Full wwPDB EM Validation Report ⓘ

Nov 25, 2024 – 03:22 PM EST

PDB ID	:	9C3H
EMDB ID	:	EMD-45170
Title	:	Structure of the CNOT3-bound human 80S ribosome with tRNA-ARG in the P-site.
Authors	:	Erzberger, J.P.; Cruz, V.E.
Deposited on	:	2024-06-01
Resolution	:	2.00 Å(reported)

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

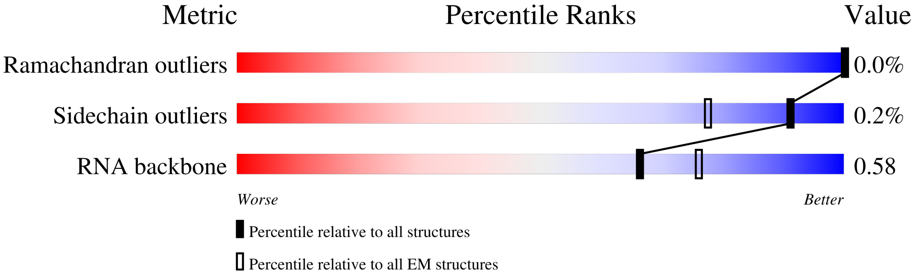
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

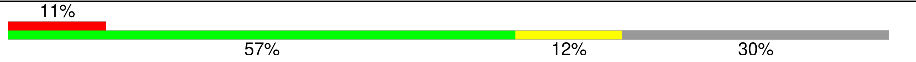
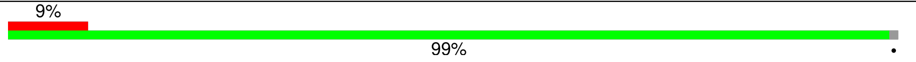
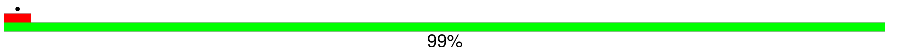
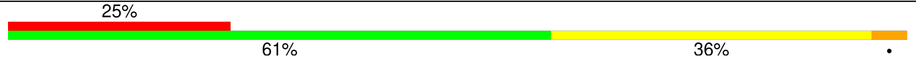
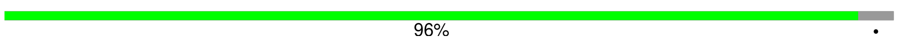
The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	L1	157	
2	L5	5069	
3	L8	297	
4	L9	121	
5	LB	403	
6	S4	76	
7	LC	427	
8	LD	257	

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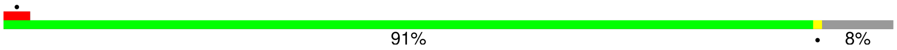
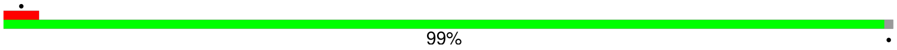
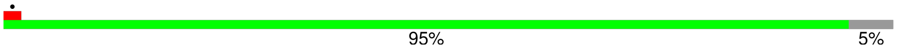
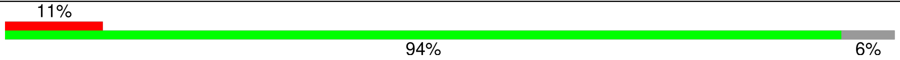
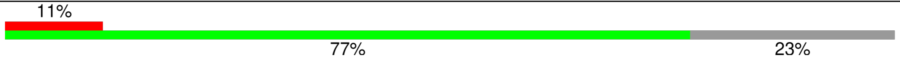
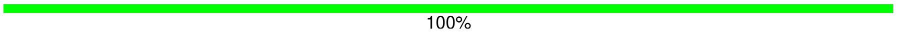
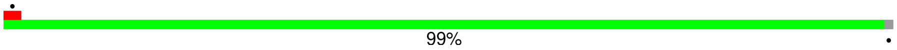
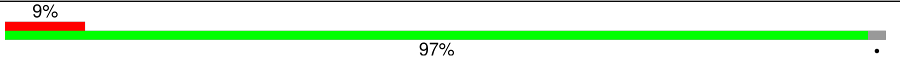
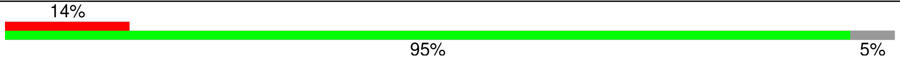
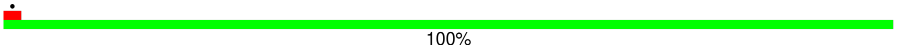
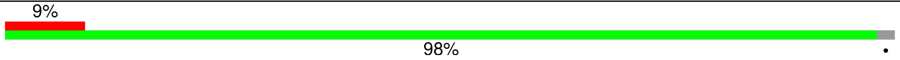
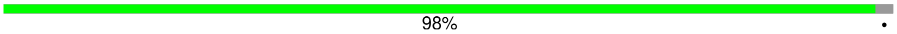
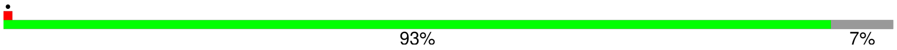
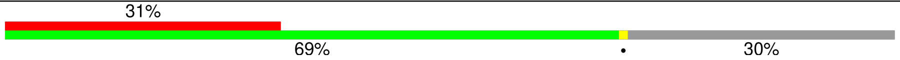
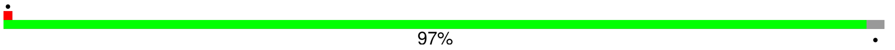
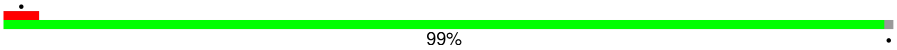
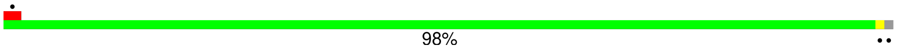
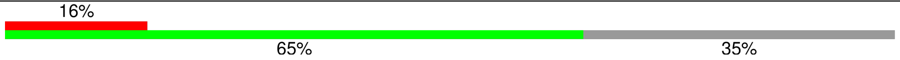
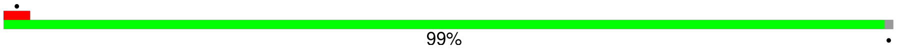
Mol	Chain	Length	Quality of chain
9	LE	145	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	135	
14	LJ	178	
15	LK	288	
16	LM	215	
17	LN	204	
18	LO	123	
19	LP	97	
20	LQ	211	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	51	
25	LV	140	
26	LW	157	
27	LY	203	
28	LZ	136	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	106	

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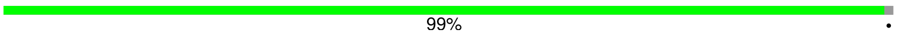
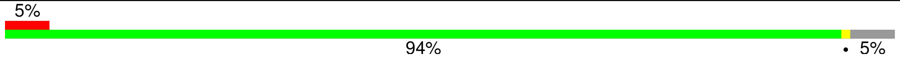
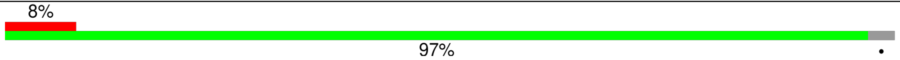
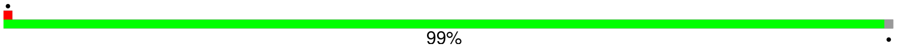
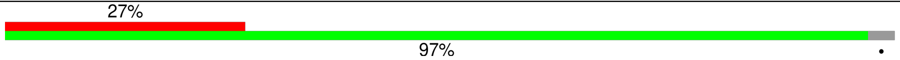
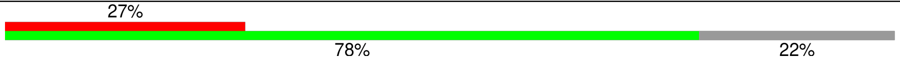
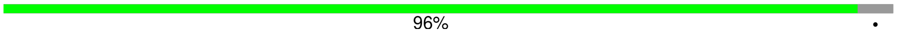
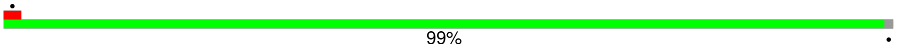
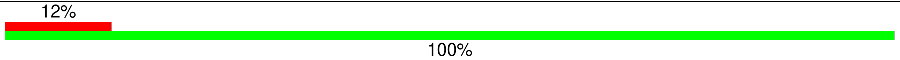
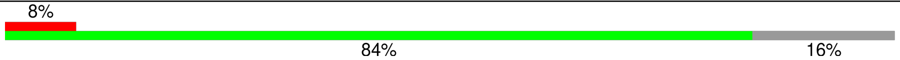
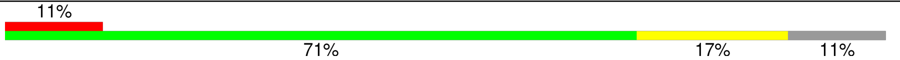
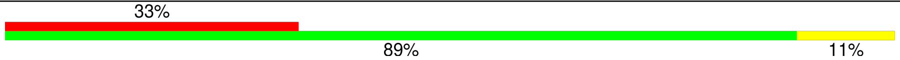
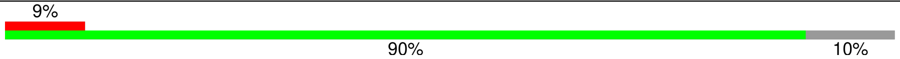
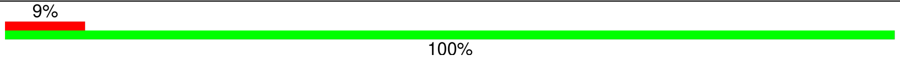
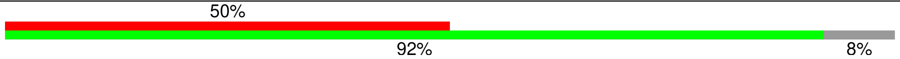
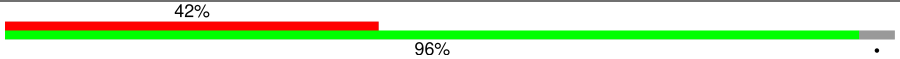
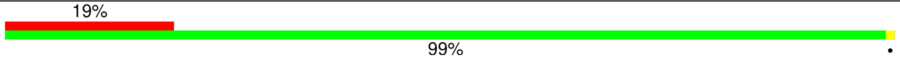
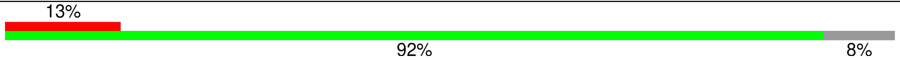
Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	184	
37	Li	105	
38	Lj	188	
39	Lk	70	
40	Ll	137	
41	Lm	128	
42	Ln	156	
43	Lo	99	
44	Lp	92	
45	Lz	214	
46	NC	25	
47	S1	264	
48	S2	1869	
49	S5	9	
50	SA	295	
51	SB	609	
52	SC	293	
53	SD	204	
54	SE	263	
55	SG	249	
56	SH	194	
57	SI	208	
58	SJ	194	

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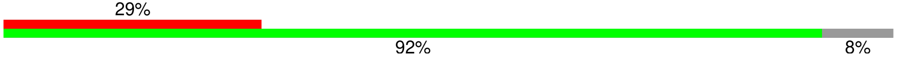
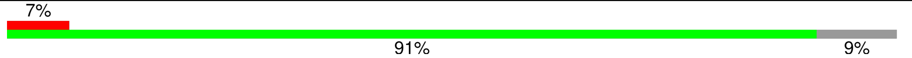
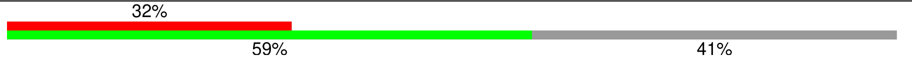
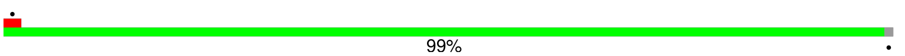
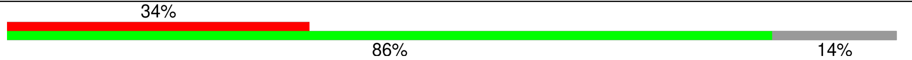
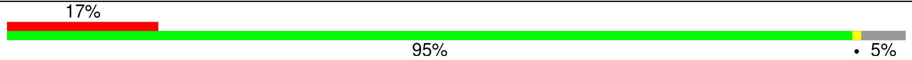
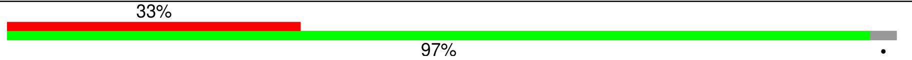
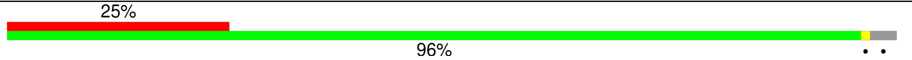
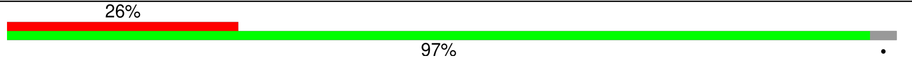
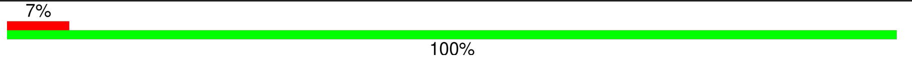
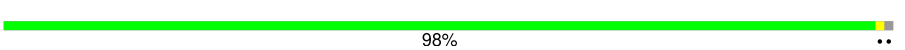
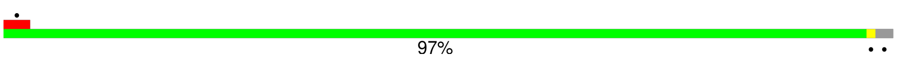
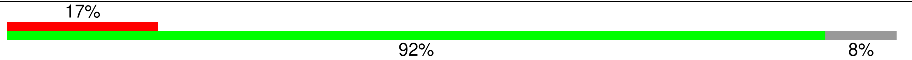
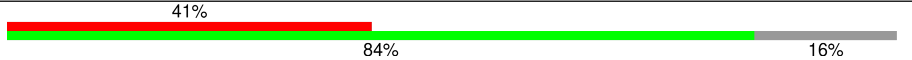
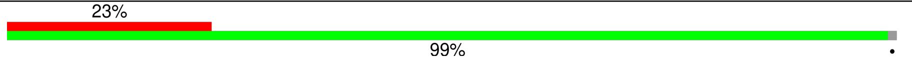
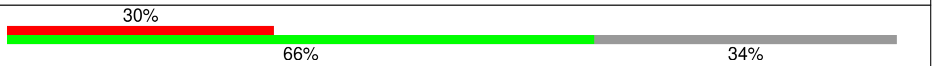
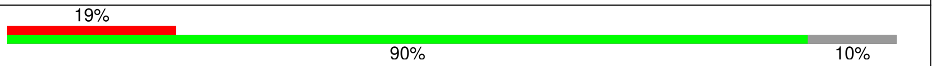
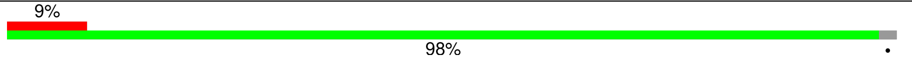
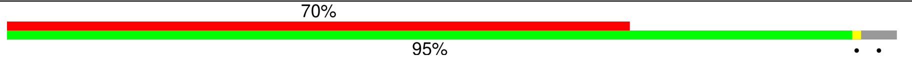
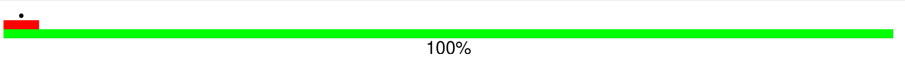
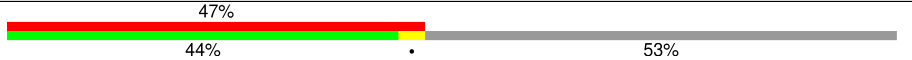
Mol	Chain	Length	Quality of chain
59	SK	243	
60	SL	158	
61	SM	165	
62	SN	151	
63	SO	151	
64	SP	145	
65	SQ	146	
66	SS	135	
67	ST	152	
68	SU	145	
69	SV	83	
70	SW	130	
71	SX	143	
72	SY	132	
73	SZ	119	
74	Sa	115	
75	Sb	84	
76	Sc	125	
77	Sd	69	
78	Se	133	
79	Sf	56	
80	Sg	317	
81	So	25	
82	Sy	132	
83	Sz	156	

2 Entry composition ⓘ

There are 88 unique types of molecules in this entry. The entry contains 222228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L1	148	3153	1408	563	1035	147	0	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L5	3531	75768	33782	13851	24605	3530	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L8	293	2386	1510	435	427	14	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L9	120	2558	1141	456	842	119	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	401	3234	2058	607	555	14	0	0

- Molecule 6 is a RNA chain called tRNA-ARG,CCG-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	S4	76	1634	732	290	536	76	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LC	365	2908	1829	580	486	13	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LD	248	1899	1189	389	315	6	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LF	225	1870	1202	358	301	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LF	173	SER	ALA	conflict	UNP P18124

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LG	216	1752	1117	337	294	4	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LH	190	1518	956	284	272	6	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LJ	167	1340	848	250	236	6	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LK	222	1780	1147	337	292	4	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LM	135	1111	713	213	178	7	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LN	203	1700	1072	359	265	4	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LO	122	1014	641	205	167	1	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 20 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	206	Total 1664	C 1041	N 345	O 274	S 4	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	186	Total 1558	C 965	N 335	O 249	S 9	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	176	Total 1460	C 930	N 284	O 235	S 11	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	157	Total 1284	C 815	N 250	O 214	S 5	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	50	Total 443	C 281	N 98	O 63	S 1	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	130	Total 972	C 615	N 183	O 169	S 5	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	110	Total 893	C 560	N 180	O 150	S 3	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LY	198	1624	1048	317	254	5	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LZ	135	1106	714	208	181	3	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	La	147	1162	736	237	186	3	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lb	104	848	526	186	132	4	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lc	101	785	498	138	142	7	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Ld	104	862	546	167	147	2	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Le	105	863	543	175	139	6	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Lf	109	875	555	174	143	3	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lg	111	882	552	182	142	6	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Lh	159	1289	808	249	223	9	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Li	102	832	521	177	129	5	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Lj	187	1512	944	314	249	5	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Lk	68	559	360	101	97	1	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Ll	124	990	614	205	167	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	2	ACE	-	acetylation	UNP P46779

- Molecule 41 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lm	100	816	524	142	148	2	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lo	52	436	272	91	67	6	1	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PHE	deletion	UNP P62987
Lo	?	-	ALA	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	GLU	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	THR	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	SER	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	TYR	deletion	UNP P62987
Lo	?	-	ASN	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Lp	88	681	430	131	113	7	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lz	211	1705	1081	329	281	14	0	0

- Molecule 46 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	NC	25	227	134	52	41	0	0

- Molecule 47 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	S1	221	1790	1135	323	318	14	0	0

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	S2	1660	35485	15869	6358	11599	1659	0	0

- Molecule 49 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	S5	9	191	85	33	64	9	0	0

- Molecule 50 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SA	220	1731	1099	303	321	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 51 is a protein called CCR4-NOT transcription complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SB	232	1937	1204	344	383	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SB	608	PRO	-	expression tag	UNP O75175
SB	609	ARG	-	expression tag	UNP O75175

- Molecule 52 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SC	219	1700	1100	292	298	10	0	0

- Molecule 53 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SD	184	1463	917	276	263	7	0	0

- Molecule 54 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SE	262	2075	1324	386	357	8	0	0

- Molecule 55 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SG	229	1853	1158	369	319	7	0	0

- Molecule 56 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SH	187	1509	963	277	268	1	0	0

- Molecule 57 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SI	207	1695	1064	334	292	5	0	0

- Molecule 58 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SJ	179	1495	953	299	241	2	0	0

- Molecule 59 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 60 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SL	143	1180	754	223	197	6	0	0

- Molecule 61 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 62 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SN	150	1207	773	229	204	1	0	0

- Molecule 63 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SO	127	956	585	189	176	6	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 64 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	SP	125	1021	647	192	175	7	0	0

- Molecule 65 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	SQ	139	1108	704	210	191	3	0	0

- Molecule 66 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	147	Total 1208	C 758	N 244	O 205	S 1	0	0

- Molecule 68 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 69 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SW	129	Total 1033	C 659	N 193	O 175	S 6	0	0

- Molecule 71 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 72 is a protein called Isoform 3 of Small ribosomal subunit protein eS24.

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

- Molecule 73 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SZ	100	Total 795	C 498	N 152	O 141	S 4	0	0

- Molecule 74 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sc	83	Total	C	N	O	S	0	0
			670	431	125	113	1		

- Molecule 77 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sd	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 78 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	55	Total	C	N	O	S	0	0
			437	271	95	70	1		

- Molecule 79 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sf	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 80 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sg	303	Total	C	N	O	S	0	0
			2364	1492	412	448	12		

- Molecule 81 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms	AltConf	Trace
81	So	25	Total C N O S 239 145 64 27 3	0	0

- Molecule 82 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms	AltConf	Trace
82	Sy	121	Total C N O S 939 590 166 174 9	0	0

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms	AltConf	Trace
83	Sz	74	Total C N O S 607 384 116 100 7	0	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
84	L1	4	Total Mg 4 4	0
84	L5	204	Total Mg 204 204	0
84	L9	3	Total Mg 3 3	0
84	S4	6	Total Mg 6 6	0
84	LD	1	Total Mg 1 1	0
84	LI	2	Total Mg 2 2	0
84	LN	1	Total Mg 1 1	0
84	LR	2	Total Mg 2 2	0
84	LV	1	Total Mg 1 1	0
84	La	1	Total Mg 1 1	0
84	Lh	1	Total Mg 1 1	0
84	S2	97	Total Mg 97 97	0

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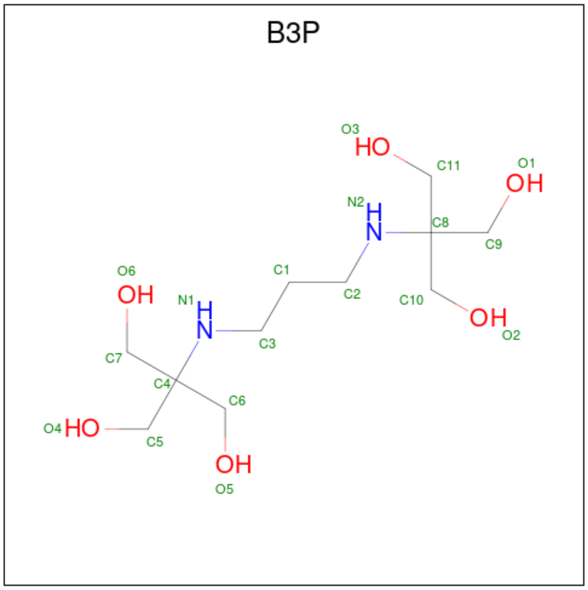
Mol	Chain	Residues	Atoms	AltConf
84	SG	1	Total Mg 1 1	0
84	ST	1	Total Mg 1 1	0
84	SX	1	Total Mg 1 1	0

- Molecule 85 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
85	L1	3	Total K 3 3	0
85	L5	42	Total K 42 42	0
85	L9	1	Total K 1 1	0
85	LC	1	Total K 1 1	0
85	LD	2	Total K 2 2	0
85	LV	1	Total K 1 1	0
85	Lz	1	Total K 1 1	0
85	S2	39	Total K 39 39	0
85	SE	1	Total K 1 1	0
85	SO	1	Total K 1 1	0
85	ST	1	Total K 1 1	0
85	Sf	1	Total K 1 1	0

- Molecule 86 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	AltConf
86	L5	1	Total C N O 19 11 2 6	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
87	LP	1	Total Zn 1 1	0
87	Le	1	Total Zn 1 1	0
87	Lg	1	Total Zn 1 1	0
87	Lo	1	Total Zn 1 1	0
87	Lp	1	Total Zn 1 1	0
87	Sa	1	Total Zn 1 1	0
87	Sf	1	Total Zn 1 1	0
87	Sz	1	Total Zn 1 1	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms	AltConf
88	L1	153	Total O 153 153	0
88	L5	4961	Total O 4961 4961	0
88	L8	25	Total O 25 25	0
88	L9	93	Total O 93 93	0
88	LB	85	Total O 85 85	0
88	S4	52	Total O 52 52	0
88	LC	104	Total O 104 104	0
88	LD	91	Total O 91 91	0
88	LE	10	Total O 10 10	0
88	LF	52	Total O 52 52	0
88	LG	16	Total O 16 16	0
88	LH	18	Total O 18 18	0
88	LI	64	Total O 64 64	0
88	LJ	3	Total O 3 3	0
88	LK	12	Total O 12 12	0
88	LM	7	Total O 7 7	0
88	LN	89	Total O 89 89	0
88	LO	13	Total O 13 13	0
88	LP	33	Total O 33 33	0
88	LQ	45	Total O 45 45	0
88	LR	23	Total O 23 23	0
88	LS	39	Total O 39 39	0

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Mol	Chain	Residues	Atoms	AltConf
88	LT	41	Total O 41 41	0
88	LU	10	Total O 10 10	0
88	LV	27	Total O 27 27	0
88	LW	7	Total O 7 7	0
88	LY	42	Total O 42 42	0
88	LZ	10	Total O 10 10	0
88	La	46	Total O 46 46	0
88	Lb	15	Total O 15 15	0
88	Lc	8	Total O 8 8	0
88	Ld	15	Total O 15 15	0
88	Le	19	Total O 19 19	0
88	Lf	33	Total O 33 33	0
88	Lg	30	Total O 30 30	0
88	Lh	42	Total O 42 42	0
88	Li	4	Total O 4 4	0
88	Lj	69	Total O 69 69	0
88	Lk	4	Total O 4 4	0
88	Ll	27	Total O 27 27	0
88	Lm	1	Total O 1 1	0
88	Ln	18	Total O 18 18	0
88	Lo	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
88	Lp	25	Total O 25 25	0
88	Lz	16	Total O 16 16	0
88	S1	25	Total O 25 25	0
88	S2	2334	Total O 2334 2334	0
88	S5	11	Total O 11 11	0
88	SA	9	Total O 9 9	0
88	SB	9	Total O 9 9	0
88	SC	36	Total O 36 36	0
88	SD	25	Total O 25 25	0
88	SE	45	Total O 45 45	0
88	SG	16	Total O 16 16	0
88	SH	6	Total O 6 6	0
88	SI	31	Total O 31 31	0
88	SJ	34	Total O 34 34	0
88	SK	6	Total O 6 6	0
88	SL	43	Total O 43 43	0
88	SM	4	Total O 4 4	0
88	SN	32	Total O 32 32	0
88	SO	33	Total O 33 33	0
88	SP	14	Total O 14 14	0
88	SQ	32	Total O 32 32	0

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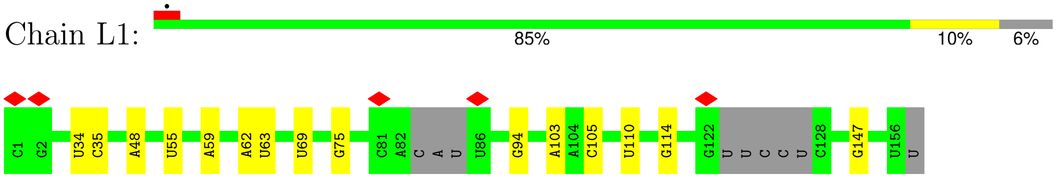
Mol	Chain	Residues	Atoms	AltConf
88	SS	5	Total O 5 5	0
88	ST	23	Total O 23 23	0
88	SU	20	Total O 20 20	0
88	SV	8	Total O 8 8	0
88	SW	39	Total O 39 39	0
88	SX	47	Total O 47 47	0
88	SY	10	Total O 10 10	0
88	SZ	12	Total O 12 12	0
88	Sa	38	Total O 38 38	0
88	Sb	11	Total O 11 11	0
88	Sc	3	Total O 3 3	0
88	Sd	2	Total O 2 2	0
88	Se	10	Total O 10 10	0
88	Sf	8	Total O 8 8	0
88	Sg	1	Total O 1 1	0
88	So	3	Total O 3 3	0

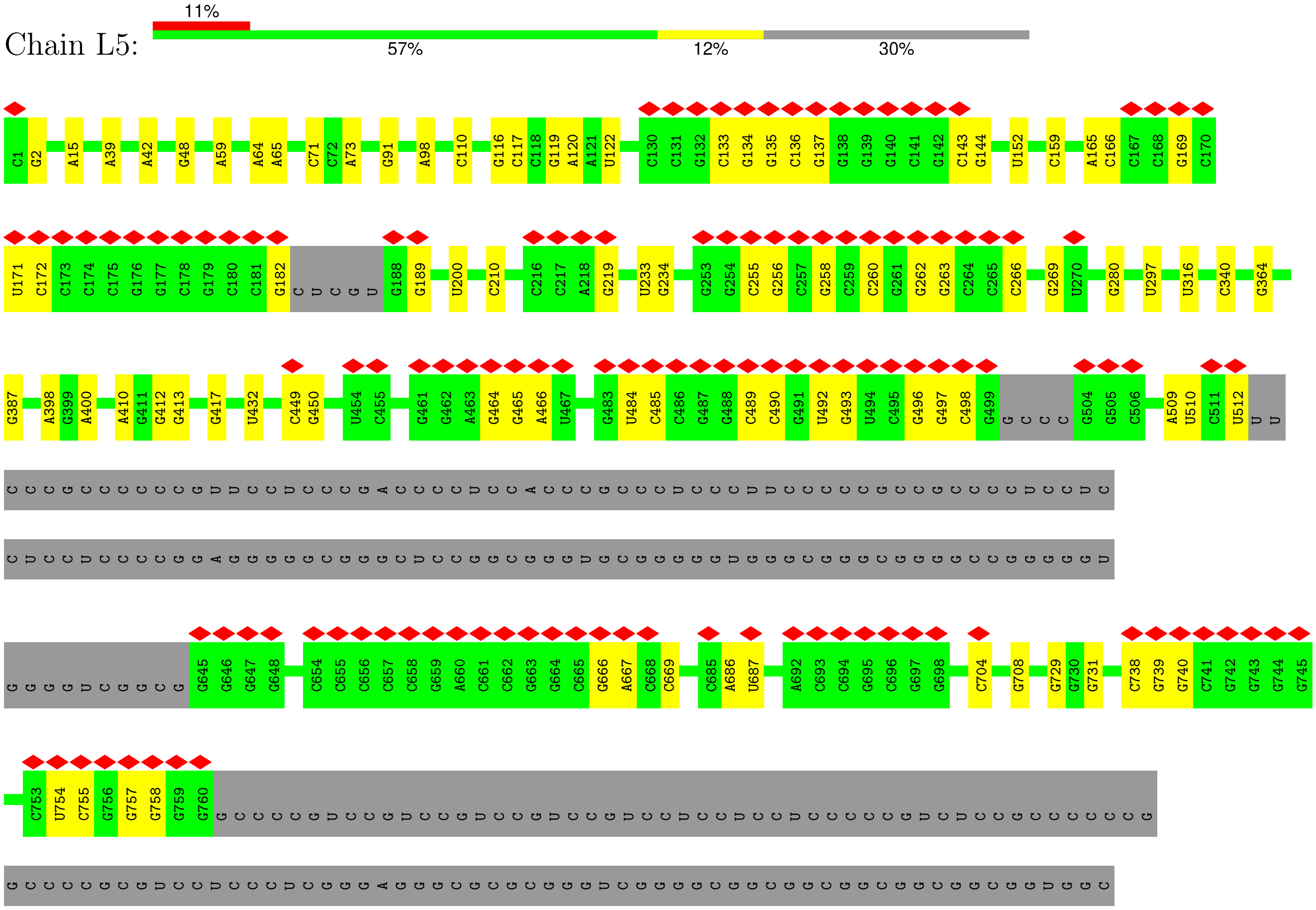
3 Residue-property plots ⓘ

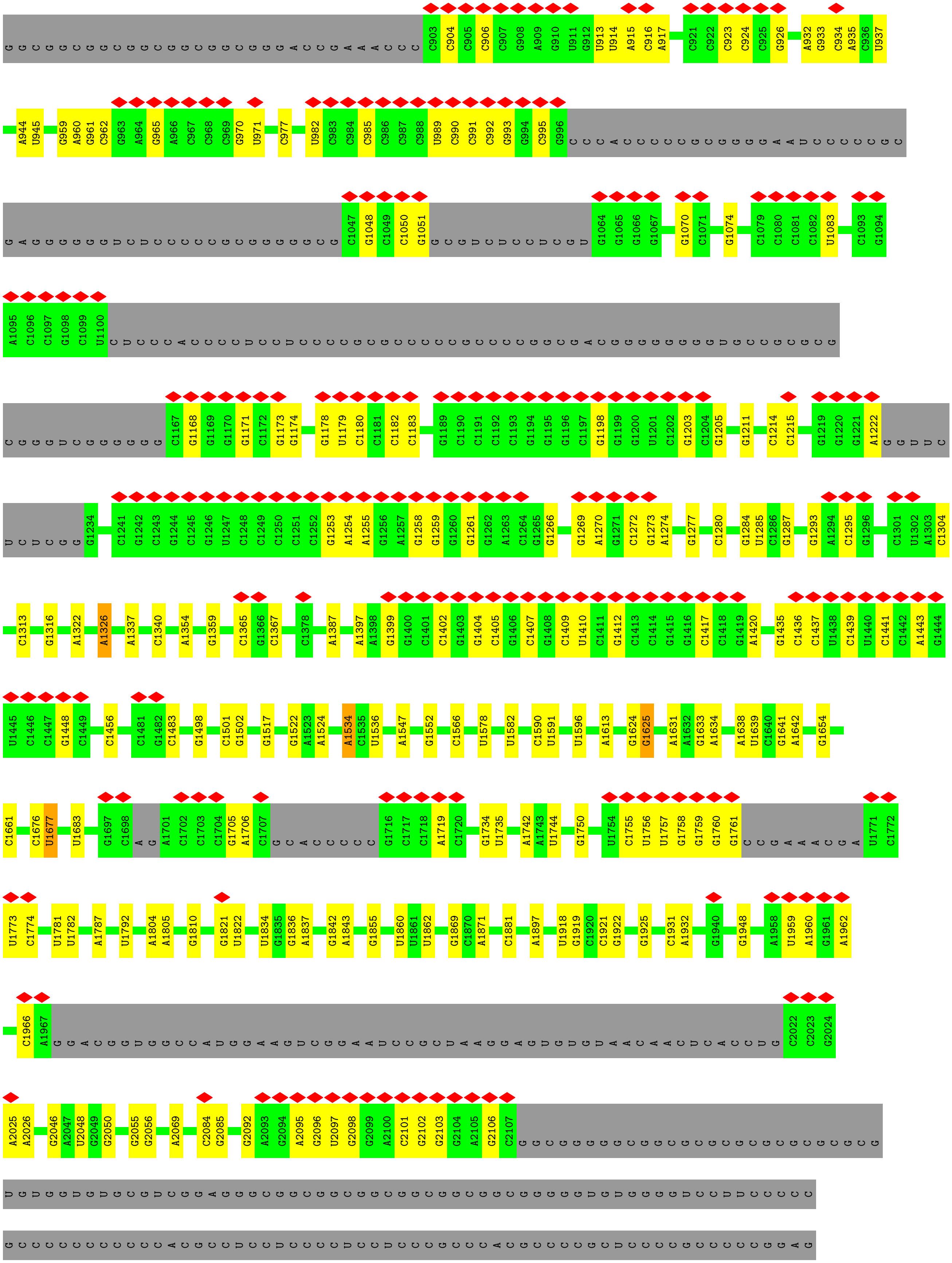
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 5.8S rRNA



- Molecule 2: 28S rRNA

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A944 U945 G959 A960 G961 C962 G963 A964 G965 A966 C967 C968 C969 G970 U971 C977 U982 C983 C984 C985 C986 C987 C988 U989 C990 C991 C992 G993 G994 C995 G996 C C C A C C C C C G C G G G G A A U C C C C C G C
G A G G G G G G U C U C C C C C G C G G G G C G C1047 G1048 C1049 C1050 G1051 G C G U C U C C U C G U G1064 G1065 G1066 G1067 G1070 C1071 G1074 C1079 C1080 C1081 C1082 U1083 C1093 G1094
A1095 C1096 C1097 G1098 C1099 U1100 C U C C C A C C C C U C C U C C C C G C G C C C C C G C C C C G G C G A C G G G G G G G U G C C G C G C G
C G G G U C G G G G G C1167 G1168 G1169 G1170 G1171 C1172 G1173 G1174 G1178 U1179 C1180 C1181 C1182 C1183 G1189 C1190 C1191 C1192 G1193 G1194 G1195 G1196 C1197 G1198 G1199 G1200 U1201 C1202 G1203 C1204 G1205 G1211 C1214 C1215 G1219 G1220 G1221 A1222 G G U U C
U C U C G G G1234 C1241 G1242 C1243 G1244 C1245 G1246 U1247 C1248 C1249 C1250 C1251 C1252 G1253 A1254 A1255 G1256 A1257 G1258 G1259 G1260 G1261 G1262 A1263 G1264 G1265 G1266 G1269 A1270 G1271 C1272 G1273 A1274 G1277 C1280 G1284 U1285 C1286 G1287 G1293 A1294 C1295 G1296 C1301 U1302 A1303 C1304
C1313 G1316 A1322 A1326 A1337 C1340 A1354 G1359 C1365 G1366 C1367 C1378 A1387 A1397 A1398 G1399 G1400 C1401 C1402 G1403 G1404 C1405 G1406 C1407 G1408 C1409 U1410 C1411 G1412 C1413 C1414 G1415 G1416 C1417 C1418 G1419 A1420 G1435 C1436 C1437 U1438 C1439 U1440 C1441 C1442 A1443 G1444
U1445 C1446 C1447 G1448 C1449 C1456 C1481 G1482 C1483 G1498 C1501 G1502 G1517 G1522 A1523 A1524 A1534 C1535 U1536 A1547 G1552 C1566 U1578 U1582 C1590 U1591 U1596 A1613 G1624 G1625 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 A1642 G1654
C1661 C1676 U1677 U1683 G1697 C1698 A G A1701 C1702 C1703 C1704 G1705 A1706 C1707 G C A C C C C G1716 C1717 C1718 A1719 C1720 G1734 U1735 A1742 A1743 U1744 G1750 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C C G A A C G A U1771 C1772
U1773 C1774 U1781 U1782 A1787 U1792 A1804 A1805 G1810 G1821 U1822 U1834 G1835 G1836 A1837 G1842 A1843 G1855 U1860 U1861 U1862 G1869 C1870 A1871 C1881 A1897 U1918 G1919 C1920 C1921 G1922 G1925 C1931 A1932 G1940 G1948 A1958 U1959 A1960 G1961 A1962
C1966 A1967 G G A C G G U G G C C A U G G A A G U C G G A A U C C G C U A A G G A G U G U G U A A C A A C U C A C C U G C2022 C2023 G2024
A2025 A2026 G2046 A2047 U2048 G2049 G2050 G2055 G2056 A2069 C2084 G2085 G2092 A2093 G2094 A2095 C2096 U2097 G2098 G2099 A2100 C2101 G2102 G2103 G2104 A2105 G2106 C2107 G G C G G G G G C G G C G C G G C G C G C G C C G C G
U G U G G U G U G C G G U C G G A G G G C G G C G G C G G C G G C G G C G G C G G G G G U G U G G G G U C C U U C C C C C
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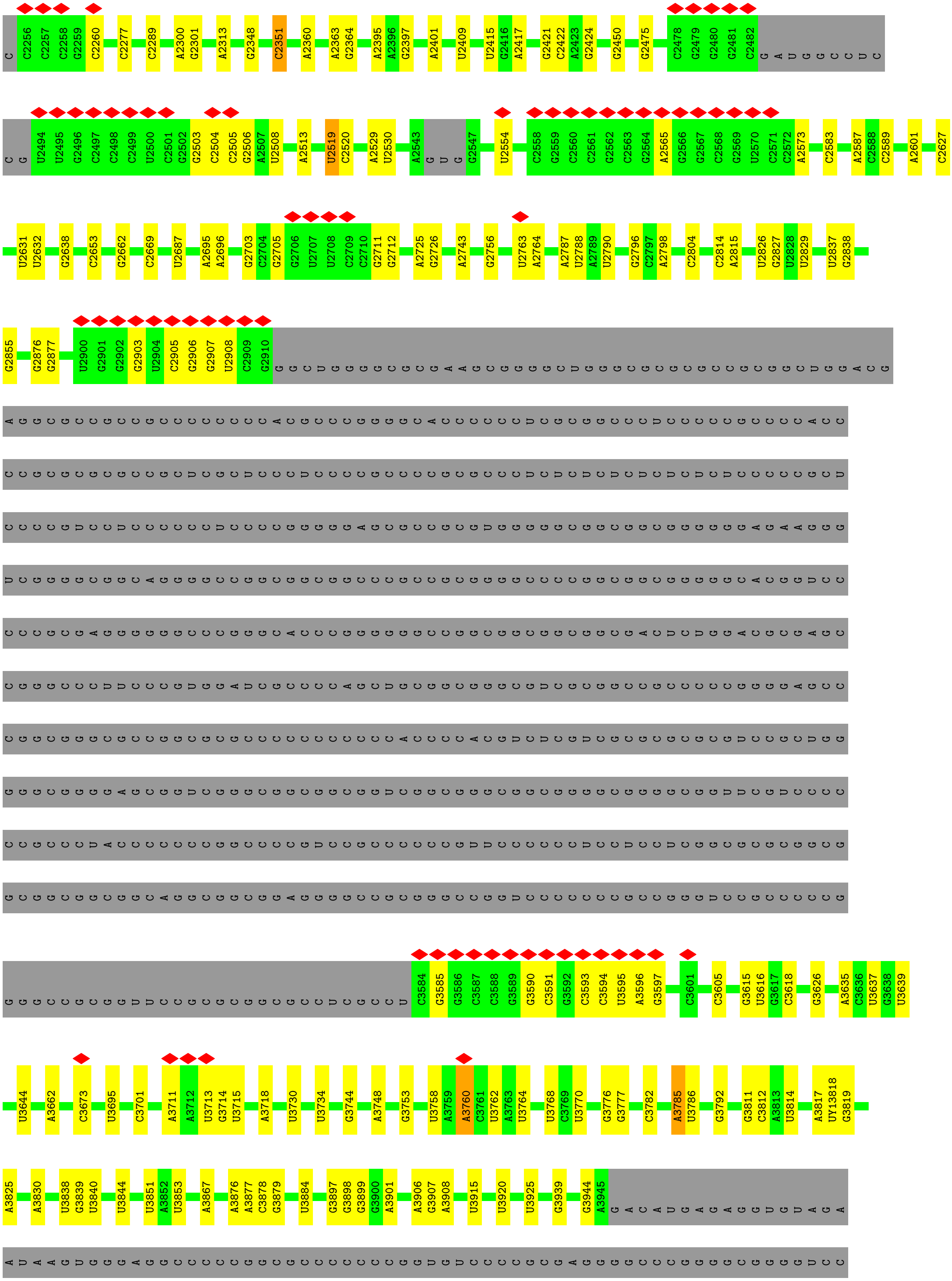
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C G
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C G G C G C G G C G C C G G C U G G C U C C C U C C C C G G C C C C G G C G C C C U C U C U C U C U C U C U C U C U C C C C G C U
C C C C G G U C C U C C C C C C C U C C C C G G G G G G A G C C G C C G C C G U G G G G G C G G C G G C G G G G G G A G A A G G G
U C G G G G G G G C A G G G G C C G G G G G G G G C C C G G C C G C G G G G C C C C C G G C G G C G G G G G C A C G G U C C
C C C G C G A G G G G G G G C C C C G G G G C A C C C G G G G G G G C C G G G C G G G C G G C G G G C G G A C U C U G G A C G C G A G C
C G G C C C C U U C C C G U G G A U C C G C C C C A G C U G C G G C G G G C G U C G C G G C C G C C C C C G G G G G A G C C
C G G C G G G C G C C G G C G C G C G C C C C C C C C C C C A C C C C A C G U C U C G U C G C G C G C G C G C G U C C G G C U G G
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C C G C C C C U A C C C C C C C G G C C C C G U C C G G C C C C C C C G G U U C C C C C C C U C C U C C U C G G G C C G C G G G C G
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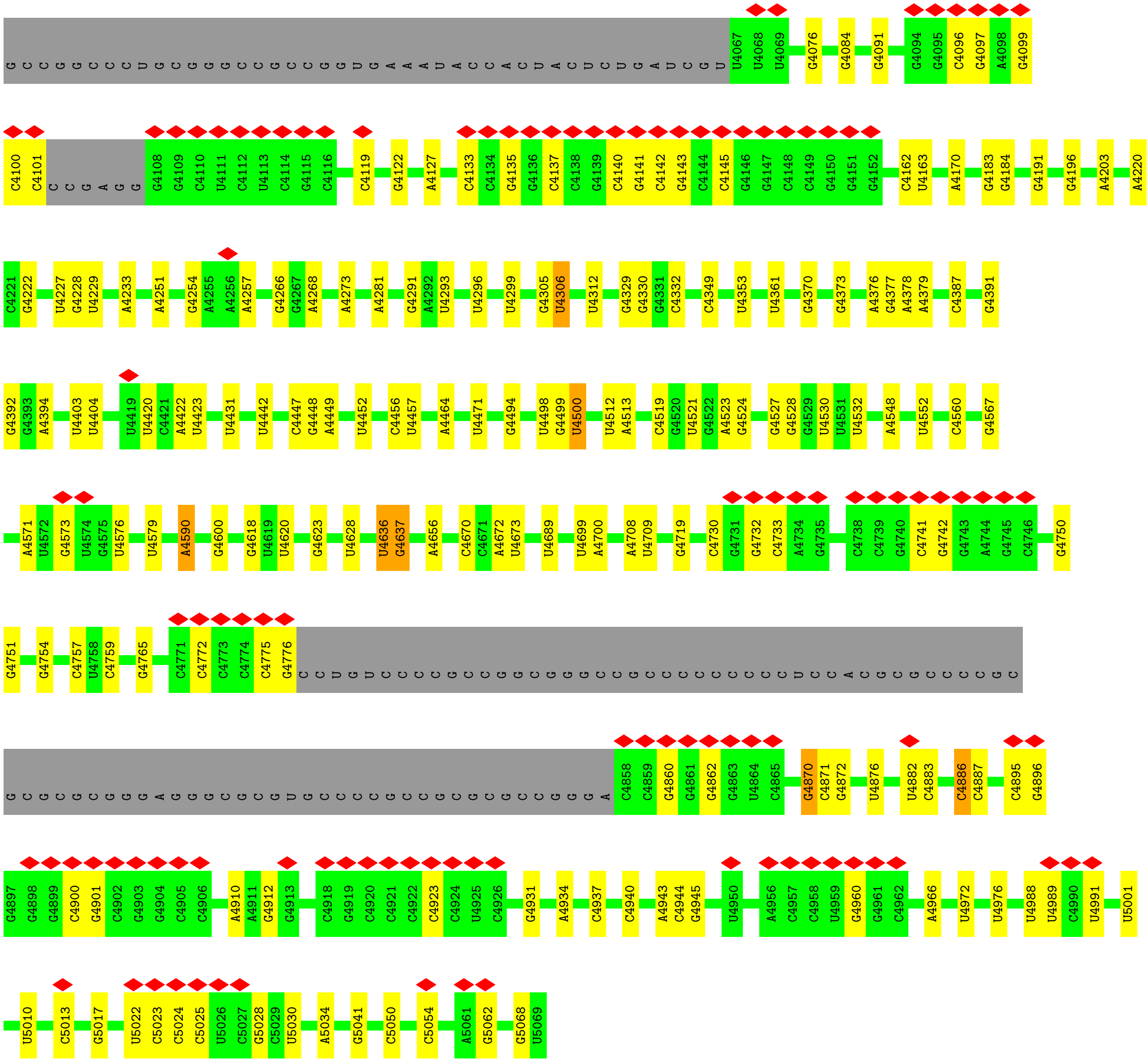
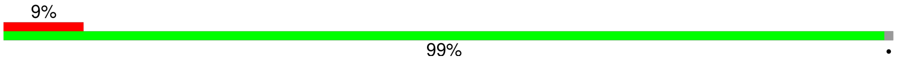
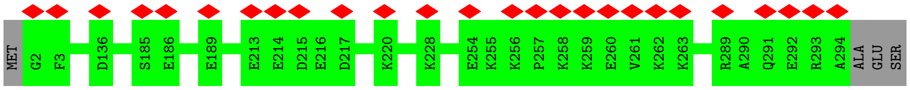


- Molecule 3: Large ribosomal subunit protein uL18

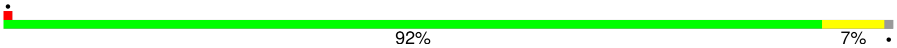
Chain L8:

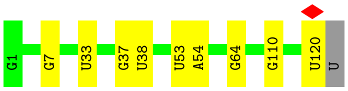




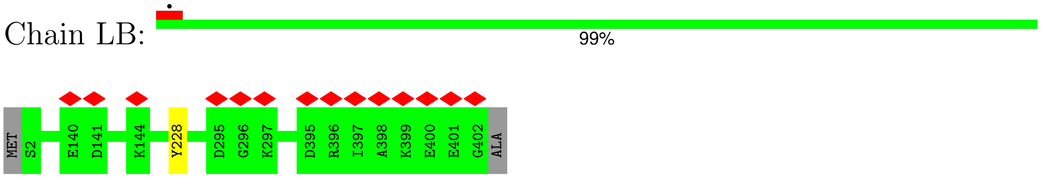
- Molecule 4: 5S rRNA

Chain L9:

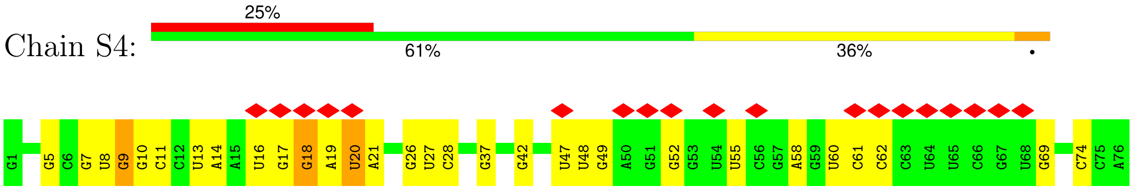




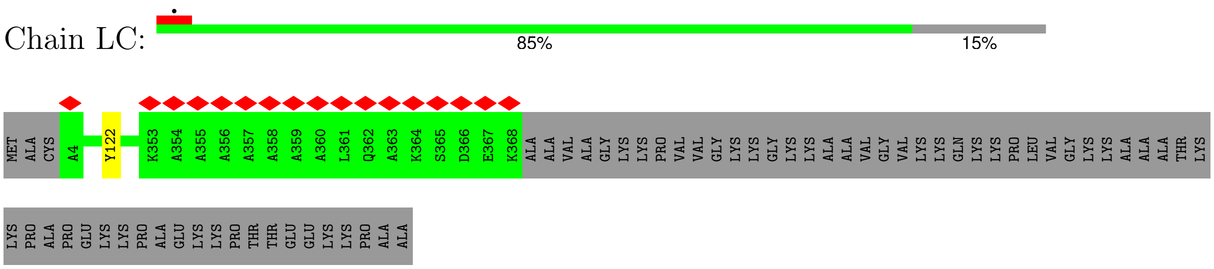
- Molecule 5: Large ribosomal subunit protein uL3



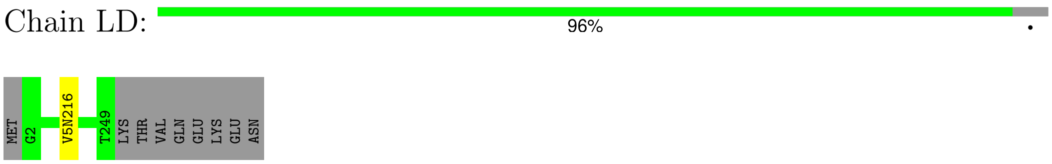
- Molecule 6: tRNA-ARG,CCG-1



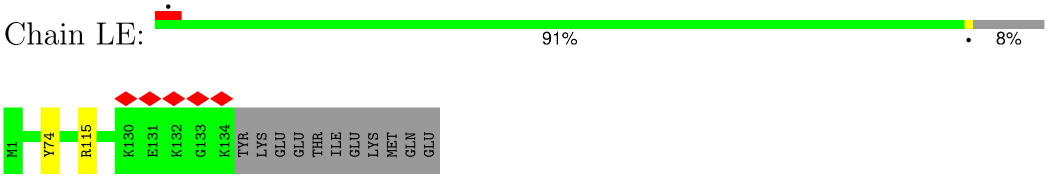
- Molecule 7: Large ribosomal subunit protein uL4



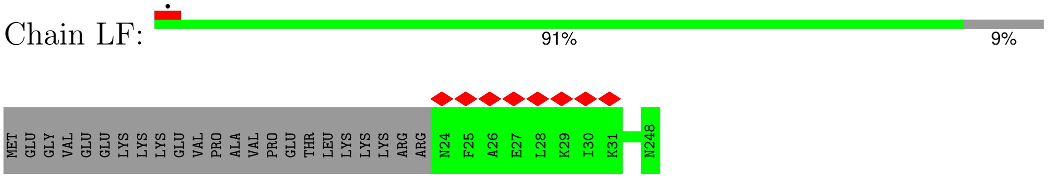
- Molecule 8: Large ribosomal subunit protein uL2



- Molecule 9: Large ribosomal subunit protein uL24

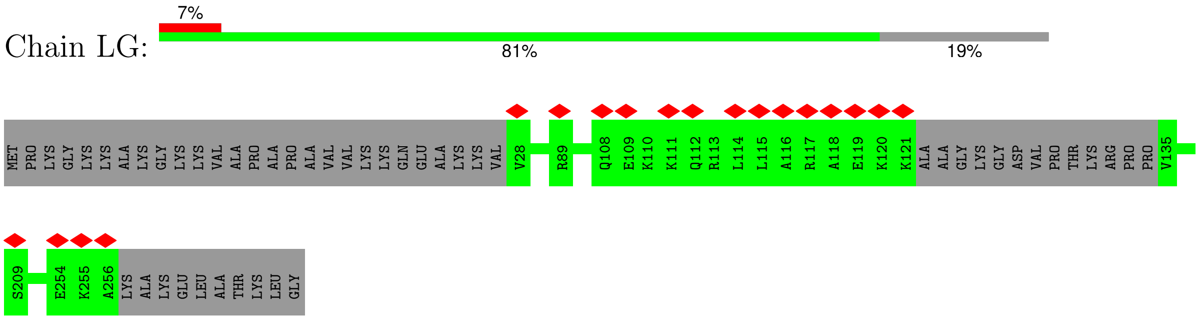


- Molecule 10: Large ribosomal subunit protein uL30



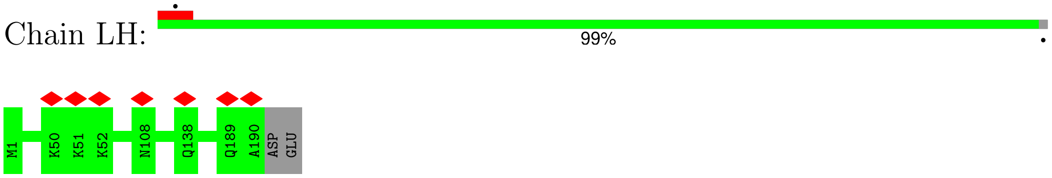
- Molecule 11: Large ribosomal subunit protein eL8

Chain LG:



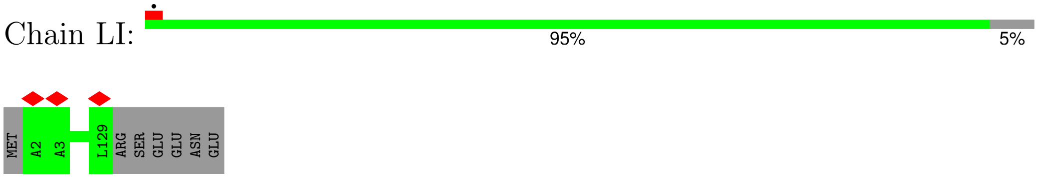
- Molecule 12: Large ribosomal subunit protein uL6

Chain LH:



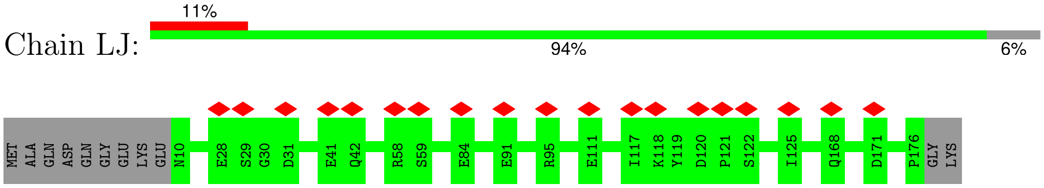
- Molecule 13: Large ribosomal subunit protein eL32

Chain LI:



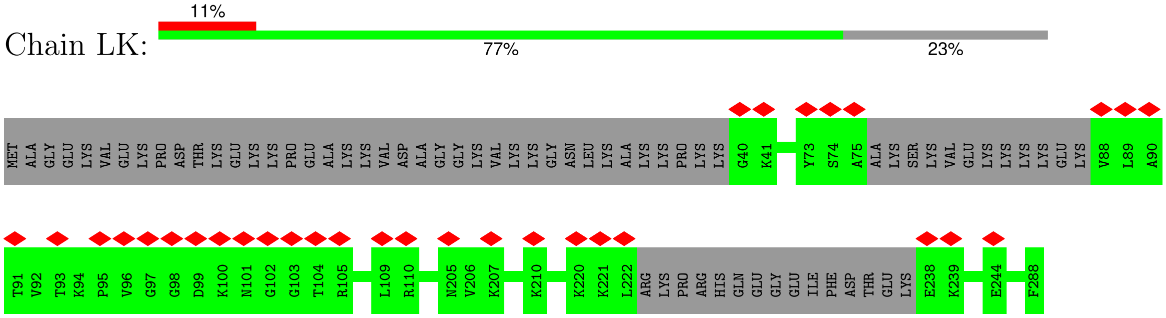
- Molecule 14: Large ribosomal subunit protein uL5

Chain LJ:



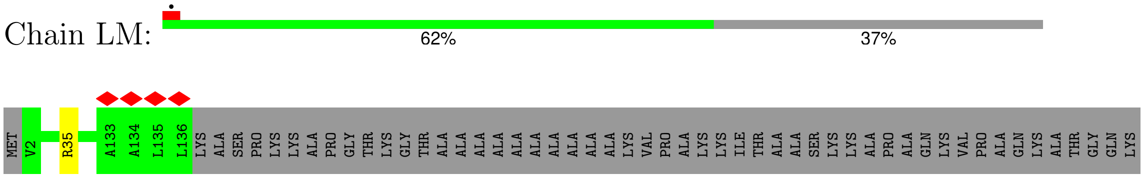
- Molecule 15: Large ribosomal subunit protein eL6

Chain LK:



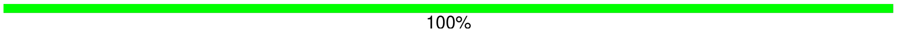
- Molecule 16: Large ribosomal subunit protein eL14

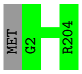
Chain LM:



- Molecule 17: Large ribosomal subunit protein eL15

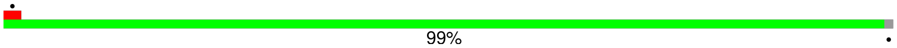
Chain LN:

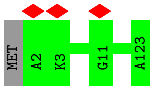




- Molecule 18: Large ribosomal subunit protein uL29

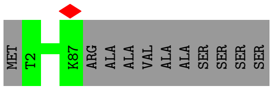
Chain LO:





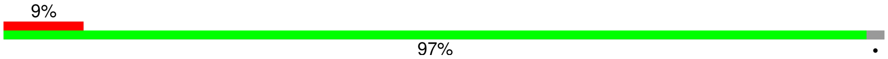
- Molecule 19: Large ribosomal subunit protein eL37

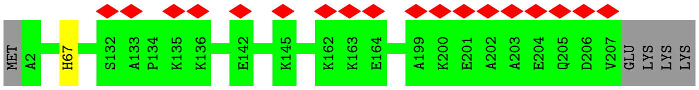
Chain LP:



- Molecule 20: Large ribosomal subunit protein eL13

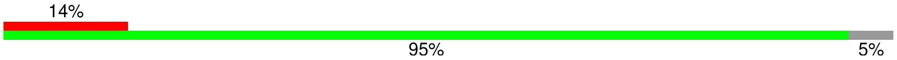
Chain LQ:

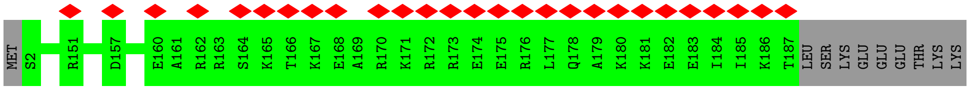




- Molecule 21: Large ribosomal subunit protein eL19

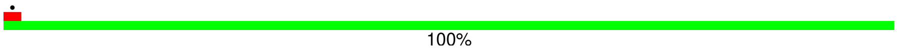
Chain LR:

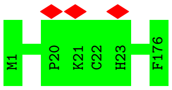




- Molecule 22: Large ribosomal subunit protein eL20

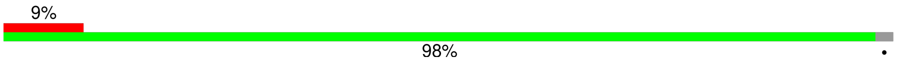
Chain LS:

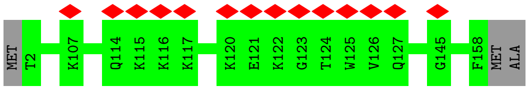




- Molecule 23: Large ribosomal subunit protein eL21

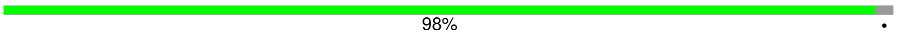
Chain LT:

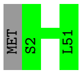




- Molecule 24: Large ribosomal subunit protein eL39

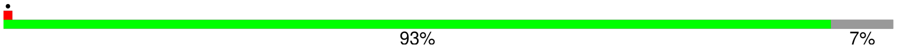
Chain LU:

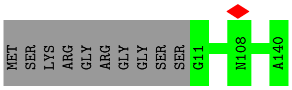




- Molecule 25: Large ribosomal subunit protein uL14

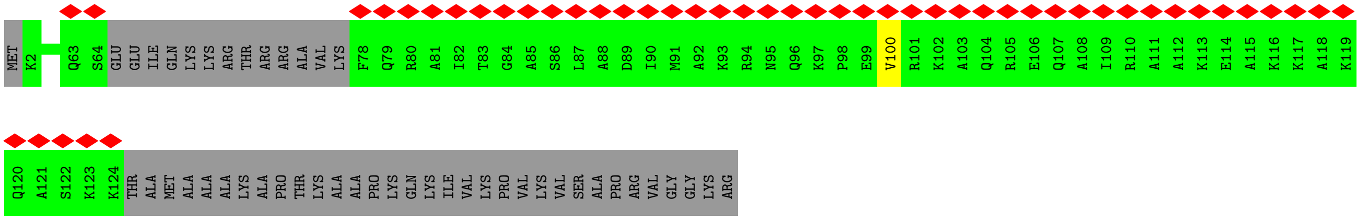
Chain LV:





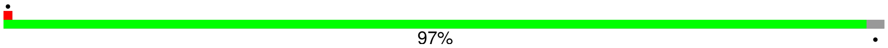
- Molecule 26: Large ribosomal subunit protein eL24

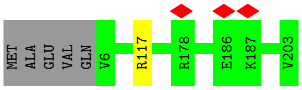
Chain LW:



- Molecule 27: Large ribosomal subunit protein uL13

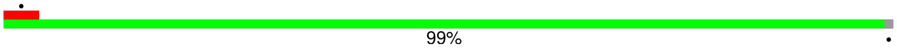
Chain LY:

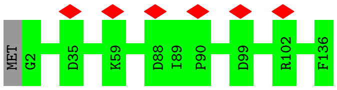




- Molecule 28: Large ribosomal subunit protein eL27

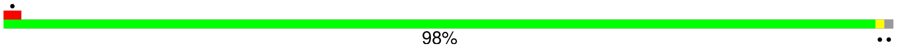
Chain LZ:

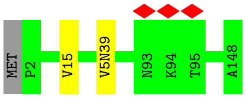




- Molecule 29: Large ribosomal subunit protein uL15

Chain La:



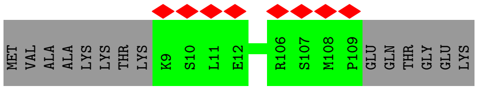


- Molecule 30: Large ribosomal subunit protein eL29

Chain Lb:

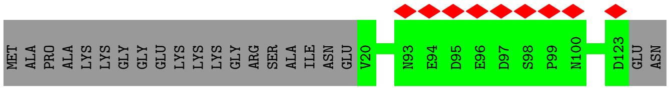
- Molecule 31: Large ribosomal subunit protein eL30

Chain Lc:



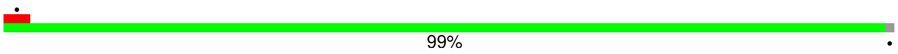
- Molecule 32: Large ribosomal subunit protein eL31

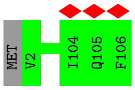
Chain Ld:



- Molecule 33: Large ribosomal subunit protein eL42

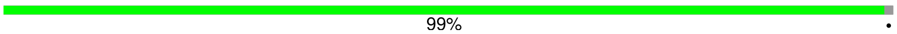
Chain Le:

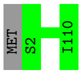




- Molecule 34: Large ribosomal subunit protein eL33

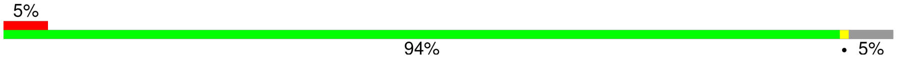
Chain Lf:

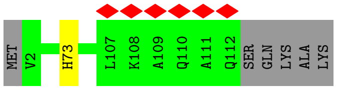




- Molecule 35: Large ribosomal subunit protein eL34

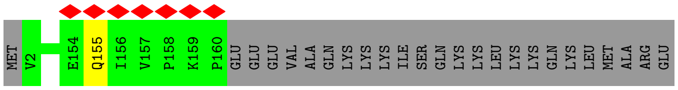
Chain Lg:





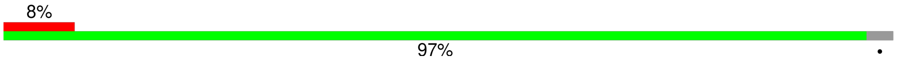
- Molecule 36: Large ribosomal subunit protein uL22

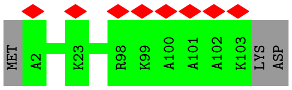
Chain Lh:



- Molecule 37: Large ribosomal subunit protein eL36

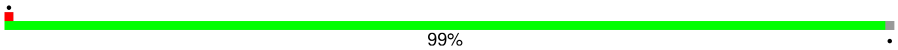
Chain Li:

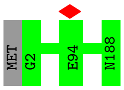




- Molecule 38: Large ribosomal subunit protein eL18

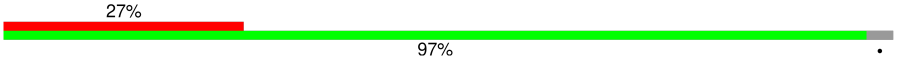
Chain Lj:

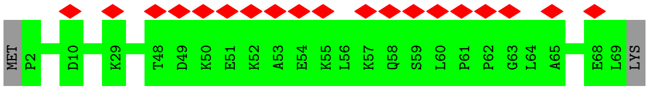




- Molecule 39: Large ribosomal subunit protein eL38

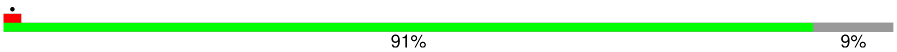
Chain Lk:

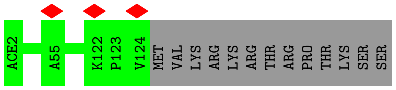




- Molecule 40: Large ribosomal subunit protein eL28

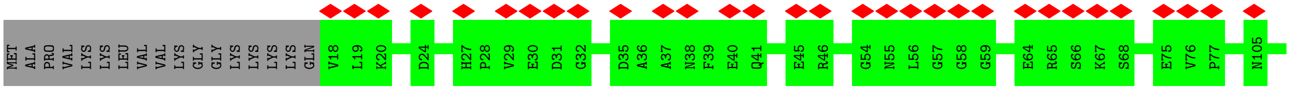
Chain Ll:

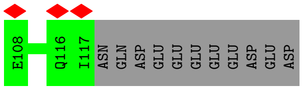




- Molecule 41: Large ribosomal subunit protein eL22

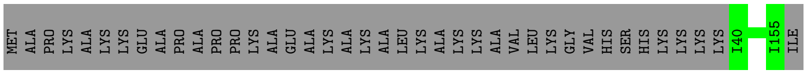
Chain Lm:





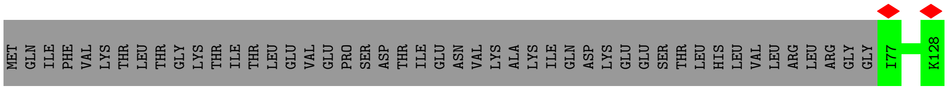
- Molecule 42: Large ribosomal subunit protein uL23

Chain Ln:



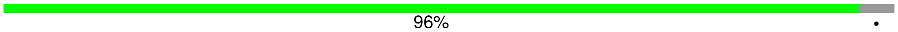
- Molecule 43: Large ribosomal subunit protein eL40

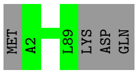
Chain Lo:



- Molecule 44: Large ribosomal subunit protein eL43

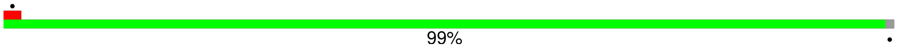
Chain Lp:

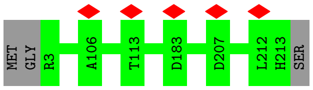




- Molecule 45: Large ribosomal subunit protein uL16

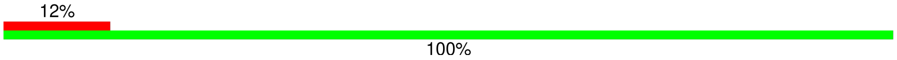
Chain Lz:

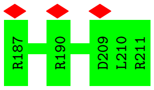




- Molecule 46: Nascent chain

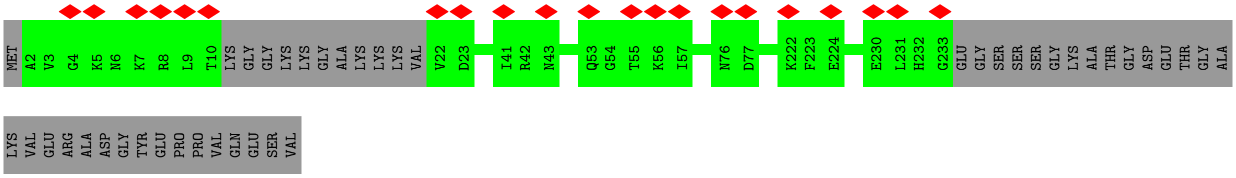
Chain NC:





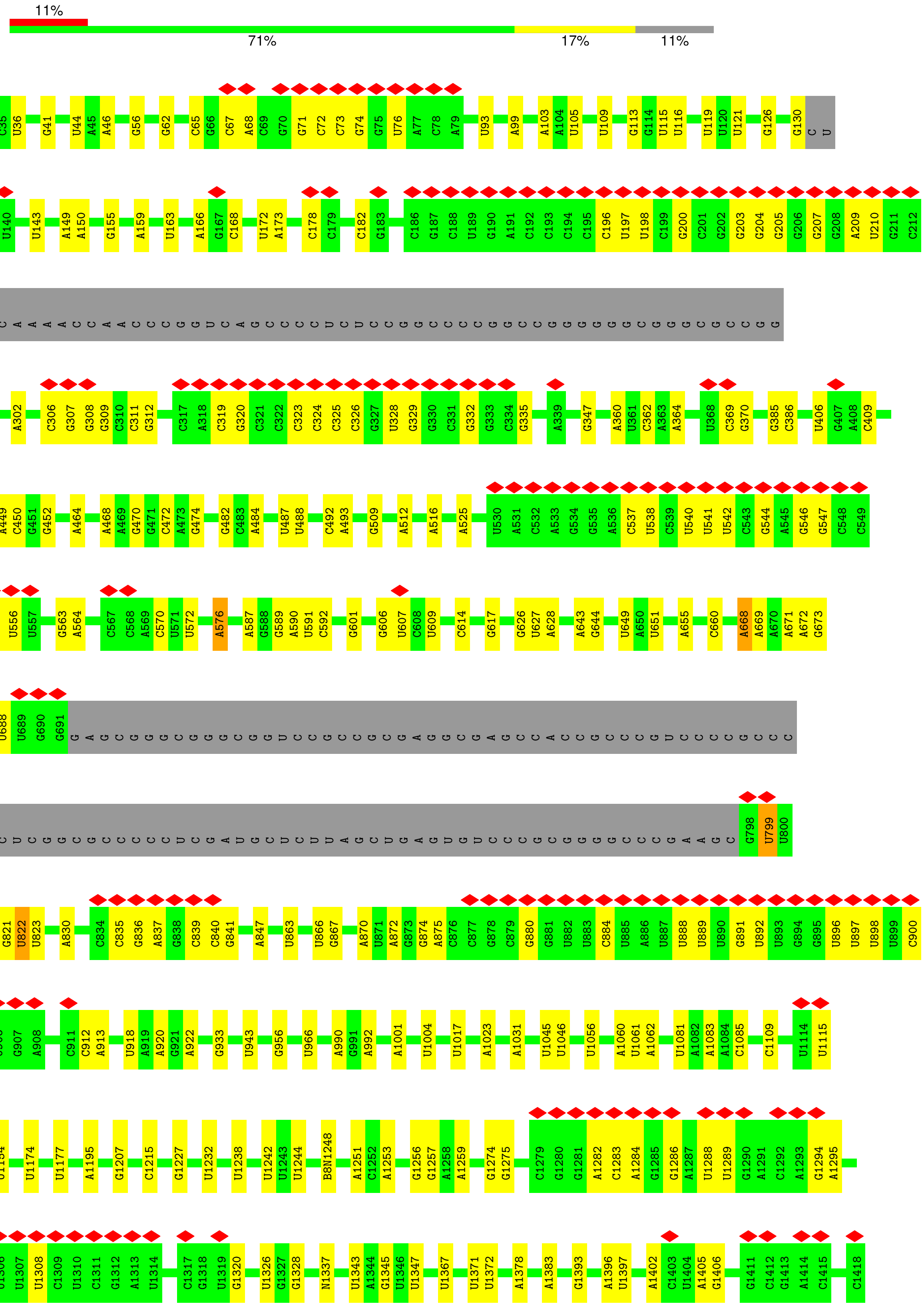
- Molecule 47: Small ribosomal subunit protein eS1

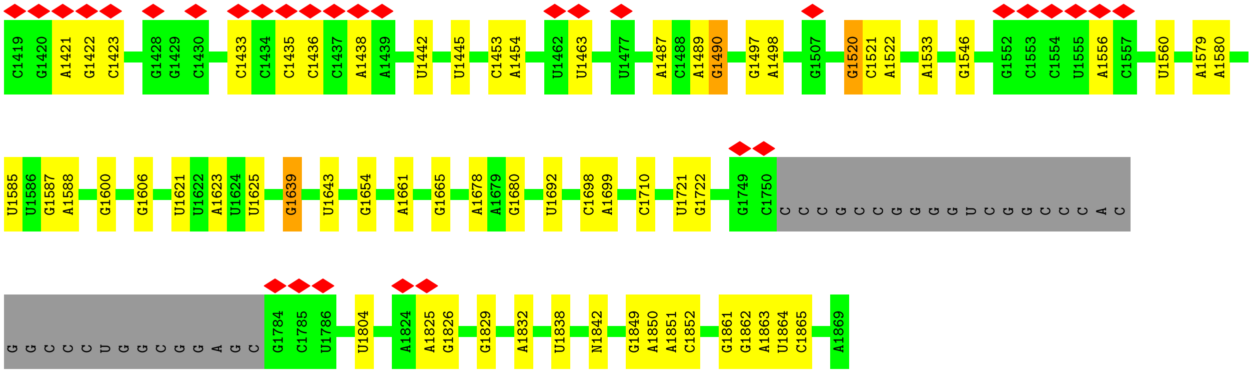
Chain S1:



- Molecule 48: 18S rRNA

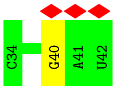
Chain S2:





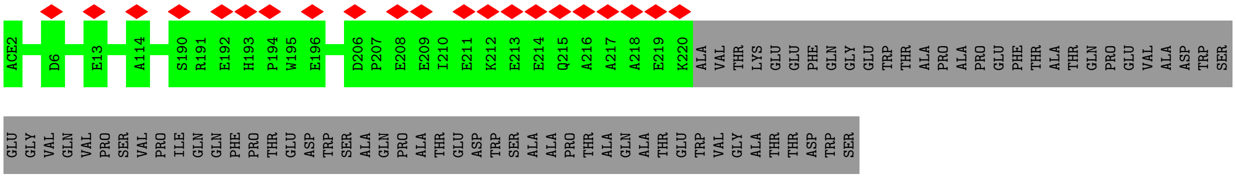
- Molecule 49: mRNA

Chain S5:



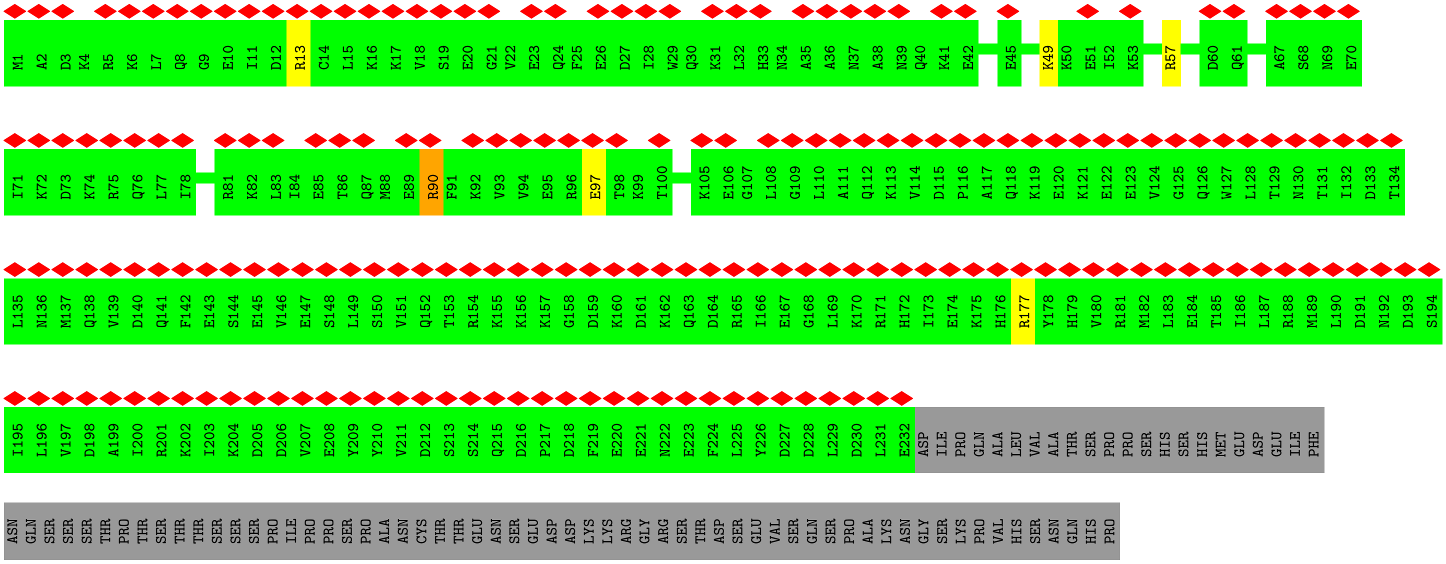
- Molecule 50: Small ribosomal subunit protein uS2

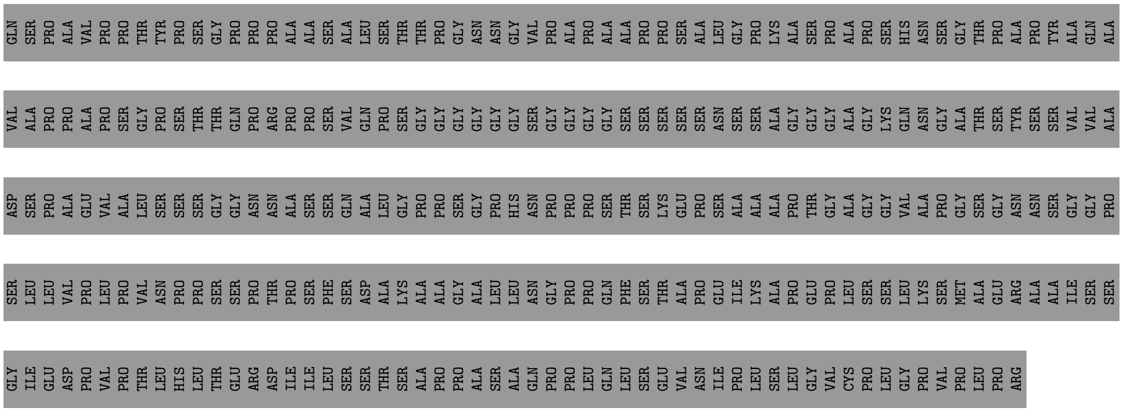
Chain SA:



- Molecule 51: CCR4-NOT transcription complex subunit 3

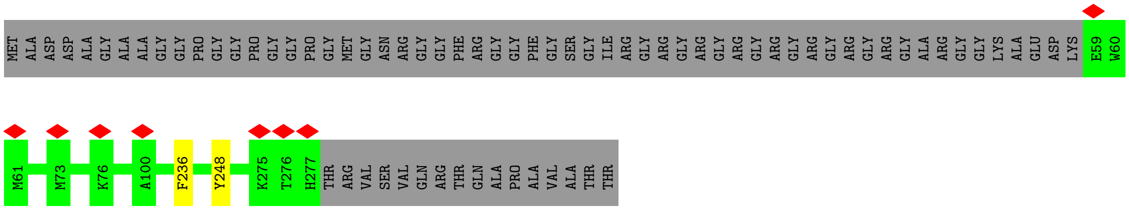
Chain SB:



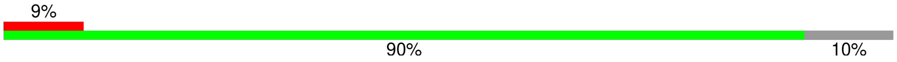


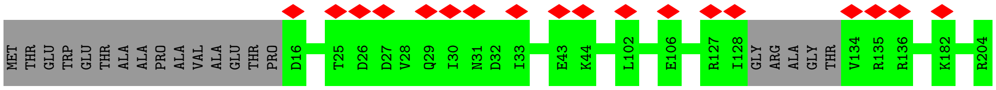
- Molecule 52: Small ribosomal subunit protein uS5

Chain SC:

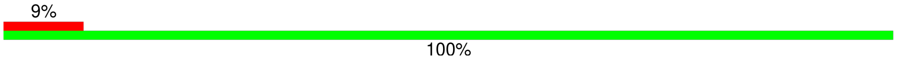



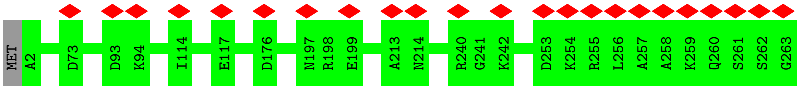
- Molecule 53: Small ribosomal subunit protein uS7

Chain SD:


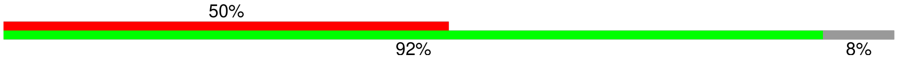


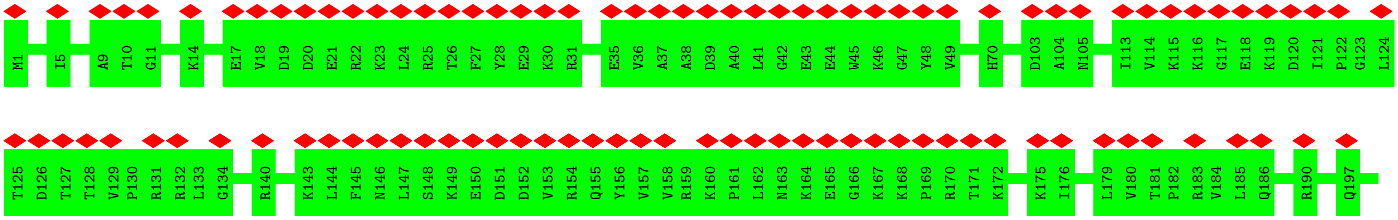
- Molecule 54: Small ribosomal subunit protein eS4, X isoform

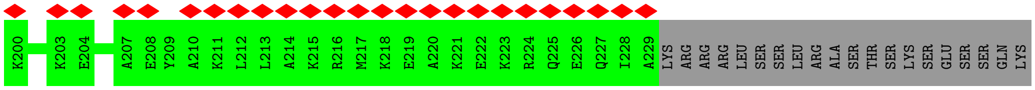
Chain SE:




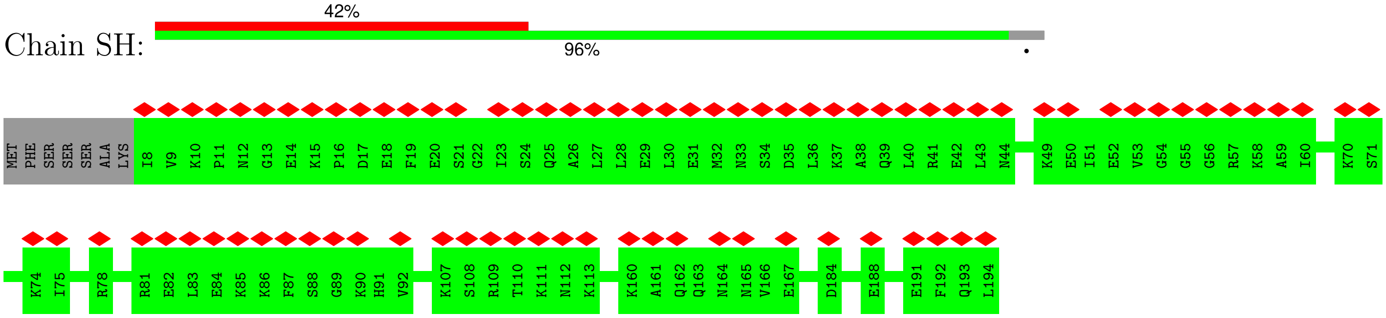
- Molecule 55: Small ribosomal subunit protein eS6

Chain SG:


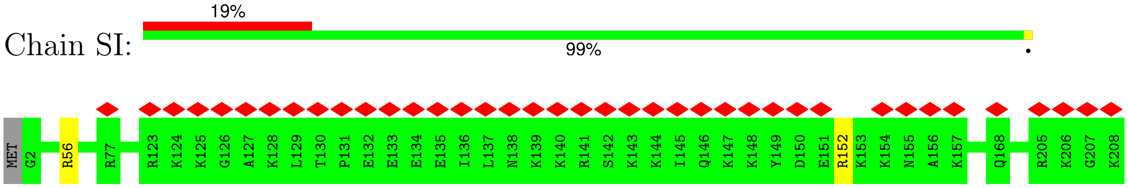




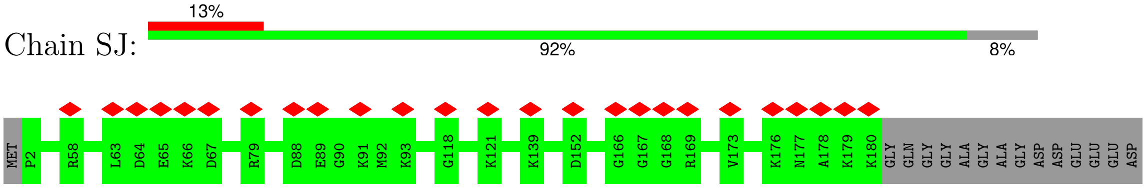
- Molecule 56: Small ribosomal subunit protein eS7



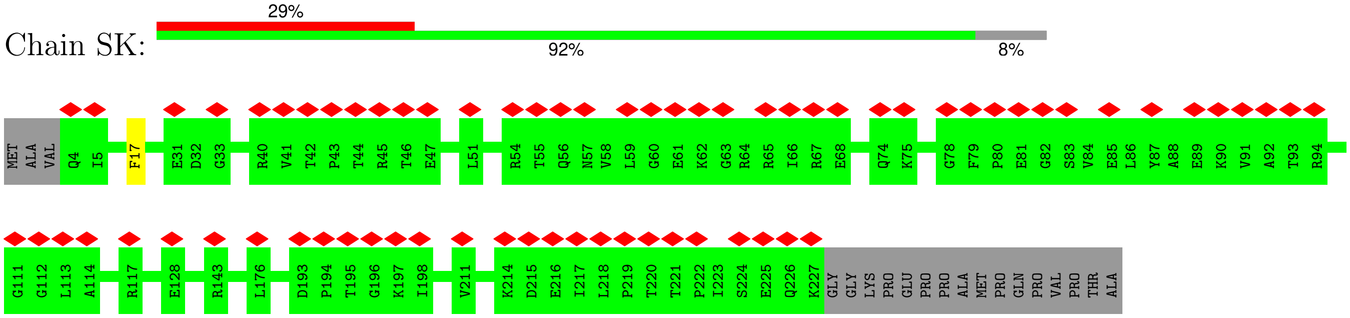
- Molecule 57: Small ribosomal subunit protein eS8



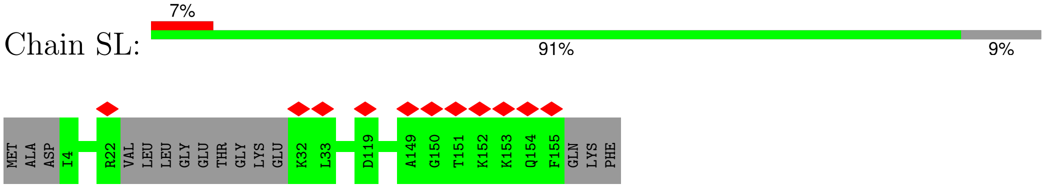
- Molecule 58: Small ribosomal subunit protein uS4



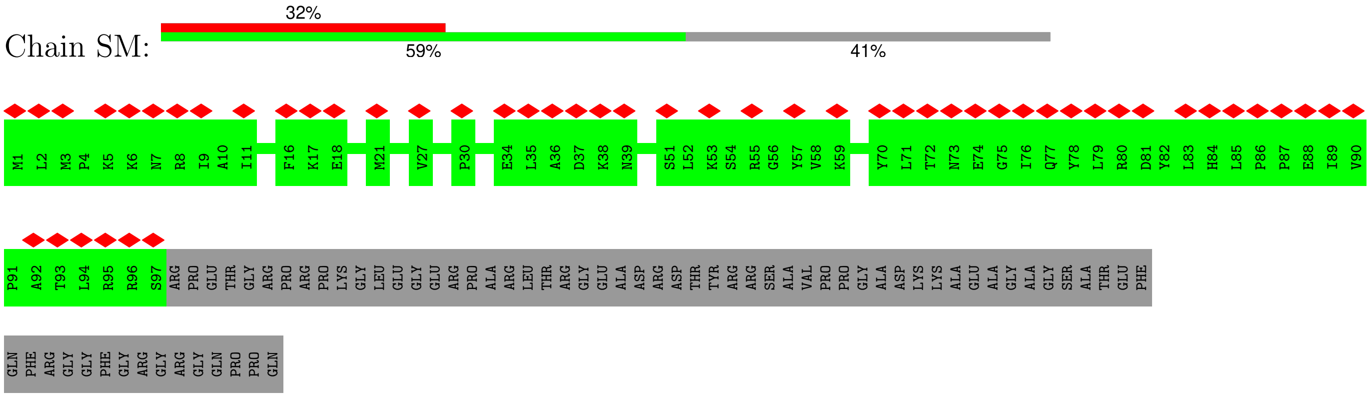
- Molecule 59: Small ribosomal subunit protein uS3



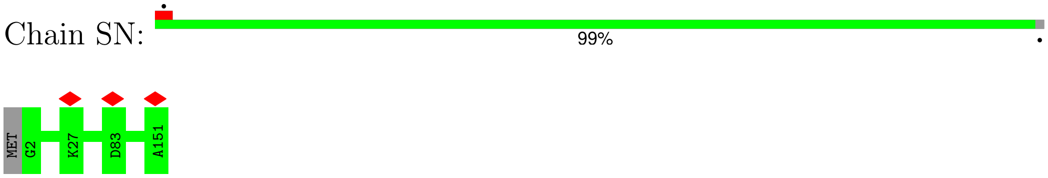
- Molecule 60: Small ribosomal subunit protein uS17



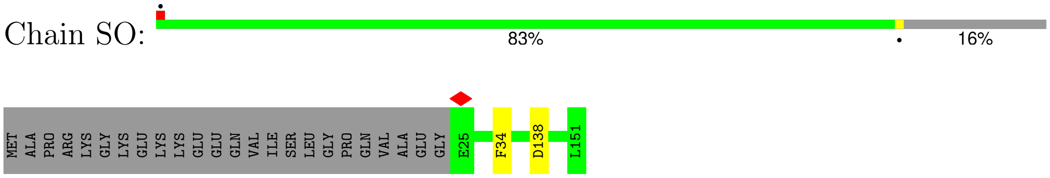
- Molecule 61: Small ribosomal subunit protein eS10



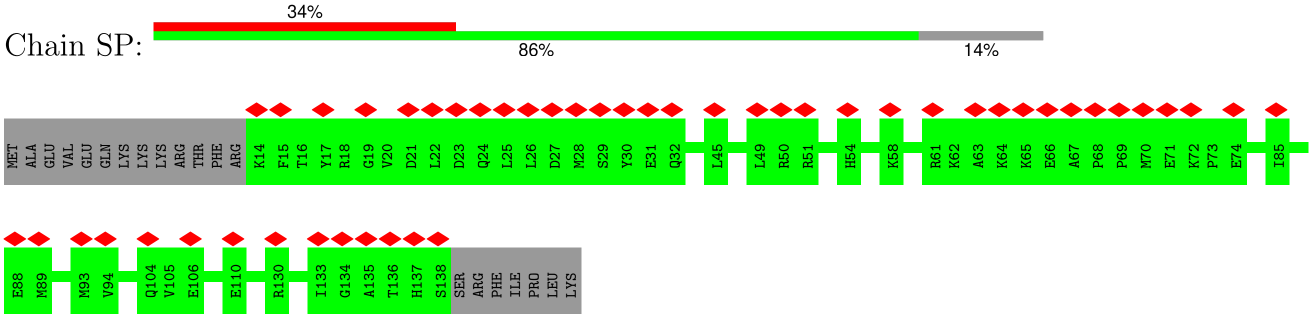
- Molecule 62: Small ribosomal subunit protein uS15



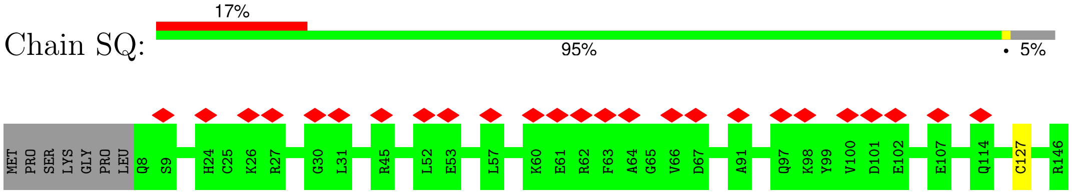
- Molecule 63: Small ribosomal subunit protein uS11



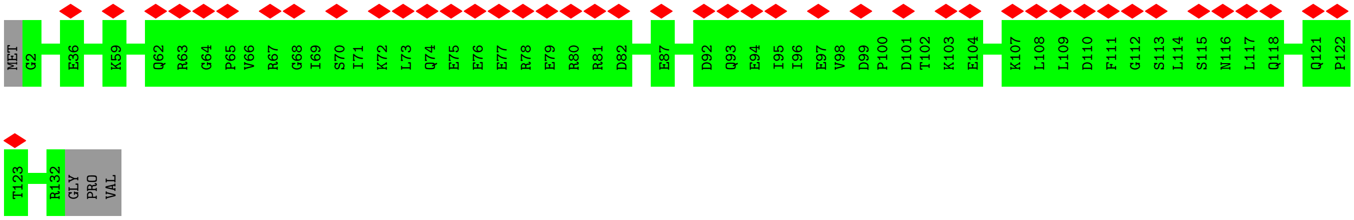
- Molecule 64: Small ribosomal subunit protein uS19



- Molecule 65: Small ribosomal subunit protein uS9

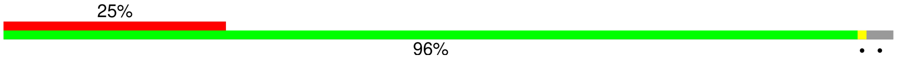


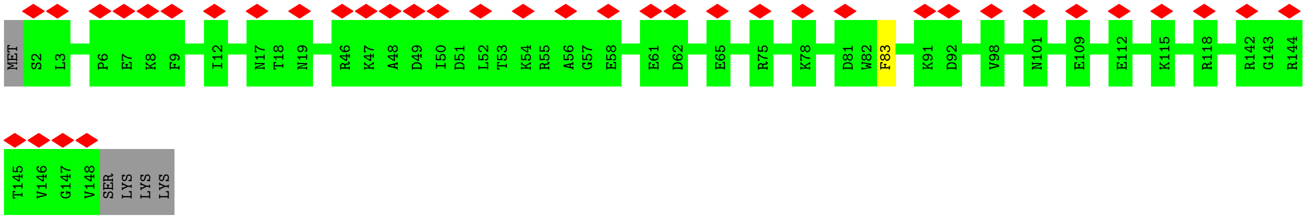
- Molecule 66: Small ribosomal subunit protein eS17



- Molecule 67: Small ribosomal subunit protein uS13

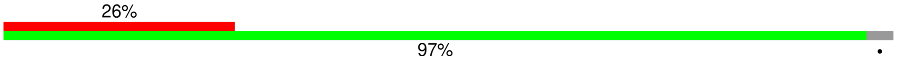
Chain ST:

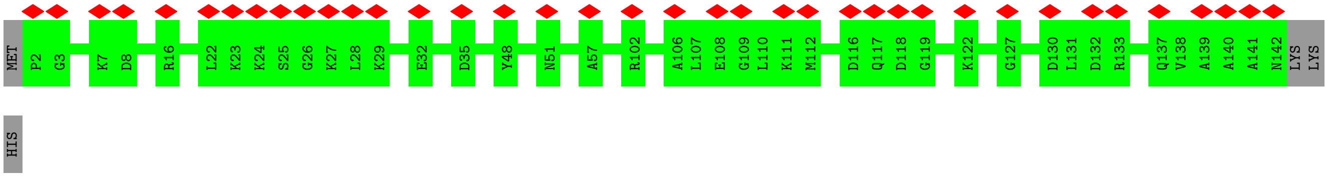




- Molecule 68: Small ribosomal subunit protein eS19

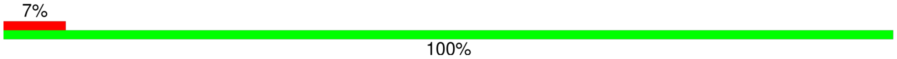
Chain SU:

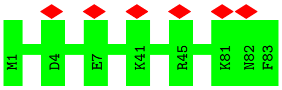




- Molecule 69: Small ribosomal subunit protein eS21

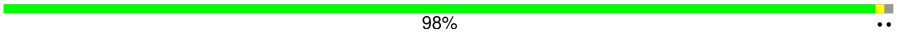
Chain SV:

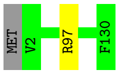




- Molecule 70: Small ribosomal subunit protein uS8

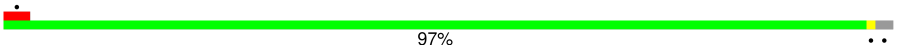
Chain SW:

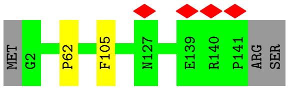




- Molecule 71: Small ribosomal subunit protein uS12

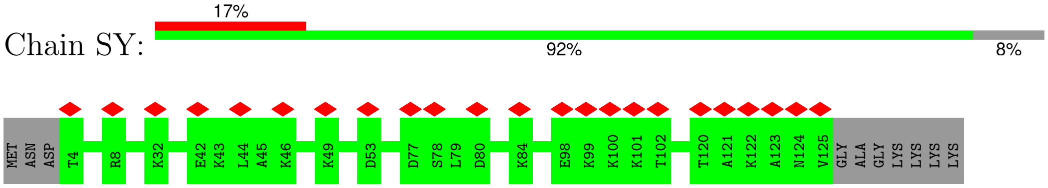
Chain SX:





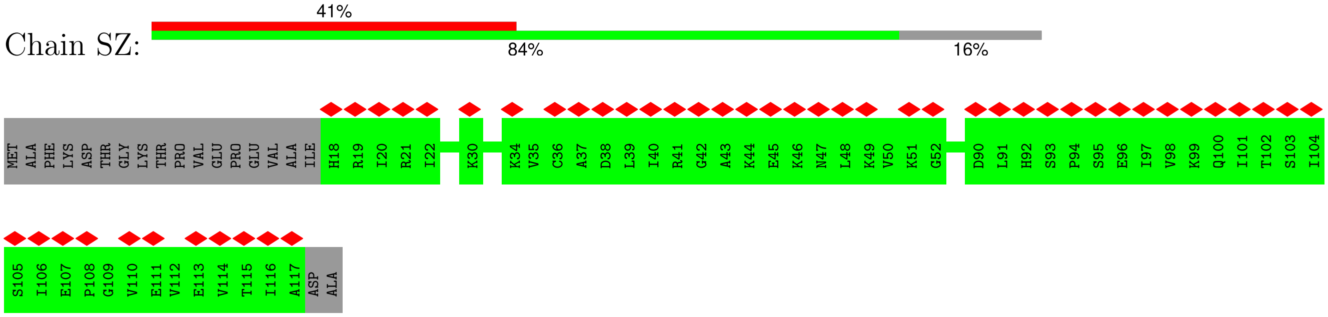
- Molecule 72: Isoform 3 of Small ribosomal subunit protein eS24

Chain SY:



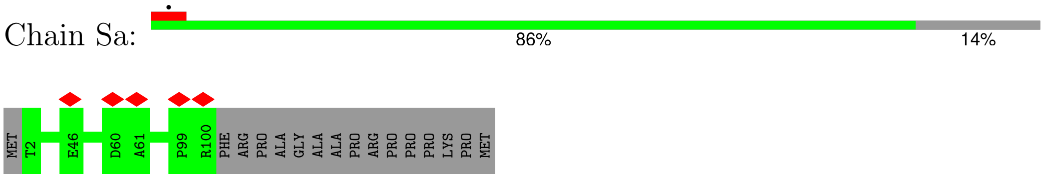
- Molecule 73: Small ribosomal subunit protein uS10

Chain SZ:



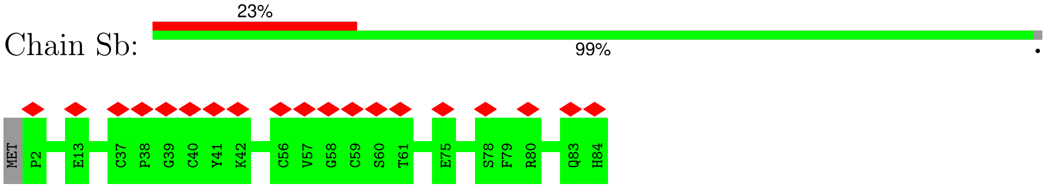
- Molecule 74: Small ribosomal subunit protein eS26

Chain Sa:



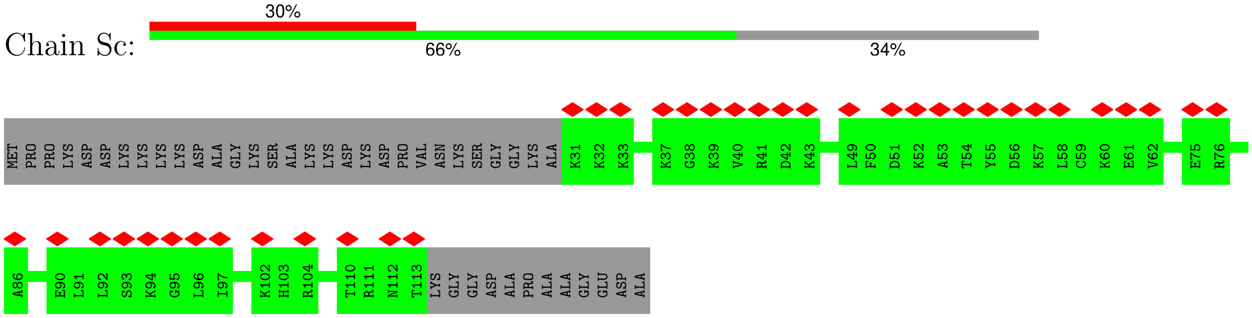
- Molecule 75: Small ribosomal subunit protein eS27

Chain Sb:



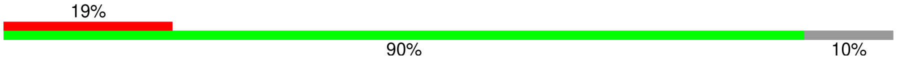
- Molecule 76: Small ribosomal subunit protein eS25

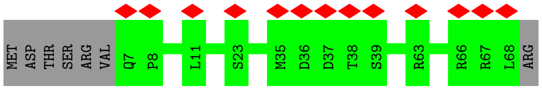
Chain Sc:



- Molecule 77: Small ribosomal subunit protein eS28

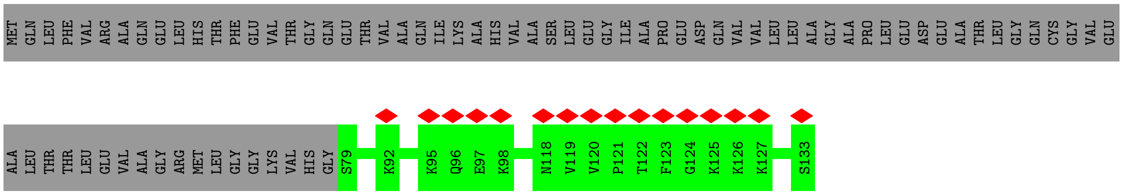
Chain Sd:





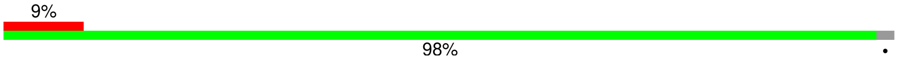
- Molecule 78: FAU ubiquitin-like and ribosomal protein S30

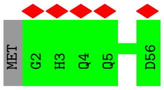
Chain Se:



- Molecule 79: Small ribosomal subunit protein uS14

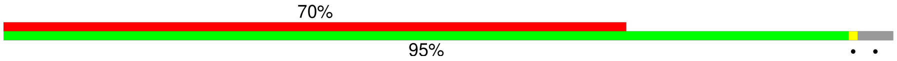
Chain Sf:

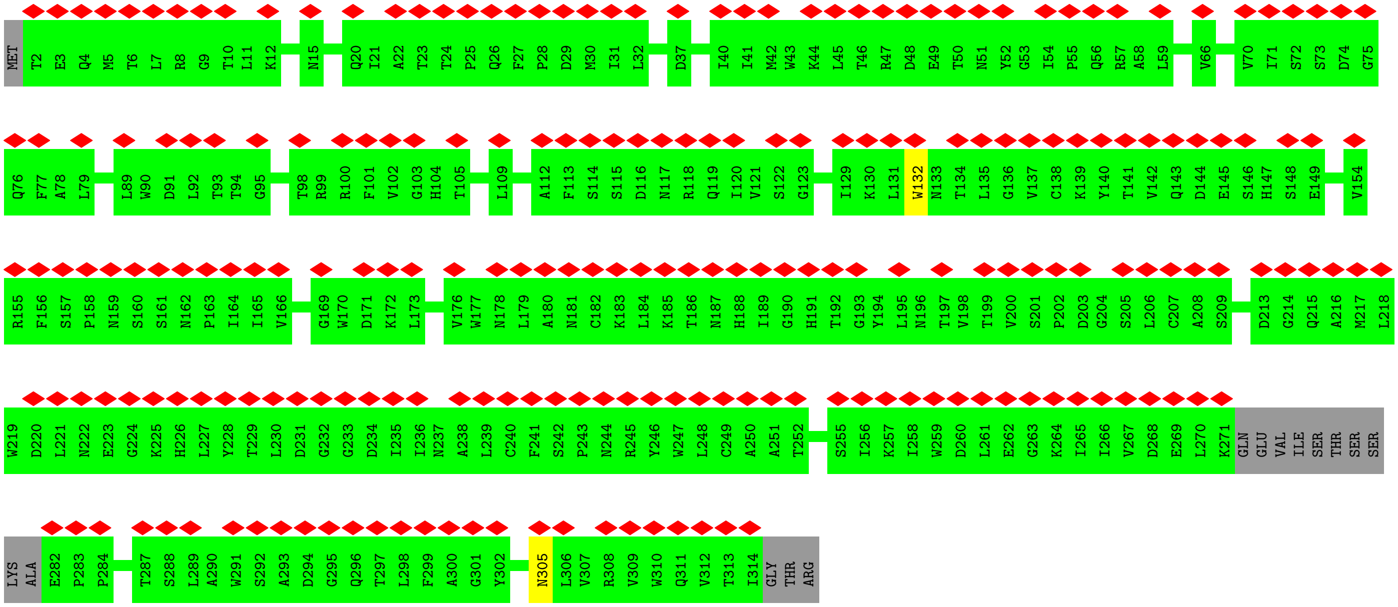




- Molecule 80: Receptor of activated protein C kinase 1

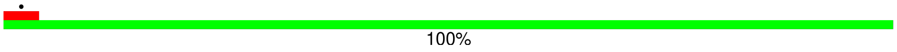
Chain Sg:

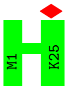




- Molecule 81: Small ribosomal subunit protein eS32

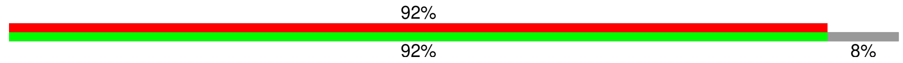
Chain So:

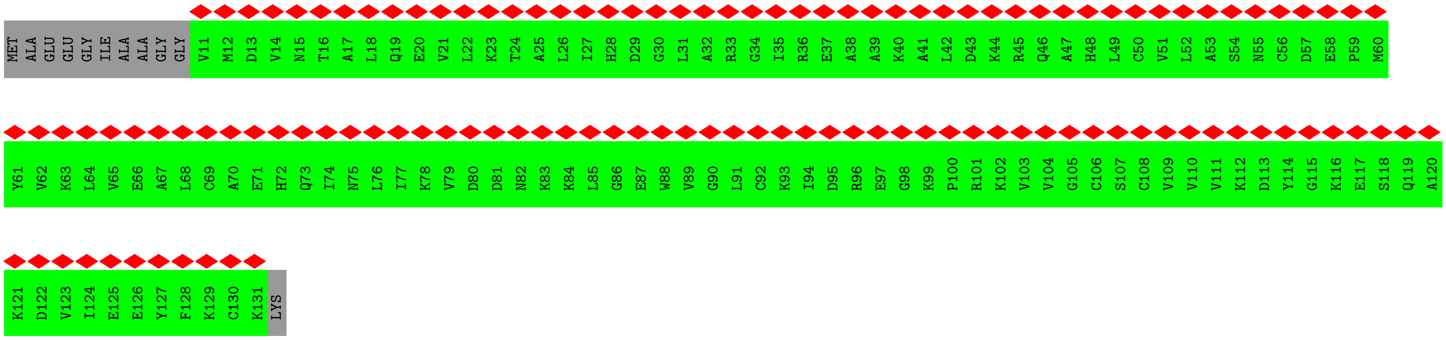




- Molecule 82: Small ribosomal subunit protein eS12

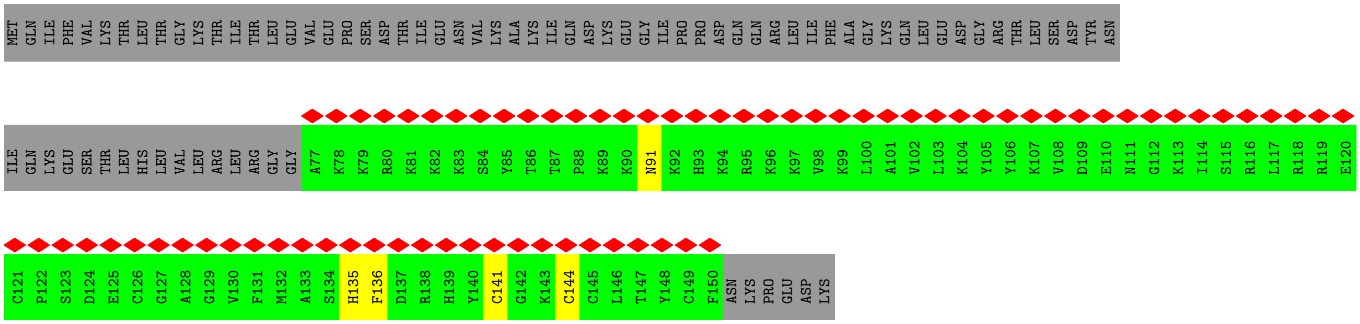
Chain Sy:





- Molecule 83: Ubiquitin-40S ribosomal protein S27a

Chain Sz:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	17	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0175	Depositor
Map size (Å)	419.328, 419.328, 419.328	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.936, 0.936, 0.936	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, UY1, A2M, PSU, M3L, B3P, JMH, 2MG, 1MG, H2U, ZN, MG, ACE, 4AC, 7MG, MLZ, V5N, B8N, OMC, MA6, 6MZ, K, OMG, 5MU, HIC, OMU, M2G, 1MA, HY3, UR3, IAS

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	L1	0.38	0/3450	0.77	0/5372
2	L5	0.38	0/81683	0.82	11/127409 (0.0%)
3	L8	0.27	0/2432	0.51	0/3256
4	L9	0.37	0/2858	0.80	0/4455
5	LB	0.26	0/3289	0.53	0/4399
6	S4	0.73	0/1530	1.07	0/2384
7	LC	0.26	0/2962	0.55	0/3977
8	LD	0.27	0/1924	0.60	0/2578
9	LE	0.25	0/1132	0.55	0/1504
10	LF	0.28	0/1905	0.55	0/2540
11	LG	0.26	0/1781	0.54	0/2397
12	LH	0.26	0/1537	0.53	0/2066
13	LI	0.27	0/1071	0.57	0/1429
14	LJ	0.26	0/1363	0.56	0/1824
15	LK	0.26	0/1814	0.54	0/2435
16	LM	0.26	0/1133	0.52	0/1516
17	LN	0.26	0/1745	0.59	0/2338
18	LO	0.26	0/1022	0.54	0/1351
19	LP	0.27	0/720	0.61	0/952
20	LQ	0.26	0/1695	0.57	0/2270
21	LR	0.25	0/1574	0.57	0/2080
22	LS	0.27	0/1500	0.56	0/2013
23	LT	0.26	0/1312	0.52	0/1753
24	LU	0.25	0/453	0.55	0/599
25	LV	0.27	0/986	0.54	0/1324
26	LW	0.26	0/907	0.51	0/1202
27	LY	0.27	0/1656	0.54	0/2216
28	LZ	0.27	0/1129	0.51	0/1507
29	La	0.26	0/1178	0.54	0/1573
30	Lb	0.25	0/850	0.54	0/1121
31	Lc	0.30	0/796	0.50	0/1068

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Ld	0.26	0/877	0.57	0/1181
33	Le	0.27	0/866	0.55	0/1141
34	Lf	0.27	0/894	0.59	0/1198
35	Lg	0.26	0/892	0.58	0/1189
36	Lh	0.26	0/1317	0.54	0/1769
37	Li	0.25	0/843	0.55	0/1115
38	Lj	0.27	0/1536	0.61	0/2052
39	Lk	0.27	0/565	0.49	0/750
40	Ll	0.28	0/1003	0.59	0/1346
41	Lm	0.27	0/830	0.51	0/1114
42	Ln	0.26	0/966	0.53	0/1301
43	Lo	0.25	0/433	0.55	0/575
44	Lp	0.25	0/691	0.57	0/919
45	Lz	0.27	0/1744	0.54	0/2331
46	NC	0.21	0/226	0.70	0/299
47	S1	0.25	0/1816	0.49	0/2427
48	S2	0.37	0/37683	0.79	5/58736 (0.0%)
49	S5	0.32	0/212	0.78	0/328
50	SA	0.26	0/1766	0.48	0/2399
51	SB	0.39	0/1959	0.69	2/2618 (0.1%)
52	SC	0.26	0/1737	0.48	0/2347
53	SD	0.25	0/1483	0.50	0/1993
54	SE	0.26	0/2117	0.53	0/2849
55	SG	0.26	0/1876	0.55	0/2499
56	SH	0.26	0/1532	0.49	0/2053
57	SI	0.25	0/1724	0.54	0/2298
58	SJ	0.25	0/1520	0.55	0/2030
59	SK	0.25	0/1773	0.53	0/2387
60	SL	0.26	0/1201	0.55	0/1604
61	SM	0.25	0/840	0.45	0/1133
62	SN	0.26	0/1231	0.54	0/1656
63	SO	0.26	0/959	0.57	0/1284
64	SP	0.26	0/1041	0.51	0/1392
65	SQ	0.26	0/1125	0.53	0/1506
66	SS	0.25	0/1078	0.51	0/1447
67	ST	0.24	0/1226	0.56	0/1643
68	SU	0.25	0/1113	0.50	0/1493
69	SV	0.26	0/643	0.51	0/860
70	SW	0.26	0/1050	0.53	0/1406
71	SX	0.25	0/1096	0.51	0/1461
72	SY	0.25	0/1019	0.54	0/1354
73	SZ	0.26	0/805	0.56	0/1081
74	Sa	0.26	0/805	0.57	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Sb	0.25	0/664	0.49	0/891
76	Sc	0.25	0/678	0.51	0/906
77	Sd	0.25	0/490	0.59	0/656
78	Se	0.26	0/442	0.55	0/582
79	Sf	0.25	0/469	0.54	0/623
80	Sg	0.24	0/2420	0.51	0/3294
81	So	0.27	0/240	0.72	0/305
82	Sy	0.25	0/949	0.46	0/1273
83	Sz	0.26	0/619	0.53	0/818
All	All	0.34	0/222471	0.72	18/325899 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	LM	0	1
51	SB	0	4
57	SI	0	1
All	All	0	6

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	417	G	O4'-C1'-N9	7.74	114.39	108.20
2	L5	4404	U	O4'-C1'-N1	6.88	113.70	108.20
2	L5	1639	U	C2-N1-C1'	6.34	125.30	117.70
48	S2	1520	G	C4-N9-C1'	6.33	134.74	126.50
2	L5	1639	U	C6-N1-C1'	-6.14	112.60	121.20
2	L5	1552	G	O4'-C1'-N9	6.14	113.11	108.20
51	SB	49	LYS	CD-CE-NZ	6.12	125.79	111.70
48	S2	1453	C	C2-N1-C1'	6.06	125.47	118.80
2	L5	2519	U	O4'-C1'-N1	6.03	113.02	108.20
2	L5	2409	U	O4'-C1'-N1	5.89	112.91	108.20
2	L5	4886	C	C2-N1-C1'	5.84	125.23	118.80
48	S2	1453	C	C6-N1-C1'	-5.50	114.20	120.80
48	S2	1396	A	O4'-C1'-N9	5.45	112.56	108.20
2	L5	4404	U	C2-N1-C1'	5.39	124.17	117.70
2	L5	4404	U	C6-N1-C1'	-5.37	113.68	121.20
2	L5	4527	G	O4'-C1'-N9	5.25	112.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1520	G	C8-N9-C1'	-5.13	120.33	127.00
51	SB	90	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	LM	35	ARG	Sidechain
51	SB	13	ARG	Sidechain
51	SB	177	ARG	Sidechain
51	SB	57	ARG	Sidechain
51	SB	90	ARG	Sidechain
57	SI	152	ARG	Sidechain

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	
3	L8	291/297 (98%)	282 (97%)	9 (3%)	0	100	100
5	LB	398/403 (99%)	394 (99%)	4 (1%)	0	100	100
7	LC	363/427 (85%)	352 (97%)	11 (3%)	0	100	100
8	LD	245/257 (95%)	237 (97%)	8 (3%)	0	100	100
9	LE	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
10	LF	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
11	LG	212/266 (80%)	209 (99%)	3 (1%)	0	100	100
12	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LI	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
14	LJ	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
15	LK	216/288 (75%)	210 (97%)	6 (3%)	0	100	100
16	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
17	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
18	LO	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
19	LP	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
20	LQ	204/211 (97%)	202 (99%)	2 (1%)	0	100	100
21	LR	184/196 (94%)	183 (100%)	1 (0%)	0	100	100
22	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	LT	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
24	LU	48/51 (94%)	48 (100%)	0	0	100	100
25	LV	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
26	LW	106/157 (68%)	103 (97%)	3 (3%)	0	100	100
27	LY	196/203 (97%)	193 (98%)	3 (2%)	0	100	100
28	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	La	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	19	14
30	Lb	99/159 (62%)	97 (98%)	2 (2%)	0	100	100
31	Lc	99/115 (86%)	99 (100%)	0	0	100	100
32	Ld	102/125 (82%)	102 (100%)	0	0	100	100
33	Le	102/106 (96%)	102 (100%)	0	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
36	Lh	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
39	Lk	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	Ll	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
41	Lm	98/128 (77%)	91 (93%)	7 (7%)	0	100	100
42	Ln	114/156 (73%)	113 (99%)	1 (1%)	0	100	100
43	Lo	50/99 (50%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Lp	86/92 (94%)	82 (95%)	4 (5%)	0	100	100
45	Lz	209/214 (98%)	209 (100%)	0	0	100	100
46	NC	23/25 (92%)	23 (100%)	0	0	100	100
47	S1	217/264 (82%)	214 (99%)	3 (1%)	0	100	100
50	SA	218/295 (74%)	217 (100%)	1 (0%)	0	100	100
51	SB	230/609 (38%)	219 (95%)	10 (4%)	1 (0%)	30	27
52	SC	217/293 (74%)	211 (97%)	6 (3%)	0	100	100
53	SD	180/204 (88%)	172 (96%)	8 (4%)	0	100	100
54	SE	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
55	SG	227/249 (91%)	222 (98%)	5 (2%)	0	100	100
56	SH	185/194 (95%)	177 (96%)	8 (4%)	0	100	100
57	SI	205/208 (99%)	203 (99%)	2 (1%)	0	100	100
58	SJ	177/194 (91%)	173 (98%)	4 (2%)	0	100	100
59	SK	222/243 (91%)	217 (98%)	5 (2%)	0	100	100
60	SL	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
61	SM	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
62	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
63	SO	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
64	SP	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
65	SQ	137/146 (94%)	135 (98%)	2 (2%)	0	100	100
66	SS	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
67	ST	145/152 (95%)	142 (98%)	3 (2%)	0	100	100
68	SU	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
69	SV	81/83 (98%)	81 (100%)	0	0	100	100
70	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
71	SX	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
72	SY	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
73	SZ	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
74	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
75	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
76	Sc	81/125 (65%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Sd	60/69 (87%)	60 (100%)	0	0	100	100
78	Se	53/133 (40%)	53 (100%)	0	0	100	100
79	Sf	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
80	Sg	299/317 (94%)	284 (95%)	15 (5%)	0	100	100
81	So	23/25 (92%)	23 (100%)	0	0	100	100
82	Sy	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
83	Sz	72/156 (46%)	63 (88%)	8 (11%)	1 (1%)	9	4
All	All	11414/13366 (85%)	11166 (98%)	245 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	SB	97	GLU
83	Sz	91	ASN
29	La	15	VAL

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	
3	L8	247/250 (99%)	247 (100%)	0	100	100
5	LB	347/348 (100%)	346 (100%)	1 (0%)	91	94
7	LC	304/348 (87%)	303 (100%)	1 (0%)	91	94
8	LD	189/198 (96%)	189 (100%)	0	100	100
9	LE	124/135 (92%)	122 (98%)	2 (2%)	58	64
10	LF	195/216 (90%)	195 (100%)	0	100	100
11	LG	187/223 (84%)	187 (100%)	0	100	100
12	LH	169/171 (99%)	169 (100%)	0	100	100
13	LI	114/121 (94%)	114 (100%)	0	100	100
14	LJ	141/149 (95%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LK	196/252 (78%)	196 (100%)	0	100	100
16	LM	115/161 (71%)	115 (100%)	0	100	100
17	LN	171/172 (99%)	171 (100%)	0	100	100
18	LO	109/110 (99%)	109 (100%)	0	100	100
19	LP	73/80 (91%)	73 (100%)	0	100	100
20	LQ	172/177 (97%)	171 (99%)	1 (1%)	84	88
21	LR	165/175 (94%)	165 (100%)	0	100	100
22	LS	157/157 (100%)	157 (100%)	0	100	100
23	LT	138/140 (99%)	138 (100%)	0	100	100
24	LU	47/48 (98%)	47 (100%)	0	100	100
25	LV	100/107 (94%)	100 (100%)	0	100	100
26	LW	90/126 (71%)	89 (99%)	1 (1%)	70	76
27	LY	170/174 (98%)	169 (99%)	1 (1%)	84	88
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	119/120 (99%)	119 (100%)	0	100	100
30	Lb	85/125 (68%)	85 (100%)	0	100	100
31	Lc	86/97 (89%)	86 (100%)	0	100	100
32	Ld	95/110 (86%)	95 (100%)	0	100	100
33	Le	92/93 (99%)	92 (100%)	0	100	100
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	95/100 (95%)	94 (99%)	1 (1%)	70	76
36	Lh	140/163 (86%)	139 (99%)	1 (1%)	81	86
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	164/165 (99%)	164 (100%)	0	100	100
39	Lk	63/65 (97%)	63 (100%)	0	100	100
40	Ll	107/120 (89%)	107 (100%)	0	100	100
41	Lm	90/115 (78%)	90 (100%)	0	100	100
42	Ln	104/133 (78%)	104 (100%)	0	100	100
43	Lo	48/90 (53%)	48 (100%)	0	100	100
44	Lp	71/75 (95%)	71 (100%)	0	100	100
45	Lz	179/181 (99%)	179 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	NC	25/25 (100%)	25 (100%)	0	100	100
47	S1	200/231 (87%)	200 (100%)	0	100	100
50	SA	182/242 (75%)	182 (100%)	0	100	100
51	SB	215/509 (42%)	215 (100%)	0	100	100
52	SC	185/225 (82%)	183 (99%)	2 (1%)	70	76
53	SD	157/170 (92%)	157 (100%)	0	100	100
54	SE	224/225 (100%)	224 (100%)	0	100	100
55	SG	199/218 (91%)	199 (100%)	0	100	100
56	SH	168/174 (97%)	168 (100%)	0	100	100
57	SI	179/180 (99%)	178 (99%)	1 (1%)	84	88
58	SJ	160/168 (95%)	160 (100%)	0	100	100
59	SK	188/202 (93%)	187 (100%)	1 (0%)	86	90
60	SL	130/142 (92%)	130 (100%)	0	100	100
61	SM	88/136 (65%)	88 (100%)	0	100	100
62	SN	130/131 (99%)	130 (100%)	0	100	100
63	SO	99/118 (84%)	98 (99%)	1 (1%)	73	78
64	SP	111/130 (85%)	111 (100%)	0	100	100
65	SQ	115/121 (95%)	114 (99%)	1 (1%)	75	81
66	SS	119/122 (98%)	119 (100%)	0	100	100
67	ST	127/132 (96%)	126 (99%)	1 (1%)	79	84
68	SU	111/115 (96%)	111 (100%)	0	100	100
69	SV	67/67 (100%)	67 (100%)	0	100	100
70	SW	112/113 (99%)	111 (99%)	1 (1%)	75	81
71	SX	111/114 (97%)	110 (99%)	1 (1%)	75	81
72	SY	107/114 (94%)	107 (100%)	0	100	100
73	SZ	92/107 (86%)	92 (100%)	0	100	100
74	Sa	86/98 (88%)	86 (100%)	0	100	100
75	Sb	75/76 (99%)	75 (100%)	0	100	100
76	Sc	74/103 (72%)	74 (100%)	0	100	100
77	Sd	55/62 (89%)	55 (100%)	0	100	100
78	Se	45/104 (43%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	Sf	48/49 (98%)	48 (100%)	0	100	100
80	Sg	263/275 (96%)	261 (99%)	2 (1%)	79	84
81	So	24/24 (100%)	24 (100%)	0	100	100
82	Sy	103/108 (95%)	103 (100%)	0	100	100
83	Sz	66/140 (47%)	62 (94%)	4 (6%)	15	12
All	All	9989/11356 (88%)	9965 (100%)	24 (0%)	91	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LB	228	TYR
7	LC	122	TYR
9	LE	74	TYR
9	LE	115	ARG
20	LQ	67	HIS
26	LW	100	VAL
27	LY	117	ARG
35	Lg	73	HIS
36	Lh	155	GLN
52	SC	236	PHE
52	SC	248	TYR
57	SI	56	ARG
59	SK	17	PHE
63	SO	34	PHE
65	SQ	127	CYS
67	ST	83	PHE
70	SW	97	ARG
71	SX	105	PHE
80	Sg	132	TRP
80	Sg	305	ASN
83	Sz	135	HIS
83	Sz	136	PHE
83	Sz	141	CYS
83	Sz	144	CYS

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

Mol	Chain	Res	Type
40	Ll	30	ASN

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Mol	Chain	Res	Type
55	SG	146	ASN
80	Sg	187	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	145/157 (92%)	12 (8%)	0
2	L5	3508/5069 (69%)	516 (14%)	10 (0%)
4	L9	119/121 (98%)	9 (7%)	0
48	S2	1649/1869 (88%)	246 (14%)	4 (0%)
49	S5	8/9 (88%)	1 (12%)	0
6	S4	75/76 (98%)	24 (32%)	2 (2%)
All	All	5504/7301 (75%)	808 (14%)	16 (0%)

All (808) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	34	U
1	L1	35	C
1	L1	48	A
1	L1	59	A
1	L1	62	A
1	L1	63	U
1	L1	94	G
1	L1	103	A
1	L1	105	C
1	L1	110	U
1	L1	114	G
1	L1	147	G
2	L5	2	G
2	L5	15	A
2	L5	39	A
2	L5	48	G
2	L5	59	A
2	L5	64	A
2	L5	65	A
2	L5	71	C
2	L5	73	A
2	L5	91	G
2	L5	98	A
2	L5	110	C

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Mol	Chain	Res	Type
2	L5	116	G
2	L5	117	C
2	L5	119	G
2	L5	120	A
2	L5	122	U
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	136	C
2	L5	137	G
2	L5	143	C
2	L5	144	G
2	L5	152	U
2	L5	159	C
2	L5	165	A
2	L5	166	C
2	L5	169	G
2	L5	171	U
2	L5	172	C
2	L5	182	G
2	L5	189	G
2	L5	200	U
2	L5	210	C
2	L5	219	G
2	L5	233	U
2	L5	234	G
2	L5	255	C
2	L5	256	G
2	L5	258	G
2	L5	260	C
2	L5	262	G
2	L5	263	G
2	L5	266	C
2	L5	269	G
2	L5	280	G
2	L5	297	U
2	L5	316	U
2	L5	340	C
2	L5	364	G
2	L5	387	G
2	L5	410	A
2	L5	412	G

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Mol	Chain	Res	Type
2	L5	413	G
2	L5	432	U
2	L5	449	C
2	L5	450	G
2	L5	465	G
2	L5	466	A
2	L5	484	U
2	L5	485	C
2	L5	489	C
2	L5	490	C
2	L5	492	U
2	L5	493	G
2	L5	496	G
2	L5	497	G
2	L5	498	C
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	666	G
2	L5	667	A
2	L5	669	C
2	L5	686	A
2	L5	687	U
2	L5	704	C
2	L5	708	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	740	G
2	L5	754	U
2	L5	755	C
2	L5	757	G
2	L5	758	G
2	L5	904	C
2	L5	906	C
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	916	C
2	L5	917	A
2	L5	923	C
2	L5	924	C

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Mol	Chain	Res	Type
2	L5	926	G
2	L5	932	A
2	L5	933	G
2	L5	934	C
2	L5	935	A
2	L5	937	U
2	L5	944	A
2	L5	945	U
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	970	G
2	L5	971	U
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	989	U
2	L5	990	C
2	L5	991	C
2	L5	992	C
2	L5	993	G
2	L5	995	C
2	L5	1048	G
2	L5	1050	C
2	L5	1051	G
2	L5	1070	G
2	L5	1074	G
2	L5	1083	U
2	L5	1168	G
2	L5	1171	G
2	L5	1173	G
2	L5	1174	G
2	L5	1178	G
2	L5	1179	U
2	L5	1180	C
2	L5	1182	C
2	L5	1183	C
2	L5	1198	G
2	L5	1203	G
2	L5	1205	G

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Mol	Chain	Res	Type
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1222	A
2	L5	1253	G
2	L5	1254	A
2	L5	1255	A
2	L5	1258	G
2	L5	1259	G
2	L5	1261	G
2	L5	1266	G
2	L5	1269	G
2	L5	1270	A
2	L5	1272	C
2	L5	1273	G
2	L5	1274	A
2	L5	1277	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1295	C
2	L5	1304	C
2	L5	1313	C
2	L5	1326	A2M
2	L5	1337	A
2	L5	1354	A
2	L5	1359	G
2	L5	1365	C
2	L5	1367	C
2	L5	1387	A
2	L5	1397	A
2	L5	1399	G
2	L5	1402	C
2	L5	1404	G
2	L5	1405	C
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1412	G
2	L5	1417	C

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Mol	Chain	Res	Type
2	L5	1420	A
2	L5	1435	G
2	L5	1436	C
2	L5	1437	C
2	L5	1439	C
2	L5	1441	C
2	L5	1443	A
2	L5	1448	G
2	L5	1483	C
2	L5	1498	G
2	L5	1501	C
2	L5	1502	G
2	L5	1534	A2M
2	L5	1547	A
2	L5	1566	C
2	L5	1578	U
2	L5	1591	U
2	L5	1596	U
2	L5	1624	G
2	L5	1625	OMG
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1676	C
2	L5	1677	PSU
2	L5	1705	G
2	L5	1706	A
2	L5	1719	A
2	L5	1734	G
2	L5	1735	U
2	L5	1742	A
2	L5	1750	G
2	L5	1755	C
2	L5	1756	U
2	L5	1757	U
2	L5	1758	G
2	L5	1759	G

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Mol	Chain	Res	Type
2	L5	1761	G
2	L5	1774	C
2	L5	1787	A
2	L5	1804	A
2	L5	1805	A
2	L5	1810	G
2	L5	1821	G
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1843	A
2	L5	1855	G
2	L5	1869	G
2	L5	1897	A
2	L5	1918	U
2	L5	1919	G
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1948	G
2	L5	1959	U
2	L5	1960	A
2	L5	1962	A
2	L5	1966	C
2	L5	2025	A
2	L5	2026	A
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C
2	L5	2085	G
2	L5	2092	G
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G

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Mol	Chain	Res	Type
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2106	G
2	L5	2260	C
2	L5	2277	C
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2313	A
2	L5	2348	G
2	L5	2351	OMC
2	L5	2360	A
2	L5	2395	A
2	L5	2397	G
2	L5	2417	A
2	L5	2421	G
2	L5	2422	OMC
2	L5	2450	G
2	L5	2475	G
2	L5	2503	G
2	L5	2504	C
2	L5	2505	C
2	L5	2506	G
2	L5	2513	A
2	L5	2519	U
2	L5	2520	C
2	L5	2529	A
2	L5	2530	U
2	L5	2554	U
2	L5	2565	A
2	L5	2573	A
2	L5	2583	C
2	L5	2587	A
2	L5	2589	C
2	L5	2601	A
2	L5	2627	C
2	L5	2631	U
2	L5	2638	G
2	L5	2653	C
2	L5	2662	G
2	L5	2669	C

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Mol	Chain	Res	Type
2	L5	2687	U
2	L5	2695	A
2	L5	2696	A
2	L5	2703	G
2	L5	2705	G
2	L5	2711	G
2	L5	2712	G
2	L5	2725	A
2	L5	2726	G
2	L5	2743	A
2	L5	2756	G
2	L5	2763	U
2	L5	2764	A
2	L5	2788	U
2	L5	2790	U
2	L5	2796	G
2	L5	2798	A
2	L5	2814	C
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U
2	L5	2838	G
2	L5	2855	G
2	L5	2877	G
2	L5	2903	G
2	L5	2905	C
2	L5	2906	G
2	L5	2907	G
2	L5	2908	U
2	L5	3585	G
2	L5	3590	G
2	L5	3591	C
2	L5	3593	C
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3605	C
2	L5	3615	G
2	L5	3616	U
2	L5	3618	C
2	L5	3626	G

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Mol	Chain	Res	Type
2	L5	3635	A
2	L5	3644	U
2	L5	3662	A
2	L5	3673	C
2	L5	3711	A
2	L5	3713	U
2	L5	3714	G
2	L5	3748	A
2	L5	3753	G
2	L5	3760	A2M
2	L5	3776	G
2	L5	3777	G
2	L5	3785	A2M
2	L5	3786	U
2	L5	3811	G
2	L5	3812	C
2	L5	3814	U
2	L5	3817	A
2	L5	3819	G
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3876	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3897	G
2	L5	3898	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3939	G
2	L5	4076	G
2	L5	4084	G
2	L5	4091	G
2	L5	4096	C
2	L5	4097	G
2	L5	4099	G
2	L5	4100	C
2	L5	4101	C

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Mol	Chain	Res	Type
2	L5	4119	C
2	L5	4122	G
2	L5	4127	A
2	L5	4133	C
2	L5	4135	G
2	L5	4137	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4145	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4203	A
2	L5	4222	G
2	L5	4229	U
2	L5	4233	A
2	L5	4251	A
2	L5	4254	G
2	L5	4257	A
2	L5	4266	G
2	L5	4268	A
2	L5	4273	A
2	L5	4281	A
2	L5	4291	G
2	L5	4305	G
2	L5	4306	OMU
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4349	C
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4379	A
2	L5	4387	C
2	L5	4391	G

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Mol	Chain	Res	Type
2	L5	4394	A
2	L5	4422	A
2	L5	4448	G
2	L5	4449	A
2	L5	4452	U
2	L5	4464	A
2	L5	4500	PSU
2	L5	4512	U
2	L5	4513	A
2	L5	4519	C
2	L5	4524	G
2	L5	4528	G
2	L5	4548	A
2	L5	4560	C
2	L5	4567	G
2	L5	4573	G
2	L5	4590	A2M
2	L5	4600	G
2	L5	4636	PSU
2	L5	4637	OMG
2	L5	4656	A
2	L5	4670	C
2	L5	4672	A
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4730	C
2	L5	4732	G
2	L5	4733	C
2	L5	4741	C
2	L5	4742	G
2	L5	4750	G
2	L5	4751	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4765	G
2	L5	4772	C
2	L5	4775	C
2	L5	4776	G
2	L5	4860	G

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Mol	Chain	Res	Type
2	L5	4862	G
2	L5	4870	OMG
2	L5	4871	C
2	L5	4876	U
2	L5	4882	U
2	L5	4883	C
2	L5	4886	C
2	L5	4887	C
2	L5	4895	C
2	L5	4896	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	A
2	L5	4912	G
2	L5	4923	C
2	L5	4931	G
2	L5	4934	A
2	L5	4937	C
2	L5	4940	C
2	L5	4943	A
2	L5	4944	C
2	L5	4945	G
2	L5	4960	G
2	L5	4966	A
2	L5	4976	U
2	L5	4988	U
2	L5	4989	U
2	L5	4991	U
2	L5	5013	C
2	L5	5017	G
2	L5	5022	U
2	L5	5023	C
2	L5	5024	C
2	L5	5025	C
2	L5	5028	G
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5062	G
2	L5	5068	G

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Mol	Chain	Res	Type
4	L9	7	G
4	L9	33	U
4	L9	37	G
4	L9	38	U
4	L9	53	U
4	L9	54	A
4	L9	64	G
4	L9	110	G
4	L9	120	U
6	S4	5	G
6	S4	7	G
6	S4	8	U
6	S4	9	1MG
6	S4	11	C
6	S4	13	U
6	S4	14	A
6	S4	16	H2U
6	S4	17	G
6	S4	18	OMG
6	S4	19	A
6	S4	20	H2U
6	S4	21	A
6	S4	28	C
6	S4	42	G
6	S4	47	H2U
6	S4	48	U
6	S4	49	G
6	S4	52	G
6	S4	60	U
6	S4	61	C
6	S4	62	C
6	S4	69	G
6	S4	74	C
48	S2	2	A
48	S2	33	G
48	S2	41	G
48	S2	44	U
48	S2	46	A
48	S2	56	G
48	S2	62	G
48	S2	65	C
48	S2	67	C

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Mol	Chain	Res	Type
48	S2	68	A
48	S2	71	G
48	S2	72	C
48	S2	73	C
48	S2	74	G
48	S2	76	U
48	S2	103	A
48	S2	113	G
48	S2	115	U
48	S2	126	G
48	S2	130	G
48	S2	143	U
48	S2	149	A
48	S2	150	A
48	S2	155	G
48	S2	163	U
48	S2	168	C
48	S2	173	A
48	S2	178	C
48	S2	182	C
48	S2	196	C
48	S2	197	U
48	S2	198	U
48	S2	200	G
48	S2	203	G
48	S2	204	G
48	S2	205	G
48	S2	207	G
48	S2	209	A
48	S2	213	G
48	S2	302	A
48	S2	306	C
48	S2	307	G
48	S2	308	G
48	S2	309	G
48	S2	311	C
48	S2	312	G
48	S2	319	C
48	S2	320	G
48	S2	323	C
48	S2	324	C
48	S2	325	C

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Mol	Chain	Res	Type
48	S2	326	C
48	S2	328	U
48	S2	329	G
48	S2	332	G
48	S2	335	G
48	S2	347	G
48	S2	360	A
48	S2	362	C
48	S2	364	A
48	S2	369	C
48	S2	370	G
48	S2	385	G
48	S2	386	C
48	S2	409	C
48	S2	438	G
48	S2	448	A
48	S2	449	A
48	S2	450	C
48	S2	452	G
48	S2	464	A
48	S2	470	G
48	S2	472	C
48	S2	474	G
48	S2	482	G
48	S2	487	U
48	S2	488	U
48	S2	492	C
48	S2	493	A
48	S2	516	A
48	S2	525	A
48	S2	537	C
48	S2	538	U
48	S2	540	U
48	S2	541	U
48	S2	542	U
48	S2	544	G
48	S2	546	G
48	S2	547	G
48	S2	553	U
48	S2	554	A
48	S2	555	A
48	S2	556	U

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Mol	Chain	Res	Type
48	S2	563	G
48	S2	564	A
48	S2	570	C
48	S2	576	A2M
48	S2	587	A
48	S2	589	G
48	S2	591	U
48	S2	592	C
48	S2	606	G
48	S2	607	U
48	S2	614	C
48	S2	617	G
48	S2	626	G
48	S2	628	A
48	S2	643	A
48	S2	655	A
48	S2	660	C
48	S2	668	A2M
48	S2	669	A
48	S2	671	A
48	S2	672	A
48	S2	673	G
48	S2	688	U
48	S2	799	OMU
48	S2	821	G
48	S2	822	PSU
48	S2	830	A
48	S2	835	C
48	S2	836	G
48	S2	837	A
48	S2	839	C
48	S2	840	C
48	S2	841	G
48	S2	847	A
48	S2	870	A
48	S2	872	A
48	S2	875	A
48	S2	880	G
48	S2	884	C
48	S2	888	U
48	S2	889	U
48	S2	891	G

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Mol	Chain	Res	Type
48	S2	892	U
48	S2	896	U
48	S2	897	U
48	S2	898	U
48	S2	900	C
48	S2	901	G
48	S2	903	A
48	S2	913	A
48	S2	920	A
48	S2	922	A
48	S2	933	G
48	S2	943	U
48	S2	956	G
48	S2	990	A
48	S2	992	A
48	S2	1001	A
48	S2	1017	U
48	S2	1023	A
48	S2	1060	A
48	S2	1061	U
48	S2	1062	A
48	S2	1083	A
48	S2	1085	C
48	S2	1109	C
48	S2	1115	U
48	S2	1116	C
48	S2	1131	G
48	S2	1154	U
48	S2	1195	A
48	S2	1207	G
48	S2	1215	C
48	S2	1227	G
48	S2	1242	U
48	S2	1251	A
48	S2	1253	A
48	S2	1256	G
48	S2	1257	G
48	S2	1259	A
48	S2	1274	G
48	S2	1275	G
48	S2	1282	A
48	S2	1283	C

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Mol	Chain	Res	Type
48	S2	1284	A
48	S2	1286	G
48	S2	1289	U
48	S2	1294	G
48	S2	1295	A
48	S2	1302	G
48	S2	1303	C
48	S2	1304	U
48	S2	1308	U
48	S2	1320	G
48	S2	1343	U
48	S2	1345	G
48	S2	1371	U
48	S2	1372	U
48	S2	1378	A
48	S2	1393	G
48	S2	1397	U
48	S2	1402	A
48	S2	1405	A
48	S2	1406	G
48	S2	1421	A
48	S2	1422	G
48	S2	1423	C
48	S2	1433	C
48	S2	1435	C
48	S2	1436	C
48	S2	1438	A
48	S2	1454	A
48	S2	1463	U
48	S2	1487	A
48	S2	1489	A
48	S2	1490	OMG
48	S2	1497	G
48	S2	1498	A
48	S2	1521	C
48	S2	1522	A
48	S2	1533	A
48	S2	1546	G
48	S2	1556	A
48	S2	1560	U
48	S2	1579	A
48	S2	1580	A

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Mol	Chain	Res	Type
48	S2	1585	U
48	S2	1587	G
48	S2	1588	A
48	S2	1600	G
48	S2	1606	G
48	S2	1621	U
48	S2	1623	A
48	S2	1639	7MG
48	S2	1654	G
48	S2	1661	A
48	S2	1665	G
48	S2	1680	G
48	S2	1698	C
48	S2	1699	A
48	S2	1721	U
48	S2	1722	G
48	S2	1825	A
48	S2	1826	G
48	S2	1829	G
48	S2	1838	U
48	S2	1849	G
48	S2	1852	C
48	S2	1861	G
48	S2	1862	G
48	S2	1863	A
48	S2	1864	U
48	S2	1865	C
49	S5	40	G

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	42	A
2	L5	464	G
2	L5	465	G
2	L5	1590	C
2	L5	1613	A
2	L5	1633	G
2	L5	2529	A
2	L5	2587	A
2	L5	3876	A
2	L5	4699	U

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Mol	Chain	Res	Type
6	S4	19	A
6	S4	60	U
48	S2	836	G
48	S2	874	G
48	S2	912	C
48	S2	1520	G

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

235 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	L5	3695	85,2,84	18,21,22	1.35	2 (11%)	21,30,33	2.15	5 (23%)
2	PSU	L5	4579	2	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
6	PSU	S4	55	6	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
2	PSU	L5	4552	2	18,21,22	1.33	2 (11%)	21,30,33	2.21	3 (14%)
33	MLZ	Le	53	33	8,9,10	0.68	0	4,9,11	0.80	0
48	PSU	S2	681	48	18,21,22	1.32	2 (11%)	21,30,33	2.08	4 (19%)
2	OMG	L5	2050	2	19,26,27	0.85	1 (5%)	21,38,41	1.08	1 (4%)
2	UR3	L5	4530	2	19,22,23	0.94	0	26,32,35	1.70	2 (7%)
2	PSU	L5	1582	2	18,21,22	1.41	2 (11%)	21,30,33	2.05	3 (14%)
48	PSU	S2	815	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
2	PSU	L5	4293	2	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
48	PSU	S2	1174	48,85	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	3758	2	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
48	PSU	S2	218	48	18,21,22	1.38	3 (16%)	21,30,33	1.96	4 (19%)
2	A2M	L5	398	2	18,25,26	1.43	2 (11%)	20,36,39	0.97	1 (5%)
2	PSU	L5	4353	2	18,21,22	1.32	3 (16%)	21,30,33	2.05	4 (19%)
2	OMC	L5	2422	2,84	19,22,23	0.79	0	25,31,34	0.74	0
2	OMC	L5	3701	85,2	19,22,23	0.77	0	25,31,34	0.87	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	OMG	L5	3944	2	19,26,27	0.90	1 (5%)	21,38,41	1.05	1 (4%)
6	2MG	S4	10	6	18,26,27	1.10	3 (16%)	16,38,41	0.81	0
48	OMG	S2	1328	48,85	19,26,27	0.88	1 (5%)	21,38,41	1.03	2 (9%)
2	PSU	L5	3844	2	18,21,22	1.38	3 (16%)	21,30,33	2.03	3 (14%)
48	MA6	S2	1851	48	19,26,27	1.11	2 (10%)	18,38,41	2.30	6 (33%)
48	PSU	S2	1238	48	18,21,22	1.39	2 (11%)	21,30,33	2.13	4 (19%)
48	PSU	S2	609	48	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
2	PSU	L5	4532	2	18,21,22	1.42	3 (16%)	21,30,33	2.03	3 (14%)
71	HY3	SX	62	71,85	7,8,9	0.98	0	7,10,12	1.08	1 (14%)
2	PSU	L5	4471	2	18,21,22	1.44	3 (16%)	21,30,33	1.95	4 (19%)
6	H2U	S4	47	6	18,21,22	0.63	0	19,30,33	0.45	0
6	5MU	S4	54	6	19,22,23	0.25	0	27,32,35	0.31	0
2	OMG	L5	3744	2	19,26,27	0.88	1 (5%)	21,38,41	1.04	2 (9%)
48	A2M	S2	468	48	18,25,26	1.41	1 (5%)	20,36,39	1.04	2 (10%)
2	PSU	L5	4423	2	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
48	OMC	S2	1703	48,84	19,22,23	0.76	0	25,31,34	0.78	0
2	OMG	L5	4370	2	19,26,27	0.85	1 (5%)	21,38,41	1.13	2 (9%)
48	OMU	S2	172	48	19,22,23	1.20	2 (10%)	25,31,34	1.89	5 (20%)
48	A2M	S2	1678	48	18,25,26	1.46	2 (11%)	20,36,39	1.06	1 (5%)
2	A2M	L5	2363	2,84	18,25,26	1.35	1 (5%)	20,36,39	1.05	1 (5%)
2	OMG	L5	3899	2	19,26,27	0.87	1 (5%)	21,38,41	1.17	1 (4%)
2	PSU	L5	4972	2	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
2	OMG	L5	4870	2	19,26,27	0.89	1 (5%)	21,38,41	1.10	1 (4%)
2	PSU	L5	3730	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
2	A2M	L5	4571	2	18,25,26	1.38	1 (5%)	20,36,39	0.97	1 (5%)
2	PSU	L5	3884	2	18,21,22	1.40	3 (16%)	21,30,33	2.03	4 (19%)
48	OMU	S2	1326	48,84	19,22,23	1.21	3 (15%)	25,31,34	1.84	5 (20%)
48	PSU	S2	1692	48	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
2	PSU	L5	3768	2	18,21,22	1.37	2 (11%)	21,30,33	2.20	4 (19%)
2	PSU	L5	3770	2	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
2	OMU	L5	2415	2	19,22,23	1.25	4 (21%)	25,31,34	1.72	5 (20%)
2	PSU	L5	3715	2	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
48	OMU	S2	121	48	19,22,23	1.19	3 (15%)	25,31,34	1.80	5 (20%)
2	OMG	L5	4392	2	19,26,27	0.83	0	21,38,41	1.14	1 (4%)
48	PSU	S2	801	48	18,21,22	1.39	3 (16%)	21,30,33	2.07	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	OMU	L5	3925	2	19,22,23	1.23	2 (10%)	25,31,34	1.85	5 (20%)
2	PSU	L5	4500	2	18,21,22	1.36	2 (11%)	21,30,33	2.11	5 (23%)
48	PSU	S2	1046	48	18,21,22	1.35	2 (11%)	21,30,33	1.91	4 (19%)
2	PSU	L5	4312	2	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
2	A2M	L5	3867	2	18,25,26	1.36	1 (5%)	20,36,39	0.93	1 (5%)
2	OMG	L5	2876	2	19,26,27	0.83	1 (5%)	21,38,41	1.09	3 (14%)
48	PSU	S2	119	48	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
2	OMG	L5	4637	85,2	19,26,27	0.86	1 (5%)	21,38,41	1.15	3 (14%)
48	OMG	S2	1490	48,84	19,26,27	0.87	1 (5%)	21,38,41	0.99	1 (4%)
48	PSU	S2	823	48	18,21,22	1.35	2 (11%)	21,30,33	2.11	5 (23%)
2	OMG	L5	4494	2	19,26,27	0.89	1 (5%)	21,38,41	1.05	2 (9%)
48	OMC	S2	174	48	19,22,23	0.79	0	25,31,34	0.83	0
48	A2M	S2	166	48	18,25,26	1.41	2 (11%)	20,36,39	1.06	1 (5%)
2	OMC	L5	2804	2	19,22,23	0.79	1 (5%)	25,31,34	0.75	0
2	PSU	L5	4431	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
1	OMG	L1	75	1	19,26,27	0.86	1 (5%)	21,38,41	1.14	2 (9%)
2	PSU	L5	1683	85,2	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
2	PSU	L5	3851	2	18,21,22	1.39	2 (11%)	21,30,33	1.98	5 (23%)
48	PSU	S2	1004	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
48	PSU	S2	1081	48	18,21,22	1.42	2 (11%)	21,30,33	2.09	5 (23%)
48	OMU	S2	428	48	19,22,23	1.18	2 (10%)	25,31,34	1.84	5 (20%)
2	PSU	L5	1792	85,2	18,21,22	1.32	2 (11%)	21,30,33	1.98	3 (14%)
6	M2G	S4	26	6	20,27,28	1.14	3 (15%)	19,40,43	0.73	0
2	PSU	L5	3920	2,84	18,21,22	1.38	2 (11%)	21,30,33	2.13	6 (28%)
2	PSU	L5	4420	2	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
2	OMC	L5	3869	2	19,22,23	0.76	0	25,31,34	0.71	0
2	PSU	L5	4628	2	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
2	OMC	L5	3841	2	19,22,23	0.78	0	25,31,34	0.79	0
2	OMG	L5	1316	2	19,26,27	0.90	1 (5%)	21,38,41	1.08	1 (4%)
2	OMG	L5	1522	2	19,26,27	0.89	1 (5%)	21,38,41	1.14	2 (9%)
2	OMG	L5	1625	85,2	19,26,27	0.96	1 (5%)	21,38,41	1.06	2 (9%)
48	A2M	S2	590	48	18,25,26	1.37	1 (5%)	20,36,39	1.31	1 (5%)
2	A2M	L5	4523	2,84	18,25,26	1.32	1 (5%)	20,36,39	1.35	3 (15%)
48	PSU	S2	1232	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	3 (14%)
2	PSU	L5	4361	2	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	2MG	L5	729	2	18,26,27	1.50	3 (16%)	16,38,41	2.00	4 (25%)
2	OMC	L5	3808	2	19,22,23	0.75	0	25,31,34	0.78	0
2	PSU	L5	4403	2	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
48	A2M	S2	27	48,84	18,25,26	1.36	1 (5%)	20,36,39	1.02	1 (5%)
2	6MZ	L5	4220	2	17,25,26	0.97	1 (5%)	15,36,39	2.38	3 (20%)
48	A2M	S2	99	48,84	18,25,26	1.38	1 (5%)	20,36,39	1.00	0
48	PSU	S2	1045	48	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
2	OMC	L5	4536	2	19,22,23	0.76	0	25,31,34	0.87	0
2	PSU	L5	4457	2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
2	A2M	L5	2787	2	18,25,26	1.36	1 (5%)	20,36,39	1.07	1 (5%)
2	OMU	L5	2837	2	19,22,23	1.25	3 (15%)	25,31,34	1.90	5 (20%)
48	PSU	S2	918	48	18,21,22	1.40	3 (16%)	21,30,33	2.10	5 (23%)
48	PSU	S2	1347	48	18,21,22	1.36	2 (11%)	21,30,33	2.16	4 (19%)
2	A2M	L5	3825	2	18,25,26	1.34	1 (5%)	20,36,39	0.94	1 (5%)
48	PSU	S2	1056	48	18,21,22	1.37	3 (16%)	21,30,33	1.97	4 (19%)
2	UY1	L5	3818	85,2	19,22,23	1.55	5 (26%)	21,31,34	1.88	5 (23%)
48	PSU	S2	651	48	18,21,22	1.36	2 (11%)	21,30,33	2.12	4 (19%)
6	PSU	S4	27	6	18,21,22	0.92	1 (5%)	21,30,33	0.66	0
2	2MG	L5	1517	2	18,26,27	1.49	3 (16%)	16,38,41	1.99	4 (25%)
48	PSU	S2	814	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
6	H2U	S4	16	6	18,21,22	0.63	0	19,30,33	0.54	0
2	OMG	L5	4499	2	19,26,27	0.87	1 (5%)	21,38,41	1.13	2 (9%)
6	H2U	S4	20	6	18,21,22	0.68	1 (5%)	19,30,33	0.51	0
48	OMG	S2	867	48	19,26,27	0.87	1 (5%)	21,38,41	1.12	2 (9%)
63	IAS	SO	138	63	6,7,8	1.10	0	3,8,10	2.15	1 (33%)
2	A2M	L5	2401	2	18,25,26	1.35	1 (5%)	20,36,39	0.86	0
2	OMU	L5	4306	2	19,22,23	1.24	3 (15%)	25,31,34	1.75	4 (16%)
2	OMG	L5	4228	2	19,26,27	0.93	1 (5%)	21,38,41	1.19	2 (9%)
2	PSU	L5	4521	85,2,84	18,21,22	1.36	2 (11%)	21,30,33	2.11	4 (19%)
2	PSU	L5	2508	2	18,21,22	1.32	3 (16%)	21,30,33	2.00	4 (19%)
2	OMU	L5	4498	2	19,22,23	1.20	3 (15%)	25,31,34	1.91	5 (20%)
2	PSU	L5	4636	2	18,21,22	1.41	3 (16%)	21,30,33	2.04	4 (19%)
2	OMC	L5	1881	2,84	19,22,23	0.77	0	25,31,34	0.96	1 (4%)
48	PSU	S2	109	48	18,21,22	1.37	3 (16%)	21,30,33	2.01	3 (14%)
48	OMU	S2	1288	48	19,22,23	1.21	2 (10%)	25,31,34	1.90	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
2	OMU	L5	4620	2	19,22,23	1.23	3 (15%)	25,31,34	1.64	5 (20%)
2	A2M	L5	3785	2	18,25,26	1.36	1 (5%)	20,36,39	1.91	2 (10%)
2	5MC	L5	3782	2,84	19,22,23	1.65	3 (15%)	26,32,35	1.04	2 (7%)
48	PSU	S2	572	48,85	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
48	A2M	S2	484	48	18,25,26	1.22	1 (5%)	20,36,39	0.81	0
48	OMC	S2	1391	48	19,22,23	0.79	0	25,31,34	0.81	0
2	OMG	L5	1760	2	19,26,27	0.89	1 (5%)	21,38,41	1.02	2 (9%)
48	PSU	S2	1445	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
2	PSU	L5	5001	2	18,21,22	1.35	2 (11%)	21,30,33	2.09	3 (14%)
43	M3L	Lo	98	43	10,11,12	1.04	0	9,14,16	0.67	0
2	OMG	L5	2424	2	19,26,27	0.86	1 (5%)	21,38,41	1.04	2 (9%)
48	PSU	S2	863	48	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
48	PSU	S2	822	48	18,21,22	1.36	2 (11%)	21,30,33	1.97	4 (19%)
2	OMC	L5	2365	2	19,22,23	0.75	0	25,31,34	0.78	0
48	PSU	S2	36	48	18,21,22	1.39	3 (16%)	21,30,33	1.97	4 (19%)
48	A2M	S2	576	48,85	18,25,26	1.32	1 (5%)	20,36,39	0.94	1 (5%)
2	OMG	L5	4618	2	19,26,27	0.89	1 (5%)	21,38,41	1.07	2 (9%)
48	A2M	S2	1031	48	18,25,26	1.35	2 (11%)	20,36,39	1.08	1 (5%)
48	OMC	S2	462	48	19,22,23	0.80	0	25,31,34	0.85	0
2	A2M	L5	1871	2,84	18,25,26	1.40	2 (11%)	20,36,39	1.13	1 (5%)
2	OMU	L5	1773	2	19,22,23	1.22	3 (15%)	25,31,34	1.84	5 (20%)
48	4AC	S2	1842	48,85	21,24,25	3.13	11 (52%)	28,34,37	0.98	1 (3%)
48	A2M	S2	159	48	18,25,26	1.39	3 (16%)	20,36,39	0.99	2 (10%)
48	PSU	S2	105	48	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	1860	2	18,21,22	1.37	3 (16%)	21,30,33	1.92	4 (19%)
2	PSU	L5	3639	2	18,21,22	1.41	2 (11%)	21,30,33	2.08	6 (28%)
48	6MZ	S2	1832	48,85,84	17,25,26	0.88	1 (5%)	15,36,39	2.54	3 (20%)
48	PSU	S2	210	48	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
2	OMC	L5	2351	2,84	19,22,23	0.78	0	25,31,34	0.92	1 (4%)
2	A2M	L5	4590	2	18,25,26	1.39	1 (5%)	20,36,39	1.03	0
1	PSU	L1	69	1	18,21,22	1.44	2 (11%)	21,30,33	2.14	5 (23%)
2	PSU	L5	4442	2	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
2	A2M	L5	1326	2	18,25,26	1.33	1 (5%)	20,36,39	0.93	0
2	PSU	L5	4689	2	18,21,22	1.42	3 (16%)	21,30,33	2.04	4 (19%)
1	PSU	L1	55	1	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	OMU	S2	627	48	19,22,23	1.20	2 (10%)	25,31,34	1.77	5 (20%)
2	OMC	L5	2824	2	19,22,23	0.78	0	25,31,34	0.74	0
48	B8N	S2	1248	48	25,29,30	3.33	8 (32%)	28,42,45	2.04	8 (28%)
2	OMU	L5	4227	2	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
48	OMC	S2	517	48	19,22,23	0.78	0	25,31,34	0.83	0
48	PSU	S2	1367	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
48	PSU	S2	93	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	3 (14%)
48	PSU	S2	34	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	PSU	L5	3734	2	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
48	PSU	S2	649	48	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
5	HIC	LB	245	5	8,11,12	1.19	0	5,14,16	1.09	0
6	OMG	S4	18	6	19,26,27	1.08	3 (15%)	21,38,41	0.73	1 (4%)
48	OMG	S2	601	48	19,26,27	0.87	1 (5%)	21,38,41	1.06	2 (9%)
2	PSU	L5	3853	2,84	18,21,22	1.40	2 (11%)	21,30,33	2.01	3 (14%)
2	A2M	L5	3718	2	18,25,26	1.26	1 (5%)	20,36,39	1.10	2 (10%)
2	OMC	L5	4456	2	19,22,23	0.78	0	25,31,34	0.88	1 (4%)
2	JMH	L5	1456	2	18,22,23	2.83	6 (33%)	23,32,35	0.91	1 (4%)
29	V5N	La	39	29	4,11,12	1.29	0	5,14,16	2.28	2 (40%)
2	OMG	L5	4623	2	19,26,27	0.92	1 (5%)	21,38,41	1.13	2 (9%)
48	PSU	S2	1244	48	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
48	OMG	S2	683	48	19,26,27	0.88	1 (5%)	21,38,41	1.12	2 (9%)
48	OMU	S2	1804	48	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
48	A2M	S2	668	48,84	18,25,26	1.40	2 (11%)	20,36,39	1.36	2 (10%)
6	1MG	S4	9	6,84	19,26,27	1.12	2 (10%)	18,39,42	1.01	1 (5%)
48	PSU	S2	1177	48	18,21,22	1.34	2 (11%)	21,30,33	2.19	4 (19%)
48	7MG	S2	1639	6,48	23,26,27	1.09	1 (4%)	27,39,42	0.85	2 (7%)
2	PSU	L5	1744	85,2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
2	A2M	L5	1524	2	18,25,26	1.37	2 (11%)	20,36,39	1.23	1 (5%)
2	A2M	L5	400	2	18,25,26	1.32	1 (5%)	20,36,39	0.99	0
48	OMU	S2	799	48	19,22,23	1.25	4 (21%)	25,31,34	1.78	5 (20%)
48	OMG	S2	644	48	19,26,27	0.89	1 (5%)	21,38,41	1.09	2 (9%)
6	1MA	S4	58	6	17,25,26	0.86	1 (5%)	17,37,40	0.77	0
2	OMG	L5	4196	6,2	19,26,27	0.83	1 (5%)	21,38,41	1.08	2 (9%)
48	PSU	S2	866	48	18,21,22	1.39	2 (11%)	21,30,33	2.05	3 (14%)
48	MA6	S2	1850	48	19,26,27	1.12	2 (10%)	18,38,41	2.21	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PSU	L5	1781	2	18,21,22	1.43	3 (16%)	21,30,33	1.99	3 (14%)
48	PSU	S2	406	48	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
2	OMC	L5	1340	2	19,22,23	0.80	0	25,31,34	0.85	1 (4%)
2	PSU	L5	2632	2	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
48	PSU	S2	966	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	OMG	L5	2364	2	19,26,27	0.82	1 (5%)	21,38,41	1.13	3 (14%)
2	PSU	L5	1862	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
48	OMU	S2	116	48	19,22,23	1.20	3 (15%)	25,31,34	1.82	5 (20%)
48	OMU	S2	1442	48	19,22,23	1.24	4 (21%)	25,31,34	1.80	4 (16%)
2	PSU	L5	4299	2	18,21,22	1.39	3 (16%)	21,30,33	1.96	4 (19%)
2	OMC	L5	2861	2	19,22,23	0.78	0	25,31,34	0.80	0
48	PSU	S2	686	48	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
30	MLZ	Lb	5	30	8,9,10	0.65	0	4,9,11	0.96	0
2	PSU	L5	3764	2	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
2	PSU	L5	1536	2	18,21,22	1.37	2 (11%)	21,30,33	1.99	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.78	0	25,31,34	0.83	0
2	PSU	L5	3637	85,2	18,21,22	1.34	2 (11%)	21,30,33	2.13	4 (19%)
2	1MA	L5	1322	2,84	17,25,26	1.12	2 (11%)	17,37,40	1.38	3 (17%)
48	OMC	S2	1710	48	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
2	PSU	L5	1677	2	18,21,22	1.44	3 (16%)	21,30,33	2.08	4 (19%)
2	A2M	L5	3760	48,2	18,25,26	1.28	1 (5%)	20,36,39	1.05	0
2	PSU	L5	5010	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
2	PSU	L5	4576	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	3 (14%)
48	PSU	S2	1625	48	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
2	A2M	L5	2815	2	18,25,26	1.30	1 (5%)	20,36,39	0.85	0
8	V5N	LD	216	8	4,11,12	1.47	1 (25%)	5,14,16	1.99	2 (40%)
2	PSU	L5	4296	2	18,21,22	1.40	2 (11%)	21,30,33	2.08	4 (19%)
2	5MC	L5	4447	85,2	19,22,23	1.70	3 (15%)	26,32,35	1.27	2 (7%)
2	PSU	L5	4673	2	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
2	A2M	L5	1534	2,84	18,25,26	1.40	1 (5%)	20,36,39	1.23	2 (10%)
48	A2M	S2	1383	48	18,25,26	1.29	1 (5%)	20,36,39	1.29	3 (15%)
48	OMG	S2	436	48	19,26,27	0.88	1 (5%)	21,38,41	1.09	2 (9%)
48	OMG	S2	509	48,84	19,26,27	0.93	1 (5%)	21,38,41	1.03	2 (9%)
2	PSU	L5	3762	2	18,21,22	1.42	2 (11%)	21,30,33	2.10	4 (19%)
48	A2M	S2	512	48	18,25,26	1.41	1 (5%)	20,36,39	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
48	4AC	S2	1337	48	21,24,25	3.20	11 (52%)	28,34,37	1.08	3 (10%)
2	A2M	L5	3830	2	18,25,26	1.42	1 (5%)	20,36,39	1.05	1 (5%)
2	OMG	L5	3792	85,2	19,26,27	0.90	1 (5%)	21,38,41	1.02	1 (4%)
6	1MG	S4	37	6	19,26,27	1.11	1 (5%)	18,39,42	0.94	1 (5%)
2	PSU	L5	1782	2	18,21,22	1.36	2 (11%)	21,30,33	2.09	3 (14%)
2	2MG	L5	4872	2	18,26,27	1.48	3 (16%)	16,38,41	1.99	4 (25%)
48	PSU	S2	1643	48,84	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	3695	85,2,84	-	0/7/25/26	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
6	PSU	S4	55	6	-	0/7/25/26	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
33	MLZ	Le	53	33	-	2/7/8/10	-
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	2050	2	-	0/5/27/28	0/3/3/3
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	48,85	-	0/7/25/26	0/2/2/2
2	PSU	L5	3758	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
2	A2M	L5	398	2	-	0/5/27/28	0/3/3/3
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2422	2,84	-	0/9/27/28	0/2/2/2
2	OMC	L5	3701	85,2	-	4/9/27/28	0/2/2/2
2	OMG	L5	3944	2	-	2/5/27/28	0/3/3/3
6	2MG	S4	10	6	-	0/5/27/28	0/3/3/3
48	OMG	S2	1328	48,85	-	0/5/27/28	0/3/3/3
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
48	MA6	S2	1851	48	-	3/7/29/30	0/3/3/3
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	609	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	HY3	SX	62	71,85	-	0/1/12/14	0/1/1/1
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
6	H2U	S4	47	6	-	2/7/38/39	0/2/2/2
6	5MU	S4	54	6	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/5/27/28	0/3/3/3
48	A2M	S2	468	48	-	0/5/27/28	0/3/3/3
2	PSU	L5	4423	2	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	48,84	-	0/9/27/28	0/2/2/2
2	OMG	L5	4370	2	-	0/5/27/28	0/3/3/3
48	OMU	S2	172	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	1678	48	-	1/5/27/28	0/3/3/3
2	A2M	L5	2363	2,84	-	1/5/27/28	0/3/3/3
2	OMG	L5	3899	2	-	0/5/27/28	0/3/3/3
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4870	2	-	3/5/27/28	0/3/3/3
2	PSU	L5	3730	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4571	2	-	0/5/27/28	0/3/3/3
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	1326	48,84	-	0/9/27/28	0/2/2/2
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3768	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3770	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	2415	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3715	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
2	OMG	L5	4392	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
48	PSU	S2	1046	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3867	2	-	1/5/27/28	0/3/3/3
2	OMG	L5	2876	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	85,2	-	0/5/27/28	0/3/3/3
48	OMG	S2	1490	48,84	-	1/5/27/28	0/3/3/3
48	PSU	S2	823	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	4494	2	-	0/5/27/28	0/3/3/3
48	OMC	S2	174	48	-	1/9/27/28	0/2/2/2
48	A2M	S2	166	48	-	0/5/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	75	1	-	0/5/27/28	0/3/3/3
2	PSU	L5	1683	85,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3851	2	-	2/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	4/9/27/28	0/2/2/2
2	PSU	L5	1792	85,2	-	0/7/25/26	0/2/2/2
6	M2G	S4	26	6	-	0/7/29/30	0/3/3/3
2	PSU	L5	3920	2,84	-	0/7/25/26	0/2/2/2
2	PSU	L5	4420	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3841	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	1316	2	-	0/5/27/28	0/3/3/3
2	OMG	L5	1522	2	-	0/5/27/28	0/3/3/3
2	OMG	L5	1625	85,2	-	1/5/27/28	0/3/3/3
48	A2M	S2	590	48	-	2/5/27/28	0/3/3/3
2	A2M	L5	4523	2,84	-	0/5/27/28	0/3/3/3
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
2	2MG	L5	729	2	-	0/5/27/28	0/3/3/3
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	27	48,84	-	0/5/27/28	0/3/3/3
2	6MZ	L5	4220	2	-	0/5/27/28	0/3/3/3
48	A2M	S2	99	48,84	-	1/5/27/28	0/3/3/3
48	PSU	S2	1045	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2787	2	-	1/5/27/28	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
2	UY1	L5	3818	85,2	-	1/9/27/28	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
6	PSU	S4	27	6	-	0/7/25/26	0/2/2/2
2	2MG	L5	1517	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
6	H2U	S4	16	6	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	4499	2	-	1/5/27/28	0/3/3/3
6	H2U	S4	20	6	-	2/7/38/39	0/2/2/2
48	OMG	S2	867	48	-	0/5/27/28	0/3/3/3
63	IAS	SO	138	63	-	1/7/7/8	-
2	A2M	L5	2401	2	-	2/5/27/28	0/3/3/3
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4228	2	-	0/5/27/28	0/3/3/3
2	PSU	L5	4521	85,2,84	-	0/7/25/26	0/2/2/2
2	PSU	L5	2508	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4636	2	-	2/7/25/26	0/2/2/2
2	OMC	L5	1881	2,84	-	0/9/27/28	0/2/2/2
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	0/9/27/28	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	3785	2	-	1/5/27/28	0/3/3/3
2	5MC	L5	3782	2,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	48,85	-	0/7/25/26	0/2/2/2
48	A2M	S2	484	48	-	0/5/27/28	0/3/3/3
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
2	OMG	L5	1760	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
43	M3L	Lo	98	43	-	0/9/10/12	-
2	OMG	L5	2424	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	822	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	2365	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	576	48,85	-	2/5/27/28	0/3/3/3
2	OMG	L5	4618	2	-	0/5/27/28	0/3/3/3
48	A2M	S2	1031	48	-	0/5/27/28	0/3/3/3
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
2	A2M	L5	1871	2,84	-	0/5/27/28	0/3/3/3
2	OMU	L5	1773	2	-	0/9/27/28	0/2/2/2
48	4AC	S2	1842	48,85	-	0/11/29/30	0/2/2/2
48	A2M	S2	159	48	-	0/5/27/28	0/3/3/3
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	48,85,84	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	S2	210	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,84	-	2/9/27/28	0/2/2/2
2	A2M	L5	4590	2	-	1/5/27/28	0/3/3/3
1	PSU	L1	69	1	-	0/7/25/26	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1326	2	-	2/5/27/28	0/3/3/3
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	55	1	-	0/7/25/26	0/2/2/2
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
48	B8N	S2	1248	48	-	4/16/34/35	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3734	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
6	OMG	S4	18	6	-	2/5/27/28	0/3/3/3
48	OMG	S2	601	48	-	0/5/27/28	0/3/3/3
2	PSU	L5	3853	2,84	-	0/7/25/26	0/2/2/2
2	A2M	L5	3718	2	-	0/5/27/28	0/3/3/3
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	JMH	L5	1456	2	-	0/7/25/26	0/2/2/2
29	V5N	La	39	29	-	0/5/10/12	0/1/1/1
2	OMG	L5	4623	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	OMG	S2	683	48	-	1/5/27/28	0/3/3/3
48	OMU	S2	1804	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	668	48,84	-	2/5/27/28	0/3/3/3
6	1MG	S4	9	6,84	-	1/3/25/26	0/3/3/3
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
48	7MG	S2	1639	6,48	-	2/7/37/38	0/3/3/3
2	PSU	L5	1744	85,2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1524	2	-	1/5/27/28	0/3/3/3
2	A2M	L5	400	2	-	0/5/27/28	0/3/3/3
48	OMU	S2	799	48	-	1/9/27/28	0/2/2/2
48	OMG	S2	644	48	-	1/5/27/28	0/3/3/3
6	1MA	S4	58	6	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	4196	6,2	-	0/5/27/28	0/3/3/3
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	MA6	S2	1850	48	-	0/7/29/30	0/3/3/3
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	1340	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	2	-	1/5/27/28	0/3/3/3
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
48	OMU	S2	1442	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
30	MLZ	Lb	5	30	-	2/7/8/10	-
2	PSU	L5	3764	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1536	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3887	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3637	85,2	-	0/7/25/26	0/2/2/2
2	1MA	L5	1322	2,84	-	0/3/25/26	0/3/3/3
48	OMC	S2	1710	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	1677	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3760	48,2	-	4/5/27/28	0/3/3/3
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	0/5/27/28	0/3/3/3
8	V5N	LD	216	8	-	1/5/10/12	0/1/1/1
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	85,2	-	4/7/25/26	0/2/2/2
2	PSU	L5	4673	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1534	2,84	-	1/5/27/28	0/3/3/3
48	A2M	S2	1383	48	-	1/5/27/28	0/3/3/3
48	OMG	S2	436	48	-	0/5/27/28	0/3/3/3
48	OMG	S2	509	48,84	-	0/5/27/28	0/3/3/3
2	PSU	L5	3762	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	512	48	-	2/5/27/28	0/3/3/3
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
2	A2M	L5	3830	2	-	0/5/27/28	0/3/3/3
2	OMG	L5	3792	85,2	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1MG	S4	37	6	-	0/3/25/26	0/3/3/3
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
2	2MG	L5	4872	2	-	0/5/27/28	0/3/3/3
48	PSU	S2	1643	48,84	-	0/7/25/26	0/2/2/2

All (423) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1248	B8N	C4-N3	-8.14	1.26	1.40
48	S2	1248	B8N	C6-N1	7.66	1.55	1.36
2	L5	1456	JMH	C2-N1	7.61	1.49	1.38
48	S2	1337	4AC	C4-N3	7.02	1.44	1.32
48	S2	1248	B8N	C4-C5	6.97	1.63	1.47
48	S2	1842	4AC	C4-N3	6.69	1.44	1.32
2	L5	1456	JMH	C6-C5	6.68	1.50	1.35
48	S2	1337	4AC	C6-C5	6.36	1.49	1.35
48	S2	1842	4AC	C6-C5	6.32	1.49	1.35
48	S2	1337	4AC	C2-N3	6.07	1.48	1.36
2	L5	3782	5MC	C5-C4	5.98	1.48	1.44
2	L5	4447	5MC	C5-C4	5.96	1.48	1.44
48	S2	1842	4AC	C2-N3	5.69	1.47	1.36
48	S2	1248	B8N	C2-N1	5.58	1.55	1.39
48	S2	1248	B8N	C6-C5	5.40	1.42	1.35
48	S2	1248	B8N	C1'-C5	-4.75	1.39	1.50
2	L5	1456	JMH	C2-N3	4.59	1.48	1.39
2	L5	729	2MG	C2-N2	4.52	1.42	1.33
2	L5	1517	2MG	C2-N2	4.51	1.42	1.33
2	L5	4872	2MG	C2-N2	4.46	1.42	1.33
48	S2	1639	7MG	C5-N7	4.45	1.41	1.35
2	L5	1871	A2M	O5'-C5'	-4.28	1.31	1.44
2	L5	2787	A2M	O5'-C5'	-4.27	1.31	1.44
48	S2	1842	4AC	C2-N1	4.17	1.48	1.40
2	L5	3760	A2M	O5'-C5'	-4.16	1.32	1.44
2	L5	3830	A2M	O5'-C5'	-4.14	1.32	1.44
48	S2	1337	4AC	C2-N1	4.11	1.48	1.40
2	L5	4523	A2M	O5'-C5'	-4.02	1.32	1.44
2	L5	3825	A2M	O5'-C5'	-4.01	1.32	1.44
2	L5	3785	A2M	O5'-C5'	-3.98	1.32	1.44
2	L5	2401	A2M	O5'-C5'	-3.96	1.32	1.44
2	L5	2815	A2M	O5'-C5'	-3.93	1.32	1.44
2	L5	2363	A2M	O5'-C5'	-3.93	1.32	1.44
48	S2	1383	A2M	O5'-C5'	-3.92	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1842	4AC	C5-C4	3.92	1.49	1.41
48	S2	99	A2M	O5'-C5'	-3.91	1.32	1.44
48	S2	27	A2M	O5'-C5'	-3.91	1.32	1.44
2	L5	1326	A2M	O5'-C5'	-3.90	1.32	1.44
2	L5	398	A2M	O5'-C5'	-3.88	1.32	1.44
2	L5	3867	A2M	O5'-C5'	-3.88	1.32	1.44
2	L5	1524	A2M	O5'-C5'	-3.86	1.32	1.44
48	S2	468	A2M	O5'-C5'	-3.86	1.33	1.44
48	S2	512	A2M	O5'-C5'	-3.81	1.33	1.44
48	S2	1337	4AC	C5-C4	3.80	1.49	1.41
2	L5	4571	A2M	O5'-C5'	-3.78	1.33	1.44
2	L5	1534	A2M	O5'-C5'	-3.77	1.33	1.44
48	S2	668	A2M	O5'-C5'	-3.76	1.33	1.44
2	L5	400	A2M	O5'-C5'	-3.75	1.33	1.44
48	S2	1031	A2M	O5'-C5'	-3.72	1.33	1.44
48	S2	1842	4AC	O2-C2	-3.72	1.16	1.23
48	S2	1678	A2M	O5'-C5'	-3.69	1.33	1.44
2	L5	3639	PSU	C6-C5	3.69	1.39	1.35
2	L5	4403	PSU	C6-C5	3.68	1.39	1.35
48	S2	166	A2M	O5'-C5'	-3.66	1.33	1.44
2	L5	3718	A2M	O5'-C5'	-3.65	1.33	1.44
48	S2	1337	4AC	C7-N4	3.63	1.44	1.37
6	S4	55	PSU	C6-C5	3.62	1.39	1.35
48	S2	484	A2M	O5'-C5'	-3.60	1.33	1.44
48	S2	159	A2M	O5'-C5'	-3.59	1.33	1.44
2	L5	3884	PSU	C6-C5	3.57	1.39	1.35
48	S2	1232	PSU	C6-C5	3.56	1.39	1.35
2	L5	1781	PSU	C6-C5	3.56	1.39	1.35
2	L5	4532	PSU	C6-C5	3.56	1.39	1.35
2	L5	2632	PSU	C6-C5	3.56	1.39	1.35
6	S4	27	PSU	C6-C5	3.54	1.39	1.35
2	L5	3853	PSU	C6-C5	3.53	1.39	1.35
2	L5	4590	A2M	O5'-C5'	-3.53	1.33	1.44
2	L5	3818	UY1	C4-N3	-3.52	1.32	1.38
2	L5	3770	PSU	C6-C5	3.51	1.39	1.35
48	S2	590	A2M	O5'-C5'	-3.51	1.34	1.44
48	S2	1367	PSU	C6-C5	3.50	1.39	1.35
2	L5	4673	PSU	C6-C5	3.50	1.39	1.35
48	S2	1692	PSU	C6-C5	3.49	1.39	1.35
48	S2	572	PSU	C6-C5	3.48	1.39	1.35
1	L1	69	PSU	C6-C5	3.48	1.39	1.35
2	L5	1536	PSU	C6-C5	3.47	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3762	PSU	C6-C5	3.47	1.39	1.35
2	L5	3844	PSU	C6-C5	3.47	1.39	1.35
48	S2	1238	PSU	C6-C5	3.46	1.39	1.35
48	S2	649	PSU	C6-C5	3.46	1.39	1.35
48	S2	576	A2M	O5'-C5'	-3.46	1.34	1.44
2	L5	4296	PSU	C6-C5	3.45	1.39	1.35
2	L5	4636	PSU	C6-C5	3.45	1.39	1.35
48	S2	866	PSU	C6-C5	3.45	1.39	1.35
48	S2	1842	4AC	C7-N4	3.45	1.44	1.37
2	L5	4299	PSU	C6-C5	3.44	1.39	1.35
48	S2	1174	PSU	C6-C5	3.44	1.39	1.35
48	S2	1337	4AC	O2-C2	-3.42	1.17	1.23
48	S2	210	PSU	C6-C5	3.42	1.39	1.35
48	S2	918	PSU	C6-C5	3.42	1.39	1.35
2	L5	4471	PSU	C6-C5	3.41	1.39	1.35
2	L5	4361	PSU	C6-C5	3.41	1.39	1.35
48	S2	1337	4AC	C4-N4	3.40	1.45	1.39
2	L5	4579	PSU	C6-C5	3.40	1.39	1.35
2	L5	4521	PSU	C6-C5	3.38	1.39	1.35
48	S2	966	PSU	C6-C5	3.38	1.39	1.35
48	S2	1004	PSU	C6-C5	3.38	1.39	1.35
48	S2	36	PSU	C6-C5	3.37	1.39	1.35
2	L5	3734	PSU	C6-C5	3.37	1.39	1.35
2	L5	3637	PSU	C6-C5	3.37	1.39	1.35
48	S2	1081	PSU	C6-C5	3.37	1.39	1.35
48	S2	93	PSU	C6-C5	3.36	1.39	1.35
2	L5	3920	PSU	C6-C5	3.35	1.39	1.35
48	S2	1046	PSU	C6-C5	3.33	1.39	1.35
2	L5	4293	PSU	C6-C5	3.33	1.39	1.35
48	S2	119	PSU	C6-C5	3.32	1.39	1.35
48	S2	801	PSU	C6-C5	3.32	1.39	1.35
2	L5	3730	PSU	C6-C5	3.32	1.39	1.35
48	S2	815	PSU	C6-C5	3.31	1.39	1.35
2	L5	3851	PSU	C6-C5	3.31	1.39	1.35
48	S2	651	PSU	C6-C5	3.31	1.39	1.35
48	S2	863	PSU	C6-C5	3.30	1.38	1.35
2	L5	3768	PSU	C6-C5	3.30	1.38	1.35
48	S2	609	PSU	C6-C5	3.30	1.38	1.35
48	S2	1056	PSU	C6-C5	3.30	1.38	1.35
48	S2	1842	4AC	C6-N1	3.29	1.45	1.38
2	L5	3695	PSU	C6-C5	3.28	1.38	1.35
2	L5	1860	PSU	C6-C5	3.27	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	5010	PSU	C6-C5	3.27	1.38	1.35
2	L5	4689	PSU	C6-C5	3.27	1.38	1.35
2	L5	4972	PSU	C6-C5	3.27	1.38	1.35
2	L5	4457	PSU	C6-C5	3.27	1.38	1.35
2	L5	1683	PSU	C6-C5	3.25	1.38	1.35
48	S2	686	PSU	C6-C5	3.24	1.38	1.35
48	S2	1045	PSU	C6-C5	3.23	1.38	1.35
48	S2	1445	PSU	C6-C5	3.23	1.38	1.35
48	S2	1625	PSU	C6-C5	3.23	1.38	1.35
2	L5	1862	PSU	C6-C5	3.23	1.38	1.35
2	L5	3764	PSU	C6-C5	3.22	1.38	1.35
48	S2	34	PSU	C6-C5	3.22	1.38	1.35
2	L5	3715	PSU	C6-C5	3.22	1.38	1.35
2	L5	4442	PSU	C6-C5	3.22	1.38	1.35
2	L5	4312	PSU	C6-C5	3.21	1.38	1.35
2	L5	1782	PSU	C6-C5	3.20	1.38	1.35
1	L1	55	PSU	C6-C5	3.19	1.38	1.35
48	S2	406	PSU	C6-C5	3.18	1.38	1.35
2	L5	4552	PSU	C6-C5	3.18	1.38	1.35
48	S2	105	PSU	C6-C5	3.18	1.38	1.35
2	L5	1322	1MA	C6-N1	3.17	1.44	1.41
2	L5	4576	PSU	C6-C5	3.17	1.38	1.35
2	L5	4431	PSU	C6-C5	3.16	1.38	1.35
48	S2	681	PSU	C6-C5	3.16	1.38	1.35
48	S2	823	PSU	C6-C5	3.16	1.38	1.35
2	L5	4423	PSU	C6-C5	3.16	1.38	1.35
2	L5	5001	PSU	C6-C5	3.16	1.38	1.35
48	S2	822	PSU	C6-C5	3.16	1.38	1.35
48	S2	1337	4AC	C6-N1	3.15	1.45	1.38
48	S2	218	PSU	C6-C5	3.15	1.38	1.35
2	L5	1582	PSU	C6-C5	3.14	1.38	1.35
48	S2	1643	PSU	C6-C5	3.14	1.38	1.35
48	S2	1347	PSU	C6-C5	3.13	1.38	1.35
2	L5	3758	PSU	C6-C5	3.13	1.38	1.35
2	L5	1744	PSU	C6-C5	3.13	1.38	1.35
2	L5	4353	PSU	C6-C5	3.12	1.38	1.35
2	L5	4447	5MC	C6-C5	3.12	1.39	1.34
48	S2	1177	PSU	C6-C5	3.12	1.38	1.35
48	S2	109	PSU	C6-C5	3.12	1.38	1.35
2	L5	4628	PSU	C6-C5	3.11	1.38	1.35
48	S2	814	PSU	C6-C5	3.10	1.38	1.35
48	S2	1244	PSU	C6-C5	3.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4500	PSU	C6-C5	3.09	1.38	1.35
2	L5	2508	PSU	C6-C5	3.02	1.38	1.35
2	L5	4420	PSU	C6-C5	3.00	1.38	1.35
1	L1	69	PSU	C4-N3	-2.96	1.33	1.38
1	L1	55	PSU	C4-N3	-2.96	1.33	1.38
2	L5	1677	PSU	C6-C5	2.93	1.38	1.35
48	S2	1842	4AC	C4-N4	2.92	1.44	1.39
48	S2	1851	MA6	C6-C5	2.92	1.49	1.44
48	S2	801	PSU	C4-N3	-2.89	1.33	1.38
48	S2	814	PSU	C4-N3	-2.89	1.33	1.38
2	L5	3920	PSU	C4-N3	-2.89	1.33	1.38
2	L5	1677	PSU	C4-N3	-2.86	1.33	1.38
2	L5	3715	PSU	C4-N3	-2.86	1.33	1.38
2	L5	3758	PSU	C4-N3	-2.84	1.33	1.38
2	L5	3639	PSU	C4-N3	-2.84	1.33	1.38
2	L5	1792	PSU	C6-C5	2.84	1.38	1.35
48	S2	406	PSU	C4-N3	-2.82	1.33	1.38
2	L5	4299	PSU	C4-N3	-2.82	1.33	1.38
48	S2	1850	MA6	C6-C5	2.82	1.49	1.44
2	L5	4471	PSU	C4-N3	-2.82	1.33	1.38
2	L5	1781	PSU	C4-N3	-2.81	1.33	1.38
2	L5	3925	OMU	C4-N3	-2.81	1.33	1.38
48	S2	93	PSU	C4-N3	-2.81	1.33	1.38
2	L5	2837	OMU	C4-N3	-2.80	1.33	1.38
48	S2	966	PSU	C4-N3	-2.80	1.33	1.38
2	L5	3851	PSU	C4-N3	-2.80	1.33	1.38
2	L5	3818	UY1	C4-C5	-2.79	1.36	1.44
2	L5	4689	PSU	C4-N3	-2.79	1.33	1.38
2	L5	3782	5MC	C6-C5	2.79	1.39	1.34
48	S2	1347	PSU	C4-N3	-2.79	1.33	1.38
2	L5	4579	PSU	C4-N3	-2.79	1.33	1.38
2	L5	4442	PSU	C4-N3	-2.78	1.33	1.38
2	L5	4293	PSU	C4-N3	-2.77	1.33	1.38
2	L5	1582	PSU	C4-N3	-2.76	1.33	1.38
48	S2	815	PSU	C4-N3	-2.76	1.33	1.38
6	S4	18	OMG	C5-C6	-2.75	1.42	1.47
2	L5	4673	PSU	C4-N3	-2.75	1.33	1.38
48	S2	609	PSU	C4-N3	-2.75	1.33	1.38
2	L5	3695	PSU	C4-N3	-2.75	1.33	1.38
48	S2	36	PSU	C4-N3	-2.75	1.33	1.38
48	S2	1045	PSU	C4-N3	-2.75	1.33	1.38
2	L5	4500	PSU	C4-N3	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	34	PSU	C4-N3	-2.74	1.33	1.38
48	S2	1081	PSU	C4-N3	-2.74	1.33	1.38
2	L5	4620	OMU	C4-N3	-2.73	1.33	1.38
2	L5	4431	PSU	C4-N3	-2.73	1.33	1.38
2	L5	1683	PSU	C4-N3	-2.73	1.33	1.38
2	L5	1782	PSU	C4-N3	-2.73	1.33	1.38
48	S2	109	PSU	C4-N3	-2.73	1.33	1.38
48	S2	218	PSU	C4-N3	-2.72	1.33	1.38
48	S2	105	PSU	C4-N3	-2.72	1.33	1.38
48	S2	686	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4498	OMU	C4-N3	-2.72	1.34	1.38
48	S2	572	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4636	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4312	PSU	C4-N3	-2.72	1.33	1.38
2	L5	2632	PSU	C4-N3	-2.72	1.33	1.38
48	S2	1238	PSU	C4-N3	-2.72	1.33	1.38
48	S2	799	OMU	C4-N3	-2.71	1.34	1.38
48	S2	1692	PSU	C4-N3	-2.71	1.33	1.38
48	S2	1804	OMU	C4-N3	-2.71	1.34	1.38
48	S2	1004	PSU	C4-N3	-2.71	1.33	1.38
48	S2	1232	PSU	C4-N3	-2.71	1.33	1.38
2	L5	3637	PSU	C4-N3	-2.70	1.33	1.38
2	L5	4296	PSU	C4-N3	-2.70	1.33	1.38
48	S2	651	PSU	C4-N3	-2.70	1.33	1.38
48	S2	210	PSU	C4-N3	-2.69	1.33	1.38
48	S2	1445	PSU	C4-N3	-2.69	1.33	1.38
2	L5	4220	6MZ	C6-C5	2.69	1.49	1.44
48	S2	1244	PSU	C4-N3	-2.69	1.33	1.38
2	L5	3768	PSU	C4-N3	-2.68	1.33	1.38
48	S2	918	PSU	C4-N3	-2.68	1.33	1.38
2	L5	4576	PSU	C4-N3	-2.68	1.33	1.38
2	L5	2415	OMU	C4-N3	-2.68	1.34	1.38
2	L5	3762	PSU	C4-N3	-2.68	1.33	1.38
2	L5	3770	PSU	C4-N3	-2.68	1.33	1.38
2	L5	4972	PSU	C4-N3	-2.68	1.33	1.38
6	S4	26	M2G	C5-C6	-2.68	1.42	1.47
2	L5	4420	PSU	C4-N3	-2.67	1.33	1.38
48	S2	509	OMG	C6-N1	-2.67	1.33	1.37
48	S2	649	PSU	C4-N3	-2.67	1.33	1.38
2	L5	3730	PSU	C4-N3	-2.67	1.33	1.38
2	L5	4628	PSU	C4-N3	-2.67	1.33	1.38
48	S2	1174	PSU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4227	OMU	C4-N3	-2.66	1.34	1.38
2	L5	1517	2MG	C6-N1	2.66	1.41	1.37
48	S2	866	PSU	C4-N3	-2.66	1.33	1.38
48	S2	1177	PSU	C4-N3	-2.66	1.33	1.38
2	L5	5010	PSU	C4-N3	-2.66	1.33	1.38
2	L5	1860	PSU	C4-N3	-2.66	1.33	1.38
48	S2	1442	OMU	C4-N3	-2.65	1.34	1.38
2	L5	4361	PSU	C4-N3	-2.65	1.33	1.38
2	L5	3844	PSU	C4-N3	-2.65	1.33	1.38
48	S2	121	OMU	C4-N3	-2.65	1.34	1.38
2	L5	4306	OMU	C4-N3	-2.64	1.34	1.38
2	L5	3734	PSU	C4-N3	-2.64	1.33	1.38
48	S2	1625	PSU	C4-N3	-2.64	1.33	1.38
48	S2	1046	PSU	C4-N3	-2.64	1.33	1.38
2	L5	4423	PSU	C4-N3	-2.64	1.33	1.38
2	L5	3884	PSU	C4-N3	-2.63	1.33	1.38
48	S2	681	PSU	C4-N3	-2.63	1.33	1.38
2	L5	1536	PSU	C4-N3	-2.63	1.33	1.38
48	S2	119	PSU	C4-N3	-2.63	1.33	1.38
2	L5	5001	PSU	C4-N3	-2.63	1.33	1.38
48	S2	822	PSU	C4-N3	-2.62	1.33	1.38
48	S2	1288	OMU	C4-N3	-2.62	1.34	1.38
48	S2	1367	PSU	C4-N3	-2.62	1.33	1.38
48	S2	627	OMU	C4-N3	-2.61	1.34	1.38
2	L5	4872	2MG	C6-N1	2.61	1.41	1.37
2	L5	2508	PSU	C4-N3	-2.61	1.34	1.38
48	S2	116	OMU	C4-N3	-2.61	1.34	1.38
48	S2	1326	OMU	C4-N3	-2.61	1.34	1.38
2	L5	729	2MG	C6-N1	2.61	1.41	1.37
2	L5	4457	PSU	C4-N3	-2.61	1.34	1.38
2	L5	3853	PSU	C4-N3	-2.60	1.34	1.38
48	S2	1056	PSU	C4-N3	-2.60	1.34	1.38
2	L5	1792	PSU	C4-N3	-2.60	1.34	1.38
6	S4	10	2MG	C5-C6	-2.60	1.42	1.47
2	L5	1744	PSU	C4-N3	-2.60	1.34	1.38
2	L5	1456	JMH	O2-C2	-2.59	1.17	1.22
48	S2	823	PSU	C4-N3	-2.59	1.34	1.38
48	S2	863	PSU	C4-N3	-2.58	1.34	1.38
2	L5	1773	OMU	C4-N3	-2.58	1.34	1.38
2	L5	1862	PSU	C4-N3	-2.58	1.34	1.38
48	S2	428	OMU	C4-N3	-2.57	1.34	1.38
2	L5	3764	PSU	C4-N3	-2.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	172	OMU	C4-N3	-2.57	1.34	1.38
2	L5	1677	PSU	O4'-C1'	-2.56	1.40	1.43
2	L5	4552	PSU	C4-N3	-2.56	1.34	1.38
2	L5	4403	PSU	C4-N3	-2.56	1.34	1.38
48	S2	1643	PSU	C4-N3	-2.55	1.34	1.38
2	L5	4353	PSU	C4-N3	-2.55	1.34	1.38
48	S2	668	A2M	O4'-C4'	-2.54	1.39	1.45
2	L5	1456	JMH	C5-C4	2.53	1.48	1.42
2	L5	4521	PSU	C4-N3	-2.53	1.34	1.38
2	L5	1456	JMH	C6-N1	2.51	1.44	1.38
2	L5	1625	OMG	C6-N1	-2.49	1.34	1.37
48	S2	1832	6MZ	C6-C5	2.48	1.48	1.44
2	L5	3818	UY1	O4-C4	-2.48	1.18	1.23
2	L5	4532	PSU	C4-N3	-2.45	1.34	1.38
2	L5	3792	OMG	C6-N1	-2.44	1.34	1.37
48	S2	644	OMG	C6-N1	-2.44	1.34	1.37
2	L5	2424	OMG	C6-N1	-2.42	1.34	1.37
2	L5	4228	OMG	C6-N1	-2.40	1.34	1.37
2	L5	4306	OMU	C2-N3	-2.38	1.33	1.38
2	L5	4494	OMG	C6-N1	-2.37	1.34	1.37
2	L5	1760	OMG	C6-N1	-2.36	1.34	1.37
48	S2	1842	4AC	O7-C7	-2.36	1.18	1.23
48	S2	867	OMG	C6-N1	-2.36	1.34	1.37
48	S2	436	OMG	C6-N1	-2.35	1.34	1.37
2	L5	3818	UY1	O2-C2	-2.34	1.18	1.23
2	L5	2415	OMU	C2-N3	-2.34	1.33	1.38
48	S2	1490	OMG	C6-N1	-2.34	1.34	1.37
2	L5	4623	OMG	C6-N1	-2.34	1.34	1.37
2	L5	4620	OMU	C2-N3	-2.34	1.33	1.38
2	L5	4618	OMG	C6-N1	-2.34	1.34	1.37
2	L5	4872	2MG	C5-C6	-2.33	1.42	1.47
48	S2	1248	B8N	O4-C4	-2.32	1.18	1.23
48	S2	683	OMG	C6-N1	-2.32	1.34	1.37
48	S2	1328	OMG	C6-N1	-2.32	1.34	1.37
2	L5	4227	OMU	C2-N3	-2.31	1.33	1.38
2	L5	4637	OMG	C6-N1	-2.30	1.34	1.37
6	S4	37	1MG	C5-C4	-2.30	1.37	1.43
2	L5	3944	OMG	C6-N1	-2.30	1.34	1.37
2	L5	1316	OMG	C6-N1	-2.30	1.34	1.37
2	L5	3744	OMG	C6-N1	-2.30	1.34	1.37
6	S4	9	1MG	C5-C4	-2.30	1.37	1.43
2	L5	4498	OMU	C2-N3	-2.29	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4447	5MC	C6-N1	-2.29	1.34	1.38
2	L5	729	2MG	C5-C6	-2.29	1.42	1.47
2	L5	2876	OMG	C6-N1	-2.29	1.34	1.37
2	L5	1522	OMG	C6-N1	-2.28	1.34	1.37
2	L5	4870	OMG	C6-N1	-2.28	1.34	1.37
48	S2	1326	OMU	C2-N3	-2.28	1.34	1.38
2	L5	4499	OMG	C6-N1	-2.28	1.34	1.37
48	S2	601	OMG	C6-N1	-2.27	1.34	1.37
2	L5	3925	OMU	C2-N3	-2.27	1.34	1.38
48	S2	159	A2M	C5'-C4'	2.25	1.58	1.51
1	L1	75	OMG	C6-N1	-2.24	1.34	1.37
2	L5	2050	OMG	C6-N1	-2.24	1.34	1.37
48	S2	1851	MA6	C6-N1	2.24	1.35	1.32
2	L5	1517	2MG	C5-C6	-2.24	1.43	1.47
48	S2	1804	OMU	C2-N3	-2.24	1.34	1.38
2	L5	4370	OMG	C6-N1	-2.23	1.34	1.37
2	L5	3782	5MC	C6-N1	-2.23	1.34	1.38
48	S2	799	OMU	C2-N3	-2.22	1.34	1.38
48	S2	1442	OMU	C2-N3	-2.22	1.34	1.38
2	L5	2364	OMG	C6-N1	-2.21	1.34	1.37
48	S2	1337	4AC	CM7-C7	2.21	1.55	1.50
48	S2	116	OMU	C5-C4	-2.21	1.38	1.43
2	L5	398	A2M	O4'-C1'	2.21	1.43	1.40
48	S2	172	OMU	C2-N3	-2.21	1.34	1.38
48	S2	116	OMU	C2-N3	-2.20	1.34	1.38
2	L5	3818	UY1	C6-N1	-2.20	1.32	1.36
48	S2	1288	OMU	C2-N3	-2.19	1.34	1.38
6	S4	26	M2G	C5-C4	-2.19	1.37	1.43
48	S2	1337	4AC	O7-C7	-2.19	1.18	1.23
48	S2	627	OMU	C2-N3	-2.18	1.34	1.38
2	L5	4299	PSU	C2-N3	-2.18	1.33	1.37
6	S4	20	H2U	C2-N3	-2.18	1.34	1.38
48	S2	121	OMU	C2-N3	-2.18	1.34	1.38
8	LD	216	V5N	O2-CB	-2.18	1.38	1.42
48	S2	1442	OMU	C5-C4	-2.17	1.39	1.43
48	S2	1248	B8N	O2-C2	-2.15	1.18	1.22
2	L5	2837	OMU	C2-N1	2.15	1.41	1.38
2	L5	1773	OMU	C2-N3	-2.14	1.34	1.38
48	S2	801	PSU	C2-N3	-2.14	1.34	1.37
6	S4	10	2MG	C8-N7	-2.13	1.31	1.34
6	S4	18	OMG	C8-N7	-2.13	1.31	1.34
6	S4	26	M2G	C8-N7	-2.13	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	799	OMU	C2-N1	2.12	1.41	1.38
48	S2	406	PSU	C2-N3	-2.12	1.34	1.37
2	L5	2415	OMU	C2-N1	2.12	1.41	1.38
2	L5	1860	PSU	C2-N3	-2.12	1.34	1.37
2	L5	3899	OMG	C6-N1	-2.12	1.34	1.37
1	L1	55	PSU	C2-N3	-2.11	1.34	1.37
2	L5	4532	PSU	C2-N1	-2.11	1.33	1.36
48	S2	34	PSU	C2-N3	-2.11	1.34	1.37
2	L5	1322	1MA	C2-N1	2.11	1.40	1.35
2	L5	2804	OMC	C6-C5	2.10	1.40	1.35
48	S2	218	PSU	C2-N3	-2.10	1.34	1.37
48	S2	1842	4AC	CM7-C7	2.10	1.54	1.50
2	L5	4471	PSU	C2-N3	-2.10	1.34	1.37
2	L5	4689	PSU	C2-N3	-2.09	1.34	1.37
2	L5	1871	A2M	O4'-C1'	2.09	1.43	1.40
48	S2	36	PSU	C2-N3	-2.09	1.34	1.37
48	S2	1850	MA6	C6-N1	2.09	1.35	1.32
48	S2	121	OMU	C5-C4	-2.08	1.39	1.43
6	S4	58	1MA	C5-C4	-2.07	1.38	1.43
48	S2	1804	OMU	C5-C4	-2.07	1.39	1.43
2	L5	2415	OMU	C5-C4	-2.07	1.39	1.43
48	S2	428	OMU	C2-N3	-2.07	1.34	1.38
2	L5	4498	OMU	C5-C4	-2.07	1.39	1.43
2	L5	4196	OMG	C6-N1	-2.06	1.34	1.37
2	L5	1781	PSU	C2-N3	-2.06	1.34	1.37
2	L5	3884	PSU	C2-N3	-2.06	1.34	1.37
2	L5	4353	PSU	C2-N3	-2.06	1.34	1.37
48	S2	918	PSU	O4'-C1'	-2.05	1.41	1.43
2	L5	4306	OMU	C2-N1	2.05	1.41	1.38
48	S2	109	PSU	C2-N3	-2.04	1.34	1.37
2	L5	4636	PSU	C2-N3	-2.04	1.34	1.37
2	L5	2837	OMU	C2-N3	-2.04	1.34	1.38
6	S4	18	OMG	C5-C4	-2.04	1.38	1.43
2	L5	4227	OMU	C2-N1	2.04	1.41	1.38
48	S2	1678	A2M	O4'-C1'	2.03	1.43	1.40
48	S2	166	A2M	C2-N3	2.03	1.35	1.32
48	S2	1056	PSU	C2-N3	-2.03	1.34	1.37
6	S4	9	1MG	C5-C6	-2.03	1.41	1.47
48	S2	799	OMU	C5-C4	-2.03	1.39	1.43
48	S2	1326	OMU	C5-C4	-2.03	1.39	1.43
2	L5	4620	OMU	C5-C4	-2.03	1.39	1.43
2	L5	3758	PSU	C2-N3	-2.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1773	OMU	C2-N1	2.02	1.41	1.38
48	S2	93	PSU	C2-N3	-2.02	1.34	1.37
48	S2	966	PSU	C2-N3	-2.02	1.34	1.37
48	S2	159	A2M	O4'-C1'	2.01	1.43	1.40
48	S2	1442	OMU	C2-N1	2.01	1.41	1.38
2	L5	2632	PSU	C2-N3	-2.01	1.34	1.37
6	S4	10	2MG	C5-C4	-2.01	1.38	1.43
2	L5	1524	A2M	C2-N3	2.01	1.35	1.32
2	L5	2508	PSU	C2-N3	-2.01	1.34	1.37
2	L5	3844	PSU	C2-N3	-2.00	1.34	1.37
48	S2	1031	A2M	C1'-N9	-2.00	1.45	1.49

All (619) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1832	6MZ	C2-N1-C6	8.53	123.22	116.60
2	L5	4220	6MZ	C2-N1-C6	7.73	122.60	116.60
2	L5	3920	PSU	N1-C2-N3	6.85	122.39	115.17
1	L1	55	PSU	N1-C2-N3	6.77	122.31	115.17
2	L5	4530	UR3	C4-N3-C2	-6.77	119.13	124.58
2	L5	3768	PSU	N1-C2-N3	6.77	122.31	115.17
48	S2	1177	PSU	N1-C2-N3	6.73	122.27	115.17
2	L5	3762	PSU	N1-C2-N3	6.69	122.23	115.17
1	L1	69	PSU	N1-C2-N3	6.69	122.22	115.17
2	L5	3695	PSU	N1-C2-N3	6.67	122.20	115.17
48	S2	1347	PSU	N1-C2-N3	6.66	122.20	115.17
2	L5	3639	PSU	N1-C2-N3	6.66	122.19	115.17
48	S2	1238	PSU	N1-C2-N3	6.64	122.17	115.17
2	L5	4673	PSU	N1-C2-N3	6.63	122.17	115.17
2	L5	1782	PSU	N1-C2-N3	6.61	122.14	115.17
48	S2	801	PSU	N1-C2-N3	6.61	122.14	115.17
2	L5	3637	PSU	N1-C2-N3	6.59	122.12	115.17
48	S2	572	PSU	N1-C2-N3	6.58	122.11	115.17
48	S2	1081	PSU	N1-C2-N3	6.57	122.10	115.17
2	L5	4521	PSU	N1-C2-N3	6.57	122.10	115.17
48	S2	1045	PSU	N1-C2-N3	6.56	122.09	115.17
2	L5	4552	PSU	N1-C2-N3	6.56	122.09	115.17
2	L5	4457	PSU	N1-C2-N3	6.55	122.08	115.17
2	L5	4442	PSU	N1-C2-N3	6.55	122.08	115.17
2	L5	4500	PSU	N1-C2-N3	6.53	122.06	115.17
2	L5	4296	PSU	N1-C2-N3	6.53	122.06	115.17
2	L5	3785	A2M	C4'-O4'-C1'	-6.52	103.96	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	651	PSU	N1-C2-N3	6.51	122.04	115.17
48	S2	815	PSU	N1-C2-N3	6.51	122.03	115.17
2	L5	4636	PSU	N1-C2-N3	6.50	122.02	115.17
2	L5	4423	PSU	N1-C2-N3	6.49	122.02	115.17
2	L5	4576	PSU	N1-C2-N3	6.49	122.02	115.17
2	L5	5001	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	406	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	1445	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	814	PSU	N1-C2-N3	6.46	121.98	115.17
2	L5	4431	PSU	N1-C2-N3	6.45	121.98	115.17
48	S2	966	PSU	N1-C2-N3	6.44	121.97	115.17
2	L5	4579	PSU	N1-C2-N3	6.43	121.95	115.17
2	L5	1781	PSU	N1-C2-N3	6.43	121.95	115.17
48	S2	1692	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	823	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	1004	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	119	PSU	N1-C2-N3	6.41	121.93	115.17
2	L5	3734	PSU	N1-C2-N3	6.41	121.93	115.17
2	L5	1677	PSU	N1-C2-N3	6.40	121.92	115.17
2	L5	3770	PSU	N1-C2-N3	6.39	121.91	115.17
48	S2	866	PSU	N1-C2-N3	6.38	121.90	115.17
2	L5	1582	PSU	N1-C2-N3	6.38	121.90	115.17
48	S2	105	PSU	N1-C2-N3	6.38	121.89	115.17
48	S2	681	PSU	N1-C2-N3	6.38	121.89	115.17
2	L5	3853	PSU	N1-C2-N3	6.37	121.89	115.17
48	S2	34	PSU	N1-C2-N3	6.37	121.89	115.17
48	S2	1367	PSU	N1-C2-N3	6.37	121.89	115.17
48	S2	918	PSU	N1-C2-N3	6.37	121.88	115.17
2	L5	3884	PSU	N1-C2-N3	6.36	121.88	115.17
48	S2	93	PSU	N1-C2-N3	6.36	121.88	115.17
48	S2	863	PSU	N1-C2-N3	6.35	121.86	115.17
2	L5	4532	PSU	N1-C2-N3	6.33	121.85	115.17
48	S2	649	PSU	N1-C2-N3	6.32	121.84	115.17
48	S2	1625	PSU	N1-C2-N3	6.32	121.83	115.17
2	L5	3851	PSU	N1-C2-N3	6.32	121.83	115.17
48	S2	1244	PSU	N1-C2-N3	6.31	121.82	115.17
48	S2	609	PSU	N1-C2-N3	6.30	121.82	115.17
2	L5	4972	PSU	N1-C2-N3	6.30	121.81	115.17
2	L5	1862	PSU	N1-C2-N3	6.29	121.81	115.17
48	S2	1232	PSU	N1-C2-N3	6.29	121.81	115.17
48	S2	686	PSU	N1-C2-N3	6.29	121.80	115.17
2	L5	2632	PSU	N1-C2-N3	6.28	121.80	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3844	PSU	N1-C2-N3	6.28	121.79	115.17
48	S2	1174	PSU	N1-C2-N3	6.28	121.79	115.17
2	L5	3758	PSU	N1-C2-N3	6.27	121.79	115.17
2	L5	4471	PSU	N1-C2-N3	6.27	121.78	115.17
48	S2	109	PSU	N1-C2-N3	6.27	121.78	115.17
2	L5	4628	PSU	N1-C2-N3	6.26	121.78	115.17
2	L5	1744	PSU	N1-C2-N3	6.25	121.76	115.17
2	L5	5010	PSU	N1-C2-N3	6.25	121.76	115.17
48	S2	210	PSU	N1-C2-N3	6.25	121.76	115.17
2	L5	4353	PSU	N1-C2-N3	6.22	121.73	115.17
2	L5	4293	PSU	N1-C2-N3	6.20	121.70	115.17
2	L5	3715	PSU	N1-C2-N3	6.19	121.70	115.17
48	S2	1643	PSU	N1-C2-N3	6.18	121.69	115.17
2	L5	3730	PSU	N1-C2-N3	6.18	121.69	115.17
2	L5	4312	PSU	N1-C2-N3	6.18	121.68	115.17
2	L5	1683	PSU	N1-C2-N3	6.16	121.67	115.17
2	L5	4361	PSU	N1-C2-N3	6.15	121.66	115.17
48	S2	36	PSU	N1-C2-N3	6.13	121.63	115.17
48	S2	1056	PSU	N1-C2-N3	6.13	121.63	115.17
2	L5	4403	PSU	N1-C2-N3	6.11	121.62	115.17
2	L5	4689	PSU	N1-C2-N3	6.11	121.62	115.17
2	L5	4299	PSU	N1-C2-N3	6.10	121.60	115.17
2	L5	4420	PSU	N1-C2-N3	6.10	121.60	115.17
48	S2	218	PSU	N1-C2-N3	6.09	121.59	115.17
2	L5	2508	PSU	N1-C2-N3	6.09	121.59	115.17
48	S2	822	PSU	N1-C2-N3	6.08	121.58	115.17
2	L5	1860	PSU	N1-C2-N3	6.06	121.56	115.17
48	S2	1850	MA6	C2-N1-C6	6.05	122.78	116.84
2	L5	3764	PSU	N1-C2-N3	6.03	121.53	115.17
2	L5	1792	PSU	N1-C2-N3	6.02	121.52	115.17
2	L5	1536	PSU	N1-C2-N3	5.97	121.46	115.17
48	S2	1851	MA6	C2-N1-C6	5.96	122.68	116.84
48	S2	1046	PSU	N1-C2-N3	5.86	121.35	115.17
48	S2	1248	B8N	C5-C4-N3	5.24	125.67	116.15
48	S2	172	OMU	C4-N3-C2	-5.16	120.20	126.61
2	L5	4498	OMU	C4-N3-C2	-5.00	120.41	126.61
48	S2	428	OMU	C4-N3-C2	-4.99	120.42	126.61
48	S2	1326	OMU	C4-N3-C2	-4.94	120.47	126.61
2	L5	4227	OMU	C4-N3-C2	-4.88	120.56	126.61
2	L5	3925	OMU	C4-N3-C2	-4.87	120.56	126.61
2	L5	4552	PSU	O2-C2-N1	-4.84	117.80	122.79
2	L5	2837	OMU	C4-N3-C2	-4.83	120.62	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3818	UY1	N1-C2-N3	4.81	120.24	115.17
2	L5	1773	OMU	C4-N3-C2	-4.77	120.69	126.61
48	S2	1442	OMU	C4-N3-C2	-4.77	120.69	126.61
48	S2	1804	OMU	C4-N3-C2	-4.75	120.72	126.61
2	L5	4872	2MG	CM2-N2-C2	-4.74	113.46	123.65
48	S2	627	OMU	C4-N3-C2	-4.74	120.73	126.61
48	S2	116	OMU	C4-N3-C2	-4.72	120.75	126.61
48	S2	590	A2M	C4'-O4'-C1'	-4.72	105.61	109.92
48	S2	1248	B8N	C4-N3-C2	-4.71	119.82	125.62
2	L5	3818	UY1	C4-N3-C2	-4.67	119.94	126.37
2	L5	4306	OMU	C4-N3-C2	-4.66	120.83	126.61
48	S2	121	OMU	C4-N3-C2	-4.66	120.83	126.61
2	L5	2837	OMU	N3-C2-N1	4.65	120.94	114.89
48	S2	1177	PSU	C4-N3-C2	-4.64	119.99	126.37
48	S2	1288	OMU	C4-N3-C2	-4.62	120.88	126.61
2	L5	4227	OMU	N3-C2-N1	4.61	120.89	114.89
2	L5	729	2MG	CM2-N2-C2	-4.57	113.82	123.65
48	S2	799	OMU	C4-N3-C2	-4.57	120.94	126.61
2	L5	3768	PSU	C4-N3-C2	-4.55	120.10	126.37
48	S2	681	PSU	C4-N3-C2	-4.53	120.13	126.37
2	L5	4498	OMU	N3-C2-N1	4.48	120.72	114.89
2	L5	3637	PSU	C4-N3-C2	-4.47	120.21	126.37
2	L5	3925	OMU	N3-C2-N1	4.47	120.71	114.89
2	L5	4353	PSU	C4-N3-C2	-4.47	120.22	126.37
48	S2	1347	PSU	C4-N3-C2	-4.46	120.22	126.37
2	L5	1517	2MG	CM2-N2-C2	-4.46	114.06	123.65
2	L5	4552	PSU	C4-N3-C2	-4.43	120.27	126.37
2	L5	3695	PSU	C4-N3-C2	-4.42	120.28	126.37
48	S2	651	PSU	C4-N3-C2	-4.42	120.29	126.37
48	S2	406	PSU	C4-N3-C2	-4.41	120.29	126.37
2	L5	1524	A2M	C4'-O4'-C1'	-4.41	105.89	109.92
2	L5	2415	OMU	C4-N3-C2	-4.40	121.15	126.61
48	S2	172	OMU	N3-C2-N1	4.39	120.60	114.89
2	L5	4447	5MC	C5-C6-N1	-4.38	118.55	123.31
48	S2	863	PSU	C4-N3-C2	-4.37	120.35	126.37
2	L5	1744	PSU	C4-N3-C2	-4.37	120.36	126.37
2	L5	4423	PSU	C4-N3-C2	-4.36	120.36	126.37
48	S2	1326	OMU	N3-C2-N1	4.36	120.56	114.89
2	L5	4420	PSU	C4-N3-C2	-4.35	120.38	126.37
2	L5	4403	PSU	C4-N3-C2	-4.35	120.38	126.37
2	L5	4500	PSU	C4-N3-C2	-4.32	120.42	126.37
48	S2	823	PSU	C4-N3-C2	-4.32	120.42	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1862	PSU	C4-N3-C2	-4.31	120.43	126.37
48	S2	1238	PSU	C4-N3-C2	-4.29	120.46	126.37
2	L5	1677	PSU	C4-N3-C2	-4.27	120.48	126.37
2	L5	5001	PSU	C4-N3-C2	-4.25	120.52	126.37
2	L5	1773	OMU	N3-C2-N1	4.24	120.41	114.89
48	S2	627	OMU	N3-C2-N1	4.23	120.40	114.89
48	S2	1442	OMU	N3-C2-N1	4.23	120.40	114.89
2	L5	3884	PSU	C4-N3-C2	-4.22	120.56	126.37
2	L5	4521	PSU	C4-N3-C2	-4.22	120.56	126.37
48	S2	799	OMU	N3-C2-N1	4.22	120.38	114.89
48	S2	1692	PSU	C4-N3-C2	-4.21	120.57	126.37
2	L5	1683	PSU	O2-C2-N1	-4.21	118.45	122.79
2	L5	4576	PSU	C4-N3-C2	-4.21	120.58	126.37
48	S2	801	PSU	C4-N3-C2	-4.21	120.58	126.37
48	S2	649	PSU	C4-N3-C2	-4.19	120.59	126.37
48	S2	815	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	3920	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	4457	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	4431	PSU	C4-N3-C2	-4.19	120.60	126.37
48	S2	1244	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	3758	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	4296	PSU	C4-N3-C2	-4.19	120.60	126.37
48	S2	105	PSU	C4-N3-C2	-4.18	120.61	126.37
2	L5	3768	PSU	O2-C2-N1	-4.18	118.48	122.79
2	L5	2508	PSU	C4-N3-C2	-4.18	120.61	126.37
1	L1	69	PSU	C4-N3-C2	-4.18	120.61	126.37
2	L5	4673	PSU	C4-N3-C2	-4.17	120.62	126.37
2	L5	1782	PSU	C4-N3-C2	-4.16	120.64	126.37
2	L5	3715	PSU	C4-N3-C2	-4.16	120.65	126.37
1	L1	55	PSU	C4-N3-C2	-4.15	120.65	126.37
2	L5	4306	OMU	N3-C2-N1	4.15	120.29	114.89
48	S2	1804	OMU	N3-C2-N1	4.15	120.29	114.89
2	L5	1683	PSU	C4-N3-C2	-4.15	120.66	126.37
48	S2	1045	PSU	C4-N3-C2	-4.14	120.66	126.37
48	S2	1081	PSU	C4-N3-C2	-4.14	120.67	126.37
2	L5	3844	PSU	C4-N3-C2	-4.12	120.69	126.37
2	L5	4689	PSU	C4-N3-C2	-4.12	120.69	126.37
2	L5	3762	PSU	C4-N3-C2	-4.12	120.69	126.37
48	S2	572	PSU	C4-N3-C2	-4.12	120.69	126.37
48	S2	686	PSU	C4-N3-C2	-4.12	120.70	126.37
48	S2	428	OMU	N3-C2-N1	4.11	120.25	114.89
48	S2	866	PSU	C4-N3-C2	-4.11	120.71	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1174	PSU	C4-N3-C2	-4.11	120.71	126.37
2	L5	3730	PSU	C4-N3-C2	-4.11	120.71	126.37
2	L5	4972	PSU	C4-N3-C2	-4.11	120.71	126.37
48	S2	1851	MA6	C10-N6-C6	-4.11	108.08	119.40
48	S2	814	PSU	C4-N3-C2	-4.10	120.72	126.37
48	S2	1004	PSU	C4-N3-C2	-4.10	120.72	126.37
2	L5	3851	PSU	C4-N3-C2	-4.10	120.72	126.37
2	L5	1582	PSU	C4-N3-C2	-4.10	120.72	126.37
48	S2	1445	PSU	C4-N3-C2	-4.09	120.73	126.37
48	S2	1347	PSU	O2-C2-N1	-4.08	118.58	122.79
2	L5	5010	PSU	C4-N3-C2	-4.07	120.76	126.37
48	S2	121	OMU	N3-C2-N1	4.07	120.19	114.89
2	L5	1792	PSU	C4-N3-C2	-4.06	120.77	126.37
2	L5	4442	PSU	C4-N3-C2	-4.06	120.78	126.37
2	L5	4361	PSU	C4-N3-C2	-4.05	120.79	126.37
48	S2	966	PSU	C4-N3-C2	-4.05	120.79	126.37
48	S2	1288	OMU	N3-C2-N1	4.05	120.16	114.89
2	L5	1517	2MG	N1-C2-N2	-4.05	112.43	116.56
48	S2	93	PSU	C4-N3-C2	-4.04	120.80	126.37
48	S2	1643	PSU	C4-N3-C2	-4.04	120.80	126.37
48	S2	918	PSU	C4-N3-C2	-4.04	120.80	126.37
2	L5	3770	PSU	C4-N3-C2	-4.04	120.81	126.37
48	S2	34	PSU	C4-N3-C2	-4.04	120.81	126.37
48	S2	119	PSU	C4-N3-C2	-4.04	120.81	126.37
2	L5	3734	PSU	C4-N3-C2	-4.03	120.81	126.37
2	L5	4579	PSU	C4-N3-C2	-4.03	120.81	126.37
48	S2	1367	PSU	C4-N3-C2	-4.03	120.82	126.37
48	S2	823	PSU	O2-C2-N1	-4.03	118.64	122.79
48	S2	1056	PSU	C4-N3-C2	-4.00	120.86	126.37
48	S2	116	OMU	C5-C4-N3	4.00	120.41	114.80
48	S2	210	PSU	C4-N3-C2	-4.00	120.86	126.37
2	L5	3764	PSU	C4-N3-C2	-3.99	120.87	126.37
2	L5	1536	PSU	C4-N3-C2	-3.98	120.88	126.37
2	L5	4312	PSU	C4-N3-C2	-3.98	120.89	126.37
2	L5	2632	PSU	C4-N3-C2	-3.98	120.89	126.37
2	L5	4293	PSU	C4-N3-C2	-3.97	120.90	126.37
48	S2	1625	PSU	C4-N3-C2	-3.96	120.92	126.37
48	S2	36	PSU	C4-N3-C2	-3.96	120.92	126.37
2	L5	729	2MG	N1-C2-N2	-3.95	112.53	116.56
48	S2	609	PSU	C4-N3-C2	-3.95	120.93	126.37
2	L5	4532	PSU	C4-N3-C2	-3.94	120.94	126.37
48	S2	1232	PSU	C4-N3-C2	-3.94	120.94	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4299	PSU	C4-N3-C2	-3.94	120.94	126.37
48	S2	1804	OMU	C5-C4-N3	3.94	120.32	114.80
2	L5	4498	OMU	C5-C4-N3	3.94	120.32	114.80
2	L5	4628	PSU	C4-N3-C2	-3.94	120.95	126.37
48	S2	1445	PSU	O2-C2-N1	-3.94	118.73	122.79
2	L5	4620	OMU	N3-C2-N1	3.93	120.01	114.89
48	S2	116	OMU	N3-C2-N1	3.93	120.01	114.89
48	S2	1244	PSU	O2-C2-N1	-3.93	118.74	122.79
48	S2	651	PSU	O2-C2-N1	-3.93	118.74	122.79
2	L5	3639	PSU	C4-N3-C2	-3.93	120.96	126.37
48	S2	109	PSU	C4-N3-C2	-3.92	120.97	126.37
2	L5	4521	PSU	O2-C2-N1	-3.92	118.74	122.79
2	L5	4620	OMU	C4-N3-C2	-3.92	121.74	126.61
48	S2	1177	PSU	O2-C2-N1	-3.91	118.75	122.79
2	L5	3853	PSU	C4-N3-C2	-3.90	121.00	126.37
48	S2	121	OMU	C5-C4-N3	3.90	120.26	114.80
48	S2	1248	B8N	C1'-C5-C4	3.89	123.52	117.61
48	S2	822	PSU	C4-N3-C2	-3.89	121.01	126.37
48	S2	1832	6MZ	N3-C2-N1	-3.89	123.40	128.67
2	L5	1744	PSU	O2-C2-N1	-3.88	118.79	122.79
48	S2	172	OMU	C5-C4-N3	3.88	120.23	114.80
2	L5	1781	PSU	C4-N3-C2	-3.87	121.04	126.37
2	L5	1582	PSU	O2-C2-N1	-3.87	118.80	122.79
48	S2	1625	PSU	O2-C2-N1	-3.86	118.81	122.79
48	S2	1046	PSU	C4-N3-C2	-3.86	121.05	126.37
2	L5	4306	OMU	C5-C4-N3	3.86	120.21	114.80
2	L5	4636	PSU	C4-N3-C2	-3.86	121.06	126.37
2	L5	2415	OMU	N3-C2-N1	3.86	119.91	114.89
48	S2	1288	OMU	C5-C4-N3	3.85	120.20	114.80
2	L5	1862	PSU	O2-C2-N1	-3.85	118.82	122.79
2	L5	4220	6MZ	N3-C2-N1	-3.85	123.45	128.67
48	S2	668	A2M	O4'-C1'-N9	-3.84	103.66	108.75
2	L5	3762	PSU	O2-C2-N1	-3.84	118.83	122.79
48	S2	428	OMU	C5-C4-N3	3.84	120.17	114.80
2	L5	4431	PSU	O2-C2-N1	-3.83	118.83	122.79
2	L5	4532	PSU	O2-C2-N1	-3.83	118.84	122.79
48	S2	218	PSU	C4-N3-C2	-3.83	121.09	126.37
2	L5	2415	OMU	C5-C4-N3	3.83	120.16	114.80
2	L5	3925	OMU	C5-C4-N3	3.83	120.16	114.80
48	S2	1326	OMU	C5-C4-N3	3.82	120.15	114.80
2	L5	5001	PSU	O2-C2-N1	-3.82	118.85	122.79
29	La	39	V5N	O-C-CA	-3.81	114.97	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	4471	PSU	C4-N3-C2	-3.81	121.12	126.37
2	L5	1860	PSU	C4-N3-C2	-3.80	121.13	126.37
48	S2	1045	PSU	O2-C2-N1	-3.80	118.87	122.79
48	S2	1442	OMU	C5-C4-N3	3.80	120.12	114.80
48	S2	1850	MA6	N3-C2-N1	-3.79	123.52	128.67
2	L5	1773	OMU	C5-C4-N3	3.79	120.11	114.80
48	S2	1174	PSU	O2-C2-N1	-3.78	118.89	122.79
2	L5	4872	2MG	N1-C2-N2	-3.76	112.72	116.56
48	S2	627	OMU	C5-C4-N3	3.76	120.06	114.80
2	L5	4423	PSU	O2-C2-N1	-3.75	118.92	122.79
48	S2	572	PSU	O2-C2-N1	-3.75	118.92	122.79
48	S2	799	OMU	C5-C4-N3	3.74	120.05	114.80
2	L5	1517	2MG	O6-C6-C5	3.74	131.74	124.32
2	L5	1782	PSU	O2-C2-N1	-3.73	118.94	122.79
48	S2	109	PSU	O2-C2-N1	-3.73	118.94	122.79
48	S2	1081	PSU	O2-C2-N1	-3.73	118.94	122.79
2	L5	4689	PSU	O2-C2-N1	-3.72	118.95	122.79
48	S2	1238	PSU	O2-C2-N1	-3.72	118.95	122.79
2	L5	729	2MG	O6-C6-C5	3.72	131.69	124.32
48	S2	863	PSU	O2-C2-N1	-3.70	118.97	122.79
2	L5	4500	PSU	O2-C2-N1	-3.70	118.97	122.79
2	L5	4227	OMU	C5-C4-N3	3.69	119.97	114.80
48	S2	1248	B8N	N3-C2-N1	3.68	121.21	116.72
1	L1	55	PSU	O2-C2-N1	-3.68	119.00	122.79
2	L5	4636	PSU	O2-C2-N1	-3.67	119.00	122.79
2	L5	1792	PSU	O2-C2-N1	-3.67	119.00	122.79
2	L5	4628	PSU	O2-C2-N1	-3.66	119.01	122.79
48	S2	119	PSU	O2-C2-N1	-3.66	119.02	122.79
2	L5	3853	PSU	O2-C2-N1	-3.65	119.02	122.79
48	S2	866	PSU	O2-C2-N1	-3.65	119.03	122.79
2	L5	4576	PSU	O2-C2-N1	-3.65	119.03	122.79
48	S2	918	PSU	O2-C2-N1	-3.63	119.05	122.79
2	L5	3695	PSU	O2-C2-N1	-3.62	119.05	122.79
63	SO	138	IAS	OD1-CG-CB	-3.61	114.88	125.38
2	L5	3734	PSU	O2-C2-N1	-3.61	119.07	122.79
2	L5	4420	PSU	O2-C2-N1	-3.60	119.07	122.79
48	S2	1232	PSU	O2-C2-N1	-3.60	119.08	122.79
2	L5	4872	2MG	O6-C6-C5	3.59	131.43	124.32
48	S2	686	PSU	O2-C2-N1	-3.59	119.09	122.79
2	L5	4312	PSU	O2-C2-N1	-3.58	119.10	122.79
2	L5	2508	PSU	O2-C2-N1	-3.57	119.11	122.79
2	L5	3637	PSU	O2-C2-N1	-3.55	119.12	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4293	PSU	O2-C2-N1	-3.55	119.12	122.79
48	S2	406	PSU	O2-C2-N1	-3.54	119.14	122.79
48	S2	1004	PSU	O2-C2-N1	-3.53	119.15	122.79
48	S2	1851	MA6	N3-C2-N1	-3.53	123.88	128.67
2	L5	2632	PSU	O2-C2-N1	-3.52	119.16	122.79
2	L5	3730	PSU	O2-C2-N1	-3.52	119.16	122.79
2	L5	4296	PSU	O2-C2-N1	-3.51	119.16	122.79
2	L5	3764	PSU	O2-C2-N1	-3.51	119.17	122.79
2	L5	5010	PSU	O2-C2-N1	-3.51	119.17	122.79
1	L1	69	PSU	O2-C2-N1	-3.51	119.17	122.79
48	S2	1643	PSU	O2-C2-N1	-3.50	119.18	122.79
2	L5	4579	PSU	O2-C2-N1	-3.50	119.18	122.79
2	L5	3770	PSU	O2-C2-N1	-3.49	119.19	122.79
48	S2	649	PSU	O2-C2-N1	-3.49	119.19	122.79
48	S2	815	PSU	O2-C2-N1	-3.48	119.20	122.79
48	S2	116	OMU	O4-C4-C5	-3.48	119.16	125.16
48	S2	814	PSU	O2-C2-N1	-3.47	119.21	122.79
2	L5	4442	PSU	O2-C2-N1	-3.47	119.22	122.79
48	S2	1692	PSU	O2-C2-N1	-3.46	119.22	122.79
2	L5	3844	PSU	O2-C2-N1	-3.45	119.23	122.79
2	L5	1677	PSU	O2-C2-N1	-3.45	119.23	122.79
2	L5	4530	UR3	C5-C4-N3	3.45	119.58	115.04
48	S2	1851	MA6	C4-C5-N7	-3.44	105.70	109.34
2	L5	2837	OMU	C5-C4-N3	3.44	119.62	114.80
48	S2	1850	MA6	C10-N6-C6	-3.44	109.91	119.40
48	S2	34	PSU	O2-C2-N1	-3.44	119.25	122.79
2	L5	4403	PSU	O2-C2-N1	-3.43	119.25	122.79
48	S2	218	PSU	O2-C2-N1	-3.43	119.25	122.79
2	L5	4457	PSU	O2-C2-N1	-3.42	119.26	122.79
2	L5	4620	OMU	C5-C4-N3	3.40	119.57	114.80
48	S2	822	PSU	O2-C2-N1	-3.40	119.28	122.79
48	S2	105	PSU	O2-C2-N1	-3.37	119.32	122.79
2	L5	3715	PSU	O2-C2-N1	-3.36	119.33	122.79
2	L5	4673	PSU	O2-C2-N1	-3.36	119.33	122.79
2	L5	3899	OMG	C8-N7-C5	3.35	108.25	102.55
2	L5	3758	PSU	O2-C2-N1	-3.34	119.34	122.79
48	S2	1367	PSU	O2-C2-N1	-3.34	119.35	122.79
48	S2	609	PSU	O2-C2-N1	-3.31	119.37	122.79
48	S2	428	OMU	O4-C4-C5	-3.29	119.48	125.16
2	L5	1536	PSU	O2-C2-N1	-3.29	119.39	122.79
2	L5	4498	OMU	O4-C4-C5	-3.28	119.50	125.16
48	S2	1056	PSU	O2-C2-N1	-3.28	119.40	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	4972	PSU	O2-C2-N1	-3.28	119.41	122.79
48	S2	93	PSU	O2-C2-N1	-3.27	119.41	122.79
8	LD	216	V5N	O-C-CA	-3.26	116.38	124.77
2	L5	4523	A2M	C4’-O4’-C1’	-3.24	106.96	109.92
48	S2	36	PSU	O2-C2-N1	-3.23	119.45	122.79
48	S2	966	PSU	O2-C2-N1	-3.18	119.51	122.79
48	S2	1383	A2M	C4’-O4’-C1’	-3.18	107.01	109.92
29	La	39	V5N	O2-CB-CA	3.18	114.48	107.49
2	L5	1522	OMG	C8-N7-C5	3.16	107.93	102.55
48	S2	121	OMU	O4-C4-C5	-3.16	119.72	125.16
48	S2	210	PSU	O2-C2-N1	-3.15	119.54	122.79
48	S2	1850	MA6	C4-C5-N7	-3.14	106.02	109.34
2	L5	4361	PSU	O2-C2-N1	-3.14	119.55	122.79
2	L5	1781	PSU	O2-C2-N1	-3.13	119.56	122.79
48	S2	683	OMG	C8-N7-C5	3.13	107.88	102.55
2	L5	4228	OMG	C8-N7-C5	3.13	107.87	102.55
2	L5	3884	PSU	O2-C2-N1	-3.12	119.57	122.79
48	S2	681	PSU	O2-C2-N1	-3.12	119.57	122.79
48	S2	1442	OMU	O4-C4-C5	-3.12	119.78	125.16
48	S2	1046	PSU	O2-C2-N1	-3.10	119.60	122.79
48	S2	1804	OMU	O4-C4-C5	-3.09	119.83	125.16
2	L5	1860	PSU	O2-C2-N1	-3.09	119.60	122.79
2	L5	4353	PSU	O2-C2-N1	-3.08	119.61	122.79
2	L5	3639	PSU	O2-C2-N1	-3.08	119.62	122.79
2	L5	4623	OMG	C8-N7-C5	3.06	107.77	102.55
2	L5	4498	OMU	O2-C2-N1	-3.06	118.81	122.80
2	L5	2050	OMG	C8-N7-C5	3.03	107.71	102.55
2	L5	3782	5MC	C5-C6-N1	-3.02	120.03	123.31
48	S2	1288	OMU	O4-C4-C5	-3.02	119.95	125.16
48	S2	801	PSU	O2-C2-N1	-3.02	119.67	122.79
2	L5	1322	1MA	N1-C6-N6	3.02	127.29	119.71
2	L5	4392	OMG	C8-N7-C5	3.02	107.68	102.55
2	L5	4618	OMG	C8-N7-C5	3.00	107.66	102.55
2	L5	4499	OMG	C8-N7-C5	2.99	107.65	102.55
2	L5	4299	PSU	O2-C2-N1	-2.99	119.70	122.79
48	S2	1326	OMU	O4-C4-C5	-2.99	120.00	125.16
1	L1	75	OMG	C8-N7-C5	2.98	107.62	102.55
2	L5	4471	PSU	O2-C2-N1	-2.97	119.73	122.79
2	L5	4196	OMG	C8-N7-C5	2.96	107.58	102.55
48	S2	644	OMG	C8-N7-C5	2.94	107.56	102.55
48	S2	172	OMU	O4-C4-C5	-2.94	120.09	125.16
2	L5	2415	OMU	O4-C4-C5	-2.94	120.09	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1773	OMU	O4-C4-C5	-2.94	120.10	125.16
2	L5	2837	OMU	O4-C4-C5	-2.93	120.12	125.16
2	L5	4370	OMG	C8-N7-C5	2.92	107.51	102.55
2	L5	2364	OMG	C8-N7-C5	2.90	107.50	102.55
2	L5	1625	OMG	C8-N7-C5	2.89	107.47	102.55
48	S2	1328	OMG	C8-N7-C5	2.88	107.45	102.55
2	L5	3792	OMG	C8-N7-C5	2.88	107.45	102.55
48	S2	1248	B8N	C31-N3-C4	2.88	121.25	117.18
2	L5	4306	OMU	O4-C4-C5	-2.88	120.20	125.16
2	L5	1534	A2M	C3'-C2'-C1'	-2.87	97.31	102.81
8	LD	216	V5N	O2-CB-CA	2.87	113.79	107.49
48	S2	436	OMG	C8-N7-C5	2.87	107.43	102.55
48	S2	601	OMG	C8-N7-C5	2.86	107.42	102.55
48	S2	1288	OMU	O3'-C3'-C2'	2.86	119.18	111.19
48	S2	627	OMU	O4-C4-C5	-2.85	120.24	125.16
2	L5	1760	OMG	C8-N7-C5	2.83	107.36	102.55
48	S2	799	OMU	O4-C4-C5	-2.83	120.29	125.16
2	L5	3925	OMU	O4-C4-C5	-2.82	120.30	125.16
2	L5	4637	OMG	C8-N7-C5	2.81	107.34	102.55
2	L5	4220	6MZ	C4-C5-N7	-2.81	106.36	109.34
48	S2	509	OMG	C8-N7-C5	2.79	107.30	102.55
48	S2	867	OMG	C8-N7-C5	2.79	107.29	102.55
2	L5	1322	1MA	CM1-N1-C6	-2.78	115.84	120.15
48	S2	172	OMU	O2-C2-N1	-2.77	119.19	122.80
2	L5	3744	OMG	C8-N7-C5	2.77	107.26	102.55
2	L5	3851	PSU	O2-C2-N1	-2.76	119.94	122.79
2	L5	3782	5MC	C5-C4-N3	-2.74	118.94	121.75
2	L5	4870	OMG	C8-N7-C5	2.73	107.20	102.55
2	L5	4523	A2M	C3'-C2'-C1'	-2.72	97.60	102.81
2	L5	3785	A2M	O4'-C1'-N9	2.71	112.34	108.75
2	L5	1322	1MA	C5-C6-N1	-2.70	110.07	113.95
2	L5	3944	OMG	C8-N7-C5	2.70	107.15	102.55
2	L5	3920	PSU	O2-C2-N1	-2.70	120.00	122.79
2	L5	4227	OMU	O4-C4-C5	-2.69	120.52	125.16
2	L5	2876	OMG	C8-N7-C5	2.69	107.13	102.55
2	L5	1316	OMG	C8-N7-C5	2.68	107.11	102.55
2	L5	4494	OMG	C8-N7-C5	2.68	107.11	102.55
48	S2	1490	OMG	C8-N7-C5	2.67	107.09	102.55
48	S2	1710	OMC	O2-C2-N3	-2.66	118.14	122.33
2	L5	3718	A2M	N3-C2-N1	2.65	132.27	128.67
48	S2	1337	4AC	C6-C5-C4	2.61	120.15	117.00
2	L5	3925	OMU	O2-C2-N1	-2.61	119.40	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	1536	PSU	C6-C5-C4	-2.61	116.41	118.17
48	S2	468	A2M	C4'-O4'-C1'	-2.60	107.54	109.92
2	L5	2424	OMG	C8-N7-C5	2.59	106.97	102.55
48	S2	918	PSU	O4'-C1'-C2'	2.57	108.70	105.15
48	S2	406	PSU	C5-C6-N1	-2.57	118.58	122.14
2	L5	3637	PSU	C5-C6-N1	-2.55	118.60	122.14
48	S2	116	OMU	O2-C2-N1	-2.55	119.48	122.80
48	S2	1832	6MZ	C4-C5-N7	-2.55	106.64	109.34
2	L5	3818	UY1	C6-N1-C2	-2.54	120.33	122.69
48	S2	1248	B8N	O4-C4-C5	-2.54	118.19	122.58
2	L5	2837	OMU	O2-C2-N1	-2.52	119.51	122.80
48	S2	1851	MA6	C10-N6-C9	-2.52	108.08	116.18
2	L5	1677	PSU	C5-C6-N1	-2.52	118.64	122.14
2	L5	4420	PSU	C5-C6-N1	-2.52	118.64	122.14
48	S2	668	A2M	C4'-O4'-C1'	-2.51	107.62	109.92
2	L5	4447	5MC	C5-C4-N3	-2.51	119.19	121.75
48	S2	428	OMU	O2-C2-N1	-2.50	119.54	122.80
48	S2	1383	A2M	C3'-C2'-C1'	-2.50	98.03	102.81
2	L5	4227	OMU	O2-C2-N1	-2.48	119.56	122.80
2	L5	4353	PSU	C5-C6-N1	-2.45	118.74	122.14
2	L5	1534	A2M	O4'-C1'-N9	-2.45	105.50	108.75
48	S2	681	PSU	C5-C6-N1	-2.44	118.75	122.14
48	S2	799	OMU	C1'-N1-C2	2.41	121.92	117.59
2	L5	3758	PSU	C5-C6-N1	-2.41	118.80	122.14
48	S2	1238	PSU	C5-C6-N1	-2.41	118.80	122.14
2	L5	3695	PSU	C5-C6-N1	-2.40	118.81	122.14
1	L1	69	PSU	O4'-C1'-C2'	2.40	108.47	105.15
2	L5	3920	PSU	O2-C2-N3	-2.39	117.61	121.86
2	L5	1517	2MG	O6-C6-N1	-2.39	117.79	120.62
48	S2	1248	B8N	O4-C4-N3	-2.38	116.12	119.99
48	S2	1639	7MG	C5-C4-N9	2.38	109.38	106.33
2	L5	4370	OMG	C5-C6-N1	2.38	118.61	114.07
2	L5	4637	OMG	C5-C6-N1	2.37	118.60	114.07
48	S2	1639	7MG	C4-C5-N7	2.37	108.18	105.38
1	L1	69	PSU	C5-C6-N1	-2.37	118.85	122.14
2	L5	4620	OMU	O2-C2-N1	-2.37	119.71	122.80
2	L5	2364	OMG	C5-C6-N1	2.36	118.58	114.07
48	S2	801	PSU	C5-C6-N1	-2.36	118.86	122.14
48	S2	627	OMU	O2-C2-N1	-2.36	119.72	122.80
2	L5	4296	PSU	C5-C6-N1	-2.35	118.88	122.14
48	S2	1177	PSU	C5-C6-N1	-2.35	118.89	122.14
48	S2	1326	OMU	O2-C2-N1	-2.34	119.75	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	4620	OMU	O4-C4-C5	-2.33	121.14	125.16
2	L5	2415	OMU	C1'-N1-C2	2.33	121.77	117.59
48	S2	815	PSU	C5-C6-N1	-2.30	118.94	122.14
6	S4	9	1MG	N2-C2-N1	-2.30	116.94	118.79
2	L5	4442	PSU	O4'-C1'-C2'	2.30	108.33	105.15
2	L5	4499	OMG	C5-C6-N1	2.30	118.45	114.07
48	S2	1347	PSU	C5-C6-N1	-2.29	118.96	122.14
2	L5	4500	PSU	C5-C6-N1	-2.29	118.96	122.14
2	L5	729	2MG	O6-C6-N1	-2.29	117.90	120.62
2	L5	3768	PSU	C5-C6-N1	-2.28	118.97	122.14
48	S2	1337	4AC	C5-C4-N3	-2.28	119.03	122.60
48	S2	651	PSU	C5-C6-N1	-2.28	118.98	122.14
2	L5	2363	A2M	N3-C2-N1	2.27	131.76	128.67
2	L5	4196	OMG	C5-C6-N1	2.26	118.38	114.07
2	L5	1871	A2M	C4'-O4'-C1'	-2.25	107.86	109.92
2	L5	3920	PSU	C5-C6-N1	-2.25	119.01	122.14
2	L5	3818	UY1	O2-C2-N1	-2.25	120.47	122.79
48	S2	1383	A2M	C2'-C3'-C4'	-2.24	97.17	101.99
2	L5	2876	OMG	C5-C6-N1	2.24	118.34	114.07
48	S2	822	PSU	O4'-C1'-C2'	2.24	108.25	105.15
48	S2	1056	PSU	C5-C6-N1	-2.24	119.04	122.14
6	S4	37	1MG	N2-C2-N1	-2.23	116.99	118.79
2	L5	3639	PSU	C5-C6-N1	-2.23	119.05	122.14
48	S2	27	A2M	C4'-O4'-C1'	-2.23	107.89	109.92
2	L5	3770	PSU	C5-C6-N1	-2.22	119.05	122.14
2	L5	3701	OMC	O2-C2-N3	-2.21	118.84	122.33
2	L5	4872	2MG	O6-C6-N1	-2.21	118.00	120.62
2	L5	4403	PSU	C5-C6-N1	-2.21	119.08	122.14
48	S2	1678	A2M	C4'-O4'-C1'	-2.20	107.91	109.92
1	L1	55	PSU	C5-C6-N1	-2.20	119.09	122.14
48	S2	686	PSU	C5-C6-N1	-2.19	119.10	122.14
48	S2	166	A2M	C4'-O4'-C1'	-2.19	107.92	109.92
2	L5	3884	PSU	C5-C6-N1	-2.19	119.10	122.14
2	L5	1773	OMU	O2'-C2'-C1'	2.19	113.14	108.99
48	S2	159	A2M	C3'-C2'-C1'	-2.18	98.63	102.81
48	S2	1045	PSU	C5-C6-N1	-2.18	119.12	122.14
2	L5	4628	PSU	O4'-C1'-C2'	2.17	108.15	105.15
2	L5	3715	PSU	C5-C6-N1	-2.17	119.13	122.14
48	S2	1850	MA6	N1-C6-N6	2.17	119.33	116.83
2	L5	3851	PSU	C5-C6-N1	-2.17	119.13	122.14
2	L5	4228	OMG	C5-C6-N1	2.17	118.20	114.07
48	S2	867	OMG	C5-C6-N1	2.16	118.19	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4494	OMG	C5-C6-N1	2.16	118.19	114.07
48	S2	1248	B8N	O4'-C1'-C2'	2.16	108.13	105.15
48	S2	823	PSU	C5-C6-N1	-2.15	119.15	122.14
2	L5	3920	PSU	O4'-C1'-C2'	2.15	108.12	105.15
48	S2	966	PSU	C5-C6-N1	-2.14	119.17	122.14
71	SX	62	HY3	O-C-CA	-2.14	119.21	124.86
2	L5	3830	A2M	N3-C2-N1	2.14	131.57	128.67
48	S2	1842	4AC	C5-C4-N3	-2.14	119.26	122.60
2	L5	3639	PSU	O4'-C1'-C2'	2.13	108.10	105.15
48	S2	1643	PSU	O4'-C1'-C2'	2.13	108.10	105.15
2	L5	4636	PSU	O4'-C1'-C2'	2.13	108.10	105.15
2	L5	1744	PSU	C5-C6-N1	-2.13	119.19	122.14
2	L5	4623	OMG	C5-C6-N1	2.13	118.13	114.07
2	L5	2351	OMC	O2-C2-N3	-2.13	118.98	122.33
48	S2	36	PSU	C5-C6-N1	-2.12	119.20	122.14
2	L5	4972	PSU	C5-C6-N1	-2.12	119.20	122.14
2	L5	4571	A2M	O4'-C1'-N9	-2.12	105.94	108.75
48	S2	210	PSU	C5-C6-N1	-2.12	119.20	122.14
48	S2	1337	4AC	N4-C4-N3	2.12	117.30	113.87
48	S2	1081	PSU	C5-C6-N1	-2.11	119.21	122.14
48	S2	1031	A2M	C4'-O4'-C1'	-2.11	107.99	109.92
48	S2	576	A2M	N3-C2-N1	2.11	131.54	128.67
2	L5	4456	OMC	O2-C2-N3	-2.11	119.00	122.33
2	L5	1340	OMC	O2-C2-N3	-2.11	119.00	122.33
48	S2	218	PSU	O4'-C1'-C2'	2.11	108.07	105.15
2	L5	398	A2M	N3-C2-N1	2.11	131.54	128.67
48	S2	436	OMG	C5-C6-N1	2.10	118.08	114.07
48	S2	683	OMG	C5-C6-N1	2.10	118.07	114.07
48	S2	1367	PSU	C5-C6-N1	-2.10	119.23	122.14
48	S2	1081	PSU	O4'-C1'-C2'	2.10	108.05	105.15
2	L5	4471	PSU	C5-C6-N1	-2.09	119.23	122.14
2	L5	4618	OMG	C5-C6-N1	2.09	118.06	114.07
48	S2	121	OMU	O2-C2-N1	-2.09	120.08	122.80
48	S2	1004	PSU	C5-C6-N1	-2.09	119.24	122.14
2	L5	2876	OMG	O6-C6-C5	-2.09	120.18	124.32
48	S2	509	OMG	C5-C6-N1	2.09	118.05	114.07
2	L5	3744	OMG	C5-C6-N1	2.08	118.05	114.07
2	L5	4689	PSU	C5-C6-N1	-2.08	119.25	122.14
2	L5	1881	OMC	O2-C2-N3	-2.08	119.05	122.33
2	L5	3762	PSU	C5-C6-N1	-2.08	119.25	122.14
48	S2	863	PSU	C5-C6-N1	-2.08	119.25	122.14
48	S2	601	OMG	C5-C6-N1	2.08	118.03	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2508	PSU	C5-C6-N1	-2.07	119.26	122.14
2	L5	3867	A2M	N3-C2-N1	2.07	131.49	128.67
2	L5	1760	OMG	C5-C6-N1	2.07	118.02	114.07
2	L5	3730	PSU	C5-C6-N1	-2.07	119.27	122.14
2	L5	3639	PSU	O2-C2-N3	-2.07	118.19	121.86
48	S2	801	PSU	O2-C2-N3	-2.07	118.19	121.86
2	L5	1456	JMH	C6-N1-C2	-2.06	120.11	121.80
48	S2	468	A2M	N3-C2-N1	2.06	131.47	128.67
48	S2	1851	MA6	C9-N6-C6	-2.06	113.72	119.40
2	L5	4299	PSU	C5-C6-N1	-2.06	119.28	122.14
2	L5	1625	OMG	C5-C6-N1	2.06	118.00	114.07
48	S2	572	PSU	C5-C6-N1	-2.06	119.28	122.14
48	S2	1692	PSU	C5-C6-N1	-2.06	119.28	122.14
48	S2	814	PSU	C5-C6-N1	-2.06	119.28	122.14
2	L5	4673	PSU	C5-C6-N1	-2.06	119.29	122.14
2	L5	1683	PSU	C5-C6-N1	-2.05	119.29	122.14
2	L5	4457	PSU	O4'-C1'-C2'	2.05	107.99	105.15
48	S2	823	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L5	1522	OMG	C5-C6-N1	2.05	117.98	114.07
2	L5	4523	A2M	N3-C2-N1	2.05	131.46	128.67
2	L5	3851	PSU	O2-C2-N3	-2.05	118.22	121.86
48	S2	34	PSU	C5-C6-N1	-2.05	119.30	122.14
2	L5	2424	OMG	C5-C6-N1	2.05	117.97	114.07
48	S2	644	OMG	C5-C6-N1	2.05	117.97	114.07
2	L5	3695	PSU	O4'-C1'-C2'	2.04	107.98	105.15
48	S2	1328	OMG	C5-C6-N1	2.04	117.96	114.07
48	S2	1445	PSU	O4'-C1'-C2'	2.04	107.97	105.15
48	S2	1850	MA6	C10-N6-C9	-2.04	109.64	116.18
2	L5	4431	PSU	C5-C6-N1	-2.04	119.31	122.14
48	S2	918	PSU	C5-C6-N1	-2.03	119.32	122.14
48	S2	159	A2M	N3-C2-N1	2.03	131.43	128.67
2	L5	4500	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	L1	75	OMG	C5-C6-N1	2.03	117.94	114.07
2	L5	4423	PSU	C5-C6-N1	-2.02	119.33	122.14
2	L5	3825	A2M	C3'-C2'-C1'	-2.02	98.93	102.81
2	L5	2364	OMG	O6-C6-C5	-2.02	120.32	124.32
2	L5	1862	PSU	C5-C6-N1	-2.02	119.34	122.14
48	S2	1046	PSU	O4'-C1'-C2'	2.02	107.94	105.15
2	L5	1860	PSU	C5-C6-N1	-2.01	119.34	122.14
2	L5	3718	A2M	C4'-O4'-C1'	-2.01	108.08	109.92
48	S2	1288	OMU	O2-C2-N1	-2.01	120.18	122.80
2	L5	4521	PSU	O4'-C1'-C2'	2.00	107.92	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	4637	OMG	O6-C6-C5	-2.00	120.35	124.32
6	S4	18	OMG	O6-C6-C5	2.00	128.29	124.32
2	L5	2787	A2M	O4'-C1'-N9	-2.00	106.09	108.75
2	L5	3818	UY1	O4'-C1'-C2'	2.00	108.06	104.56

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L5	3701	OMC	C2'-C1'-N1-C6
2	L5	3760	A2M	C1'-C2'-O2'-CM'
2	L5	4590	A2M	C4'-C5'-O5'-P
6	S4	18	OMG	C1'-C2'-O2'-CM2
6	S4	47	H2U	O4'-C4'-C5'-O5'
6	S4	47	H2U	C3'-C4'-C5'-O5'
48	S2	1248	B8N	O4'-C4'-C5'-O5'
48	S2	1383	A2M	C1'-C2'-O2'-CM'
48	S2	1678	A2M	C1'-C2'-O2'-CM'
48	S2	1832	6MZ	C5-C6-N6-C9
48	S2	1832	6MZ	N1-C6-N6-C9
48	S2	1851	MA6	C5-C6-N6-C10
2	L5	4636	PSU	C3'-C4'-C5'-O5'
2	L5	4870	OMG	O4'-C4'-C5'-O5'
6	S4	16	H2U	O4'-C4'-C5'-O5'
48	S2	576	A2M	C3'-C4'-C5'-O5'
2	L5	3701	OMC	C2'-C1'-N1-C2
2	L5	3760	A2M	O4'-C4'-C5'-O5'
2	L5	4500	PSU	O4'-C4'-C5'-O5'
2	L5	4636	PSU	O4'-C4'-C5'-O5'
2	L5	4870	OMG	C3'-C4'-C5'-O5'
48	S2	512	A2M	O4'-C4'-C5'-O5'
48	S2	576	A2M	O4'-C4'-C5'-O5'
48	S2	1639	7MG	C3'-C4'-C5'-O5'
48	S2	1851	MA6	N1-C6-N6-C10
2	L5	3760	A2M	C3'-C4'-C5'-O5'
2	L5	4500	PSU	C3'-C4'-C5'-O5'
48	S2	1248	B8N	C3'-C4'-C5'-O5'
2	L5	3851	PSU	C3'-C4'-C5'-O5'
6	S4	16	H2U	C3'-C4'-C5'-O5'
48	S2	668	A2M	O4'-C4'-C5'-O5'
48	S2	1639	7MG	O4'-C4'-C5'-O5'
48	S2	1248	B8N	N34-C33-C34-O36

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Mol	Chain	Res	Type	Atoms
48	S2	627	OMU	O4'-C4'-C5'-O5'
48	S2	668	A2M	C3'-C4'-C5'-O5'
2	L5	4447	5MC	C2'-C1'-N1-C6
6	S4	18	OMG	O4'-C4'-C5'-O5'
6	S4	20	H2U	O4'-C4'-C5'-O5'
33	Le	53	MLZ	CE-CD-CG-CB
48	S2	627	OMU	C3'-C4'-C5'-O5'
2	L5	1534	A2M	C4'-C5'-O5'-P
6	S4	58	1MA	O4'-C4'-C5'-O5'
48	S2	428	OMU	C2'-C1'-N1-C6
48	S2	1248	B8N	N34-C33-C34-O35
6	S4	20	H2U	C3'-C4'-C5'-O5'
48	S2	512	A2M	C3'-C4'-C5'-O5'
2	L5	3851	PSU	O4'-C4'-C5'-O5'
48	S2	590	A2M	C3'-C4'-C5'-O5'
2	L5	3818	UY1	C4'-C5'-O5'-P
2	L5	2364	OMG	O4'-C4'-C5'-O5'
30	Lb	5	MLZ	C-CA-CB-CG
2	L5	4447	5MC	O4'-C1'-N1-C6
30	Lb	5	MLZ	N-CA-CB-CG
63	SO	138	IAS	CA-CB-CG-OD1
2	L5	1326	A2M	C4'-C5'-O5'-P
48	S2	590	A2M	O4'-C4'-C5'-O5'
48	S2	799	OMU	C3'-C4'-C5'-O5'
48	S2	428	OMU	O4'-C1'-N1-C6
2	L5	3869	OMC	C3'-C2'-O2'-CM2
2	L5	4500	PSU	C4'-C5'-O5'-P
48	S2	644	OMG	C4'-C5'-O5'-P
2	L5	3701	OMC	O4'-C1'-N1-C2
2	L5	3701	OMC	O4'-C1'-N1-C6
6	S4	9	1MG	C4'-C5'-O5'-P
2	L5	3785	A2M	O4'-C4'-C5'-O5'
2	L5	4447	5MC	O4'-C1'-N1-C2
2	L5	4870	OMG	C4'-C5'-O5'-P
48	S2	1490	OMG	C4'-C5'-O5'-P
2	L5	4447	5MC	C2'-C1'-N1-C2
2	L5	2401	A2M	C3'-C2'-O2'-CM'
2	L5	3944	OMG	C3'-C2'-O2'-CM2
2	L5	4499	OMG	C3'-C2'-O2'-CM2
48	S2	1851	MA6	C4'-C5'-O5'-P
6	S4	58	1MA	C3'-C4'-C5'-O5'
48	S2	683	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L5	1326	A2M	C3'-C4'-C5'-O5'
2	L5	2401	A2M	C3'-C4'-C5'-O5'
48	S2	174	OMC	C3'-C2'-O2'-CM2
48	S2	428	OMU	O4'-C1'-N1-C2
48	S2	1081	PSU	C4'-C5'-O5'-P
2	L5	1524	A2M	C3'-C4'-C5'-O5'
2	L5	3944	OMG	C3'-C4'-C5'-O5'
48	S2	99	A2M	O4'-C4'-C5'-O5'
33	Le	53	MLZ	CG-CD-CE-NZ
2	L5	2351	OMC	O4'-C4'-C5'-O5'
2	L5	3867	A2M	C3'-C4'-C5'-O5'
2	L5	3844	PSU	C4'-C5'-O5'-P
6	S4	16	H2U	C4'-C5'-O5'-P
2	L5	1625	OMG	C3'-C2'-O2'-CM2
2	L5	2363	A2M	C3'-C2'-O2'-CM'
8	LD	216	V5N	O-C-CA-CB
2	L5	3760	A2M	C4'-C5'-O5'-P
2	L5	2351	OMC	C2'-C1'-N1-C2
48	S2	428	OMU	C2'-C1'-N1-C2
2	L5	2787	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 429 ligands modelled in this entry, 428 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	B3P	L5	5129	-	18,18,18	0.72	0	23,23,23	0.97	1 (4%)

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
86	B3P	L5	5129	-	-	9/28/28/28	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	L5	5129	B3P	C11-C8-C10	-2.51	104.51	110.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

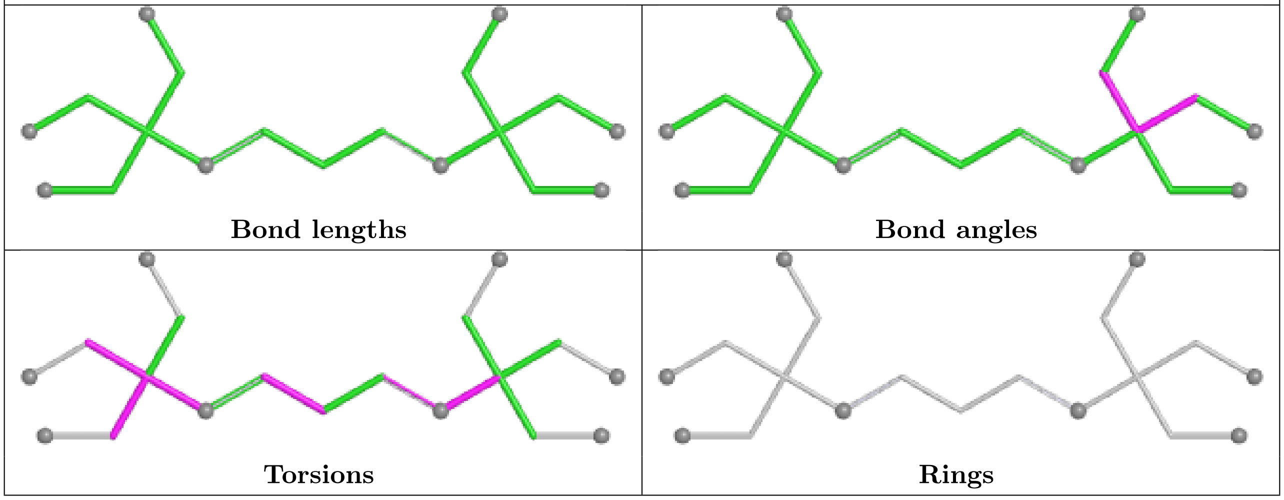
Mol	Chain	Res	Type	Atoms
86	L5	5129	B3P	N1-C4-C7-O6
86	L5	5129	B3P	C1-C2-N2-C8
86	L5	5129	B3P	C5-C4-N1-C3
86	L5	5129	B3P	C7-C4-N1-C3
86	L5	5129	B3P	C10-C8-N2-C2
86	L5	5129	B3P	C11-C8-N2-C2
86	L5	5129	B3P	C2-C1-C3-N1
86	L5	5129	B3P	C6-C4-C7-O6
86	L5	5129	B3P	N1-C4-C6-O5

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand B3P L5 5129



Bond lengths

Bond angles

Torsions

Rings

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.

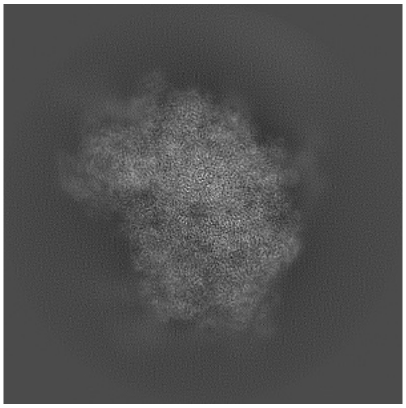
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45170. These allow visual inspection of the internal detail of the map and identification of artifacts.

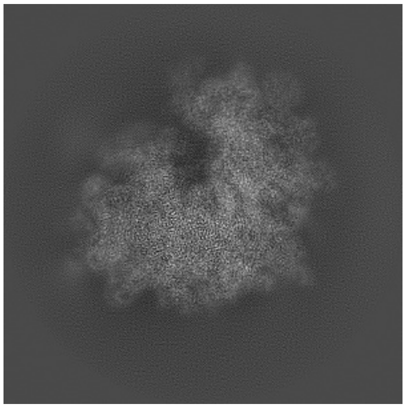
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

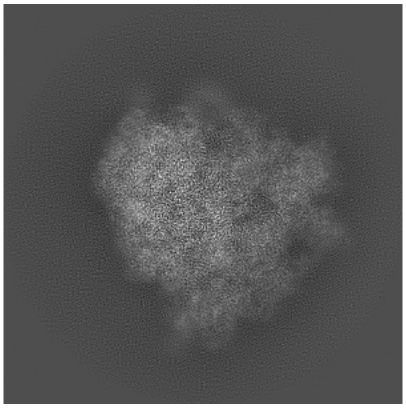
6.1.1 Primary map



X

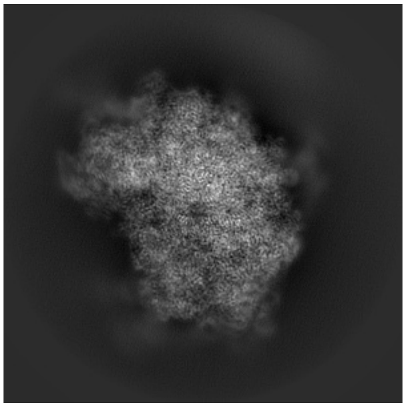


Y

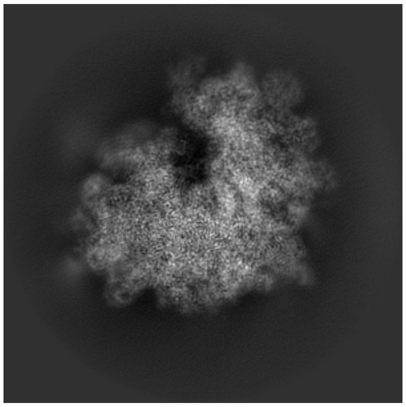


Z

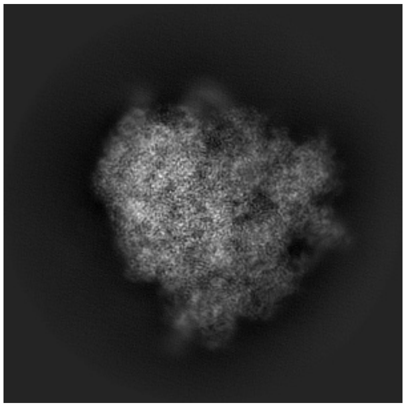
6.1.2 Raw map



X



Y

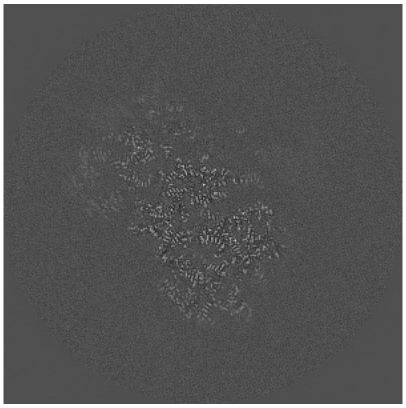


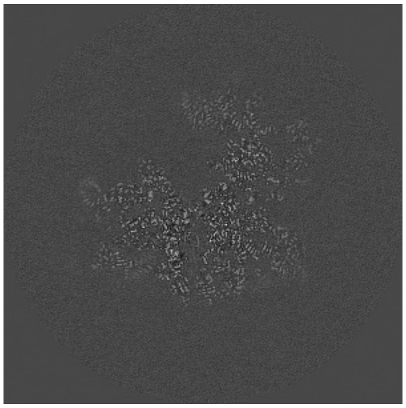
Z

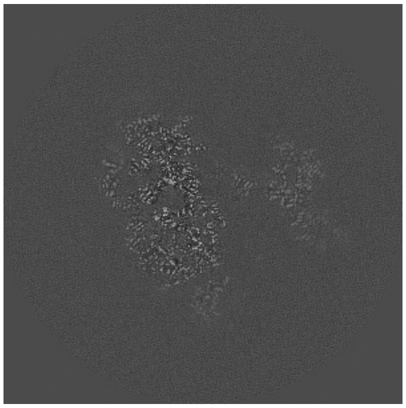
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

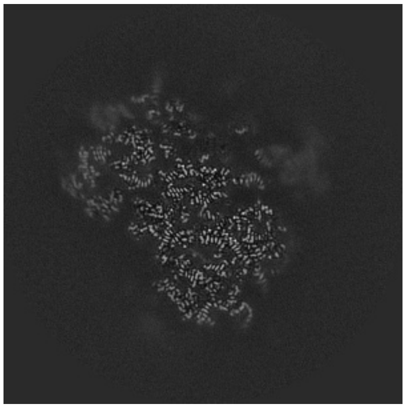
6.2.1 Primary map

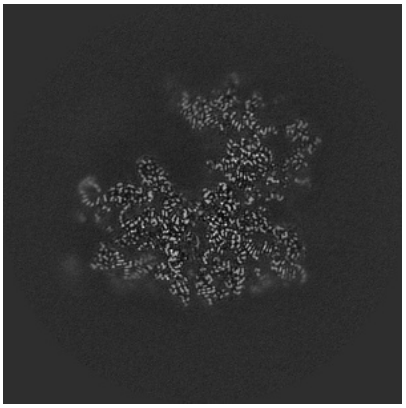

X Index: 224

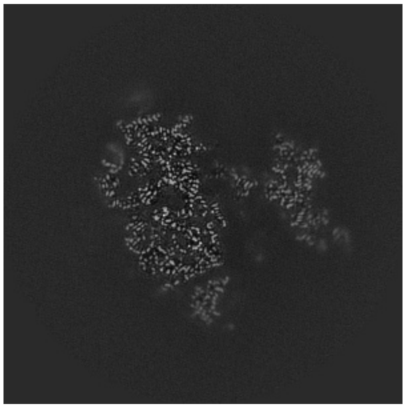

Y Index: 224


Z Index: 224

6.2.2 Raw map


X Index: 224

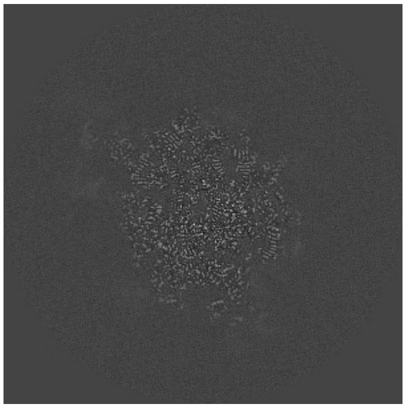

Y Index: 224

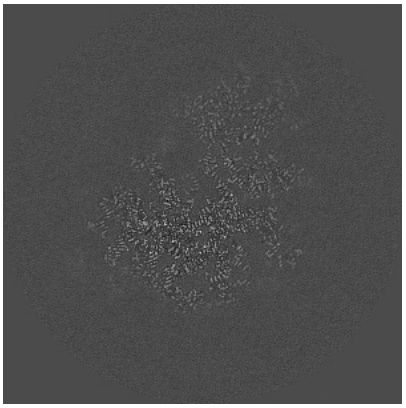

Z Index: 224

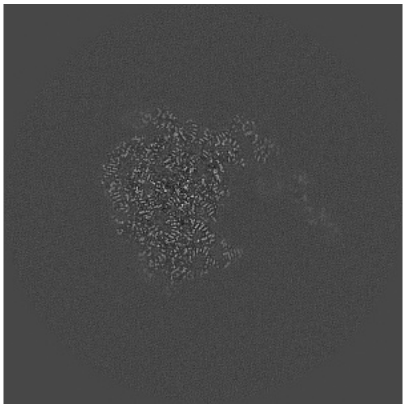
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

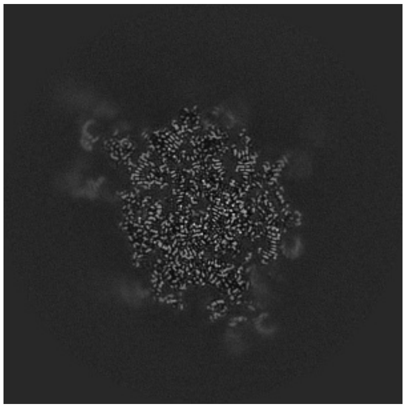
6.3.1 Primary map

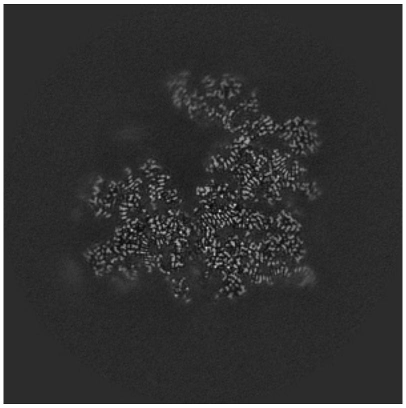

X Index: 200

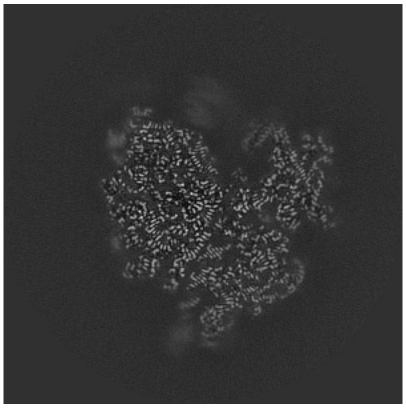

Y Index: 238


Z Index: 190

6.3.2 Raw map


X Index: 200

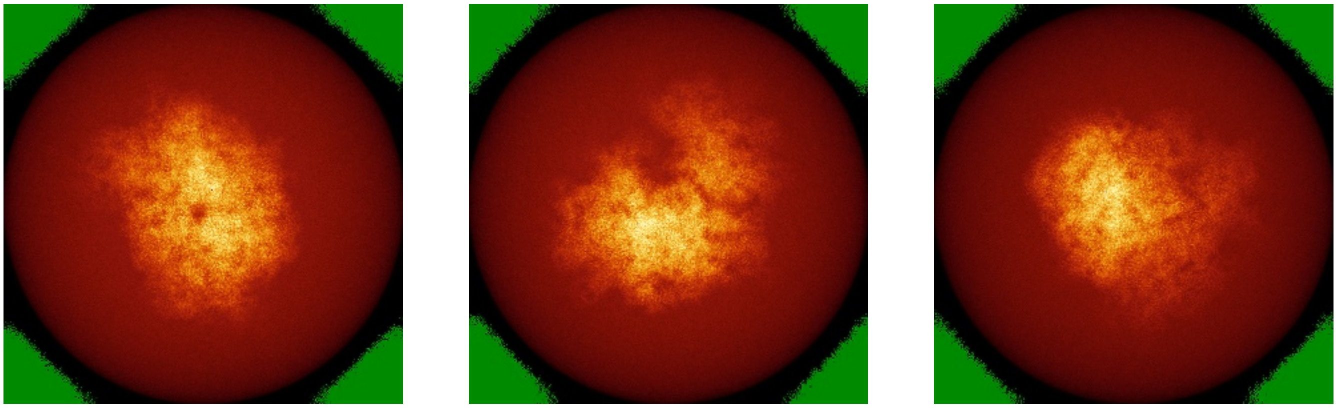

Y Index: 215


Z Index: 252

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

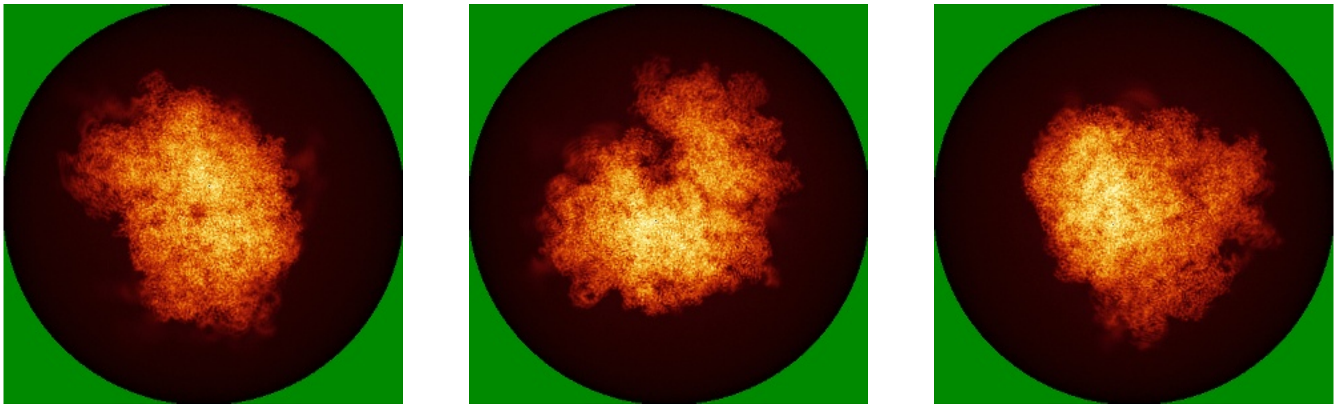
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

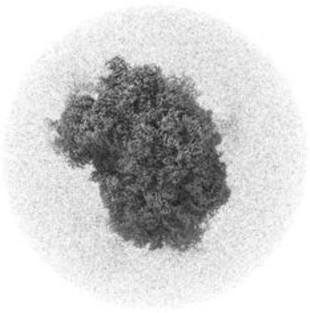


X Y Z

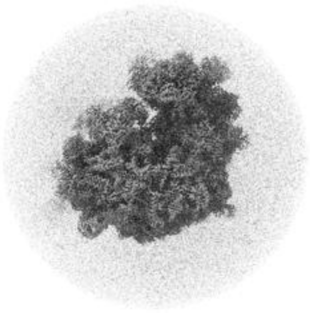
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

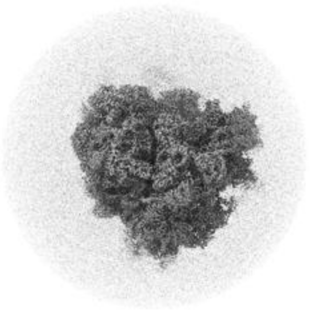
6.5.1 Primary map



X



Y

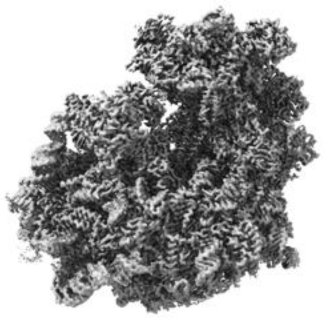


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y

Z

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

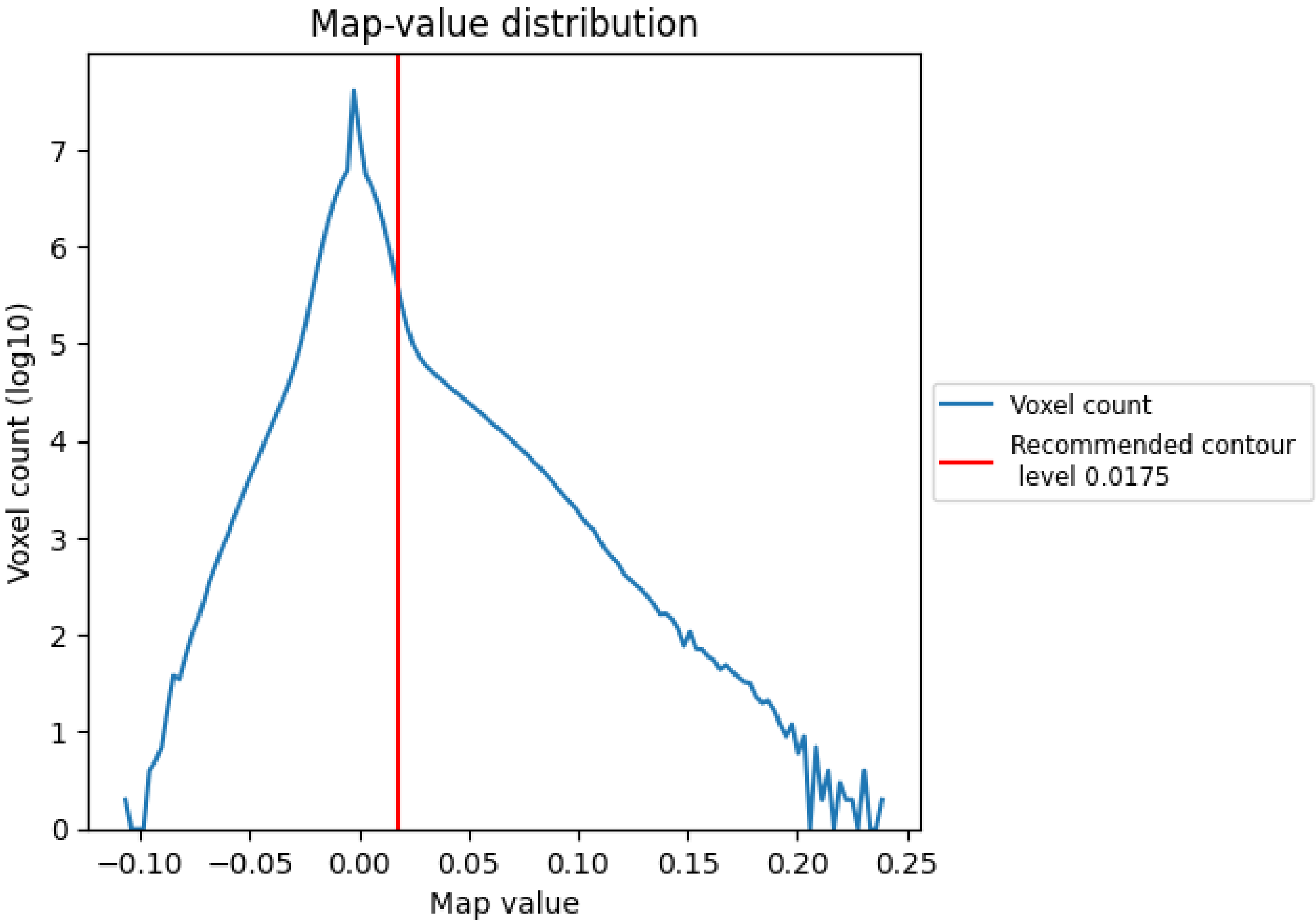
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

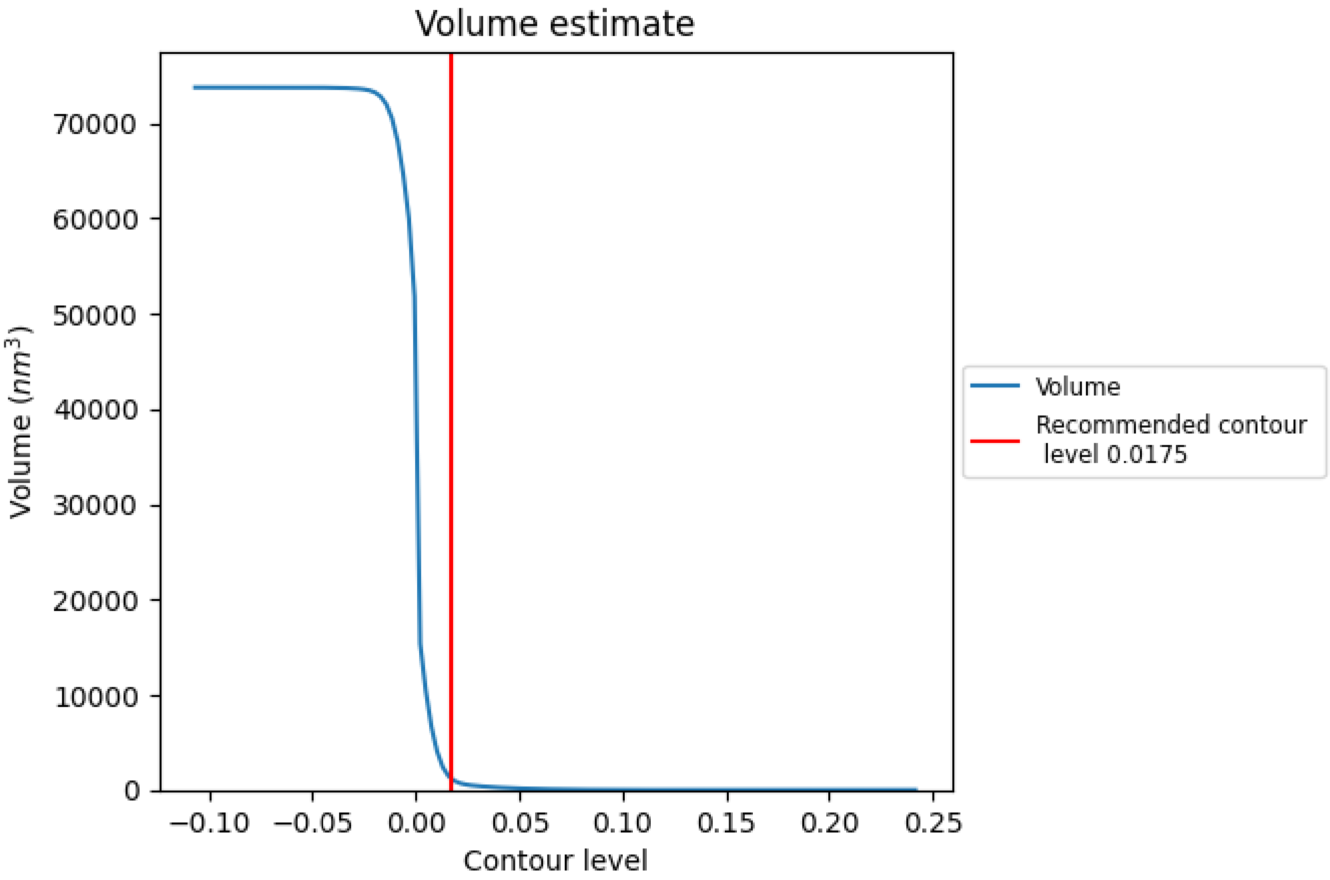
This section contains the results of statistical analysis of the map.

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.

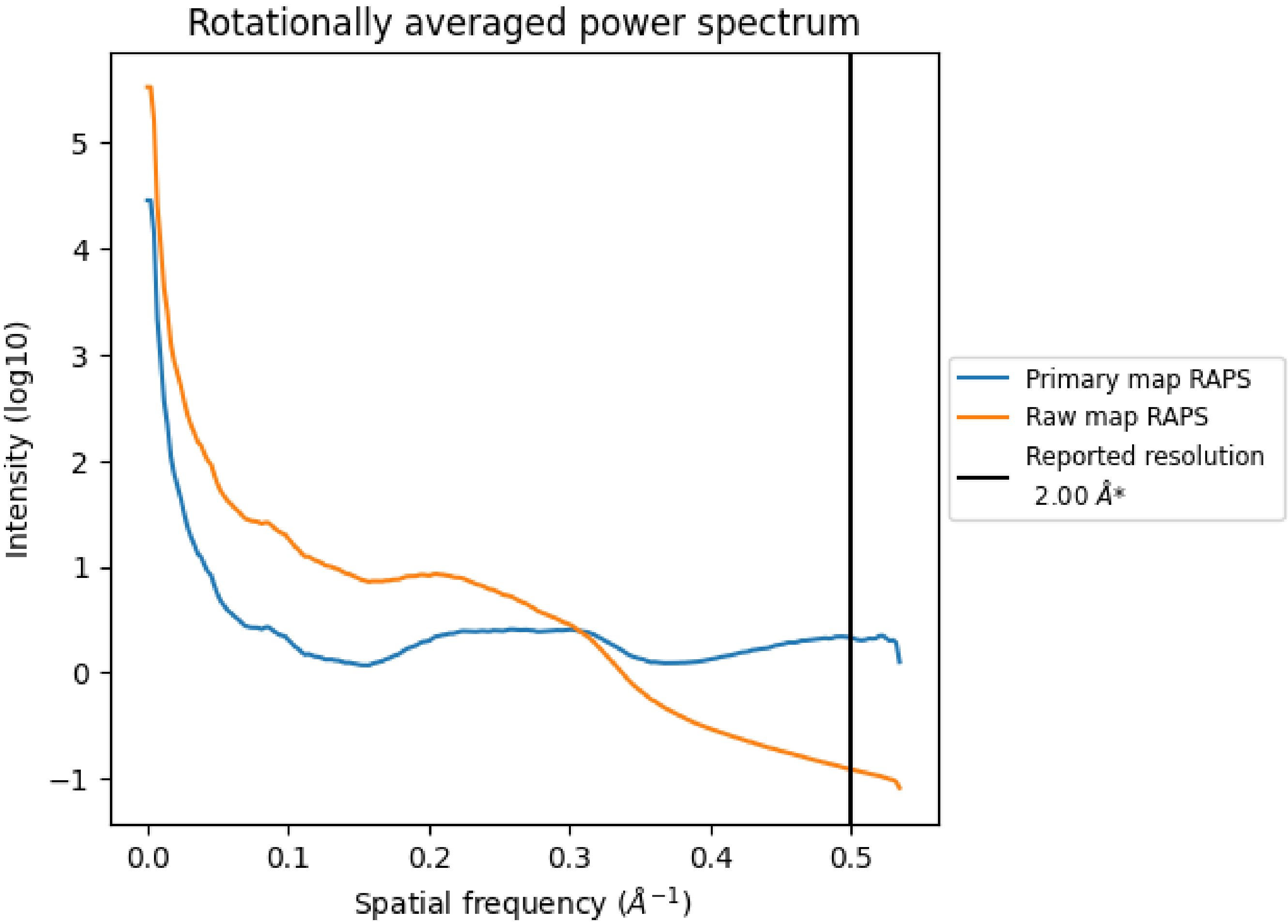
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1154 nm^3; this corresponds to an approximate mass of 1042 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 ⓘ

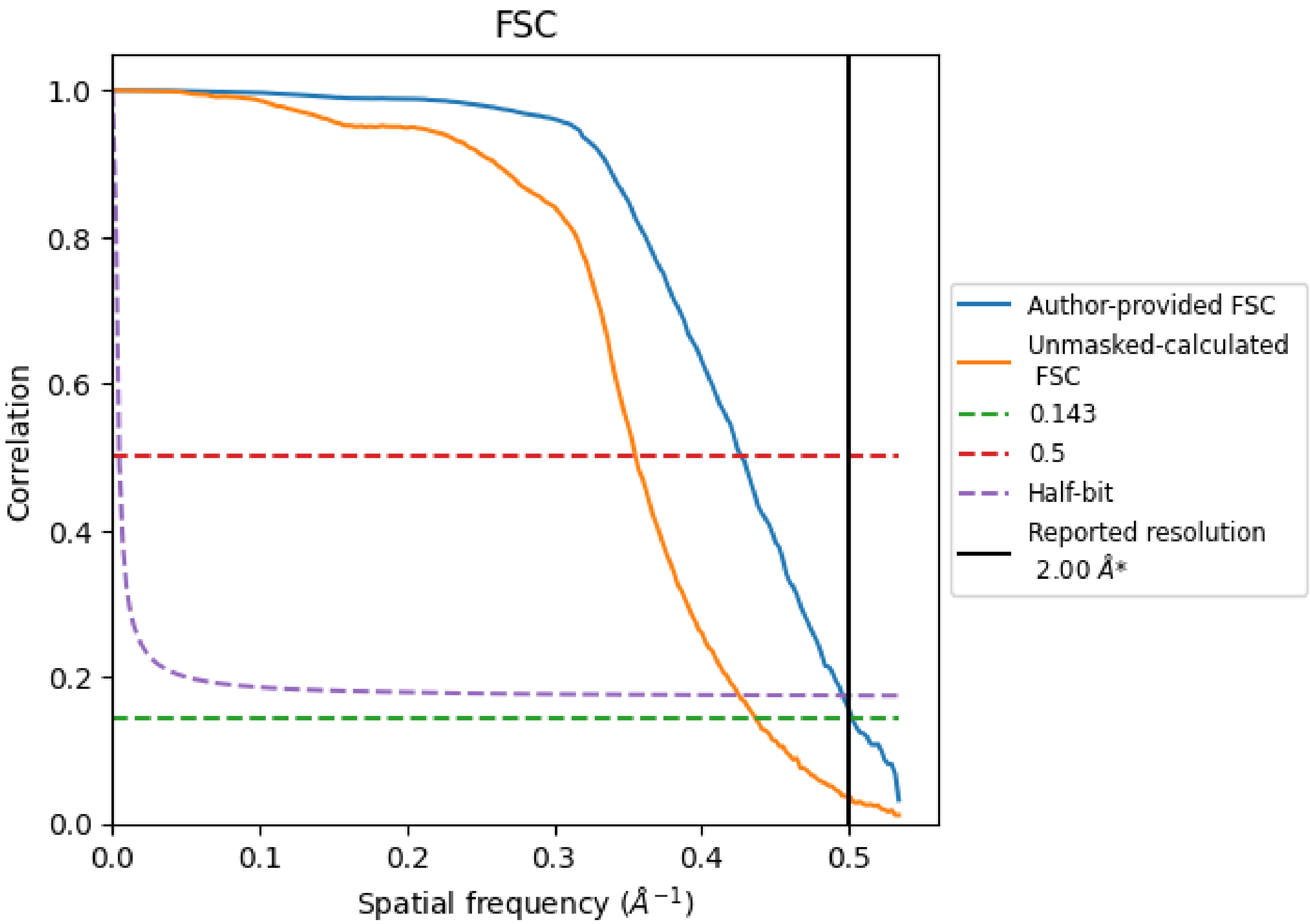


*Reported resolution corresponds to spatial frequency of 0.500 $Å^{-1}$

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.500 Å^{-1}

8.2 Resolution estimates ⓘ

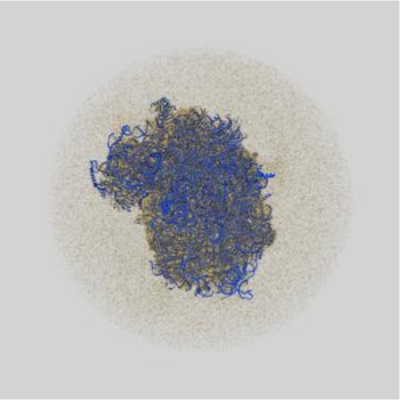
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	1.99	2.34	2.02
Unmasked-calculated*	2.29	2.81	2.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.29 differs from the reported value 2.0 by more than 10 %

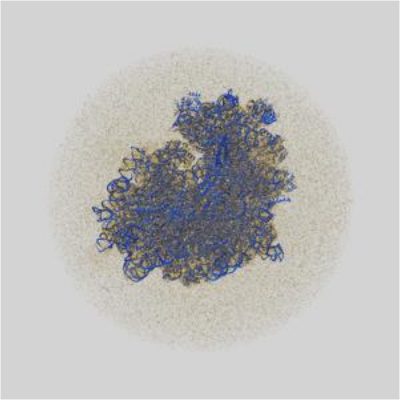
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45170 and PDB model 9C3H. Per-residue inclusion information can be found in section 3 on page 26.

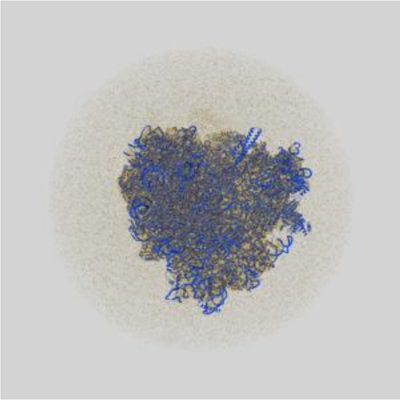
9.1 Map-model overlay



X



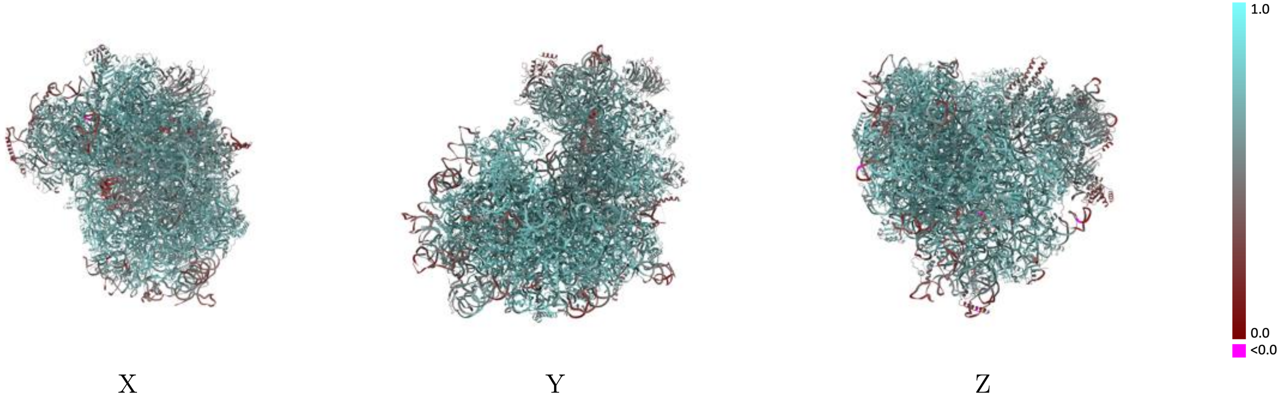
Y



Z

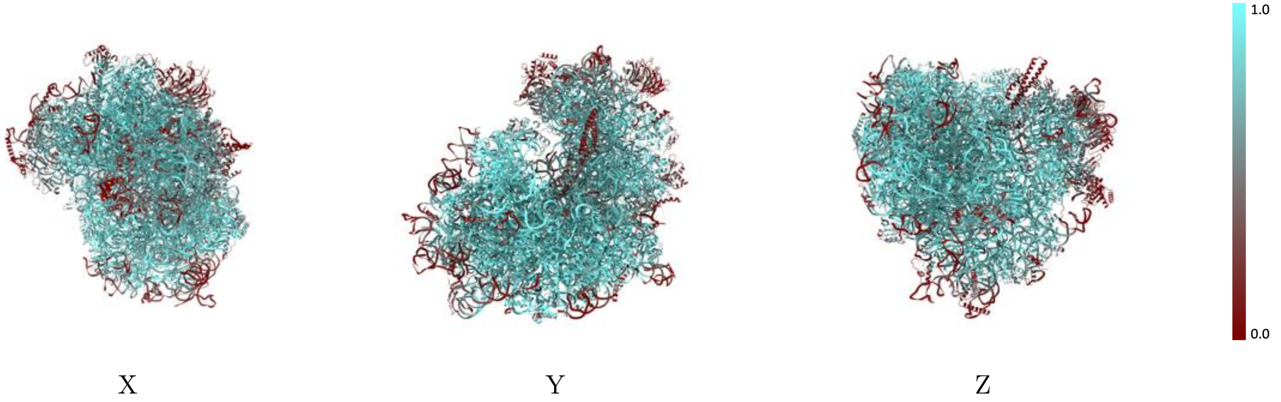
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



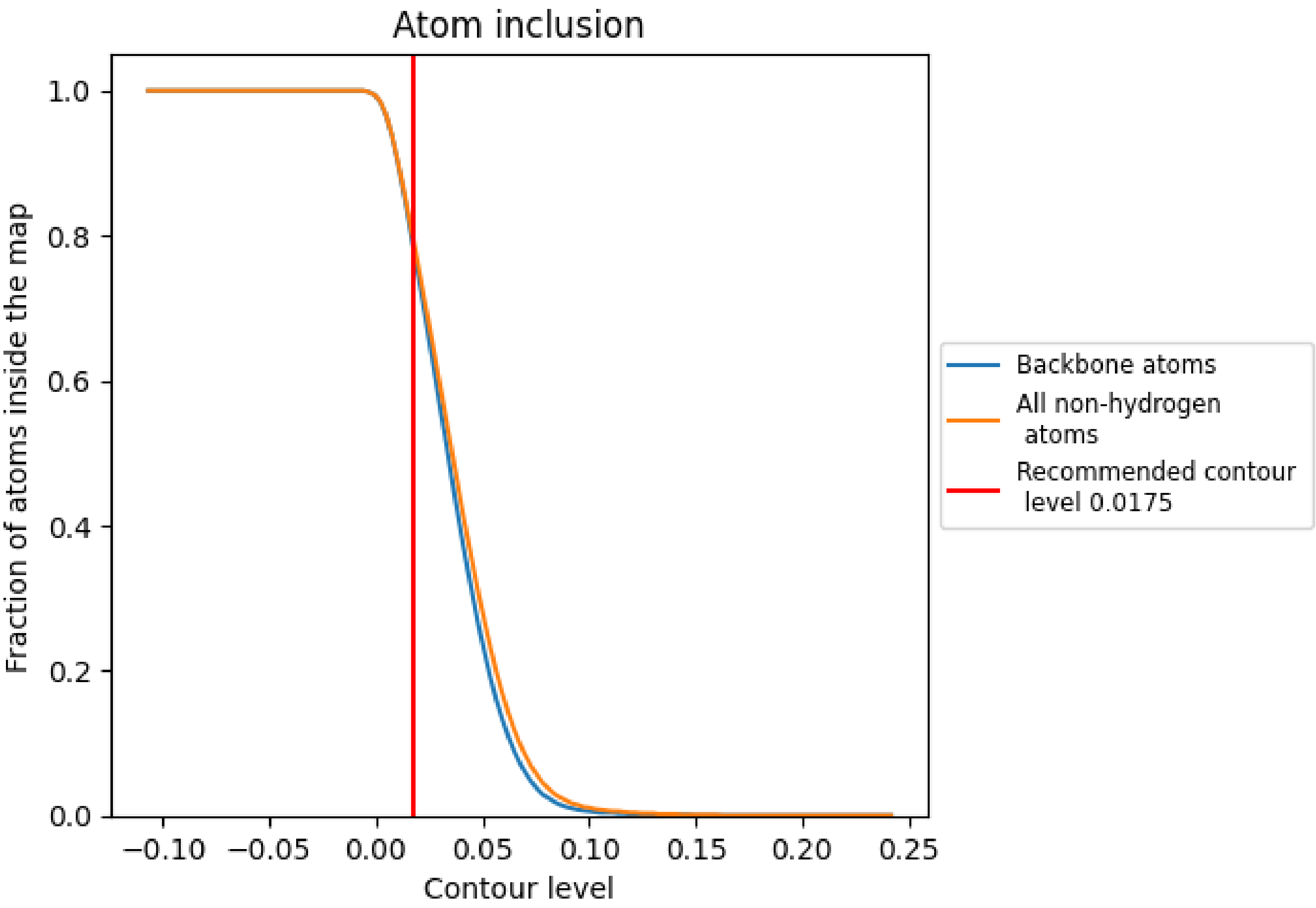
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0175).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.6840
L1	0.9300	0.7300
L5	0.8260	0.6900
L8	0.8170	0.6940
L9	0.9590	0.7290
LB	0.9070	0.7620
LC	0.9150	0.7580
LD	0.9670	0.7980
LE	0.8660	0.7310
LF	0.9190	0.7660
LG	0.8140	0.6910
LH	0.8680	0.7170
LI	0.9440	0.7780
LJ	0.7340	0.6530
LK	0.7900	0.6870
LM	0.8760	0.7220
LN	0.9900	0.7950
LO	0.8420	0.7120
LP	0.9570	0.7860
LQ	0.8410	0.7190
LR	0.7860	0.6910
LS	0.9430	0.7700
LT	0.8500	0.7320
LU	0.9290	0.7620
LV	0.9450	0.7820
LW	0.5460	0.5580
LY	0.9220	0.7670
LZ	0.8460	0.7070
La	0.9480	0.7810
Lb	0.7250	0.6580
Lc	0.8530	0.7260
Ld	0.8530	0.7320
Le	0.8710	0.7520
Lf	0.9610	0.7890
Lg	0.8900	0.7490

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Chain	Atom inclusion	Q-score
Lh	0.8950	0.7620
Li	0.8220	0.7050
Lj	0.9580	0.7850
Lk	0.6380	0.6390
Ll	0.9330	0.7610
Lm	0.5580	0.5820
Ln	0.8940	0.7330
Lo	0.8970	0.7570
Lp	0.9380	0.7800
Lz	0.8890	0.7440
NC	0.7850	0.7310
S1	0.7900	0.7010
S2	0.8130	0.6640
S4	0.6970	0.6070
S5	0.6810	0.6390
SA	0.8100	0.6880
SB	0.1950	0.4830
SC	0.8710	0.7160
SD	0.7280	0.6620
SE	0.7310	0.6680
SG	0.4090	0.5340
SH	0.4950	0.5730
SI	0.7380	0.6670
SJ	0.7400	0.6660
SK	0.5540	0.5990
SL	0.8510	0.7180
SM	0.4130	0.5430
SN	0.8860	0.7330
SO	0.9000	0.7400
SP	0.4790	0.5850
SQ	0.6670	0.6440
SS	0.5800	0.6090
ST	0.5820	0.6090
SU	0.5910	0.6100
SV	0.8040	0.6990
SW	0.9320	0.7530
SX	0.9010	0.7420
SY	0.5650	0.6070
SZ	0.4730	0.5500
Sa	0.8770	0.7360
Sb	0.6980	0.6580
Sc	0.4800	0.5800

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Chain	Atom inclusion	Q-score
Sd	0.6380	0.6400
Se	0.6070	0.6140
Sf	0.7870	0.6790
Sg	0.2680	0.5080
So	0.8580	0.7470
Sy	0.0440	0.2790
Sz	0.0850	0.3440