-C5	-2.29	119.90	124.37
2	2	601	OMG	N1-C2-N3	-2.29	119.05	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	354	OMU	O2-C2-N1	-2.28	119.75	122.79
2	2	512	A2M	O4'-C1'-C2'	-2.28	102.64	106.59
2	2	1337	4AC	C5-C4-N3	-2.28	118.93	122.59
2	2	93	PSU	O2-C2-N1	-2.27	120.29	122.79
2	2	668	A2M	C1'-N9-C4	-2.27	122.65	126.64
2	2	354	OMU	C2'-C1'-N1	-2.27	109.82	114.22
2	2	1490	OMG	C5-C6-N1	2.25	117.92	113.95
2	2	509	OMG	N2-C2-N1	2.24	121.49	116.71
2	2	1490	OMG	C8-N7-C5	2.24	107.25	102.99
2	2	484	A2M	C2-N1-C6	2.23	122.56	118.75
35	A	2	SAC	C2A-C1A-N	2.23	119.87	116.10
35	A	2	SAC	O-C-CA	-2.22	118.96	124.78
2	2	354	OMU	O4-C4-C5	-2.22	121.27	125.16
2	2	1177	PSU	C5-C6-N1	-2.21	118.79	122.11
2	2	1639	7MG	C5-C4-N9	-2.20	103.50	106.35
2	2	119	PSU	O2-C2-N1	-2.19	120.38	122.79
2	2	1347	PSU	C3'-C2'-C1'	2.18	104.18	101.64
2	2	428	OMU	O2-C2-N1	-2.18	119.89	122.79
2	2	1056	PSU	O2-C2-N1	-2.16	120.41	122.79
2	2	1442	OMU	O2-C2-N1	-2.16	119.91	122.79
2	2	822	PSU	O4'-C1'-C2'	2.16	108.19	105.14
2	2	436	OMG	C2-N1-C6	-2.16	121.12	125.10
2	2	649	PSU	C6-C5-C4	2.16	119.70	118.20
2	2	1842	4AC	O7-C7-CM7	-2.15	118.06	122.06
2	2	1238	PSU	O2-C2-N1	-2.14	120.43	122.79
2	2	1850	MA6	C4-C5-N7	-2.14	107.17	109.40
27	O	138	IAS	CA-CB-CG	-2.13	105.28	114.50
2	2	296	PSU	C6-C5-C4	2.11	119.68	118.20
2	2	1337	4AC	O2-C2-N3	-2.11	118.89	122.33
2	2	109	PSU	C5-C4-N3	2.11	121.35	116.58
2	2	1625	PSU	C6-C5-C4	2.10	119.66	118.20
2	2	36	PSU	C3'-C2'-C1'	2.09	104.07	101.64
2	2	166	A2M	O4'-C1'-C2'	-2.09	102.97	106.59
2	2	27	A2M	C2-N1-C6	2.08	122.31	118.75
2	2	576	A2M	O4'-C1'-C2'	-2.06	103.01	106.59
2	2	436	OMG	N1-C2-N3	-2.06	119.47	123.32
2	2	1232	PSU	O2-C2-N1	-2.05	120.54	122.79
2	2	644	OMG	N1-C2-N3	-2.04	119.50	123.32
2	2	1081	PSU	O4-C4-N3	-2.04	116.20	120.12
2	2	1081	PSU	C5-C4-N3	2.03	121.17	116.58
2	2	1248	B8N	O36-C34-O35	-2.03	119.49	124.09
2	2	1337	4AC	C6-C5-C4	2.02	119.44	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	681	PSU	C6-C5-C4	2.02	119.61	118.20
2	2	1383	A2M	C2'-C3'-C4'	-2.02	97.61	101.99
2	2	172	OMU	O2'-C2'-C1'	2.01	113.01	109.08
2	2	1248	B8N	O4'-C1'-C2'	2.01	107.98	105.14
2	2	109	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	X	62	HY3	O-C-CA-C3
2	2	27	A2M	C1'-C2'-O2'-CM'
2	2	116	OMU	C1'-C2'-O2'-CM2
2	2	174	OMC	C1'-C2'-O2'-CM2
2	2	468	A2M	C1'-C2'-O2'-CM'
2	2	484	A2M	C1'-C2'-O2'-CM'
2	2	1248	B8N	O4'-C4'-C5'-O5'
2	2	1248	B8N	C3'-C4'-C5'-O5'
2	2	1678	A2M	C1'-C2'-O2'-CM'
2	2	1850	MA6	C5-C6-N6-C9
2	2	1851	MA6	O4'-C4'-C5'-O5'
2	2	1851	MA6	C5-C6-N6-C9
2	2	1851	MA6	N1-C6-N6-C9
27	O	138	IAS	CA-CB-CG-OD1
2	2	668	A2M	O4'-C4'-C5'-O5'
2	2	668	A2M	C3'-C4'-C5'-O5'
2	2	1447	OMG	C3'-C4'-C5'-O5'
2	2	1851	MA6	C3'-C4'-C5'-O5'
17	V	1	AME	CT2-CT1-N-CA
17	V	1	AME	OT-CT1-N-CA
2	2	1850	MA6	N1-C6-N6-C9
2	2	172	OMU	C3'-C2'-O2'-CM2
17	V	1	AME	N-CA-CB-CG
2	2	1447	OMG	O4'-C4'-C5'-O5'
2	2	1851	MA6	C5-C6-N6-C10
2	2	576	A2M	C3'-C4'-C5'-O5'
2	2	428	OMU	C2'-C1'-N1-C6
2	2	99	A2M	O4'-C4'-C5'-O5'
2	2	1337	4AC	O7-C7-N4-C4
2	2	1337	4AC	CM7-C7-N4-C4
2	2	1842	4AC	O7-C7-N4-C4
2	2	1842	4AC	CM7-C7-N4-C4

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Mol	Chain	Res	Type	Atoms
2	2	644	OMG	C4'-C5'-O5'-P
2	2	428	OMU	O4'-C1'-N1-C6
2	2	1851	MA6	C4'-C5'-O5'-P
2	2	1490	OMG	C4'-C5'-O5'-P
2	2	428	OMU	O4'-C1'-N1-C2
2	2	1347	PSU	O4'-C4'-C5'-O5'
2	2	99	A2M	C3'-C4'-C5'-O5'
2	2	576	A2M	O4'-C4'-C5'-O5'
2	2	428	OMU	C2'-C1'-N1-C2
27	O	138	IAS	OXT-C-CA-N
2	2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 173 ligands modelled in this entry, 173 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

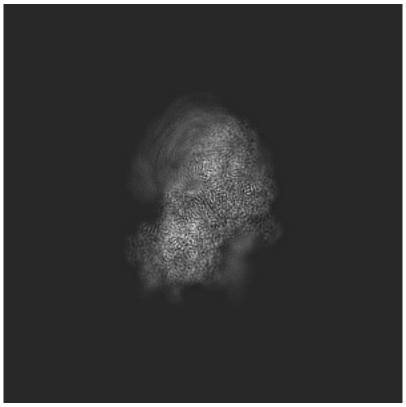
6 Map visualisation

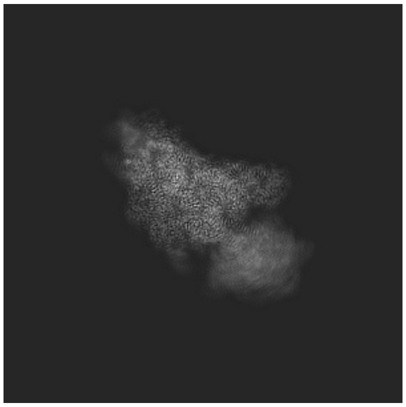
This section contains visualisations of the EMDB entry EMD-14317. These allow visual inspection of the internal detail of the map and identification of artifacts.

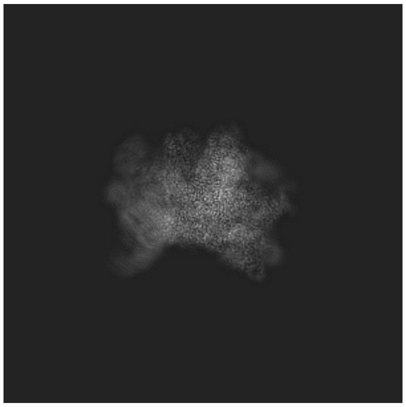
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

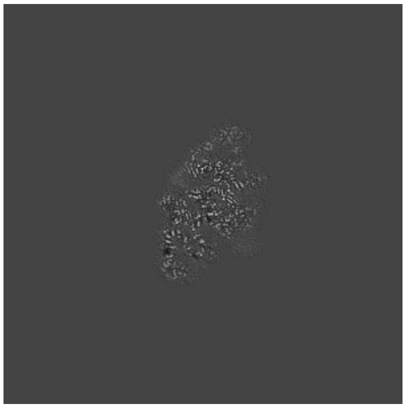

Y

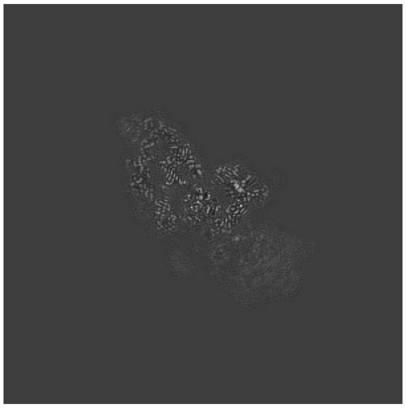

Z

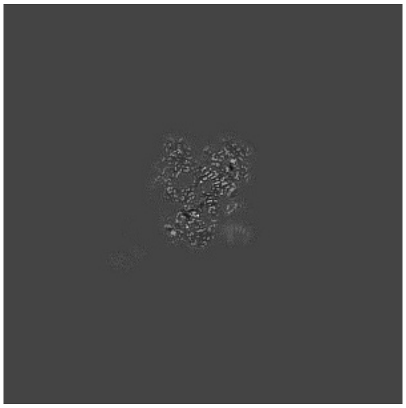
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 256

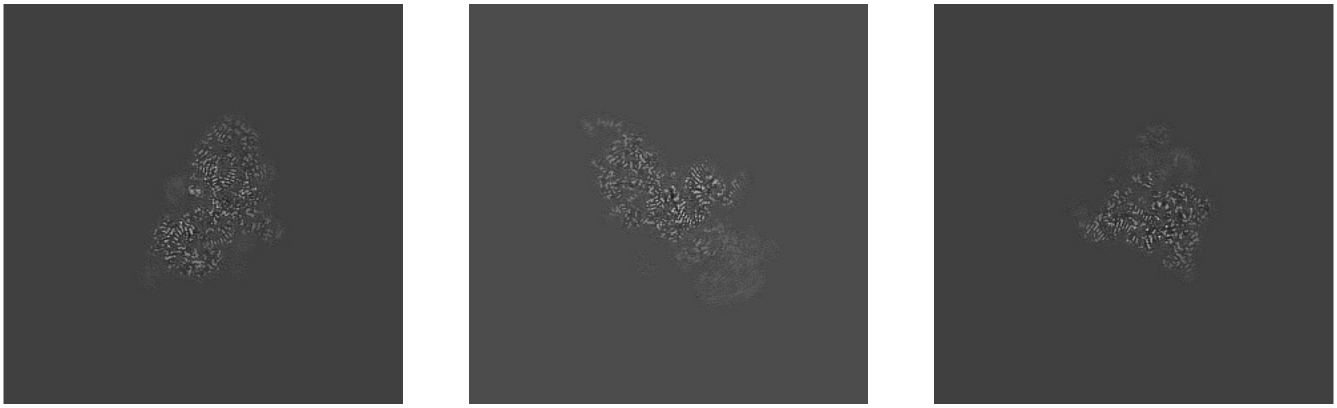

Y Index: 256


Z Index: 256

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

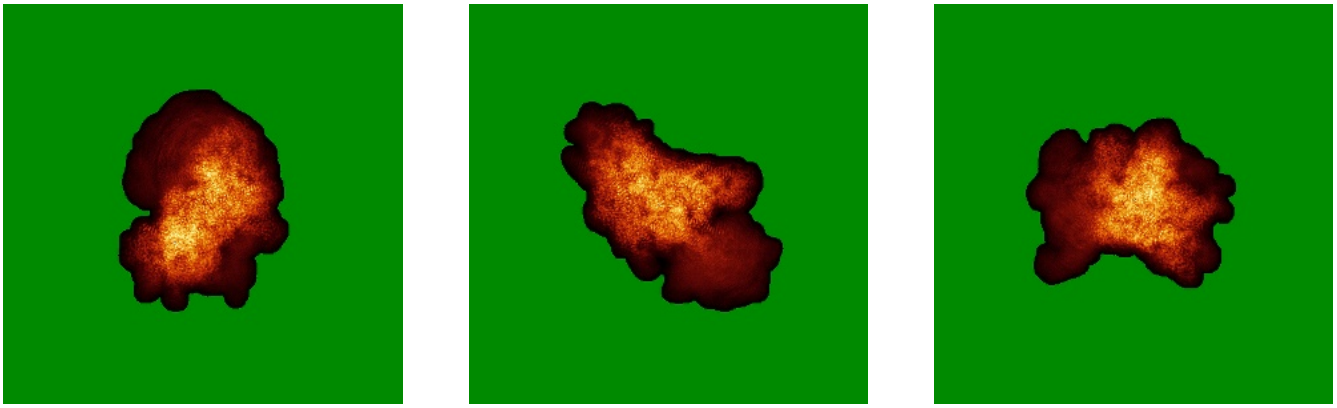


X Index: 279 Y Index: 264 Z Index: 213

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

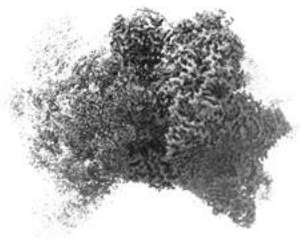
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

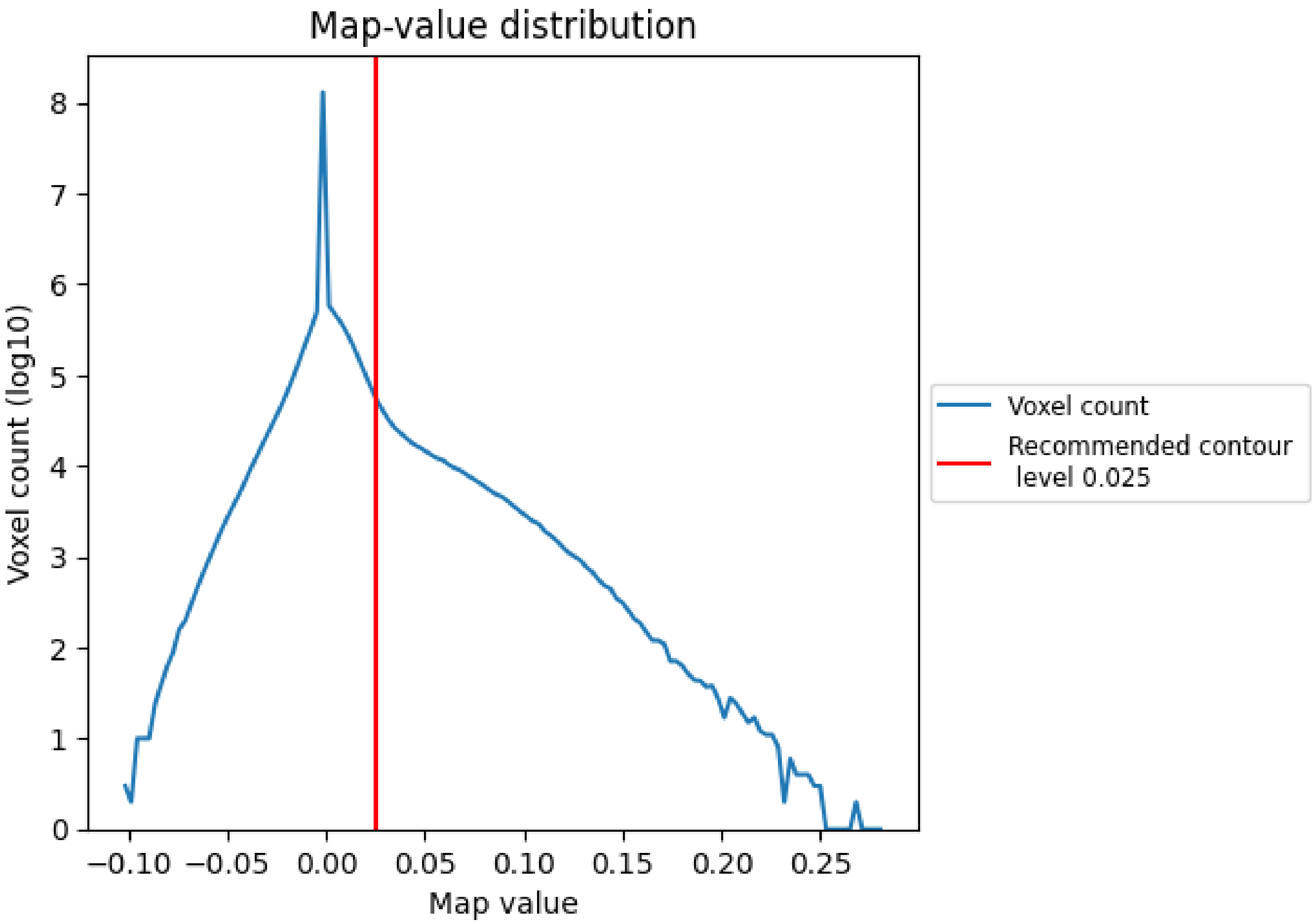
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

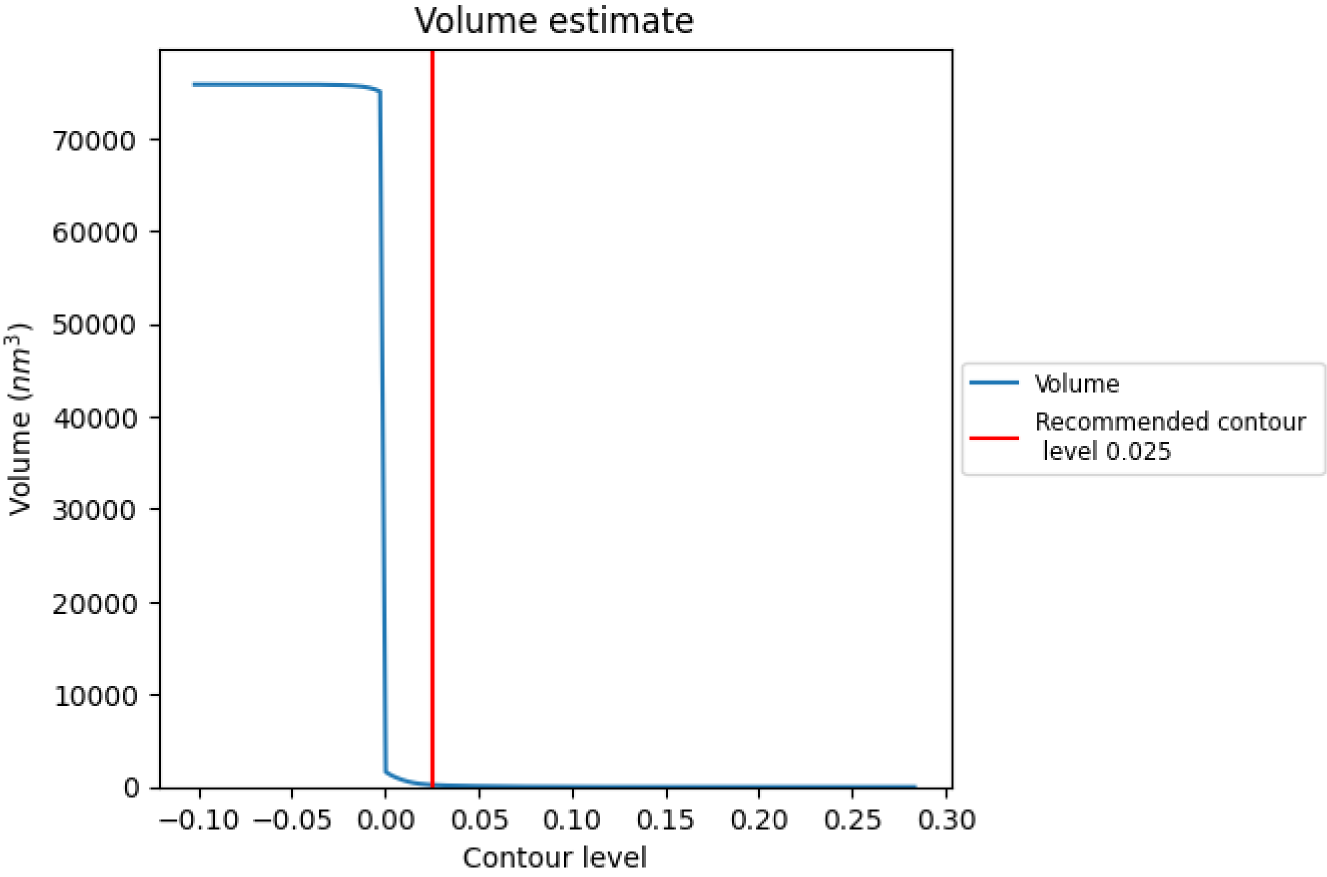
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

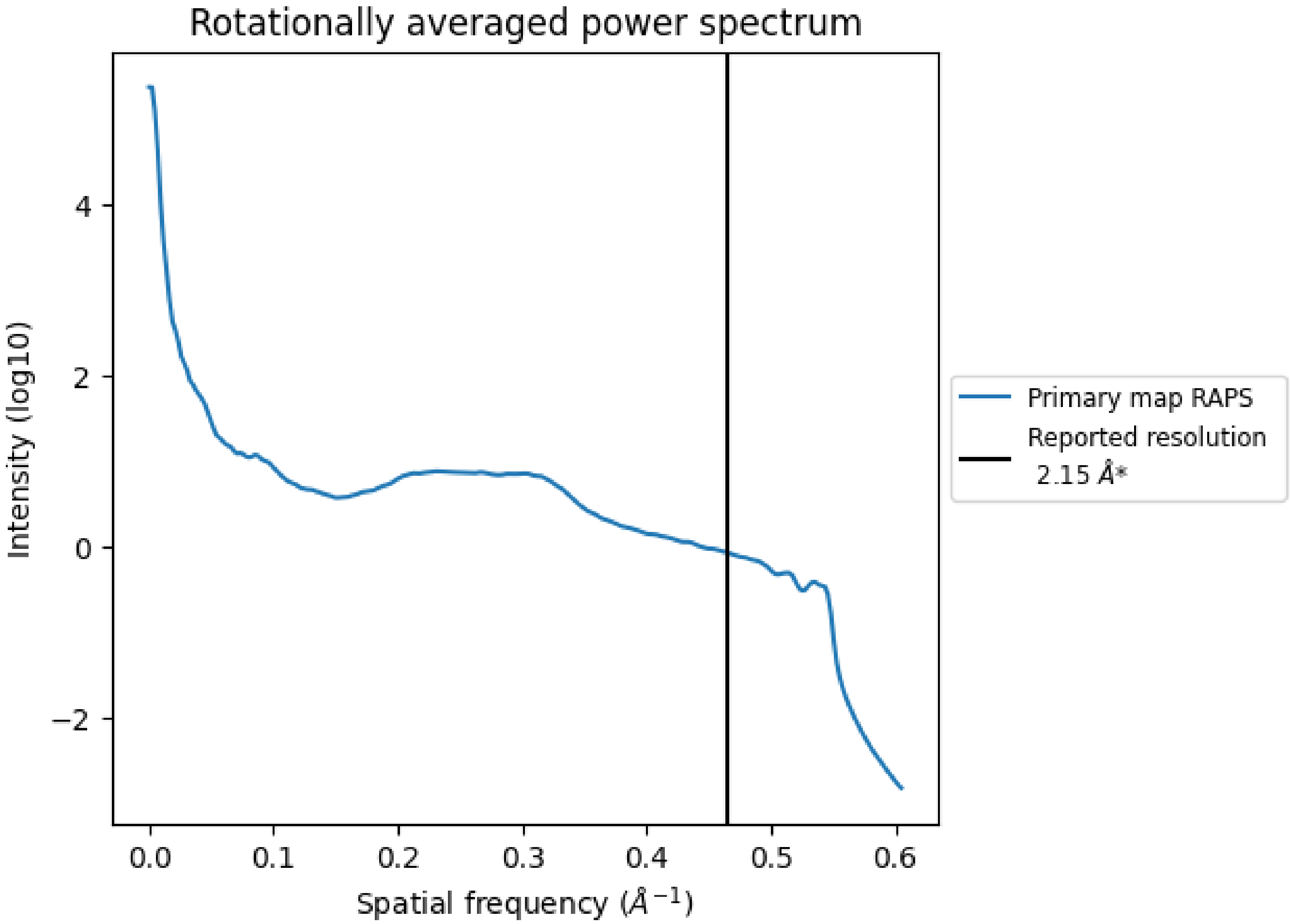
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 225 nm^3; this corresponds to an approximate mass of 203 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

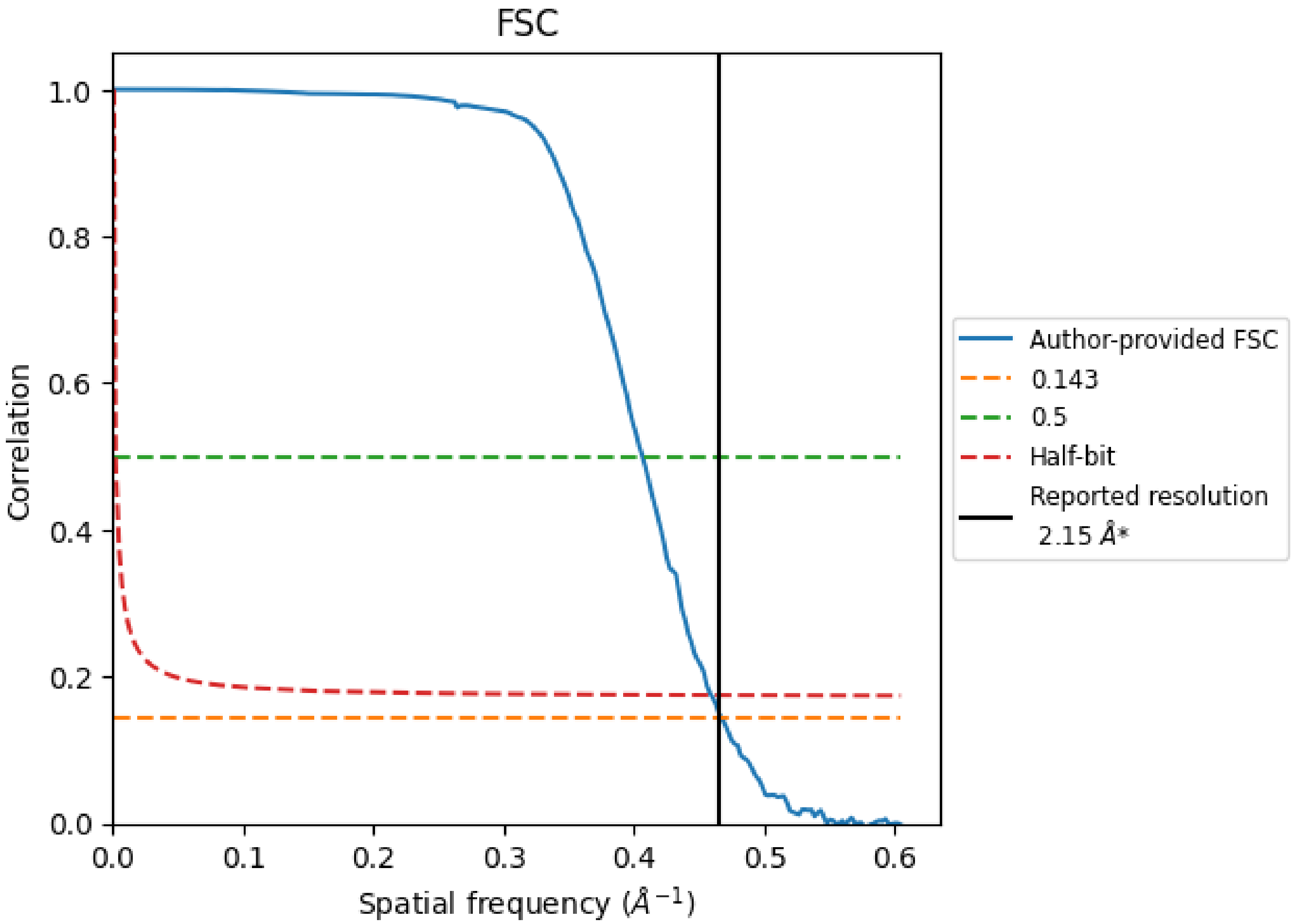


*Reported resolution corresponds to spatial frequency of 0.465 $\AA^{-1}$

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.465 Å^{-1}

8.2 Resolution estimates ⓘ

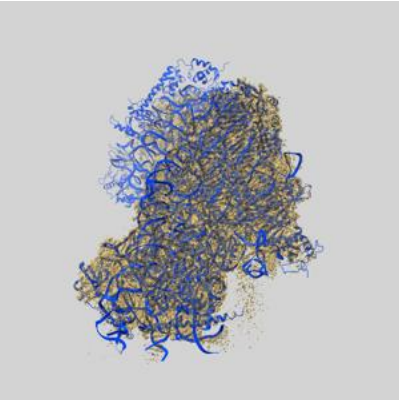
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.14	2.46	2.18
Unmasked-calculated*	-	-	-

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

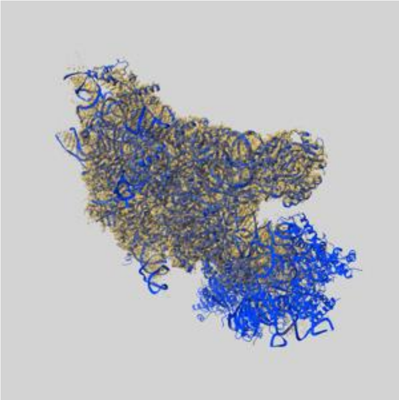
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14317 and PDB model 7R4X. Per-residue inclusion information can be found in section 3 on page 13.

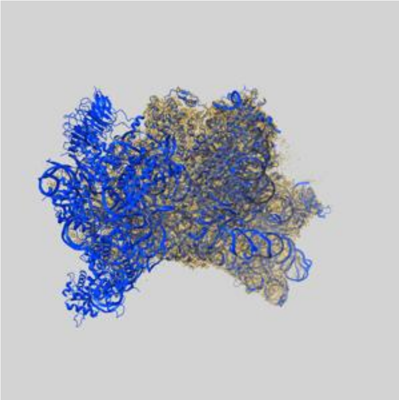
9.1 Map-model overlay (i)



X



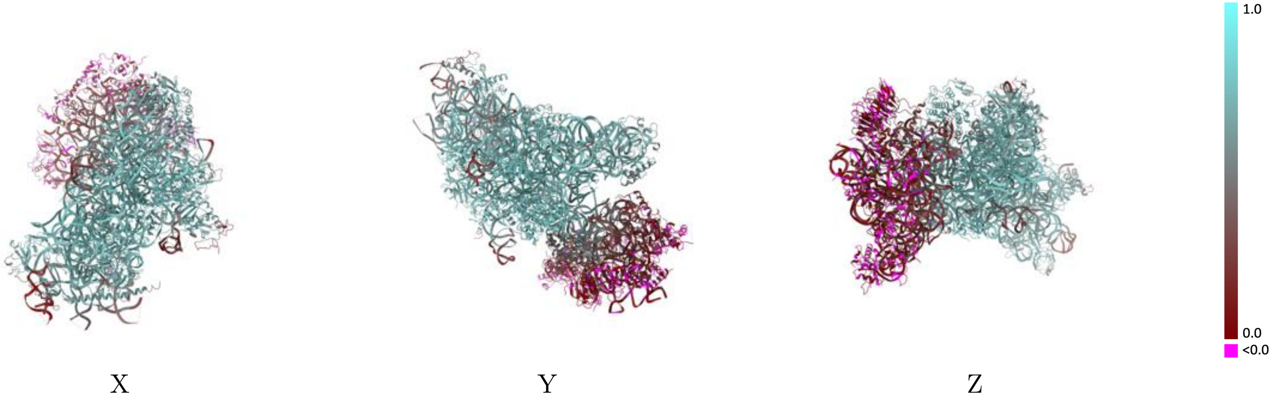
Y



Z

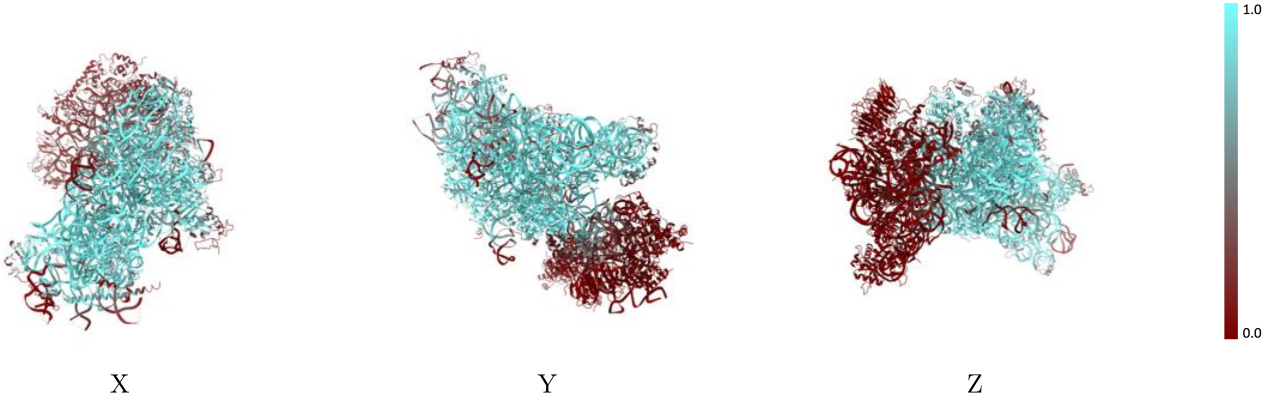
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



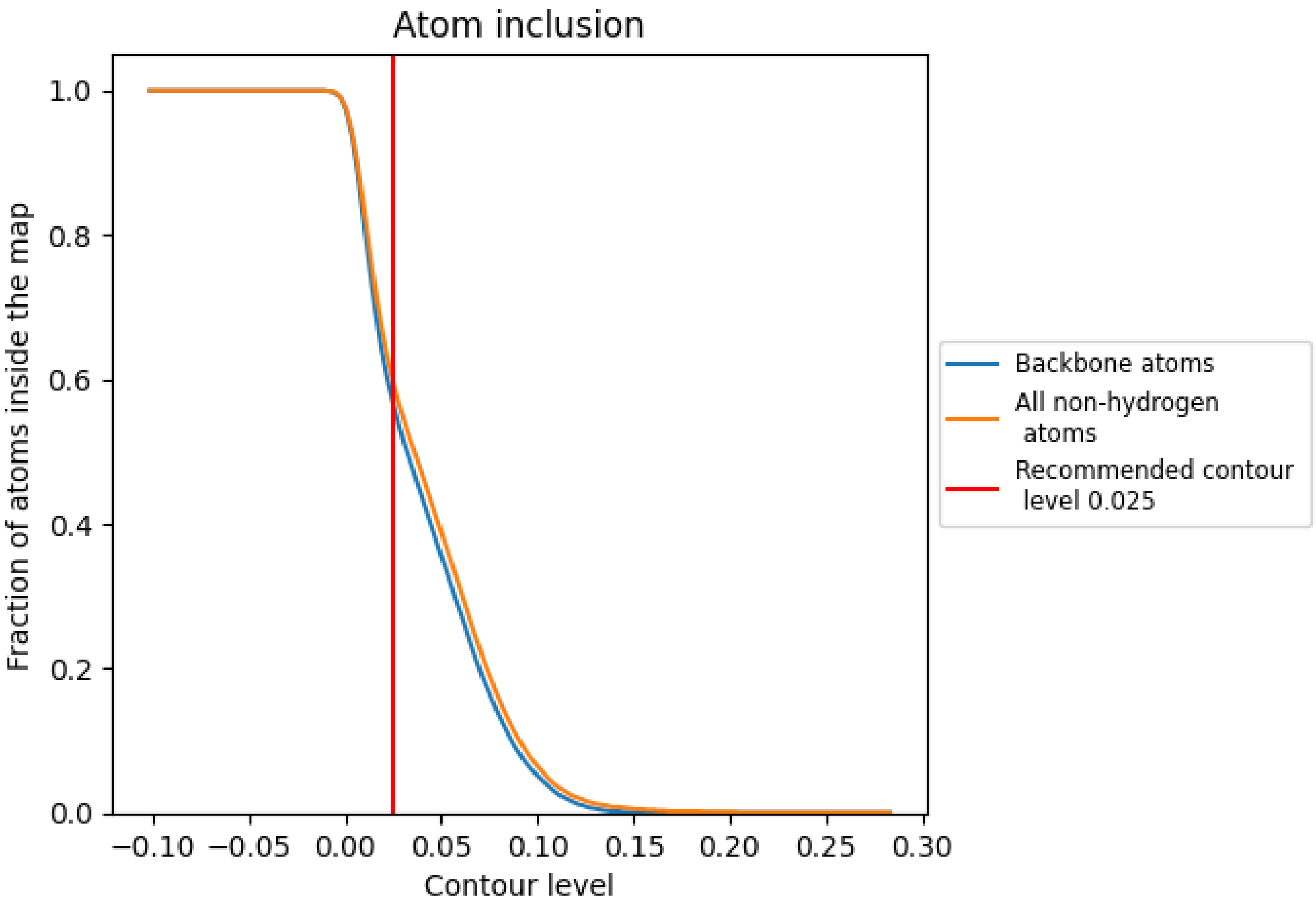
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 60% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5950	0.5210
2	0.6770	0.5580
A	0.9030	0.7170
B	0.7650	0.6480
C	0.9130	0.7440
D	0.1730	0.3590
E	0.9420	0.7390
F	0.0210	0.1930
G	0.6250	0.6060
H	0.5390	0.5700
I	0.7720	0.6420
J	0.8950	0.7330
K	0.0290	0.1770
L	0.8970	0.7170
M	0.0010	0.0580
N	0.8610	0.6950
O	0.8390	0.6690
P	0.0060	0.1180
Q	0.0500	0.1560
R	0.2950	0.4730
S	0.0050	0.0860
T	0.0050	0.1020
U	0.1150	0.2440
V	0.8940	0.7250
W	0.9680	0.7720
X	0.9490	0.7620
Y	0.8870	0.7050
Z	0.0000	0.0570
a	0.8450	0.6970
b	0.7610	0.6650
c	0.0490	0.2810
d	0.2170	0.3440
e	0.7350	0.6540
f	0.0000	0.0280
g	0.0070	0.1120
n	0.8010	0.6940