Full wwPDB EM Validation Report ⓘ

Jul 3, 2023 – 04:41 PM EDT

PDB ID	:	8FLE
EMDB ID	:	EMD-29276
Title	:	Human nuclear pre-60S ribosomal subunit (State L2)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.48 Å(reported)

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

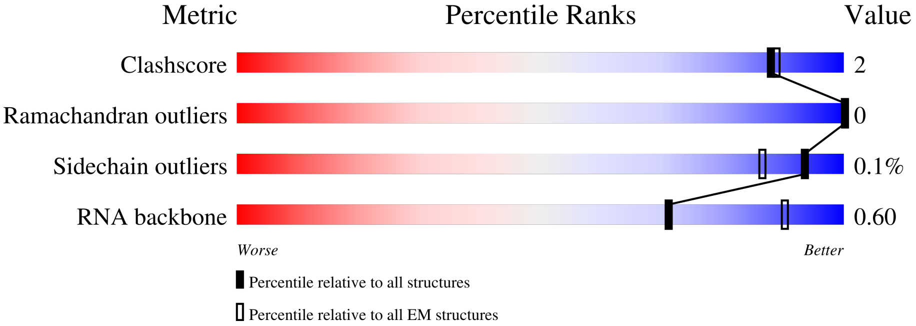
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

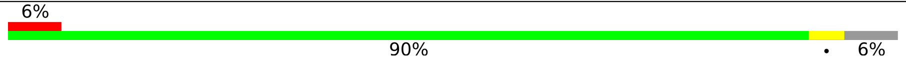
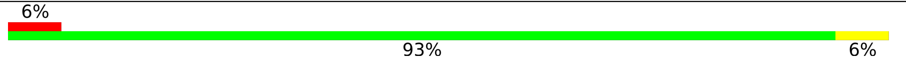
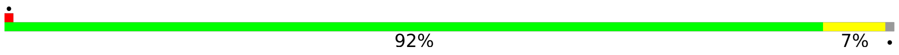
The reported resolution of this entry is 2.48 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BE	214	
2	L1	157	
3	L3	5070	
4	L4	121	
5	L5	178	
6	L6	211	
7	L7	203	

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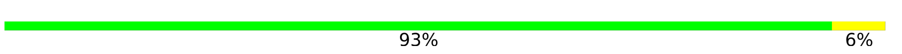
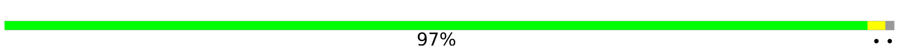
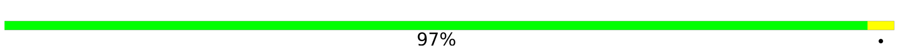
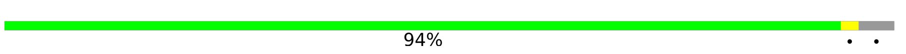
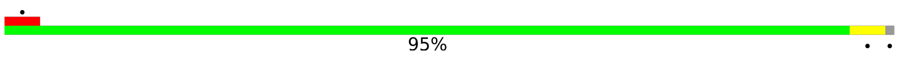
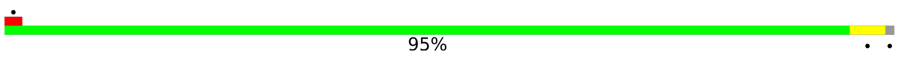
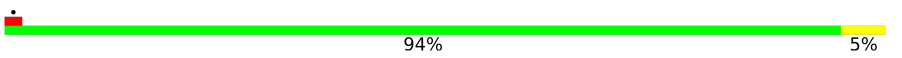
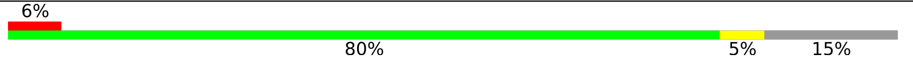
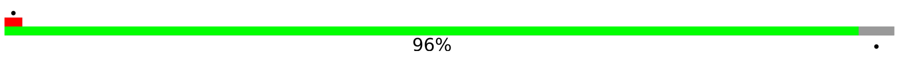
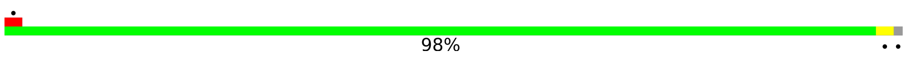
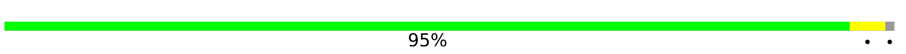
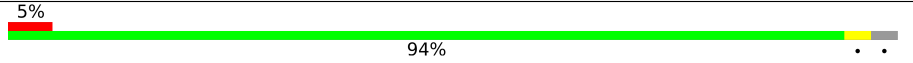
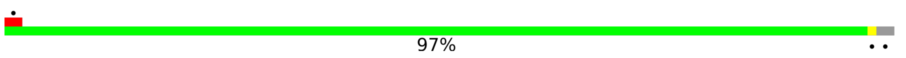
Mol	Chain	Length	Quality of chain
8	L8	215	 59% • 37%
9	L9	204	 93% 6%
10	LA	184	 • 80% • 17%
11	LB	188	 97% • •
12	LC	176	 97% •
13	LD	196	 • 76% • 21%
14	LE	160	 94% • •
15	LF	128	 • 73% 7% 20%
16	LG	140	 • 95% • •
17	LH	156	 • 88% • 8%
18	LI	145	 • 87% 6% 8%
19	LJ	136	 88% 11% •
20	LK	148	 • 95% • •
21	LL	137	 • 83% 8% 9%
22	LM	159	 6% 53% 5% • 41%
23	LN	403	 • 94% 5%
24	LO	115	 • 75% 8% 17%
25	LP	125	 6% 80% 5% 15%
26	LQ	135	 • 90% 5% 5%
27	LR	117	 • 96% •
28	LS	123	 • 98% • •
29	LT	110	 95% • •
30	LU	105	 5% 94% • •
31	LV	106	 • 97% • •
32	LW	97	 80% 8% 11%

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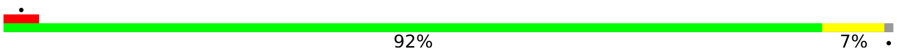
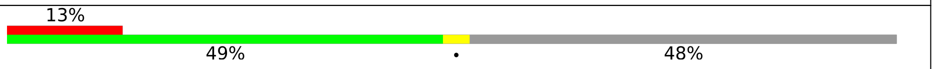
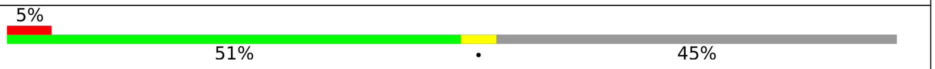
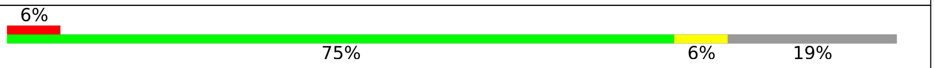
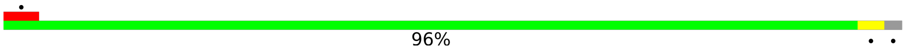
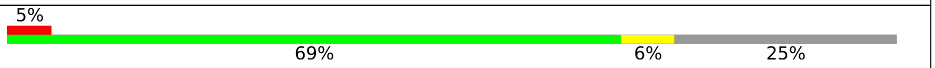
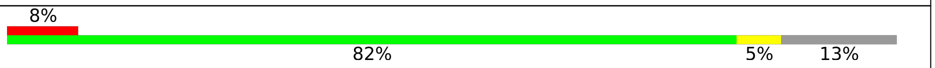
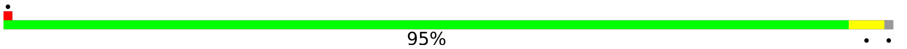
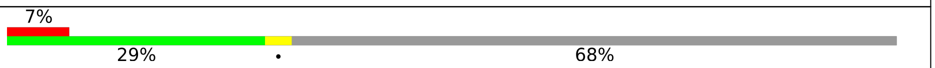
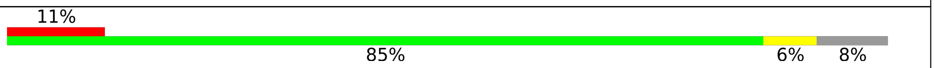
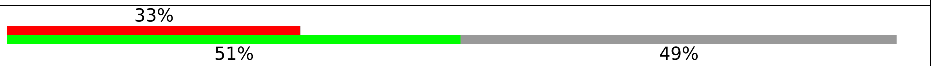
Mol	Chain	Length	Quality of chain
33	LX	92	
34	LY	70	
35	LZ	51	
36	NK	129	
37	NL	478	
38	NP	134	
39	SA	427	
40	SB	297	
41	SC	288	
42	SD	248	
43	SE	266	
44	SF	257	
45	SG	192	
46	SH	293	
47	SI	255	
48	SK	245	
49	SM	588	
50	SQ	239	
51	SR	634	
52	SV	163	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 144139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BE	160	1295	827	242	218	8	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	154	3278	1463	581	1080	154	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L3	3372	72381	32259	13258	23492	3372	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L4	120	2561	1141	456	844	120	0	0

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L5	168	1349	853	251	239	6	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L6	210	1701	1064	352	281	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L7	201	1650	1063	321	261	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L8	135	1111	713	213	178	7	0	0

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L9	203	1701	1072	359	266	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LA	153	1242	776	241	216	9	0	0

- Molecule 11 is a protein called 60S ribosomal protein L18.

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

- Molecule 12 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LC	176	1461	930	284	236	11	0	0

- Molecule 13 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LD	154	1289	805	277	198	9	0	0

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LG	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 17 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 18 is a protein called 60S ribosomal protein L26.

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

- Molecule 19 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 20 is a protein called 60S ribosomal protein L27a.

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

- Molecule 21 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LL	125	Total 1002	C 622	N 207	O 168	S 5	0	0

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LM	94	Total 775	C 483	N 170	O 118	S 4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LN	402	Total 3239	C 2061	N 608	O 556	S 14	0	0

- Molecule 24 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LO	95	Total 738	C 468	N 131	O 133	S 6	0	0

- Molecule 25 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LP	106	Total 879	C 555	N 170	O 152	S 2	0	0

- Molecule 26 is a protein called 60S ribosomal protein L32.

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

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LR	112	Total 888	C 555	N 183	O 144	S 6	0	0

- Molecule 28 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LS	122	1015	641	205	168	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LT	109	876	555	174	144	3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L36.

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

- Molecule 31 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LV	104	851	533	174	138	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L37.

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

- Molecule 33 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LX	91	708	445	136	120	7	0	0

- Molecule 34 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LY	69	569	366	103	99	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LZ	50	444	281	98	64	1	0	0

- Molecule 36 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	NK	67	581	363	128	88	2	0	0

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	NL	263	2175	1347	433	393	2	0	0

- Molecule 38 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	NP	108	876	537	182	153	4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	SA	358	2853	1797	570	473	13	0	0

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	SB	292	2376	1499	433	430	14	0	0

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	SC	217	1747	1124	332	287	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L7.

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

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 44 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 45 is a protein called 60S ribosomal protein L9.

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

- Molecule 46 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SH	93	Total	C	N	O	S	1	0
			781	506	133	139	3		

- Molecule 47 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SI	234	Total	C	N	O	S	2	0
			1944	1259	365	316	4		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 49 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SM	399	3278	2120	576	571	11	0	0

- Molecule 50 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	SQ	123	610	364	123	123	0	0

- Molecule 51 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SR	243	2002	1238	377	375	12	0	0

- Molecule 52 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SV	139	1184	754	229	191	10	0	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	L1	5	5	5	0
53	L3	72	72	72	0
53	L4	3	3	3	0
53	LG	1	1	1	0
53	LQ	1	1	1	0
53	LR	1	1	1	0
53	LT	1	1	1	0
53	LW	1	1	1	0
53	SA	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
53	SF	1	Total Mg 1 1	0

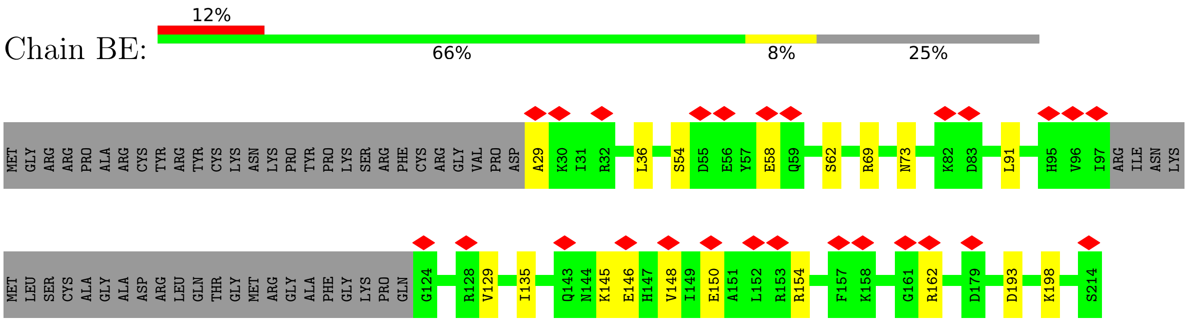
- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
54	LR	1	Total Zn 1 1	0
54	LV	1	Total Zn 1 1	0
54	LW	1	Total Zn 1 1	0
54	LX	1	Total Zn 1 1	0
54	NP	1	Total Zn 1 1	0
54	SV	1	Total Zn 1 1	0

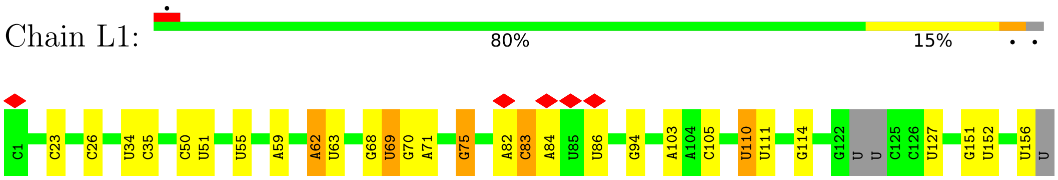
3 Residue-property plots ⓘ

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

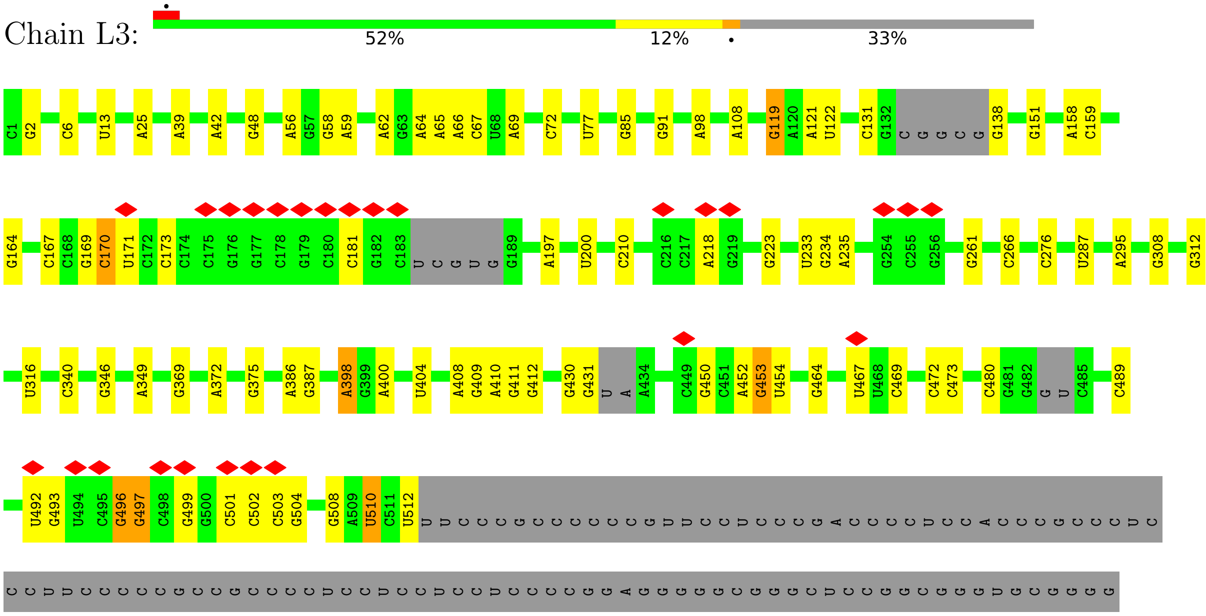
- Molecule 1: 60S ribosomal protein L10

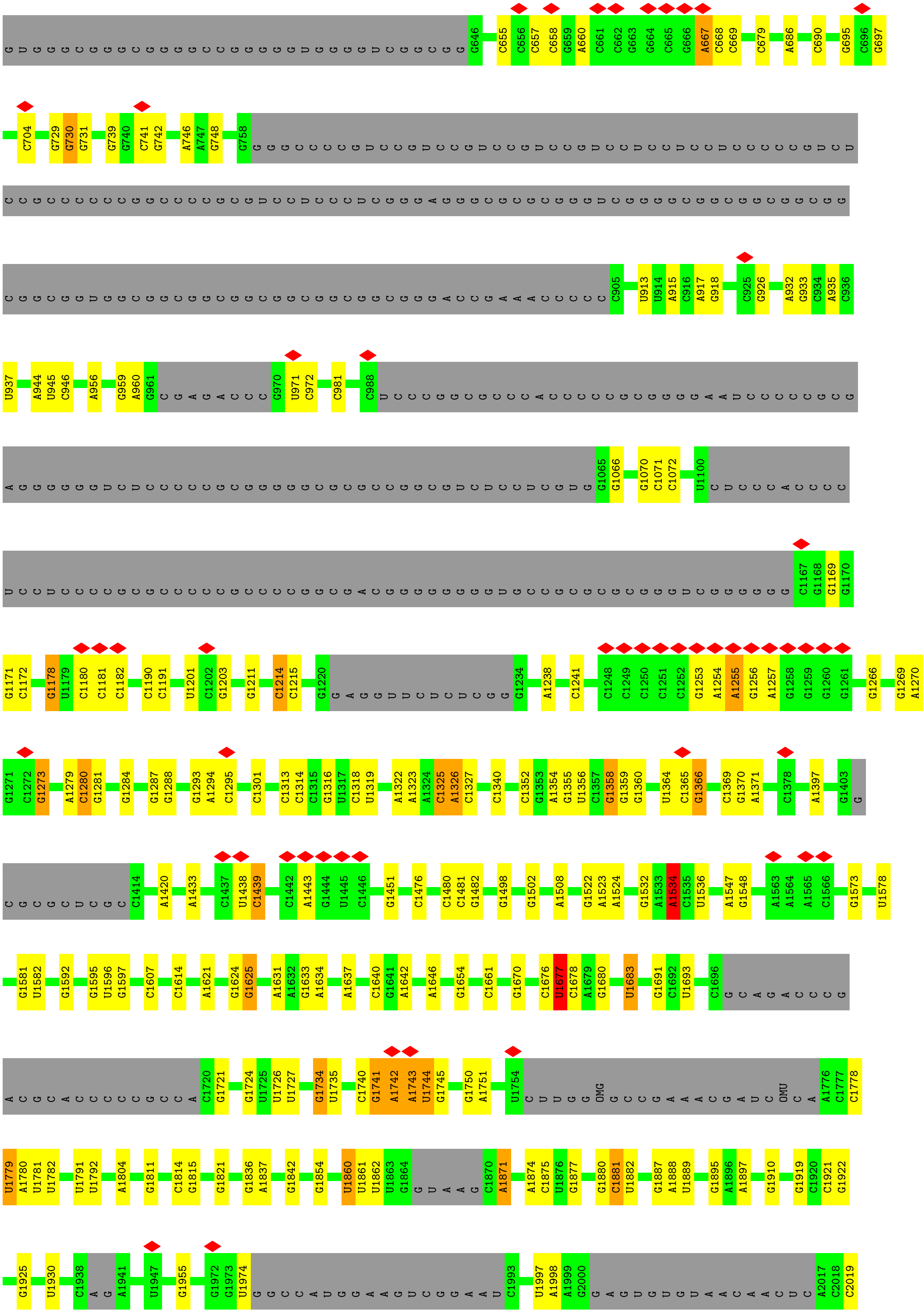


- Molecule 2: 5.8S rRNA



- Molecule 3: 28S rRNA

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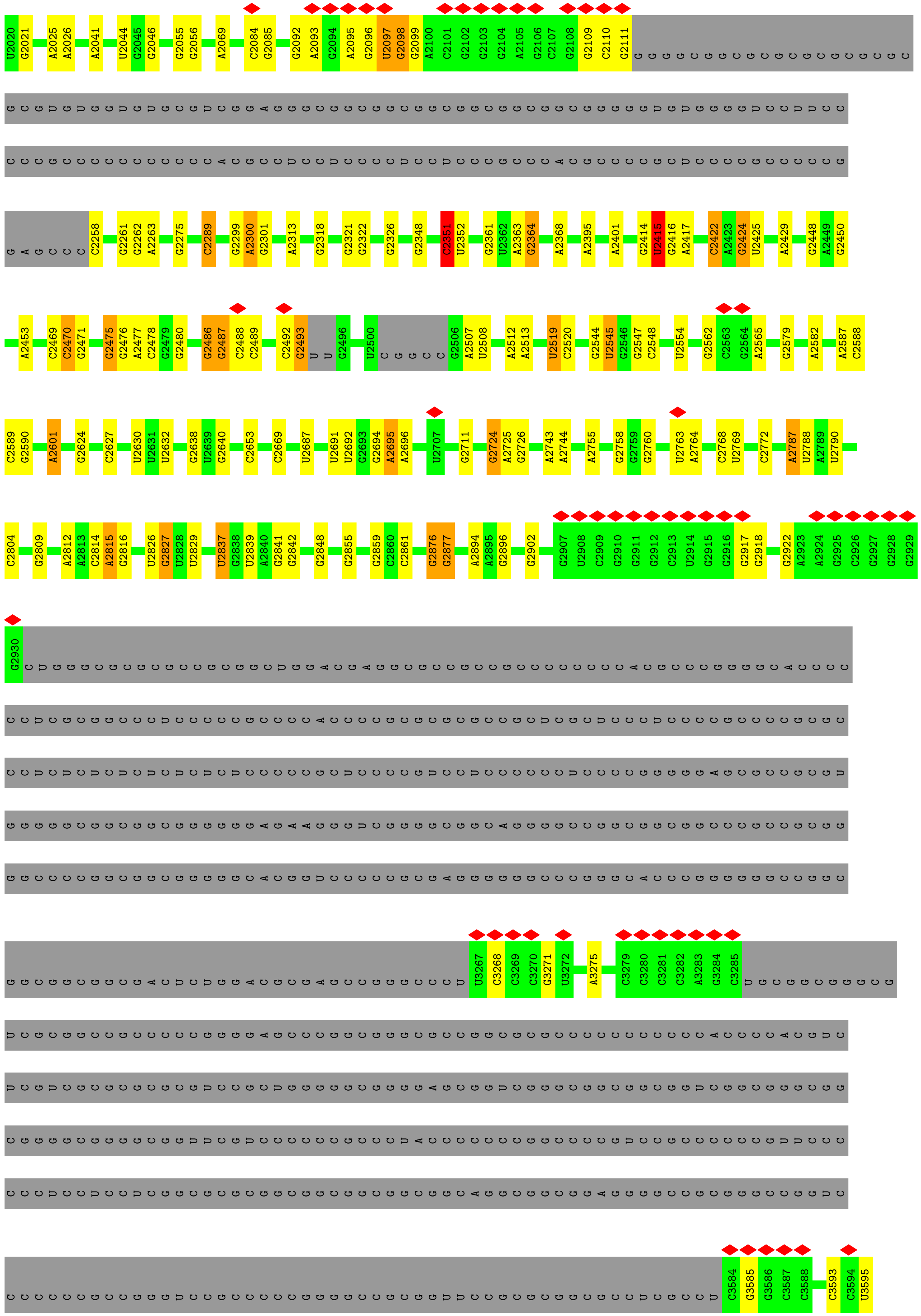
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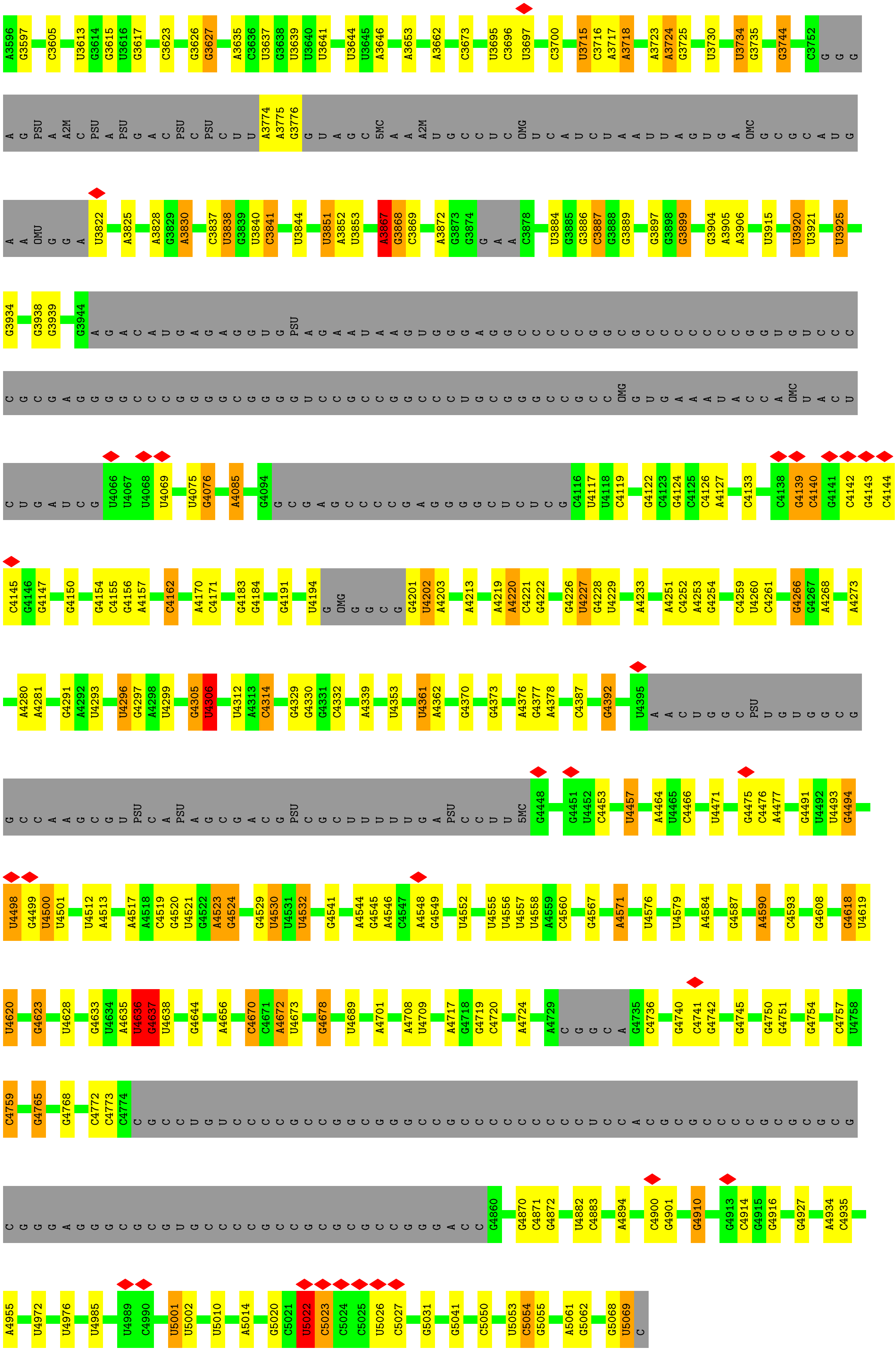
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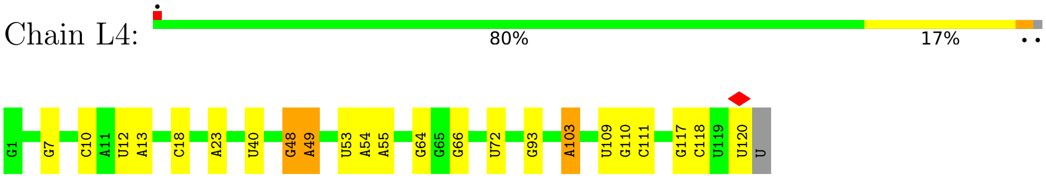
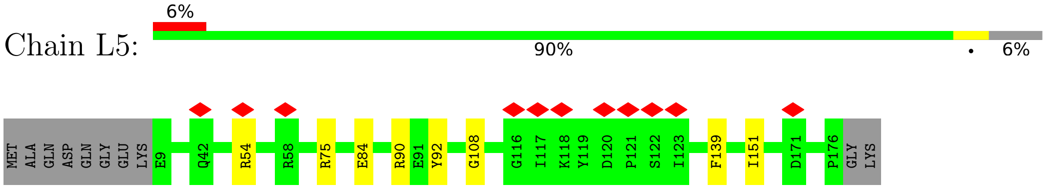
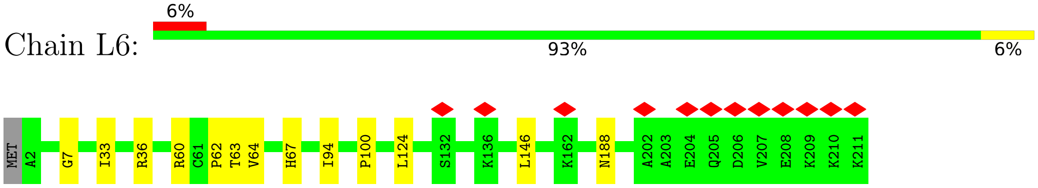
- Molecule 4: 5S rRNA



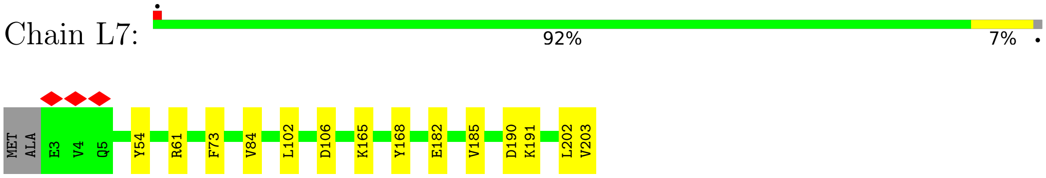
- Molecule 5: 60S ribosomal protein L11



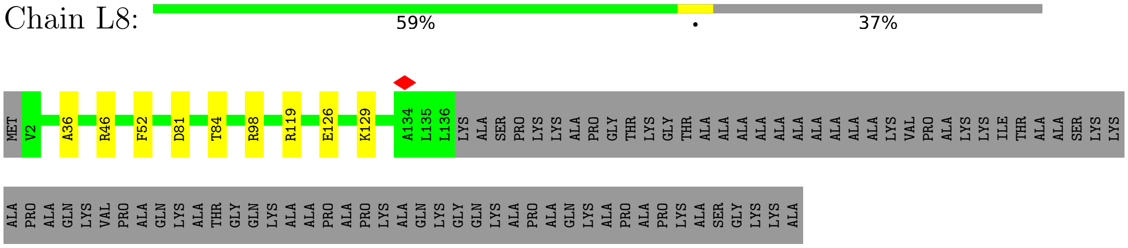
- Molecule 6: 60S ribosomal protein L13



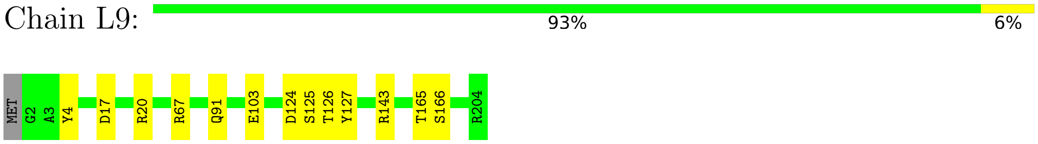
- Molecule 7: 60S ribosomal protein L13a



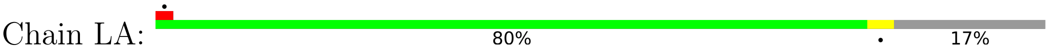
- Molecule 8: 60S ribosomal protein L14

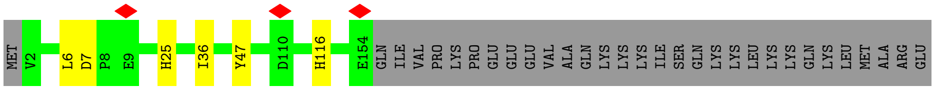


- Molecule 9: 60S ribosomal protein L15



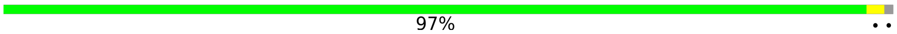
- Molecule 10: 60S ribosomal protein L17

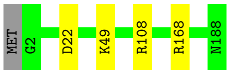




- Molecule 11: 60S ribosomal protein L18

Chain LB:





- Molecule 12: 60S ribosomal protein L18a

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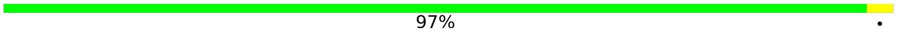
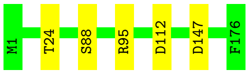


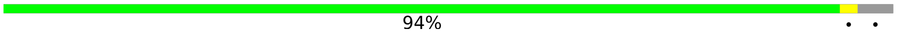


- Molecule 13: 60S ribosomal protein L19

Chain LD:

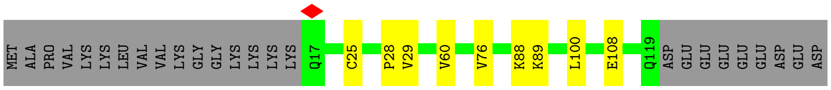
- Molecule 14: 60S ribosomal protein L21

Chain LE:



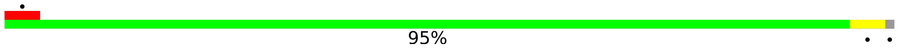
- Molecule 15: 60S ribosomal protein L22

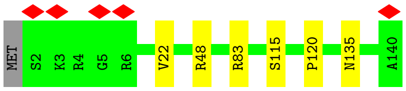
Chain LF:



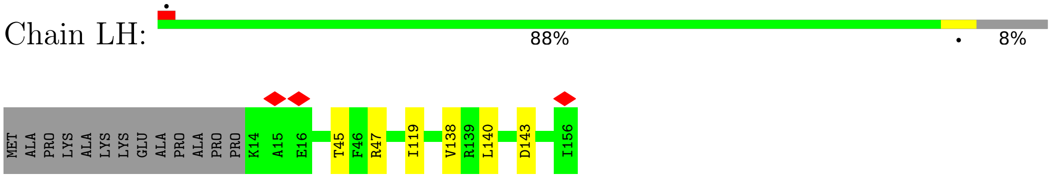
- Molecule 16: 60S ribosomal protein L23

Chain LG:

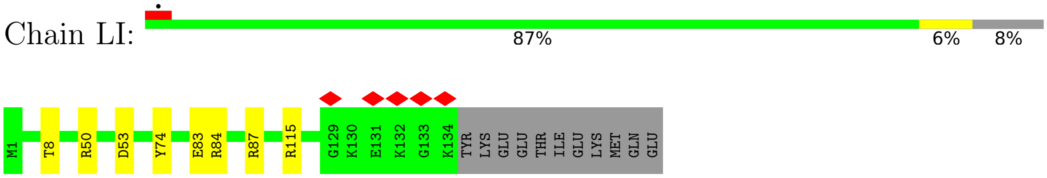




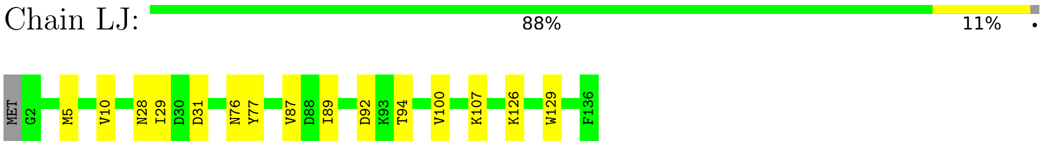
- Molecule 17: 60S ribosomal protein L23a



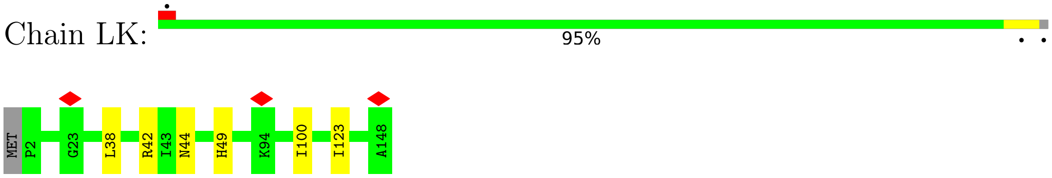
- Molecule 18: 60S ribosomal protein L26



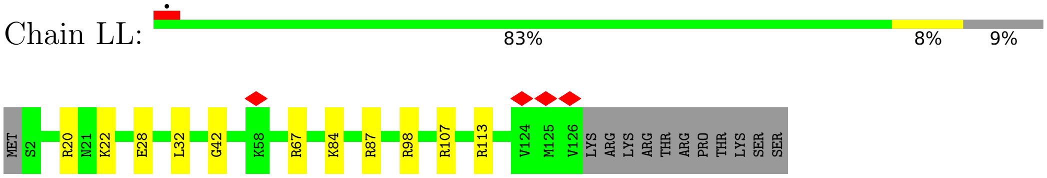
- Molecule 19: 60S ribosomal protein L27



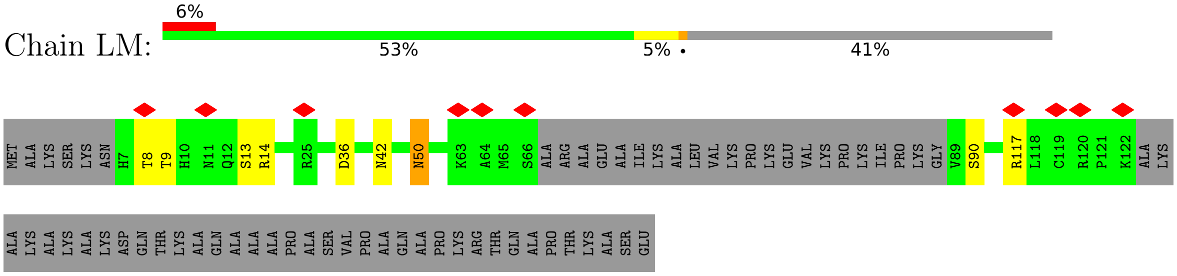
- Molecule 20: 60S ribosomal protein L27a



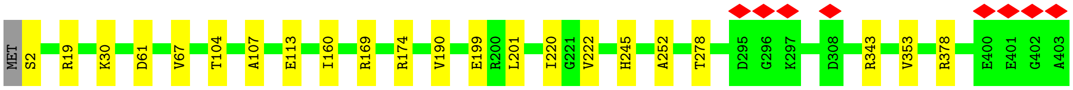
- Molecule 21: 60S ribosomal protein L28



- Molecule 22: 60S ribosomal protein L29



- Molecule 23: 60S ribosomal protein L3



- Molecule 24: 60S ribosomal protein L30

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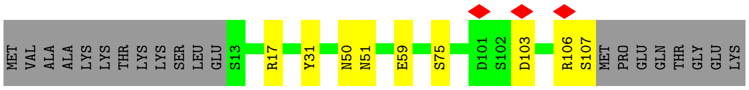
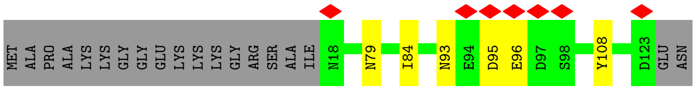


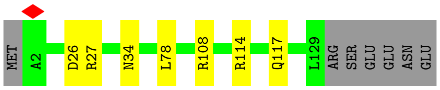
- Molecule 25: 60S ribosomal protein L31

Chain LP:



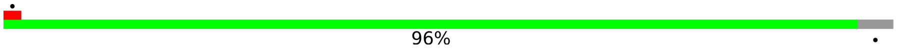
- Molecule 26: 60S ribosomal protein L32

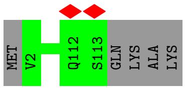
Chain LQ:



- Molecule 27: 60S ribosomal protein L34

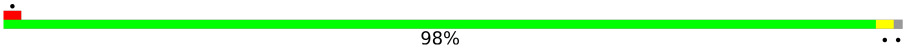
Chain LR:

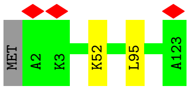




- Molecule 28: 60S ribosomal protein L35

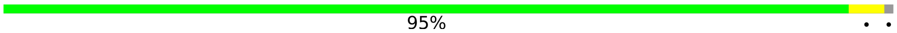
Chain LS:

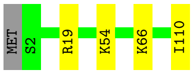




- Molecule 29: 60S ribosomal protein L35a

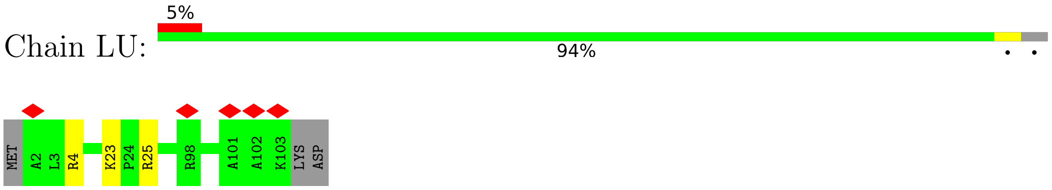
Chain LT:





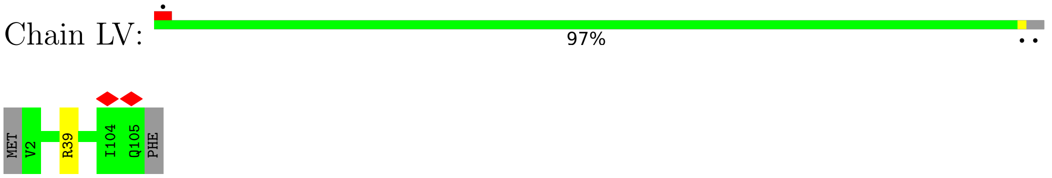
- Molecule 30: 60S ribosomal protein L36

Chain LU:



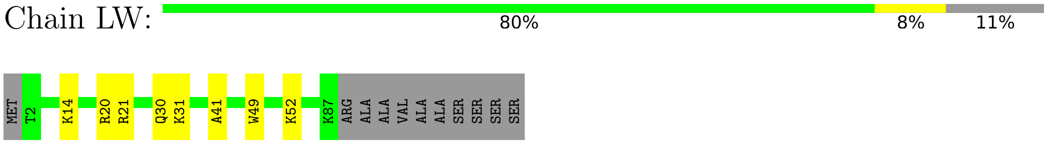
- Molecule 31: 60S ribosomal protein L36a

Chain LV:



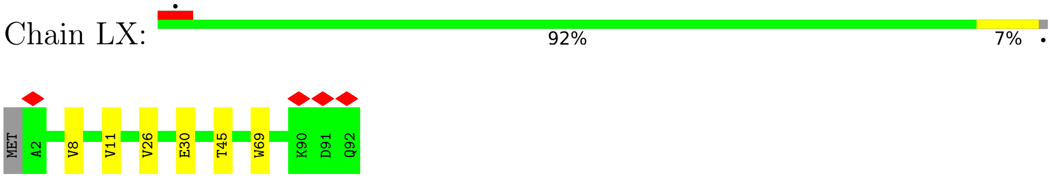
- Molecule 32: 60S ribosomal protein L37

Chain LW:



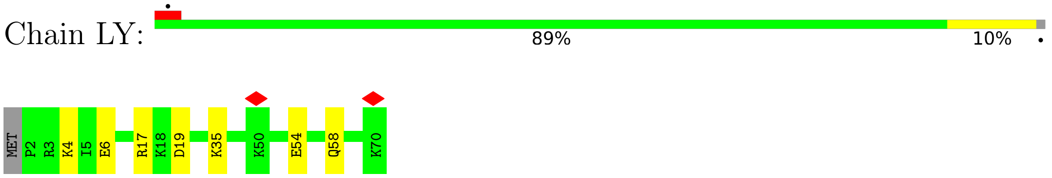
- Molecule 33: 60S ribosomal protein L37a

Chain LX:



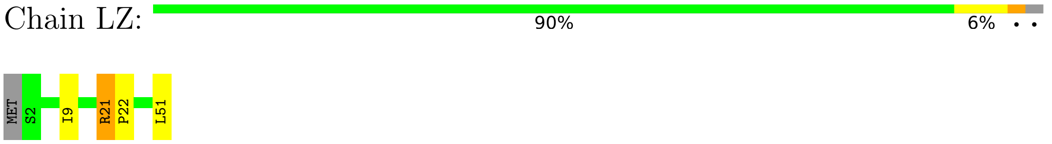
- Molecule 34: 60S ribosomal protein L38

Chain LY:



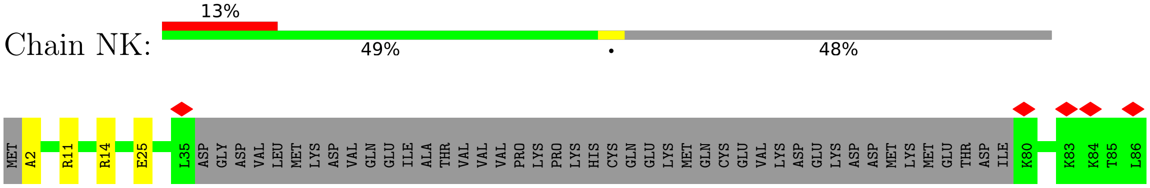
- Molecule 35: 60S ribosomal protein L39

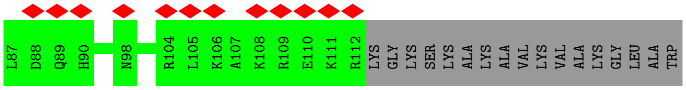
Chain LZ:



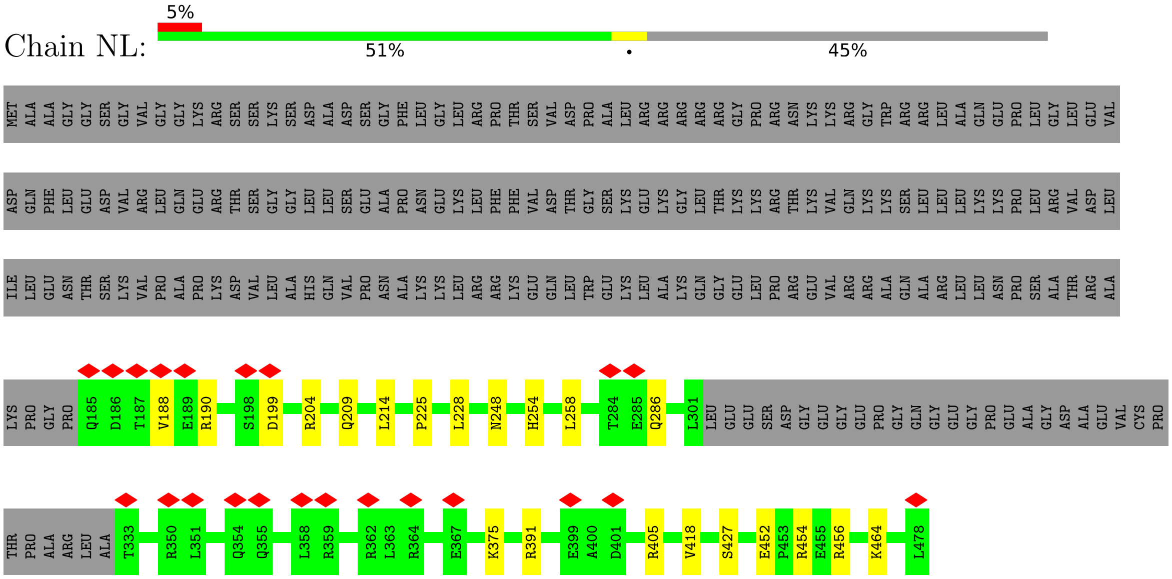
- Molecule 36: Protein LLP homolog

Chain NK:

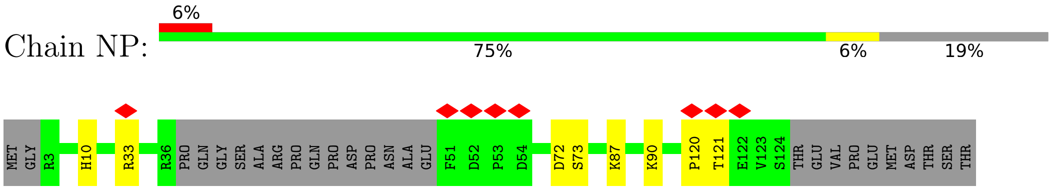




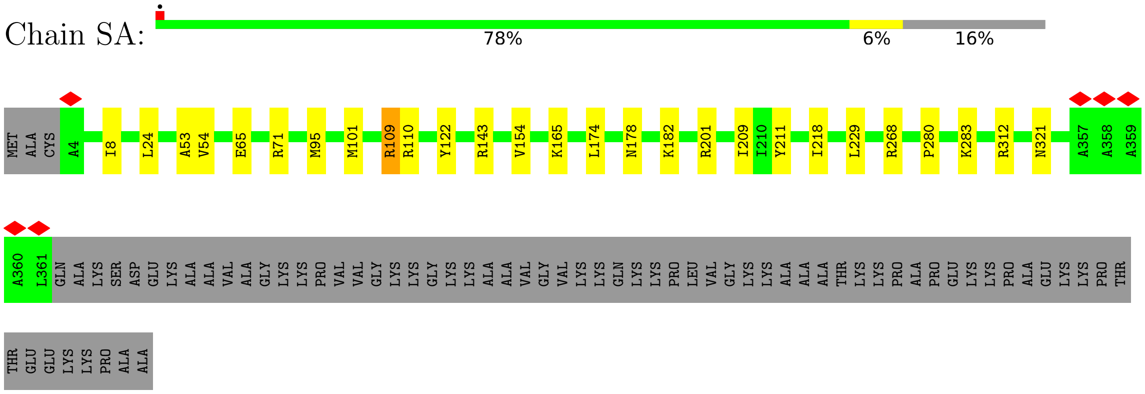
- Molecule 37: Ribosome biogenesis protein NOP53



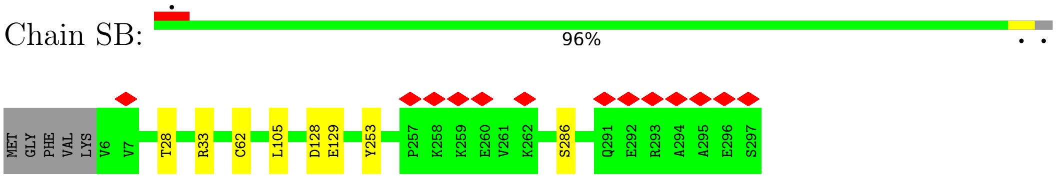
- Molecule 38: Zinc finger protein 593



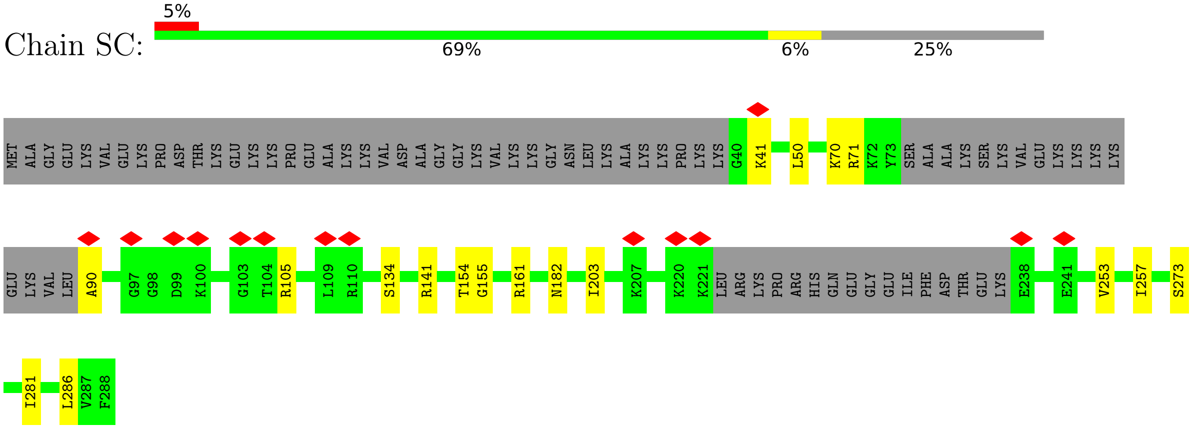
- Molecule 39: 60S ribosomal protein L4



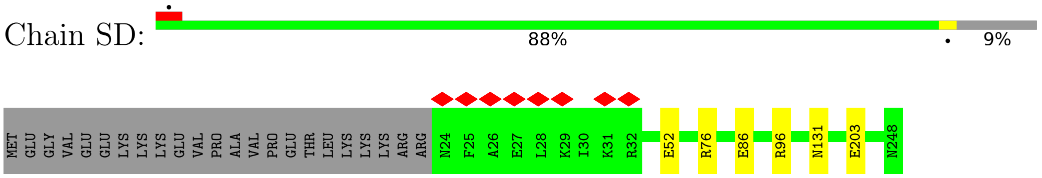
- Molecule 40: 60S ribosomal protein L5



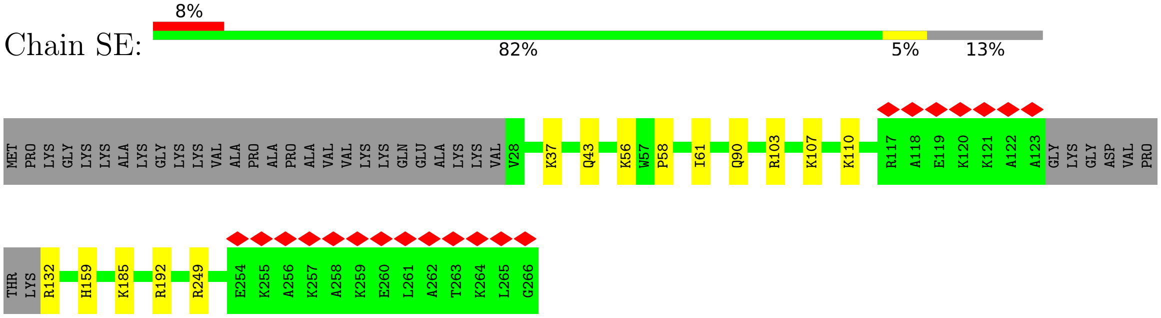
- Molecule 41: 60S ribosomal protein L6



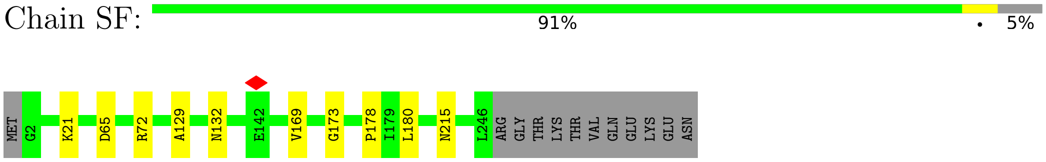
- Molecule 42: 60S ribosomal protein L7



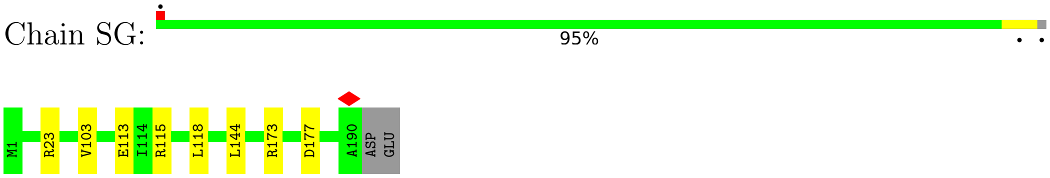
- Molecule 43: 60S ribosomal protein L7a



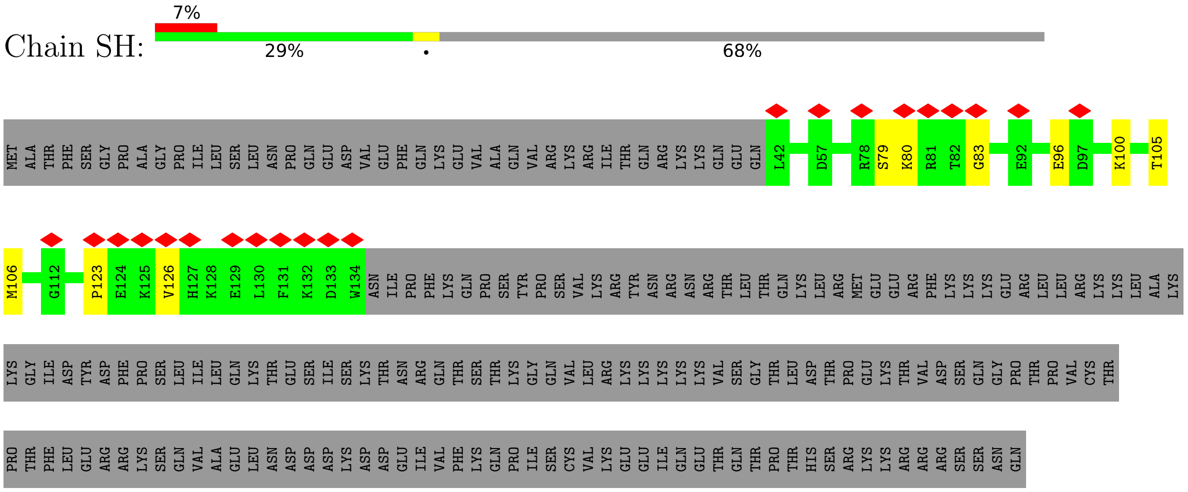
- Molecule 44: 60S ribosomal protein L8



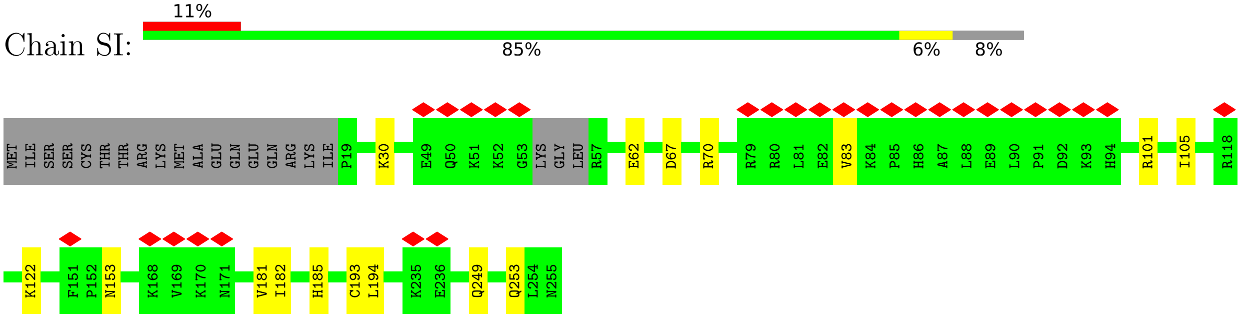
- Molecule 45: 60S ribosomal protein L9



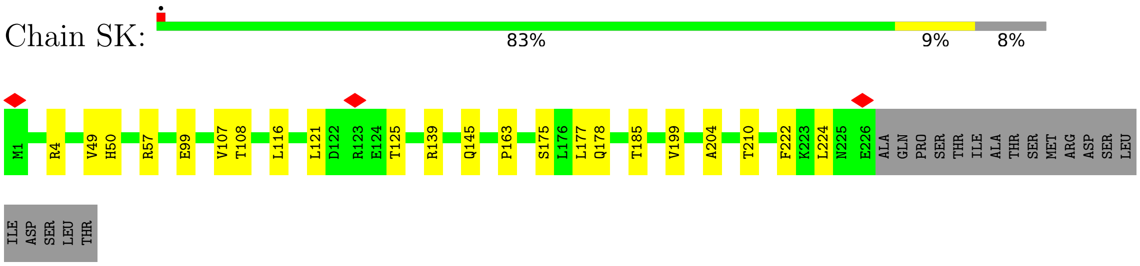
- Molecule 46: MKI67 FHA domain-interacting nucleolar phosphoprotein



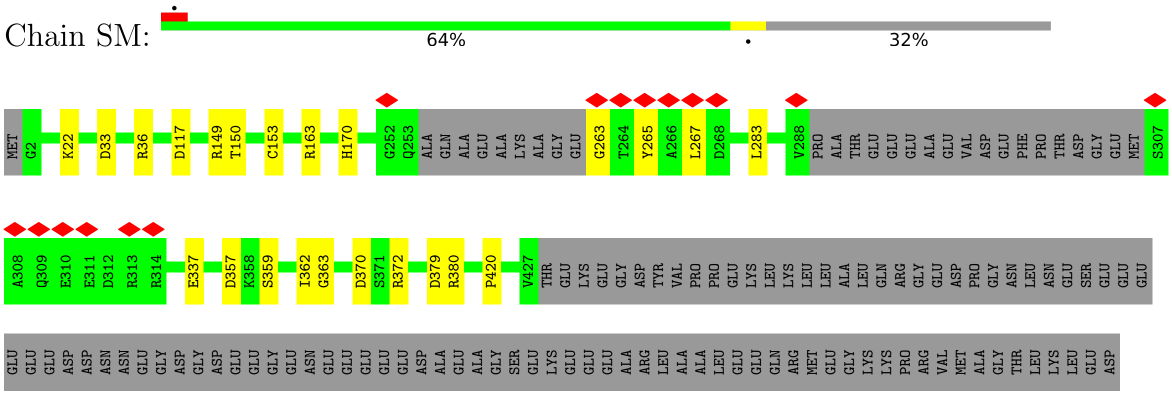
- Molecule 47: 60S ribosomal protein L7-like 1

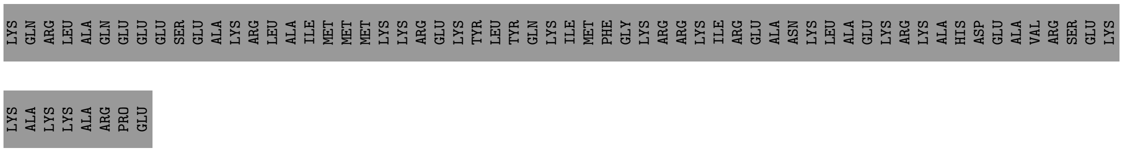


- Molecule 48: Eukaryotic translation initiation factor 6



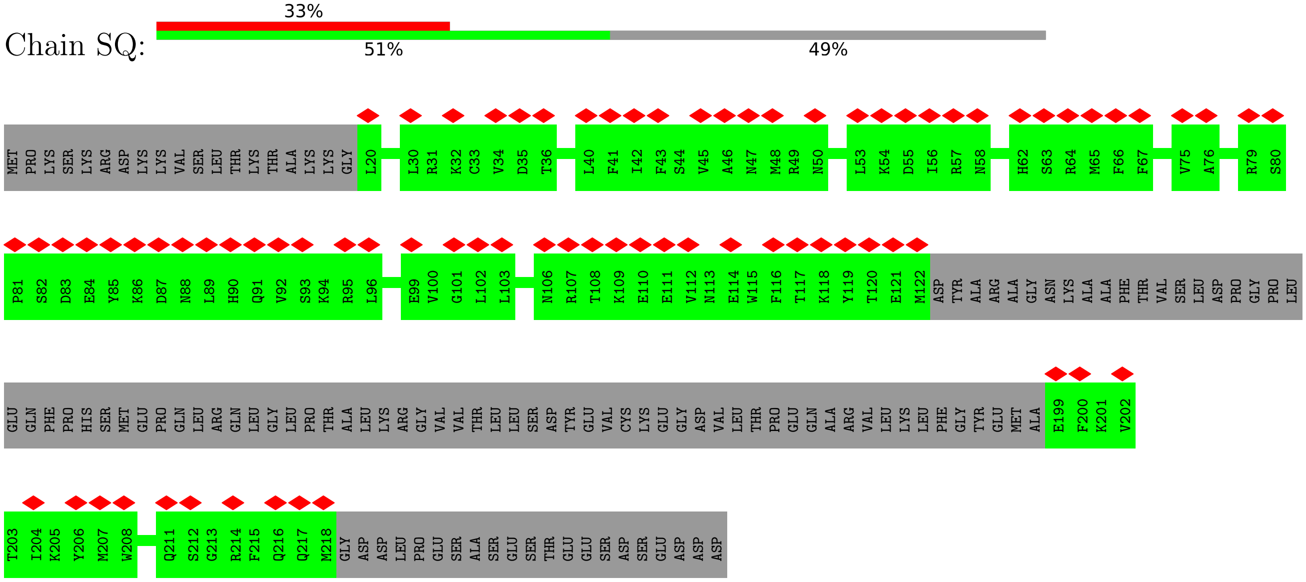
- Molecule 49: Pescadillo homolog





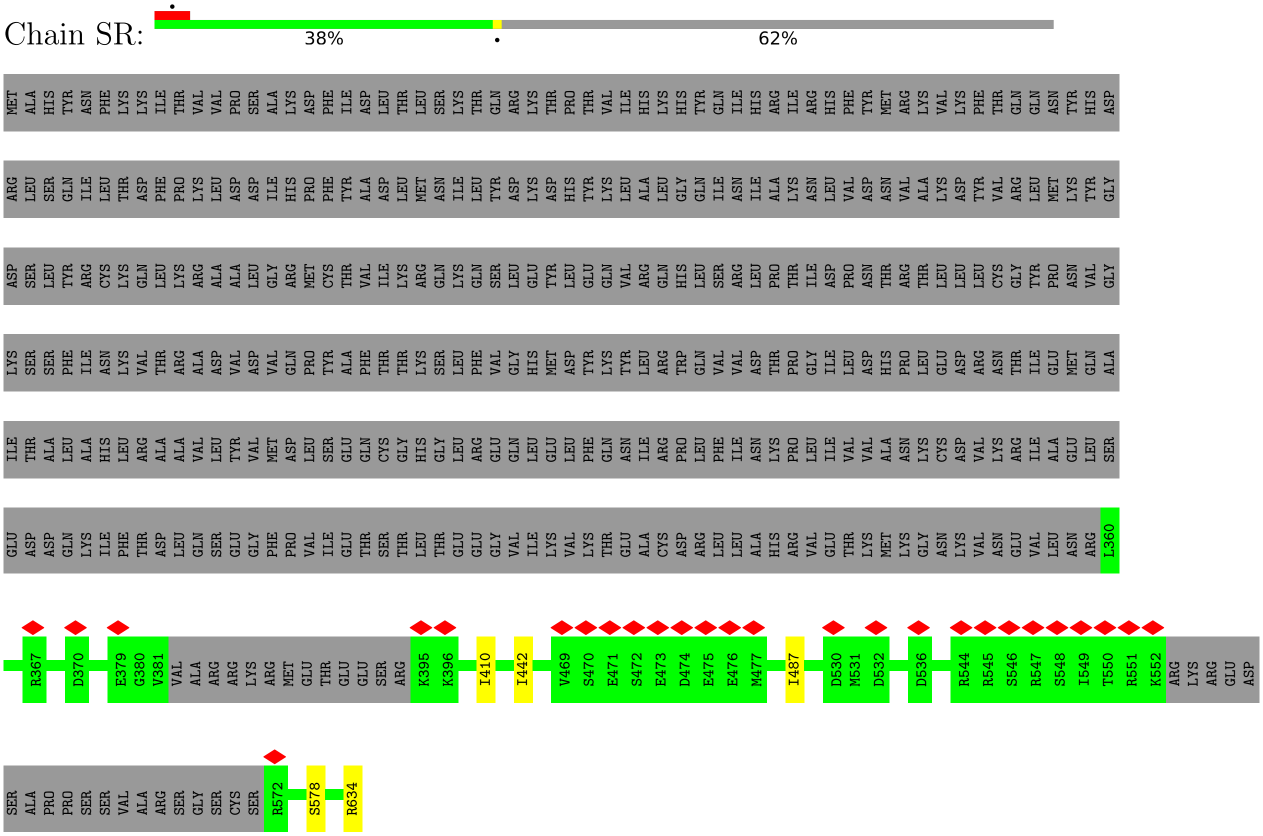
- Molecule 50: mRNA turnover protein 4 homolog

Chain SQ:



- Molecule 51: GTP-binding protein 4

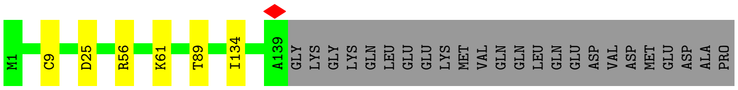
Chain SR:



- Molecule 52: Probable ribosome biogenesis protein RLP24

Chain SV:


82%
15%


M1
C9
D25
R56
K61
T89
I134
A139
GLY
LYS
GLY
LYS
GLN
LEU
GLU
GLU
LYS
MET
VAL
GLN
GLN
LEU
GLN
GLU
ASP
VAL
ASP
MET
GLU
ASP
ALA
PRO

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	123749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.008	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.193	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, MG, OMU, UR3, 6MZ, ZN, OMC, PSU, OMG, 1MA, A2M

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	BE	0.26	0/1323	0.55	0/1767
2	L1	0.64	0/3589	0.76	0/5589
3	L3	0.59	0/78428	0.79	11/122316 (0.0%)
4	L4	0.84	0/2861	0.84	3/4459 (0.1%)
5	L5	0.30	0/1372	0.57	0/1836
6	L6	0.29	0/1732	0.61	0/2315
7	L7	0.33	0/1682	0.58	0/2250
8	L8	0.30	0/1133	0.53	0/1516
9	L9	0.35	0/1746	0.64	0/2338
10	LA	0.31	0/1268	0.54	0/1701
11	LB	0.35	0/1536	0.66	0/2052
12	LC	0.38	0/1501	0.59	0/2013
13	LD	0.27	0/1305	0.60	0/1727
14	LE	0.38	0/1291	0.58	0/1724
15	LF	0.33	0/856	0.52	0/1149
16	LG	0.32	0/1048	0.59	0/1402
17	LH	0.29	0/1175	0.52	0/1572
18	LI	0.32	0/1132	0.60	0/1504
19	LJ	0.35	0/1130	0.57	0/1507
20	LK	0.34	0/1191	0.56	0/1591
21	LL	0.29	0/1017	0.60	0/1364
22	LM	0.29	0/788	0.59	0/1040
23	LN	0.32	0/3294	0.55	0/4406
24	LO	0.30	0/748	0.49	0/1004
25	LP	0.32	0/894	0.60	0/1204
26	LQ	0.31	0/1071	0.58	0/1429
27	LR	0.32	0/898	0.62	0/1197
28	LS	0.29	0/1023	0.56	0/1351
29	LT	0.34	0/895	0.62	0/1198
30	LU	0.28	0/843	0.60	0/1115
31	LV	0.36	0/864	0.61	0/1140
32	LW	0.34	0/720	0.67	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LX	0.29	0/718	0.56	0/953
34	LY	0.29	0/575	0.52	0/761
35	LZ	0.31	0/454	0.63	0/599
36	NK	0.26	0/587	0.60	0/767
37	NL	0.27	0/2207	0.59	0/2955
38	NP	0.27	0/893	0.61	0/1194
39	SA	0.32	0/2907	0.59	0/3905
40	SB	0.38	0/2421	0.55	0/3241
41	SC	0.28	0/1781	0.56	0/2388
42	SD	0.33	0/1905	0.57	0/2539
43	SE	0.32	0/1903	0.56	0/2559
44	SF	0.32	0/1914	0.61	0/2567
45	SG	0.30	0/1537	0.55	0/2066
46	SH	0.29	0/805	0.53	0/1085
47	SI	0.26	0/1991	0.53	0/2671
48	SK	0.30	0/1745	0.53	0/2374
49	SM	0.33	0/3357	0.53	0/4529
50	SQ	0.23	0/608	0.44	0/845
51	SR	0.29	0/2026	0.56	0/2690
52	SV	0.33	0/1207	0.57	0/1600
All	All	0.50	0/151895	0.71	14/222016 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	1881	C	C2-N1-C1’	8.03	127.63	118.80
3	L3	2486	G	N1-C6-O6	-6.36	116.08	119.90
3	L3	1881	C	C6-N1-C2	-6.21	117.81	120.30
3	L3	170	C	C6-N1-C2	-6.21	117.82	120.30
3	L3	1881	C	N1-C2-O2	5.89	122.43	118.90
3	L3	2469	C	C2-N1-C1’	5.84	125.22	118.80
3	L3	2486	G	C5-C6-O6	5.78	132.07	128.60
3	L3	5022	U	O4’-C1’-N1	5.75	112.80	108.20
4	L4	48	G	N3-C4-N9	5.53	129.31	126.00
3	L3	1881	C	N3-C2-O2	-5.50	118.05	121.90
3	L3	2519	U	O4’-C1’-N1	5.47	112.58	108.20
3	L3	1881	C	C6-N1-C1’	-5.31	114.42	120.80
4	L4	48	G	O4’-C1’-N9	5.21	112.37	108.20
4	L4	48	G	N3-C4-C5	-5.19	126.00	128.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BE	1295	0	1331	15	0
2	L1	3278	0	1665	14	0
3	L3	72381	0	36675	255	0
4	L4	2561	0	1295	9	0
5	L5	1349	0	1383	6	0
6	L6	1701	0	1818	10	0
7	L7	1650	0	1794	11	0
8	L8	1111	0	1174	8	0
9	L9	1701	0	1749	9	0
10	LA	1242	0	1269	4	0
11	LB	1512	0	1628	4	0
12	LC	1461	0	1502	4	0
13	LD	1289	0	1429	6	0
14	LE	1264	0	1328	3	0
15	LF	842	0	864	6	0
16	LG	1034	0	1097	4	0
17	LH	1156	0	1268	5	0
18	LI	1115	0	1205	8	0
19	LJ	1107	0	1182	8	0
20	LK	1162	0	1213	4	0
21	LL	1002	0	1068	9	0
22	LM	775	0	841	8	0
23	LN	3239	0	3377	19	0
24	LO	738	0	774	5	0
25	LP	879	0	924	3	0
26	LQ	1053	0	1147	5	0
27	LR	888	0	977	0	0
28	LS	1015	0	1148	2	0
29	LT	876	0	912	3	0
30	LU	832	0	917	2	0
31	LV	851	0	920	1	0
32	LW	705	0	737	7	0
33	LX	708	0	756	6	0
34	LY	569	0	637	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	LZ	444	0	483	5	0
36	NK	581	0	656	4	0
37	NL	2175	0	2235	16	0
38	NP	876	0	881	6	0
39	SA	2853	0	3028	24	0
40	SB	2376	0	2403	6	0
41	SC	1747	0	1897	13	0
42	SD	1870	0	1996	6	0
43	SE	1869	0	2014	12	0
44	SF	1876	0	1970	8	0
45	SG	1518	0	1601	5	0
46	SH	781	0	768	4	0
47	SI	1944	0	2077	12	0
48	SK	1721	0	1695	11	0
49	SM	3278	0	3332	17	0
50	SQ	610	0	257	0	0
51	SR	2002	0	2072	6	0
52	SV	1184	0	1248	5	0
53	L1	5	0	0	0	0
53	L3	72	0	0	0	0
53	L4	3	0	0	0	0
53	LG	1	0	0	0	0
53	LQ	1	0	0	0	0
53	LR	1	0	0	0	0
53	LT	1	0	0	0	0
53	LW	1	0	0	0	0
53	SA	1	0	0	0	0
53	SF	1	0	0	0	0
54	LR	1	0	0	0	0
54	LV	1	0	0	0	0
54	LW	1	0	0	0	0
54	LX	1	0	0	0	0
54	NP	1	0	0	0	0
54	SV	1	0	0	0	0
All	All	144139	0	108617	462	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (462) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:SA:109:ARG:O	39:SA:109:ARG:HG2	1.50	1.05
3:L3:3867:A2M:H8	3:L3:3867:A2M:H5”	1.51	0.93
4:L4:40:U:O2	5:L5:75:ARG:NH1	2.06	0.88
3:L3:4220:6MZ:O1P	14:LE:2:THR:OG1	1.92	0.87
4:L4:72:U:O2	4:L4:103:A:N6	2.12	0.83
3:L3:4156:G:OP2	3:L3:4157:A:O2’	1.97	0.82
3:L3:2300:A:N6	39:SA:178:ASN:OD1	2.13	0.82
39:SA:109:ARG:O	39:SA:109:ARG:CG	2.26	0.81
3:L3:2263:A:OP1	21:LL:107:ARG:NH2	2.13	0.81
49:SM:357:ASP:OD2	49:SM:359:SER:OG	1.99	0.80
3:L3:1480:C:O2’	3:L3:1482:G:OP2	2.00	0.80
5:L5:84:GLU:OE2	5:L5:92:TYR:OH	2.00	0.79
37:NL:418:VAL:O	47:SI:30:LYS:NZ	2.16	0.79
5:L5:90:ARG:NH2	5:L5:108:GLY:O	2.16	0.78
3:L3:4517:A:OP2	23:LN:2:SER:OG	2.02	0.78
3:L3:1214:C:N4	22:LM:90:SER:O	2.16	0.78
3:L3:480:C:OP2	21:LL:67:ARG:NH1	2.18	0.77
4:L4:55:A:O2’	5:L5:151:ILE:O	2.03	0.77
32:LW:14:LYS:NZ	35:LZ:51:LEU:OXT	2.17	0.77
3:L3:2275:G:OP2	39:SA:312:ARG:NH1	2.18	0.77
3:L3:679:C:OP1	21:LL:84:LYS:NZ	2.13	0.76
37:NL:199:ASP:OD2	37:NL:204:ARG:NH1	2.18	0.76
3:L3:3776:G:OP2	3:L3:3776:G:N2	2.17	0.75
3:L3:4085:A:OP2	17:LH:45:THR:OG1	2.04	0.75
3:L3:2545:U:O2’	3:L3:2547:G:N7	2.19	0.75
46:SH:96:GLU:OE2	46:SH:100:LYS:NZ	2.19	0.75
3:L3:4633:G:O2’	3:L3:4635:A:OP2	2.03	0.75
3:L3:1889:U:OP1	29:LT:19:ARG:NH2	2.20	0.74
3:L3:3717:A:OP2	3:L3:3735:G:N2	2.21	0.73
48:SK:121:LEU:O	48:SK:139:ARG:NH2	2.22	0.73
3:L3:2725:A:N6	13:LD:88:ARG:O	2.22	0.72
3:L3:2520:C:O2	3:L3:2640:G:N2	2.22	0.72
38:NP:33:ARG:NH1	52:SV:25:ASP:OD2	2.22	0.72
2:L1:51:U:OP2	35:LZ:21:ARG:NH2	2.23	0.72
3:L3:1071:C:O2	41:SC:70:LYS:NZ	2.20	0.72
48:SK:4:ARG:NH2	48:SK:210:THR:O	2.23	0.72
3:L3:695:G:O2’	3:L3:697:G:OP2	2.08	0.71
19:LJ:126:LYS:NZ	37:NL:286:GLN:O	2.23	0.71
3:L3:1433:A:N6	3:L3:1451:G:O2’	2.24	0.71
3:L3:2480:G:OP1	49:SM:22:LYS:NZ	2.23	0.71
2:L1:75:OMG:OP2	18:LI:74:TYR:OH	2.08	0.71
48:SK:99:GLU:OE1	48:SK:125:THR:OG1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:2896:G:OP1	13:LD:136:ARG:NH1	2.24	0.70
3:L3:375:G:OP2	32:LW:52:LYS:NZ	2.23	0.70
3:L3:1998:A:N3	3:L3:2019:C:O2'	2.24	0.70
2:L1:71:A:O2'	2:L1:83:C:N4	2.25	0.70
3:L3:2487:G:OP1	37:NL:456:ARG:NH2	2.23	0.70
1:BE:29:ALA:N	1:BE:62:SER:HG	1.89	0.70
3:L3:2475:G:O6	17:LH:47:ARG:NH1	2.25	0.70
3:L3:2763:U:O2'	37:NL:391:ARG:NH2	2.26	0.69
3:L3:4476:C:O2'	45:SG:173:ARG:NH2	2.25	0.69
39:SA:54:VAL:HG11	39:SA:101:MET:HE1	1.74	0.69
49:SM:370:ASP:OD2	49:SM:372:ARG:NH2	2.26	0.69
18:LI:83:GLU:OE2	18:LI:84:ARG:NH2	2.26	0.68
24:LO:103:ASP:OD1	24:LO:106:ARG:NH2	2.27	0.68
3:L3:386:A:O2'	18:LI:87:ARG:NH1	2.27	0.68
4:L4:12:U:O3'	4:L4:109:U:O2'	2.08	0.68
3:L3:1280:C:O2'	39:SA:321:ASN:OD1	2.09	0.68
3:L3:1744:PSU:H2'	3:L3:1745:G:H8	1.58	0.67
3:L3:489:C:O2'	3:L3:667:A:N6	2.27	0.67
2:L1:110:U:OP2	32:LW:20:ARG:NH2	2.28	0.67
3:L3:508:G:O2'	3:L3:510:U:OP2	2.01	0.67
3:L3:408:A:O2'	3:L3:411:G:OP2	2.10	0.67
3:L3:85:G:O2'	11:LB:168:ARG:NH1	2.28	0.67
49:SM:337:GLU:OE1	49:SM:380:ARG:NH2	2.28	0.66
9:L9:17:ASP:OD1	9:L9:20:ARG:NH2	2.28	0.66
16:LG:115:SER:OG	48:SK:145:GLN:OE1	2.13	0.65
23:LN:160:ILE:HD11	23:LN:190:VAL:HG13	1.77	0.65
35:LZ:21:ARG:NH1	35:LZ:22:PRO:O	2.30	0.65
19:LJ:92:ASP:OD1	19:LJ:94:THR:OG1	2.05	0.65
3:L3:404:U:O3'	18:LI:87:ARG:NH2	2.30	0.65
3:L3:937:U:OP1	8:L8:46:ARG:NH1	2.29	0.65
3:L3:2448:G:O2'	44:SF:21:LYS:NZ	2.28	0.65
34:LY:4:LYS:NZ	34:LY:6:GLU:OE2	2.28	0.65
3:L3:2841:G:OP1	38:NP:10:HIS:NE2	2.26	0.65
3:L3:2848:G:O2'	3:L3:3838:U:O4	2.07	0.65
1:BE:193:ASP:OD1	3:L3:1751:A:O2'	2.12	0.65
6:L6:146:LEU:HD12	6:L6:146:LEU:O	1.96	0.65
3:L3:121:A:OP1	43:SE:110:LYS:NZ	2.27	0.64
3:L3:1874:A:O2'	3:L3:4219:A:N3	2.26	0.64
3:L3:3906:A:OP1	39:SA:71:ARG:NH1	2.30	0.64
3:L3:1743:A:O2'	3:L3:1744:PSU:H5"	1.96	0.64
3:L3:2300:A:N7	39:SA:143:ARG:NH1	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:1325:C:H2’	3:L3:1326:A2M:H5’	1.79	0.64
3:L3:3673:C:OP1	9:L9:67:ARG:NH2	2.30	0.64
3:L3:4765:G:OP1	45:SG:23:ARG:NE	2.29	0.64
47:SI:153:ASN:ND2	49:SM:263:GLY:O	2.30	0.64
3:L3:119:G:O4’	43:SE:132:ARG:NH1	2.31	0.63
3:L3:4117:U:O4’	43:SE:43:GLN:NE2	2.31	0.63
3:L3:2601:A:N6	3:L3:2744:A:OP2	2.31	0.63
4:L4:23:A:N3	4:L4:118:C:O2’	2.26	0.63
16:LG:115:SER:O	16:LG:135:ASN:ND2	2.32	0.62
3:L3:1744:PSU:H2’	3:L3:1745:G:C8	2.34	0.62
3:L3:2318:G:N2	3:L3:2321:G:OP2	2.22	0.62
3:L3:4314:C:O2’	22:LM:36:ASP:OD1	2.15	0.62
29:LT:54:LYS:O	29:LT:66:LYS:NZ	2.28	0.62
37:NL:427:SER:OG	49:SM:379:ASP:OD1	2.18	0.62
3:L3:2724:G:O2’	3:L3:2726:G:OP2	2.16	0.61
3:L3:235:A:OP1	39:SA:201:ARG:NH2	2.33	0.61
1:BE:150:GLU:OE2	1:BE:154:ARG:NH2	2.33	0.61
4:L4:117:G:OP1	40:SB:253:TYR:OH	2.14	0.61
3:L3:1255:A:OP1	3:L3:1257:A:N6	2.34	0.60
20:LK:38:LEU:O	20:LK:42:ARG:NH1	2.34	0.60
3:L3:935:A:O2’	8:L8:46:ARG:NH1	2.35	0.60
1:BE:54:SER:HB2	1:BE:135:ILE:HD11	1.82	0.60
23:LN:199:GLU:OE1	23:LN:199:GLU:N	2.34	0.60
3:L3:1724:G:N2	22:LM:13:SER:O	2.31	0.60
3:L3:3734:PSU:H2’	3:L3:3735:G:O4’	2.02	0.60
3:L3:4985:U:O2	23:LN:174:ARG:NH1	2.35	0.59
37:NL:452:GLU:OE2	37:NL:454:ARG:NH1	2.36	0.59
3:L3:4678:G:OP2	36:NK:14:ARG:NH1	2.36	0.59
3:L3:4259:C:OP2	5:L5:54:ARG:NH2	2.36	0.59
3:L3:2262:G:OP2	21:LL:98:ARG:NH1	2.32	0.59
3:L3:4124:G:N2	43:SE:43:GLN:O	2.36	0.59
3:L3:690:C:OP1	21:LL:87:ARG:NH1	2.36	0.58
3:L3:67:C:OP2	3:L3:312:G:N2	2.34	0.58
3:L3:3700:C:O2’	3:L3:3774:A:N3	2.33	0.58
43:SE:90:GLN:NE2	47:SI:62:GLU:OE2	2.36	0.58
3:L3:4213:A:H2’	22:LM:9:THR:HG21	1.85	0.58
3:L3:346:G:OP1	18:LI:8:THR:HG23	2.04	0.58
3:L3:1534:A2M:HM’3	3:L3:1637:A:C4	2.39	0.58
3:L3:431:G:N2	3:L3:3889:G:OP2	2.37	0.57
23:LN:353:VAL:HG23	36:NK:25:GLU:HG3	1.84	0.57
47:SI:67:ASP:OD1	47:SI:70:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4623:OMG:OP1	23:LN:19:ARG:NH2	2.34	0.57
35:LZ:9:ILE:HD12	35:LZ:51:LEU:HD21	1.87	0.57
38:NP:72:ASP:OD1	38:NP:73:SER:N	2.37	0.57
3:L3:4910:G:N2	7:L7:106:ASP:O	2.37	0.57
3:L3:1366:G:N2	3:L3:1371:A:OP2	2.38	0.57
3:L3:3718:A2M:H2	3:L3:3934:G:O4’	2.05	0.57
3:L3:5053:U:O2’	3:L3:5054:C:OP2	2.19	0.56
3:L3:2493:G:O4’	49:SM:36:ARG:NH2	2.38	0.56
3:L3:4678:G:N7	36:NK:11:ARG:NH2	2.53	0.56
21:LL:28:GLU:OE2	21:LL:42:GLY:N	2.37	0.56
2:L1:69:PSU:H2’	2:L1:70:G:O4’	2.06	0.56
3:L3:5022:U:O2’	3:L3:5023:C:OP2	2.19	0.56
3:L3:2588:C:OP1	3:L3:2768:C:O2’	2.21	0.56
9:L9:126:THR:HG23	9:L9:127:TYR:CD2	2.41	0.56
19:LJ:29:ILE:O	19:LJ:31:ASP:N	2.39	0.56
45:SG:113:GLU:OE1	45:SG:115:ARG:NH2	2.38	0.56
3:L3:1273:G:N7	22:LM:117:ARG:NH1	2.53	0.56
2:L1:62:A:OP1	28:LS:52:LYS:NZ	2.39	0.55
3:L3:2758:G:OP1	37:NL:405:ARG:NH1	2.39	0.55
3:L3:2876:OMG:HM22	3:L3:2877:G:H5’	1.87	0.55
24:LO:17:ARG:NH1	24:LO:107:SER:OG	2.39	0.55
39:SA:65:GLU:OE1	39:SA:65:GLU:N	2.39	0.55
3:L3:2922:G:O2’	3:L3:3275:A:N6	2.39	0.55
3:L3:3617:G:O6	38:NP:87:LYS:NZ	2.33	0.55
3:L3:3623:C:O2	13:LD:82:LYS:NZ	2.39	0.55
7:L7:182:GLU:OE2	8:L8:119:ARG:NH2	2.40	0.55
3:L3:369:G:N2	3:L3:372:A:OP2	2.35	0.55
3:L3:2695:A:OP1	34:LY:35:LYS:NZ	2.40	0.55
3:L3:1238:A:O2’	42:SD:52:GLU:OE2	2.25	0.55
3:L3:1741:G:H3’	3:L3:1742:A:H5”	1.89	0.55
3:L3:4126:C:OP1	43:SE:37:LYS:NZ	2.34	0.55
3:L3:4529:G:O2’	3:L3:4530:UR3:H5’	2.07	0.55
3:L3:1595:G:N2	51:SR:634:ARG:OXT	2.28	0.54
3:L3:1326:A2M:H2’	3:L3:1327:C:C6	2.42	0.54
3:L3:1573:G:OP1	13:LD:92:LYS:NZ	2.39	0.54
7:L7:190:ASP:OD1	7:L7:191:LYS:N	2.40	0.54
3:L3:1734:G:N2	3:L3:1735:U:O4	2.32	0.54
3:L3:4520:G:OP2	23:LN:2:SER:N	2.40	0.54
23:LN:113:GLU:OE2	23:LN:169:ARG:NH1	2.41	0.54
3:L3:5001:PSU:H2’	3:L3:5002:U:O4’	2.07	0.54
3:L3:2351:OMC:HM22	3:L3:2352:U:H5’	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:36:LEU:HD11	1:BE:69:ARG:HG2	1.89	0.54
12:LC:24:THR:HG23	12:LC:24:THR:O	2.08	0.54
1:BE:145:LYS:O	1:BE:148:VAL:HG22	2.08	0.53
48:SK:107:VAL:HG12	48:SK:108:THR:HG23	1.90	0.53
21:LL:32:LEU:O	21:LL:113:ARG:NH1	2.40	0.53
3:L3:2351:OMC:HM23	39:SA:95:MET:HG3	1.91	0.53
3:L3:4934:A:O2’	3:L3:4935:C:OP2	2.19	0.53
3:L3:5068:G:N2	3:L3:5069:U:O4	2.33	0.53
33:LX:26:VAL:HG21	44:SF:180:LEU:HD11	1.90	0.53
3:L3:2361:G:O6	10:LA:25:HIS:ND1	2.41	0.53
22:LM:50:ASN:O	22:LM:50:ASN:ND2	2.41	0.53
3:L3:151:G:OP2	9:L9:4:TYR:OH	2.24	0.53
3:L3:2414:G:O2’	3:L3:2415:OMU:O5’	2.15	0.53
2:L1:26:C:O2’	39:SA:53:ALA:O	2.24	0.53
3:L3:1325:C:C2’	3:L3:1326:A2M:H5’	2.38	0.52
3:L3:1364:U:OP2	6:L6:36:ARG:NH2	2.41	0.52
39:SA:154:VAL:HG11	39:SA:174:LEU:HD11	1.91	0.52
3:L3:453:G:H1	3:L3:1293:G:H22	1.57	0.52
3:L3:2624:G:N7	15:LF:88:LYS:NZ	2.56	0.52
3:L3:3718:A2M:H2	3:L3:3934:G:C1’	2.38	0.52
3:L3:4546:A:N7	44:SF:215:ASN:ND2	2.56	0.52
3:L3:1677:PSU:H4’	3:L3:1680:G:C2	2.45	0.52
3:L3:1326:A2M:H2’	3:L3:1327:C:H6	1.75	0.52
7:L7:202:LEU:O	7:L7:202:LEU:HD23	2.10	0.52
3:L3:1860:PSU:H2’	3:L3:1861:U:C6	2.44	0.52
3:L3:4717:A:OP2	23:LN:30:LYS:NZ	2.40	0.52
3:L3:1508:A:OP1	39:SA:110:ARG:NH2	2.40	0.52
3:L3:2368:A:N6	3:L3:2827:G:O2’	2.43	0.52
48:SK:116:LEU:HD13	48:SK:177:LEU:HD21	1.92	0.52
3:L3:2562:G:O2’	3:L3:2565:A:N6	2.43	0.51
49:SM:170:HIS:HB3	49:SM:283:LEU:HD11	1.92	0.51
3:L3:1548:G:O2’	3:L3:2812:A:N3	2.41	0.51
14:LE:94:GLU:OE1	14:LE:94:GLU:N	2.43	0.51
1:BE:198:LYS:NZ	3:L3:1780:A:O2’	2.35	0.51
3:L3:2590:G:O2’	3:L3:2755:A:N6	2.40	0.51
3:L3:2815:A2M:H2’	3:L3:2816:G:C8	2.46	0.51
3:L3:4620:OMU:OP2	3:L3:4670:C:N4	2.35	0.51
18:LI:53:ASP:OD2	18:LI:115:ARG:NH2	2.43	0.51
3:L3:2258:C:N3	41:SC:90:ALA:N	2.58	0.50
3:L3:4139:G:H21	3:L3:4140:C:N4	2.09	0.50
3:L3:4280:A:N6	40:SB:28:THR:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LQ:26:ASP:OD1	26:LQ:27:ARG:N	2.44	0.50
33:LX:45:THR:HG23	33:LX:45:THR:O	2.12	0.50
39:SA:209:ILE:HB	39:SA:229:LEU:HD13	1.92	0.50
3:L3:4637:OMG:H2'	3:L3:4638:U:C6	2.47	0.50
23:LN:378:ARG:NH1	52:SV:9:CYS:SG	2.84	0.50
40:SB:62:CYS:HB3	40:SB:105:LEU:HD22	1.93	0.50
29:LT:110:ILE:O	41:SC:141:ARG:NH2	2.45	0.50
41:SC:161:ARG:O	41:SC:182:ASN:ND2	2.45	0.50
2:L1:83:C:H41	18:LI:50:ARG:HH21	1.58	0.50
3:L3:1778:C:O2'	3:L3:1779:PSU:H5"	2.11	0.50
39:SA:8:ILE:HD11	39:SA:24:LEU:HD13	1.94	0.50
3:L3:4252:C:OP2	3:L3:4253:A:O2'	2.25	0.50
6:L6:62:PRO:O	6:L6:63:THR:HG23	2.12	0.50
3:L3:4075:U:OP1	43:SE:249:ARG:NH1	2.44	0.49
3:L3:1607:C:O2'	3:L3:3828:A:N3	2.43	0.49
3:L3:1814:C:O2'	22:LM:42:ASN:OD1	2.24	0.49
47:SI:253:GLN:O	49:SM:149:ARG:NH1	2.41	0.49
3:L3:2470:C:O2'	43:SE:56:LYS:NZ	2.31	0.49
3:L3:4670:C:O2'	3:L3:4672:A:OP2	2.27	0.49
33:LX:26:VAL:HG22	44:SF:178:PRO:HD2	1.94	0.49
3:L3:62:A:N3	3:L3:77:U:O2'	2.40	0.49
3:L3:1621:A:OP2	32:LW:30:GLN:NE2	2.45	0.49
10:LA:36:ILE:HD11	10:LA:47:TYR:HD2	1.77	0.49
23:LN:220:ILE:HG12	23:LN:278:THR:HG23	1.95	0.49
47:SI:249:GLN:OE1	49:SM:267:LEU:HD21	2.13	0.49
3:L3:1369:C:OP2	3:L3:1370:G:O2'	2.20	0.49
3:L3:2322:G:OP2	26:LQ:34:ASN:ND2	2.45	0.49
23:LN:222:VAL:O	23:LN:343:ARG:NH1	2.46	0.49
3:L3:122:U:O4	43:SE:107:LYS:NZ	2.33	0.49
3:L3:4894:A:OP1	8:L8:129:LYS:NZ	2.42	0.48
2:L1:50:C:O2'	51:SR:578:SER:OG	2.22	0.48
3:L3:3939:G:O2'	3:L3:4076:G:N2	2.41	0.48
3:L3:4635:A:H3'	3:L3:4636:PSU:H4'	1.94	0.48
15:LF:25:CYS:O	15:LF:29:VAL:HG22	2.13	0.48
49:SM:150:THR:OG1	49:SM:153:CYS:SG	2.57	0.48
3:L3:1532:G:OP2	32:LW:31:LYS:NZ	2.44	0.48
41:SC:253:VAL:HG12	41:SC:257:ILE:HD12	1.95	0.48
34:LY:54:GLU:OE2	34:LY:58:GLN:NE2	2.41	0.48
39:SA:211:TYR:OH	39:SA:218:ILE:HD11	2.14	0.48
3:L3:3868:G:O2'	3:L3:3869:OMC:H5"	2.13	0.48
12:LC:95:ARG:NH2	12:LC:112:ASP:OD2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NP:120:PRO:O	38:NP:121:THR:OG1	2.20	0.48
1:BE:162:ARG:NH2	12:LC:88:SER:OG	2.47	0.48
40:SB:128:ASP:OD1	40:SB:129:GLU:N	2.44	0.48
41:SC:161:ARG:NH1	41:SC:273:SER:OG	2.47	0.48
41:SC:203:ILE:O	41:SC:203:ILE:HG22	2.14	0.48
46:SH:123:PRO:O	46:SH:126:VAL:HG12	2.13	0.48
3:L3:295:A:OP2	31:LV:39:ARG:NH1	2.41	0.47
3:L3:4927:G:OP2	3:L3:4927:G:N2	2.29	0.47
35:LZ:9:ILE:HG23	35:LZ:51:LEU:HD21	1.96	0.47
49:SM:265:TYR:HB3	49:SM:362:ILE:HD11	1.96	0.47
3:L3:1355:G:OP1	11:LB:108:ARG:NH1	2.41	0.47
33:LX:69:TRP:NE1	44:SF:173:GLY:O	2.45	0.47
41:SC:281:ILE:CG2	41:SC:286:LEU:HD11	2.45	0.47
3:L3:4476:C:O2'	3:L3:4477:A:OP2	2.27	0.47
3:L3:4541:G:N2	3:L3:4544:A:OP2	2.37	0.47
3:L3:4202:U:O2'	3:L3:4203:A:OP2	2.26	0.47
2:L1:50:C:HO2'	51:SR:578:SER:HG	1.50	0.47
3:L3:2861:OMC:H1'	3:L3:2861:OMC:HM23	1.44	0.47
34:LY:17:ARG:NH2	34:LY:19:ASP:OD2	2.47	0.47
19:LJ:5:MET:O	19:LJ:28:ASN:ND2	2.44	0.47
23:LN:107:ALA:HB2	23:LN:201:LEU:HG	1.96	0.47
42:SD:203:GLU:OE1	42:SD:203:GLU:N	2.44	0.47
48:SK:175:SER:O	48:SK:178:GLN:NE2	2.48	0.47
37:NL:188:VAL:O	49:SM:163:ARG:NH1	2.48	0.47
37:NL:190:ARG:NH2	49:SM:117:ASP:OD1	2.46	0.47
3:L3:2097:U:O3'	3:L3:2098:G:H4'	2.15	0.47
3:L3:4494:OMG:HM21	16:LG:22:VAL:HG21	1.96	0.47
3:L3:3925:OMU:HM23	3:L3:3925:OMU:H1'	1.52	0.46
3:L3:4593:C:OP2	36:NK:2:ALA:N	2.48	0.46
4:L4:7:G:OP1	40:SB:33:ARG:NH1	2.48	0.46
11:LB:22:ASP:OD2	39:SA:283:LYS:NZ	2.35	0.46
3:L3:1646:A:O2'	32:LW:49:TRP:O	2.27	0.46
3:L3:4524:G:C2	23:LN:252:ALA:HB1	2.49	0.46
24:LO:50:ASN:ND2	24:LO:75:SER:O	2.48	0.46
25:LP:84:ILE:HD11	25:LP:108:TYR:CE1	2.49	0.46
3:L3:2630:U:O4	15:LF:89:LYS:NZ	2.43	0.46
3:L3:3718:A2M:HM'3	3:L3:3718:A2M:H1'	1.70	0.46
19:LJ:10:VAL:HG11	19:LJ:129:TRP:HZ3	1.80	0.46
43:SE:58:PRO:HD2	43:SE:61:ILE:HD12	1.96	0.46
44:SF:65:ASP:OD2	44:SF:72:ARG:NE	2.48	0.46
46:SH:105:THR:HG23	46:SH:106:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:223:G:OP2	39:SA:165:LYS:NZ	2.49	0.46
3:L3:3744:OMG:HM23	3:L3:3744:OMG:H1'	1.63	0.46
3:L3:3938:G:N2	3:L3:4171:C:OP2	2.47	0.46
3:L3:4296:PSU:H2'	3:L3:4297:G:O4'	2.15	0.46
21:LL:20:ARG:NH1	26:LQ:78:LEU:O	2.46	0.46
24:LO:50:ASN:OD1	24:LO:51:ASN:N	2.49	0.46
3:L3:1279:A:O2'	3:L3:1281:G:N7	2.43	0.46
3:L3:1340:OMC:HM23	3:L3:1340:OMC:H1'	1.49	0.46
3:L3:4872:G:O6	8:L8:98:ARG:NH1	2.49	0.46
47:SI:182:ILE:HD11	47:SI:194:LEU:HD13	1.98	0.46
3:L3:730:G:OP2	42:SD:76:ARG:NE	2.49	0.46
3:L3:3723:A:H2'	3:L3:3724:A2M:H8	1.98	0.46
9:L9:124:ASP:OD1	9:L9:125:SER:N	2.47	0.46
19:LJ:100:VAL:HG13	19:LJ:107:LYS:HA	1.97	0.46
3:L3:4724:A:O2'	23:LN:104:THR:HG22	2.16	0.46
8:L8:81:ASP:HB3	8:L8:84:THR:HG22	1.98	0.46
3:L3:3641:U:OP2	3:L3:3646:A:N6	2.42	0.46
6:L6:7:GLY:O	20:LK:49:HIS:NE2	2.48	0.46
24:LO:31:TYR:OH	24:LO:59:GLU:OE1	2.21	0.46
43:SE:103:ARG:NH2	43:SE:192:ARG:O	2.48	0.46
4:L4:48:G:O2'	4:L4:49:A:C8	2.68	0.45
9:L9:103:GLU:OE2	9:L9:165:THR:HG21	2.17	0.45
17:LH:143:ASP:N	17:LH:143:ASP:OD1	2.49	0.45
41:SC:50:LEU:HD23	41:SC:50:LEU:H	1.80	0.45
2:L1:83:C:H41	18:LI:50:ARG:NH2	2.14	0.45
3:L3:2815:A2M:HM'3	3:L3:2815:A2M:H1'	1.80	0.45
2:L1:152:U:OP1	3:L3:4162:C:N4	2.49	0.45
3:L3:4361:PSU:H2'	3:L3:4362:A:O4'	2.16	0.45
7:L7:54:TYR:OH	7:L7:73:PHE:O	2.33	0.45
44:SF:129:ALA:O	44:SF:169:VAL:HG11	2.15	0.45
3:L3:469:C:N3	41:SC:105:ARG:NH1	2.65	0.45
3:L3:2424:OMG:HM23	3:L3:2424:OMG:H1'	1.65	0.45
23:LN:67:VAL:O	23:LN:67:VAL:HG22	2.17	0.45
37:NL:254:HIS:CE1	37:NL:258:LEU:HD11	2.52	0.45
41:SC:154:THR:HG23	41:SC:155:GLY:N	2.31	0.45
3:L3:2804:OMC:HM23	3:L3:2804:OMC:H1'	1.70	0.45
3:L3:3718:A2M:H2	3:L3:3934:G:H1'	1.97	0.45
51:SR:442:ILE:HD13	52:SV:89:THR:HG21	1.98	0.45
19:LJ:76:ASN:OD1	19:LJ:77:TYR:N	2.50	0.45
49:SM:33:ASP:OD1	49:SM:36:ARG:NH1	2.50	0.45
3:L3:308:G:OP2	3:L3:308:G:N2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:496:G:O2'	3:L3:497:G:OP1	2.27	0.45
10:LA:6:LEU:HD12	10:LA:116:HIS:CD2	2.52	0.45
3:L3:1326:A2M:H1'	3:L3:1326:A2M:HM'3	1.65	0.45
3:L3:1677:PSU:H4'	3:L3:1680:G:N1	2.31	0.45
3:L3:1727:U:OP1	42:SD:131:ASN:ND2	2.48	0.45
3:L3:3841:OMC:HM23	3:L3:3841:OMC:H1'	1.66	0.45
3:L3:1178:G:H21	40:SB:286:SER:HB3	1.82	0.44
3:L3:4201:G:O2'	3:L3:4202:U:OP2	2.28	0.44
3:L3:4637:OMG:HM23	3:L3:4637:OMG:H1'	1.53	0.44
3:L3:4768:G:OP1	7:L7:168:TYR:OH	2.30	0.44
4:L4:13:A:P	4:L4:109:U:HO2'	2.37	0.44
15:LF:60:VAL:HG11	15:LF:76:VAL:HG13	2.00	0.44
1:BE:146:GLU:OE1	1:BE:146:GLU:N	2.46	0.44
3:L3:2579:G:N2	3:L3:2582:A:OP2	2.29	0.44
19:LJ:87:VAL:HG11	19:LJ:89:ILE:HD12	1.99	0.44
37:NL:225:PRO:HD2	37:NL:228:LEU:HD12	1.98	0.44
44:SF:132:ASN:O	44:SF:169:VAL:HG12	2.17	0.44
48:SK:49:VAL:HG12	48:SK:50:HIS:O	2.18	0.44
3:L3:2364:OMG:HM23	3:L3:2364:OMG:H1'	1.74	0.44
3:L3:4759:C:O2	7:L7:165:LYS:NZ	2.43	0.44
15:LF:108:GLU:N	15:LF:108:GLU:OE1	2.51	0.44
3:L3:3851:PSU:H2'	3:L3:3852:A:O4'	2.17	0.44
3:L3:1366:G:C2	6:L6:33:ILE:HD13	2.53	0.44
3:L3:1482:G:N7	6:L6:188:ASN:ND2	2.65	0.44
3:L3:2837:OMU:HM23	3:L3:2837:OMU:H1'	1.60	0.44
32:LW:21:ARG:NH2	32:LW:41:ALA:O	2.40	0.44
2:L1:75:OMG:HM23	2:L1:75:OMG:H1'	1.50	0.43
3:L3:4392:OMG:HM23	3:L3:4392:OMG:H1'	1.74	0.43
3:L3:3887:OMC:H6	3:L3:3887:OMC:C5'	2.31	0.43
1:BE:36:LEU:HD11	1:BE:69:ARG:CG	2.48	0.43
3:L3:3268:C:OP1	37:NL:375:LYS:NZ	2.47	0.43
45:SG:118:LEU:HD21	45:SG:177:ASP:OD2	2.18	0.43
47:SI:193:CYS:SG	47:SI:194:LEU:N	2.91	0.43
48:SK:163:PRO:HG3	48:SK:185:THR:HG22	1.99	0.43
3:L3:1877:G:H1'	22:LM:8:THR:HG23	1.99	0.43
13:LD:7:GLN:OE1	13:LD:7:GLN:N	2.50	0.43
51:SR:487:ILE:HA	52:SV:134:ILE:HD11	2.00	0.43
1:BE:58:GLU:N	1:BE:58:GLU:OE1	2.52	0.43
6:L6:100:PRO:O	30:LU:25:ARG:NH2	2.50	0.43
25:LP:95:ASP:OD1	25:LP:96:GLU:N	2.52	0.43
3:L3:1860:PSU:H2'	3:L3:1861:U:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4305:G:O2'	3:L3:4306:OMU:O5'	2.32	0.43
47:SI:83:VAL:O	47:SI:83:VAL:HG12	2.19	0.43
1:BE:29:ALA:N	1:BE:62:SER:OG	2.51	0.43
3:L3:2326:G:OP1	26:LQ:108:ARG:NH2	2.52	0.43
33:LX:8:VAL:O	33:LX:11:VAL:HG22	2.19	0.43
3:L3:748:G:N2	12:LC:147:ASP:O	2.52	0.43
3:L3:1895:G:OP1	42:SD:96:ARG:NH2	2.52	0.43
3:L3:4618:OMG:HM22	3:L3:4619:U:H5'	2.01	0.43
7:L7:185:VAL:HG13	8:L8:126:GLU:HG3	2.01	0.43
37:NL:248:ASN:ND2	49:SM:420:PRO:O	2.52	0.42
3:L3:3830:A2M:HM'3	3:L3:3830:A2M:H1'	1.81	0.42
14:LE:136:ARG:NH2	42:SD:86:GLU:OE2	2.52	0.42
3:L3:3886:G:H2'	3:L3:3887:OMC:H5'	2.01	0.42
39:SA:122:TYR:HE1	39:SA:280:PRO:CB	2.33	0.42
48:SK:199:VAL:HG23	48:SK:204:ALA:HB2	2.00	0.42
3:L3:398:A2M:HM'3	3:L3:398:A2M:H1'	1.81	0.42
3:L3:1438:U:O2'	3:L3:1439:C:OP1	2.32	0.42
3:L3:3715:PSU:H2'	3:L3:3716:C:O4'	2.19	0.42
3:L3:4457:PSU:H1'	23:LN:252:ALA:HB3	2.00	0.42
3:L3:1358:G:O2'	3:L3:1360:G:O6	2.30	0.42
3:L3:4587:G:OP1	7:L7:61:ARG:NH1	2.51	0.42
17:LH:119:ILE:HD12	17:LH:140:LEU:HD22	2.02	0.42
26:LQ:114:ARG:NH1	26:LQ:117:GLN:OE1	2.50	0.42
46:SH:79:SER:O	46:SH:83:GLY:N	2.47	0.42
3:L3:981:C:OP2	41:SC:71:ARG:NH2	2.53	0.42
3:L3:3605:C:OP2	13:LD:71:ARG:NE	2.45	0.42
3:L3:3920:PSU:H2'	3:L3:3921:U:C6	2.55	0.42
9:L9:165:THR:HG22	9:L9:166:SER:N	2.34	0.42
17:LH:138:VAL:HG23	17:LH:138:VAL:O	2.20	0.42
47:SI:101:ARG:NH1	47:SI:122:LYS:O	2.52	0.42
1:BE:36:LEU:HD13	1:BE:73:ASN:HB2	2.02	0.42
3:L3:3613:U:OP2	38:NP:90:LYS:NZ	2.49	0.42
3:L3:4500:PSU:H2'	3:L3:4501:U:C6	2.55	0.42
7:L7:84:VAL:HG11	7:L7:102:LEU:HD22	2.02	0.42
47:SI:181:VAL:O	47:SI:185:HIS:ND1	2.45	0.42
3:L3:655:C:OP2	39:SA:268:ARG:NH2	2.53	0.42
3:L3:2809:G:O2'	3:L3:4644:G:OP1	2.35	0.42
1:BE:36:LEU:HD21	1:BE:69:ARG:HH11	1.85	0.42
3:L3:1190:C:H2'	3:L3:1191:C:C6	2.54	0.42
6:L6:94:ILE:HG23	6:L6:124:LEU:HD21	2.02	0.42
1:BE:91:LEU:HD11	1:BE:129:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:3627:OMG:HM23	3:L3:3627:OMG:H1’	1.71	0.41
3:L3:3904:G:O3’	39:SA:71:ARG:HD3	2.20	0.41
3:L3:1352:C:O2’	3:L3:1356:U:OP1	2.38	0.41
3:L3:4636:PSU:N1	25:LP:79:ASN:OD1	2.53	0.41
43:SE:159:HIS:ND1	43:SE:185:LYS:HA	2.35	0.41
3:L3:4745:G:H22	3:L3:4955:A:H2	1.67	0.41
47:SI:105:ILE:HG13	47:SI:105:ILE:O	2.21	0.41
3:L3:4260:U:H2’	3:L3:4261:C:C6	2.55	0.41
10:LA:7:ASP:OD1	10:LA:7:ASP:N	2.47	0.41
49:SM:362:ILE:HG22	49:SM:363:GLY:N	2.36	0.41
3:L3:398:A2M:O5’	3:L3:398:A2M:H8	2.20	0.41
3:L3:1871:A2M:H1’	3:L3:1871:A2M:HM’3	1.76	0.41
3:L3:4266:G:H2’	3:L3:4266:G:N3	2.36	0.41
3:L3:4571:A2M:H8	3:L3:4571:A2M:O5’	2.21	0.41
3:L3:5022:U:HO2’	3:L3:5023:C:P	2.42	0.41
5:L5:139:PHE:HA	5:L5:151:ILE:HD13	2.02	0.41
39:SA:54:VAL:HG11	39:SA:101:MET:CE	2.44	0.41
3:L3:72:C:N3	6:L6:60:ARG:NH1	2.69	0.41
3:L3:287:U:O2’	9:L9:91:GLN:OE1	2.37	0.41
3:L3:2691:U:C2	3:L3:2692:U:C5	3.08	0.41
16:LG:83:ARG:NH1	16:LG:120:PRO:O	2.48	0.41
3:L3:1693:U:OP2	11:LB:49:LYS:NZ	2.46	0.41
3:L3:3899:OMG:HM23	3:L3:3899:OMG:H1’	1.61	0.41
6:L6:64:VAL:O	6:L6:67:HIS:ND1	2.54	0.41
7:L7:203:VAL:HG22	7:L7:203:VAL:O	2.21	0.41
37:NL:209:GLN:HB2	37:NL:214:LEU:HD11	2.03	0.41
52:SV:56:ARG:HG3	52:SV:61:LYS:HB2	2.02	0.41
3:L3:131:C:N4	3:L3:138:G:O6	2.54	0.41
3:L3:1288:G:OP1	41:SC:134:SER:OG	2.35	0.41
3:L3:1881:C:O2	3:L3:1881:C:H2’	2.20	0.41
3:L3:2859:G:H21	3:L3:3837:C:H1’	1.85	0.41
3:L3:3724:A2M:HM’2	3:L3:3725:G:O4’	2.21	0.41
3:L3:4155:C:OP2	37:NL:464:LYS:NZ	2.39	0.41
3:L3:4457:PSU:O4	23:LN:252:ALA:HB3	2.20	0.41
8:L8:36:ALA:HB2	8:L8:52:PHE:CE1	2.56	0.41
15:LF:28:PRO:HB3	15:LF:100:LEU:HD11	2.02	0.41
33:LX:26:VAL:HG12	33:LX:30:GLU:HG3	2.02	0.41
3:L3:158:A:N1	3:L3:276:C:O2’	2.44	0.41
48:SK:222:PHE:O	48:SK:224:LEU:N	2.53	0.41
2:L1:68:G:O2’	2:L1:69:PSU:H5”	2.22	0.40
3:L3:1683:PSU:OP1	20:LK:44:ASN:ND2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4226:G:O2'	3:L3:4227:OMU:H5"	2.20	0.40
23:LN:61:ASP:OD2	51:SR:410:ILE:HG23	2.21	0.40
45:SG:103:VAL:HG11	45:SG:144:LEU:HD21	2.03	0.40
3:L3:2289:C:O2'	21:LL:22:LYS:NZ	2.37	0.40
3:L3:2299:G:OP1	39:SA:182:LYS:NZ	2.47	0.40
20:LK:100:ILE:HD13	20:LK:123:ILE:HB	2.03	0.40
3:L3:3717:A:H2'	3:L3:3718:A2M:H8	2.04	0.40
3:L3:4494:OMG:O5'	3:L3:4494:OMG:H8	2.04	0.40
9:L9:143:ARG:HH11	28:LS:95:LEU:HD23	1.86	0.40
3:L3:1481:C:N3	30:LU:4:ARG:NH1	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BE	156/214 (73%)	151 (97%)	5 (3%)	0	100	100
5	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
6	L6	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
7	L7	199/203 (98%)	199 (100%)	0	0	100	100
8	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
9	L9	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
10	LA	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
11	LB	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
12	LC	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
13	LD	152/196 (78%)	152 (100%)	0	0	100	100
14	LE	150/160 (94%)	143 (95%)	7 (5%)	0	100	100
15	LF	101/128 (79%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LG	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
17	LH	141/156 (90%)	141 (100%)	0	0	100	100
18	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
19	LJ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
20	LK	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
21	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
22	LM	90/159 (57%)	88 (98%)	2 (2%)	0	100	100
23	LN	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
24	LO	93/115 (81%)	92 (99%)	1 (1%)	0	100	100
25	LP	104/125 (83%)	104 (100%)	0	0	100	100
26	LQ	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
27	LR	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
28	LS	120/123 (98%)	120 (100%)	0	0	100	100
29	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
30	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
31	LV	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
32	LW	84/97 (87%)	84 (100%)	0	0	100	100
33	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
34	LY	67/70 (96%)	67 (100%)	0	0	100	100
35	LZ	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
36	NK	63/129 (49%)	63 (100%)	0	0	100	100
37	NL	259/478 (54%)	258 (100%)	1 (0%)	0	100	100
38	NP	104/134 (78%)	103 (99%)	1 (1%)	0	100	100
39	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
40	SB	290/297 (98%)	287 (99%)	3 (1%)	0	100	100
41	SC	211/288 (73%)	205 (97%)	6 (3%)	0	100	100
42	SD	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
43	SE	228/266 (86%)	225 (99%)	3 (1%)	0	100	100
44	SF	243/257 (95%)	233 (96%)	10 (4%)	0	100	100
45	SG	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
46	SH	92/293 (31%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	SI	232/255 (91%)	227 (98%)	5 (2%)	0	100	100
48	SK	224/245 (91%)	216 (96%)	8 (4%)	0	100	100
49	SM	393/588 (67%)	388 (99%)	5 (1%)	0	100	100
50	SQ	119/239 (50%)	117 (98%)	2 (2%)	0	100	100
51	SR	237/634 (37%)	236 (100%)	1 (0%)	0	100	100
52	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	8025/10060 (80%)	7885 (98%)	140 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BE	137/181 (76%)	137 (100%)	0	100	100
5	L5	142/149 (95%)	142 (100%)	0	100	100
6	L6	176/177 (99%)	176 (100%)	0	100	100
7	L7	173/174 (99%)	173 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	171/172 (99%)	171 (100%)	0	100	100
10	LA	134/163 (82%)	134 (100%)	0	100	100
11	LB	164/165 (99%)	164 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LD	138/175 (79%)	138 (100%)	0	100	100
14	LE	136/140 (97%)	136 (100%)	0	100	100
15	LF	93/115 (81%)	93 (100%)	0	100	100
16	LG	106/107 (99%)	105 (99%)	1 (1%)	78	91
17	LH	124/133 (93%)	124 (100%)	0	100	100
18	LI	124/135 (92%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LJ	117/118 (99%)	117 (100%)	0	100	100
20	LK	120/121 (99%)	120 (100%)	0	100	100
21	LL	109/121 (90%)	109 (100%)	0	100	100
22	LM	80/126 (64%)	78 (98%)	2 (2%)	47	71
23	LN	347/348 (100%)	347 (100%)	0	100	100
24	LO	80/97 (82%)	80 (100%)	0	100	100
25	LP	97/110 (88%)	96 (99%)	1 (1%)	76	89
26	LQ	114/121 (94%)	114 (100%)	0	100	100
27	LR	96/100 (96%)	96 (100%)	0	100	100
28	LS	109/110 (99%)	109 (100%)	0	100	100
29	LT	88/89 (99%)	88 (100%)	0	100	100
30	LU	86/89 (97%)	85 (99%)	1 (1%)	71	87
31	LV	92/94 (98%)	92 (100%)	0	100	100
32	LW	73/80 (91%)	73 (100%)	0	100	100
33	LX	74/75 (99%)	74 (100%)	0	100	100
34	LY	64/65 (98%)	64 (100%)	0	100	100
35	LZ	47/48 (98%)	46 (98%)	1 (2%)	53	76
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	NL	227/402 (56%)	227 (100%)	0	100	100
38	NP	92/114 (81%)	92 (100%)	0	100	100
39	SA	298/348 (86%)	297 (100%)	1 (0%)	92	97
40	SB	246/250 (98%)	246 (100%)	0	100	100
41	SC	192/252 (76%)	191 (100%)	1 (0%)	88	95
42	SD	194/215 (90%)	194 (100%)	0	100	100
43	SE	198/223 (89%)	198 (100%)	0	100	100
44	SF	188/199 (94%)	188 (100%)	0	100	100
45	SG	169/171 (99%)	169 (100%)	0	100	100
46	SH	86/274 (31%)	85 (99%)	1 (1%)	71	87
47	SI	211/228 (92%)	211 (100%)	0	100	100
48	SK	196/213 (92%)	195 (100%)	1 (0%)	88	95
49	SM	354/509 (70%)	354 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	SR	218/574 (38%)	218 (100%)	0	100	100
52	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	6941/8452 (82%)	6931 (100%)	10 (0%)	93	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LG	48	ARG
22	LM	14	ARG
22	LM	50	ASN
25	LP	93	ASN
30	LU	23	LYS
35	LZ	21	ARG
39	SA	109	ARG
41	SC	41	LYS
46	SH	80	LYS
48	SK	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
8	L8	69	HIS
10	LA	116	HIS
12	LC	122	HIS
22	LM	49	HIS
23	LN	42	HIS
23	LN	322	HIS
25	LP	93	ASN
36	NK	90	HIS
38	NP	13	HIS
41	SC	136	HIS
41	SC	190	HIS
47	SI	225	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	19 (12%)	0
3	L3	3339/5070 (65%)	423 (12%)	6 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L4	119/121 (98%)	12 (10%)	0
All	All	3610/5348 (67%)	454 (12%)	6 (0%)

All (454) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	62	A
2	L1	63	U
2	L1	82	A
2	L1	83	C
2	L1	84	A
2	L1	86	U
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	110	U
2	L1	111	U
2	L1	114	G
2	L1	127	U
2	L1	151	G
2	L1	156	U
3	L3	2	G
3	L3	6	C
3	L3	13	U
3	L3	25	A
3	L3	39	A
3	L3	42	A
3	L3	48	G
3	L3	56	A
3	L3	58	G
3	L3	59	A
3	L3	64	A
3	L3	65	A
3	L3	66	A
3	L3	69	A
3	L3	91	G
3	L3	98	A
3	L3	108	A

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Mol	Chain	Res	Type
3	L3	119	G
3	L3	159	C
3	L3	164	G
3	L3	167	C
3	L3	169	G
3	L3	170	C
3	L3	171	U
3	L3	173	C
3	L3	181	C
3	L3	197	A
3	L3	200	U
3	L3	210	C
3	L3	218	A
3	L3	233	U
3	L3	234	G
3	L3	261	G
3	L3	266	C
3	L3	316	U
3	L3	340	C
3	L3	349	A
3	L3	387	G
3	L3	409	G
3	L3	410	A
3	L3	412	G
3	L3	430	G
3	L3	450	G
3	L3	452	A
3	L3	453	G
3	L3	454	U
3	L3	464	G
3	L3	467	U
3	L3	472	C
3	L3	473	C
3	L3	492	U
3	L3	493	G
3	L3	496	G
3	L3	497	G
3	L3	499	G
3	L3	501	C
3	L3	502	C
3	L3	503	C
3	L3	504	G

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Mol	Chain	Res	Type
3	L3	510	U
3	L3	512	U
3	L3	657	C
3	L3	658	C
3	L3	660	A
3	L3	667	A
3	L3	668	C
3	L3	669	C
3	L3	686	A
3	L3	704	C
3	L3	729	G
3	L3	730	G
3	L3	731	G
3	L3	739	G
3	L3	741	C
3	L3	742	G
3	L3	746	A
3	L3	913	U
3	L3	915	A
3	L3	917	A
3	L3	918	G
3	L3	926	G
3	L3	932	A
3	L3	933	G
3	L3	944	A
3	L3	945	U
3	L3	946	C
3	L3	956	A
3	L3	959	G
3	L3	960	A
3	L3	971	U
3	L3	972	C
3	L3	1066	G
3	L3	1070	G
3	L3	1072	C
3	L3	1169	G
3	L3	1171	G
3	L3	1172	C
3	L3	1178	G
3	L3	1180	C
3	L3	1181	C
3	L3	1182	C

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Mol	Chain	Res	Type
3	L3	1201	U
3	L3	1203	G
3	L3	1211	G
3	L3	1214	C
3	L3	1215	C
3	L3	1241	C
3	L3	1253	G
3	L3	1254	A
3	L3	1255	A
3	L3	1256	G
3	L3	1266	G
3	L3	1269	G
3	L3	1270	A
3	L3	1273	G
3	L3	1280	C
3	L3	1284	G
3	L3	1287	G
3	L3	1294	A
3	L3	1295	C
3	L3	1301	C
3	L3	1313	C
3	L3	1314	C
3	L3	1318	C
3	L3	1319	U
3	L3	1323	A
3	L3	1325	C
3	L3	1354	A
3	L3	1358	G
3	L3	1359	G
3	L3	1365	C
3	L3	1366	G
3	L3	1397	A
3	L3	1420	A
3	L3	1439	C
3	L3	1443	A
3	L3	1476	C
3	L3	1498	G
3	L3	1502	G
3	L3	1523	A
3	L3	1534	A2M
3	L3	1547	A
3	L3	1578	U

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Mol	Chain	Res	Type
3	L3	1581	G
3	L3	1592	G
3	L3	1596	U
3	L3	1597	G
3	L3	1614	C
3	L3	1624	G
3	L3	1625	OMG
3	L3	1631	A
3	L3	1633	G
3	L3	1634	A
3	L3	1640	C
3	L3	1642	A
3	L3	1654	G
3	L3	1661	C
3	L3	1670	G
3	L3	1676	C
3	L3	1677	PSU
3	L3	1678	C
3	L3	1691	G
3	L3	1721	G
3	L3	1726	U
3	L3	1734	G
3	L3	1740	C
3	L3	1741	G
3	L3	1742	A
3	L3	1743	A
3	L3	1750	G
3	L3	1791	U
3	L3	1804	A
3	L3	1811	G
3	L3	1815	G
3	L3	1821	G
3	L3	1836	G
3	L3	1837	A
3	L3	1842	G
3	L3	1854	G
3	L3	1875	C
3	L3	1880	G
3	L3	1882	U
3	L3	1887	G
3	L3	1888	A
3	L3	1897	A

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Mol	Chain	Res	Type
3	L3	1910	G
3	L3	1919	G
3	L3	1921	C
3	L3	1922	G
3	L3	1925	G
3	L3	1930	U
3	L3	1955	G
3	L3	1974	U
3	L3	1997	U
3	L3	2021	G
3	L3	2025	A
3	L3	2026	A
3	L3	2041	A
3	L3	2044	U
3	L3	2046	G
3	L3	2055	G
3	L3	2056	G
3	L3	2069	A
3	L3	2084	C
3	L3	2085	G
3	L3	2092	G
3	L3	2093	A
3	L3	2095	A
3	L3	2096	G
3	L3	2097	U
3	L3	2098	G
3	L3	2099	G
3	L3	2109	G
3	L3	2110	C
3	L3	2111	G
3	L3	2261	G
3	L3	2289	C
3	L3	2300	A
3	L3	2301	G
3	L3	2313	A
3	L3	2348	G
3	L3	2351	OMC
3	L3	2395	A
3	L3	2415	OMU
3	L3	2416	G
3	L3	2417	A
3	L3	2422	OMC

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Mol	Chain	Res	Type
3	L3	2425	U
3	L3	2429	A
3	L3	2450	G
3	L3	2453	A
3	L3	2470	C
3	L3	2471	G
3	L3	2475	G
3	L3	2476	G
3	L3	2477	A
3	L3	2478	C
3	L3	2486	G
3	L3	2487	G
3	L3	2488	C
3	L3	2489	C
3	L3	2492	C
3	L3	2493	G
3	L3	2507	A
3	L3	2512	A
3	L3	2513	A
3	L3	2519	U
3	L3	2544	G
3	L3	2545	U
3	L3	2548	C
3	L3	2554	U
3	L3	2587	A
3	L3	2589	C
3	L3	2601	A
3	L3	2627	C
3	L3	2638	G
3	L3	2653	C
3	L3	2669	C
3	L3	2687	U
3	L3	2694	G
3	L3	2695	A
3	L3	2696	A
3	L3	2711	G
3	L3	2724	G
3	L3	2743	A
3	L3	2760	G
3	L3	2764	A
3	L3	2769	U
3	L3	2772	C

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Mol	Chain	Res	Type
3	L3	2787	A2M
3	L3	2788	U
3	L3	2790	U
3	L3	2814	C
3	L3	2826	U
3	L3	2827	G
3	L3	2829	U
3	L3	2842	G
3	L3	2855	G
3	L3	2877	G
3	L3	2894	A
3	L3	2902	G
3	L3	2917	G
3	L3	2918	G
3	L3	3271	G
3	L3	3585	G
3	L3	3593	C
3	L3	3595	U
3	L3	3597	G
3	L3	3615	G
3	L3	3626	G
3	L3	3635	A
3	L3	3644	U
3	L3	3653	A
3	L3	3662	A
3	L3	3696	C
3	L3	3697	U
3	L3	3775	A
3	L3	3838	U
3	L3	3840	U
3	L3	3867	A2M
3	L3	3868	G
3	L3	3872	A
3	L3	3887	OMC
3	L3	3897	G
3	L3	3905	A
3	L3	3915	U
3	L3	4069	U
3	L3	4076	G
3	L3	4085	A
3	L3	4119	C
3	L3	4122	G

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Mol	Chain	Res	Type
3	L3	4127	A
3	L3	4133	C
3	L3	4139	G
3	L3	4140	C
3	L3	4142	C
3	L3	4143	G
3	L3	4144	C
3	L3	4145	C
3	L3	4147	G
3	L3	4150	G
3	L3	4154	G
3	L3	4162	C
3	L3	4170	A
3	L3	4183	G
3	L3	4184	G
3	L3	4191	G
3	L3	4194	U
3	L3	4202	U
3	L3	4221	C
3	L3	4222	G
3	L3	4229	U
3	L3	4233	A
3	L3	4251	A
3	L3	4254	G
3	L3	4266	G
3	L3	4268	A
3	L3	4273	A
3	L3	4281	A
3	L3	4291	G
3	L3	4305	G
3	L3	4306	OMU
3	L3	4314	C
3	L3	4329	G
3	L3	4330	G
3	L3	4332	C
3	L3	4339	A
3	L3	4373	G
3	L3	4376	A
3	L3	4377	G
3	L3	4378	A
3	L3	4387	C
3	L3	4453	C

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Mol	Chain	Res	Type
3	L3	4464	A
3	L3	4466	C
3	L3	4475	G
3	L3	4491	G
3	L3	4498	OMU
3	L3	4512	U
3	L3	4513	A
3	L3	4519	C
3	L3	4523	A2M
3	L3	4524	G
3	L3	4532	PSU
3	L3	4545	G
3	L3	4548	A
3	L3	4549	G
3	L3	4555	U
3	L3	4556	U
3	L3	4557	U
3	L3	4558	U
3	L3	4560	C
3	L3	4567	G
3	L3	4584	A
3	L3	4590	A2M
3	L3	4608	G
3	L3	4636	PSU
3	L3	4637	OMG
3	L3	4656	A
3	L3	4670	C
3	L3	4672	A
3	L3	4678	G
3	L3	4701	A
3	L3	4708	A
3	L3	4709	U
3	L3	4719	G
3	L3	4720	C
3	L3	4736	C
3	L3	4740	G
3	L3	4741	C
3	L3	4742	G
3	L3	4750	G
3	L3	4751	G
3	L3	4754	G
3	L3	4757	C

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Mol	Chain	Res	Type
3	L3	4759	C
3	L3	4765	G
3	L3	4772	C
3	L3	4773	C
3	L3	4870	G
3	L3	4871	C
3	L3	4882	U
3	L3	4883	C
3	L3	4900	C
3	L3	4901	G
3	L3	4910	G
3	L3	4914	C
3	L3	4916	G
3	L3	4976	U
3	L3	5014	A
3	L3	5020	G
3	L3	5022	U
3	L3	5023	C
3	L3	5026	U
3	L3	5027	C
3	L3	5031	G
3	L3	5041	G
3	L3	5050	C
3	L3	5054	C
3	L3	5055	G
3	L3	5061	A
3	L3	5062	G
3	L3	5069	U
4	L4	10	C
4	L4	18	C
4	L4	49	A
4	L4	53	U
4	L4	54	A
4	L4	64	G
4	L4	66	G
4	L4	93	G
4	L4	103	A
4	L4	110	G
4	L4	111	C
4	L4	120	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L3	496	G
3	L3	502	C
3	L3	503	C
3	L3	1625	OMG
3	L3	1633	G
3	L3	2095	A

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

110 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	$\#\|Z\| > 2$
3	OMU	L3	2837	3	19,22,23	1.97	6 (31%)	26,31,34	1.84	5 (19%)
2	PSU	L1	69	2	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
3	A2M	L3	1871	3	18,25,26	1.21	2 (11%)	18,36,39	1.36	2 (11%)
3	PSU	L3	4628	3	18,21,22	1.01	2 (11%)	22,30,33	1.89	6 (27%)
3	PSU	L3	3734	3	18,21,22	1.07	1 (5%)	22,30,33	1.87	5 (22%)
3	OMC	L3	4456	3	19,22,23	0.66	0	26,31,34	0.58	0
2	PSU	L1	55	2	18,21,22	1.03	1 (5%)	22,30,33	1.84	5 (22%)
3	OMU	L3	4227	3	19,22,23	1.93	5 (26%)	26,31,34	1.84	5 (19%)
3	OMU	L3	4498	3	19,22,23	2.09	7 (36%)	26,31,34	1.69	5 (19%)
2	OMG	L1	75	2	18,26,27	1.23	2 (11%)	19,38,41	0.85	1 (5%)
3	PSU	L3	3884	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMG	L3	4637	3	18,26,27	1.24	3 (16%)	19,38,41	0.83	1 (5%)
3	OMG	L3	4392	3	18,26,27	1.25	3 (16%)	19,38,41	0.87	1 (5%)
3	OMC	L3	2861	3	19,22,23	0.60	0	26,31,34	0.63	0
3	OMG	L3	1625	3	18,26,27	1.24	2 (11%)	19,38,41	0.84	1 (5%)
3	PSU	L3	5010	3	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
3	PSU	L3	4312	3	18,21,22	1.04	1 (5%)	22,30,33	1.90	4 (18%)
3	OMG	L3	2876	3	18,26,27	1.20	2 (11%)	19,38,41	0.81	1 (5%)
3	PSU	L3	1677	3	18,21,22	1.03	2 (11%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMC	L3	3841	3	19,22,23	0.63	0	26,31,34	0.79	1 (3%)
3	A2M	L3	3825	3	18,25,26	1.20	3 (16%)	18,36,39	1.26	2 (11%)
3	PSU	L3	4532	3	18,21,22	1.05	1 (5%)	22,30,33	1.92	5 (22%)
3	A2M	L3	2401	3	18,25,26	1.25	3 (16%)	18,36,39	1.32	2 (11%)
3	A2M	L3	1326	3	18,25,26	1.28	3 (16%)	18,36,39	1.44	3 (16%)
3	PSU	L3	4521	3	18,21,22	1.03	1 (5%)	22,30,33	1.79	5 (22%)
3	OMG	L3	3744	3	18,26,27	1.20	2 (11%)	19,38,41	0.85	1 (5%)
3	PSU	L3	1862	3	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	L3	4299	3	18,21,22	0.98	1 (5%)	22,30,33	1.94	5 (22%)
3	PSU	L3	4579	3	18,21,22	0.99	2 (11%)	22,30,33	1.77	4 (18%)
3	PSU	L3	4296	3	18,21,22	1.07	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	L3	4353	3	18,21,22	1.04	2 (11%)	22,30,33	1.87	6 (27%)
3	A2M	L3	400	3	18,25,26	1.21	3 (16%)	18,36,39	1.32	2 (11%)
3	OMG	L3	2364	3	18,26,27	1.27	3 (16%)	19,38,41	0.86	1 (5%)
3	OMU	L3	4306	3	19,22,23	1.92	5 (26%)	26,31,34	1.90	4 (15%)
3	OMG	L3	3899	3	18,26,27	1.28	3 (16%)	19,38,41	0.87	1 (5%)
3	A2M	L3	4523	3	18,25,26	1.21	3 (16%)	18,36,39	1.23	2 (11%)
3	PSU	L3	3695	3	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
3	PSU	L3	4689	3	18,21,22	1.03	1 (5%)	22,30,33	1.87	3 (13%)
3	PSU	L3	4457	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	4 (18%)
3	PSU	L3	3853	3	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
3	OMC	L3	2824	3	19,22,23	0.61	0	26,31,34	0.67	0
3	PSU	L3	5001	3	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	L3	4370	3	18,26,27	1.30	3 (16%)	19,38,41	1.03	1 (5%)
3	PSU	L3	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
3	OMC	L3	3869	3	19,22,23	0.65	0	26,31,34	0.67	0
3	PSU	L3	3637	3	18,21,22	1.04	1 (5%)	22,30,33	1.82	3 (13%)
3	OMG	L3	4499	3	18,26,27	1.11	2 (11%)	19,38,41	0.85	1 (5%)
3	A2M	L3	2787	3	18,25,26	1.23	3 (16%)	18,36,39	1.39	1 (5%)
3	PSU	L3	4500	3	18,21,22	1.06	1 (5%)	22,30,33	1.81	5 (22%)
3	A2M	L3	1524	3	18,25,26	1.24	3 (16%)	18,36,39	1.31	2 (11%)
3	PSU	L3	4576	3	18,21,22	1.05	1 (5%)	22,30,33	1.82	5 (22%)
3	PSU	L3	1779	3	18,21,22	1.05	1 (5%)	22,30,33	1.83	5 (22%)
3	OMU	L3	4620	3	19,22,23	1.95	5 (26%)	26,31,34	1.59	4 (15%)
3	OMC	L3	3701	3	19,22,23	0.56	0	26,31,34	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	A2M	L3	1534	3,53	18,25,26	1.24	3 (16%)	18,36,39	1.39	3 (16%)
3	PSU	L3	1536	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	L3	3822	3	18,21,22	1.13	1 (5%)	22,30,33	1.83	5 (22%)
3	OMG	L3	1522	3	18,26,27	1.26	3 (16%)	19,38,41	0.89	1 (5%)
3	PSU	L3	1781	3	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
3	A2M	L3	2815	3	18,25,26	1.23	3 (16%)	18,36,39	1.24	2 (11%)
3	A2M	L3	4590	3	18,25,26	1.29	3 (16%)	18,36,39	1.40	2 (11%)
3	PSU	L3	4293	3	18,21,22	0.96	1 (5%)	22,30,33	1.69	3 (13%)
3	A2M	L3	2363	3,53	18,25,26	1.24	3 (16%)	18,36,39	1.30	1 (5%)
3	OMC	L3	2365	3	19,22,23	0.64	0	26,31,34	0.68	0
3	PSU	L3	1782	3	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
3	OMU	L3	2415	3	19,22,23	1.96	6 (31%)	26,31,34	1.79	5 (19%)
3	UR3	L3	4530	3	19,22,23	1.18	3 (15%)	26,32,35	1.20	1 (3%)
3	PSU	L3	4471	3	18,21,22	1.08	1 (5%)	22,30,33	1.79	5 (22%)
3	PSU	L3	2508	3	18,21,22	1.01	1 (5%)	22,30,33	1.89	4 (18%)
3	OMG	L3	4618	3	18,26,27	1.24	3 (16%)	19,38,41	0.90	1 (5%)
3	A2M	L3	3830	3	18,25,26	1.21	3 (16%)	18,36,39	1.33	2 (11%)
3	PSU	L3	3730	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
3	OMC	L3	2351	3,53	19,22,23	0.71	1 (5%)	26,31,34	0.84	1 (3%)
3	OMG	L3	4494	3	18,26,27	1.26	2 (11%)	19,38,41	0.82	1 (5%)
3	OMG	L3	3627	3	18,26,27	1.23	3 (16%)	19,38,41	0.89	1 (5%)
3	PSU	L3	4673	3	18,21,22	1.06	2 (11%)	22,30,33	1.79	4 (18%)
3	PSU	L3	4493	3	18,21,22	1.03	1 (5%)	22,30,33	1.81	2 (9%)
3	A2M	L3	3724	3	18,25,26	1.23	3 (16%)	18,36,39	1.30	2 (11%)
3	OMG	L3	4623	3	18,26,27	1.22	2 (11%)	19,38,41	0.97	1 (5%)
3	PSU	L3	1860	3	18,21,22	0.98	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	L3	1340	3	19,22,23	0.68	0	26,31,34	0.78	0
3	OMC	L3	2804	3	19,22,23	0.65	0	26,31,34	0.66	0
3	PSU	L3	3715	3	18,21,22	1.05	1 (5%)	22,30,33	1.83	6 (27%)
3	A2M	L3	3867	3	18,25,26	1.24	3 (16%)	18,36,39	1.40	1 (5%)
3	OMC	L3	4536	3	19,22,23	0.64	0	26,31,34	0.70	0
3	PSU	L3	4972	3	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	L3	1582	3	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	L3	3844	3	18,21,22	1.07	1 (5%)	22,30,33	1.85	5 (22%)
3	1MA	L3	1322	3	16,25,26	0.89	2 (12%)	18,37,40	1.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	OMU	L3	3925	3	19,22,23	1.94	6 (31%)	26,31,34	1.90	5 (19%)
3	OMC	L3	3887	3	19,22,23	0.64	0	26,31,34	0.66	0
3	PSU	L3	2632	3	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
3	6MZ	L3	4220	3	18,25,26	1.09	2 (11%)	16,36,39	1.98	4 (25%)
3	PSU	L3	4552	3	18,21,22	1.00	1 (5%)	22,30,33	1.80	5 (22%)
3	OMC	L3	2422	3,53	19,22,23	0.63	0	26,31,34	0.73	1 (3%)
3	PSU	L3	1683	3	18,21,22	1.13	2 (11%)	22,30,33	1.95	4 (18%)
3	A2M	L3	3718	3	18,25,26	1.29	3 (16%)	18,36,39	1.19	1 (5%)
3	PSU	L3	1792	3	18,21,22	1.03	1 (5%)	22,30,33	1.85	4 (18%)
3	A2M	L3	4571	3	18,25,26	1.21	3 (16%)	18,36,39	1.21	1 (5%)
3	PSU	L3	2839	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	OMG	L3	2424	3	18,26,27	1.24	3 (16%)	19,38,41	0.79	1 (5%)
3	PSU	L3	4636	3	18,21,22	1.06	1 (5%)	22,30,33	1.95	5 (22%)
23	HIC	LN	245	23	8,11,12	1.59	2 (25%)	6,14,16	1.12	0
3	PSU	L3	3851	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMG	L3	1316	3	18,26,27	1.22	3 (16%)	19,38,41	0.90	1 (5%)
3	A2M	L3	398	3	18,25,26	1.25	3 (16%)	18,36,39	1.32	2 (11%)
3	PSU	L3	3920	3,53	18,21,22	1.05	2 (11%)	22,30,33	1.83	5 (22%)
3	PSU	L3	4361	3	18,21,22	1.07	1 (5%)	22,30,33	1.87	4 (18%)
3	PSU	L3	1744	3	18,21,22	1.07	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	L3	4228	3	18,26,27	1.34	3 (16%)	19,38,41	0.98	1 (5%)

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
3	OMU	L3	2837	3	-	1/9/27/28	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
3	A2M	L3	1871	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3734	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	4456	3	-	0/9/27/28	0/2/2/2
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
3	OMU	L3	4227	3	-	1/9/27/28	0/2/2/2
3	OMU	L3	4498	3	-	0/9/27/28	0/2/2/2
2	OMG	L1	75	2	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	3884	3	-	2/7/25/26	0/2/2/2
3	OMG	L3	4637	3	-	1/5/27/28	0/3/3/3
3	OMG	L3	4392	3	-	1/5/27/28	0/3/3/3
3	OMC	L3	2861	3	-	1/9/27/28	0/2/2/2
3	OMG	L3	1625	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4312	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2876	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	1677	3	-	4/7/25/26	0/2/2/2
3	OMC	L3	3841	3	-	1/9/27/28	0/2/2/2
3	A2M	L3	3825	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	4532	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2401	3	-	2/5/27/28	0/3/3/3
3	A2M	L3	1326	3	-	3/5/27/28	0/3/3/3
3	PSU	L3	4521	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	3744	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	1862	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4296	3	-	2/7/25/26	0/2/2/2
3	PSU	L3	4353	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	400	3	-	1/5/27/28	0/3/3/3
3	OMG	L3	2364	3	-	3/5/27/28	0/3/3/3
3	OMU	L3	4306	3	-	5/9/27/28	0/2/2/2
3	OMG	L3	3899	3	-	1/5/27/28	0/3/3/3
3	A2M	L3	4523	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3853	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	5001	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4370	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	3639	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	3637	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4499	3	-	0/5/27/28	0/3/3/3
3	A2M	L3	2787	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	4500	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	1524	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L3	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1779	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	4620	3	-	0/9/27/28	0/2/2/2
3	OMC	L3	3701	3	-	6/9/27/28	0/2/2/2
3	A2M	L3	1534	3,53	-	2/5/27/28	0/3/3/3
3	PSU	L3	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3822	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1522	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	1781	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2815	3	-	1/5/27/28	0/3/3/3
3	A2M	L3	4590	3	-	3/5/27/28	0/3/3/3
3	PSU	L3	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	2363	3,53	-	0/5/27/28	0/3/3/3
3	OMC	L3	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	1782	3	-	0/7/25/26	0/2/2/2
3	OMU	L3	2415	3	-	3/9/27/28	0/2/2/2
3	UR3	L3	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4618	3	-	2/5/27/28	0/3/3/3
3	A2M	L3	3830	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	3730	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2351	3,53	-	4/9/27/28	0/2/2/2
3	OMG	L3	4494	3	-	0/5/27/28	0/3/3/3
3	OMG	L3	3627	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3724	3	-	1/5/27/28	0/3/3/3
3	OMG	L3	4623	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	1340	3	-	1/9/27/28	0/2/2/2
3	OMC	L3	2804	3	-	1/9/27/28	0/2/2/2
3	PSU	L3	3715	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3867	3	-	2/5/27/28	0/3/3/3
3	OMC	L3	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L3	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	3844	3	-	1/7/25/26	0/2/2/2
3	1MA	L3	1322	3	-	2/3/25/26	0/3/3/3
3	OMU	L3	3925	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L3	3887	3	-	2/9/27/28	0/2/2/2
3	PSU	L3	2632	3	-	0/7/25/26	0/2/2/2
3	6MZ	L3	4220	3	-	0/5/27/28	0/3/3/3
3	PSU	L3	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L3	2422	3,53	-	1/9/27/28	0/2/2/2
3	PSU	L3	1683	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	3718	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	1792	3	-	0/7/25/26	0/2/2/2
3	A2M	L3	4571	3	-	2/5/27/28	0/3/3/3
3	PSU	L3	2839	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	2424	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	4636	3	-	4/7/25/26	0/2/2/2
23	HIC	LN	245	23	-	2/5/6/8	0/1/1/1
3	PSU	L3	3851	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	1316	3	-	1/5/27/28	0/3/3/3
3	A2M	L3	398	3	-	1/5/27/28	0/3/3/3
3	PSU	L3	3920	3,53	-	0/7/25/26	0/2/2/2
3	PSU	L3	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L3	1744	3	-	0/7/25/26	0/2/2/2
3	OMG	L3	4228	3	-	0/5/27/28	0/3/3/3

All (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4498	OMU	C6-N1	4.87	1.49	1.38
3	L3	4620	OMU	C6-N1	4.57	1.49	1.38
3	L3	2415	OMU	C6-N1	4.52	1.48	1.38
3	L3	4227	OMU	C6-N1	4.51	1.48	1.38
3	L3	2837	OMU	C6-N1	4.44	1.48	1.38
3	L3	4306	OMU	C6-N1	4.42	1.48	1.38
3	L3	3925	OMU	C6-N1	4.38	1.48	1.38
3	L3	4498	OMU	C2-N1	4.23	1.45	1.38
3	L3	4498	OMU	C5-C4	4.06	1.52	1.43
3	L3	2837	OMU	C5-C4	3.87	1.52	1.43
3	L3	4306	OMU	C2-N1	3.87	1.44	1.38
3	L3	3925	OMU	C2-N1	3.87	1.44	1.38
3	L3	2837	OMU	C2-N1	3.86	1.44	1.38
3	L3	2415	OMU	C2-N1	3.86	1.44	1.38
3	L3	4620	OMU	C2-N1	3.80	1.44	1.38
3	L3	3925	OMU	C5-C4	3.79	1.52	1.43
3	L3	4227	OMU	C5-C4	3.75	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	2415	OMU	C5-C4	3.69	1.51	1.43
3	L3	4620	OMU	C5-C4	3.67	1.51	1.43
3	L3	4227	OMU	C2-N1	3.65	1.44	1.38
3	L3	3822	PSU	C6-C5	3.64	1.39	1.35
3	L3	4306	OMU	C5-C4	3.43	1.51	1.43
3	L3	1744	PSU	C6-C5	3.39	1.39	1.35
23	LN	245	HIC	CD2-CG	3.37	1.41	1.36
3	L3	4500	PSU	C6-C5	3.36	1.39	1.35
3	L3	1782	PSU	C6-C5	3.33	1.39	1.35
3	L3	4494	OMG	C8-N7	-3.30	1.29	1.35
3	L3	1781	PSU	C6-C5	3.29	1.39	1.35
3	L3	4306	OMU	O4-C4	-3.29	1.18	1.24
3	L3	3695	PSU	C6-C5	3.28	1.39	1.35
3	L3	3734	PSU	C6-C5	3.28	1.39	1.35
3	L3	1779	PSU	C6-C5	3.26	1.39	1.35
3	L3	1871	A2M	O4'-C1'	3.24	1.45	1.41
3	L3	4228	OMG	C8-N7	-3.22	1.29	1.35
3	L3	3730	PSU	C6-C5	3.18	1.39	1.35
3	L3	4576	PSU	C6-C5	3.18	1.39	1.35
3	L3	1326	A2M	O4'-C1'	3.18	1.45	1.41
3	L3	2632	PSU	C6-C5	3.16	1.39	1.35
3	L3	3715	PSU	C6-C5	3.16	1.39	1.35
3	L3	5010	PSU	C6-C5	3.15	1.39	1.35
3	L3	1625	OMG	C8-N7	-3.14	1.29	1.35
3	L3	4361	PSU	C6-C5	3.12	1.39	1.35
3	L3	4530	UR3	C2-N1	-3.11	1.34	1.38
3	L3	2364	OMG	C8-N7	-3.11	1.29	1.35
3	L3	4493	PSU	C6-C5	3.10	1.38	1.35
3	L3	5001	PSU	C6-C5	3.09	1.38	1.35
3	L3	4370	OMG	C8-N7	-3.09	1.29	1.35
3	L3	4471	PSU	C6-C5	3.09	1.38	1.35
2	L1	75	OMG	C8-N7	-3.08	1.29	1.35
3	L3	4392	OMG	C8-N7	-3.08	1.29	1.35
3	L3	4972	PSU	C6-C5	3.08	1.38	1.35
3	L3	4673	PSU	C6-C5	3.08	1.38	1.35
3	L3	2876	OMG	C8-N7	-3.08	1.29	1.35
3	L3	3724	A2M	O4'-C1'	3.08	1.45	1.41
3	L3	3844	PSU	C6-C5	3.07	1.38	1.35
3	L3	1862	PSU	C6-C5	3.07	1.38	1.35
3	L3	4532	PSU	C6-C5	3.07	1.38	1.35
3	L3	3899	OMG	C8-N7	-3.05	1.29	1.35
3	L3	4636	PSU	C6-C5	3.05	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4618	OMG	C8-N7	-3.04	1.29	1.35
3	L3	398	A2M	O4'-C1'	3.03	1.45	1.41
3	L3	4457	PSU	C6-C5	3.03	1.38	1.35
3	L3	3851	PSU	C6-C5	3.03	1.38	1.35
3	L3	4620	OMU	O4-C4	-3.02	1.18	1.24
3	L3	4637	OMG	C8-N7	-3.01	1.29	1.35
3	L3	3853	PSU	C6-C5	2.99	1.38	1.35
3	L3	2839	PSU	C6-C5	2.99	1.38	1.35
3	L3	1522	OMG	C8-N7	-2.99	1.29	1.35
3	L3	2424	OMG	C8-N7	-2.98	1.29	1.35
3	L3	4590	A2M	O4'-C1'	2.98	1.45	1.41
3	L3	4623	OMG	C8-N7	-2.98	1.29	1.35
2	L1	69	PSU	C6-C5	2.98	1.38	1.35
3	L3	4227	OMU	O4-C4	-2.98	1.18	1.24
3	L3	3884	PSU	C6-C5	2.96	1.38	1.35
3	L3	4521	PSU	C6-C5	2.96	1.38	1.35
3	L3	3637	PSU	C6-C5	2.95	1.38	1.35
3	L3	400	A2M	O4'-C1'	2.92	1.45	1.41
3	L3	3744	OMG	C8-N7	-2.92	1.30	1.35
3	L3	3925	OMU	O4-C4	-2.92	1.18	1.24
3	L3	3627	OMG	C8-N7	-2.92	1.30	1.35
3	L3	1316	OMG	C8-N7	-2.91	1.30	1.35
3	L3	3718	A2M	O4'-C1'	2.91	1.45	1.41
3	L3	2401	A2M	O4'-C1'	2.90	1.45	1.41
3	L3	3867	A2M	O4'-C1'	2.89	1.45	1.41
2	L1	55	PSU	C6-C5	2.88	1.38	1.35
3	L3	2815	A2M	O4'-C1'	2.88	1.45	1.41
3	L3	1582	PSU	C6-C5	2.87	1.38	1.35
3	L3	4571	A2M	O4'-C1'	2.87	1.45	1.41
3	L3	3830	A2M	O4'-C1'	2.87	1.45	1.41
3	L3	4296	PSU	C6-C5	2.87	1.38	1.35
3	L3	1536	PSU	C6-C5	2.87	1.38	1.35
3	L3	2508	PSU	C6-C5	2.87	1.38	1.35
3	L3	3920	PSU	C6-C5	2.86	1.38	1.35
3	L3	2415	OMU	O4-C4	-2.86	1.19	1.24
3	L3	2837	OMU	O4-C4	-2.85	1.19	1.24
3	L3	1792	PSU	C6-C5	2.85	1.38	1.35
3	L3	4312	PSU	C6-C5	2.85	1.38	1.35
3	L3	4228	OMG	C5-C6	-2.85	1.41	1.47
3	L3	4689	PSU	C6-C5	2.84	1.38	1.35
3	L3	2363	A2M	C8-N7	-2.84	1.29	1.34
3	L3	1860	PSU	C6-C5	2.84	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	4353	PSU	C6-C5	2.83	1.38	1.35
3	L3	4523	A2M	O4'-C1'	2.83	1.45	1.41
3	L3	3639	PSU	C6-C5	2.82	1.38	1.35
3	L3	2787	A2M	C8-N7	-2.82	1.29	1.34
3	L3	4552	PSU	C6-C5	2.82	1.38	1.35
3	L3	3825	A2M	O4'-C1'	2.81	1.45	1.41
3	L3	2364	OMG	C5-C6	-2.80	1.41	1.47
3	L3	3718	A2M	C8-N7	-2.79	1.29	1.34
3	L3	2363	A2M	O4'-C1'	2.79	1.45	1.41
3	L3	4220	6MZ	C8-N7	-2.76	1.29	1.34
3	L3	2424	OMG	C5-C6	-2.75	1.41	1.47
3	L3	1534	A2M	C8-N7	-2.74	1.29	1.34
3	L3	4499	OMG	C8-N7	-2.74	1.30	1.35
3	L3	4590	A2M	C8-N7	-2.74	1.29	1.34
3	L3	4306	OMU	O2-C2	-2.73	1.18	1.23
3	L3	3744	OMG	C5-C6	-2.72	1.41	1.47
3	L3	1524	A2M	C8-N7	-2.72	1.29	1.34
3	L3	3899	OMG	C5-C6	-2.71	1.41	1.47
3	L3	4392	OMG	C5-C6	-2.71	1.41	1.47
3	L3	4530	UR3	C4-N3	-2.70	1.34	1.40
3	L3	4571	A2M	C8-N7	-2.69	1.29	1.34
3	L3	3867	A2M	C8-N7	-2.69	1.29	1.34
3	L3	4579	PSU	C6-C5	2.69	1.38	1.35
3	L3	4637	OMG	C5-C6	-2.69	1.42	1.47
3	L3	4498	OMU	C2-N3	2.68	1.42	1.38
3	L3	4498	OMU	O4-C4	-2.68	1.19	1.24
3	L3	3627	OMG	C5-C6	-2.67	1.42	1.47
3	L3	4628	PSU	C6-C5	2.67	1.38	1.35
3	L3	1534	A2M	O4'-C1'	2.67	1.44	1.41
3	L3	1522	OMG	C5-C6	-2.66	1.42	1.47
3	L3	4370	OMG	C5-C6	-2.65	1.42	1.47
3	L3	2815	A2M	C8-N7	-2.65	1.30	1.34
3	L3	1316	OMG	C5-C6	-2.64	1.42	1.47
2	L1	75	OMG	C5-C6	-2.61	1.42	1.47
3	L3	398	A2M	C8-N7	-2.61	1.30	1.34
3	L3	3825	A2M	C8-N7	-2.61	1.30	1.34
3	L3	4494	OMG	C5-C6	-2.60	1.42	1.47
3	L3	400	A2M	C8-N7	-2.59	1.30	1.34
3	L3	2787	A2M	O4'-C1'	2.59	1.44	1.41
3	L3	2401	A2M	C8-N7	-2.58	1.30	1.34
3	L3	1625	OMG	C5-C6	-2.57	1.42	1.47
3	L3	4523	A2M	C8-N7	-2.56	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L3	1524	A2M	O4'-C1'	2.55	1.44	1.41
3	L3	4618	OMG	C5-C6	-2.55	1.42	1.47
3	L3	2876	OMG	C5-C6	-2.53	1.42	1.47
3	L3	3830	A2M	C8-N7	-2.52	1.30	1.34
3	L3	4623	OMG	C5-C6	-2.51	1.42	1.47
3	L3	4227	OMU	O2-C2	-2.51	1.18	1.23
3	L3	1683	PSU	C6-C5	2.49	1.38	1.35
3	L3	4530	UR3	C2-N3	-2.48	1.34	1.39
3	L3	1871	A2M	C8-N7	-2.48	1.30	1.34
3	L3	3724	A2M	C8-N7	-2.47	1.30	1.34
3	L3	1326	A2M	C8-N7	-2.47	1.30	1.34
3	L3	4293	PSU	C6-C5	2.47	1.38	1.35
3	L3	3718	A2M	C4-N3	-2.42	1.32	1.35
3	L3	3925	OMU	O2-C2	-2.40	1.18	1.23
3	L3	2415	OMU	O2-C2	-2.40	1.18	1.23
3	L3	1677	PSU	C6-C5	2.40	1.38	1.35
3	L3	1326	A2M	C4-N3	-2.34	1.32	1.35
3	L3	2837	OMU	O2-C2	-2.34	1.18	1.23
3	L3	2401	A2M	C4-N3	-2.33	1.32	1.35
3	L3	1322	1MA	C8-N7	-2.31	1.31	1.35
3	L3	4499	OMG	C5-C6	-2.31	1.42	1.47
3	L3	4370	OMG	C5-C4	-2.30	1.37	1.43
3	L3	2837	OMU	C2-N3	2.29	1.42	1.38
3	L3	4590	A2M	C4-N3	-2.29	1.32	1.35
3	L3	4620	OMU	O2-C2	-2.28	1.18	1.23
3	L3	1534	A2M	C4-N3	-2.25	1.32	1.35
3	L3	4299	PSU	C6-C5	2.23	1.37	1.35
3	L3	4228	OMG	C5-C4	-2.22	1.37	1.43
3	L3	1524	A2M	C4-N3	-2.22	1.32	1.35
3	L3	1677	PSU	O4'-C1'	-2.22	1.40	1.43
3	L3	3899	OMG	C5-C4	-2.21	1.37	1.43
3	L3	398	A2M	C4-N3	-2.20	1.32	1.35
3	L3	2787	A2M	C4-N3	-2.20	1.32	1.35
3	L3	2415	OMU	C2-N3	2.18	1.41	1.38
3	L3	4618	OMG	C5-C4	-2.18	1.37	1.43
3	L3	1683	PSU	C4-C5	-2.15	1.38	1.44
3	L3	4220	6MZ	C6-N6	2.15	1.38	1.35
3	L3	4498	OMU	C4-N3	2.14	1.42	1.38
3	L3	1322	1MA	C5-C4	-2.13	1.37	1.43
3	L3	1522	OMG	C5-C4	-2.12	1.37	1.43
3	L3	2815	A2M	C4-N3	-2.12	1.32	1.35
3	L3	3724	A2M	C4-N3	-2.09	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	LN	245	HIC	CZ-NE2	-2.09	1.42	1.48
3	L3	4353	PSU	C4-C5	-2.08	1.38	1.44
3	L3	1316	OMG	C5-C4	-2.08	1.37	1.43
3	L3	2364	OMG	C5-C4	-2.08	1.37	1.43
3	L3	4498	OMU	O2-C2	-2.08	1.19	1.23
3	L3	2424	OMG	C5-C4	-2.07	1.37	1.43
3	L3	4628	PSU	C4-C5	-2.07	1.38	1.44
3	L3	3627	OMG	C5-C4	-2.06	1.37	1.43
3	L3	3830	A2M	C4-N3	-2.06	1.32	1.35
3	L3	4296	PSU	C4-C5	-2.05	1.38	1.44
3	L3	3867	A2M	C4-N3	-2.05	1.32	1.35
3	L3	4673	PSU	C4-C5	-2.04	1.38	1.44
3	L3	4523	A2M	C4-N3	-2.04	1.32	1.35
3	L3	2351	OMC	C4-N3	-2.04	1.30	1.34
3	L3	4637	OMG	C5-C4	-2.04	1.37	1.43
3	L3	4571	A2M	C4-N3	-2.03	1.32	1.35
3	L3	3925	OMU	C2-N3	2.03	1.41	1.38
3	L3	4392	OMG	C5-C4	-2.02	1.37	1.43
3	L3	3825	A2M	C4-N3	-2.02	1.32	1.35
3	L3	2363	A2M	C4-N3	-2.02	1.32	1.35
3	L3	3920	PSU	C4-C5	-2.01	1.38	1.44
3	L3	400	A2M	C4-N3	-2.00	1.32	1.35
3	L3	4579	PSU	C4-C5	-2.00	1.38	1.44

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L3	3925	OMU	C4-N3-C2	-5.65	119.13	126.58
3	L3	4227	OMU	C4-N3-C2	-5.62	119.16	126.58
3	L3	2837	OMU	C4-N3-C2	-5.52	119.30	126.58
3	L3	4220	6MZ	C2-N1-C6	5.49	121.30	116.59
3	L3	4306	OMU	C4-N3-C2	-5.47	119.37	126.58
3	L3	4299	PSU	C4-N3-C2	-5.15	118.92	126.34
3	L3	2415	OMU	C4-N3-C2	-5.13	119.81	126.58
3	L3	4312	PSU	N1-C2-N3	5.08	120.88	115.13
3	L3	4296	PSU	C4-N3-C2	-5.07	119.04	126.34
3	L3	4636	PSU	C4-N3-C2	-5.06	119.04	126.34
3	L3	4498	OMU	C4-N3-C2	-5.00	119.98	126.58
3	L3	4689	PSU	C4-N3-C2	-4.99	119.15	126.34
3	L3	2508	PSU	C4-N3-C2	-4.98	119.17	126.34
3	L3	4299	PSU	N1-C2-N3	4.97	120.76	115.13
3	L3	1683	PSU	C4-N3-C2	-4.97	119.18	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4532	PSU	C4-N3-C2	-4.93	119.23	126.34
3	L3	1792	PSU	C4-N3-C2	-4.93	119.24	126.34
3	L3	4493	PSU	C4-N3-C2	-4.92	119.25	126.34
3	L3	4689	PSU	N1-C2-N3	4.89	120.67	115.13
3	L3	5010	PSU	C4-N3-C2	-4.87	119.33	126.34
3	L3	1582	PSU	C4-N3-C2	-4.86	119.33	126.34
3	L3	3637	PSU	C4-N3-C2	-4.85	119.34	126.34
3	L3	4361	PSU	N1-C2-N3	4.85	120.63	115.13
3	L3	4532	PSU	N1-C2-N3	4.84	120.62	115.13
3	L3	4312	PSU	C4-N3-C2	-4.83	119.38	126.34
3	L3	4636	PSU	N1-C2-N3	4.82	120.59	115.13
3	L3	4628	PSU	C4-N3-C2	-4.82	119.40	126.34
3	L3	3851	PSU	C4-N3-C2	-4.81	119.41	126.34
3	L3	1683	PSU	N1-C2-N3	4.81	120.58	115.13
3	L3	1781	PSU	C4-N3-C2	-4.80	119.43	126.34
3	L3	4353	PSU	C4-N3-C2	-4.80	119.43	126.34
3	L3	1744	PSU	C4-N3-C2	-4.77	119.46	126.34
3	L3	4628	PSU	N1-C2-N3	4.76	120.53	115.13
3	L3	4361	PSU	C4-N3-C2	-4.75	119.49	126.34
3	L3	3695	PSU	C4-N3-C2	-4.75	119.49	126.34
3	L3	1677	PSU	C4-N3-C2	-4.75	119.49	126.34
3	L3	4457	PSU	N1-C2-N3	4.74	120.50	115.13
3	L3	4353	PSU	N1-C2-N3	4.74	120.50	115.13
3	L3	3730	PSU	C4-N3-C2	-4.73	119.52	126.34
3	L3	4457	PSU	C4-N3-C2	-4.73	119.53	126.34
3	L3	3639	PSU	C4-N3-C2	-4.73	119.53	126.34
3	L3	3734	PSU	C4-N3-C2	-4.71	119.55	126.34
3	L3	1536	PSU	C4-N3-C2	-4.71	119.55	126.34
3	L3	2632	PSU	C4-N3-C2	-4.70	119.57	126.34
2	L1	55	PSU	C4-N3-C2	-4.70	119.57	126.34
3	L3	5010	PSU	N1-C2-N3	4.69	120.44	115.13
3	L3	4552	PSU	C4-N3-C2	-4.68	119.60	126.34
3	L3	1862	PSU	C4-N3-C2	-4.68	119.60	126.34
3	L3	3844	PSU	N1-C2-N3	4.67	120.42	115.13
3	L3	3715	PSU	C4-N3-C2	-4.67	119.61	126.34
3	L3	3920	PSU	C4-N3-C2	-4.67	119.61	126.34
3	L3	3851	PSU	N1-C2-N3	4.67	120.42	115.13
3	L3	2508	PSU	N1-C2-N3	4.66	120.41	115.13
3	L3	3730	PSU	N1-C2-N3	4.66	120.41	115.13
3	L3	1677	PSU	N1-C2-N3	4.66	120.41	115.13
3	L3	3734	PSU	N1-C2-N3	4.65	120.39	115.13
3	L3	1779	PSU	C4-N3-C2	-4.64	119.65	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3637	PSU	N1-C2-N3	4.64	120.39	115.13
3	L3	4306	OMU	N3-C2-N1	4.64	121.04	114.89
3	L3	1782	PSU	C4-N3-C2	-4.63	119.67	126.34
3	L3	1860	PSU	C4-N3-C2	-4.63	119.67	126.34
3	L3	1779	PSU	N1-C2-N3	4.63	120.37	115.13
3	L3	4296	PSU	N1-C2-N3	4.62	120.37	115.13
3	L3	2839	PSU	N1-C2-N3	4.62	120.37	115.13
3	L3	4576	PSU	N1-C2-N3	4.62	120.37	115.13
3	L3	4576	PSU	C4-N3-C2	-4.62	119.68	126.34
2	L1	69	PSU	C4-N3-C2	-4.62	119.68	126.34
3	L3	4293	PSU	C4-N3-C2	-4.62	119.69	126.34
3	L3	4972	PSU	N1-C2-N3	4.62	120.36	115.13
3	L3	3884	PSU	N1-C2-N3	4.61	120.36	115.13
3	L3	4500	PSU	C4-N3-C2	-4.61	119.70	126.34
3	L3	3822	PSU	N1-C2-N3	4.60	120.34	115.13
3	L3	4521	PSU	C4-N3-C2	-4.60	119.71	126.34
3	L3	1782	PSU	N1-C2-N3	4.60	120.34	115.13
3	L3	1862	PSU	N1-C2-N3	4.59	120.33	115.13
3	L3	3920	PSU	N1-C2-N3	4.59	120.33	115.13
3	L3	4493	PSU	N1-C2-N3	4.59	120.33	115.13
2	L1	69	PSU	N1-C2-N3	4.58	120.32	115.13
3	L3	3715	PSU	N1-C2-N3	4.58	120.32	115.13
3	L3	4972	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L3	3844	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L3	1781	PSU	N1-C2-N3	4.58	120.31	115.13
3	L3	4500	PSU	N1-C2-N3	4.57	120.31	115.13
3	L3	4579	PSU	C4-N3-C2	-4.57	119.76	126.34
3	L3	4471	PSU	N1-C2-N3	4.56	120.30	115.13
3	L3	5001	PSU	N1-C2-N3	4.56	120.30	115.13
3	L3	5001	PSU	C4-N3-C2	-4.56	119.77	126.34
3	L3	4530	UR3	C4-N3-C2	-4.56	120.27	124.56
3	L3	3639	PSU	N1-C2-N3	4.55	120.29	115.13
3	L3	3695	PSU	N1-C2-N3	4.54	120.27	115.13
3	L3	4673	PSU	C4-N3-C2	-4.54	119.80	126.34
3	L3	2839	PSU	C4-N3-C2	-4.54	119.80	126.34
3	L3	1792	PSU	N1-C2-N3	4.52	120.25	115.13
3	L3	1744	PSU	N1-C2-N3	4.50	120.23	115.13
3	L3	4552	PSU	N1-C2-N3	4.50	120.23	115.13
3	L3	1860	PSU	N1-C2-N3	4.50	120.23	115.13
3	L3	3925	OMU	N3-C2-N1	4.50	120.86	114.89
3	L3	1536	PSU	N1-C2-N3	4.49	120.22	115.13
3	L3	3822	PSU	C4-N3-C2	-4.49	119.87	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4471	PSU	C4-N3-C2	-4.49	119.87	126.34
2	L1	55	PSU	N1-C2-N3	4.49	120.22	115.13
3	L3	3884	PSU	C4-N3-C2	-4.48	119.88	126.34
3	L3	1582	PSU	N1-C2-N3	4.48	120.21	115.13
3	L3	2632	PSU	N1-C2-N3	4.47	120.20	115.13
3	L3	4673	PSU	N1-C2-N3	4.47	120.19	115.13
3	L3	3853	PSU	C4-N3-C2	-4.46	119.92	126.34
3	L3	4620	OMU	C4-N3-C2	-4.45	120.71	126.58
3	L3	4521	PSU	N1-C2-N3	4.44	120.16	115.13
3	L3	4579	PSU	N1-C2-N3	4.42	120.14	115.13
3	L3	3853	PSU	N1-C2-N3	4.28	119.98	115.13
3	L3	4590	A2M	N3-C2-N1	-4.24	122.06	128.68
3	L3	2363	A2M	N3-C2-N1	-4.20	122.11	128.68
3	L3	3724	A2M	N3-C2-N1	-4.20	122.12	128.68
3	L3	4293	PSU	N1-C2-N3	4.19	119.88	115.13
3	L3	2415	OMU	N3-C2-N1	4.19	120.45	114.89
3	L3	400	A2M	N3-C2-N1	-4.19	122.13	128.68
3	L3	2837	OMU	N3-C2-N1	4.16	120.42	114.89
3	L3	1524	A2M	N3-C2-N1	-4.15	122.18	128.68
3	L3	3830	A2M	N3-C2-N1	-4.15	122.20	128.68
3	L3	1871	A2M	N3-C2-N1	-4.12	122.24	128.68
3	L3	3825	A2M	N3-C2-N1	-4.11	122.26	128.68
3	L3	398	A2M	N3-C2-N1	-4.10	122.28	128.68
3	L3	4227	OMU	C5-C4-N3	4.09	120.96	114.84
3	L3	2787	A2M	N3-C2-N1	-4.08	122.30	128.68
3	L3	4523	A2M	N3-C2-N1	-4.06	122.33	128.68
3	L3	2815	A2M	N3-C2-N1	-4.01	122.41	128.68
3	L3	4227	OMU	N3-C2-N1	4.00	120.20	114.89
3	L3	2401	A2M	N3-C2-N1	-3.99	122.44	128.68
3	L3	4220	6MZ	N3-C2-N1	-3.96	122.49	128.68
3	L3	3867	A2M	N3-C2-N1	-3.93	122.54	128.68
3	L3	4571	A2M	N3-C2-N1	-3.91	122.57	128.68
3	L3	4498	OMU	N3-C2-N1	3.89	120.06	114.89
3	L3	1534	A2M	N3-C2-N1	-3.86	122.64	128.68
3	L3	1326	A2M	N3-C2-N1	-3.84	122.67	128.68
3	L3	2837	OMU	C5-C4-N3	3.66	120.32	114.84
3	L3	3925	OMU	C5-C4-N3	3.65	120.30	114.84
3	L3	4306	OMU	C5-C4-N3	3.60	120.23	114.84
3	L3	3718	A2M	N3-C2-N1	-3.56	123.11	128.68
3	L3	4620	OMU	N3-C2-N1	3.50	119.54	114.89
3	L3	4498	OMU	C5-C4-N3	3.47	120.03	114.84
3	L3	2415	OMU	C5-C4-N3	3.46	120.02	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4620	OMU	C5-C4-N3	3.40	119.93	114.84
3	L3	4227	OMU	O4-C4-C5	-3.34	119.29	125.16
3	L3	3925	OMU	O4-C4-C5	-3.24	119.45	125.16
3	L3	2837	OMU	O4-C4-C5	-3.09	119.72	125.16
3	L3	3844	PSU	O2-C2-N1	-3.03	119.45	122.79
3	L3	2415	OMU	O4-C4-C5	-3.03	119.84	125.16
3	L3	3822	PSU	O2-C2-N1	-3.02	119.47	122.79
3	L3	3884	PSU	O2-C2-N1	-2.98	119.51	122.79
3	L3	2508	PSU	O2-C2-N1	-2.92	119.58	122.79
3	L3	4370	OMG	O6-C6-C5	2.91	130.06	124.37
2	L1	55	PSU	O2-C2-N1	-2.91	119.58	122.79
3	L3	4498	OMU	O4-C4-C5	-2.91	120.04	125.16
3	L3	1536	PSU	O2-C2-N1	-2.88	119.62	122.79
3	L3	4306	OMU	O4-C4-C5	-2.87	120.11	125.16
3	L3	4299	PSU	O2-C2-N1	-2.86	119.64	122.79
3	L3	1860	PSU	O2-C2-N1	-2.83	119.67	122.79
3	L3	4579	PSU	O2-C2-N1	-2.82	119.68	122.79
3	L3	1677	PSU	O2-C2-N1	-2.82	119.69	122.79
3	L3	3639	PSU	O2-C2-N1	-2.81	119.70	122.79
3	L3	3853	PSU	O2-C2-N1	-2.79	119.72	122.79
3	L3	4220	6MZ	C9-N6-C6	-2.78	120.47	122.87
2	L1	69	PSU	O2-C2-N1	-2.77	119.74	122.79
3	L3	4620	OMU	O4-C4-C5	-2.76	120.30	125.16
3	L3	4361	PSU	O2-C2-N1	-2.76	119.75	122.79
3	L3	1782	PSU	O2-C2-N1	-2.74	119.78	122.79
3	L3	1779	PSU	O2-C2-N1	-2.73	119.78	122.79
3	L3	4500	PSU	O2-C2-N1	-2.72	119.80	122.79
3	L3	4623	OMG	O6-C6-C5	2.71	129.67	124.37
3	L3	1683	PSU	C6-C5-C4	2.70	120.08	118.20
3	L3	3734	PSU	O2-C2-N1	-2.69	119.83	122.79
3	L3	3884	PSU	C6-N1-C2	-2.68	119.94	122.68
3	L3	3730	PSU	O2-C2-N1	-2.67	119.85	122.79
3	L3	4457	PSU	O2-C2-N1	-2.67	119.85	122.79
3	L3	2839	PSU	O2-C2-N1	-2.66	119.86	122.79
3	L3	4972	PSU	O2-C2-N1	-2.66	119.86	122.79
3	L3	4576	PSU	O2-C2-N1	-2.66	119.87	122.79
3	L3	1862	PSU	O2-C2-N1	-2.65	119.87	122.79
3	L3	4628	PSU	O2-C2-N1	-2.65	119.87	122.79
3	L3	4636	PSU	C6-C5-C4	2.64	120.05	118.20
3	L3	4636	PSU	O2-C2-N1	-2.64	119.88	122.79
3	L3	4296	PSU	O2-C2-N1	-2.64	119.89	122.79
3	L3	4532	PSU	O2-C2-N1	-2.64	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4312	PSU	O2-C2-N1	-2.63	119.89	122.79
3	L3	2839	PSU	C6-N1-C2	-2.61	120.02	122.68
3	L3	4532	PSU	C6-C5-C4	2.59	120.01	118.20
3	L3	1316	OMG	O6-C6-C5	2.57	129.40	124.37
3	L3	4220	6MZ	C4-C5-N7	-2.57	106.72	109.40
3	L3	4471	PSU	O2-C2-N1	-2.56	119.97	122.79
3	L3	1683	PSU	O2-C2-N1	-2.54	119.99	122.79
3	L3	3734	PSU	C6-C5-C4	2.54	119.97	118.20
3	L3	1781	PSU	O2-C2-N1	-2.53	120.01	122.79
3	L3	4579	PSU	C6-N1-C2	-2.53	120.10	122.68
3	L3	3695	PSU	O2-C2-N1	-2.52	120.01	122.79
3	L3	3715	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L3	4353	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L3	4457	PSU	C6-N1-C2	-2.46	120.17	122.68
3	L3	4293	PSU	O2-C2-N1	-2.45	120.10	122.79
3	L3	4312	PSU	C6-N1-C2	-2.44	120.19	122.68
3	L3	5010	PSU	C6-C5-C4	2.44	119.91	118.20
3	L3	2401	A2M	C4-C5-N7	-2.44	106.86	109.40
3	L3	1522	OMG	O6-C6-C5	2.43	129.13	124.37
3	L3	1779	PSU	C6-N1-C2	-2.43	120.20	122.68
3	L3	5001	PSU	C6-N1-C2	-2.43	120.20	122.68
3	L3	4361	PSU	C6-N1-C2	-2.42	120.20	122.68
3	L3	3822	PSU	C6-N1-C2	-2.42	120.21	122.68
3	L3	4228	OMG	O6-C6-C5	2.42	129.09	124.37
3	L3	4628	PSU	C6-N1-C2	-2.41	120.22	122.68
3	L3	1860	PSU	C6-N1-C2	-2.41	120.22	122.68
3	L3	5001	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L3	4673	PSU	O2-C2-N1	-2.40	120.14	122.79
3	L3	4618	OMG	O6-C6-C5	2.40	129.06	124.37
3	L3	3920	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L3	4972	PSU	C6-N1-C2	-2.40	120.23	122.68
3	L3	4392	OMG	O6-C6-C5	2.40	129.06	124.37
3	L3	4552	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L3	4673	PSU	C6-N1-C2	-2.39	120.24	122.68
3	L3	5010	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L3	3841	OMC	C1'-N1-C2	2.39	123.76	118.42
3	L3	2632	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L3	3851	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L3	1792	PSU	O2-C2-N1	-2.38	120.17	122.79
3	L3	1326	A2M	C4-C5-N7	-2.38	106.92	109.40
3	L3	3637	PSU	C6-C5-C4	2.37	119.86	118.20
3	L3	3822	PSU	C6-C5-C4	2.37	119.85	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L3	3899	OMG	O6-C6-C5	2.36	128.99	124.37
3	L3	3695	PSU	C6-C5-C4	2.36	119.85	118.20
3	L3	4471	PSU	C6-N1-C2	-2.35	120.28	122.68
3	L3	3844	PSU	C6-C5-C4	2.34	119.83	118.20
3	L3	3730	PSU	C6-N1-C2	-2.34	120.29	122.68
3	L3	1744	PSU	O2-C2-N1	-2.33	120.22	122.79
3	L3	3744	OMG	O6-C6-C5	2.33	128.91	124.37
3	L3	4521	PSU	O2-C2-N1	-2.32	120.23	122.79
3	L3	4494	OMG	O6-C6-C5	2.32	128.91	124.37
3	L3	4689	PSU	C6-N1-C2	-2.31	120.32	122.68
2	L1	75	OMG	O6-C6-C5	2.31	128.88	124.37
3	L3	3925	OMU	O2-C2-N1	-2.31	119.72	122.79
3	L3	2351	OMC	C1'-N1-C2	2.31	123.57	118.42
3	L3	4499	OMG	O6-C6-C5	2.31	128.88	124.37
3	L3	1677	PSU	C6-C5-C4	2.31	119.81	118.20
3	L3	3627	OMG	O6-C6-C5	2.30	128.87	124.37
3	L3	1625	OMG	O6-C6-C5	2.30	128.87	124.37
3	L3	3844	PSU	C6-N1-C2	-2.30	120.33	122.68
3	L3	4498	OMU	O2-C2-N1	-2.29	119.75	122.79
3	L3	4628	PSU	C6-C5-C4	2.27	119.78	118.20
3	L3	4576	PSU	C6-N1-C2	-2.27	120.37	122.68
3	L3	2876	OMG	O6-C6-C5	2.26	128.79	124.37
3	L3	2837	OMU	O2-C2-N1	-2.26	119.78	122.79
3	L3	3639	PSU	C6-C5-C4	2.26	119.78	118.20
2	L1	69	PSU	C6-N1-C2	-2.25	120.38	122.68
3	L3	2364	OMG	O6-C6-C5	2.25	128.77	124.37
3	L3	2424	OMG	O6-C6-C5	2.25	128.76	124.37
3	L3	3715	PSU	C6-N1-C2	-2.24	120.39	122.68
3	L3	1534	A2M	C4-C5-N7	-2.23	107.07	109.40
3	L3	1782	PSU	C6-N1-C2	-2.23	120.40	122.68
2	L1	69	PSU	O4'-C1'-C2'	2.23	108.29	105.14
3	L3	4590	A2M	C4-C5-N7	-2.23	107.08	109.40
3	L3	4500	PSU	C6-N1-C2	-2.23	120.41	122.68
3	L3	1326	A2M	O4'-C4'-C3'	-2.22	100.72	105.11
3	L3	2815	A2M	C4-C5-N7	-2.21	107.09	109.40
3	L3	1582	PSU	O2-C2-N1	-2.21	120.36	122.79
3	L3	398	A2M	C4-C5-N7	-2.21	107.10	109.40
3	L3	3920	PSU	C6-C5-C4	2.19	119.73	118.20
3	L3	4637	OMG	O6-C6-C5	2.19	128.65	124.37
3	L3	3715	PSU	O4'-C1'-C2'	2.19	108.23	105.14
3	L3	1322	1MA	C5-C6-N1	-2.19	110.63	113.90
3	L3	1862	PSU	C6-N1-C2	-2.18	120.46	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	3920	PSU	C6-N1-C2	-2.17	120.46	122.68
3	L3	4552	PSU	C6-N1-C2	-2.16	120.47	122.68
3	L3	1781	PSU	C6-C5-C4	2.16	119.71	118.20
3	L3	3853	PSU	C6-N1-C2	-2.16	120.47	122.68
3	L3	2415	OMU	O2-C2-N1	-2.16	119.92	122.79
3	L3	4500	PSU	C6-C5-C4	2.16	119.71	118.20
3	L3	2632	PSU	C6-N1-C2	-2.15	120.48	122.68
3	L3	3830	A2M	C4-C5-N7	-2.15	107.16	109.40
3	L3	1677	PSU	C6-N1-C2	-2.15	120.49	122.68
3	L3	4353	PSU	C6-N1-C2	-2.15	120.49	122.68
3	L3	1782	PSU	C6-C5-C4	2.14	119.69	118.20
3	L3	2422	OMC	C1'-N1-C2	2.14	123.19	118.42
3	L3	1744	PSU	C6-C5-C4	2.14	119.69	118.20
3	L3	400	A2M	C4-C5-N7	-2.13	107.17	109.40
3	L3	3734	PSU	C6-N1-C2	-2.13	120.50	122.68
3	L3	4636	PSU	O4'-C1'-C2'	2.12	108.14	105.14
3	L3	1792	PSU	C6-C5-C4	2.12	119.68	118.20
3	L3	1582	PSU	C6-C5-C4	2.12	119.68	118.20
3	L3	2508	PSU	C6-C5-C4	2.11	119.67	118.20
2	L1	55	PSU	C6-C5-C4	2.11	119.67	118.20
3	L3	4521	PSU	C6-C5-C4	2.11	119.67	118.20
3	L3	1322	1MA	N1-C6-N6	2.10	125.12	119.77
3	L3	5010	PSU	C6-N1-C2	-2.10	120.53	122.68
3	L3	4521	PSU	C6-N1-C2	-2.10	120.53	122.68
3	L3	1536	PSU	C6-N1-C2	-2.09	120.55	122.68
2	L1	55	PSU	C6-N1-C2	-2.09	120.55	122.68
3	L3	3639	PSU	C6-N1-C2	-2.09	120.55	122.68
3	L3	4628	PSU	O4'-C1'-C2'	2.08	108.08	105.14
3	L3	4532	PSU	C6-N1-C2	-2.08	120.55	122.68
3	L3	3730	PSU	C6-C5-C4	2.08	119.65	118.20
3	L3	3695	PSU	C6-N1-C2	-2.07	120.56	122.68
3	L3	4576	PSU	C6-C5-C4	2.07	119.64	118.20
3	L3	3851	PSU	C6-N1-C2	-2.07	120.57	122.68
3	L3	3715	PSU	C6-C5-C4	2.06	119.64	118.20
3	L3	4353	PSU	C6-C5-C4	2.05	119.63	118.20
3	L3	4299	PSU	C6-C5-C4	2.04	119.63	118.20
3	L3	4471	PSU	C6-C5-C4	2.04	119.62	118.20
3	L3	4227	OMU	O2-C2-N1	-2.03	120.08	122.79
3	L3	1524	A2M	C4-C5-N7	-2.03	107.28	109.40
3	L3	3724	A2M	C4-C5-N7	-2.03	107.29	109.40
3	L3	4523	A2M	C4-C5-N7	-2.03	107.29	109.40
3	L3	1779	PSU	C6-C5-C4	2.02	119.61	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	4552	PSU	C6-C5-C4	2.02	119.61	118.20
3	L3	3825	A2M	C4-C5-N7	-2.02	107.30	109.40
3	L3	4353	PSU	O4'-C1'-C2'	2.01	107.98	105.14
3	L3	4299	PSU	C6-N1-C2	-2.01	120.63	122.68
3	L3	1534	A2M	C3'-C2'-C1'	-2.00	99.12	102.89
3	L3	1871	A2M	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
3	L3	398	A2M	C1'-C2'-O2'-CM'
3	L3	400	A2M	C1'-C2'-O2'-CM'
3	L3	1316	OMG	C1'-C2'-O2'-CM2
3	L3	1326	A2M	C1'-C2'-O2'-CM'
3	L3	1340	OMC	C1'-C2'-O2'-CM2
3	L3	1677	PSU	C2'-C1'-C5-C6
3	L3	1871	A2M	C1'-C2'-O2'-CM'
3	L3	2364	OMG	C1'-C2'-O2'-CM2
3	L3	2424	OMG	C1'-C2'-O2'-CM2
3	L3	2787	A2M	C3'-C4'-C5'-O5'
3	L3	2804	OMC	C1'-C2'-O2'-CM2
3	L3	2815	A2M	C1'-C2'-O2'-CM'
3	L3	2837	OMU	C1'-C2'-O2'-CM2
3	L3	2861	OMC	C1'-C2'-O2'-CM2
3	L3	3627	OMG	C1'-C2'-O2'-CM2
3	L3	3701	OMC	C2'-C1'-N1-C2
3	L3	3701	OMC	C2'-C1'-N1-C6
3	L3	3718	A2M	C1'-C2'-O2'-CM'
3	L3	3744	OMG	C1'-C2'-O2'-CM2
3	L3	3830	A2M	C1'-C2'-O2'-CM'
3	L3	3841	OMC	C1'-C2'-O2'-CM2
3	L3	3867	A2M	C3'-C4'-C5'-O5'
3	L3	3887	OMC	C3'-C4'-C5'-O5'
3	L3	3887	OMC	O4'-C4'-C5'-O5'
3	L3	3899	OMG	C1'-C2'-O2'-CM2
3	L3	3925	OMU	C1'-C2'-O2'-CM2
3	L3	4227	OMU	C1'-C2'-O2'-CM2
3	L3	4392	OMG	C1'-C2'-O2'-CM2
3	L3	4571	A2M	C1'-C2'-O2'-CM'
3	L3	4636	PSU	C2'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
3	L3	4637	OMG	C1'-C2'-O2'-CM2
23	LN	245	HIC	CA-CB-CG-ND1
23	LN	245	HIC	CA-CB-CG-CD2
3	L3	4590	A2M	C4'-C5'-O5'-P
3	L3	1862	PSU	C3'-C4'-C5'-O5'
3	L3	4523	A2M	O4'-C4'-C5'-O5'
3	L3	1677	PSU	C3'-C4'-C5'-O5'
3	L3	1677	PSU	O4'-C4'-C5'-O5'
3	L3	1862	PSU	O4'-C4'-C5'-O5'
3	L3	2787	A2M	O4'-C4'-C5'-O5'
3	L3	3867	A2M	O4'-C4'-C5'-O5'
3	L3	4523	A2M	C3'-C4'-C5'-O5'
3	L3	4306	OMU	C3'-C4'-C5'-O5'
3	L3	2401	A2M	C3'-C4'-C5'-O5'
3	L3	3701	OMC	O4'-C4'-C5'-O5'
3	L3	4306	OMU	O4'-C4'-C5'-O5'
3	L3	2364	OMG	O4'-C4'-C5'-O5'
3	L3	2415	OMU	O4'-C4'-C5'-O5'
3	L3	1326	A2M	C3'-C4'-C5'-O5'
3	L3	2401	A2M	O4'-C4'-C5'-O5'
3	L3	3701	OMC	C3'-C4'-C5'-O5'
3	L3	3724	A2M	C1'-C2'-O2'-CM'
3	L3	4306	OMU	C4'-C5'-O5'-P
3	L3	1322	1MA	O4'-C4'-C5'-O5'
3	L3	1625	OMG	C3'-C4'-C5'-O5'
3	L3	4618	OMG	O4'-C4'-C5'-O5'
3	L3	2415	OMU	C4'-C5'-O5'-P
3	L3	3701	OMC	O4'-C1'-N1-C6
3	L3	3844	PSU	C4'-C5'-O5'-P
3	L3	2351	OMC	C2'-C1'-N1-C6
3	L3	3884	PSU	O4'-C1'-C5-C4
3	L3	4370	OMG	C3'-C2'-O2'-CM2
3	L3	4571	A2M	C3'-C2'-O2'-CM'
3	L3	4590	A2M	C3'-C2'-O2'-CM'
3	L3	2351	OMC	O4'-C4'-C5'-O5'
3	L3	4636	PSU	C4'-C5'-O5'-P
3	L3	4296	PSU	C3'-C4'-C5'-O5'
3	L3	1322	1MA	C3'-C4'-C5'-O5'
3	L3	2364	OMG	C3'-C4'-C5'-O5'
3	L3	2415	OMU	C3'-C4'-C5'-O5'
3	L3	4296	PSU	O4'-C4'-C5'-O5'
3	L3	1677	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
3	L3	3884	PSU	O4'-C1'-C5-C6
3	L3	4636	PSU	O4'-C1'-C5-C6
3	L3	2351	OMC	C2'-C1'-N1-C2
3	L3	4306	OMU	C2'-C1'-N1-C2
3	L3	3701	OMC	O4'-C1'-N1-C2
3	L3	4590	A2M	C3'-C4'-C5'-O5'
3	L3	4636	PSU	O4'-C4'-C5'-O5'
3	L3	2351	OMC	C3'-C2'-O2'-CM2
3	L3	1326	A2M	O4'-C4'-C5'-O5'
3	L3	1534	A2M	O4'-C4'-C5'-O5'
3	L3	2422	OMC	O4'-C4'-C5'-O5'
3	L3	4618	OMG	C3'-C4'-C5'-O5'
3	L3	1534	A2M	C4'-C5'-O5'-P
3	L3	4306	OMU	C2'-C1'-N1-C6

There are no ring outliers.

53 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	2837	OMU	1	0
2	L1	69	PSU	2	0
3	L3	1871	A2M	1	0
3	L3	3734	PSU	1	0
3	L3	4227	OMU	1	0
2	L1	75	OMG	2	0
3	L3	4637	OMG	2	0
3	L3	4392	OMG	1	0
3	L3	2861	OMC	1	0
3	L3	2876	OMG	1	0
3	L3	1677	PSU	2	0
3	L3	3841	OMC	1	0
3	L3	1326	A2M	5	0
3	L3	3744	OMG	1	0
3	L3	4296	PSU	1	0
3	L3	2364	OMG	1	0
3	L3	4306	OMU	1	0
3	L3	3899	OMG	1	0
3	L3	4457	PSU	2	0
3	L3	5001	PSU	1	0
3	L3	3869	OMC	1	0
3	L3	4500	PSU	1	0
3	L3	1779	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L3	4620	OMU	1	0
3	L3	1534	A2M	1	0
3	L3	2815	A2M	2	0
3	L3	2415	OMU	1	0
3	L3	4530	UR3	1	0
3	L3	4618	OMG	1	0
3	L3	3830	A2M	1	0
3	L3	2351	OMC	2	0
3	L3	4494	OMG	2	0
3	L3	3627	OMG	1	0
3	L3	3724	A2M	2	0
3	L3	4623	OMG	1	0
3	L3	1860	PSU	2	0
3	L3	1340	OMC	1	0
3	L3	2804	OMC	1	0
3	L3	3715	PSU	1	0
3	L3	3867	A2M	1	0
3	L3	3925	OMU	1	0
3	L3	3887	OMC	2	0
3	L3	4220	6MZ	1	0
3	L3	1683	PSU	1	0
3	L3	3718	A2M	5	0
3	L3	4571	A2M	1	0
3	L3	2424	OMG	1	0
3	L3	4636	PSU	2	0
3	L3	3851	PSU	1	0
3	L3	398	A2M	2	0
3	L3	3920	PSU	1	0
3	L3	4361	PSU	1	0
3	L3	1744	PSU	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 93 ligands modelled in this entry, 93 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

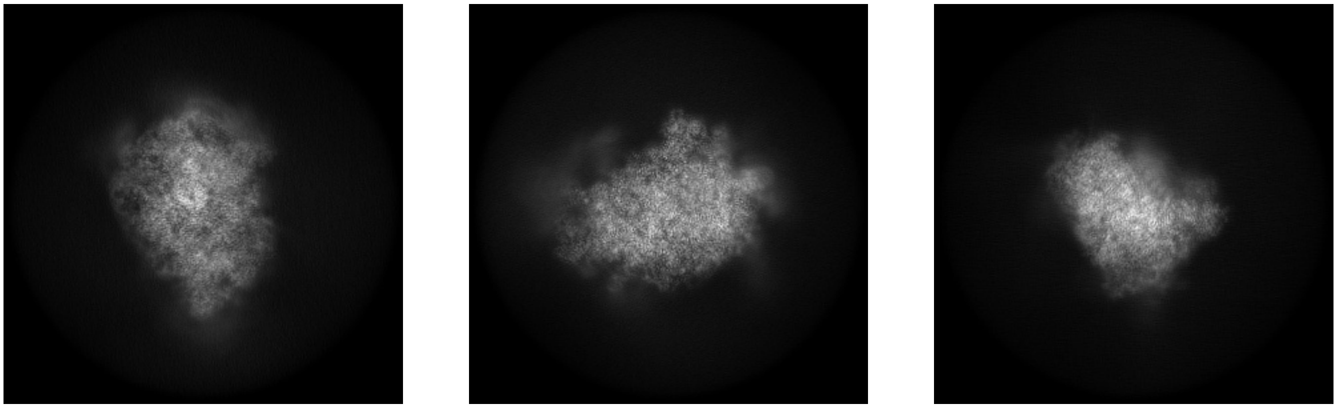
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-29276. 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.

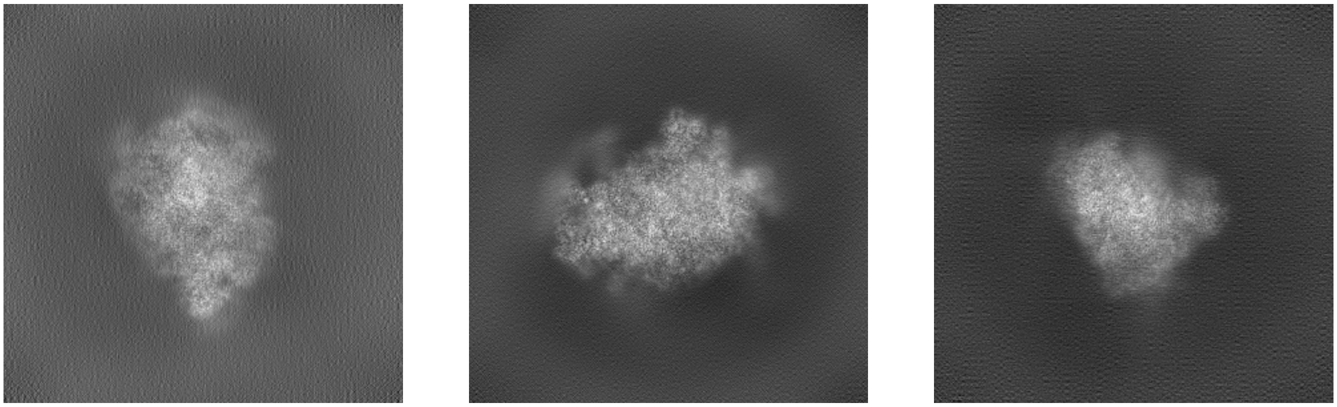
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

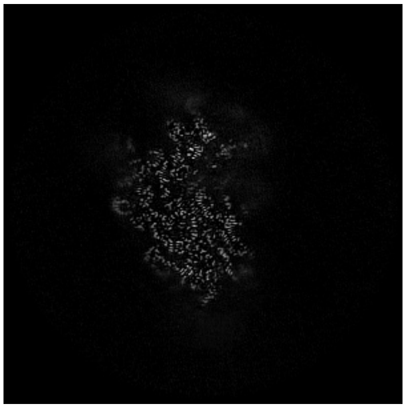


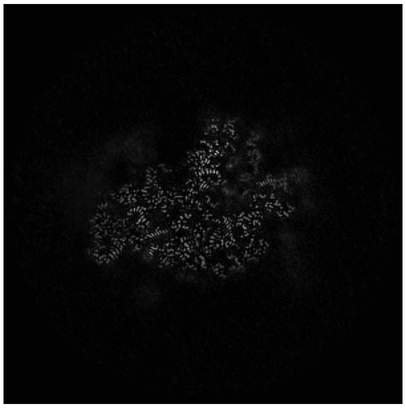
X Y Z

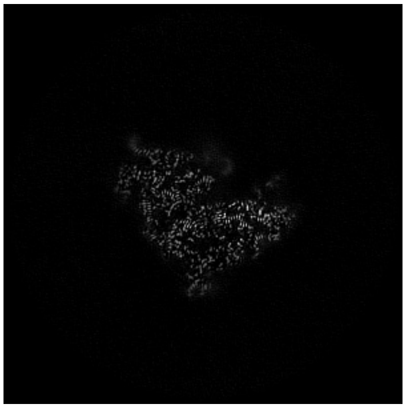
The images above show the map projected in three orthogonal directions.

6.2 Central slices

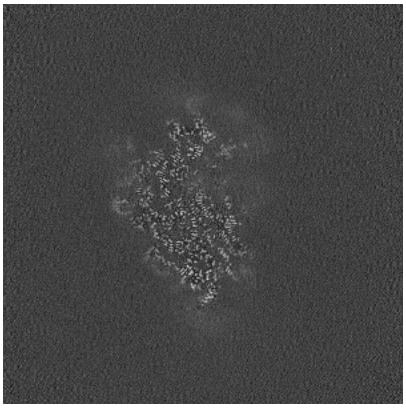
6.2.1 Primary map

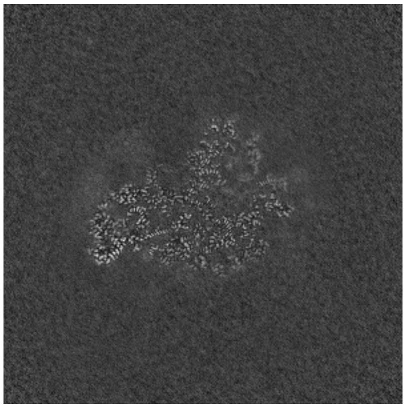

X Index: 240

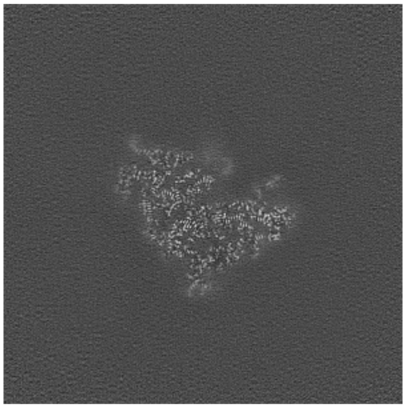

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

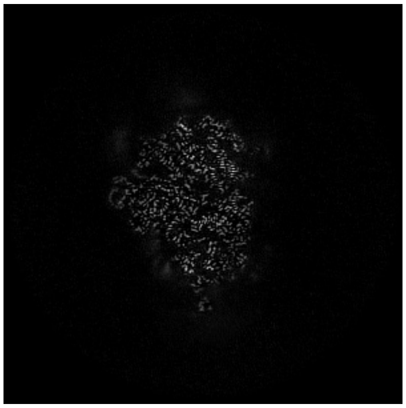

Y Index: 240


Z Index: 240

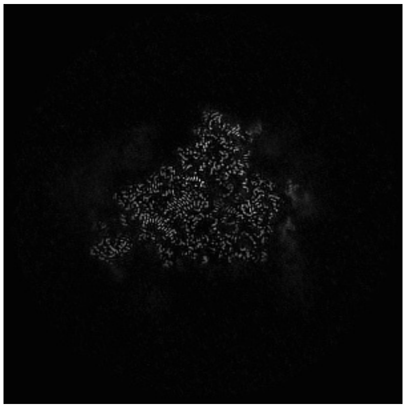
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

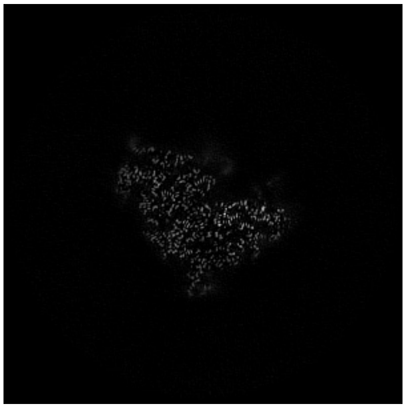
6.3.1 Primary map



X Index: 226

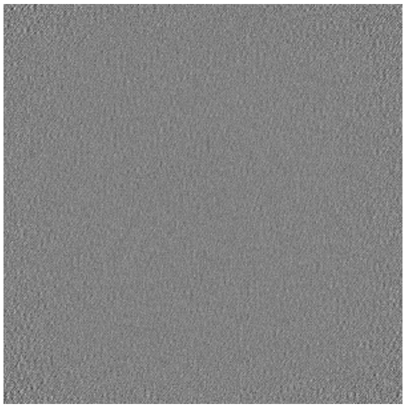


Y Index: 227

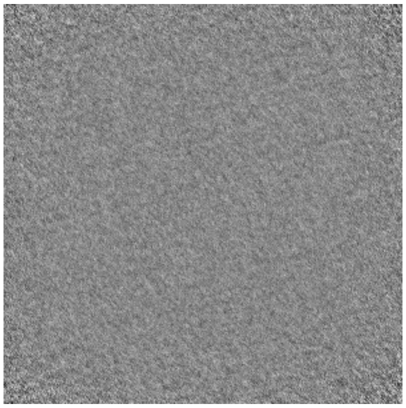


Z Index: 239

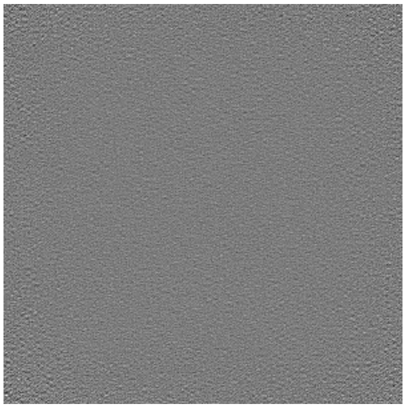
6.3.2 Raw map



X Index: 0



Y Index: 0

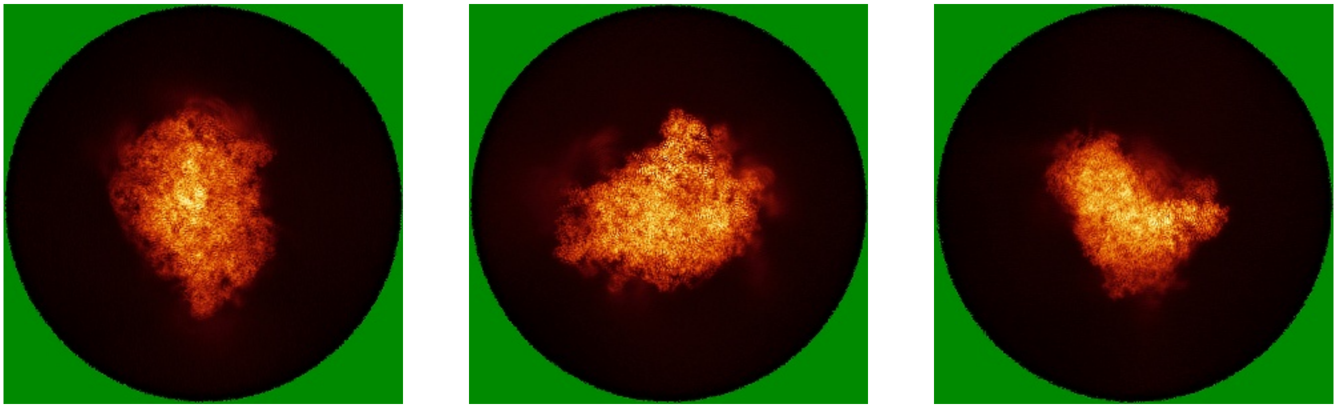


Z Index: 0

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

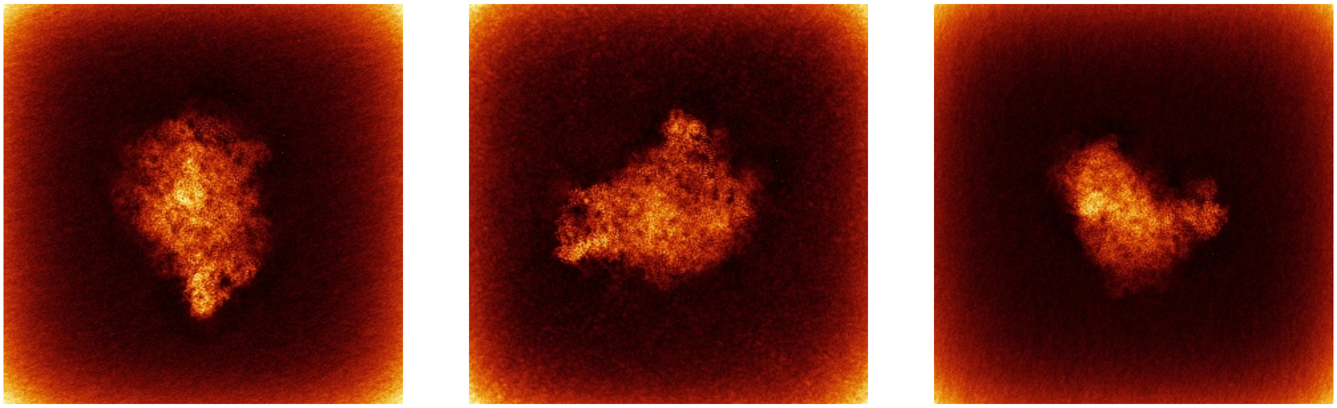
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

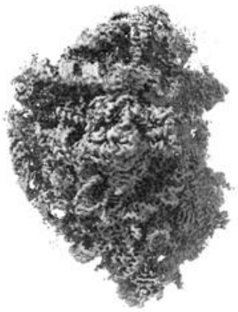


X Y Z

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

6.5.1 Primary map


X

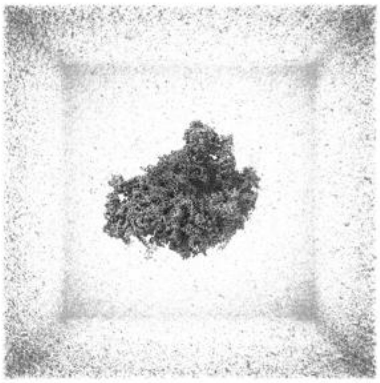

Y

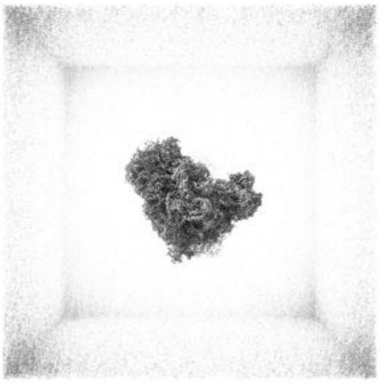

Z

The images above show the 3D surface view of the map at the recommended contour level 0.95. 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.

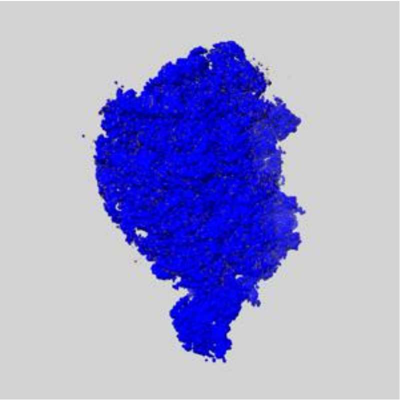
6.6 Mask visualisation ⓘ

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

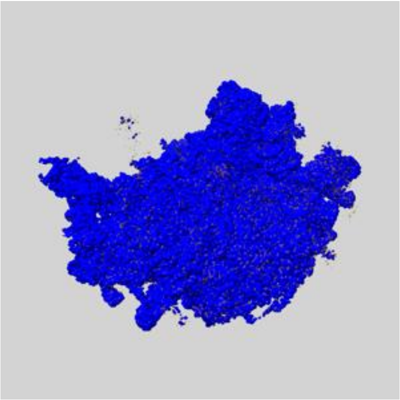
A mask typically either:

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

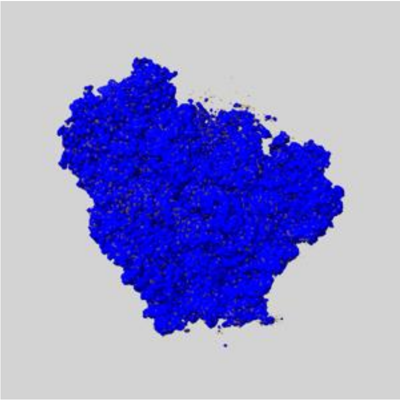
6.6.1 emd_29276_msk_1.map ⓘ



X



Y

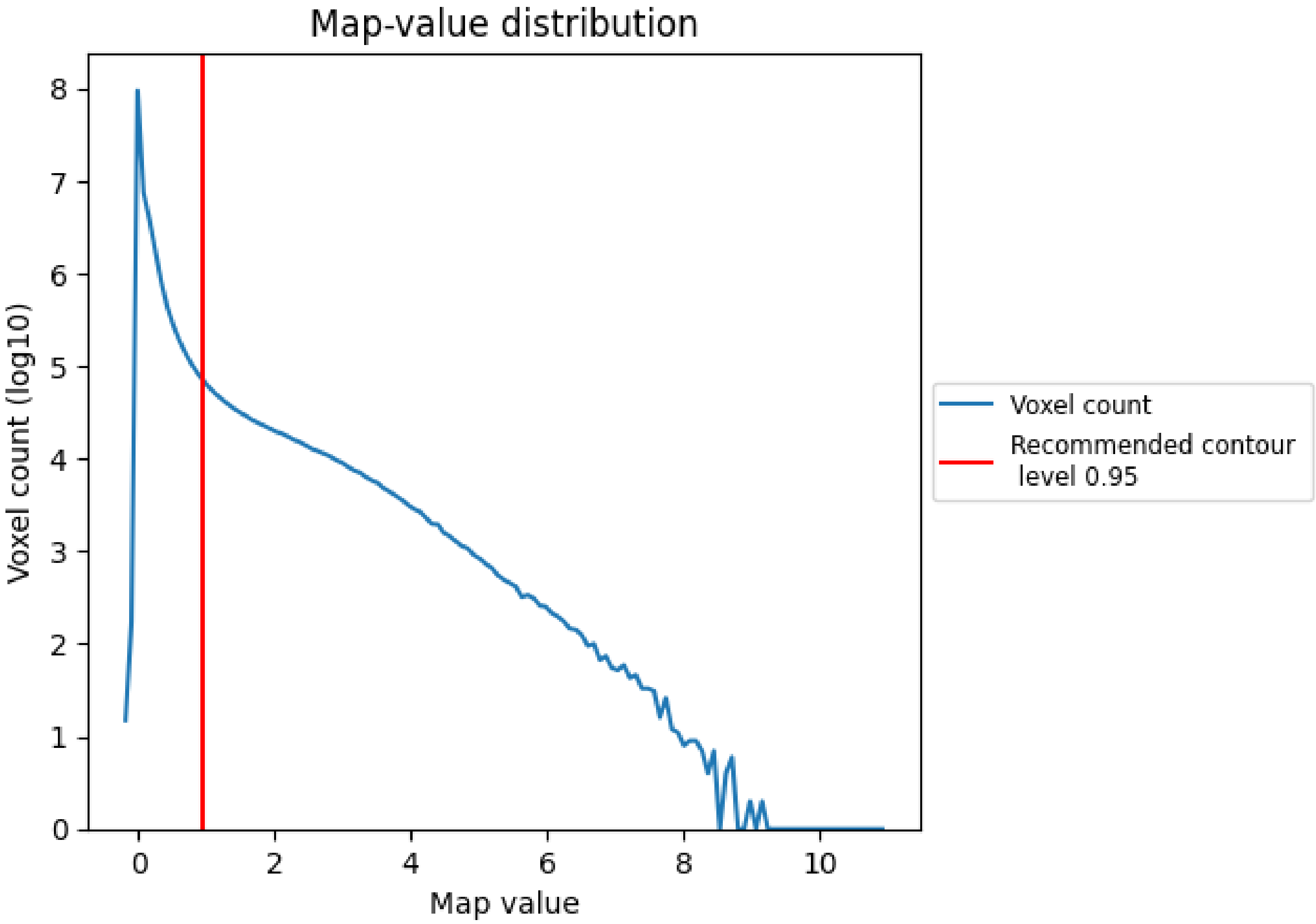


Z

7 Map analysis ⓘ

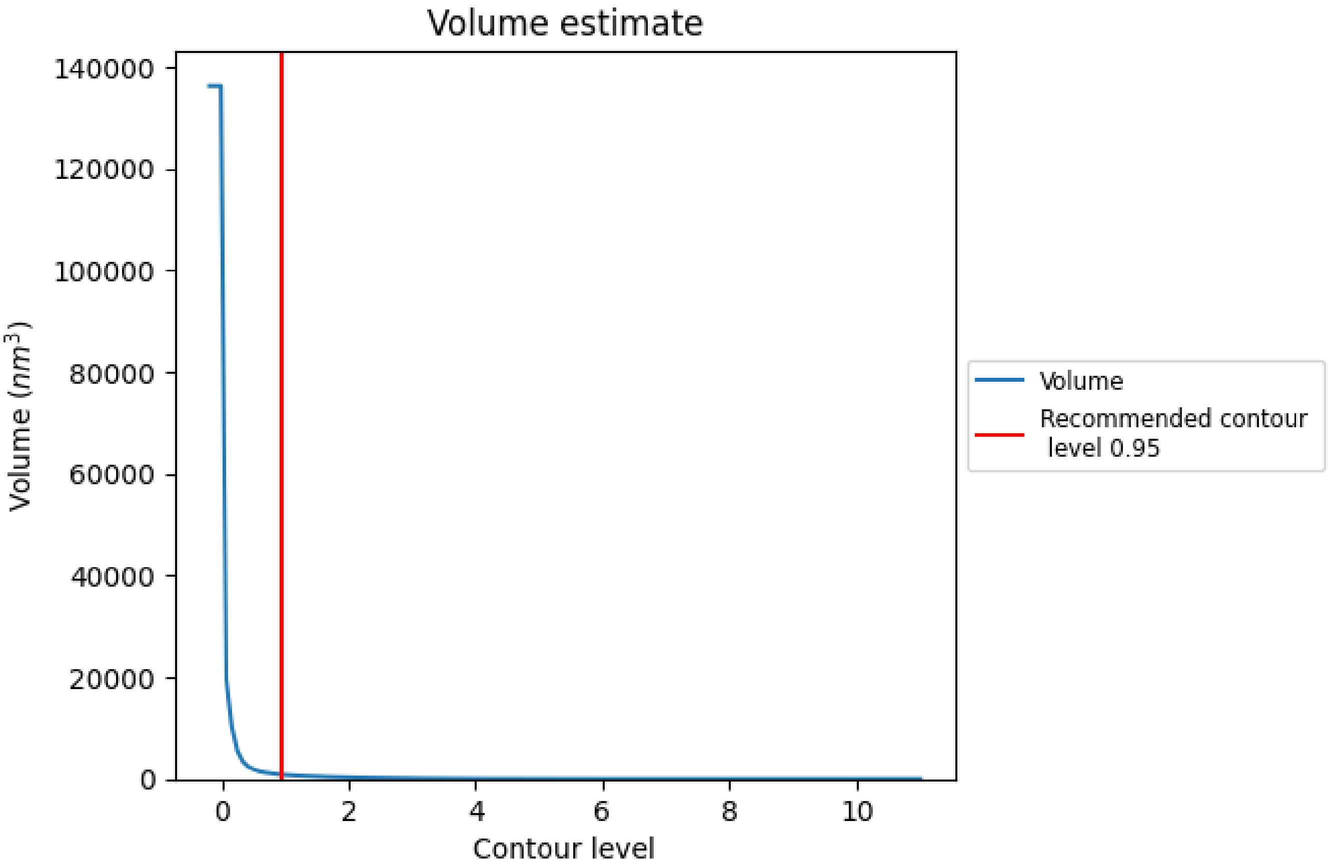
This section contains the results of statistical analysis of the map.

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.

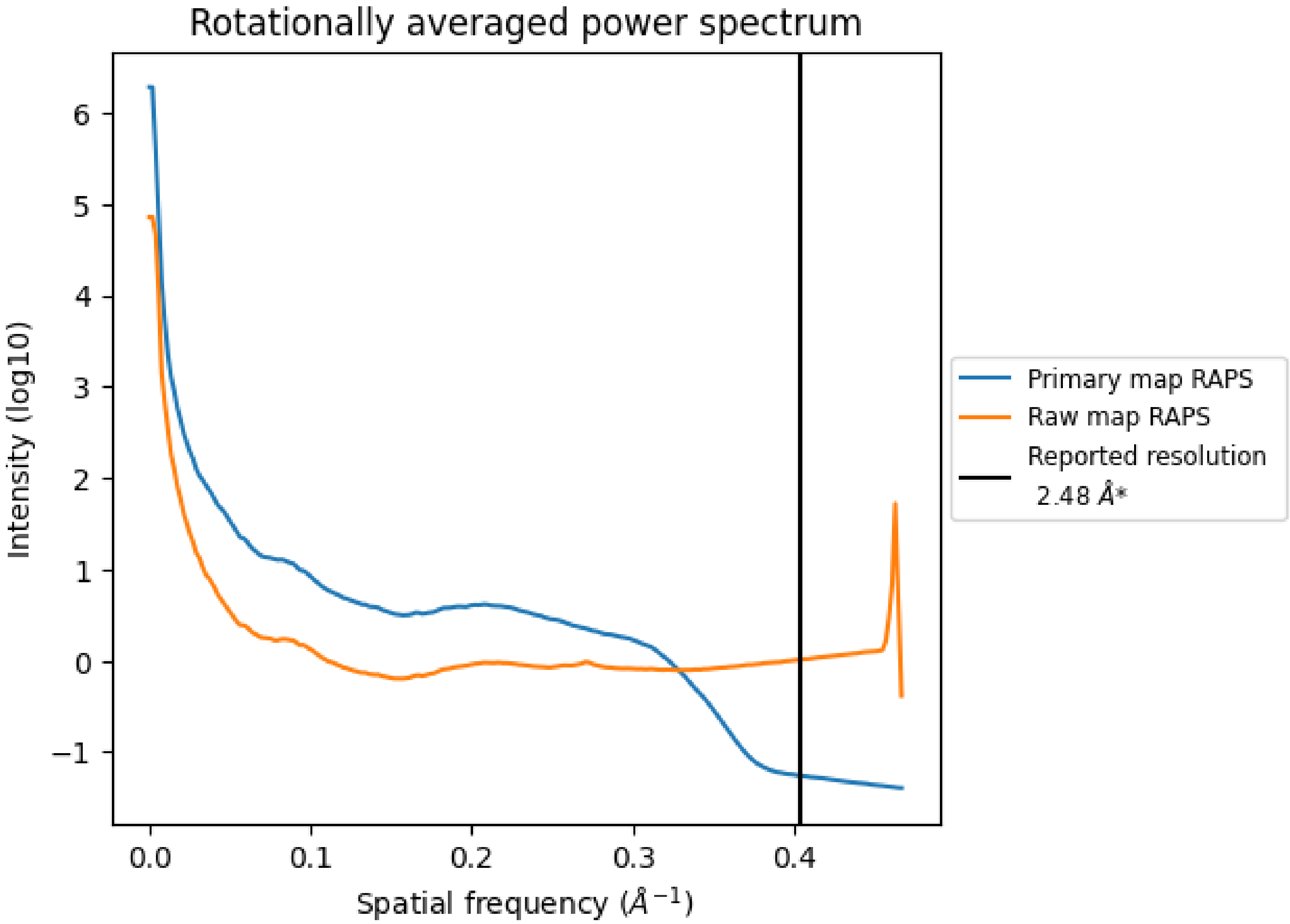
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 881 nm^3; this corresponds to an approximate mass of 795 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 ⓘ

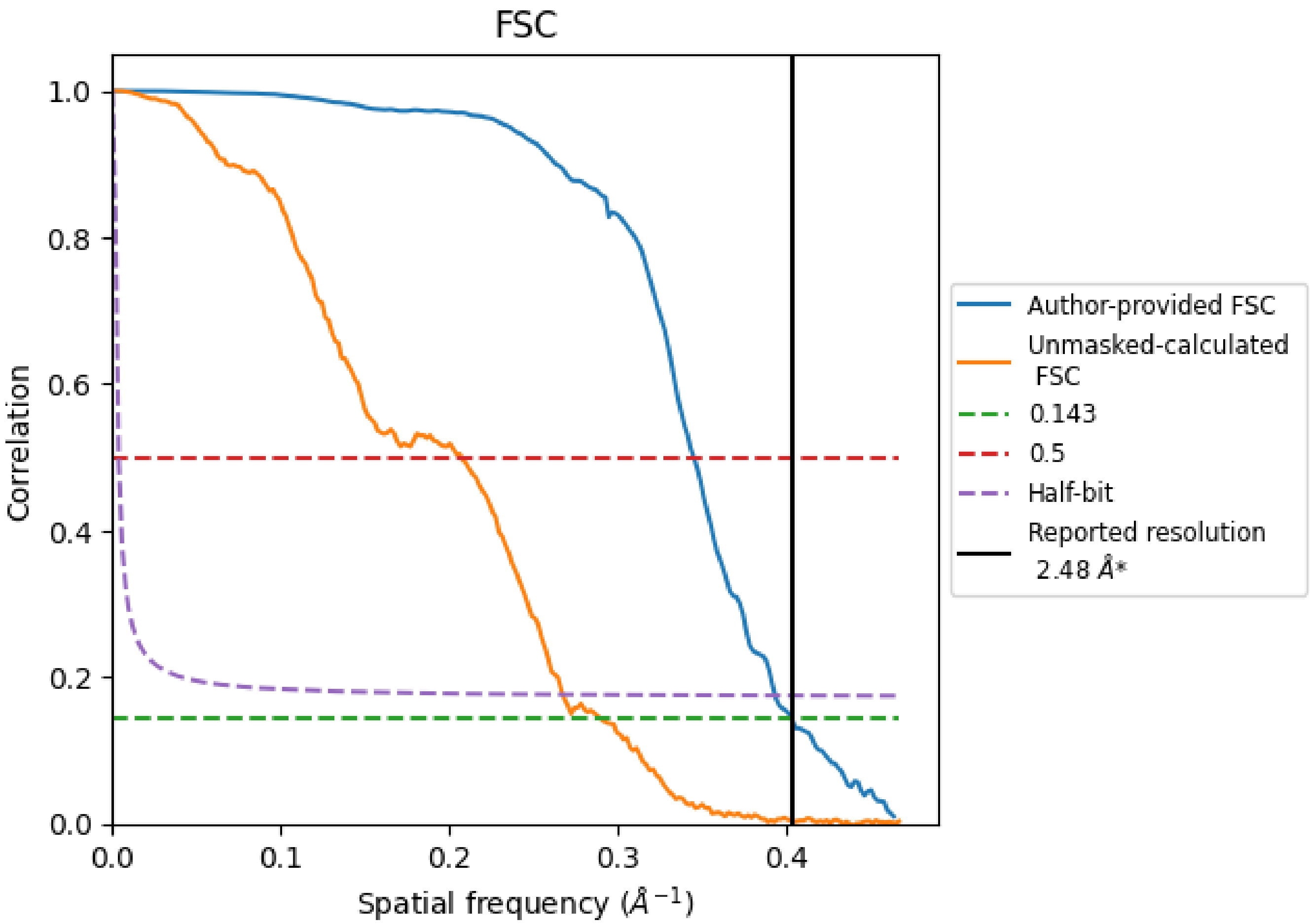


*Reported resolution corresponds to spatial frequency of 0.403 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.403 $Å^{-1}$

8.2 Resolution estimates ⓘ

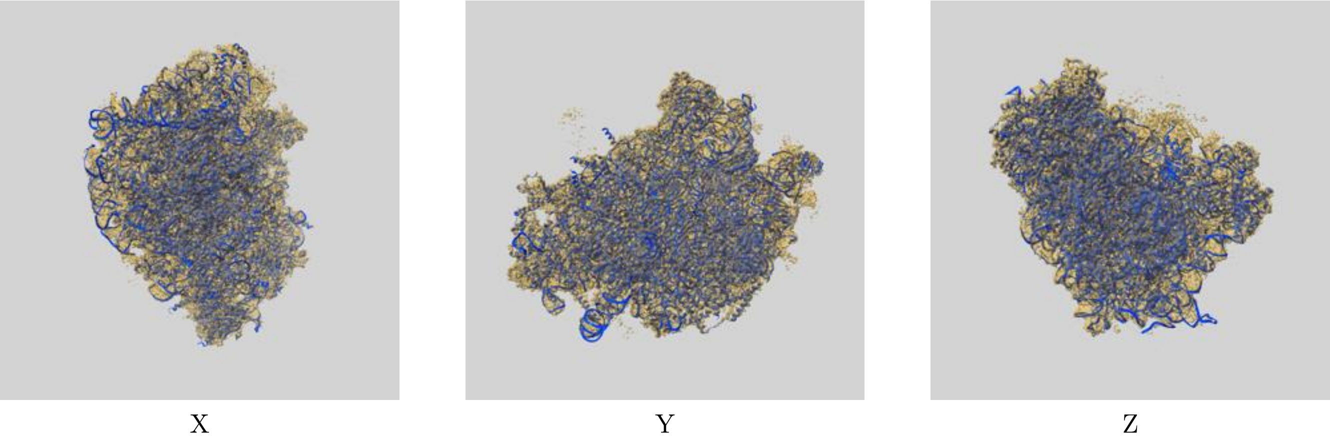
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.90	2.54
Unmasked-calculated*	3.46	4.83	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.48 by more than 10 %

9 Map-model fit ⓘ

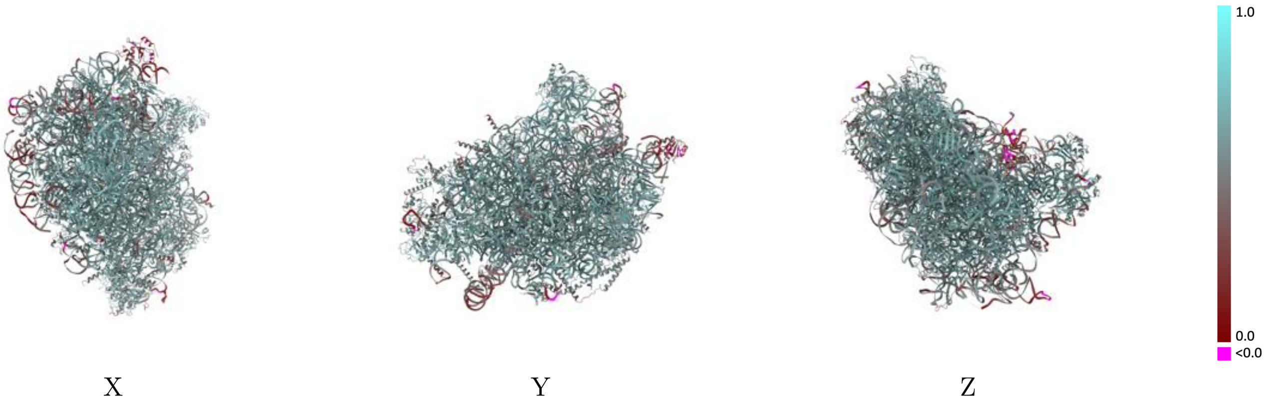
This section contains information regarding the fit between EMDB map EMD-29276 and PDB model 8FLE. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay ⓘ



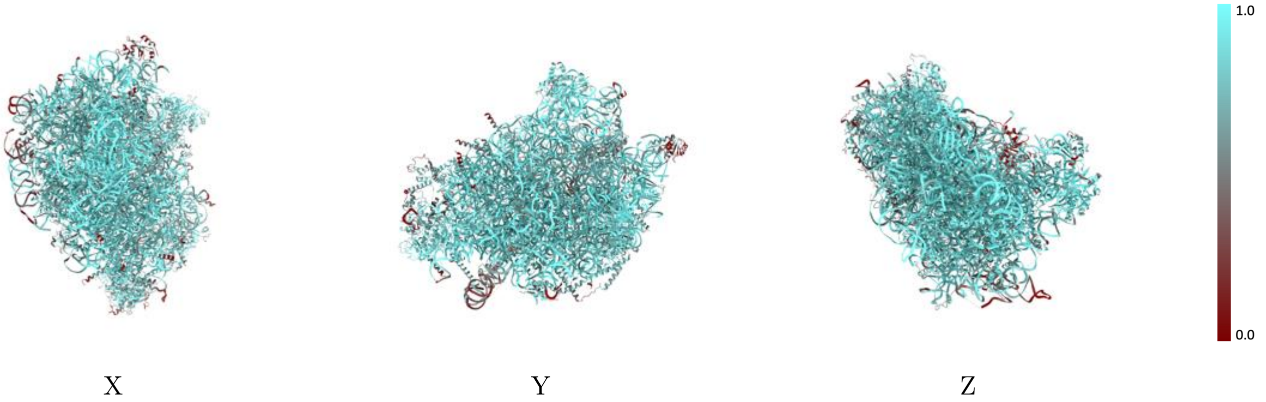
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



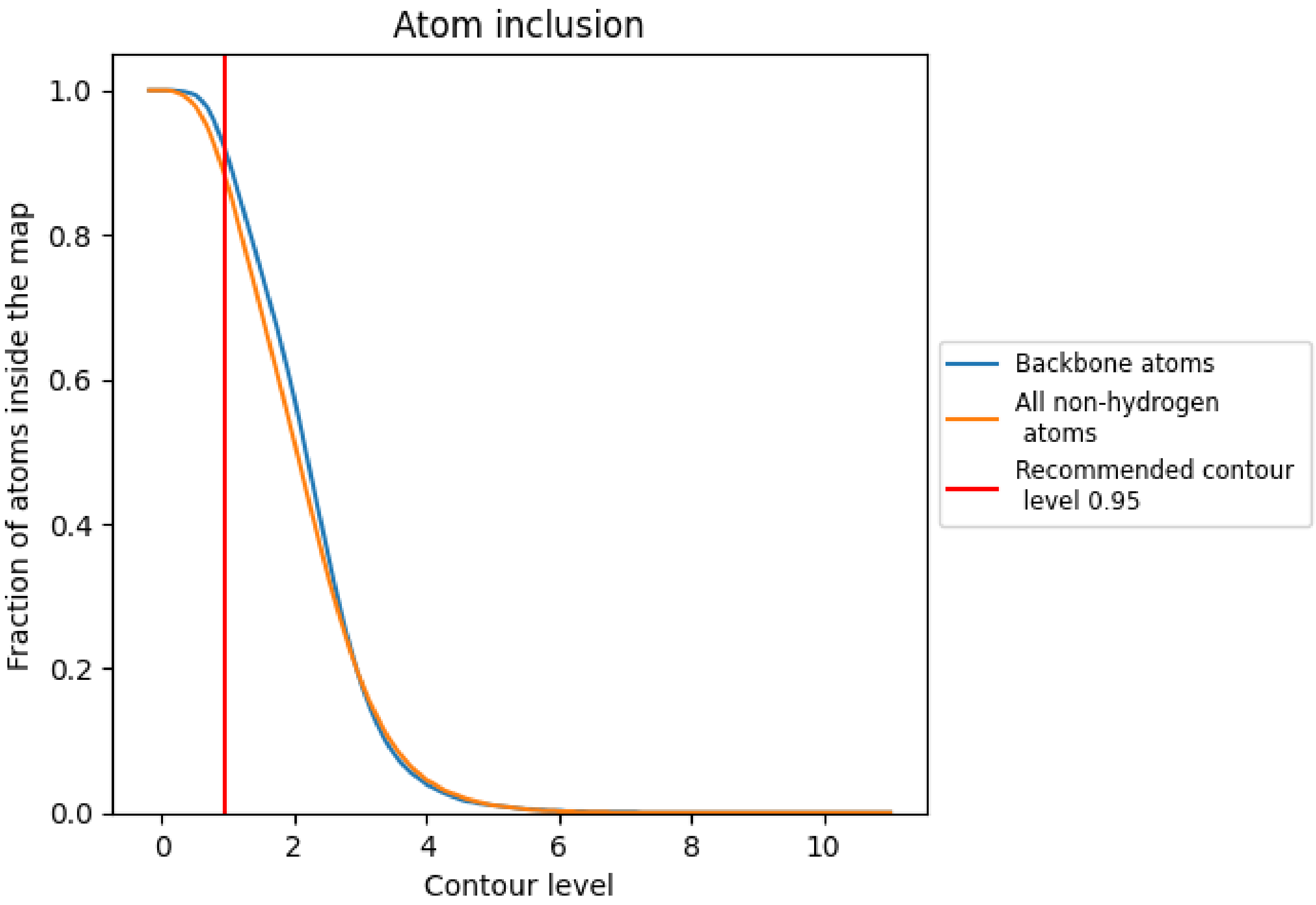
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.5910
BE	0.6340	0.4630
L1	0.9560	0.6260
L3	0.9070	0.5800
L4	0.9920	0.6380
L5	0.8060	0.5720
L6	0.8240	0.5890
L7	0.9070	0.6230
L8	0.9240	0.6220
L9	0.9650	0.6560
LA	0.8830	0.6220
LB	0.9210	0.6360
LC	0.9620	0.6550
LD	0.8480	0.5940
LE	0.9030	0.6140
LF	0.8110	0.5770
LG	0.8770	0.6110
LH	0.8640	0.6240
LI	0.8500	0.5980
LJ	0.9210	0.6250
LK	0.9220	0.6340
LL	0.8860	0.6110
LM	0.7470	0.5640
LN	0.8960	0.6220
LO	0.8040	0.5820
LP	0.8480	0.5970
LQ	0.9070	0.6260
LR	0.8940	0.6230
LS	0.8580	0.6080
LT	0.9310	0.6370
LU	0.7990	0.5850
LV	0.8870	0.6240
LW	0.9450	0.6410
LX	0.8160	0.6050
LY	0.7500	0.5750

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Chain	Atom inclusion	Q-score
LZ	0.9340	0.6320
NK	0.6030	0.5120
NL	0.7690	0.5820
NP	0.7680	0.5830
SA	0.8970	0.6210
SB	0.8830	0.6110
SC	0.7870	0.5700
SD	0.8910	0.6180
SE	0.8450	0.5940
SF	0.9110	0.6380
SG	0.8980	0.6120
SH	0.5860	0.5030
SI	0.6760	0.5460
SK	0.8710	0.5970
SM	0.8800	0.6250
SQ	0.3620	0.2410
SR	0.7230	0.5450
SV	0.8370	0.5950