



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 05:23 PM EDT

PDB ID : 9YGM / pdb\_00009ygm  
EMDB ID : EMD-72933  
Title : Babesia divergens ribosome structure by single-particle cryo-EM (3D class3, E-site tRNA)  
Authors : Gutierrez-Vargas, C.; Izhaki-Tavor, L.S.; Leger-Abraham, M.  
Deposited on : 2025-09-29  
Resolution : 2.70 Å (reported)  
Based on initial models : 5XXU, ., 3J7A, 5XXB

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

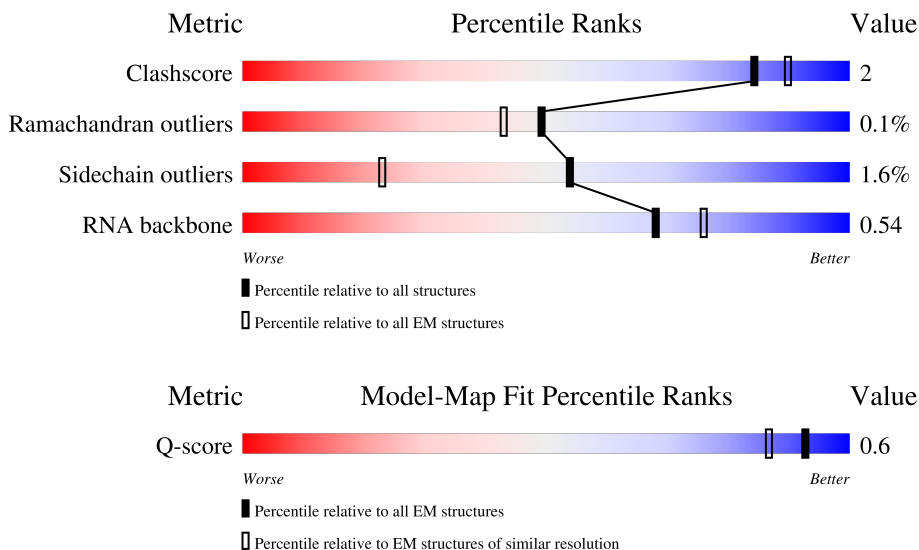
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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

Mol	Chain	Length	Quality of chain
1	L3	122	 77% 16% 7%
2	LB	257	 92% . .
3	LC	395	 91% 5% .

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Mol	Chain	Length	Quality of chain
4	LE	171	94%
5	LF	190	96%
6	LG	212	65% 5% 30%
7	LJ	203	96%
8	LK	139	87% 6% 7%
9	LP	306	91% 6%
10	LQ	222	82% 16%
11	LU	194	77% 22%
12	LV	122	77% 20%
13	LZ	146	90% 5%
14	La	123	93%
15	Lb	59	88% 10%
16	Ld	108	81% 5% 14%
17	Le	117	86% 10%
18	Lf	132	90% 5% 5%
19	Lg	115	93% 6%
20	LD	360	90% 6% 5%
21	LI	202	96%
22	LL	133	90% 6%
23	LM	147	98%
24	LN	204	94% 5%
25	LO	227	88% 5% 7%
26	LR	194	85% 5% 10%
27	LS	188	96%
28	LT	160	92%









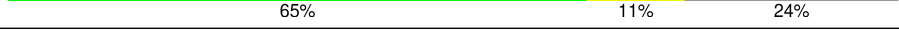

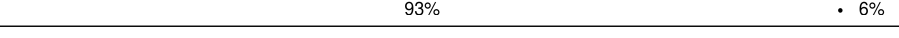
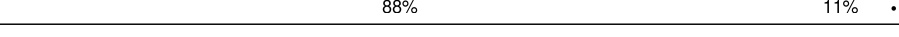

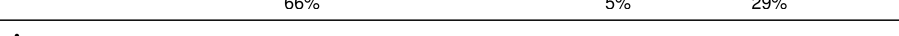


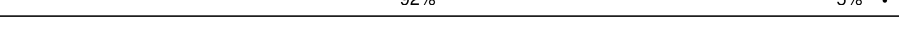

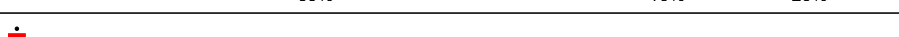






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Mol	Chain	Length	Quality of chain
29	LX	137	85% 5% 10%
30	Lc	259	78% 5% 17%
31	Lh	150	63% 34%
32	Li	116	88% 5% 7%
33	Lj	98	88% 9%
34	Lk	70	83% 10% 7%
35	Ll	59	80% 17%
36	Lm	55	91% 9%
37	Lp	94	90% 7% 3%
38	Lo	105	92% 8%
39	LH	285	5% 76% 21%
40	SA	264	72% 8% 19%
41	SB	274	66% 5% 28%
42	SD	184	94% 6%
43	SE	266	93% 7%
44	SF	196	91% 8%
45	SG	239	85% 5% 10%
46	SI	194	15% 84% 7% 8%
47	SJ	130	93% 6% 1%
48	SK	192	86% 7% 6%
49	SP	145	86% 13% 1%
50	ST	151	94% 5% 1%
51	SU	156	90% 6% 4%
52	SY	79	96% 4% 1%
53	Sb	115	78% 6% 16%



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Mol	Chain	Length	Quality of chain
54	Sc	82	
55	Se	61	
56	SC	223	
57	SH	192	
58	SL	149	
59	SM	120	
60	SQ	135	
61	SR	154	
62	SS	66	
63	SW	149	
64	Sd	67	
65	Sg	323	
66	SN	113	
67	SZ	135	
68	Sa	104	
69	Sf	77	
70	Ln	39	
71	SV	134	
72	SO	157	
73	L4	159	
74	L5	3326	
75	S7	74	
76	S1	1728	
77	LA	217	
78	LW	153	

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Mol	Chain	Length	Quality of chain
79	LY	156	
80	SX	174	

## 2 Entry composition [i](#)

There are 84 unique types of molecules in this entry. The entry contains 189052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L3	122	2610	1163	476	849	122	0	0

- Molecule 2 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	LB	248	1892	1179	382	326	5	0	0

- Molecule 3 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	LC	381	3036	1934	565	522	15	0	0

- Molecule 4 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LE	166	1345	850	250	239	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LF	186	1469	934	263	266	6	0	0

- Molecule 6 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LG	149	1163	753	200	205	5	0	0

- Molecule 7 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LJ	196	1544	970	307	256	11	0	0

- Molecule 8 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LK	129	973	620	179	168	6	0	0

- Molecule 9 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LP	289	2351	1488	436	417	10	0	0

- Molecule 10 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LQ	186	1449	911	285	248	5	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LQ	?	-	VAL	deletion	UNP A0AAD9G7R0
LQ	?	-	ASP	deletion	UNP A0AAD9G7R0
LQ	?	-	PHE	deletion	UNP A0AAD9G7R0
LQ	?	-	HIS	deletion	UNP A0AAD9G7R0
LQ	?	-	GLU	deletion	UNP A0AAD9G7R0
LQ	?	-	LYS	deletion	UNP A0AAD9G7R0
LQ	?	-	ASP	deletion	UNP A0AAD9G7R0
LQ	?	-	MET	deletion	UNP A0AAD9G7R0
LQ	?	-	MET	deletion	UNP A0AAD9G7R0
LQ	?	-	MET	deletion	UNP A0AAD9G7R0
LQ	?	-	HIS	deletion	UNP A0AAD9G7R0
LQ	?	-	VAL	deletion	UNP A0AAD9G7R0
LQ	?	-	SER	deletion	UNP A0AAD9G7R0
LQ	?	-	THR	deletion	UNP A0AAD9G7R0
LQ	?	-	GLU	deletion	UNP A0AAD9G7R0
LQ	?	-	SER	deletion	UNP A0AAD9G7R0
LQ	?	-	ARG	deletion	UNP A0AAD9G7R0

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Chain	Residue	Modelled	Actual	Comment	Reference
LQ	?	-	ARG	deletion	UNP A0AAD9G7R0
LQ	?	-	SER	deletion	UNP A0AAD9G7R0
LQ	?	-	SER	deletion	UNP A0AAD9G7R0
LQ	?	-	ASP	deletion	UNP A0AAD9G7R0
LQ	?	-	SER	deletion	UNP A0AAD9G7R0
LQ	?	-	ALA	deletion	UNP A0AAD9G7R0
LQ	?	-	GLY	deletion	UNP A0AAD9G7R0
LQ	?	-	GLU	deletion	UNP A0AAD9G7R0

- Molecule 11 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LU	152	1231	777	242	207	5	0	0

- Molecule 12 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LV	97	799	513	141	144	1	0	0

- Molecule 13 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LZ	138	1120	707	217	190	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	La	119	985	623	194	165	3	0	0

- Molecule 15 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Lb	53	431	267	95	66	3	0	0

- Molecule 16 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ld	93	Total	C	N	O	S	0	0
			706	444	126	127	9		

- Molecule 17 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Le	105	Total	C	N	O	S	0	0
			869	550	169	147	3		

- Molecule 18 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Lf	125	Total	C	N	O	S	0	0
			1026	647	212	165	2		

- Molecule 19 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Lg	108	Total	C	N	O	S	0	0
			879	563	167	144	5		

- Molecule 20 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LD	343	Total	C	N	O	S	0	0
			2634	1657	512	453	12		

- Molecule 21 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LI	201	Total	C	N	O	S	0	0
			1628	1038	317	264	9		

- Molecule 22 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL	128	Total	C	N	O	S	0	0
			1018	657	183	175	3		

- Molecule 23 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LM	146	1159	737	230	186	6	0	0

- Molecule 24 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LN	202	1708	1073	360	266	9	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LN	1	MET	-	insertion	UNP A0AAD9LIN3
LN	2	GLY	-	insertion	UNP A0AAD9LIN3
LN	3	ALA	-	insertion	UNP A0AAD9LIN3
LN	4	TYR	-	insertion	UNP A0AAD9LIN3
LN	5	ARG	-	insertion	UNP A0AAD9LIN3
LN	6	TYR	-	insertion	UNP A0AAD9LIN3

- Molecule 25 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LO	212	1706	1094	325	279	8	0	0

- Molecule 26 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LR	175	1433	891	300	231	11	0	0

- Molecule 27 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LS	184	1484	944	279	253	8	0	0

- Molecule 28 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LT	154	1238	784	241	207	6	0	0

- Molecule 29 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LX	123	1020	633	206	176	5	0	0

- Molecule 30 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lc	215	1759	1133	332	288	6	0	0

- Molecule 31 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lh	99	808	495	180	128	5	0	0

- Molecule 32 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Li	108	847	530	166	146	5	0	0

- Molecule 33 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Lj	89	703	428	155	113	7	0	0

- Molecule 34 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Lk	65	525	333	99	92	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Ll	49	431	275	93	63	0	0

- Molecule 36 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Lm	50	407	252	85	63	7	0	0

- Molecule 37 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Lp	93	733	455	145	128	5	0	0

- Molecule 38 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Lo	97	782	492	155	129	6	0	0

- Molecule 39 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LH	224	1817	1164	337	308	8	0	0

- Molecule 40 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	SA	215	1742	1107	313	309	13	0	0

- Molecule 41 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	SB	196	1553	997	269	277	10	0	0

- Molecule 42 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	SD	178	1474	934	287	246	7	0	0

- Molecule 43 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SE	258	Total	C	N	O	S	0	0
			2060	1306	383	363	8		

- Molecule 44 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SF	180	Total	C	N	O	S	0	0
			1361	873	241	240	7		

- Molecule 45 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SG	216	Total	C	N	O	S	0	0
			1760	1100	343	307	10		

- Molecule 46 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SI	178	Total	C	N	O	S	0	0
			1430	916	260	251	3		

- Molecule 47 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SJ	129	Total	C	N	O	S	0	0
			1033	661	190	176	6		

- Molecule 48 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SK	181	Total	C	N	O	S	0	0
			1462	914	289	252	7		

- Molecule 49 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SP	143	Total	C	N	O	S	0	0
			1124	709	224	189	2		

- Molecule 50 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	ST	149	Total	C	N	O	S	0	0
			1213	777	228	203	5		

- Molecule 51 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SU	151	Total	C	N	O	S	0	0
			1237	794	230	203	10		

- Molecule 52 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SY	78	Total	C	N	O	S	0	0
			600	368	107	121	4		

- Molecule 53 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Sb	97	Total	C	N	O	S	0	0
			777	477	165	129	6		

- Molecule 54 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Sc	69	Total	C	N	O	S	0	0
			540	341	100	93	6		

- Molecule 55 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Se	40	Total	C	N	O	0	0
			324	199	73	52		

- Molecule 56 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SC	209	Total	C	N	O	S	0	0
			1627	1027	305	289	6		

- Molecule 57 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SH	187	1474	922	281	261	10	0	0

- Molecule 58 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SL	134	1055	666	207	179	3	0	0

- Molecule 59 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SM	98	778	484	143	145	6	0	0

- Molecule 60 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SQ	115	875	550	149	170	6	0	0

- Molecule 61 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SR	144	1147	710	226	204	7	0	0

- Molecule 62 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SS	50	412	260	84	64	4	0	0

- Molecule 63 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SW	115	942	612	166	159	5	0	0

- Molecule 64 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Sd	63	488	301	99	87	1	0	0

- Molecule 65 is a protein called Receptor for activated C kinase 1, RACK1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Sg	322	2489	1570	428	477	14	0	0

- Molecule 66 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SN	96	801	528	135	133	5	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	?	-	GLY	deletion	UNP A0AAD9G6F1
SN	?	-	GLU	deletion	UNP A0AAD9G6F1
SN	?	-	LEU	deletion	UNP A0AAD9G6F1
SN	?	-	ARG	deletion	UNP A0AAD9G6F1
SN	?	-	PHE	deletion	UNP A0AAD9G6F1
SN	?	-	MET	deletion	UNP A0AAD9G6F1
SN	?	-	THR	deletion	UNP A0AAD9G6F1
SN	?	-	VAL	deletion	UNP A0AAD9G6F1
SN	?	-	LEU	deletion	UNP A0AAD9G6F1
SN	?	-	THR	deletion	UNP A0AAD9G6F1
SN	?	-	TYR	deletion	UNP A0AAD9G6F1
SN	?	-	TYR	deletion	UNP A0AAD9G6F1
SN	?	-	PHE	deletion	UNP A0AAD9G6F1
SN	?	-	VAL	deletion	UNP A0AAD9G6F1
SN	?	-	GLY	deletion	UNP A0AAD9G6F1
SN	?	-	SER	deletion	UNP A0AAD9G6F1
SN	?	-	LEU	deletion	UNP A0AAD9G6F1
SN	?	-	HIS	deletion	UNP A0AAD9G6F1
SN	?	-	GLY	deletion	UNP A0AAD9G6F1
SN	?	-	ARG	deletion	UNP A0AAD9G6F1
SN	?	-	ALA	deletion	UNP A0AAD9G6F1

- Molecule 67 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SZ	96	Total	C	N	O	S	0	0
			790	508	147	132	3		

- Molecule 68 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sa	75	Total	C	N	O	S	0	0
			601	382	106	109	4		

- Molecule 69 is a protein called 40S ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sf	64	Total	C	N	O	S	0	0
			509	325	95	83	6		

- Molecule 70 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ln	38	Total	C	N	O	S	0	0
			349	213	89	45	2		

- Molecule 71 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SV	79	Total	C	N	O	S	0	0
			644	407	128	107	2		

- Molecule 72 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SO	126	Total	C	N	O	S	0	0
			950	585	188	173	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	144	IAS	ASP	conflict	UNP A0AAD9GIK0

- Molecule 73 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
73	L4	151	3209	1437	573	1048	151	0	0

- Molecule 74 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
74	L5	2871	61299	27392	10965	20071	2871	0	0

- Molecule 75 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
75	S7	68	1446	646	255	478	67	0	0

- Molecule 76 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
76	S1	1550	33088	14798	5892	10848	1550	0	0

- Molecule 77 is a protein called 60S ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	LA	217	1716	1089	308	311	8	0	0

- Molecule 78 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	LW	118	963	612	181	167	3	0	0

- Molecule 79 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	LY	59	491	319	91	80	1	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	?	-	VAL	deletion	UNP A0AAD9LE14
LY	?	-	CYS	deletion	UNP A0AAD9LE14
LY	?	-	PRO	deletion	UNP A0AAD9LE14
LY	?	-	LYS	deletion	UNP A0AAD9LE14
LY	?	-	VAL	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	CYS	deletion	UNP A0AAD9LE14
LY	?	-	ASN	deletion	UNP A0AAD9LE14
LY	?	-	ASN	deletion	UNP A0AAD9LE14
LY	?	-	PHE	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	GLN	deletion	UNP A0AAD9LE14
LY	?	-	TRP	deletion	UNP A0AAD9LE14
LY	?	-	PRO	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	HIS	deletion	UNP A0AAD9LE14
LY	?	-	ASN	deletion	UNP A0AAD9LE14
LY	?	-	ASN	deletion	UNP A0AAD9LE14
LY	?	-	CYS	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	ALA	deletion	UNP A0AAD9LE14
LY	?	-	LEU	deletion	UNP A0AAD9LE14
LY	?	-	PHE	deletion	UNP A0AAD9LE14
LY	?	-	VAL	deletion	UNP A0AAD9LE14
LY	?	-	THR	deletion	UNP A0AAD9LE14
LY	?	-	MET	deletion	UNP A0AAD9LE14
LY	?	-	VAL	deletion	UNP A0AAD9LE14
LY	?	-	THR	deletion	UNP A0AAD9LE14
LY	?	-	LEU	deletion	UNP A0AAD9LE14
LY	?	-	THR	deletion	UNP A0AAD9LE14
LY	?	-	LYS	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	ASP	deletion	UNP A0AAD9LE14
LY	?	-	ILE	deletion	UNP A0AAD9LE14
LY	?	-	PHE	deletion	UNP A0AAD9LE14
LY	?	-	ILE	deletion	UNP A0AAD9LE14
LY	?	-	ILE	deletion	UNP A0AAD9LE14
LY	?	-	LEU	deletion	UNP A0AAD9LE14
LY	?	-	ALA	deletion	UNP A0AAD9LE14
LY	?	-	PHE	deletion	UNP A0AAD9LE14
LY	?	-	LEU	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14
LY	?	-	SER	deletion	UNP A0AAD9LE14

- Molecule 80 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	SX	159	1300	818	251	226	5	0	0

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
81	L3	1	1	1	0
81	L4	1	1	1	0
81	L5	133	133	133	0
81	S1	1	1	1	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	Lh	1	1	1	0
82	Lj	1	1	1	0
82	Lm	1	1	1	0
82	Lp	1	1	1	0
82	Lo	1	1	1	0

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
83	L5	25	25	25	0
83	S1	1	1	1	0

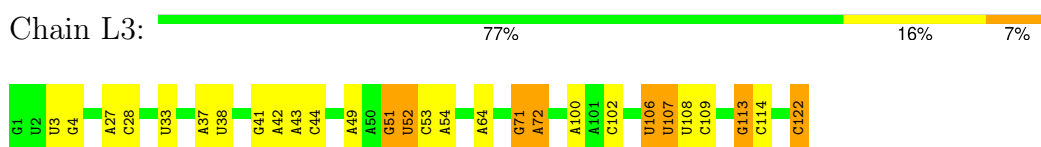
- Molecule 84 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
84	SA	2	Total 2	O 2	0
84	L5	25	Total 25	O 25	0
84	S1	7	Total 7	O 7	0

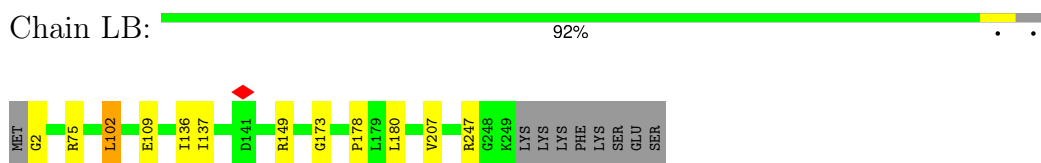
### 3 Residue-property plots [i](#)

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

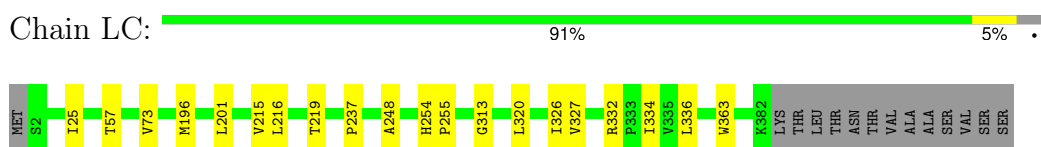
- Molecule 1: 5S ribosomal RNA



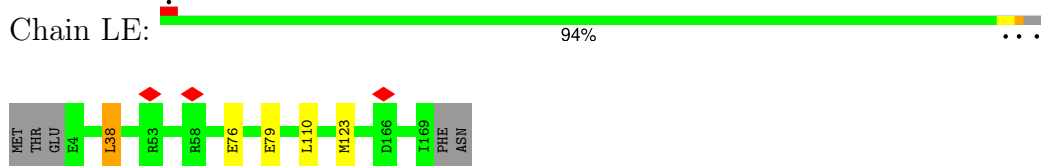
- Molecule 2: 60S ribosomal protein uL2



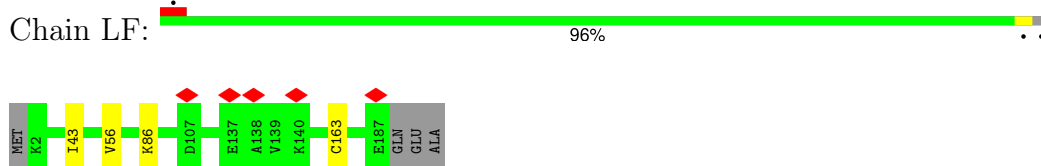
- Molecule 3: 60S ribosomal protein uL3



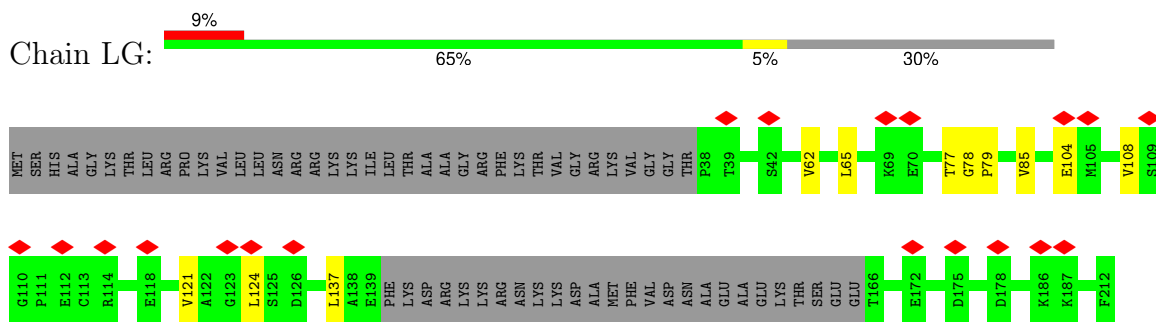
- Molecule 4: 60S ribosomal protein uL5



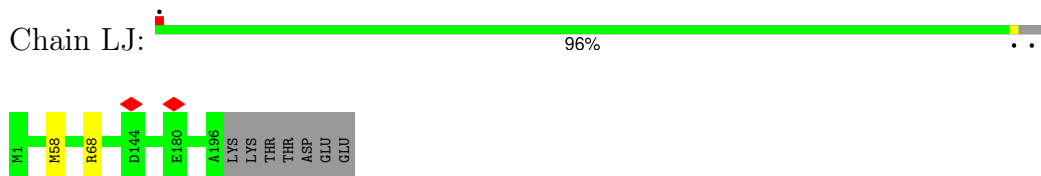
- Molecule 5: 60S ribosomal protein uL6



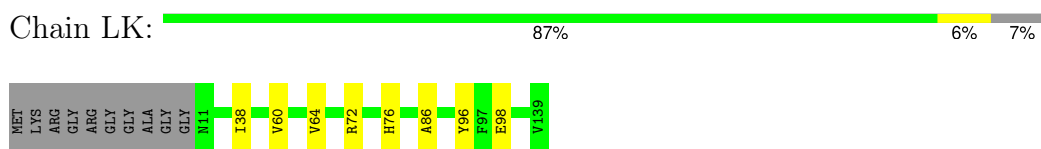
- Molecule 6: 60S ribosomal protein eL6



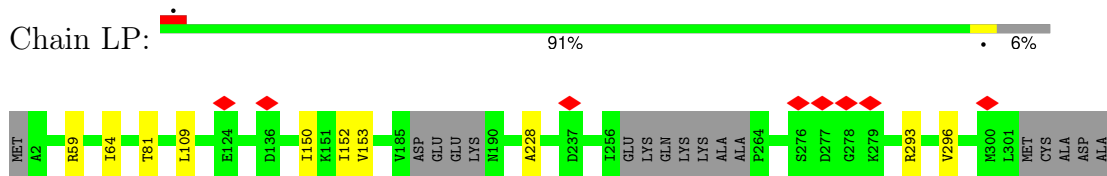
• Molecule 7: 60S ribosomal protein eL13



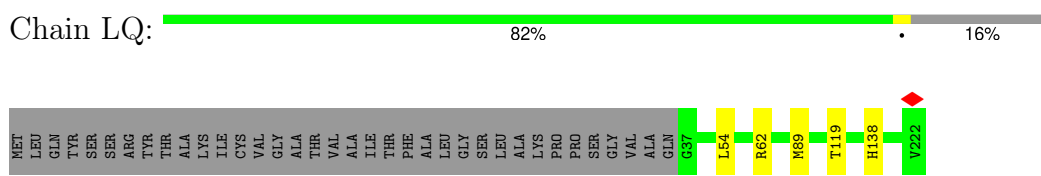
• Molecule 8: 60S ribosomal protein uL14



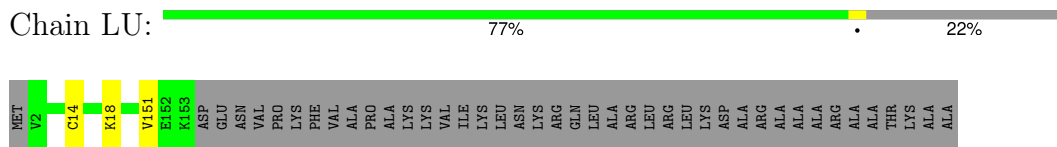
• Molecule 9: 60S ribosomal protein uL18



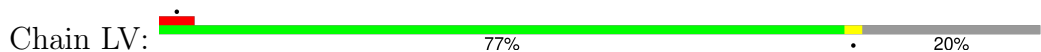
• Molecule 10: 60S ribosomal protein eL18



• Molecule 11: 60S ribosomal protein uL22



• Molecule 12: 60S ribosomal protein eL22

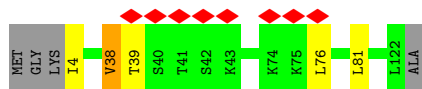




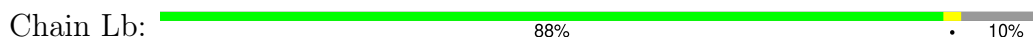
• Molecule 13: 60S ribosomal protein eL27



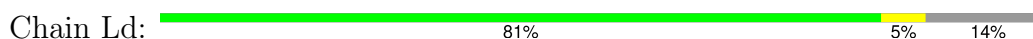
• Molecule 14: 60S ribosomal protein uL29



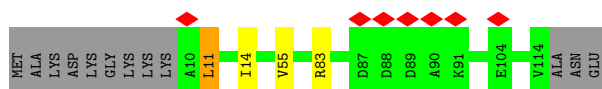
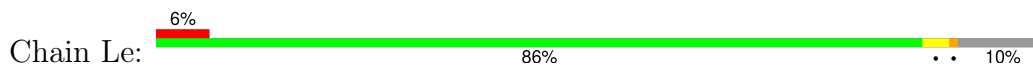
• Molecule 15: 60S ribosomal protein eL29



• Molecule 16: 60S ribosomal protein eL30



• Molecule 17: 60S ribosomal protein eL31

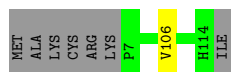


• Molecule 18: 60S ribosomal protein eL32

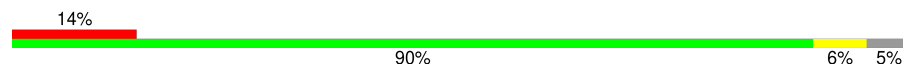


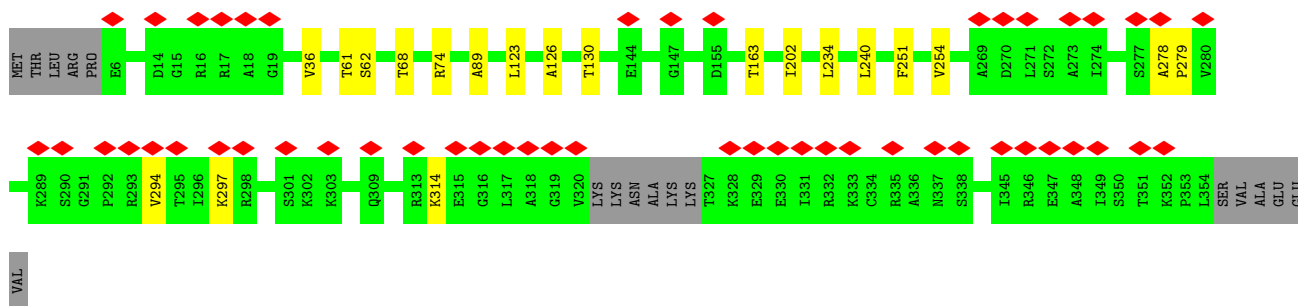
• Molecule 19: 60S ribosomal protein eL33

Chain Lg:  93% • 6%



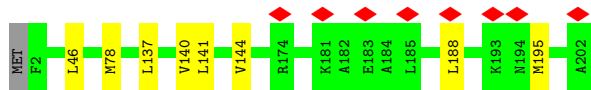
• Molecule 20: 60S ribosomal protein uL4

Chain LD:  14% 90% 6% 5%



• Molecule 21: 60S ribosomal protein uL13

Chain LI:  96% •



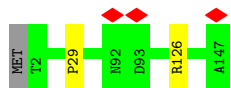
• Molecule 22: 60S ribosomal protein eL14

Chain LL:  90% 6% •



• Molecule 23: 60S ribosomal protein uL15

Chain LM:  98% ••

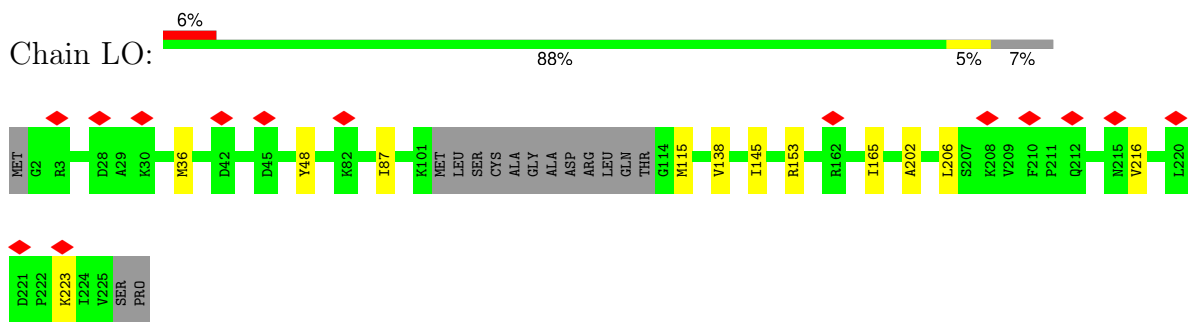


• Molecule 24: 60S ribosomal protein eL15

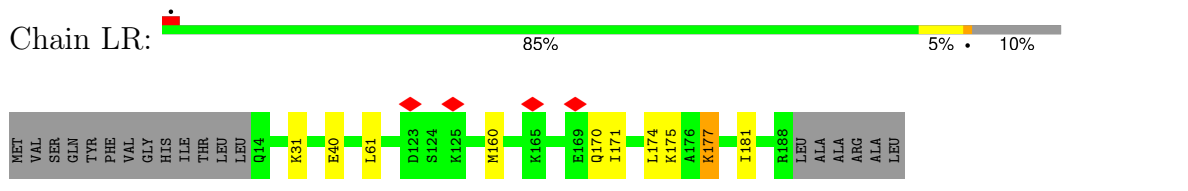
Chain LN:  94% •



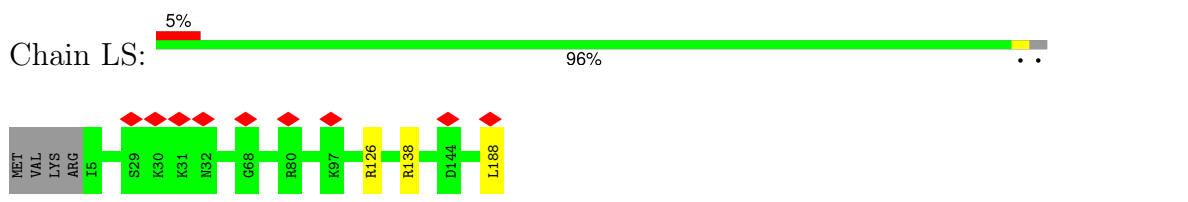
• Molecule 25: 60S ribosomal protein uL16



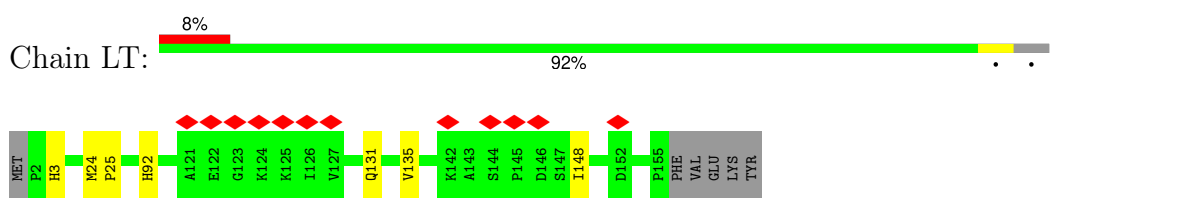
• Molecule 26: 60S ribosomal protein eL19



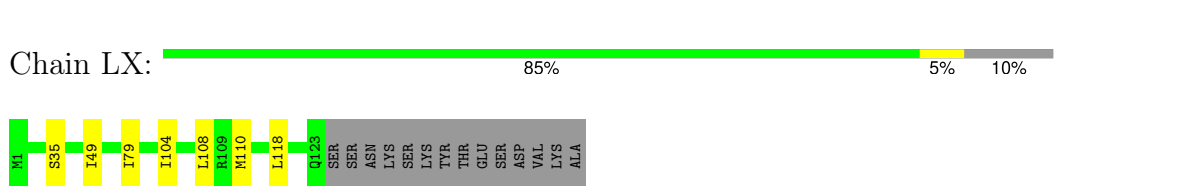
• Molecule 27: 60S ribosomal protein eL20



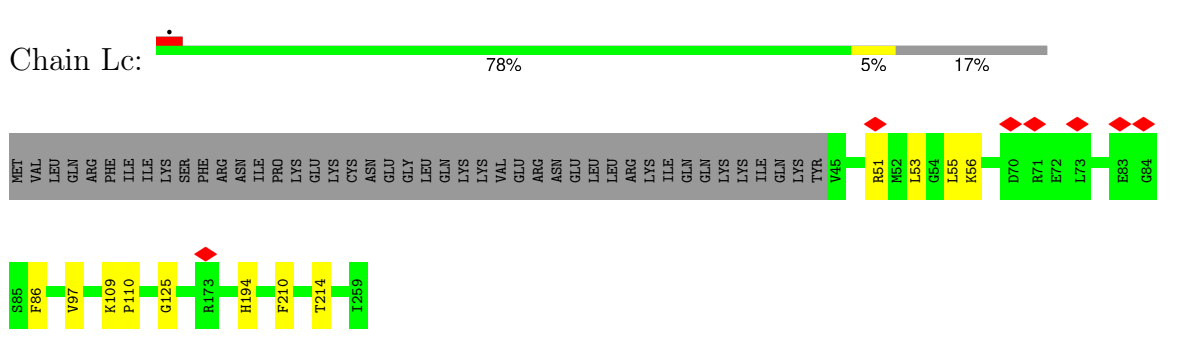
• Molecule 28: 60S ribosomal protein eL21



• Molecule 29: 60S ribosomal protein uL24

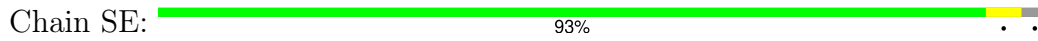


• Molecule 30: 60S ribosomal protein uL30

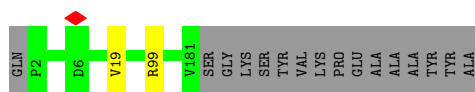




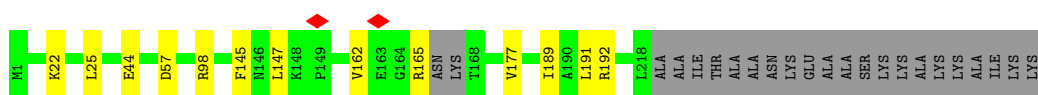
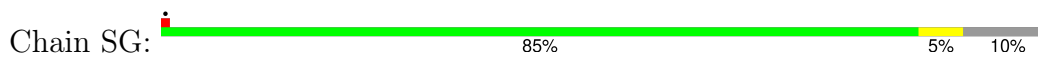




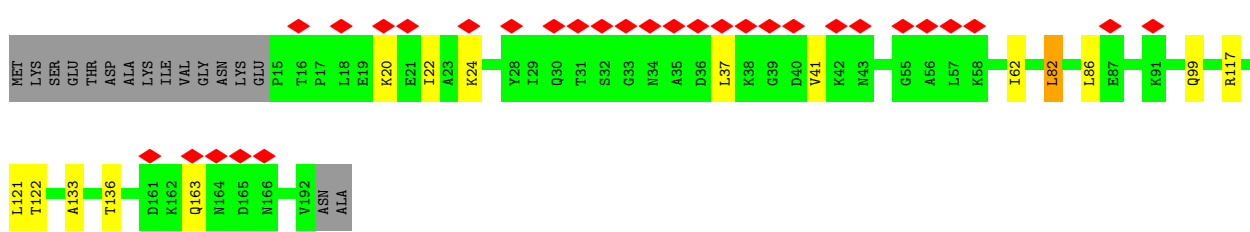
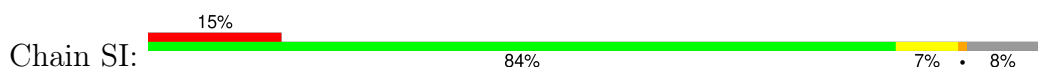
• Molecule 44: 40S ribosomal protein uS5



• Molecule 45: 40S ribosomal protein eS6



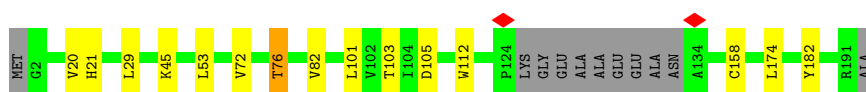
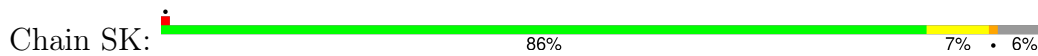
• Molecule 46: 40S ribosomal protein eS7



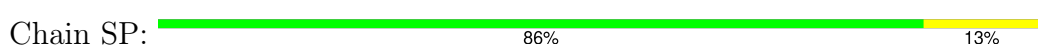
• Molecule 47: 40S ribosomal protein uS8



• Molecule 48: 40S ribosomal protein eS8



• Molecule 49: 40S ribosomal protein uS12





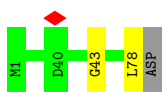
- Molecule 50: 40S ribosomal protein uS15



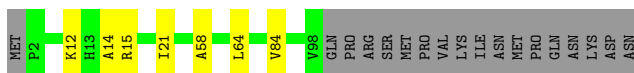
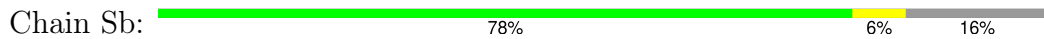
- Molecule 51: 40S ribosomal protein uS17



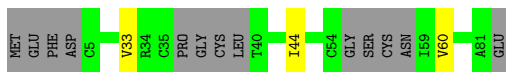
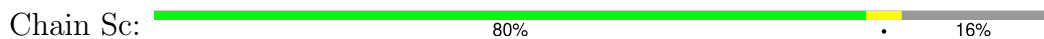
- Molecule 52: 40S ribosomal protein eS21



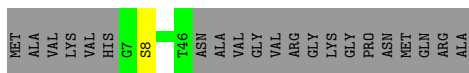
- Molecule 53: 40S ribosomal protein eS26



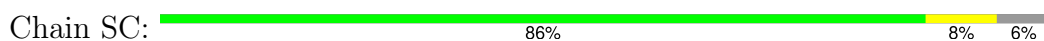
- Molecule 54: 40S ribosomal protein eS27



- Molecule 55: 40S ribosomal protein eS30



- Molecule 56: 40S ribosomal protein uS3

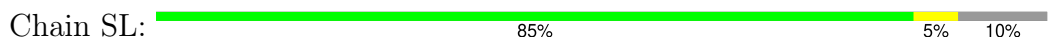




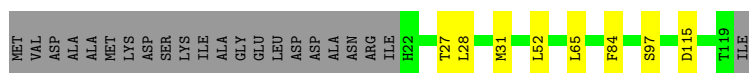
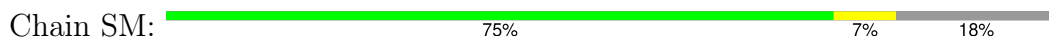
• Molecule 57: 40S ribosomal protein uS7



• Molecule 58: 40S ribosomal protein uS9



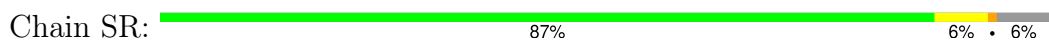
• Molecule 59: 40S ribosomal protein uS10



• Molecule 60: 40S ribosomal protein eS12



• Molecule 61: 40S ribosomal protein uS13



• Molecule 62: 40S ribosomal protein uS14

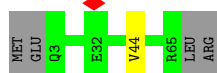


• Molecule 63: 40S ribosomal protein uS19

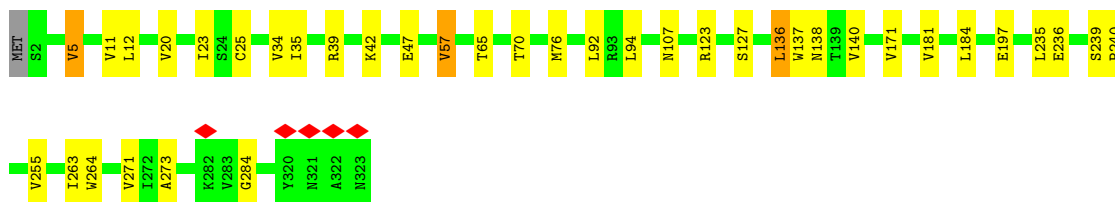
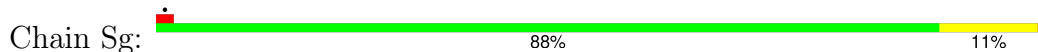




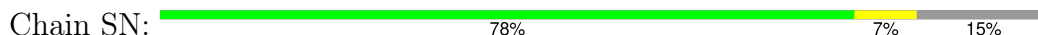
• Molecule 64: 40S ribosomal protein eS28



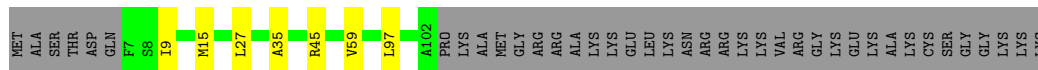
• Molecule 65: Receptor for activated C kinase 1, RACK1 protein



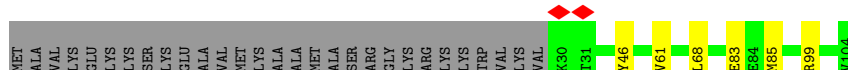
• Molecule 66: 40S ribosomal protein eS10



• Molecule 67: 40S ribosomal protein eS24



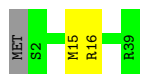
• Molecule 68: 40S ribosomal protein eS25



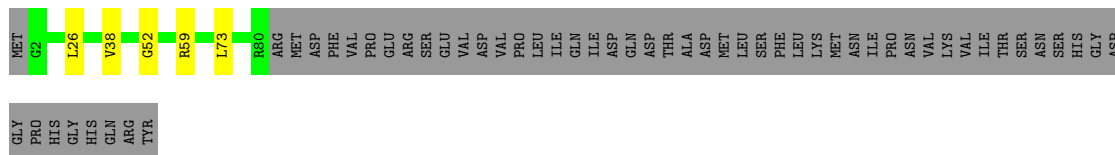
• Molecule 69: 40S ribosomal protein eS31



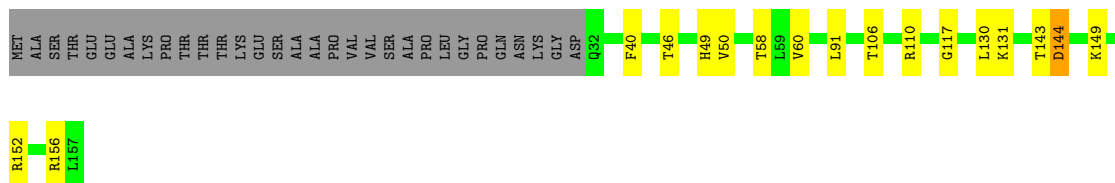
• Molecule 70: 60S ribosomal protein eL41



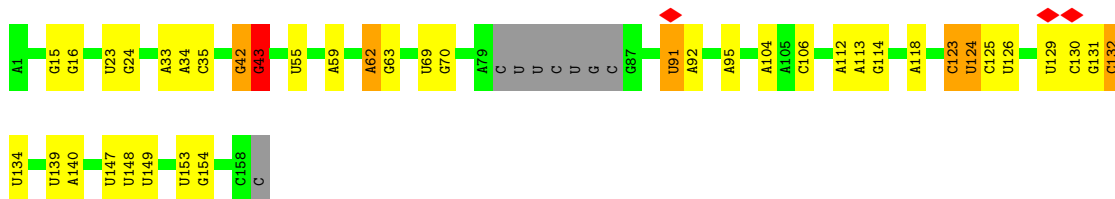
• Molecule 71: 40S ribosomal protein eS17



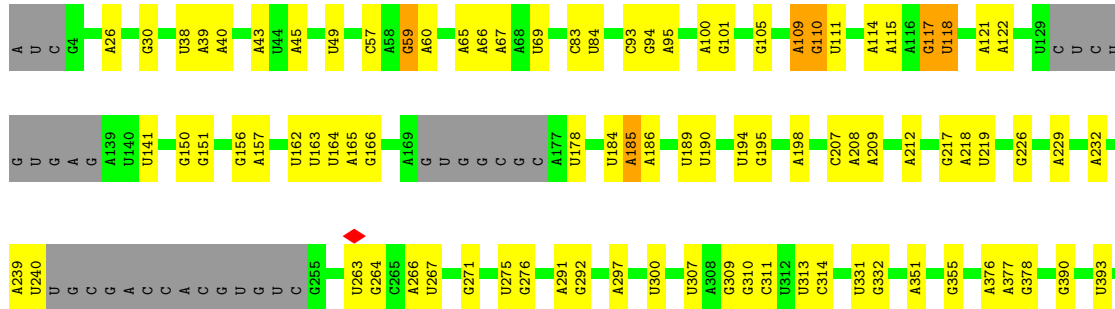
• Molecule 72: 40S ribosomal protein uS11



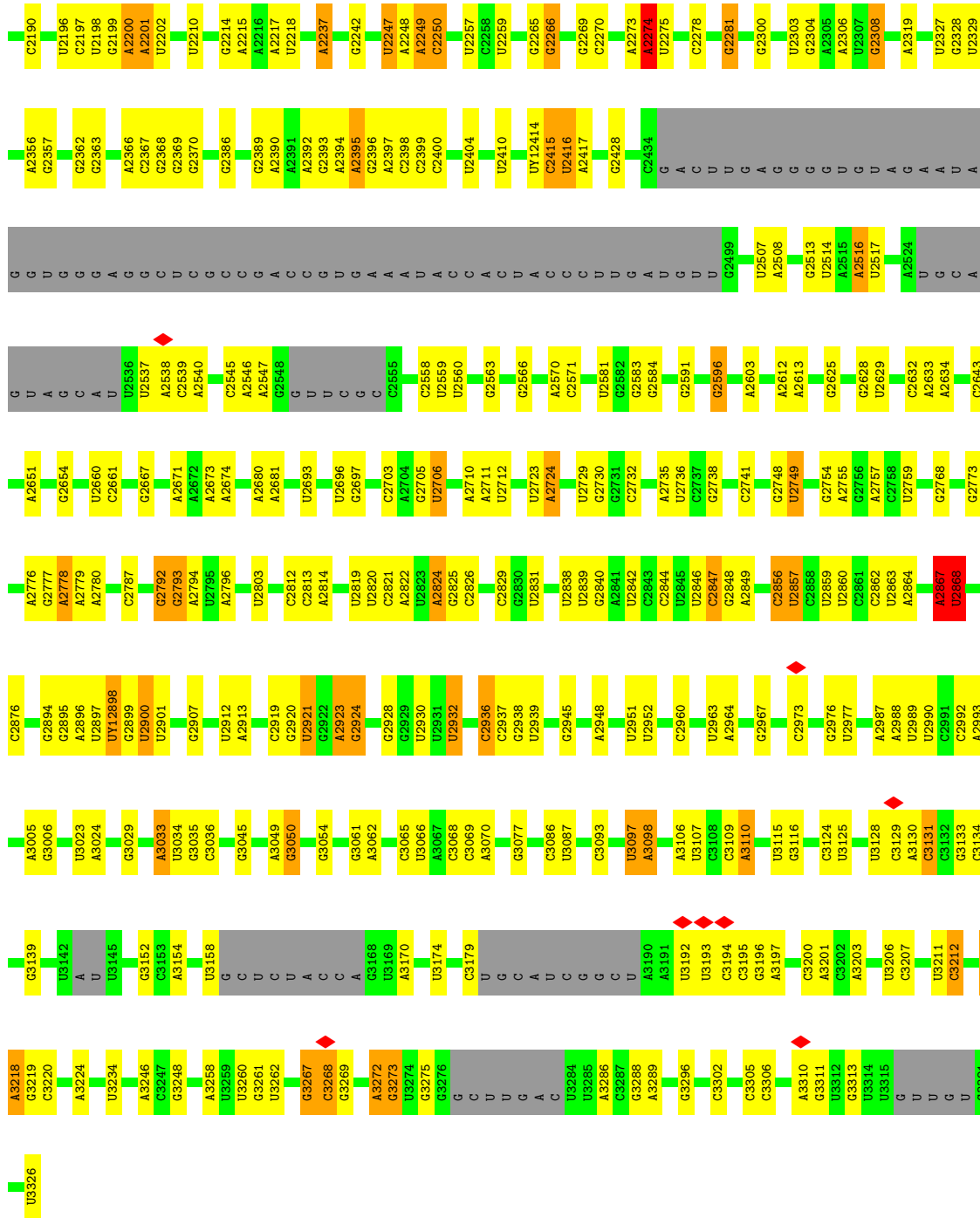
• Molecule 73: 5.8S ribosomal RNA



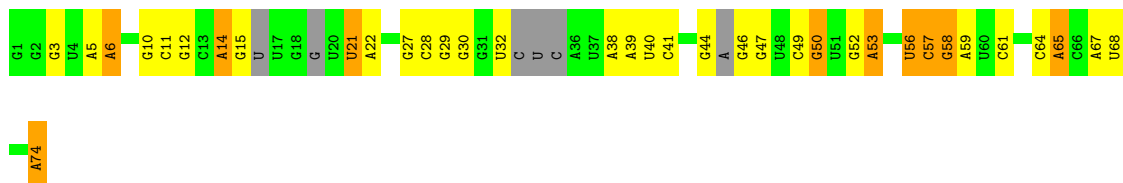
• Molecule 74: 28S ribosomal RNA





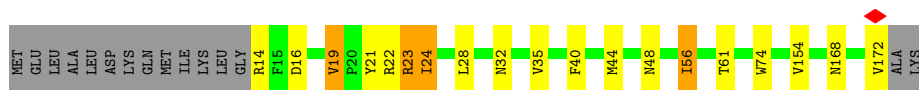


• Molecule 75: E-site tRNA









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	261009	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	40.365	Depositor
Minimum map value	-1.689	Depositor
Average map value	0.522	Depositor
Map value standard deviation	1.452	Depositor
Recommended contour level	4	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, A2M, OMC, PSU, K, IAS, 5MC, MA6, ZN, OMG, B8N, 1MA, 7MG, MG, OMU, 4AC

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	L3	0.25	0/2918	0.28	0/4549
2	LB	0.22	0/1930	0.28	0/2589
3	LC	0.22	0/3110	0.27	0/4183
4	LE	0.17	0/1365	0.27	0/1821
5	LF	0.16	0/1488	0.24	0/2005
6	LG	0.17	0/1183	0.29	0/1588
7	LJ	0.19	0/1567	0.25	0/2092
8	LK	0.21	0/989	0.28	0/1333
9	LP	0.18	0/2394	0.23	0/3203
10	LQ	0.20	0/1470	0.26	0/1962
11	LU	0.21	0/1256	0.26	0/1685
12	LV	0.14	0/813	0.24	0/1090
13	LZ	0.17	0/1134	0.23	0/1511
14	La	0.18	0/993	0.24	0/1320
15	Lb	0.20	0/438	0.29	0/575
16	Ld	0.18	0/716	0.25	0/961
17	Le	0.19	0/885	0.24	0/1191
18	Lf	0.20	0/1043	0.24	0/1389
19	Lg	0.23	0/901	0.26	0/1203
20	LD	0.19	0/2672	0.26	0/3587
21	LI	0.21	0/1661	0.26	0/2219
22	LL	0.17	0/1033	0.24	0/1385
23	LM	0.23	0/1189	0.25	0/1586
24	LN	0.24	0/1744	0.28	0/2323
25	LO	0.17	0/1749	0.24	0/2349
26	LR	0.20	0/1451	0.26	0/1918
27	LS	0.18	0/1516	0.24	0/2039
28	LT	0.20	0/1266	0.25	0/1700
29	LX	0.19	0/1035	0.27	0/1375
30	Lc	0.20	0/1793	0.28	0/2395
31	Lh	0.21	0/818	0.24	0/1089
32	Li	0.19	0/857	0.27	0/1142

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Lj	0.23	0/718	0.31	0/951
34	Lk	0.18	0/532	0.24	0/716
35	Ll	0.20	0/441	0.22	0/585
36	Lm	0.17	0/412	0.26	0/547
37	Lp	0.24	0/744	0.31	0/991
38	Lo	0.20	0/792	0.26	0/1042
39	LH	0.17	0/1850	0.24	0/2484
40	SA	0.30	0/1767	0.29	0/2368
41	SB	0.25	0/1587	0.28	0/2155
42	SD	0.32	0/1499	0.29	0/1997
43	SE	0.33	0/2101	0.32	0/2830
44	SF	0.33	0/1390	0.31	0/1880
45	SG	0.26	0/1783	0.27	0/2373
46	SI	0.22	0/1450	0.26	0/1949
47	SJ	0.36	0/1053	0.35	0/1414
48	SK	0.35	0/1487	0.32	0/1985
49	SP	0.35	0/1143	0.37	0/1527
50	ST	0.32	0/1239	0.28	0/1662
51	SU	0.38	0/1263	0.30	0/1689
52	SY	0.28	0/607	0.28	0/818
53	Sb	0.33	0/788	0.32	0/1052
54	Sc	0.29	0/547	0.30	0/729
55	Se	0.27	0/329	0.28	0/437
56	SC	0.33	0/1648	0.29	0/2211
57	SH	0.44	0/1494	0.36	0/2006
58	SL	0.45	0/1069	0.36	0/1428
59	SM	0.34	0/790	0.31	0/1065
60	SQ	0.21	0/883	0.31	0/1192
61	SR	0.39	0/1162	0.30	0/1562
62	SS	0.44	0/423	0.39	0/566
63	SW	0.37	0/961	0.31	0/1289
64	Sd	0.36	0/492	0.29	0/657
65	Sg	0.33	0/2546	0.35	0/3461
66	SN	0.33	0/827	0.37	0/1127
67	SZ	0.32	0/805	0.30	0/1074
68	Sa	0.39	0/608	0.38	0/815
69	Sf	0.23	0/518	0.32	0/689
70	Ln	0.37	0/354	0.34	0/458
71	SV	0.37	0/652	0.31	0/865
72	SO	0.31	0/953	0.36	0/1278
73	L4	0.27	0/3559	0.35	2/5538 (0.0%)
74	L5	0.29	1/67551 (0.0%)	0.31	15/105251 (0.0%)
75	S7	0.19	0/1611	0.27	0/2500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	S1	0.50	0/36450	0.34	2/56755 (0.0%)
77	LA	0.20	0/1740	0.47	0/2340
78	LW	0.24	0/977	0.46	0/1311
79	LY	0.32	0/505	0.57	0/676
80	SX	0.48	0/1328	0.58	0/1786
All	All	0.33	1/200805 (0.0%)	0.31	19/293438 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
66	SN	0	1
79	LY	0	1
80	SX	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	1472	A2M	O3'-P	5.17	1.61	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2868	U	OP1-P-OP2	-13.83	78.10	119.60
74	L5	1874	U	OP1-P-OP2	-12.82	81.15	119.60
74	L5	2867	A	OP2-P-O3'	-12.57	70.29	108.00
74	L5	1873	G	OP2-P-O3'	-12.43	70.70	108.00
76	S1	411	A	OP1-P-O3'	-10.98	75.05	108.00
74	L5	1874	U	O5'-P-OP1	-10.82	75.53	108.00
74	L5	2930	U	OP1-P-O3'	-10.77	75.68	108.00
74	L5	1908	A	OP2-P-O3'	-10.47	76.58	108.00
74	L5	2930	U	OP2-P-O3'	-10.26	77.21	108.00
74	L5	1908	A	OP1-P-O3'	-9.96	78.12	108.00
74	L5	2868	U	O5'-P-OP1	-9.82	78.53	108.00
73	L4	91	U	OP1-P-O3'	-9.33	80.00	108.00
76	S1	411	A	OP2-P-O3'	-9.14	80.59	108.00
74	L5	1874	U	O5'-P-OP2	8.64	133.92	108.00
74	L5	2867	A	OP1-P-O3'	8.54	133.63	108.00
74	L5	2868	U	O5'-P-OP2	8.07	132.21	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	L4	91	U	OP2-P-O3'	-7.21	86.39	108.00
74	L5	1873	G	O3'-P-O5'	-6.81	93.78	104.00
74	L5	1873	G	OP1-P-O3'	6.78	128.34	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
79	LY	50	ARG	Sidechain
66	SN	53	THR	Peptide
80	SX	14	ARG	Sidechain

## 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	L3	2610	0	1323	14	0
2	LB	1892	0	1951	8	0
3	LC	3036	0	3146	16	0
4	LE	1345	0	1395	3	0
5	LF	1469	0	1561	2	0
6	LG	1163	0	1249	7	0
7	LJ	1544	0	1669	1	0
8	LK	973	0	1030	4	0
9	LP	2351	0	2400	8	0
10	LQ	1449	0	1576	2	0
11	LU	1231	0	1273	2	0
12	LV	799	0	836	2	0
13	LZ	1120	0	1216	4	0
14	La	985	0	1110	2	0
15	Lb	431	0	469	0	0
16	Ld	706	0	726	2	0
17	Le	869	0	914	2	0
18	Lf	1026	0	1108	3	0
19	Lg	879	0	915	0	0
20	LD	2634	0	2814	13	0
21	LI	1628	0	1736	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	LL	1018	0	1102	5	0
23	LM	1159	0	1193	2	0
24	LN	1708	0	1803	5	0
25	LO	1706	0	1756	7	0
26	LR	1433	0	1546	5	0
27	LS	1484	0	1552	3	0
28	LT	1238	0	1297	2	0
29	LX	1020	0	1086	4	0
30	Lc	1759	0	1876	8	0
31	Lh	808	0	860	2	0
32	Li	847	0	923	3	0
33	Lj	703	0	716	2	0
34	Lk	525	0	568	5	0
35	Ll	431	0	471	1	0
36	Lm	407	0	445	0	0
37	Lp	733	0	759	3	0
38	Lo	782	0	855	0	0
39	LH	1817	0	1929	4	0
40	SA	1742	0	1850	10	0
41	SB	1553	0	1605	8	0
42	SD	1474	0	1553	2	0
43	SE	2060	0	2139	7	0
44	SF	1361	0	1420	0	0
45	SG	1760	0	1881	6	0
46	SI	1430	0	1539	7	0
47	SJ	1033	0	1070	4	0
48	SK	1462	0	1512	9	0
49	SP	1124	0	1198	15	0
50	ST	1213	0	1288	3	0
51	SU	1237	0	1306	6	0
52	SY	600	0	590	1	0
53	Sb	777	0	821	4	0
54	Sc	540	0	567	1	0
55	Se	324	0	350	0	0
56	SC	1627	0	1728	8	0
57	SH	1474	0	1532	8	0
58	SL	1055	0	1125	3	0
59	SM	778	0	798	5	0
60	SQ	875	0	909	6	0
61	SR	1147	0	1188	8	0
62	SS	412	0	407	4	0
63	SW	942	0	1010	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Sd	488	0	513	1	0
65	Sg	2489	0	2448	18	0
66	SN	801	0	812	3	0
67	SZ	790	0	823	6	0
68	Sa	601	0	638	3	0
69	Sf	509	0	544	4	0
70	Ln	349	0	393	0	0
71	SV	644	0	693	5	0
72	SO	950	0	988	8	0
73	L4	3209	0	1631	13	0
74	L5	61299	0	30924	246	0
75	S7	1446	0	737	23	0
76	S1	33088	0	16684	164	0
77	LA	1716	0	1811	33	0
78	LW	963	0	1033	13	0
79	LY	491	0	505	7	0
80	SX	1300	0	1317	11	0
81	L3	1	0	0	0	0
81	L4	1	0	0	0	0
81	L5	133	0	0	0	0
81	S1	1	0	0	0	0
82	Lh	1	0	0	0	0
82	Lj	1	0	0	0	0
82	Lm	1	0	0	0	0
82	Lo	1	0	0	0	0
82	Lp	1	0	0	0	0
83	L5	25	0	0	0	0
83	S1	1	0	0	0	0
84	L5	25	0	0	0	0
84	S1	7	0	0	0	0
84	SA	2	0	0	0	0
All	All	189052	0	143034	772	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 (772) 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)
56:SC:27:LEU:HD12	56:SC:39:VAL:HG21	1.77	0.67
76:S1:472:G:HO2'	76:S1:473:U:H6	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:LA:35:ILE:HG22	77:LA:37:LEU:HD21	1.78	0.65
76:S1:482:U:H2'	76:S1:483:G:C8	2.31	0.65
74:L5:2793:G:O4'	74:L5:2847:5MC:HM53	1.97	0.65
78:LW:38:ARG:HG3	78:LW:38:ARG:HH11	1.62	0.65
65:Sg:92:LEU:HD21	65:Sg:127:SER:HB3	1.79	0.65
77:LA:179:ARG:O	77:LA:183:VAL:HG23	1.97	0.65
63:SW:111:ILE:HA	63:SW:115:MET:HE2	1.78	0.64
77:LA:119:ILE:HD13	77:LA:134:PRO:HG3	1.81	0.63
78:LW:106:ILE:O	78:LW:110:VAL:HG23	1.98	0.63
40:SA:127:VAL:HG21	40:SA:176:ALA:HB3	1.82	0.62
41:SB:78:VAL:HG21	41:SB:120:ILE:HD12	1.81	0.62
80:SX:28:LEU:HD22	80:SX:154:VAL:CG1	2.30	0.62
46:SI:22:ILE:HD11	46:SI:62:ILE:HG21	1.82	0.60
9:LP:296:VAL:HG23	25:LO:206:LEU:HD11	1.82	0.60
76:S1:1364:C:H3'	76:S1:1365:U:C5'	2.30	0.60
77:LA:35:ILE:HG23	77:LA:203:LEU:CD2	2.32	0.60
2:LB:137:ILE:HD11	2:LB:149:ARG:HB3	1.83	0.60
49:SP:6:PRO:O	76:S1:1028:U:OP2	2.19	0.60
30:Lc:55:LEU:HD21	30:Lc:194:HIS:HB2	1.84	0.59
40:SA:156:VAL:HG12	40:SA:160:LYS:HB2	1.85	0.58
72:SO:106:THR:HG21	72:SO:110:ARG:HE	1.67	0.58
74:L5:1636:G:H2'	74:L5:1637:U:O4'	2.04	0.58
50:ST:144:GLU:HG2	50:ST:145:THR:HG23	1.86	0.57
74:L5:2741:C:H42	75:S7:74:A:H8	1.50	0.57
3:LC:196:MET:HE1	3:LC:201:LEU:HD13	1.86	0.57
61:SR:103:ASN:O	61:SR:107:THR:HG23	2.04	0.57
41:SB:37:MET:HE1	41:SB:157:LEU:HD21	1.86	0.57
74:L5:117:G:H4'	74:L5:118:U:OP1	2.05	0.57
22:LL:5:THR:H	27:LS:188:LEU:HD13	1.69	0.57
39:LH:72:VAL:HG21	78:LW:37:ARG:HD3	1.86	0.57
6:LG:65:LEU:HD11	6:LG:77:THR:HG22	1.87	0.56
32:Li:88:LYS:HA	32:Li:97:ALA:HB2	1.87	0.56
74:L5:2513:G:H2'	74:L5:2514:U:O2	2.06	0.56
74:L5:520:U:H2'	74:L5:521:G:C8	2.40	0.56
72:SO:143:THR:O	72:SO:144:IAS:HB3	2.06	0.56
59:SM:84:PHE:HB3	62:SS:50:PHE:HB3	1.87	0.56
3:LC:219:THR:HG22	3:LC:327:VAL:HG23	1.88	0.55
37:Lp:78:THR:O	37:Lp:82:ILE:HG23	2.07	0.55
56:SC:13:PHE:HB3	59:SM:31:MET:HE3	1.87	0.55
56:SC:36:TYR:OH	56:SC:39:VAL:HG23	2.07	0.55
76:S1:1368:G:H4'	76:S1:1369:A:H5'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S1:1216:G:H1	76:S1:1249:G:H22	1.55	0.55
76:S1:1158:G:H2'	76:S1:1159:A:O4'	2.08	0.54
74:L5:714:C:H3'	74:L5:715:G:H5''	1.89	0.54
74:L5:3260:U:H2'	74:L5:3261:G:O4'	2.08	0.54
51:SU:72:MET:HE3	51:SU:118:GLY:HA2	1.90	0.54
74:L5:399:A:H4'	74:L5:400:A:OP1	2.07	0.54
74:L5:2778:A:O2'	74:L5:2779:A:H2'	2.08	0.54
74:L5:2516:A:H3'	78:LW:40:THR:HG21	1.89	0.54
76:S1:1096:A:H2'	76:S1:1097:G:C8	2.42	0.53
77:LA:190:VAL:HG21	77:LA:197:TRP:CE2	2.43	0.53
49:SP:53:VAL:HG13	49:SP:72:VAL:CG2	2.39	0.53
3:LC:237:PRO:HD3	74:L5:2856:OMC:HM21	1.89	0.53
79:LY:20:VAL:HG13	79:LY:39:ILE:HG13	1.90	0.53
3:LC:57:THR:HG22	3:LC:73:VAL:HG22	1.90	0.53
76:S1:1532:A:N3	76:S1:1532:A:C2'	2.71	0.53
77:LA:95:ASN:O	77:LA:99:VAL:HG23	2.09	0.53
76:S1:966:G:H2'	76:S1:967:G:C8	2.44	0.52
80:SX:28:LEU:HD22	80:SX:154:VAL:HG11	1.91	0.52
74:L5:114:A:H2'	74:L5:115:A:O4'	2.09	0.52
74:L5:1157:C:H2'	74:L5:1158:A2M:H8	1.91	0.52
8:LK:38:ILE:HD12	8:LK:60:VAL:HG21	1.92	0.52
53:Sb:58:ALA:HB2	72:SO:131:LYS:HB3	1.91	0.52
76:S1:483:G:H1	76:S1:512:C:H5	1.57	0.52
77:LA:9:LEU:O	77:LA:13:ILE:HG13	2.10	0.52
76:S1:796:G:H2'	76:S1:797:G:C8	2.45	0.52
7:LJ:58:MET:HE2	7:LJ:68:ARG:HB3	1.93	0.51
47:SJ:28:ARG:HB3	47:SJ:29:PRO:HD3	1.90	0.51
56:SC:10:ARG:HH22	76:S1:1449:A:H62	1.57	0.51
76:S1:808:U:H2'	76:S1:809:C:C6	2.46	0.51
76:S1:1269:A:H2'	76:S1:1270:A:C8	2.45	0.51
9:LP:64:ILE:HG13	9:LP:109:LEU:HD22	1.92	0.51
22:LL:6:LYS:HZ2	27:LS:188:LEU:HD12	1.75	0.51
27:LS:126:ARG:O	74:L5:1320:G:H1'	2.11	0.51
76:S1:1095:G:C2	76:S1:1096:A:C8	2.98	0.51
77:LA:68:GLY:HA3	77:LA:72:HIS:HB2	1.93	0.51
4:LE:38:LEU:HD12	4:LE:123:MET:HE1	1.92	0.51
43:SE:25:LEU:HD13	76:S1:715:A:C5	2.45	0.51
61:SR:107:THR:HG22	61:SR:110:ARG:HH22	1.76	0.51
74:L5:1723:A:H2'	74:L5:1724:A:C8	2.46	0.51
26:LR:177:LYS:O	26:LR:181:ILE:HG23	2.10	0.51
74:L5:3268:C:OP1	74:L5:3268:C:H3'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:SA:105:ILE:HD13	40:SA:211:LEU:HD13	1.92	0.51
43:SE:209:GLY:HA3	51:SU:38:MET:HE1	1.92	0.51
48:SK:76:THR:HG21	48:SK:105:ASP:O	2.10	0.51
76:S1:301:A:H2'	76:S1:302:G:O4'	2.11	0.51
74:L5:522:G:H2'	74:L5:523:U:O4'	2.11	0.51
74:L5:567:G:O2'	74:L5:568:C:H5'	2.11	0.51
76:S1:560:A:H2'	76:S1:561:A:C8	2.46	0.51
74:L5:194:U:H2'	74:L5:195:G:O4'	2.11	0.51
76:S1:1465:C:H4'	76:S1:1471:G:C6	2.46	0.51
76:S1:1504:G:N3	76:S1:1504:G:H2'	2.26	0.51
74:L5:185:A:H2'	74:L5:186:A:H5'	1.93	0.50
74:L5:520:U:C4	74:L5:557:G:O6	2.64	0.50
72:SO:91:LEU:HD12	72:SO:130:LEU:HD11	1.93	0.50
74:L5:309:G:H2'	74:L5:310:G:C8	2.46	0.50
76:S1:1006:G:H2'	76:S1:1008:G:N7	2.25	0.50
76:S1:1081:C:H5	76:S1:1554:G:H1	1.60	0.50
33:Lj:18:THR:OG1	74:L5:826:A2M:H8	2.12	0.50
74:L5:649:C:H2'	74:L5:649:C:O2	2.10	0.50
74:L5:3124:C:H2'	74:L5:3125:U:O4'	2.11	0.50
20:LD:36:VAL:HG21	20:LD:240:LEU:HD21	1.93	0.50
74:L5:882:C:H4'	74:L5:883:U:OP2	2.12	0.50
76:S1:1269:A:O2'	76:S1:1270:A:P	2.69	0.50
21:LI:141:LEU:HA	21:LI:144:VAL:HG22	1.93	0.50
49:SP:34:LEU:HD21	76:S1:1057:A:H5''	1.93	0.50
76:S1:380:A:H2'	76:S1:381:C:C6	2.46	0.50
6:LG:121:VAL:HG12	6:LG:121:VAL:O	2.11	0.50
30:Lc:55:LEU:HD21	30:Lc:194:HIS:CB	2.42	0.50
57:SH:67:HIS:HA	76:S1:1091:C:OP1	2.12	0.50
74:L5:925:G:H5'	74:L5:926:A:OP1	2.12	0.50
74:L5:2249:A:H4'	74:L5:2250:C:OP1	2.12	0.50
74:L5:2357:G:H22	74:L5:2389:G:H1'	1.77	0.50
77:LA:48:PHE:CE2	77:LA:158:LEU:HD22	2.47	0.50
22:LL:13:LEU:HD12	22:LL:26:CYS:O	2.12	0.50
29:LX:49:ILE:HD13	29:LX:79:ILE:HD13	1.94	0.50
56:SC:27:LEU:HD22	56:SC:71:LEU:HD21	1.93	0.50
75:S7:14:A:C6	75:S7:15:G:C6	3.00	0.50
14:La:38:VAL:HG12	14:La:39:THR:H	1.77	0.49
77:LA:87:GLU:O	77:LA:91:LYS:HG3	2.12	0.49
68:Sa:61:VAL:HG23	68:Sa:99:ARG:HG3	1.94	0.49
65:Sg:12:LEU:CD1	65:Sg:57:VAL:HG13	2.41	0.49
74:L5:2813:C:H5	74:L5:2829:C:H42	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S1:472:G:O2'	76:S1:473:U:H6	1.95	0.49
21:LI:195:MET:HA	21:LI:195:MET:HE3	1.94	0.49
74:L5:2612:A:H4'	74:L5:2613:A:O5'	2.13	0.49
76:S1:810:G:H2'	76:S1:811:U:C6	2.48	0.49
78:LW:45:ASN:OD1	78:LW:45:ASN:C	2.55	0.49
74:L5:2106:A:H1'	74:L5:2107:G:OP2	2.11	0.49
76:S1:819:U:H2'	76:S1:820:G:C8	2.47	0.49
65:Sg:263:ILE:HB	65:Sg:273:ALA:HB3	1.94	0.49
75:S7:56:U:H1'	75:S7:58:G:C8	2.46	0.49
76:S1:849:A:H2'	76:S1:850:G:C8	2.47	0.49
56:SC:27:LEU:HD12	56:SC:39:VAL:CG2	2.43	0.49
74:L5:562:C:H2'	74:L5:563:G:O4'	2.13	0.49
74:L5:749:G:H2'	74:L5:750:C:C6	2.48	0.49
74:L5:2274:A2M:H2	74:L5:2951:U:O2	2.12	0.49
76:S1:1577:G:H1	76:S1:1683:A:H62	1.60	0.49
61:SR:28:VAL:HG23	61:SR:56:LYS:O	2.13	0.49
76:S1:24:U:H5	76:S1:570:A:N1	2.10	0.49
74:L5:667:C:H2'	74:L5:668:A:H8	1.78	0.49
76:S1:16:G:H2'	76:S1:17:C:C6	2.47	0.49
76:S1:1532:A:N3	76:S1:1532:A:H2'	2.27	0.49
9:LP:59:ARG:HG2	9:LP:81:THR:HG23	1.95	0.48
74:L5:745:G:O2'	74:L5:746:U:H2'	2.12	0.48
74:L5:3023:U:O2'	74:L5:3024:A:H5'	2.13	0.48
76:S1:26:A:H2'	76:S1:27:U:C6	2.49	0.48
51:SU:72:MET:HE1	51:SU:152:GLN:HG3	1.95	0.48
74:L5:2190:C:H5	74:L5:2237:A:H62	1.61	0.48
74:L5:3272:A:O2'	74:L5:3273:G:O4'	2.30	0.48
74:L5:3272:A:N3	74:L5:3272:A:H2'	2.27	0.48
76:S1:1589:C:O2	76:S1:1589:C:O4'	2.31	0.48
76:S1:426:C:H2'	76:S1:426:C:O2	2.12	0.48
40:SA:51:THR:HG23	40:SA:56:LEU:HD23	1.96	0.48
48:SK:101:LEU:HD11	48:SK:182:TYR:CG	2.49	0.48
48:SK:158:CYS:HB2	48:SK:174:LEU:HD21	1.96	0.48
49:SP:109:ARG:HG3	49:SP:114:VAL:HG22	1.95	0.48
76:S1:1232:U:O4'	76:S1:1232:U:O2	2.31	0.48
77:LA:119:ILE:N	77:LA:120:PRO:HD3	2.29	0.48
32:Li:10:GLU:HG3	32:Li:31:LEU:HD11	1.95	0.48
49:SP:53:VAL:HG13	49:SP:72:VAL:HG23	1.96	0.48
50:ST:92:VAL:HG11	50:ST:149:LEU:HD12	1.95	0.48
74:L5:1471:U:H2'	74:L5:1472:A2M:H8	1.95	0.48
76:S1:1216:G:H22	76:S1:1249:G:N2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LO:115:MET:HA	25:LO:115:MET:HE2	1.96	0.48
57:SH:129:VAL:HG13	57:SH:133:ARG:HD3	1.94	0.48
58:SL:34:ILE:CG2	80:SX:24:ILE:HD11	2.44	0.48
74:L5:1744:C:O2'	74:L5:1745:G:P	2.72	0.48
76:S1:150:A:H2'	76:S1:151:A:O4'	2.14	0.48
76:S1:1032:G:O2'	76:S1:1033:G:H5'	2.14	0.48
20:LD:163:THR:HG21	74:L5:208:A:H2'	1.96	0.48
71:SV:73:LEU:H	71:SV:73:LEU:HD12	1.79	0.48
74:L5:643:A:H2'	74:L5:644:C:C6	2.48	0.48
74:L5:855:A:H2'	74:L5:856:A:O4'	2.14	0.48
2:LB:109:GLU:OE1	2:LB:136:ILE:HG22	2.14	0.48
34:Lk:5:LEU:HD13	34:Lk:11:TYR:HA	1.96	0.48
76:S1:1528:C:O5'	76:S1:1528:C:O2	2.32	0.48
76:S1:1538:U:H2'	76:S1:1539:G:C8	2.49	0.48
45:SG:177:VAL:HG22	76:S1:135:A:H8	1.79	0.47
49:SP:19:ARG:O	49:SP:20:ARG:HB3	2.14	0.47
74:L5:3267:G:H3'	74:L5:3268:C:H5''	1.95	0.47
73:L4:123:C:H1'	73:L4:124:U:OP2	2.13	0.47
74:L5:1759:C:H2'	74:L5:1760:U:O2	2.15	0.47
76:S1:713:U:HO2'	76:S1:714:G:H8	1.61	0.47
21:LI:188:LEU:HD11	22:LL:121:ARG:HB2	1.95	0.47
45:SG:22:LYS:HA	45:SG:25:LEU:HD23	1.96	0.47
65:Sg:284:GLY:CA	71:SV:26:LEU:HD22	2.44	0.47
74:L5:752:U:H4'	74:L5:753:G:OP2	2.14	0.47
76:S1:1499:U:C2'	76:S1:1500:G:H5'	2.44	0.47
1:L3:44:C:H4'	9:LP:152:ILE:HD12	1.96	0.47
31:Lh:79:VAL:HG12	31:Lh:80:ARG:NH1	2.29	0.47
80:SX:56:ILE:HD12	80:SX:74:TRP:CH2	2.49	0.47
3:LC:313:GLY:HA2	74:L5:3306:C:H4'	1.95	0.47
49:SP:29:TYR:O	49:SP:30:LYS:HB3	2.14	0.47
76:S1:996:U:H2'	76:S1:997:C:C6	2.50	0.47
77:LA:110:LEU:HD21	77:LA:150:ILE:HD11	1.97	0.47
80:SX:24:ILE:HD12	80:SX:24:ILE:H	1.80	0.47
20:LD:123:LEU:HD11	20:LD:234:LEU:HD12	1.96	0.47
41:SB:61:ILE:HD11	41:SB:177:MET:SD	2.55	0.47
65:Sg:20:VAL:HG11	65:Sg:23:ILE:HD11	1.97	0.47
76:S1:19:A:H2'	76:S1:20:G:O4'	2.15	0.47
12:LV:36:PRO:HB2	12:LV:64:ARG:HE	1.80	0.47
29:LX:110:MET:HE1	29:LX:118:LEU:HD12	1.97	0.47
34:Lk:15:LEU:HD21	34:Lk:57:PRO:CD	2.45	0.47
58:SL:34:ILE:HG23	80:SX:24:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Sg:25:CYS:SG	65:Sg:34:VAL:HG22	2.54	0.47
73:L4:69:U:H2'	73:L4:70:G:O4'	2.14	0.47
74:L5:185:A:C2	74:L5:229:A:C2	3.02	0.47
74:L5:674:U:H2'	74:L5:675:C:C6	2.49	0.47
74:L5:1460:C:O2	74:L5:1460:C:O4'	2.30	0.47
76:S1:137:G:O2'	76:S1:138:G:H5'	2.14	0.47
23:LM:126:ARG:HD3	32:Li:17:THR:HG21	1.95	0.47
25:LO:153:ARG:HA	25:LO:165:ILE:HD11	1.96	0.47
43:SE:58:LEU:O	67:SZ:15:MET:HE1	2.15	0.47
30:Lc:51:ARG:O	30:Lc:55:LEU:HD23	2.15	0.47
74:L5:207:C:H2'	74:L5:208:A:O4'	2.15	0.47
74:L5:1557:A:H2'	74:L5:1558:A:C8	2.50	0.47
74:L5:1792:G:H2'	74:L5:1793:U:O4'	2.15	0.47
76:S1:1701:4AC:H5	76:S1:1701:4AC:O7	2.15	0.47
77:LA:122:TYR:O	77:LA:123:LEU:HD23	2.15	0.47
76:S1:1021:C:H2'	76:S1:1021:C:O2	2.15	0.47
76:S1:1216:G:H22	76:S1:1249:G:H22	1.62	0.47
9:LP:153:VAL:HG21	74:L5:2723:U:C4	2.50	0.46
76:S1:789:U:O2	76:S1:789:U:O4'	2.33	0.46
77:LA:95:ASN:C	77:LA:97:THR:N	2.73	0.46
5:LF:43:ILE:CG1	5:LF:56:VAL:HG13	2.45	0.46
20:LD:68:THR:HG21	74:L5:2395:A:H2'	1.97	0.46
66:SN:6:MET:HE2	66:SN:12:PRO:HG3	1.98	0.46
67:SZ:9:ILE:HD12	67:SZ:45:ARG:HG2	1.97	0.46
76:S1:12:U:H2'	76:S1:13:C:C6	2.50	0.46
77:LA:44:ARG:O	77:LA:45:ASP:C	2.58	0.46
3:LC:320:LEU:HD12	3:LC:336:LEU:HD13	1.97	0.46
20:LD:294:VAL:HG23	74:L5:1385:C:H5''	1.97	0.46
74:L5:1386:A:H2'	74:L5:1387:A:C8	2.50	0.46
6:LG:121:VAL:HA	6:LG:124:LEU:HD23	1.97	0.46
48:SK:82:VAL:HG11	48:SK:103:THR:HG23	1.97	0.46
60:SQ:51:VAL:HG21	60:SQ:131:VAL:HG21	1.96	0.46
60:SQ:127:MET:O	60:SQ:131:VAL:HG23	2.15	0.46
65:Sg:284:GLY:HA3	71:SV:26:LEU:HD22	1.96	0.46
75:S7:27:G:H22	75:S7:40:U:H3	1.64	0.46
76:S1:1368:G:C4'	76:S1:1369:A:H5'	2.46	0.46
78:LW:74:ILE:HG12	78:LW:109:ALA:HB1	1.98	0.46
1:L3:51:G:O2'	1:L3:52:U:P	2.74	0.46
9:LP:150:ILE:HG22	9:LP:150:ILE:O	2.16	0.46
74:L5:632:U:H4'	74:L5:633:A:O5'	2.15	0.46
43:SE:35:PRO:HD3	76:S1:421:C:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SR:5:ILE:HD11	68:Sa:46:TYR:CG	2.50	0.46
63:SW:131:MET:O	63:SW:132:HIS:HB2	2.15	0.46
74:L5:670:G:H1	74:L5:1460:C:H5	1.64	0.46
6:LG:77:THR:O	6:LG:77:THR:HG23	2.16	0.46
42:SD:5:TYR:CE1	43:SE:18:ILE:HD13	2.50	0.46
48:SK:72:VAL:HG21	48:SK:112:TRP:CE2	2.51	0.46
62:SS:37:CYS:HB2	62:SS:40:CYS:SG	2.56	0.46
74:L5:555:C:H2'	74:L5:556:U:O4'	2.16	0.46
76:S1:1407:G:H2'	76:S1:1408:A:C8	2.51	0.46
73:L4:132:C:H4'	73:L4:133:A:OP1	2.16	0.46
74:L5:2362:G:H2'	74:L5:2363:G:C8	2.51	0.46
76:S1:864:A:H2'	76:S1:865:A:C8	2.51	0.46
76:S1:1097:G:H2'	76:S1:1098:C:O4'	2.16	0.46
74:L5:1744:C:O2'	74:L5:1745:G:H8	1.99	0.46
76:S1:1406:U:H2'	76:S1:1406:U:O2	2.15	0.46
20:LD:126:ALA:O	20:LD:130:THR:HG23	2.16	0.46
46:SI:82:LEU:CD2	46:SI:86:LEU:HD13	2.46	0.46
74:L5:624:G:H2'	74:L5:625:U:C6	2.50	0.46
74:L5:2131:U:C6	74:L5:2135:U:C4	3.04	0.46
76:S1:1192:G:O2'	76:S1:1193:G:H5'	2.16	0.46
60:SQ:77:ILE:HG21	60:SQ:131:VAL:CG1	2.46	0.45
76:S1:1248:C:H2'	76:S1:1249:G:O4'	2.16	0.45
1:L3:122:C:O2	1:L3:122:C:O4'	2.34	0.45
73:L4:24:G:H1'	74:L5:351:A:C4	2.52	0.45
74:L5:3097:U:H4'	74:L5:3098:A:OP1	2.15	0.45
75:S7:38:A:C2	75:S7:39:A:C8	3.04	0.45
80:SX:16:ASP:O	80:SX:23:ARG:NH2	2.49	0.45
8:LK:86:ALA:HA	8:LK:96:TYR:HB3	1.99	0.45
40:SA:126:ASP:HB3	40:SA:134:MET:HE3	1.98	0.45
65:Sg:39:ARG:HA	65:Sg:70:THR:HB	1.97	0.45
74:L5:3033:A:H2	74:L5:3061:G:H21	1.63	0.45
74:L5:3115:U:H2'	74:L5:3116:G:O4'	2.16	0.45
3:LC:248:ALA:HB3	74:L5:2857:PSU:H1'	1.99	0.45
47:SJ:28:ARG:O	47:SJ:59:GLY:O	2.34	0.45
49:SP:53:VAL:HG22	49:SP:72:VAL:HG21	1.98	0.45
74:L5:657:1MA:HM11	74:L5:2846:U:OP1	2.16	0.45
74:L5:1173:G:O4'	74:L5:1195:A:H2	1.99	0.45
76:S1:1296:G:H4'	76:S1:1297:U:OP2	2.16	0.45
76:S1:1532:A:H4'	76:S1:1533:G:OP1	2.16	0.45
3:LC:363:TRP:O	74:L5:3258:A:H4'	2.16	0.45
49:SP:6:PRO:HB2	49:SP:11:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SP:59:ILE:HD11	49:SP:84:THR:HG21	1.98	0.45
74:L5:424:A:H2'	74:L5:425:G:O4'	2.17	0.45
74:L5:715:G:C5	74:L5:716:U:C5	3.05	0.45
74:L5:1663:U:O2'	74:L5:1664:G:H5'	2.17	0.45
74:L5:2813:C:H2'	74:L5:2814:A:O4'	2.16	0.45
75:S7:5:A:H2'	75:S7:6:A:C8	2.52	0.45
76:S1:694:U:O2	76:S1:694:U:O4'	2.35	0.45
76:S1:893:U:H2'	76:S1:894:C:O4'	2.17	0.45
3:LC:215:VAL:HG13	3:LC:334:ILE:CG2	2.46	0.45
23:LM:29:PRO:HA	74:L5:946:G:H5'	1.98	0.45
45:SG:145:PHE:HB2	45:SG:147:LEU:HD13	1.97	0.45
57:SH:68:GLY:O	57:SH:69:ARG:C	2.60	0.45
63:SW:84:LEU:O	63:SW:120:ILE:HD11	2.17	0.45
76:S1:1273:A:H2'	76:S1:1274:G:O4'	2.16	0.45
76:S1:1420:A:H2'	76:S1:1421:G:O4'	2.16	0.45
76:S1:1595:A:O2'	76:S1:1596:U:H5'	2.16	0.45
11:LU:14:CYS:SG	11:LU:151:VAL:HG22	2.57	0.45
74:L5:2247:U:O2	74:L5:2247:U:O4'	2.33	0.45
74:L5:2838:U:H2'	74:L5:2839:U:O4'	2.17	0.45
74:L5:2859:U:H2'	74:L5:2860:U:C6	2.52	0.45
76:S1:956:U:H3'	76:S1:957:G:C5'	2.47	0.45
76:S1:1437:A:H2'	76:S1:1438:A:O4'	2.17	0.45
80:SX:32:ASN:HB3	80:SX:35:VAL:HG12	1.99	0.45
2:LB:2:GLY:HA2	2:LB:207:VAL:HG23	1.99	0.45
67:SZ:9:ILE:HG23	67:SZ:27:LEU:HD11	1.99	0.45
74:L5:1614:A:H2'	74:L5:1615:G:C8	2.51	0.45
74:L5:1727:U:H2'	74:L5:1728:C:C6	2.52	0.45
74:L5:2190:C:O2	74:L5:2190:C:C2'	2.64	0.45
74:L5:2516:A:OP2	78:LW:41:HIS:HB2	2.17	0.45
74:L5:3133:G:H2'	74:L5:3134:C:O2	2.16	0.45
76:S1:737:G:H2'	76:S1:737:G:N3	2.32	0.45
76:S1:1183:U:O5'	76:S1:1183:U:O2	2.35	0.45
76:S1:1492:U:O2	76:S1:1492:U:O4'	2.34	0.45
3:LC:254:HIS:HA	3:LC:255:PRO:C	2.40	0.45
14:La:81:LEU:HD11	78:LW:58:ARG:NH2	2.32	0.45
43:SE:179:LEU:HD12	43:SE:179:LEU:N	2.32	0.45
59:SM:28:LEU:HD12	59:SM:28:LEU:N	2.32	0.45
74:L5:1526:A:C4	74:L5:1527:A:C8	3.05	0.45
74:L5:1961:G:H21	74:L5:3289:A:H8	1.63	0.45
76:S1:30:G:H2'	76:S1:31:C:C6	2.52	0.45
79:LY:12:LEU:HG	79:LY:13:CYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SN:49:HIS:O	66:SN:52:MET:O	2.35	0.45
74:L5:509:U:H2'	74:L5:510:C:O2	2.17	0.45
74:L5:639:U:H2'	74:L5:640:C:C6	2.52	0.45
80:SX:168:ASN:O	80:SX:172:VAL:HG23	2.17	0.45
17:Le:11:LEU:HD12	17:Le:11:LEU:O	2.17	0.44
18:Lf:76:VAL:HG13	18:Lf:81:GLU:HB2	1.99	0.44
57:SH:122:VAL:O	57:SH:123:ARG:HB3	2.17	0.44
73:L4:15:G:H2'	73:L4:16:G:O4'	2.17	0.44
74:L5:2976:G:H2'	74:L5:2977:U:C6	2.52	0.44
76:S1:29:U:O5'	76:S1:29:U:O2	2.35	0.44
21:LI:46:LEU:HD12	21:LI:140:VAL:HG22	2.00	0.44
74:L5:988:U:H2'	74:L5:989:G:O4'	2.17	0.44
74:L5:2867:A:O2'	74:L5:2868:U:P	2.74	0.44
74:L5:3272:A:H2	74:L5:3288:G:H21	1.63	0.44
76:S1:478:G:O3'	76:S1:479:G:O4'	2.36	0.44
76:S1:1246:A:H4'	76:S1:1247:A:O5'	2.17	0.44
76:S1:1402:A:H2'	76:S1:1403:C:C6	2.51	0.44
1:L3:3:U:H2'	1:L3:4:G:H8	1.82	0.44
1:L3:113:G:H2'	1:L3:114:C:C6	2.53	0.44
20:LD:61:THR:HG22	20:LD:62:SER:N	2.32	0.44
22:LL:87:ALA:O	22:LL:91:THR:HG23	2.16	0.44
24:LN:80:VAL:HG23	24:LN:89:ILE:HD11	2.00	0.44
74:L5:1145:A:H2'	74:L5:1146:U:H6	1.83	0.44
74:L5:1580:G:C6	74:L5:1582:A:C6	3.06	0.44
74:L5:1807:G:H2'	74:L5:1808:A:C8	2.52	0.44
76:S1:1688:G:H1'	76:S1:1709:MA6:H2	1.99	0.44
40:SA:127:VAL:HG23	40:SA:177:SER:HB3	1.99	0.44
74:L5:1749:C:H3'	74:L5:1750:G:H5'	1.99	0.44
74:L5:2181:A:C5	74:L5:2182:U:C6	3.05	0.44
75:S7:30:G:N2	75:S7:38:A:C2	2.85	0.44
76:S1:456:A:N1	76:S1:474:A:N1	2.65	0.44
76:S1:1171:C:O4'	76:S1:1171:C:O2	2.35	0.44
76:S1:1175:U:O2'	76:S1:1176:U:H5'	2.17	0.44
76:S1:1417:U:OP2	76:S1:1455:U:H5	1.99	0.44
24:LN:7:MET:SD	39:LH:182:LEU:HD23	2.57	0.44
76:S1:139:A:O2'	76:S1:140:U:P	2.75	0.44
76:S1:490:A:H2'	76:S1:491:C:O4'	2.18	0.44
76:S1:887:C:H2'	76:S1:888:A:O4'	2.18	0.44
76:S1:905:G:H4'	76:S1:1704:A:H4'	1.98	0.44
77:LA:7:ASP:O	77:LA:11:GLU:HG3	2.17	0.44
79:LY:38:PHE:CD1	79:LY:44:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LX:108:LEU:H	29:LX:108:LEU:HD23	1.83	0.44
42:SD:77:LEU:CD2	42:SD:86:MET:HE1	2.47	0.44
60:SQ:117:ILE:HG22	60:SQ:118:ASP:N	2.33	0.44
74:L5:2138:A:H1'	74:L5:2274:A2M:H61	1.82	0.44
74:L5:2200:A:H4'	74:L5:2201:A:O5'	2.18	0.44
74:L5:2270:C:O2	74:L5:2270:C:O4'	2.35	0.44
76:S1:1149:G:H2'	76:S1:1150:U:C6	2.53	0.44
72:SO:49:HIS:NE2	72:SO:58:THR:HG23	2.33	0.44
74:L5:668:A:H2'	74:L5:669:A:C8	2.53	0.44
75:S7:49:C:H2'	75:S7:50:G:C1'	2.48	0.44
76:S1:128:G:H2'	76:S1:128:G:N3	2.32	0.44
77:LA:12:ALA:O	77:LA:16:ILE:HG13	2.17	0.44
3:LC:25:ILE:HD11	3:LC:332:ARG:HH11	1.83	0.44
71:SV:52:GLY:HA3	76:S1:1320:C:O2'	2.18	0.44
74:L5:804:G:H2'	74:L5:805:C:H6	1.82	0.44
74:L5:2612:A:H4'	74:L5:2613:A:N3	2.33	0.44
75:S7:61:C:H5'	77:LA:44:ARG:HG2	1.99	0.44
1:L3:51:G:HO2'	1:L3:52:U:P	2.41	0.44
8:LK:64:VAL:HG23	8:LK:76:HIS:CD2	2.53	0.44
17:Le:14:ILE:HG22	17:Le:83:ARG:NH1	2.33	0.44
67:SZ:35:ALA:HA	76:S1:502:A:H4'	1.99	0.44
73:L4:33:A:H2'	74:L5:59:G:H2'	1.99	0.44
74:L5:411:U:O2'	74:L5:412:U:H5'	2.18	0.44
74:L5:510:C:O2	74:L5:510:C:O4'	2.36	0.44
74:L5:1720:G:H2'	74:L5:1721:A:C8	2.53	0.44
75:S7:57:C:HO2'	75:S7:58:G:C1'	2.30	0.44
76:S1:15:U:H2'	76:S1:16:G:O4'	2.17	0.44
76:S1:1196:OMG:HM23	76:S1:1196:OMG:H1'	1.78	0.44
76:S1:1559:U:H2'	76:S1:1560:PSU:O4'	2.18	0.44
78:LW:114:TYR:CE1	78:LW:150:ILE:HG12	2.53	0.44
6:LG:78:GLY:O	6:LG:79:PRO:C	2.59	0.43
30:Lc:109:LYS:HB3	30:Lc:110:PRO:HD3	1.99	0.43
34:Lk:31:ARG:NH2	74:L5:1770:A:OP1	2.51	0.43
40:SA:32:LEU:HD21	40:SA:46:THR:OG1	2.18	0.43
46:SI:133:ALA:O	46:SI:136:THR:HG22	2.18	0.43
48:SK:29:LEU:HD12	48:SK:29:LEU:C	2.42	0.43
71:SV:26:LEU:HD23	71:SV:59:ARG:HG2	2.00	0.43
74:L5:1207:A:H2'	74:L5:1208:C:C6	2.53	0.43
76:S1:1085:A:H2'	76:S1:1086:C:H6	1.83	0.43
76:S1:1244:U:H2'	76:S1:1245:U:O4'	2.17	0.43
76:S1:1543:A:O4'	76:S1:1543:A:N3	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:109:GLU:OE1	2:LB:137:ILE:C	2.61	0.43
40:SA:123:ALA:HB2	40:SA:165:ARG:HG3	2.00	0.43
46:SI:37:LEU:O	46:SI:41:VAL:HG23	2.17	0.43
74:L5:1026:U:H3'	74:L5:1027:A:C5'	2.49	0.43
75:S7:52:G:H21	77:LA:160:LYS:CE	2.30	0.43
79:LY:29:ILE:CD1	79:LY:35:VAL:HG13	2.48	0.43
58:SL:143:ARG:HB2	76:S1:1512:C:H4'	2.01	0.43
59:SM:52:LEU:HD13	59:SM:97:SER:HB2	2.00	0.43
74:L5:83:C:H2'	74:L5:84:U:O4'	2.18	0.43
74:L5:94:G:H2'	74:L5:95:A:C8	2.52	0.43
74:L5:118:U:O2	74:L5:118:U:O4'	2.36	0.43
76:S1:138:G:H1'	76:S1:139:A:H5'	2.00	0.43
76:S1:455:U:H2'	76:S1:456:A:C8	2.53	0.43
76:S1:1183:U:O2	76:S1:1183:U:O4'	2.36	0.43
77:LA:68:GLY:HA2	77:LA:112:SER:OG	2.19	0.43
26:LR:174:LEU:O	26:LR:177:LYS:HG3	2.18	0.43
41:SB:192:ILE:HD12	41:SB:192:ILE:N	2.34	0.43
73:L4:148:U:H2'	73:L4:149:U:C6	2.53	0.43
74:L5:954:C:H2'	74:L5:955:U:C6	2.53	0.43
74:L5:1219:G:H2'	74:L5:1220:A:C8	2.54	0.43
74:L5:2399:C:H2'	74:L5:2400:C:C6	2.53	0.43
74:L5:2559:U:O2	74:L5:2559:U:O4'	2.35	0.43
75:S7:67:A:H2'	75:S7:68:U:C6	2.53	0.43
45:SG:57:ASP:CG	45:SG:98:ARG:HE	2.27	0.43
60:SQ:33:LEU:HD11	60:SQ:112:VAL:CG1	2.49	0.43
60:SQ:33:LEU:HD11	60:SQ:112:VAL:HG11	2.01	0.43
61:SR:107:THR:HG22	61:SR:110:ARG:NH2	2.33	0.43
72:SO:50:VAL:HG21	72:SO:91:LEU:HD11	2.00	0.43
74:L5:100:A:H3'	74:L5:101:G:H21	1.84	0.43
76:S1:390:A:H4'	76:S1:391:G:O5'	2.17	0.43
49:SP:35:GLY:C	49:SP:37:ARG:H	2.26	0.43
54:Sc:33:VAL:HG21	54:Sc:44:ILE:HD12	1.99	0.43
65:Sg:5:VAL:HG12	65:Sg:273:ALA:HB2	2.00	0.43
67:SZ:9:ILE:HD12	67:SZ:45:ARG:CG	2.49	0.43
74:L5:1387:A:H2'	74:L5:1388:U:O4'	2.18	0.43
74:L5:2723:U:H2'	74:L5:2724:A2M:O4'	2.19	0.43
74:L5:2862:C:O2'	74:L5:2863:U:H5'	2.19	0.43
74:L5:3217:G:H4'	74:L5:3217:G:OP1	2.18	0.43
75:S7:46:G:C6	75:S7:57:C:C6	3.07	0.43
76:S1:1312:U:O2'	76:S1:1313:A:H5'	2.19	0.43
76:S1:1500:G:H1'	76:S1:1501:A:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:LA:188:TYR:CE2	77:LA:192:LEU:HD11	2.53	0.43
13:LZ:24:ILE:N	13:LZ:24:ILE:HD12	2.34	0.43
30:Lc:210:PHE:CE1	30:Lc:214:THR:HG21	2.54	0.43
33:Lj:4:CYS:HA	33:Lj:9:GLY:HA3	2.00	0.43
49:SP:7:ARG:O	49:SP:7:ARG:HG2	2.18	0.43
53:Sb:12:LYS:HG3	53:Sb:15:ARG:HB2	2.01	0.43
74:L5:3275:G:C6	74:L5:3286:A:C6	3.07	0.43
76:S1:820:G:H2'	76:S1:821:U:C6	2.54	0.43
76:S1:820:G:H1	76:S1:842:U:H3	1.66	0.43
13:LZ:53:VAL:HA	13:LZ:57:MET:HE1	2.00	0.43
40:SA:32:LEU:HD23	40:SA:96:CYS:SG	2.59	0.43
65:Sg:42:LYS:CD	65:Sg:65:THR:HG22	2.48	0.43
66:SN:69:TRP:H	66:SN:69:TRP:CD1	2.35	0.43
73:L4:125:C:O2	73:L4:125:C:O4'	2.35	0.43
74:L5:638:U:H2'	74:L5:639:U:C6	2.53	0.43
74:L5:1726:U:O2	74:L5:1726:U:O4'	2.34	0.43
74:L5:1819:A:H2'	74:L5:1820:G:C8	2.54	0.43
76:S1:137:G:H2'	76:S1:138:G:C8	2.54	0.43
76:S1:147:G:H2'	76:S1:148:C:C6	2.53	0.43
76:S1:1417:U:H2'	76:S1:1418:C:C6	2.54	0.43
80:SX:40:PHE:CE2	80:SX:44:MET:HE3	2.53	0.43
4:LE:76:GLU:O	4:LE:79:GLU:HG2	2.19	0.43
46:SI:20:LYS:O	46:SI:24:LYS:HG2	2.18	0.43
48:SK:21:HIS:HB2	76:S1:99:U:O2	2.17	0.43
74:L5:2415:C:C2'	74:L5:2416:U:H5'	2.49	0.43
74:L5:2895:G:C2	74:L5:2896:A:N7	2.87	0.43
74:L5:3219:G:H2'	74:L5:3220:C:O4'	2.18	0.43
76:S1:1337:G:O2'	76:S1:1338:C:H5'	2.19	0.43
43:SE:71:VAL:CG1	43:SE:84:THR:HA	2.49	0.43
73:L4:147:U:H2'	73:L4:148:U:C6	2.53	0.43
74:L5:642:A:H2'	74:L5:643:A:C8	2.53	0.43
74:L5:1633:C:H2'	74:L5:1634:G:C8	2.54	0.43
74:L5:1685:A:H2'	74:L5:1686:G:C8	2.54	0.43
74:L5:2369:G:H2'	74:L5:2370:G:C8	2.53	0.43
74:L5:2813:C:O2	74:L5:2813:C:O4'	2.36	0.43
76:S1:779:U:O2'	76:S1:780:A:H5'	2.19	0.43
76:S1:978:G:HO2'	76:S1:979:U:P	2.41	0.43
76:S1:1081:C:O2	76:S1:1081:C:O4'	2.34	0.43
77:LA:156:PHE:CE2	77:LA:166:VAL:HG21	2.54	0.43
16:Ld:23:SER:HG	16:Ld:100:ASP:CG	2.27	0.42
24:LN:108:ARG:HB2	24:LN:161:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SP:13:ARG:O	49:SP:13:ARG:HG2	2.17	0.42
74:L5:511:U:H2'	74:L5:512:G:C8	2.54	0.42
74:L5:680:A:H2'	74:L5:681:C:C6	2.53	0.42
74:L5:1134:C:H2'	74:L5:1135:C:C6	2.54	0.42
24:LN:172:ARG:HD3	74:L5:30:G:H5''	2.01	0.42
26:LR:40:GLU:HG3	26:LR:61:LEU:HD22	2.01	0.42
26:LR:160:MET:N	26:LR:160:MET:HE2	2.34	0.42
74:L5:275:U:H2'	74:L5:276:G:C8	2.54	0.42
74:L5:2198:U:O2	74:L5:2198:U:O5'	2.37	0.42
74:L5:2703:C:O2	74:L5:2703:C:O5'	2.38	0.42
74:L5:2812:C:H2'	74:L5:2813:C:O2	2.19	0.42
76:S1:117:C:H1'	76:S1:370:A:C5	2.54	0.42
76:S1:1133:A:H5'	76:S1:1134:C:OP2	2.19	0.42
76:S1:1266:G:C2	76:S1:1267:C:C6	3.07	0.42
76:S1:1489:U:H2'	76:S1:1491:C:O2'	2.19	0.42
76:S1:1496:U:H2'	76:S1:1497:C:C6	2.54	0.42
79:LY:8:ILE:HD12	79:LY:8:ILE:O	2.17	0.42
1:L3:71:G:H2'	1:L3:72:A:O5'	2.19	0.42
3:LC:215:VAL:HG11	3:LC:326:ILE:HB	2.01	0.42
5:LF:43:ILE:HD11	5:LF:56:VAL:CG1	2.49	0.42
25:LO:36:MET:HE2	25:LO:87:ILE:HB	2.02	0.42
39:LH:63:ARG:N	39:LH:63:ARG:HD2	2.34	0.42
40:SA:36:VAL:HG22	40:SA:231:VAL:O	2.20	0.42
74:L5:1365:A:H2'	74:L5:1366:U:C6	2.54	0.42
74:L5:1594:C:O2	74:L5:1594:C:O4'	2.36	0.42
74:L5:2126:C:O2	74:L5:2126:C:H2'	2.20	0.42
75:S7:11:C:H2'	75:S7:12:G:C8	2.55	0.42
79:LY:49:GLN:O	79:LY:50:ARG:CB	2.67	0.42
74:L5:1972:C:H2'	74:L5:1973:G:C8	2.54	0.42
78:LW:121:VAL:HG22	78:LW:135:VAL:HG13	2.00	0.42
1:L3:106:U:O2'	25:LO:202:ALA:CB	2.68	0.42
11:LU:18:LYS:HG3	74:L5:390:G:H4'	2.01	0.42
12:LV:69:ILE:HD12	12:LV:69:ILE:N	2.34	0.42
20:LD:294:VAL:HG11	20:LD:297:LYS:HE3	1.99	0.42
65:Sg:255:VAL:HG21	65:Sg:264:TRP:HZ3	1.85	0.42
74:L5:882:C:H5''	74:L5:883:U:O5'	2.19	0.42
75:S7:3:G:H22	75:S7:68:U:H3	1.67	0.42
76:S1:1549:U:H2'	76:S1:1550:C:C6	2.55	0.42
1:L3:71:G:C2'	1:L3:72:A:O5'	2.67	0.42
2:LB:178:PRO:HB2	2:LB:180:LEU:HD13	2.01	0.42
57:SH:48:ARG:O	57:SH:49:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SH:52:THR:HG22	57:SH:132:LEU:HD13	2.02	0.42
74:L5:376:A:H4'	74:L5:377:A:OP1	2.19	0.42
76:S1:1294:C:O2'	76:S1:1295:C:H5'	2.19	0.42
77:LA:42:THR:HB	77:LA:47:ARG:HE	1.84	0.42
1:L3:42:A:C4	1:L3:43:A:C8	3.07	0.42
46:SI:117:ARG:HG3	76:S1:785:U:O4'	2.19	0.42
47:SJ:76:SER:HB3	47:SJ:77:PRO:HD3	2.00	0.42
59:SM:65:LEU:N	59:SM:65:LEU:HD12	2.34	0.42
67:SZ:59:VAL:HG22	67:SZ:97:LEU:HD11	2.02	0.42
72:SO:46:THR:HG21	72:SO:117:GLY:HA3	2.01	0.42
74:L5:109:A:H4'	74:L5:110:G:OP1	2.19	0.42
74:L5:551:C:H2'	74:L5:552:U:O4'	2.20	0.42
74:L5:1366:U:H2'	74:L5:1367:U:C6	2.55	0.42
74:L5:1760:U:O2	74:L5:1760:U:O4'	2.37	0.42
74:L5:2138:A:H1'	74:L5:2274:A2M:N6	2.35	0.42
74:L5:2936:OMC:HM22	74:L5:2937:C:O4'	2.20	0.42
76:S1:1506:G:H5''	76:S1:1507:7MG:OP1	2.19	0.42
77:LA:119:ILE:N	77:LA:120:PRO:CD	2.83	0.42
1:L3:106:U:C4'	1:L3:107:U:OP2	2.67	0.42
9:LP:293:ARG:O	9:LP:296:VAL:HG12	2.20	0.42
47:SJ:125:ILE:O	47:SJ:125:ILE:HG23	2.20	0.42
69:Sf:19:LYS:O	69:Sf:20:LYS:C	2.63	0.42
74:L5:1034:A:H2'	74:L5:1035:G:O4'	2.19	0.42
74:L5:3049:A:H2'	74:L5:3050:G:O4'	2.20	0.42
76:S1:1326:G:H1	76:S1:1336:C:H5	1.67	0.42
77:LA:47:ARG:HD3	77:LA:158:LEU:O	2.19	0.42
1:L3:49:A:OP1	9:LP:228:ALA:HB3	2.19	0.42
6:LG:62:VAL:HG11	6:LG:85:VAL:HG11	2.02	0.42
20:LD:74:ARG:O	74:L5:814:OMG:H4'	2.19	0.42
25:LO:87:ILE:HG12	25:LO:138:VAL:HG22	2.00	0.42
51:SU:67:ARG:NH1	76:S1:279:U:O2	2.52	0.42
65:Sg:92:LEU:N	65:Sg:92:LEU:HD12	2.35	0.42
74:L5:962:G:O2'	74:L5:1140:G:H4'	2.20	0.42
74:L5:2696:U:H2'	74:L5:2697:G:O4'	2.20	0.42
76:S1:807:U:H2'	76:S1:808:U:O4'	2.19	0.42
77:LA:36:SER:O	77:LA:37:LEU:HD23	2.20	0.42
1:L3:27:A:H2'	1:L3:28:C:O4'	2.20	0.42
18:Lf:20:PHE:CG	18:Lf:42:VAL:HG21	2.55	0.42
20:LD:251:PHE:O	20:LD:254:VAL:HG12	2.19	0.42
48:SK:20:VAL:O	48:SK:20:VAL:HG13	2.19	0.42
49:SP:6:PRO:O	49:SP:7:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Sg:171:VAL:HG22	65:Sg:181:VAL:HG22	2.01	0.42
74:L5:803:U:O5'	74:L5:803:U:O2	2.38	0.42
74:L5:1916:A:O2'	74:L5:3029:G:H4'	2.20	0.42
74:L5:2660:U:H2'	74:L5:2661:C:C6	2.55	0.42
74:L5:2825:G:C6	74:L5:2826:C:C5	3.08	0.42
76:S1:126:U:H3'	76:S1:127:C:O2	2.20	0.42
76:S1:406:C:H2'	76:S1:407:G:O4'	2.20	0.42
76:S1:713:U:O2'	76:S1:714:G:P	2.77	0.42
76:S1:1320:C:N4	76:S1:1322:PSU:H1'	2.34	0.42
21:LI:78:MET:SD	21:LI:137:LEU:HD11	2.59	0.41
37:Lp:70:SER:OG	37:Lp:73:THR:HG22	2.20	0.41
74:L5:291:A:H2'	74:L5:292:G:C8	2.55	0.41
74:L5:652:U:H2'	74:L5:653:C:C6	2.54	0.41
74:L5:1613:U:C2	74:L5:1614:A:N7	2.88	0.41
74:L5:1729:C:H2'	74:L5:1730:G:H8	1.85	0.41
76:S1:331:U:H2'	76:S1:333:A:H5'	2.02	0.41
76:S1:368:U:H2'	76:S1:369:G:O4'	2.20	0.41
76:S1:727:U:H2'	76:S1:728:G:C8	2.55	0.41
3:LC:248:ALA:HB1	74:L5:2924:G:N3	2.35	0.41
13:LZ:57:MET:HE3	13:LZ:65:ARG:HD3	2.01	0.41
62:SS:22:CYS:O	62:SS:23:PHE:HB2	2.20	0.41
74:L5:38:U:H2'	74:L5:39:A:O4'	2.20	0.41
74:L5:1348:G:O2'	74:L5:1349:U:H5'	2.20	0.41
74:L5:3065:C:H2'	74:L5:3066:U:O4'	2.20	0.41
75:S7:46:G:N1	75:S7:57:C:C6	2.88	0.41
75:S7:64:C:H2'	75:S7:65:A:C1'	2.51	0.41
76:S1:1071:G:H2'	76:S1:1072:A:C8	2.55	0.41
4:LE:38:LEU:HD11	4:LE:110:LEU:CD1	2.50	0.41
10:LQ:54:LEU:HD23	10:LQ:62:ARG:HG2	2.02	0.41
28:LT:148:ILE:HD11	30:Lc:86:PHE:HE2	1.86	0.41
48:SK:45:LYS:CE	48:SK:53:LEU:HD13	2.50	0.41
50:ST:89:TYR:CE2	50:ST:150:LEU:HD12	2.55	0.41
61:SR:30:VAL:HG21	76:S1:1471:G:C5	2.55	0.41
65:Sg:12:LEU:HD12	65:Sg:57:VAL:HG13	2.03	0.41
74:L5:1627:C:OP1	78:LW:136:ARG:NH1	2.54	0.41
74:L5:1712:U:O2'	74:L5:1713:U:H5'	2.21	0.41
74:L5:2142:A:H2'	74:L5:2143:A:C8	2.56	0.41
75:S7:27:G:C2	75:S7:41:C:N3	2.88	0.41
75:S7:52:G:H2'	75:S7:53:A:C8	2.55	0.41
76:S1:420:U:H2'	76:S1:421:C:O4'	2.20	0.41
76:S1:898:A:H2'	76:S1:899:A2M:H8	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S1:1521:C:H2'	76:S1:1522:G:O4'	2.20	0.41
77:LA:33:LEU:HD12	77:LA:204:THR:O	2.21	0.41
3:LC:216:LEU:N	3:LC:216:LEU:HD12	2.35	0.41
53:Sb:14:ALA:HB2	76:S1:1000:C:H4'	2.01	0.41
57:SH:66:MET:O	57:SH:67:HIS:HB2	2.21	0.41
74:L5:667:C:H2'	74:L5:668:A:C8	2.55	0.41
74:L5:843:U:H2'	74:L5:844:G:O4'	2.21	0.41
74:L5:882:C:H3'	74:L5:883:U:H4'	2.02	0.41
74:L5:1010:U:H2'	74:L5:1011:U:H6	1.85	0.41
74:L5:2938:G:H2'	74:L5:2939:U:C6	2.56	0.41
74:L5:2989:U:H2'	74:L5:2990:U:C6	2.56	0.41
76:S1:1173:C:O2	76:S1:1173:C:O5'	2.38	0.41
41:SB:58:LEU:O	41:SB:62:LYS:HG2	2.21	0.41
51:SU:131:LYS:HB2	76:S1:310:G:H3'	2.02	0.41
53:Sb:21:ILE:HD12	53:Sb:21:ILE:C	2.45	0.41
69:Sf:40:LEU:N	69:Sf:40:LEU:HD22	2.35	0.41
69:Sf:73:LEU:C	69:Sf:73:LEU:HD12	2.45	0.41
73:L4:42:G:HO2'	73:L4:43:OMG:P	2.42	0.41
76:S1:481:A:H2'	76:S1:482:U:O4'	2.21	0.41
76:S1:548:A:H4'	76:S1:549:A:OP2	2.21	0.41
77:LA:64:VAL:HG22	77:LA:108:ALA:HB3	2.02	0.41
26:LR:171:ILE:O	26:LR:175:LYS:HG2	2.20	0.41
41:SB:107:ILE:HD12	41:SB:118:LYS:HD3	2.01	0.41
45:SG:162:VAL:HG13	45:SG:165:ARG:HB2	2.01	0.41
65:Sg:138:ASN:CG	65:Sg:140:VAL:HG22	2.46	0.41
73:L4:118:A:N1	73:L4:139:U:H5	2.19	0.41
74:L5:954:C:O2'	74:L5:1429:A:H1'	2.21	0.41
74:L5:1622:C:H4'	74:L5:1856:A:H4'	2.02	0.41
74:L5:2399:C:H1'	74:L5:2796:A:C2	2.56	0.41
74:L5:2963:U:C2	74:L5:2964:A:C8	3.09	0.41
74:L5:2992:C:H2'	74:L5:2993:A:H8	1.86	0.41
74:L5:3130:A:O2'	74:L5:3131:C:P	2.79	0.41
75:S7:5:A:C6	75:S7:6:A:C6	3.08	0.41
76:S1:1698:U:H2'	76:S1:1699:U:C6	2.55	0.41
78:LW:39:ASN:ND2	78:LW:43:PHE:HE1	2.19	0.41
29:LX:35:SER:HA	29:LX:104:ILE:HD11	2.02	0.41
37:Lp:79:ILE:O	37:Lp:83:THR:HG22	2.20	0.41
65:Sg:136:LEU:HD11	65:Sg:184:LEU:HD21	2.02	0.41
72:SO:40:PHE:CD1	72:SO:40:PHE:C	2.97	0.41
74:L5:423:A:C2	74:L5:2356:A:H4'	2.56	0.41
74:L5:1972:C:C4	74:L5:2090:G:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:2190:C:O2	74:L5:2190:C:H2'	2.20	0.41
74:L5:2937:C:H2'	74:L5:2938:G:C8	2.56	0.41
74:L5:3134:C:O2	74:L5:3134:C:O4'	2.38	0.41
75:S7:14:A:H2'	75:S7:15:G:O4'	2.21	0.41
76:S1:127:C:O2	76:S1:127:C:O4'	2.37	0.41
76:S1:903:A:H2'	76:S1:904:A:O4'	2.21	0.41
76:S1:1364:C:C3'	76:S1:1365:U:C5'	2.99	0.41
76:S1:1517:U:H3	76:S1:1543:A:H2	1.66	0.41
1:L3:37:A:C2	1:L3:41:G:C2	3.09	0.41
8:LK:64:VAL:O	8:LK:72:ARG:HG3	2.20	0.41
18:Lf:86:LEU:HD13	18:Lf:86:LEU:O	2.21	0.41
24:LN:192:TRP:O	24:LN:196:GLN:HG2	2.20	0.41
41:SB:69:VAL:HG21	41:SB:188:LEU:HB2	2.03	0.41
41:SB:188:LEU:HD23	52:SY:43:GLY:O	2.21	0.41
56:SC:18:VAL:HG11	62:SS:20:ARG:NH1	2.35	0.41
56:SC:82:SER:OG	56:SC:85:THR:HG21	2.21	0.41
61:SR:140:THR:HG21	76:S1:1100:U:O4	2.20	0.41
65:Sg:35:ILE:HG22	65:Sg:76:MET:HE3	2.02	0.41
76:S1:1474:G:N2	76:S1:1501:A:OP2	2.54	0.41
77:LA:116:LEU:N	77:LA:117:PRO:CD	2.83	0.41
78:LW:45:ASN:OD1	78:LW:46:ARG:N	2.53	0.41
80:SX:19:VAL:HG13	80:SX:21:TYR:H	1.86	0.41
2:LB:173:GLY:H	74:L5:2172:C:H42	1.69	0.41
30:Lc:97:VAL:O	30:Lc:125:GLY:HA2	2.20	0.41
34:Lk:15:LEU:HD21	34:Lk:57:PRO:HD3	2.03	0.41
35:Ll:31:LEU:HD12	35:Ll:32:PRO:HD2	2.03	0.41
39:LH:71:TYR:O	74:L5:2516:A:H2'	2.19	0.41
45:SG:189:ILE:HD13	45:SG:192:ARG:NH2	2.36	0.41
51:SU:120:ILE:HD12	51:SU:156:PHE:CZ	2.56	0.41
61:SR:27:LYS:HE3	76:S1:1465:C:OP1	2.21	0.41
68:Sa:83:GLU:O	68:Sa:85:MET:O	2.39	0.41
74:L5:150:G:C4	74:L5:151:G:C8	3.09	0.41
74:L5:557:G:H2'	74:L5:558:U:O4'	2.21	0.41
74:L5:642:A:H2'	74:L5:643:A:H8	1.85	0.41
74:L5:1622:C:H2'	74:L5:1623:A:O4'	2.21	0.41
74:L5:2100:A:H2'	74:L5:2101:A:C8	2.55	0.41
74:L5:2724:A2M:O5'	74:L5:2724:A2M:H8	2.21	0.41
74:L5:2792:OMG:H2'	74:L5:2847:5MC:HM52	2.03	0.41
74:L5:2824:A:C4	74:L5:2825:G:C8	3.09	0.41
74:L5:3086:C:H2'	74:L5:3087:U:C6	2.56	0.41
74:L5:3212:C:O2	74:L5:3212:C:H3'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S1:656:G:H2'	76:S1:657:G:C1'	2.51	0.41
76:S1:1328:C:O2	76:S1:1328:C:O5'	2.38	0.41
79:LY:31:ARG:C	79:LY:33:GLY:N	2.79	0.41
2:LB:247:ARG:HE	2:LB:247:ARG:HA	1.85	0.41
3:LC:248:ALA:HB1	74:L5:2924:G:C2	2.56	0.41
10:LQ:119:THR:HG22	10:LQ:138:HIS:HB3	2.03	0.41
20:LD:202:ILE:N	20:LD:202:ILE:HD12	2.35	0.41
74:L5:239:A:H2'	74:L5:240:U:C6	2.56	0.41
74:L5:711:G:H2'	74:L5:712:C:O4'	2.21	0.41
74:L5:753:G:C8	74:L5:753:G:OP1	2.75	0.41
74:L5:1761:U:H2'	74:L5:1762:G:O4'	2.21	0.41
74:L5:2266:G:H1'	74:L5:2304:G:C6	2.56	0.41
74:L5:2920:G:H2'	74:L5:2921:PSU:O4'	2.21	0.41
74:L5:3218:A:H3'	74:L5:3219:G:H21	1.86	0.41
75:S7:61:C:C5'	77:LA:44:ARG:HG2	2.51	0.41
76:S1:722:C:C2	76:S1:723:A:C8	3.09	0.41
13:LZ:46:ILE:HD12	13:LZ:46:ILE:N	2.36	0.40
20:LD:89:ALA:HB3	74:L5:1461:U:H4'	2.03	0.40
20:LD:278:ALA:N	20:LD:279:PRO:HD2	2.37	0.40
25:LO:48:TYR:CG	25:LO:145:ILE:HD11	2.56	0.40
30:Lc:53:LEU:O	30:Lc:56:LYS:HG2	2.21	0.40
34:Lk:11:TYR:HB2	34:Lk:41:LEU:HD22	2.02	0.40
49:SP:19:ARG:C	49:SP:21:ARG:H	2.29	0.40
57:SH:128:ASP:O	64:Sd:44:VAL:HA	2.21	0.40
69:Sf:46:ASN:OD1	69:Sf:69:LEU:HD22	2.21	0.40
74:L5:709:U:H2'	74:L5:710:C:C6	2.56	0.40
74:L5:801:G:H2'	74:L5:802:U:C6	2.55	0.40
74:L5:1874:U:H5'	74:L5:1875:C:OP1	2.21	0.40
74:L5:2710:A:H2'	74:L5:2711:A:O4'	2.21	0.40
74:L5:2748:G:H3'	74:L5:2749:U:C5'	2.50	0.40
74:L5:3130:A:N3	74:L5:3130:A:H2'	2.36	0.40
75:S7:21:U:N3	75:S7:22:A:C5	2.89	0.40
76:S1:721:U:O2	76:S1:721:U:O4'	2.36	0.40
76:S1:797:G:H2'	76:S1:798:U:O4'	2.21	0.40
76:S1:1546:A:C2'	76:S1:1547:C:H5'	2.51	0.40
73:L4:55:U:H3	73:L4:62:A:H2	1.70	0.40
74:L5:162:U:H2'	74:L5:163:U:O4'	2.21	0.40
74:L5:1520:C:H2'	74:L5:1521:A:C8	2.56	0.40
74:L5:1760:U:O2	74:L5:1760:U:O5'	2.39	0.40
74:L5:2186:U:H1'	74:L5:2308:G:N2	2.36	0.40
74:L5:2673:A:H2'	74:L5:2674:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S1:91:A:C6	76:S1:371:G:C6	3.09	0.40
77:LA:95:ASN:O	77:LA:97:THR:N	2.55	0.40
31:Lh:20:GLN:HB3	31:Lh:32:VAL:HG22	2.03	0.40
46:SI:122:THR:HG23	76:S1:608:U:OP2	2.21	0.40
65:Sg:239:SER:OG	65:Sg:240:PRO:HD2	2.21	0.40
74:L5:748:A:H1'	74:L5:749:G:O5'	2.21	0.40
74:L5:748:A:O2'	74:L5:749:G:H8	2.05	0.40
74:L5:888:U:H3'	74:L5:889:G:C5'	2.51	0.40
74:L5:2102:C:H1'	74:L5:3272:A:C8	2.57	0.40
74:L5:2182:U:C4	74:L5:2183:U:C5	3.09	0.40
76:S1:713:U:O2'	76:S1:714:G:H8	2.04	0.40
76:S1:1085:A:H2'	76:S1:1086:C:C6	2.56	0.40
76:S1:1166:G:H2'	76:S1:1167:A:O4'	2.22	0.40
2:LB:102:LEU:HD23	2:LB:102:LEU:N	2.36	0.40
3:LC:25:ILE:HD11	3:LC:332:ARG:NH1	2.36	0.40
28:LT:24:MET:HB3	28:LT:25:PRO:HD2	2.03	0.40
73:L4:139:U:O2	73:L4:139:U:O4'	2.38	0.40
74:L5:212:A:N6	74:L5:226:G:H2'	2.36	0.40
74:L5:660:C:H4'	74:L5:661:A2M:O5'	2.21	0.40
74:L5:1668:U:H2'	74:L5:1669:U:C6	2.57	0.40
74:L5:2201:A:OP2	74:L5:2202:U:OP2	2.39	0.40
74:L5:2269:G:H3'	74:L5:2270:C:O2	2.22	0.40
74:L5:2392:A:H2'	74:L5:2393:G:O4'	2.22	0.40
74:L5:3109:C:H2'	74:L5:3110:A:O4'	2.21	0.40
77:LA:205:ILE:HG13	77:LA:215:ILE:HD11	2.04	0.40
6:LG:137:LEU:C	6:LG:137:LEU:HD13	2.47	0.40
16:Ld:87:TYR:CD2	74:L5:1735:A:N7	2.90	0.40
74:L5:1024:G:H2'	74:L5:1025:C:C6	2.56	0.40
74:L5:1826:A:H2'	74:L5:1827:G:H8	1.87	0.40
74:L5:2196:U:H2'	74:L5:2197:C:C6	2.56	0.40
74:L5:2398:C:O2	74:L5:2796:A:N1	2.54	0.40
77:LA:38:LYS:O	77:LA:39:ASP:C	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LB	246/257 (96%)	239 (97%)	7 (3%)	0	100	100
3	LC	379/395 (96%)	370 (98%)	9 (2%)	0	100	100
4	LE	164/171 (96%)	161 (98%)	3 (2%)	0	100	100
5	LF	184/190 (97%)	181 (98%)	3 (2%)	0	100	100
6	LG	145/212 (68%)	142 (98%)	3 (2%)	0	100	100
7	LJ	194/203 (96%)	191 (98%)	3 (2%)	0	100	100
8	LK	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
9	LP	283/306 (92%)	279 (99%)	4 (1%)	0	100	100
10	LQ	184/222 (83%)	181 (98%)	3 (2%)	0	100	100
11	LU	150/194 (77%)	146 (97%)	4 (3%)	0	100	100
12	LV	95/122 (78%)	92 (97%)	3 (3%)	0	100	100
13	LZ	134/146 (92%)	132 (98%)	2 (2%)	0	100	100
14	La	117/123 (95%)	114 (97%)	3 (3%)	0	100	100
15	Lb	51/59 (86%)	48 (94%)	3 (6%)	0	100	100
16	Ld	91/108 (84%)	89 (98%)	2 (2%)	0	100	100
17	Le	103/117 (88%)	102 (99%)	1 (1%)	0	100	100
18	Lf	123/132 (93%)	122 (99%)	1 (1%)	0	100	100
19	Lg	106/115 (92%)	103 (97%)	3 (3%)	0	100	100
20	LD	339/360 (94%)	333 (98%)	6 (2%)	0	100	100
21	LI	199/202 (98%)	196 (98%)	3 (2%)	0	100	100
22	LL	126/133 (95%)	123 (98%)	3 (2%)	0	100	100
23	LM	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
24	LN	200/204 (98%)	198 (99%)	2 (1%)	0	100	100
25	LO	208/227 (92%)	201 (97%)	7 (3%)	0	100	100
26	LR	173/194 (89%)	168 (97%)	5 (3%)	0	100	100
27	LS	182/188 (97%)	178 (98%)	4 (2%)	0	100	100
28	LT	152/160 (95%)	149 (98%)	3 (2%)	0	100	100
29	LX	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
30	Lc	213/259 (82%)	205 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	Lh	97/150 (65%)	93 (96%)	4 (4%)	0	100	100
32	Li	106/116 (91%)	103 (97%)	3 (3%)	0	100	100
33	Lj	87/98 (89%)	84 (97%)	3 (3%)	0	100	100
34	Lk	63/70 (90%)	61 (97%)	1 (2%)	1 (2%)	7	20
35	Ll	47/59 (80%)	46 (98%)	1 (2%)	0	100	100
36	Lm	48/55 (87%)	48 (100%)	0	0	100	100
37	Lp	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
38	Lo	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
39	LH	220/285 (77%)	218 (99%)	2 (1%)	0	100	100
40	SA	213/264 (81%)	211 (99%)	2 (1%)	0	100	100
41	SB	194/274 (71%)	184 (95%)	9 (5%)	1 (0%)	24	48
42	SD	176/184 (96%)	174 (99%)	2 (1%)	0	100	100
43	SE	256/266 (96%)	248 (97%)	8 (3%)	0	100	100
44	SF	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
45	SG	212/239 (89%)	209 (99%)	3 (1%)	0	100	100
46	SI	176/194 (91%)	171 (97%)	5 (3%)	0	100	100
47	SJ	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
48	SK	177/192 (92%)	175 (99%)	2 (1%)	0	100	100
49	SP	141/145 (97%)	131 (93%)	10 (7%)	0	100	100
50	ST	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
51	SU	149/156 (96%)	143 (96%)	6 (4%)	0	100	100
52	SY	76/79 (96%)	73 (96%)	3 (4%)	0	100	100
53	Sb	95/115 (83%)	85 (90%)	10 (10%)	0	100	100
54	Sc	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
55	Se	38/61 (62%)	37 (97%)	1 (3%)	0	100	100
56	SC	207/223 (93%)	204 (99%)	3 (1%)	0	100	100
57	SH	183/192 (95%)	176 (96%)	7 (4%)	0	100	100
58	SL	130/149 (87%)	125 (96%)	5 (4%)	0	100	100
59	SM	96/120 (80%)	92 (96%)	4 (4%)	0	100	100
60	SQ	113/135 (84%)	110 (97%)	3 (3%)	0	100	100
61	SR	142/154 (92%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SS	48/66 (73%)	46 (96%)	2 (4%)	0	100	100
63	SW	113/149 (76%)	111 (98%)	2 (2%)	0	100	100
64	Sd	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
65	Sg	320/323 (99%)	302 (94%)	18 (6%)	0	100	100
66	SN	94/113 (83%)	88 (94%)	6 (6%)	0	100	100
67	SZ	94/135 (70%)	91 (97%)	3 (3%)	0	100	100
68	Sa	73/104 (70%)	64 (88%)	9 (12%)	0	100	100
69	Sf	62/77 (80%)	55 (89%)	7 (11%)	0	100	100
70	Ln	36/39 (92%)	34 (94%)	1 (3%)	1 (3%)	4	9
71	SV	77/134 (58%)	77 (100%)	0	0	100	100
72	SO	123/157 (78%)	119 (97%)	4 (3%)	0	100	100
77	LA	215/217 (99%)	188 (87%)	20 (9%)	7 (3%)	3	7
78	LW	116/153 (76%)	105 (90%)	9 (8%)	2 (2%)	7	19
79	LY	57/156 (36%)	52 (91%)	2 (4%)	3 (5%)	1	3
80	SX	157/174 (90%)	153 (98%)	4 (2%)	0	100	100
All	All	10722/12219 (88%)	10394 (97%)	313 (3%)	15 (0%)	49	73

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
77	LA	44	ARG
79	LY	32	ASP
79	LY	50	ARG
70	Ln	16	ARG
77	LA	13	ILE
77	LA	39	ASP
77	LA	96	LYS
78	LW	59	HIS
79	LY	31	ARG
77	LA	40	TYR
77	LA	93	ASN
34	Lk	27	LYS
41	SB	192	ILE
77	LA	154	VAL
78	LW	51	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	LB	189/198 (96%)	187 (99%)	2 (1%)	65	85
3	LC	333/345 (96%)	333 (100%)	0	100	100
4	LE	146/151 (97%)	145 (99%)	1 (1%)	76	90
5	LF	167/170 (98%)	165 (99%)	2 (1%)	63	84
6	LG	129/181 (71%)	127 (98%)	2 (2%)	55	80
7	LJ	163/170 (96%)	163 (100%)	0	100	100
8	LK	100/104 (96%)	99 (99%)	1 (1%)	68	86
9	LP	248/261 (95%)	248 (100%)	0	100	100
10	LQ	157/184 (85%)	156 (99%)	1 (1%)	78	91
11	LU	132/163 (81%)	132 (100%)	0	100	100
12	LV	89/111 (80%)	89 (100%)	0	100	100
13	LZ	124/129 (96%)	123 (99%)	1 (1%)	73	88
14	La	109/111 (98%)	106 (97%)	3 (3%)	38	68
15	Lb	47/52 (90%)	46 (98%)	1 (2%)	47	75
16	Ld	79/94 (84%)	77 (98%)	2 (2%)	42	71
17	Le	96/105 (91%)	94 (98%)	2 (2%)	47	75
18	Lf	110/117 (94%)	109 (99%)	1 (1%)	70	87
19	Lg	93/99 (94%)	92 (99%)	1 (1%)	65	85
20	LD	273/288 (95%)	272 (100%)	1 (0%)	84	93
21	LI	171/172 (99%)	171 (100%)	0	100	100
22	LL	108/110 (98%)	107 (99%)	1 (1%)	70	87
23	LM	120/121 (99%)	120 (100%)	0	100	100
24	LN	175/176 (99%)	173 (99%)	2 (1%)	65	85
25	LO	176/188 (94%)	174 (99%)	2 (1%)	65	85
26	LR	149/164 (91%)	146 (98%)	3 (2%)	48	76
27	LS	160/164 (98%)	159 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LT	133/139 (96%)	129 (97%)	4 (3%)	36	66
29	LX	115/128 (90%)	115 (100%)	0	100	100
30	Lc	185/228 (81%)	185 (100%)	0	100	100
31	Lh	85/125 (68%)	84 (99%)	1 (1%)	63	84
32	Li	93/100 (93%)	92 (99%)	1 (1%)	65	85
33	Lj	72/78 (92%)	72 (100%)	0	100	100
34	Lk	58/62 (94%)	58 (100%)	0	100	100
35	Ll	45/54 (83%)	45 (100%)	0	100	100
36	Lm	46/49 (94%)	46 (100%)	0	100	100
37	Lp	75/76 (99%)	72 (96%)	3 (4%)	28	56
38	Lo	86/90 (96%)	86 (100%)	0	100	100
39	LH	195/243 (80%)	192 (98%)	3 (2%)	57	81
40	SA	198/237 (84%)	188 (95%)	10 (5%)	21	48
41	SB	173/238 (73%)	172 (99%)	1 (1%)	78	91
42	SD	158/163 (97%)	156 (99%)	2 (1%)	61	83
43	SE	228/235 (97%)	226 (99%)	2 (1%)	70	87
44	SF	146/157 (93%)	144 (99%)	2 (1%)	59	82
45	SG	193/208 (93%)	191 (99%)	2 (1%)	68	86
46	SI	160/173 (92%)	156 (98%)	4 (2%)	42	71
47	SJ	113/114 (99%)	111 (98%)	2 (2%)	51	78
48	SK	158/164 (96%)	157 (99%)	1 (1%)	78	91
49	SP	116/118 (98%)	115 (99%)	1 (1%)	70	87
50	ST	131/132 (99%)	130 (99%)	1 (1%)	73	88
51	SU	137/140 (98%)	133 (97%)	4 (3%)	37	67
52	SY	67/68 (98%)	66 (98%)	1 (2%)	57	81
53	Sb	86/104 (83%)	84 (98%)	2 (2%)	44	73
54	Sc	62/73 (85%)	61 (98%)	1 (2%)	55	80
55	Se	33/48 (69%)	32 (97%)	1 (3%)	36	66
56	SC	173/186 (93%)	165 (95%)	8 (5%)	24	51
57	SH	159/162 (98%)	157 (99%)	2 (1%)	61	83
58	SL	110/122 (90%)	105 (96%)	5 (4%)	24	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	SM	91/108 (84%)	89 (98%)	2 (2%)	45	74
60	SQ	99/116 (85%)	95 (96%)	4 (4%)	28	56
61	SR	123/131 (94%)	121 (98%)	2 (2%)	55	80
62	SS	44/58 (76%)	43 (98%)	1 (2%)	44	73
63	SW	103/132 (78%)	101 (98%)	2 (2%)	50	77
64	Sd	50/54 (93%)	50 (100%)	0	100	100
65	Sg	280/281 (100%)	267 (95%)	13 (5%)	24	51
66	SN	91/105 (87%)	89 (98%)	2 (2%)	45	74
67	SZ	84/115 (73%)	84 (100%)	0	100	100
68	Sa	67/90 (74%)	66 (98%)	1 (2%)	57	81
69	Sf	57/68 (84%)	57 (100%)	0	100	100
70	Ln	34/35 (97%)	33 (97%)	1 (3%)	37	67
71	SV	67/118 (57%)	66 (98%)	1 (2%)	57	81
72	SO	98/122 (80%)	94 (96%)	4 (4%)	27	56
77	LA	192/192 (100%)	184 (96%)	8 (4%)	26	55
78	LW	108/135 (80%)	101 (94%)	7 (6%)	15	37
79	LY	52/126 (41%)	46 (88%)	6 (12%)	5	14
80	SX	139/151 (92%)	132 (95%)	7 (5%)	22	48
All	All	9411/10479 (90%)	9256 (98%)	155 (2%)	54	80

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LB	75	ARG
2	LB	102	LEU
4	LE	38	LEU
5	LF	86	LYS
5	LF	163	CYS
6	LG	104	GLU
6	LG	108	VAL
8	LK	98	GLU
10	LQ	89	MET
13	LZ	108	ARG
14	La	4	ILE
14	La	38	VAL
14	La	76	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	Lb	25	LYS
16	Ld	19	LEU
16	Ld	22	LYS
17	Le	11	LEU
17	Le	55	VAL
18	Lf	49	THR
19	Lg	106	VAL
20	LD	314	LYS
22	LL	64	VAL
24	LN	39	VAL
24	LN	64	VAL
25	LO	216	VAL
25	LO	223	LYS
26	LR	31	LYS
26	LR	170	GLN
26	LR	177	LYS
27	LS	138	ARG
28	LT	3	HIS
28	LT	92	HIS
28	LT	131	GLN
28	LT	135	VAL
31	Lh	32	VAL
32	Li	80	GLN
37	Lp	32	LEU
37	Lp	82	ILE
37	Lp	89	GLN
39	LH	48	ILE
39	LH	175	HIS
39	LH	234	MET
40	SA	46	THR
40	SA	96	CYS
40	SA	119	SER
40	SA	127	VAL
40	SA	139	CYS
40	SA	150	LEU
40	SA	153	THR
40	SA	156	VAL
40	SA	188	ILE
40	SA	222	LYS
41	SB	166	CYS
42	SD	2	VAL
42	SD	161	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	SE	170	ILE
43	SE	266	HIS
44	SF	19	VAL
44	SF	99	ARG
45	SG	44	GLU
45	SG	191	LEU
46	SI	82	LEU
46	SI	99	GLN
46	SI	121	LEU
46	SI	163	GLN
47	SJ	71	LYS
47	SJ	74	VAL
48	SK	76	THR
49	SP	69	ARG
50	ST	11	ILE
51	SU	65	ARG
51	SU	72	MET
51	SU	84	MET
51	SU	145	ILE
52	SY	78	LEU
53	Sb	64	LEU
53	Sb	84	VAL
54	Sc	60	VAL
55	Se	8	SER
56	SC	14	ILE
56	SC	33	GLU
56	SC	44	THR
56	SC	68	ILE
56	SC	148	ARG
56	SC	178	GLN
56	SC	204	THR
56	SC	208	ASP
57	SH	50	ARG
57	SH	97	LEU
58	SL	13	VAL
58	SL	23	VAL
58	SL	72	ARG
58	SL	88	ARG
58	SL	116	VAL
59	SM	27	THR
59	SM	115	ASP
60	SQ	60	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
60	SQ	71	CYS
60	SQ	104	ARG
60	SQ	122	GLU
61	SR	27	LYS
61	SR	138	THR
62	SS	53	VAL
63	SW	38	VAL
63	SW	130	VAL
65	Sg	5	VAL
65	Sg	11	VAL
65	Sg	47	GLU
65	Sg	57	VAL
65	Sg	94	LEU
65	Sg	107	ASN
65	Sg	123	ARG
65	Sg	136	LEU
65	Sg	137	TRP
65	Sg	197	GLU
65	Sg	235	LEU
65	Sg	236	GLU
65	Sg	271	VAL
66	SN	63	VAL
66	SN	79	GLN
68	Sa	68	LEU
70	Ln	15	MET
71	SV	38	VAL
72	SO	60	VAL
72	SO	149	LYS
72	SO	152	ARG
72	SO	156	ARG
77	LA	16	ILE
77	LA	67	PHE
77	LA	102	LEU
77	LA	141	ASP
77	LA	154	VAL
77	LA	166	VAL
77	LA	208	THR
77	LA	215	ILE
78	LW	37	ARG
78	LW	38	ARG
78	LW	45	ASN
78	LW	47	THR

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Mol	Chain	Res	Type
78	LW	91	ASN
78	LW	110	VAL
78	LW	116	VAL
79	LY	13	CYS
79	LY	14	SER
79	LY	20	VAL
79	LY	48	LYS
79	LY	56	VAL
79	LY	64	LYS
80	SX	19	VAL
80	SX	22	ARG
80	SX	23	ARG
80	SX	24	ILE
80	SX	48	ASN
80	SX	56	ILE
80	SX	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	LB	205	ASN
2	LB	211	HIS
3	LC	311	HIS
5	LF	97	HIS
7	LJ	76	GLN
9	LP	253	ASN
11	LU	25	HIS
15	Lb	6	ASN
15	Lb	9	ASN
17	Le	100	HIS
24	LN	77	ASN
24	LN	149	GLN
25	LO	59	GLN
26	LR	14	GLN
26	LR	134	ASN
27	LS	127	ASN
29	LX	115	HIS
30	Lc	61	HIS
30	Lc	123	HIS
32	Li	24	HIS
33	Lj	27	ASN
34	Lk	59	HIS

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Mol	Chain	Res	Type
39	LH	81	GLN
39	LH	228	GLN
39	LH	255	HIS
42	SD	102	ASN
43	SE	207	HIS
45	SG	119	GLN
45	SG	180	GLN
46	SI	68	HIS
46	SI	147	GLN
48	SK	52	ASN
50	ST	49	GLN
50	ST	58	ASN
51	SU	87	ASN
51	SU	90	HIS
51	SU	116	ASN
57	SH	70	ASN
58	SL	14	GLN
61	SR	100	ASN
65	Sg	124	GLN
68	Sa	94	GLN
77	LA	118	GLN
77	LA	196	ASN
80	SX	89	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L3	121/122 (99%)	15 (12%)	3 (2%)
73	L4	149/159 (93%)	25 (16%)	3 (2%)
74	L5	2850/3326 (85%)	462 (16%)	19 (0%)
75	S7	63/74 (85%)	17 (26%)	0
76	S1	1531/1728 (88%)	233 (15%)	9 (0%)
All	All	4714/5409 (87%)	752 (15%)	34 (0%)

All (752) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L3	33	U
1	L3	38	U
1	L3	52	U
1	L3	53	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L3	54	A
1	L3	64	A
1	L3	72	A
1	L3	100	A
1	L3	102	C
1	L3	106	U
1	L3	107	U
1	L3	108	U
1	L3	109	C
1	L3	113	G
1	L3	122	C
73	L4	23	U
73	L4	34	A
73	L4	35	C
73	L4	43	OMG
73	L4	59	A
73	L4	62	A
73	L4	63	G
73	L4	91	U
73	L4	92	A
73	L4	95	A
73	L4	104	A
73	L4	106	C
73	L4	112	A
73	L4	113	A
73	L4	114	G
73	L4	124	U
73	L4	126	U
73	L4	129	U
73	L4	130	C
73	L4	131	G
73	L4	133	A
73	L4	134	U
73	L4	140	A
73	L4	153	U
73	L4	154	G
74	L5	26	A
74	L5	40	A
74	L5	43	A
74	L5	45	A
74	L5	49	U
74	L5	57	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	59	G
74	L5	60	A
74	L5	65	A
74	L5	66	A
74	L5	67	A
74	L5	69	U
74	L5	93	C
74	L5	105	G
74	L5	109	A
74	L5	110	G
74	L5	111	U
74	L5	117	G
74	L5	118	U
74	L5	121	A
74	L5	122	A
74	L5	141	U
74	L5	156	G
74	L5	157	A
74	L5	164	U
74	L5	165	A
74	L5	166	G
74	L5	178	U
74	L5	184	U
74	L5	185	A
74	L5	189	U
74	L5	190	U
74	L5	198	A
74	L5	209	A
74	L5	217	G
74	L5	218	A
74	L5	219	U
74	L5	232	A
74	L5	263	U
74	L5	264	G
74	L5	266	A
74	L5	267	U
74	L5	271	G
74	L5	297	A
74	L5	300	U
74	L5	307	U
74	L5	311	C
74	L5	313	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	314	C
74	L5	331	U
74	L5	332	G
74	L5	355	G
74	L5	378	G
74	L5	393	U
74	L5	396	U
74	L5	397	A
74	L5	399	A
74	L5	400	A
74	L5	403	A
74	L5	413	G
74	L5	422	G
74	L5	423	A
74	L5	439	C
74	L5	442	C
74	L5	444	G
74	L5	445	C
74	L5	487	C
74	L5	506	G
74	L5	514	C
74	L5	515	G
74	L5	516	U
74	L5	517	G
74	L5	520	U
74	L5	521	G
74	L5	524	U
74	L5	536	U
74	L5	539	C
74	L5	540	C
74	L5	541	G
74	L5	544	U
74	L5	547	U
74	L5	549	U
74	L5	557	G
74	L5	563	G
74	L5	568	C
74	L5	574	G
74	L5	630	C
74	L5	633	A
74	L5	649	C
74	L5	661	A2M

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	672	A
74	L5	689	A
74	L5	693	C
74	L5	694	C
74	L5	702	C
74	L5	703	A
74	L5	714	C
74	L5	715	G
74	L5	716	U
74	L5	724	G
74	L5	727	A
74	L5	728	G
74	L5	729	A
74	L5	743	G
74	L5	745	G
74	L5	746	U
74	L5	747	U
74	L5	748	A
74	L5	749	G
74	L5	751	G
74	L5	752	U
74	L5	753	G
74	L5	773	A
74	L5	774	C
74	L5	777	U
74	L5	778	U
74	L5	782	U
74	L5	783	U
74	L5	789	C
74	L5	790	G
74	L5	793	U
74	L5	794	G
74	L5	795	A
74	L5	808	G
74	L5	815	A
74	L5	826	A2M
74	L5	839	A
74	L5	845	A
74	L5	851	G
74	L5	858	G
74	L5	870	U
74	L5	883	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	889	G
74	L5	905	A
74	L5	916	G
74	L5	917	OMG
74	L5	918	G
74	L5	920	C
74	L5	923	A
74	L5	925	G
74	L5	926	A
74	L5	930	A
74	L5	932	C
74	L5	933	G
74	L5	943	G
74	L5	944	U
74	L5	946	G
74	L5	953	U
74	L5	968	C
74	L5	969	U
74	L5	971	A
74	L5	990	G
74	L5	996	U
74	L5	998	G
74	L5	1003	A
74	L5	1005	U
74	L5	1026	U
74	L5	1027	A
74	L5	1035	G
74	L5	1040	A
74	L5	1066	U
74	L5	1072	A
74	L5	1074	C
74	L5	1091	C
74	L5	1101	G
74	L5	1123	G
74	L5	1124	A
74	L5	1129	G
74	L5	1142	G
74	L5	1156	G
74	L5	1169	U
74	L5	1178	C
74	L5	1184	A
74	L5	1188	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	1203	A
74	L5	1206	U
74	L5	1207	A
74	L5	1217	C
74	L5	1219	G
74	L5	1221	U
74	L5	1226	U
74	L5	1234	G
74	L5	1238	G
74	L5	1243	U
74	L5	1332	G
74	L5	1334	U
74	L5	1338	G
74	L5	1341	C
74	L5	1342	A
74	L5	1356	A
74	L5	1371	U
74	L5	1381	G
74	L5	1410	G
74	L5	1425	G
74	L5	1440	G
74	L5	1442	G
74	L5	1454	G
74	L5	1457	G
74	L5	1460	C
74	L5	1473	G
74	L5	1478	U
74	L5	1504	A
74	L5	1506	G
74	L5	1507	U
74	L5	1525	G
74	L5	1559	G
74	L5	1576	A
74	L5	1580	G
74	L5	1582	A
74	L5	1583	U
74	L5	1585	G
74	L5	1602	G
74	L5	1605	A
74	L5	1607	A
74	L5	1608	G
74	L5	1611	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	1623	A
74	L5	1637	U
74	L5	1638	C
74	L5	1639	G
74	L5	1647	U
74	L5	1648	G
74	L5	1649	G
74	L5	1657	C
74	L5	1660	A
74	L5	1661	A
74	L5	1663	U
74	L5	1675	C
74	L5	1701	U
74	L5	1722	A
74	L5	1726	U
74	L5	1737	C
74	L5	1744	C
74	L5	1745	G
74	L5	1749	C
74	L5	1750	G
74	L5	1770	A
74	L5	1771	U
74	L5	1778	U
74	L5	1796	G
74	L5	1801	G
74	L5	1818	A
74	L5	1829	G
74	L5	1842	G
74	L5	1843	C
74	L5	1860	A
74	L5	1861	C
74	L5	1862	A
74	L5	1863	A
74	L5	1864	C
74	L5	1871	A
74	L5	1874	U
74	L5	1887	C
74	L5	1899	G
74	L5	1900	A
74	L5	1901	U
74	L5	1907	A
74	L5	1914	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	1927	G
74	L5	1948	G
74	L5	1972	C
74	L5	1973	G
74	L5	2096	U
74	L5	2104	G
74	L5	2105	G
74	L5	2106	A
74	L5	2107	G
74	L5	2115	G
74	L5	2116	G
74	L5	2125	A
74	L5	2138	A
74	L5	2143	A
74	L5	2152	A
74	L5	2154	G
74	L5	2185	C
74	L5	2199	G
74	L5	2201	A
74	L5	2214	G
74	L5	2215	A
74	L5	2217	A
74	L5	2218	U
74	L5	2237	A
74	L5	2242	G
74	L5	2247	U
74	L5	2248	A
74	L5	2249	A
74	L5	2250	C
74	L5	2265	G
74	L5	2266	G
74	L5	2273	A
74	L5	2274	A2M
74	L5	2275	U
74	L5	2278	C
74	L5	2281	OMG
74	L5	2300	G
74	L5	2303	U
74	L5	2306	A
74	L5	2308	G
74	L5	2327	U
74	L5	2328	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	2329	U
74	L5	2366	A
74	L5	2367	C
74	L5	2368	G
74	L5	2386	G
74	L5	2390	A
74	L5	2394	A
74	L5	2395	A
74	L5	2396	G
74	L5	2397	A
74	L5	2404	U
74	L5	2415	C
74	L5	2416	U
74	L5	2417	A
74	L5	2428	G
74	L5	2507	U
74	L5	2508	A
74	L5	2516	A
74	L5	2517	U
74	L5	2537	U
74	L5	2538	A
74	L5	2539	C
74	L5	2540	A
74	L5	2545	C
74	L5	2546	A
74	L5	2547	A
74	L5	2558	C
74	L5	2560	U
74	L5	2563	G
74	L5	2566	G
74	L5	2570	A
74	L5	2571	C
74	L5	2583	G
74	L5	2584	G
74	L5	2591	G
74	L5	2596	OMG
74	L5	2603	A
74	L5	2625	G
74	L5	2628	G
74	L5	2629	U
74	L5	2632	C
74	L5	2633	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	2634	A
74	L5	2643	C
74	L5	2651	A
74	L5	2654	G
74	L5	2667	G
74	L5	2671	A
74	L5	2680	A
74	L5	2681	A
74	L5	2693	U
74	L5	2705	G
74	L5	2706	OMU
74	L5	2729	U
74	L5	2730	G
74	L5	2732	C
74	L5	2735	A
74	L5	2736	U
74	L5	2738	G
74	L5	2749	U
74	L5	2754	G
74	L5	2755	A
74	L5	2757	A
74	L5	2759	U
74	L5	2768	G
74	L5	2773	G
74	L5	2776	A
74	L5	2777	G
74	L5	2778	A
74	L5	2780	A
74	L5	2787	C
74	L5	2793	G
74	L5	2794	A
74	L5	2819	U
74	L5	2821	C
74	L5	2822	A
74	L5	2824	A
74	L5	2840	G
74	L5	2844	C
74	L5	2848	G
74	L5	2849	A
74	L5	2864	A
74	L5	2868	U
74	L5	2876	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	2898	UY1
74	L5	2900	PSU
74	L5	2907	G
74	L5	2912	U
74	L5	2913	A
74	L5	2919	C
74	L5	2923	A2M
74	L5	2924	G
74	L5	2928	G
74	L5	2932	PSU
74	L5	2945	G
74	L5	2948	A
74	L5	2960	C
74	L5	2967	G
74	L5	2973	C
74	L5	2987	A
74	L5	2988	A
74	L5	3005	A
74	L5	3006	G
74	L5	3033	A
74	L5	3034	U
74	L5	3035	G
74	L5	3036	C
74	L5	3045	G
74	L5	3050	G
74	L5	3054	G
74	L5	3062	A
74	L5	3068	C
74	L5	3069	C
74	L5	3070	A
74	L5	3077	G
74	L5	3093	C
74	L5	3098	A
74	L5	3106	A
74	L5	3107	U
74	L5	3110	A
74	L5	3128	U
74	L5	3129	C
74	L5	3131	C
74	L5	3139	G
74	L5	3152	G
74	L5	3154	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	L5	3158	U
74	L5	3170	A
74	L5	3174	U
74	L5	3179	C
74	L5	3192	U
74	L5	3193	U
74	L5	3194	C
74	L5	3195	C
74	L5	3196	G
74	L5	3197	A
74	L5	3200	C
74	L5	3201	A
74	L5	3203	A
74	L5	3206	U
74	L5	3207	C
74	L5	3211	U
74	L5	3212	C
74	L5	3217	G
74	L5	3218	A
74	L5	3224	A
74	L5	3234	U
74	L5	3246	A
74	L5	3248	G
74	L5	3262	U
74	L5	3267	G
74	L5	3268	C
74	L5	3269	G
74	L5	3272	A
74	L5	3273	G
74	L5	3296	G
74	L5	3302	C
74	L5	3305	C
74	L5	3310	A
74	L5	3311	G
74	L5	3313	G
74	L5	3326	U
75	S7	6	A
75	S7	10	G
75	S7	14	A
75	S7	21	U
75	S7	28	C
75	S7	29	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
75	S7	32	U
75	S7	44	G
75	S7	47	G
75	S7	50	G
75	S7	53	A
75	S7	56	U
75	S7	57	C
75	S7	58	G
75	S7	59	A
75	S7	65	A
75	S7	74	A
76	S1	17	C
76	S1	25	C
76	S1	34	G
76	S1	47	A
76	S1	50	C
76	S1	57	G
76	S1	65	A
76	S1	68	A
76	S1	102	C
76	S1	112	A
76	S1	113	G
76	S1	114	U
76	S1	128	G
76	S1	135	A
76	S1	139	A
76	S1	140	U
76	S1	147	G
76	S1	152	U
76	S1	165	A
76	S1	171	U
76	S1	173	G
76	S1	174	A
76	S1	187	G
76	S1	231	C
76	S1	245	G
76	S1	248	U
76	S1	251	C
76	S1	289	C
76	S1	291	G
76	S1	295	G
76	S1	302	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	S1	310	G
76	S1	311	C
76	S1	319	G
76	S1	332	A
76	S1	333	A
76	S1	334	C
76	S1	342	U
76	S1	353	U
76	S1	373	A
76	S1	374	A
76	S1	375	C
76	S1	377	G
76	S1	389	A
76	S1	391	G
76	S1	396	G
76	S1	397	C
76	S1	399	G
76	S1	407	G
76	S1	412	U
76	S1	417	C
76	S1	421	C
76	S1	433	A
76	S1	441	A
76	S1	442	C
76	S1	450	A
76	S1	473	U
76	S1	474	A
76	S1	476	U
76	S1	477	U
76	S1	479	G
76	S1	489	G
76	S1	496	A
76	S1	505	A
76	S1	507	A
76	S1	526	G
76	S1	530	G
76	S1	534	C
76	S1	537	G
76	S1	548	A
76	S1	549	A
76	S1	551	U
76	S1	554	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	S1	563	A
76	S1	564	G
76	S1	575	A
76	S1	579	G
76	S1	580	U
76	S1	588	A
76	S1	589	A
76	S1	591	A
76	S1	592	A
76	S1	593	G
76	S1	607	U
76	S1	608	U
76	S1	610	U
76	S1	613	G
76	S1	617	U
76	S1	618	G
76	S1	654	U
76	S1	655	U
76	S1	657	G
76	S1	658	G
76	S1	666	C
76	S1	670	U
76	S1	678	G
76	S1	682	A
76	S1	692	G
76	S1	693	U
76	S1	701	A
76	S1	702	G
76	S1	712	U
76	S1	713	U
76	S1	714	G
76	S1	716	A
76	S1	736	A
76	S1	737	G
76	S1	738	A
76	S1	739	G
76	S1	781	A
76	S1	784	G
76	S1	788	A
76	S1	811	U
76	S1	823	A
76	S1	824	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	S1	837	U
76	S1	838	A
76	S1	839	G
76	S1	846	U
76	S1	858	A
76	S1	860	U
76	S1	867	G
76	S1	885	U
76	S1	891	A
76	S1	917	A
76	S1	918	A
76	S1	929	U
76	S1	930	A
76	S1	935	C
76	S1	951	A
76	S1	953	C
76	S1	956	U
76	S1	957	G
76	S1	964	A
76	S1	965	G
76	S1	978	G
76	S1	979	U
76	S1	990	A
76	S1	1001	A
76	S1	1017	A
76	S1	1021	C
76	S1	1022	U
76	S1	1025	G
76	S1	1036	G
76	S1	1051	G
76	S1	1063	A
76	S1	1064	A
76	S1	1071	G
76	S1	1075	G
76	S1	1083	C
76	S1	1085	A
76	S1	1092	G
76	S1	1110	U
76	S1	1119	A
76	S1	1121	A
76	S1	1124	G
76	S1	1125	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	S1	1127	A
76	S1	1142	A
76	S1	1143	G
76	S1	1151	U
76	S1	1156	OMU
76	S1	1169	A
76	S1	1170	G
76	S1	1171	C
76	S1	1188	G
76	S1	1194	U
76	S1	1211	U
76	S1	1226	U
76	S1	1231	C
76	S1	1239	U
76	S1	1240	U
76	S1	1246	A
76	S1	1265	U
76	S1	1270	A
76	S1	1271	C
76	S1	1274	G
76	S1	1286	A
76	S1	1297	U
76	S1	1321	U
76	S1	1333	A
76	S1	1340	A
76	S1	1345	G
76	S1	1348	U
76	S1	1358	A
76	S1	1360	A
76	S1	1361	OMG
76	S1	1364	C
76	S1	1365	U
76	S1	1366	G
76	S1	1391	G
76	S1	1392	C
76	S1	1393	A
76	S1	1404	A
76	S1	1415	C
76	S1	1419	G
76	S1	1430	C
76	S1	1440	G
76	S1	1448	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	S1	1450	A
76	S1	1455	U
76	S1	1469	A
76	S1	1489	U
76	S1	1492	U
76	S1	1500	G
76	S1	1501	A
76	S1	1505	A
76	S1	1507	7MG
76	S1	1516	G
76	S1	1522	G
76	S1	1533	G
76	S1	1548	G
76	S1	1554	G
76	S1	1563	A
76	S1	1566	C
76	S1	1567	A
76	S1	1589	C
76	S1	1590	G
76	S1	1597	C
76	S1	1612	G
76	S1	1683	A
76	S1	1688	G
76	S1	1690	A
76	S1	1694	A
76	S1	1697	U
76	S1	1708	G
76	S1	1710	MA6
76	S1	1720	G
76	S1	1721	G
76	S1	1722	A
76	S1	1723	U
76	S1	1724	C
76	S1	1727	PSU

All (34) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L3	51	G
1	L3	71	G
1	L3	106	U
73	L4	42	G

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Mol	Chain	Res	Type
73	L4	123	C
73	L4	132	C
74	L5	117	G
74	L5	399	A
74	L5	515	G
74	L5	632	U
74	L5	748	A
74	L5	782	U
74	L5	882	C
74	L5	925	G
74	L5	943	G
74	L5	1873	G
74	L5	2095	C
74	L5	2106	A
74	L5	2200	A
74	L5	2249	A
74	L5	2820	U
74	L5	2867	A
74	L5	3097	U
74	L5	3194	C
74	L5	3217	G
76	S1	172	C
76	S1	294	U
76	S1	390	A
76	S1	665	C
76	S1	978	G
76	S1	989	G
76	S1	1210	U
76	S1	1269	A
76	S1	1500	G

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

65 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
74	1MA	L5	657	81,74	21,25,26	2.79	6 (28%)	30,37,40	2.68	7 (23%)
74	OMU	L5	2410	74	19,22,23	2.83	6 (31%)	25,31,34	1.90	7 (28%)
74	A2M	L5	661	74	22,25,26	3.53	9 (40%)	30,36,39	2.66	10 (33%)
74	PSU	L5	2842	74	18,21,22	2.26	7 (38%)	21,30,33	2.13	5 (23%)
74	PSU	L5	2921	81,83,74	18,21,22	2.27	7 (38%)	21,30,33	2.14	4 (19%)
76	4AC	S1	1701	76	21,24,25	3.06	10 (47%)	28,34,37	1.01	3 (10%)
74	PSU	L5	2581	74	18,21,22	2.28	6 (33%)	21,30,33	2.11	3 (14%)
76	PSU	S1	686	76	18,21,22	2.39	7 (38%)	21,30,33	2.16	4 (19%)
74	OMC	L5	2936	74	19,22,23	2.93	8 (42%)	25,31,34	0.72	0
74	OMG	L5	2792	74	23,26,27	2.36	8 (34%)	32,38,41	2.05	10 (31%)
74	OMU	L5	2712	74	19,22,23	2.85	6 (31%)	25,31,34	1.87	5 (20%)
74	OMG	L5	1872	74	23,26,27	2.38	8 (34%)	32,38,41	1.98	9 (28%)
74	OMC	L5	2856	74	19,22,23	2.91	8 (42%)	25,31,34	0.67	0
74	PSU	L5	2901	74	18,21,22	2.22	6 (33%)	21,30,33	2.07	5 (23%)
74	A2M	L5	2923	81,74	22,25,26	3.55	9 (40%)	30,36,39	2.65	11 (36%)
76	A2M	S1	899	76	22,25,26	3.59	9 (40%)	30,36,39	2.63	9 (30%)
74	OMG	L5	917	83,74	23,26,27	2.44	8 (34%)	32,38,41	2.06	10 (31%)
74	A2M	L5	658	74	22,25,26	3.53	9 (40%)	30,36,39	2.62	10 (33%)
76	PSU	S1	1106	76	18,21,22	2.51	8 (44%)	21,30,33	2.16	4 (19%)
76	OMU	S1	1156	76	19,22,23	2.75	6 (31%)	25,31,34	1.89	4 (16%)
74	PSU	L5	2932	74	18,21,22	2.26	6 (33%)	21,30,33	2.12	4 (19%)
74	PSU	L5	2831	74	18,21,22	2.24	6 (33%)	21,30,33	2.11	4 (19%)
76	PSU	S1	1215	76	18,21,22	2.44	7 (38%)	21,30,33	2.19	5 (23%)
76	OMU	S1	1309	76	19,22,23	2.68	6 (31%)	25,31,34	2.05	5 (20%)
74	UY1	L5	2898	81,74	19,22,23	4.35	8 (42%)	21,31,34	1.99	5 (23%)
76	OMG	S1	1361	76	23,26,27	2.34	7 (30%)	32,38,41	1.95	9 (28%)
74	OMG	L5	2281	74	23,26,27	2.37	8 (34%)	32,38,41	1.98	9 (28%)
76	7MG	S1	1507	76	23,26,27	3.16	10 (43%)	27,39,42	2.24	9 (33%)
76	MA6	S1	1710	76	23,26,27	1.49	4 (17%)	33,38,41	3.13	12 (36%)
74	UY1	L5	2414	74	19,22,23	4.27	8 (42%)	21,31,34	2.17	6 (28%)
76	OMG	S1	1196	76	23,26,27	2.33	8 (34%)	32,38,41	2.02	9 (28%)
74	PSU	L5	2897	81,74	18,21,22	2.27	6 (33%)	21,30,33	2.08	4 (19%)
74	OMG	L5	2899	74	23,26,27	2.42	9 (39%)	32,38,41	2.03	9 (28%)
72	IAS	SO	144	72	6,7,8	1.23	0	4,8,10	2.22	2 (50%)
74	OMG	L5	814	74	23,26,27	2.37	8 (34%)	32,38,41	2.07	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
73	OMG	L4	43	73	23,26,27	2.40	9 (39%)	32,38,41	2.04	9 (28%)
74	OMU	L5	2706	74	19,22,23	2.83	6 (31%)	25,31,34	1.86	5 (20%)
74	A2M	L5	945	74	22,25,26	3.52	9 (40%)	30,36,39	2.67	13 (43%)
76	A2M	S1	28	76	22,25,26	3.58	10 (45%)	30,36,39	2.64	10 (33%)
74	PSU	L5	2210	74	18,21,22	2.22	6 (33%)	21,30,33	2.10	3 (14%)
76	OMC	S1	1571	76	19,22,23	2.83	8 (42%)	25,31,34	0.74	0
76	PSU	S1	1112	76	18,21,22	2.49	7 (38%)	21,30,33	2.14	4 (19%)
74	A2M	L5	2319	74	22,25,26	3.51	9 (40%)	30,36,39	2.64	11 (36%)
74	PSU	L5	2257	74	18,21,22	2.33	6 (33%)	21,30,33	2.03	3 (14%)
74	PSU	L5	2259	74	18,21,22	2.19	6 (33%)	21,30,33	2.03	3 (14%)
74	OMG	L5	2596	74	23,26,27	2.43	7 (30%)	32,38,41	2.01	9 (28%)
74	PSU	L5	2803	74	18,21,22	2.27	7 (38%)	21,30,33	2.15	5 (23%)
74	A2M	L5	1158	74	22,25,26	3.58	10 (45%)	30,36,39	2.61	10 (33%)
74	PSU	L5	2952	74	18,21,22	2.28	6 (33%)	21,30,33	2.13	4 (19%)
76	MA6	S1	1709	76	23,26,27	1.47	5 (21%)	33,38,41	3.11	11 (33%)
76	PSU	S1	1560	76	18,21,22	2.53	8 (44%)	21,30,33	2.16	3 (14%)
74	PSU	L5	2857	74	18,21,22	2.30	7 (38%)	21,30,33	2.08	4 (19%)
76	PSU	S1	1727	76	18,21,22	2.43	8 (44%)	21,30,33	2.24	4 (19%)
74	5MC	L5	2847	83,74	19,22,23	4.03	9 (47%)	26,32,35	1.16	1 (3%)
74	A2M	L5	2274	74	22,25,26	3.44	9 (40%)	30,36,39	2.80	14 (46%)
76	OMU	S1	547	76	19,22,23	2.89	7 (36%)	25,31,34	1.85	5 (20%)
76	A2M	S1	83	76	22,25,26	3.54	9 (40%)	30,36,39	2.65	11 (36%)
74	A2M	L5	826	81,74	22,25,26	3.54	9 (40%)	30,36,39	2.62	11 (36%)
74	A2M	L5	1472	81,74	22,25,26	3.56	9 (40%)	30,36,39	2.87	14 (46%)
76	PSU	S1	1322	76	18,21,22	2.39	8 (44%)	21,30,33	2.15	6 (28%)
76	A2M	S1	1678	76	22,25,26	3.59	10 (45%)	30,36,39	2.64	9 (30%)
74	PSU	L5	2900	74	18,21,22	2.21	6 (33%)	21,30,33	2.02	3 (14%)
76	B8N	S1	1116	76	25,29,30	3.43	7 (28%)	28,42,45	2.01	8 (28%)
74	OMG	L5	2894	74	23,26,27	2.42	9 (39%)	32,38,41	2.05	9 (28%)
74	A2M	L5	2724	74	22,25,26	3.56	9 (40%)	30,36,39	2.68	13 (43%)

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
74	1MA	L5	657	81,74	-	2/7/25/26	0/3/3/3
74	OMU	L5	2410	74	-	2/9/27/28	0/2/2/2
74	A2M	L5	661	74	-	2/9/27/28	0/3/3/3
74	PSU	L5	2842	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	2921	81,83,74	-	0/7/25/26	0/2/2/2
76	4AC	S1	1701	76	-	0/11/29/30	0/2/2/2
74	PSU	L5	2581	74	-	0/7/25/26	0/2/2/2
76	PSU	S1	686	76	-	0/7/25/26	0/2/2/2
74	OMC	L5	2936	74	-	0/9/27/28	0/2/2/2
74	OMG	L5	2792	74	-	0/9/27/28	0/3/3/3
74	OMU	L5	2712	74	-	0/9/27/28	0/2/2/2
74	OMG	L5	1872	74	-	0/9/27/28	0/3/3/3
74	OMC	L5	2856	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	2901	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	2923	81,74	-	2/9/27/28	0/3/3/3
76	A2M	S1	899	76	-	0/9/27/28	0/3/3/3
74	OMG	L5	917	83,74	-	1/9/27/28	0/3/3/3
74	A2M	L5	658	74	-	2/9/27/28	0/3/3/3
76	PSU	S1	1106	76	-	0/7/25/26	0/2/2/2
76	OMU	S1	1156	76	-	2/9/27/28	0/2/2/2
74	PSU	L5	2932	74	-	2/7/25/26	0/2/2/2
74	PSU	L5	2831	74	-	0/7/25/26	0/2/2/2
76	PSU	S1	1215	76	-	0/7/25/26	0/2/2/2
76	OMU	S1	1309	76	-	2/9/27/28	0/2/2/2
74	UY1	L5	2898	81,74	-	4/9/27/28	0/2/2/2
76	OMG	S1	1361	76	-	1/9/27/28	0/3/3/3
74	OMG	L5	2281	74	-	2/9/27/28	0/3/3/3
76	7MG	S1	1507	76	-	0/7/37/38	0/3/3/3
76	MA6	S1	1710	76	-	2/11/29/30	0/3/3/3
74	UY1	L5	2414	74	-	1/9/27/28	0/2/2/2
76	OMG	S1	1196	76	-	1/9/27/28	0/3/3/3
74	PSU	L5	2897	81,74	-	2/7/25/26	0/2/2/2
74	OMG	L5	2899	74	-	1/9/27/28	0/3/3/3
72	IAS	SO	144	72	-	2/5/6/8	-
74	OMG	L5	814	74	-	0/9/27/28	0/3/3/3
73	OMG	L4	43	73	-	1/9/27/28	0/3/3/3
74	OMU	L5	2706	74	-	0/9/27/28	0/2/2/2
74	A2M	L5	945	74	-	0/9/27/28	0/3/3/3
76	A2M	S1	28	76	-	0/9/27/28	0/3/3/3
74	PSU	L5	2210	74	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	OMC	S1	1571	76	-	0/9/27/28	0/2/2/2
76	PSU	S1	1112	76	-	0/7/25/26	0/2/2/2
74	A2M	L5	2319	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	2257	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	2259	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	2596	74	-	3/9/27/28	0/3/3/3
74	PSU	L5	2803	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	1158	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	2952	74	-	0/7/25/26	0/2/2/2
76	MA6	S1	1709	76	-	0/11/29/30	0/3/3/3
76	PSU	S1	1560	76	-	0/7/25/26	0/2/2/2
74	PSU	L5	2857	74	-	0/7/25/26	0/2/2/2
76	PSU	S1	1727	76	-	2/7/25/26	0/2/2/2
74	5MC	L5	2847	83,74	-	3/7/25/26	0/2/2/2
74	A2M	L5	2274	74	-	2/9/27/28	0/3/3/3
76	OMU	S1	547	76	-	0/9/27/28	0/2/2/2
76	A2M	S1	83	76	-	2/9/27/28	0/3/3/3
74	A2M	L5	826	81,74	-	1/9/27/28	0/3/3/3
74	A2M	L5	1472	81,74	-	0/9/27/28	0/3/3/3
76	PSU	S1	1322	76	-	2/7/25/26	0/2/2/2
76	A2M	S1	1678	76	-	0/9/27/28	0/3/3/3
74	PSU	L5	2900	74	-	3/7/25/26	0/2/2/2
76	B8N	S1	1116	76	-	4/16/34/35	0/2/2/2
74	OMG	L5	2894	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	2724	74	-	2/9/27/28	0/3/3/3

All (487) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2898	UY1	C6-C5	11.37	1.47	1.35
74	L5	2414	UY1	C6-C5	11.05	1.47	1.35
74	L5	2898	UY1	C2-N1	9.77	1.49	1.36
74	L5	2414	UY1	C2-N1	9.61	1.49	1.36
74	L5	1472	A2M	C2'-C1'	-9.48	1.29	1.53
74	L5	2847	5MC	C6-C5	9.41	1.49	1.34
76	S1	28	A2M	C2'-C1'	-9.34	1.30	1.53
74	L5	826	A2M	C2'-C1'	-9.30	1.30	1.53
74	L5	2724	A2M	C2'-C1'	-9.30	1.30	1.53
76	S1	1678	A2M	C2'-C1'	-9.28	1.30	1.53
74	L5	1158	A2M	C2'-C1'	-9.26	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	661	A2M	C2'-C1'	-9.25	1.30	1.53
74	L5	2923	A2M	C2'-C1'	-9.23	1.30	1.53
76	S1	899	A2M	C2'-C1'	-9.22	1.30	1.53
76	S1	83	A2M	C2'-C1'	-9.15	1.30	1.53
74	L5	658	A2M	C2'-C1'	-9.11	1.30	1.53
74	L5	945	A2M	C2'-C1'	-9.04	1.30	1.53
74	L5	2274	A2M	C2'-C1'	-8.99	1.31	1.53
74	L5	2319	A2M	C2'-C1'	-8.97	1.31	1.53
74	L5	1472	A2M	O4'-C1'	8.84	1.62	1.42
76	S1	1116	B8N	C4-N3	-8.74	1.25	1.40
74	L5	1158	A2M	O4'-C1'	8.63	1.61	1.42
74	L5	2724	A2M	O4'-C1'	8.56	1.61	1.42
76	S1	899	A2M	O4'-C1'	8.55	1.61	1.42
74	L5	2923	A2M	O4'-C1'	8.54	1.61	1.42
74	L5	2319	A2M	O4'-C1'	8.53	1.61	1.42
76	S1	83	A2M	O4'-C1'	8.52	1.61	1.42
74	L5	826	A2M	O4'-C1'	8.51	1.61	1.42
76	S1	1678	A2M	O4'-C1'	8.50	1.61	1.42
74	L5	657	1MA	C2-N3	8.46	1.46	1.30
74	L5	945	A2M	O4'-C1'	8.45	1.61	1.42
74	L5	661	A2M	O4'-C1'	8.42	1.61	1.42
74	L5	658	A2M	O4'-C1'	8.37	1.61	1.42
74	L5	2847	5MC	C5-C4	8.35	1.50	1.44
76	S1	28	A2M	O4'-C1'	8.28	1.61	1.42
74	L5	2274	A2M	O4'-C1'	8.19	1.60	1.42
76	S1	1116	B8N	C6-N1	7.69	1.55	1.36
76	S1	1507	7MG	C8-N9	7.45	1.50	1.45
74	L5	2898	UY1	C2-N3	7.29	1.49	1.37
76	S1	1116	B8N	C4-C5	7.28	1.64	1.47
74	L5	2414	UY1	C2-N3	7.19	1.49	1.37
74	L5	2712	OMU	C2-N1	6.83	1.49	1.38
76	S1	547	OMU	C2-N1	6.83	1.49	1.38
74	L5	658	A2M	O4'-C4'	-6.80	1.29	1.45
76	S1	1678	A2M	O4'-C4'	-6.74	1.30	1.45
76	S1	899	A2M	O4'-C4'	-6.74	1.30	1.45
76	S1	28	A2M	O4'-C4'	-6.72	1.30	1.45
76	S1	83	A2M	O4'-C4'	-6.70	1.30	1.45
74	L5	657	1MA	C4-N3	6.68	1.49	1.35
74	L5	2410	OMU	C2-N1	6.68	1.48	1.38
74	L5	945	A2M	O4'-C4'	-6.66	1.30	1.45
74	L5	661	A2M	O4'-C4'	-6.62	1.30	1.45
74	L5	2706	OMU	C2-N1	6.62	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	1158	A2M	O4'-C4'	-6.57	1.30	1.45
74	L5	2596	OMG	C4-N3	6.57	1.49	1.34
76	S1	547	OMU	C2-N3	6.56	1.49	1.38
74	L5	826	A2M	O4'-C4'	-6.55	1.30	1.45
76	S1	1560	PSU	C2-N1	-6.54	1.28	1.36
74	L5	2923	A2M	O4'-C4'	-6.52	1.30	1.45
74	L5	2724	A2M	O4'-C4'	-6.49	1.30	1.45
74	L5	2894	OMG	C4-N3	6.47	1.49	1.34
76	S1	1701	4AC	C4-N3	6.45	1.43	1.32
74	L5	2281	OMG	C4-N3	6.45	1.49	1.34
74	L5	2706	OMU	C2-N3	6.45	1.49	1.38
74	L5	917	OMG	C4-N3	6.44	1.49	1.34
76	S1	1156	OMU	C2-N1	6.44	1.48	1.38
74	L5	1472	A2M	O4'-C4'	-6.44	1.30	1.45
74	L5	2410	OMU	C2-N3	6.44	1.49	1.38
74	L5	2319	A2M	O4'-C4'	-6.43	1.30	1.45
74	L5	2712	OMU	C2-N3	6.40	1.49	1.38
74	L5	1872	OMG	C4-N3	6.40	1.48	1.34
74	L5	2899	OMG	C4-N3	6.39	1.48	1.34
73	L4	43	OMG	C4-N3	6.38	1.48	1.34
74	L5	2274	A2M	O4'-C4'	-6.33	1.30	1.45
76	S1	1727	PSU	C2-N1	-6.31	1.28	1.36
74	L5	2792	OMG	C4-N3	6.31	1.48	1.34
74	L5	2847	5MC	C2-N3	6.30	1.48	1.36
76	S1	1215	PSU	C2-N1	-6.30	1.28	1.36
74	L5	2936	OMC	C2-N3	6.29	1.48	1.36
74	L5	814	OMG	C4-N3	6.27	1.48	1.34
76	S1	1106	PSU	C2-N1	-6.26	1.28	1.36
76	S1	1112	PSU	C2-N1	-6.24	1.28	1.36
74	L5	2856	OMC	C2-N3	6.24	1.48	1.36
76	S1	1309	OMU	C2-N1	6.23	1.48	1.38
76	S1	1322	PSU	C2-N1	-6.23	1.28	1.36
76	S1	1116	B8N	C2-N1	6.17	1.57	1.39
76	S1	1361	OMG	C4-N3	6.14	1.48	1.34
76	S1	1196	OMG	C4-N3	6.11	1.48	1.34
74	L5	2257	PSU	C2-N1	-6.11	1.28	1.36
76	S1	1571	OMC	C2-N3	6.10	1.48	1.36
76	S1	1156	OMU	C2-N3	6.05	1.48	1.38
76	S1	686	PSU	C2-N1	-6.02	1.28	1.36
76	S1	1701	4AC	C6-C5	6.00	1.49	1.35
74	L5	2936	OMC	C6-C5	5.95	1.48	1.35
74	L5	2847	5MC	C4-N3	5.89	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	1309	OMU	C2-N3	5.87	1.48	1.38
74	L5	2856	OMC	C6-C5	5.87	1.48	1.35
74	L5	2857	PSU	C2-N1	-5.83	1.29	1.36
74	L5	2581	PSU	C2-N1	-5.81	1.29	1.36
76	S1	1571	OMC	C6-C5	5.79	1.48	1.35
74	L5	2900	PSU	C2-N1	-5.79	1.29	1.36
76	S1	1116	B8N	C6-C5	5.76	1.43	1.35
74	L5	2932	PSU	C2-N1	-5.76	1.29	1.36
74	L5	2901	PSU	C2-N1	-5.75	1.29	1.36
74	L5	2210	PSU	C2-N1	-5.74	1.29	1.36
74	L5	2803	PSU	C2-N1	-5.73	1.29	1.36
74	L5	2259	PSU	C2-N1	-5.73	1.29	1.36
76	S1	547	OMU	C6-C5	5.72	1.48	1.35
74	L5	2952	PSU	C2-N1	-5.71	1.29	1.36
74	L5	2842	PSU	C2-N1	-5.71	1.29	1.36
76	S1	1507	7MG	C5-N7	5.68	1.42	1.35
74	L5	2897	PSU	C2-N1	-5.67	1.29	1.36
74	L5	2712	OMU	C6-C5	5.64	1.48	1.35
74	L5	2706	OMU	C6-C5	5.64	1.48	1.35
74	L5	2410	OMU	C6-C5	5.63	1.48	1.35
74	L5	2921	PSU	C2-N1	-5.62	1.29	1.36
74	L5	2831	PSU	C2-N1	-5.61	1.29	1.36
76	S1	1156	OMU	C6-C5	5.55	1.47	1.35
74	L5	2596	OMG	C2-N3	5.45	1.46	1.33
74	L5	917	OMG	C2-N3	5.40	1.46	1.33
76	S1	1507	7MG	C2-N3	5.40	1.46	1.33
76	S1	1701	4AC	C2-N3	5.40	1.47	1.36
76	S1	1507	7MG	C4-N3	5.36	1.46	1.34
74	L5	2899	OMG	C2-N3	5.36	1.46	1.33
74	L5	2894	OMG	C2-N3	5.32	1.46	1.33
76	S1	1309	OMU	C6-C5	5.28	1.47	1.35
73	L4	43	OMG	C2-N3	5.22	1.45	1.33
74	L5	1872	OMG	C2-N3	5.22	1.45	1.33
74	L5	2792	OMG	C2-N3	5.22	1.45	1.33
74	L5	814	OMG	C2-N3	5.17	1.45	1.33
74	L5	2281	OMG	C2-N3	5.14	1.45	1.33
74	L5	2414	UY1	C1'-C5	-5.14	1.38	1.50
74	L5	2847	5MC	C2-N1	5.12	1.50	1.40
74	L5	2898	UY1	C6-N1	5.04	1.44	1.36
76	S1	1196	OMG	C2-N3	4.98	1.45	1.33
74	L5	2936	OMC	C4-N3	4.92	1.44	1.34
74	L5	2414	UY1	C6-N1	4.92	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2856	OMC	C4-N3	4.92	1.44	1.34
74	L5	2898	UY1	C1'-C5	-4.88	1.39	1.50
76	S1	1361	OMG	C2-N3	4.75	1.44	1.33
74	L5	917	OMG	C2-N2	4.75	1.45	1.34
74	L5	2899	OMG	C2-N2	4.69	1.45	1.34
74	L5	2894	OMG	C2-N2	4.68	1.45	1.34
74	L5	2936	OMC	C4-N4	4.68	1.45	1.33
73	L4	43	OMG	C2-N2	4.67	1.45	1.34
74	L5	2856	OMC	C4-N4	4.67	1.45	1.33
74	L5	2596	OMG	C2-N2	4.65	1.45	1.34
76	S1	1571	OMC	C4-N3	4.65	1.43	1.34
76	S1	1507	7MG	C2-N2	4.64	1.45	1.34
74	L5	2847	5MC	C6-N1	4.51	1.45	1.38
74	L5	814	OMG	C2-N2	4.51	1.44	1.34
74	L5	2281	OMG	C2-N2	4.47	1.44	1.34
74	L5	1872	OMG	C2-N2	4.47	1.44	1.34
76	S1	1571	OMC	C4-N4	4.46	1.44	1.33
76	S1	1701	4AC	C4-N4	4.41	1.46	1.39
74	L5	2792	OMG	C2-N2	4.37	1.44	1.34
76	S1	1196	OMG	C2-N2	4.34	1.44	1.34
74	L5	2724	A2M	C6-N6	4.31	1.45	1.34
76	S1	1361	OMG	C2-N2	4.29	1.44	1.34
76	S1	1560	PSU	C4-N3	-4.28	1.30	1.38
76	S1	1701	4AC	C7-N4	4.28	1.45	1.37
76	S1	1112	PSU	C4-N3	-4.28	1.30	1.38
74	L5	945	A2M	C6-N6	4.27	1.45	1.34
74	L5	658	A2M	C6-N6	4.26	1.45	1.34
76	S1	1507	7MG	C4-N9	4.26	1.43	1.37
74	L5	2319	A2M	C6-N6	4.26	1.45	1.34
76	S1	1106	PSU	C4-N3	-4.24	1.30	1.38
74	L5	826	A2M	C6-N6	4.24	1.45	1.34
74	L5	2923	A2M	C6-N6	4.24	1.45	1.34
74	L5	661	A2M	C6-N6	4.23	1.45	1.34
74	L5	1472	A2M	C6-N6	4.23	1.45	1.34
74	L5	2847	5MC	C4-N4	4.23	1.44	1.34
74	L5	1158	A2M	C6-N6	4.22	1.45	1.34
76	S1	1215	PSU	C4-N3	-4.16	1.31	1.38
74	L5	2274	A2M	C6-N6	4.16	1.44	1.34
76	S1	1106	PSU	O4-C4	-4.14	1.15	1.23
76	S1	28	A2M	C6-N6	4.14	1.44	1.34
76	S1	1678	A2M	C6-N6	4.13	1.44	1.34
74	L5	2936	OMC	C2-N1	4.13	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	83	A2M	C6-N6	4.13	1.44	1.34
76	S1	686	PSU	C4-N3	-4.12	1.31	1.38
74	L5	2856	OMC	C2-N1	4.12	1.48	1.40
76	S1	1571	OMC	C2-N1	4.09	1.48	1.40
76	S1	1560	PSU	O4-C4	-4.08	1.15	1.23
76	S1	899	A2M	C6-N6	4.03	1.44	1.34
76	S1	1112	PSU	O4-C4	-3.99	1.16	1.23
76	S1	1727	PSU	C4-N3	-3.98	1.31	1.38
74	L5	657	1MA	C2-N1	3.96	1.44	1.35
76	S1	686	PSU	O4-C4	-3.90	1.16	1.23
76	S1	1322	PSU	C4-N3	-3.87	1.31	1.38
74	L5	2921	PSU	C4-N3	-3.86	1.31	1.38
76	S1	1215	PSU	O4-C4	-3.86	1.16	1.23
74	L5	2952	PSU	C4-N3	-3.83	1.31	1.38
74	L5	2257	PSU	O4-C4	-3.80	1.16	1.23
76	S1	1322	PSU	O4-C4	-3.79	1.16	1.23
74	L5	2897	PSU	C4-N3	-3.79	1.31	1.38
74	L5	2842	PSU	C4-N3	-3.78	1.31	1.38
76	S1	1116	B8N	O4-C4	-3.77	1.15	1.23
74	L5	2921	PSU	O4-C4	-3.76	1.16	1.23
74	L5	2952	PSU	O4-C4	-3.76	1.16	1.23
74	L5	2831	PSU	C4-N3	-3.75	1.31	1.38
76	S1	1361	OMG	C5-N7	-3.75	1.31	1.39
74	L5	2581	PSU	C4-N3	-3.75	1.31	1.38
74	L5	2257	PSU	C4-N3	-3.74	1.31	1.38
74	L5	2897	PSU	O4-C4	-3.74	1.16	1.23
74	L5	2803	PSU	C4-N3	-3.74	1.31	1.38
76	S1	1727	PSU	O4-C4	-3.74	1.16	1.23
74	L5	2581	PSU	O4-C4	-3.73	1.16	1.23
74	L5	2857	PSU	C4-N3	-3.72	1.31	1.38
74	L5	2932	PSU	C4-N3	-3.72	1.31	1.38
74	L5	2857	PSU	O4-C4	-3.72	1.16	1.23
74	L5	657	1MA	C5-C6	3.70	1.53	1.43
74	L5	2842	PSU	O4-C4	-3.70	1.16	1.23
74	L5	2831	PSU	O4-C4	-3.69	1.16	1.23
74	L5	2803	PSU	O4-C4	-3.69	1.16	1.23
74	L5	2932	PSU	O4-C4	-3.68	1.16	1.23
76	S1	899	A2M	C5-C4	-3.64	1.32	1.39
76	S1	1710	MA6	C5-C4	-3.63	1.32	1.39
74	L5	2901	PSU	O4-C4	-3.63	1.16	1.23
74	L5	2900	PSU	C4-N3	-3.61	1.32	1.38
74	L5	2210	PSU	C4-N3	-3.60	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	1507	7MG	C2-N1	3.59	1.46	1.37
74	L5	2210	PSU	O4-C4	-3.59	1.16	1.23
76	S1	28	A2M	C5-C4	-3.58	1.32	1.39
74	L5	2900	PSU	O4-C4	-3.56	1.16	1.23
74	L5	2259	PSU	C4-N3	-3.55	1.32	1.38
74	L5	2898	UY1	C4-N3	3.54	1.45	1.38
74	L5	2259	PSU	O4-C4	-3.54	1.16	1.23
74	L5	2901	PSU	C4-N3	-3.52	1.32	1.38
76	S1	547	OMU	C4-N3	3.51	1.44	1.38
76	S1	1112	PSU	C2-N3	-3.50	1.31	1.37
76	S1	1196	OMG	C5-N7	-3.50	1.32	1.39
76	S1	1560	PSU	C2-N3	-3.49	1.31	1.37
76	S1	1678	A2M	C5-C4	-3.46	1.32	1.39
74	L5	917	OMG	C5-N7	-3.44	1.32	1.39
76	S1	1701	4AC	C5-C4	3.40	1.48	1.41
74	L5	2274	A2M	C5-C4	-3.40	1.33	1.39
74	L5	2281	OMG	C5-N7	-3.39	1.32	1.39
74	L5	2414	UY1	C4-N3	3.39	1.45	1.38
76	S1	1709	MA6	C5-C4	-3.38	1.33	1.39
76	S1	1106	PSU	C2-N3	-3.38	1.31	1.37
74	L5	1872	OMG	C5-N7	-3.37	1.32	1.39
74	L5	2319	A2M	C5-C4	-3.35	1.33	1.39
76	S1	1215	PSU	C2-N3	-3.34	1.32	1.37
76	S1	1309	OMU	O4-C4	-3.31	1.18	1.24
74	L5	1158	A2M	C5-C4	-3.31	1.33	1.39
74	L5	661	A2M	C5-C4	-3.31	1.33	1.39
74	L5	826	A2M	C5-C4	-3.31	1.33	1.39
76	S1	899	A2M	C5-N7	-3.30	1.33	1.39
74	L5	1472	A2M	C5-C4	-3.29	1.33	1.39
76	S1	83	A2M	C5-C4	-3.29	1.33	1.39
76	S1	1727	PSU	C2-N3	-3.28	1.32	1.37
74	L5	2724	A2M	C5-C4	-3.28	1.33	1.39
74	L5	2596	OMG	C5-N7	-3.27	1.32	1.39
76	S1	1701	4AC	C2-N1	3.27	1.46	1.40
74	L5	2923	A2M	C5-C4	-3.26	1.33	1.39
73	L4	43	OMG	C5-N7	-3.26	1.32	1.39
76	S1	1701	4AC	O2-C2	-3.25	1.17	1.23
74	L5	2792	OMG	C5-N7	-3.25	1.32	1.39
74	L5	658	A2M	C5-C4	-3.24	1.33	1.39
76	S1	1710	MA6	C6-N6	3.23	1.45	1.36
74	L5	2899	OMG	C5-N7	-3.23	1.32	1.39
74	L5	2894	OMG	C5-N7	-3.23	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	1309	OMU	O2-C2	-3.23	1.17	1.23
74	L5	945	A2M	C5-C4	-3.22	1.33	1.39
74	L5	2712	OMU	C4-N3	3.22	1.44	1.38
76	S1	1156	OMU	O4-C4	-3.22	1.18	1.24
74	L5	814	OMG	C5-N7	-3.20	1.32	1.39
74	L5	2706	OMU	C4-N3	3.19	1.44	1.38
76	S1	1709	MA6	C6-N6	3.19	1.45	1.36
76	S1	28	A2M	O3'-C3'	-3.15	1.35	1.43
76	S1	28	A2M	C5-N7	-3.15	1.33	1.39
76	S1	686	PSU	C2-N3	-3.13	1.32	1.37
76	S1	1571	OMC	O2-C2	-3.11	1.17	1.23
74	L5	2410	OMU	C4-N3	3.11	1.43	1.38
74	L5	2936	OMC	O2-C2	-3.10	1.17	1.23
76	S1	1678	A2M	C5-N7	-3.09	1.33	1.39
74	L5	1158	A2M	O3'-C3'	-3.08	1.35	1.43
74	L5	658	A2M	O3'-C3'	-3.07	1.35	1.43
74	L5	2724	A2M	O2'-C2'	3.07	1.50	1.42
74	L5	945	A2M	O3'-C3'	-3.06	1.35	1.43
76	S1	899	A2M	O3'-C3'	-3.06	1.35	1.43
76	S1	1678	A2M	O3'-C3'	-3.06	1.35	1.43
74	L5	2923	A2M	O3'-C3'	-3.04	1.35	1.43
74	L5	945	A2M	O2'-C2'	3.03	1.50	1.42
76	S1	1322	PSU	C2-N3	-3.02	1.32	1.37
76	S1	1156	OMU	O2-C2	-3.02	1.17	1.23
74	L5	1158	A2M	C5-N7	-3.01	1.33	1.39
76	S1	1106	PSU	C4-C5	-3.01	1.36	1.44
76	S1	83	A2M	C5-N7	-3.01	1.33	1.39
74	L5	826	A2M	C5-N7	-3.01	1.33	1.39
74	L5	2923	A2M	C5-N7	-3.00	1.33	1.39
76	S1	1112	PSU	C4-C5	-3.00	1.36	1.44
74	L5	658	A2M	O2'-C2'	2.99	1.50	1.42
74	L5	1472	A2M	C5-N7	-2.99	1.33	1.39
74	L5	2856	OMC	O2-C2	-2.99	1.18	1.23
74	L5	2319	A2M	O3'-C3'	-2.99	1.35	1.43
76	S1	1678	A2M	O2'-C2'	2.99	1.50	1.42
74	L5	2897	PSU	C2-N3	-2.99	1.32	1.37
76	S1	1710	MA6	C5-N7	-2.98	1.33	1.39
74	L5	2410	OMU	O2-C2	-2.98	1.17	1.23
74	L5	2706	OMU	O2-C2	-2.97	1.17	1.23
76	S1	1322	PSU	C4-C5	-2.97	1.36	1.44
74	L5	661	A2M	C5-N7	-2.96	1.33	1.39
76	S1	83	A2M	O3'-C3'	-2.96	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	1361	OMG	O6-C6	-2.95	1.18	1.23
74	L5	2952	PSU	C2-N3	-2.95	1.32	1.37
76	S1	83	A2M	O2'-C2'	2.94	1.49	1.42
74	L5	2936	OMC	C6-N1	2.94	1.45	1.38
74	L5	2319	A2M	O2'-C2'	2.94	1.49	1.42
74	L5	1158	A2M	O2'-C2'	2.94	1.49	1.42
76	S1	1507	7MG	O6-C6	-2.93	1.18	1.23
74	L5	658	A2M	C5-N7	-2.93	1.33	1.39
74	L5	2898	UY1	O4-C4	-2.92	1.18	1.23
74	L5	2921	PSU	C2-N3	-2.92	1.32	1.37
74	L5	2410	OMU	O4-C4	-2.91	1.18	1.24
76	S1	1560	PSU	C4-C5	-2.91	1.36	1.44
74	L5	2259	PSU	C6-C5	2.91	1.38	1.35
74	L5	2319	A2M	C5-N7	-2.91	1.33	1.39
74	L5	661	A2M	O3'-C3'	-2.91	1.35	1.43
74	L5	2857	PSU	C2-N3	-2.91	1.32	1.37
76	S1	686	PSU	C4-C5	-2.90	1.36	1.44
74	L5	945	A2M	C5-N7	-2.90	1.33	1.39
76	S1	1196	OMG	O6-C6	-2.90	1.18	1.23
74	L5	2724	A2M	O3'-C3'	-2.90	1.35	1.43
76	S1	899	A2M	O2'-C2'	2.90	1.49	1.42
76	S1	547	OMU	O2-C2	-2.89	1.17	1.23
74	L5	2712	OMU	O2-C2	-2.89	1.17	1.23
74	L5	2724	A2M	C5-N7	-2.89	1.33	1.39
76	S1	1156	OMU	C4-N3	2.89	1.43	1.38
76	S1	1507	7MG	C5-C6	2.88	1.50	1.43
74	L5	661	A2M	O2'-C2'	2.88	1.49	1.42
74	L5	2274	A2M	C5-N7	-2.87	1.33	1.39
76	S1	28	A2M	O2'-C2'	2.87	1.49	1.42
74	L5	2210	PSU	C6-C5	2.87	1.38	1.35
74	L5	2581	PSU	C2-N3	-2.87	1.32	1.37
74	L5	2856	OMC	C6-N1	2.87	1.44	1.38
74	L5	2706	OMU	O4-C4	-2.87	1.18	1.24
74	L5	657	1MA	C5-N7	-2.87	1.33	1.39
76	S1	1709	MA6	C5-N7	-2.87	1.33	1.39
74	L5	826	A2M	O3'-C3'	-2.86	1.35	1.43
76	S1	899	A2M	C8-N9	-2.85	1.32	1.37
74	L5	2923	A2M	O2'-C2'	2.85	1.49	1.42
74	L5	2803	PSU	C2-N3	-2.85	1.32	1.37
74	L5	2842	PSU	C2-N3	-2.84	1.32	1.37
74	L5	2712	OMU	O4-C4	-2.84	1.19	1.24
74	L5	2831	PSU	C6-C5	2.83	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S1	1507	7MG	C6-N1	2.83	1.44	1.38
74	L5	2257	PSU	C2-N3	-2.83	1.32	1.37
76	S1	28	A2M	C8-N9	-2.82	1.32	1.37
74	L5	2257	PSU	C4-C5	-2.82	1.36	1.44
74	L5	2581	PSU	C6-C5	2.82	1.38	1.35
74	L5	2932	PSU	C2-N3	-2.81	1.32	1.37
74	L5	2210	PSU	C2-N3	-2.80	1.32	1.37
74	L5	2900	PSU	C2-N3	-2.79	1.32	1.37
74	L5	2792	OMG	O6-C6	-2.78	1.18	1.23
76	S1	1701	4AC	C6-N1	2.78	1.44	1.38
74	L5	2831	PSU	C2-N3	-2.78	1.32	1.37
74	L5	2274	A2M	O3'-C3'	-2.76	1.36	1.43
74	L5	2842	PSU	C6-C5	2.76	1.38	1.35
76	S1	1571	OMC	C6-N1	2.75	1.44	1.38
74	L5	2932	PSU	C6-C5	2.75	1.38	1.35
76	S1	1215	PSU	C4-C5	-2.74	1.36	1.44
74	L5	2901	PSU	C6-C5	2.74	1.38	1.35
76	S1	1701	4AC	O7-C7	-2.74	1.17	1.23
74	L5	1872	OMG	O6-C6	-2.74	1.18	1.23
73	L4	43	OMG	O6-C6	-2.74	1.18	1.23
74	L5	2274	A2M	O2'-C2'	2.73	1.49	1.42
74	L5	2952	PSU	C6-C5	2.73	1.38	1.35
74	L5	2281	OMG	O6-C6	-2.73	1.18	1.23
76	S1	1678	A2M	C8-N9	-2.72	1.32	1.37
74	L5	2414	UY1	O4-C4	-2.72	1.18	1.23
74	L5	2803	PSU	C6-C5	2.72	1.38	1.35
74	L5	2921	PSU	C6-C5	2.71	1.38	1.35
74	L5	814	OMG	O6-C6	-2.71	1.18	1.23
74	L5	2857	PSU	C6-C5	2.71	1.38	1.35
74	L5	2899	OMG	O6-C6	-2.70	1.18	1.23
74	L5	2894	OMG	O6-C6	-2.70	1.18	1.23
74	L5	2596	OMG	O6-C6	-2.69	1.18	1.23
74	L5	2897	PSU	C6-C5	2.69	1.38	1.35
74	L5	826	A2M	O2'-C2'	2.68	1.49	1.42
76	S1	547	OMU	O4-C4	-2.67	1.19	1.24
74	L5	2259	PSU	C2-N3	-2.67	1.33	1.37
74	L5	2901	PSU	C2-N3	-2.67	1.33	1.37
74	L5	917	OMG	O6-C6	-2.66	1.18	1.23
74	L5	2803	PSU	C4-C5	-2.65	1.37	1.44
76	S1	83	A2M	C8-N9	-2.65	1.33	1.37
74	L5	2952	PSU	C4-C5	-2.64	1.37	1.44
74	L5	2900	PSU	C6-C5	2.64	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	826	A2M	C8-N9	-2.64	1.33	1.37
74	L5	2257	PSU	C6-C5	2.64	1.38	1.35
74	L5	1158	A2M	C8-N9	-2.62	1.33	1.37
74	L5	2831	PSU	C4-C5	-2.61	1.37	1.44
74	L5	2897	PSU	C4-C5	-2.61	1.37	1.44
76	S1	1710	MA6	C8-N9	-2.60	1.33	1.37
74	L5	2901	PSU	C4-C5	-2.60	1.37	1.44
74	L5	2724	A2M	C8-N9	-2.59	1.33	1.37
74	L5	2581	PSU	C4-C5	-2.59	1.37	1.44
74	L5	2921	PSU	C4-C5	-2.58	1.37	1.44
76	S1	1309	OMU	C4-N3	2.58	1.43	1.38
74	L5	2932	PSU	C4-C5	-2.58	1.37	1.44
74	L5	2857	PSU	C4-C5	-2.57	1.37	1.44
76	S1	1709	MA6	C8-N9	-2.56	1.33	1.37
76	S1	1361	OMG	C4-N9	-2.56	1.31	1.38
74	L5	1472	A2M	O2'-C2'	2.56	1.48	1.42
74	L5	2319	A2M	C8-N9	-2.55	1.33	1.37
74	L5	2842	PSU	C4-C5	-2.54	1.37	1.44
74	L5	917	OMG	C2-N1	2.53	1.43	1.37
74	L5	661	A2M	C8-N9	-2.53	1.33	1.37
74	L5	1472	A2M	C8-N9	-2.52	1.33	1.37
74	L5	2899	OMG	C2-N1	2.52	1.43	1.37
74	L5	2923	A2M	C8-N9	-2.52	1.33	1.37
74	L5	2596	OMG	C2-N1	2.51	1.43	1.37
74	L5	2210	PSU	C4-C5	-2.50	1.37	1.44
74	L5	945	A2M	C8-N9	-2.47	1.33	1.37
74	L5	658	A2M	C8-N9	-2.44	1.33	1.37
76	S1	1727	PSU	C6-N1	-2.44	1.32	1.36
76	S1	1727	PSU	C4-C5	-2.43	1.37	1.44
74	L5	814	OMG	C2-N1	2.43	1.43	1.37
74	L5	2900	PSU	C4-C5	-2.42	1.37	1.44
74	L5	2894	OMG	C2-N1	2.41	1.43	1.37
74	L5	2259	PSU	C4-C5	-2.40	1.37	1.44
76	S1	1727	PSU	O4'-C1'	-2.40	1.40	1.43
74	L5	2274	A2M	C8-N9	-2.37	1.33	1.37
74	L5	2792	OMG	C2-N1	2.37	1.43	1.37
73	L4	43	OMG	C2-N1	2.37	1.43	1.37
74	L5	2856	OMC	C5-C4	2.37	1.48	1.42
74	L5	2414	UY1	O2-C2	-2.36	1.18	1.23
76	S1	1196	OMG	C4-N9	-2.35	1.32	1.38
76	S1	686	PSU	C6-C5	2.32	1.37	1.35
74	L5	2792	OMG	C5-C6	2.31	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2281	OMG	C2-N1	2.31	1.43	1.37
74	L5	2936	OMC	C5-C4	2.30	1.48	1.42
74	L5	2899	OMG	C5-C6	2.29	1.53	1.44
74	L5	814	OMG	C4-N9	-2.29	1.32	1.38
74	L5	1872	OMG	C2-N1	2.28	1.43	1.37
76	S1	1215	PSU	C6-C5	2.28	1.37	1.35
76	S1	1112	PSU	C6-N1	-2.27	1.32	1.36
74	L5	2596	OMG	C5-C6	2.27	1.52	1.44
74	L5	2894	OMG	C5-C6	2.27	1.52	1.44
74	L5	814	OMG	C5-C6	2.26	1.52	1.44
74	L5	2898	UY1	O2-C2	-2.25	1.18	1.23
74	L5	1872	OMG	C5-C6	2.25	1.52	1.44
74	L5	917	OMG	C5-C6	2.25	1.52	1.44
73	L4	43	OMG	C5-C6	2.24	1.52	1.44
74	L5	2847	5MC	O2-C2	-2.24	1.19	1.23
73	L4	43	OMG	C4-N9	-2.23	1.32	1.38
76	S1	1112	PSU	O4'-C1'	-2.22	1.40	1.43
76	S1	1106	PSU	O4'-C1'	-2.22	1.40	1.43
74	L5	2857	PSU	O4'-C1'	-2.21	1.40	1.43
74	L5	2281	OMG	C5-C6	2.18	1.52	1.44
76	S1	1560	PSU	C6-N1	-2.18	1.32	1.36
76	S1	1571	OMC	C5-C4	2.17	1.48	1.42
74	L5	2847	5MC	CM5-C5	2.17	1.55	1.50
76	S1	1322	PSU	C6-C5	2.16	1.37	1.35
76	S1	1106	PSU	C6-N1	-2.16	1.32	1.36
74	L5	2803	PSU	O4'-C1'	-2.15	1.40	1.43
76	S1	1560	PSU	O4'-C1'	-2.15	1.40	1.43
74	L5	657	1MA	C4-N9	-2.15	1.32	1.38
74	L5	2921	PSU	O4'-C1'	-2.15	1.40	1.43
74	L5	917	OMG	C6-N1	2.15	1.42	1.38
76	S1	1215	PSU	C6-N1	-2.15	1.32	1.36
76	S1	686	PSU	C6-N1	-2.15	1.32	1.36
76	S1	1322	PSU	C6-N1	-2.14	1.32	1.36
76	S1	28	A2M	C4-N9	-2.14	1.33	1.37
76	S1	1196	OMG	C5-C6	2.12	1.52	1.44
74	L5	2894	OMG	C6-N1	2.12	1.42	1.38
76	S1	1196	OMG	C2-N1	2.12	1.42	1.37
76	S1	1106	PSU	C6-C5	2.12	1.37	1.35
76	S1	1116	B8N	O4'-C1'	-2.11	1.40	1.43
74	L5	2894	OMG	C4-N9	-2.11	1.32	1.38
74	L5	2899	OMG	C6-N1	2.10	1.42	1.38
74	L5	1472	A2M	O3'-C3'	-2.09	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2842	PSU	O4'-C1'	-2.09	1.41	1.43
76	S1	1727	PSU	C6-C5	2.08	1.37	1.35
74	L5	2792	OMG	C4-N9	-2.08	1.32	1.38
76	S1	1709	MA6	C4-N9	-2.08	1.33	1.37
76	S1	1361	OMG	C2-N1	2.06	1.42	1.37
76	S1	1678	A2M	C4-N9	-2.05	1.33	1.37
73	L4	43	OMG	C6-N1	2.04	1.42	1.38
74	L5	1872	OMG	C4-N9	-2.03	1.32	1.38
76	S1	1560	PSU	C6-C5	2.03	1.37	1.35
74	L5	2899	OMG	C4-N9	-2.02	1.32	1.38
76	S1	1322	PSU	O4'-C1'	-2.02	1.41	1.43
74	L5	1158	A2M	C4-N9	-2.02	1.33	1.37
76	S1	547	OMU	C5-C4	2.01	1.48	1.43
74	L5	2281	OMG	C4-N9	-2.00	1.33	1.38

All (437) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	1709	MA6	N1-C6-N6	-11.44	102.91	116.86
76	S1	1710	MA6	N1-C6-N6	-10.99	103.47	116.86
74	L5	657	1MA	C1'-N9-C8	-8.00	103.99	126.73
76	S1	1709	MA6	C5-C6-N6	7.31	136.90	125.33
74	L5	2274	A2M	N6-C6-N1	-7.09	102.58	118.38
74	L5	657	1MA	C1'-N9-C4	7.06	147.34	126.49
76	S1	83	A2M	N6-C6-N1	-6.99	102.81	118.38
76	S1	1727	PSU	N1-C2-N3	6.97	122.53	115.17
74	L5	661	A2M	N6-C6-N1	-6.95	102.89	118.38
76	S1	1678	A2M	N6-C6-N1	-6.88	103.05	118.38
76	S1	28	A2M	N6-C6-N1	-6.88	103.06	118.38
74	L5	826	A2M	N6-C6-N1	-6.87	103.08	118.38
74	L5	2319	A2M	N6-C6-N1	-6.85	103.12	118.38
74	L5	658	A2M	N6-C6-N1	-6.85	103.12	118.38
74	L5	1472	A2M	N6-C6-N1	-6.82	103.18	118.38
76	S1	899	A2M	N6-C6-N1	-6.75	103.34	118.38
74	L5	1158	A2M	N6-C6-N1	-6.73	103.38	118.38
74	L5	945	A2M	N6-C6-N1	-6.73	103.39	118.38
74	L5	2923	A2M	N6-C6-N1	-6.72	103.40	118.38
74	L5	2724	A2M	N6-C6-N1	-6.72	103.42	118.38
76	S1	1710	MA6	C5-C6-N6	6.66	135.88	125.33
76	S1	1215	PSU	N1-C2-N3	6.51	122.04	115.17
74	L5	2921	PSU	N1-C2-N3	6.34	121.86	115.17
76	S1	1309	OMU	C4-N3-C2	-6.33	118.76	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	686	PSU	N1-C2-N3	6.30	121.81	115.17
76	S1	1106	PSU	N1-C2-N3	6.29	121.81	115.17
76	S1	1560	PSU	N1-C2-N3	6.29	121.80	115.17
74	L5	2952	PSU	N1-C2-N3	6.25	121.76	115.17
76	S1	1322	PSU	N1-C2-N3	6.24	121.75	115.17
76	S1	1112	PSU	N1-C2-N3	6.23	121.74	115.17
74	L5	2803	PSU	N1-C2-N3	6.21	121.72	115.17
74	L5	2932	PSU	N1-C2-N3	6.20	121.71	115.17
74	L5	2842	PSU	N1-C2-N3	6.20	121.71	115.17
74	L5	2581	PSU	N1-C2-N3	6.17	121.68	115.17
76	S1	1710	MA6	N1-C2-N3	-6.15	119.27	128.58
74	L5	2831	PSU	N1-C2-N3	6.13	121.63	115.17
74	L5	2210	PSU	N1-C2-N3	6.08	121.59	115.17
74	L5	2897	PSU	N1-C2-N3	6.08	121.58	115.17
74	L5	2857	PSU	N1-C2-N3	6.06	121.56	115.17
76	S1	1156	OMU	C4-N3-C2	-5.95	119.22	126.61
74	L5	1158	A2M	N3-C2-N1	-5.91	119.64	128.58
76	S1	28	A2M	N3-C2-N1	-5.90	119.65	128.58
74	L5	2712	OMU	C4-N3-C2	-5.88	119.32	126.61
76	S1	1678	A2M	N3-C2-N1	-5.87	119.70	128.58
74	L5	2901	PSU	N1-C2-N3	5.86	121.35	115.17
74	L5	2900	PSU	N1-C2-N3	5.86	121.35	115.17
74	L5	2259	PSU	N1-C2-N3	5.84	121.33	115.17
74	L5	2257	PSU	N1-C2-N3	5.83	121.32	115.17
76	S1	899	A2M	N3-C2-N1	-5.81	119.78	128.58
76	S1	1709	MA6	N1-C2-N3	-5.80	119.81	128.58
74	L5	2706	OMU	C4-N3-C2	-5.79	119.43	126.61
74	L5	2319	A2M	N3-C2-N1	-5.78	119.83	128.58
76	S1	547	OMU	C4-N3-C2	-5.77	119.44	126.61
74	L5	661	A2M	N3-C2-N1	-5.71	119.94	128.58
74	L5	917	OMG	C5-C4-N3	-5.70	119.32	128.39
74	L5	2274	A2M	N3-C2-N1	-5.69	119.97	128.58
74	L5	826	A2M	N3-C2-N1	-5.65	120.03	128.58
74	L5	2724	A2M	N3-C2-N1	-5.63	120.06	128.58
76	S1	28	A2M	C5-C6-N6	5.63	137.23	123.29
74	L5	2923	A2M	N3-C2-N1	-5.63	120.06	128.58
74	L5	658	A2M	N3-C2-N1	-5.62	120.07	128.58
74	L5	2596	OMG	C5-C4-N3	-5.62	119.45	128.39
74	L5	2281	OMG	C5-C4-N3	-5.61	119.47	128.39
74	L5	945	A2M	N3-C2-N1	-5.60	120.11	128.58
74	L5	1472	A2M	N3-C2-N1	-5.59	120.12	128.58
74	L5	2274	A2M	C5-C6-N6	5.57	137.07	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	1678	A2M	C5-C6-N6	5.56	137.06	123.29
74	L5	661	A2M	C5-C6-N6	5.56	137.04	123.29
74	L5	1158	A2M	C5-C6-N6	5.52	136.96	123.29
74	L5	658	A2M	C5-C6-N6	5.51	136.93	123.29
74	L5	1872	OMG	C5-C4-N3	-5.50	119.63	128.39
74	L5	2319	A2M	C5-C6-N6	5.50	136.91	123.29
76	S1	83	A2M	C5-C6-N6	5.50	136.90	123.29
74	L5	657	1MA	N1-C2-N3	-5.49	119.47	126.00
76	S1	83	A2M	N3-C2-N1	-5.48	120.28	128.58
74	L5	2899	OMG	C5-C4-N3	-5.47	119.69	128.39
76	S1	83	A2M	C5-C4-N3	-5.47	119.19	126.72
74	L5	826	A2M	C5-C6-N6	5.47	136.82	123.29
74	L5	1472	A2M	C5-C6-N6	5.46	136.81	123.29
74	L5	2792	OMG	C5-C4-N3	-5.44	119.73	128.39
74	L5	2923	A2M	C5-C6-N6	5.39	136.64	123.29
74	L5	2410	OMU	C4-N3-C2	-5.39	119.92	126.61
74	L5	2724	A2M	C5-C6-N6	5.39	136.63	123.29
74	L5	945	A2M	C5-C6-N6	5.35	136.54	123.29
76	S1	1116	B8N	C5-C4-N3	5.35	125.86	116.15
76	S1	899	A2M	C5-C6-N6	5.28	136.35	123.29
76	S1	1196	OMG	C5-C4-N3	-5.27	120.00	128.39
76	S1	899	A2M	C5-C4-N3	-5.27	119.46	126.72
74	L5	2894	OMG	C5-C4-N3	-5.27	120.01	128.39
76	S1	1710	MA6	C5-C4-N3	-5.15	119.63	126.72
74	L5	2414	UY1	C4-N3-C2	-5.13	119.30	126.37
74	L5	1472	A2M	C5-C4-N3	-5.10	119.69	126.72
73	L4	43	OMG	C5-C4-N3	-5.09	120.28	128.39
74	L5	826	A2M	C5-C4-N3	-5.08	119.72	126.72
74	L5	2898	UY1	C4-N3-C2	-5.06	119.39	126.37
76	S1	1507	7MG	C5-C6-N1	5.06	119.84	110.94
74	L5	814	OMG	C5-C4-N3	-5.05	120.36	128.39
74	L5	945	A2M	C5-C4-N3	-5.02	119.81	126.72
74	L5	2923	A2M	C5-C4-N3	-5.00	119.84	126.72
74	L5	661	A2M	C5-C4-N3	-4.99	119.84	126.72
76	S1	1361	OMG	C5-C4-N3	-4.96	120.50	128.39
74	L5	658	A2M	C5-C4-N3	-4.95	119.91	126.72
74	L5	2274	A2M	C5-C4-N3	-4.93	119.93	126.72
74	L5	2724	A2M	C5-C4-N3	-4.89	119.98	126.72
76	S1	1678	A2M	C5-C4-N3	-4.85	120.04	126.72
74	L5	2319	A2M	C5-C4-N3	-4.82	120.08	126.72
74	L5	2414	UY1	N1-C2-N3	4.71	120.14	115.17
76	S1	28	A2M	C5-C4-N3	-4.69	120.26	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	1727	PSU	C4-N3-C2	-4.69	119.91	126.37
74	L5	1158	A2M	C5-C4-N3	-4.66	120.30	126.72
74	L5	2281	OMG	C2-N3-C4	4.64	120.30	112.30
74	L5	917	OMG	C2-N3-C4	4.64	120.29	112.30
74	L5	2899	OMG	C2-N3-C4	4.61	120.25	112.30
76	S1	686	PSU	C4-N3-C2	-4.59	120.05	126.37
76	S1	1112	PSU	C4-N3-C2	-4.59	120.05	126.37
76	S1	1106	PSU	C4-N3-C2	-4.58	120.06	126.37
76	S1	1116	B8N	C4-N3-C2	-4.57	120.00	125.62
74	L5	2894	OMG	C2-N3-C4	4.53	120.10	112.30
76	S1	1507	7MG	C2-N3-C4	4.53	120.09	112.30
76	S1	1215	PSU	C4-N3-C2	-4.51	120.16	126.37
74	L5	1472	A2M	O3'-C3'-C4'	4.51	124.03	111.08
76	S1	1560	PSU	C4-N3-C2	-4.49	120.18	126.37
74	L5	657	1MA	C5-C4-N3	-4.49	120.66	127.27
73	L4	43	OMG	C2-N3-C4	4.49	120.03	112.30
74	L5	2952	PSU	C4-N3-C2	-4.47	120.21	126.37
74	L5	2921	PSU	C4-N3-C2	-4.46	120.23	126.37
74	L5	2803	PSU	C4-N3-C2	-4.46	120.23	126.37
74	L5	2898	UY1	N1-C2-N3	4.45	119.87	115.17
76	S1	1322	PSU	C4-N3-C2	-4.45	120.24	126.37
76	S1	1709	MA6	C5-C4-N3	-4.45	120.59	126.72
74	L5	2596	OMG	C2-N3-C4	4.45	119.96	112.30
74	L5	2831	PSU	C4-N3-C2	-4.42	120.28	126.37
74	L5	1872	OMG	C2-N3-C4	4.42	119.92	112.30
76	S1	1196	OMG	C2-N3-C4	4.42	119.90	112.30
74	L5	2842	PSU	C4-N3-C2	-4.41	120.29	126.37
74	L5	2897	PSU	C4-N3-C2	-4.41	120.29	126.37
74	L5	2792	OMG	C2-N3-C4	4.41	119.89	112.30
76	S1	1361	OMG	C2-N3-C4	4.40	119.88	112.30
74	L5	2932	PSU	C4-N3-C2	-4.39	120.32	126.37
74	L5	2724	A2M	N9-C8-N7	-4.37	107.74	113.94
74	L5	2210	PSU	C4-N3-C2	-4.36	120.37	126.37
74	L5	2581	PSU	C4-N3-C2	-4.35	120.38	126.37
74	L5	814	OMG	C2-N3-C4	4.33	119.76	112.30
76	S1	1507	7MG	C4-C5-N7	4.31	110.47	105.38
76	S1	1309	OMU	C5-C4-N3	4.30	120.83	114.80
74	L5	2857	PSU	C4-N3-C2	-4.29	120.46	126.37
76	S1	1710	MA6	N9-C8-N7	-4.29	107.85	113.94
76	S1	1156	OMU	C5-C4-N3	4.26	120.76	114.80
74	L5	2259	PSU	C4-N3-C2	-4.22	120.56	126.37
74	L5	2274	A2M	N9-C8-N7	-4.22	107.95	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	1507	7MG	C5-C4-N3	-4.21	120.24	128.13
76	S1	1727	PSU	O2-C2-N1	-4.19	118.46	122.79
74	L5	2901	PSU	C4-N3-C2	-4.17	120.63	126.37
74	L5	814	OMG	C1'-N9-C4	-4.15	114.24	126.49
74	L5	826	A2M	N9-C8-N7	-4.13	108.07	113.94
74	L5	2257	PSU	C4-N3-C2	-4.12	120.70	126.37
74	L5	2900	PSU	C4-N3-C2	-4.12	120.70	126.37
74	L5	2319	A2M	N9-C8-N7	-4.09	108.13	113.94
74	L5	945	A2M	N9-C8-N7	-4.07	108.16	113.94
76	S1	1309	OMU	N3-C2-N1	4.05	120.16	114.89
74	L5	1472	A2M	N9-C8-N7	-4.04	108.20	113.94
76	S1	1709	MA6	N9-C8-N7	-4.04	108.20	113.94
74	L5	2923	A2M	N9-C8-N7	-4.01	108.25	113.94
74	L5	2712	OMU	N3-C2-N1	4.01	120.11	114.89
74	L5	2410	OMU	N3-C2-N1	4.00	120.10	114.89
74	L5	658	A2M	N9-C8-N7	-3.95	108.33	113.94
74	L5	657	1MA	C2-N3-C4	3.95	120.28	112.53
74	L5	661	A2M	N9-C8-N7	-3.95	108.33	113.94
74	L5	1158	A2M	N9-C8-N7	-3.94	108.34	113.94
73	L4	43	OMG	C1'-N9-C4	-3.94	114.86	126.49
76	S1	1678	A2M	N9-C8-N7	-3.93	108.36	113.94
76	S1	1322	PSU	O2-C2-N1	-3.92	118.75	122.79
74	L5	2706	OMU	N3-C2-N1	3.90	119.96	114.89
74	L5	2932	PSU	O2-C2-N1	-3.88	118.78	122.79
74	L5	2901	PSU	O2-C2-N1	-3.81	118.86	122.79
74	L5	814	OMG	C1'-N9-C8	3.81	137.56	126.73
76	S1	547	OMU	N3-C2-N1	3.81	119.85	114.89
74	L5	2894	OMG	C1'-N9-C4	-3.81	115.24	126.49
76	S1	83	A2M	N9-C8-N7	-3.80	108.55	113.94
76	S1	28	A2M	N9-C8-N7	-3.79	108.55	113.94
76	S1	1361	OMG	C1'-N9-C4	-3.77	115.36	126.49
76	S1	1710	MA6	C2-N3-C4	3.76	121.03	111.83
76	S1	1196	OMG	C1'-N9-C4	-3.76	115.39	126.49
76	S1	899	A2M	N9-C8-N7	-3.75	108.61	113.94
74	L5	2712	OMU	C5-C4-N3	3.75	120.05	114.80
74	L5	2706	OMU	C5-C4-N3	3.75	120.05	114.80
76	S1	1116	B8N	N3-C2-N1	3.72	121.27	116.72
74	L5	2210	PSU	O2-C2-N1	-3.70	118.97	122.79
74	L5	2803	PSU	O2-C2-N1	-3.70	118.97	122.79
76	S1	547	OMU	C5-C4-N3	3.69	119.97	114.80
76	S1	1116	B8N	C1'-C5-C4	3.68	123.20	117.61
74	L5	2259	PSU	O2-C2-N1	-3.68	118.99	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2842	PSU	O2-C2-N1	-3.68	118.99	122.79
76	S1	1215	PSU	O2-C2-N1	-3.68	118.99	122.79
76	S1	1361	OMG	C1'-N9-C8	3.68	137.19	126.73
74	L5	2831	PSU	O2-C2-N1	-3.66	119.01	122.79
76	S1	1560	PSU	O2-C2-N1	-3.66	119.01	122.79
76	S1	1156	OMU	N3-C2-N1	3.64	119.64	114.89
74	L5	2792	OMG	C1'-N9-C4	-3.64	115.72	126.49
74	L5	2257	PSU	O2-C2-N1	-3.64	119.03	122.79
73	L4	43	OMG	C1'-N9-C8	3.64	137.07	126.73
76	S1	1196	OMG	C1'-N9-C8	3.60	136.96	126.73
74	L5	2581	PSU	O2-C2-N1	-3.60	119.08	122.79
74	L5	2596	OMG	N9-C4-N3	3.59	133.13	125.95
76	S1	686	PSU	O2-C2-N1	-3.57	119.11	122.79
74	L5	2847	5MC	C5-C6-N1	-3.54	119.47	123.31
76	S1	899	A2M	C2-N3-C4	3.53	120.46	111.83
74	L5	2894	OMG	C1'-N9-C8	3.53	136.77	126.73
74	L5	2900	PSU	O2-C2-N1	-3.53	119.15	122.79
74	L5	2952	PSU	O2-C2-N1	-3.52	119.16	122.79
74	L5	2414	UY1	C6-C5-C4	3.52	120.55	118.17
74	L5	2857	PSU	O2-C2-N1	-3.51	119.17	122.79
74	L5	2921	PSU	O2-C2-N1	-3.51	119.17	122.79
74	L5	2410	OMU	C5-C4-N3	3.50	119.71	114.80
76	S1	1710	MA6	C4-C5-C6	3.50	119.53	115.91
74	L5	917	OMG	N9-C4-N3	3.50	132.94	125.95
76	S1	83	A2M	C2-N3-C4	3.48	120.32	111.83
76	S1	1106	PSU	O2-C2-N1	-3.47	119.21	122.79
74	L5	2792	OMG	C1'-N9-C8	3.45	136.52	126.73
74	L5	2281	OMG	N9-C4-N3	3.44	132.84	125.95
74	L5	826	A2M	C2-N3-C4	3.43	120.20	111.83
76	S1	1709	MA6	C2-N1-C6	3.42	120.19	111.83
74	L5	2274	A2M	C2-N3-C4	3.42	120.19	111.83
76	S1	899	A2M	N3-C4-N9	3.42	132.98	127.17
74	L5	661	A2M	C2-N3-C4	3.42	120.17	111.83
74	L5	1472	A2M	C2-N3-C4	3.39	120.11	111.83
74	L5	945	A2M	C2-N3-C4	3.38	120.10	111.83
74	L5	2923	A2M	C2-N3-C4	3.38	120.07	111.83
76	S1	1709	MA6	C4-C5-C6	3.36	119.39	115.91
74	L5	658	A2M	C2-N3-C4	3.36	120.04	111.83
76	S1	1678	A2M	C2-N3-C4	3.36	120.04	111.83
76	S1	1112	PSU	O2-C2-N1	-3.35	119.33	122.79
74	L5	2319	A2M	C2-N3-C4	3.35	120.02	111.83
74	L5	2897	PSU	O2-C2-N1	-3.34	119.34	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2724	A2M	C2-N3-C4	3.34	119.98	111.83
76	S1	28	A2M	C2-N3-C4	3.32	119.95	111.83
74	L5	2899	OMG	N9-C4-N3	3.32	132.59	125.95
76	S1	1710	MA6	C2-N1-C6	3.30	119.89	111.83
74	L5	2792	OMG	C2-N1-C6	-3.30	119.12	125.11
74	L5	1872	OMG	N9-C4-N3	3.29	132.54	125.95
76	S1	83	A2M	N3-C4-N9	3.29	132.77	127.17
76	S1	1709	MA6	C2-N3-C4	3.28	119.83	111.83
74	L5	1158	A2M	C2-N3-C4	3.27	119.81	111.83
74	L5	2923	A2M	C2'-C1'-N9	-3.26	108.39	113.75
74	L5	657	1MA	N9-C8-N7	-3.26	107.36	113.40
74	L5	917	OMG	C2-N1-C6	-3.24	119.23	125.11
74	L5	2899	OMG	C1'-N9-C4	-3.23	116.94	126.49
74	L5	2274	A2M	C4'-O4'-C1'	-3.22	102.36	109.47
74	L5	2899	OMG	C2-N1-C6	-3.21	119.28	125.11
76	S1	1507	7MG	O6-C6-C5	-3.21	119.75	127.62
74	L5	1472	A2M	C2'-C3'-C4'	3.20	108.88	101.99
74	L5	1872	OMG	C1'-N9-C4	-3.19	117.07	126.49
74	L5	2596	OMG	C2-N1-C6	-3.18	119.34	125.11
74	L5	2414	UY1	C6-N1-C2	-3.16	119.75	122.69
74	L5	2792	OMG	N9-C4-N3	3.15	132.25	125.95
74	L5	826	A2M	N3-C4-N9	3.15	132.52	127.17
74	L5	945	A2M	N3-C4-N9	3.14	132.50	127.17
74	L5	2894	OMG	N9-C4-N3	3.13	132.20	125.95
76	S1	1710	MA6	N3-C4-N9	3.12	132.47	127.17
74	L5	1472	A2M	N3-C4-N9	3.11	132.46	127.17
74	L5	2898	UY1	C6-N1-C2	-3.10	119.81	122.69
74	L5	2923	A2M	N3-C4-N9	3.10	132.44	127.17
74	L5	2724	A2M	N3-C4-N9	3.09	132.42	127.17
74	L5	917	OMG	C1'-N9-C4	-3.08	117.40	126.49
74	L5	1872	OMG	C2-N1-C6	-3.08	119.53	125.11
76	S1	1507	7MG	C5-C4-N9	3.07	110.27	106.33
74	L5	2596	OMG	C1'-N9-C4	-3.05	117.47	126.49
76	S1	1309	OMU	O4-C4-C5	-3.05	119.90	125.16
74	L5	2281	OMG	C2-N1-C6	-3.05	119.58	125.11
76	S1	547	OMU	O4-C4-C5	-3.03	119.94	125.16
76	S1	1507	7MG	C2-N1-C6	-3.02	119.64	125.11
74	L5	661	A2M	N3-C4-N9	3.01	132.29	127.17
74	L5	814	OMG	C2-N1-C6	-3.01	119.65	125.11
74	L5	1872	OMG	C1'-N9-C8	3.00	135.26	126.73
74	L5	2894	OMG	C2-N1-C6	-3.00	119.67	125.11
76	S1	1196	OMG	C2-N1-C6	-2.99	119.69	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2899	OMG	C1'-N9-C8	2.98	135.19	126.73
74	L5	658	A2M	N3-C4-N9	2.96	132.20	127.17
76	S1	1678	A2M	N3-C4-N9	2.96	132.19	127.17
74	L5	1472	A2M	O3'-C3'-C2'	2.96	119.46	111.19
74	L5	2724	A2M	C5-N7-C8	2.95	108.09	103.45
74	L5	814	OMG	N9-C8-N7	-2.94	107.94	113.40
74	L5	2319	A2M	N3-C4-N9	2.92	132.14	127.17
74	L5	2712	OMU	O4-C4-C5	-2.92	120.12	125.16
76	S1	28	A2M	N3-C4-N9	2.92	132.13	127.17
73	L4	43	OMG	N9-C4-N3	2.92	131.78	125.95
74	L5	2274	A2M	C5-N7-C8	2.91	108.02	103.45
74	L5	2706	OMU	O4-C4-C5	-2.91	120.14	125.16
72	SO	144	IAS	CA-CB-CG	-2.90	96.80	113.44
74	L5	2281	OMG	C1'-N9-C4	-2.90	117.91	126.49
76	S1	1196	OMG	N9-C4-N3	2.90	131.75	125.95
74	L5	1472	A2M	C5-N7-C8	2.89	107.99	103.45
76	S1	1710	MA6	C5-N7-C8	2.89	107.98	103.45
74	L5	826	A2M	C5-N7-C8	2.87	107.96	103.45
76	S1	1116	B8N	O4-C4-N3	-2.87	115.33	119.99
73	L4	43	OMG	C2-N1-C6	-2.87	119.91	125.11
73	L4	43	OMG	N9-C8-N7	-2.86	108.09	113.40
74	L5	2274	A2M	O4'-C1'-N9	2.85	113.57	108.09
74	L5	814	OMG	N9-C4-N3	2.85	131.65	125.95
74	L5	917	OMG	C1'-N9-C8	2.85	134.83	126.73
74	L5	1158	A2M	N3-C4-N9	2.83	131.98	127.17
74	L5	2894	OMG	N9-C8-N7	-2.80	108.21	113.40
76	S1	1156	OMU	O4-C4-C5	-2.79	120.34	125.16
76	S1	28	A2M	C2'-C1'-N9	-2.77	109.19	113.75
76	S1	83	A2M	C5-N7-C8	2.76	107.78	103.45
74	L5	945	A2M	C5-N7-C8	2.75	107.78	103.45
76	S1	1507	7MG	N9-C4-N3	2.75	129.49	125.46
74	L5	2319	A2M	C5-N7-C8	2.75	107.77	103.45
74	L5	2274	A2M	N3-C4-N9	2.75	131.84	127.17
74	L5	917	OMG	N9-C8-N7	-2.75	108.31	113.40
74	L5	2792	OMG	N9-C8-N7	-2.74	108.33	113.40
74	L5	2596	OMG	C1'-N9-C8	2.73	134.50	126.73
74	L5	661	A2M	C5-N7-C8	2.73	107.74	103.45
76	S1	1361	OMG	N9-C4-N3	2.73	131.41	125.95
76	S1	1196	OMG	N9-C8-N7	-2.72	108.36	113.40
74	L5	2899	OMG	C5-C6-N1	2.72	120.17	113.25
74	L5	2281	OMG	C1'-N9-C8	2.72	134.45	126.73
74	L5	2923	A2M	C5-N7-C8	2.72	107.72	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	658	A2M	C5-N7-C8	2.71	107.72	103.45
74	L5	2319	A2M	C2'-C1'-N9	-2.71	109.30	113.75
74	L5	2792	OMG	C5-C6-N1	2.70	120.12	113.25
74	L5	945	A2M	C2'-C1'-N9	-2.68	109.34	113.75
74	L5	917	OMG	O6-C6-C5	-2.68	119.46	126.53
74	L5	2596	OMG	N9-C8-N7	-2.67	108.45	113.40
76	S1	1361	OMG	C2-N1-C6	-2.67	120.27	125.11
74	L5	2410	OMU	O4-C4-C5	-2.66	120.57	125.16
74	L5	2596	OMG	C5-C6-N1	2.66	120.03	113.25
74	L5	2894	OMG	C5-C6-N1	2.66	120.03	113.25
74	L5	2899	OMG	N9-C8-N7	-2.65	108.48	113.40
74	L5	2281	OMG	C5-C6-N1	2.65	119.99	113.25
74	L5	917	OMG	C5-C6-N1	2.65	119.99	113.25
74	L5	2898	UY1	C6-C5-C4	2.63	119.95	118.17
76	S1	1709	MA6	N3-C4-N9	2.62	131.63	127.17
76	S1	1196	OMG	C5-C6-N1	2.62	119.92	113.25
73	L4	43	OMG	C5-C6-N1	2.61	119.91	113.25
74	L5	2899	OMG	O6-C6-C5	-2.61	119.63	126.53
76	S1	1678	A2M	C5-N7-C8	2.61	107.55	103.45
72	SO	144	IAS	OD2-CG-CB	2.60	122.09	114.00
74	L5	2724	A2M	C4-N9-C8	2.60	108.47	105.74
74	L5	1872	OMG	N9-C8-N7	-2.60	108.58	113.40
74	L5	814	OMG	C5-C6-N1	2.58	119.82	113.25
74	L5	1158	A2M	C5-N7-C8	2.58	107.50	103.45
74	L5	2894	OMG	O6-C6-C5	-2.58	119.73	126.53
74	L5	1872	OMG	C5-C6-N1	2.57	119.81	113.25
76	S1	899	A2M	C5-N7-C8	2.56	107.48	103.45
76	S1	1709	MA6	C5-N7-C8	2.56	107.47	103.45
76	S1	1701	4AC	CM7-C7-N4	2.54	119.37	115.27
76	S1	1361	OMG	O6-C6-C5	-2.53	119.86	126.53
74	L5	2281	OMG	N9-C8-N7	-2.53	108.71	113.40
74	L5	2414	UY1	O2-C2-N1	-2.52	120.19	122.79
74	L5	2596	OMG	O6-C6-C5	-2.51	119.91	126.53
76	S1	1361	OMG	C5-C6-N1	2.50	119.62	113.25
76	S1	1309	OMU	C1'-N1-C2	2.48	122.06	117.59
76	S1	28	A2M	C5-N7-C8	2.48	107.35	103.45
74	L5	2281	OMG	O6-C6-C5	-2.47	120.02	126.53
74	L5	814	OMG	O6-C6-C5	-2.47	120.02	126.53
76	S1	1361	OMG	N9-C8-N7	-2.43	108.89	113.40
73	L4	43	OMG	O6-C6-C5	-2.42	120.14	126.53
74	L5	1872	OMG	O6-C6-C5	-2.42	120.14	126.53
74	L5	2274	A2M	O4'-C1'-C2'	-2.40	102.45	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2706	OMU	O2-C2-N1	-2.40	119.67	122.80
74	L5	1158	A2M	C2'-C1'-N9	-2.39	109.82	113.75
74	L5	2792	OMG	O6-C6-C5	-2.38	120.24	126.53
74	L5	2724	A2M	C3'-C2'-C1'	2.36	107.33	102.81
74	L5	2274	A2M	C4-C5-N7	-2.35	107.89	110.58
74	L5	2898	UY1	O2-C2-N1	-2.33	120.38	122.79
76	S1	83	A2M	C6-C5-C4	2.33	120.35	117.18
74	L5	2414	UY1	CM2-O2'-C2'	2.31	120.41	114.47
76	S1	1709	MA6	C4-N9-C8	2.31	108.16	105.74
76	S1	1507	7MG	N9-C8-N7	2.29	106.62	103.37
76	S1	1116	B8N	C31-N3-C4	2.29	120.42	117.18
76	S1	1196	OMG	O6-C6-C5	-2.29	120.50	126.53
74	L5	2410	OMU	O2-C2-N1	-2.28	119.83	122.80
74	L5	2712	OMU	O2-C2-N1	-2.27	119.84	122.80
74	L5	826	A2M	C4-N9-C8	2.25	108.10	105.74
74	L5	2410	OMU	O4'-C4'-C5'	2.25	116.54	109.33
74	L5	945	A2M	C4-N9-C8	2.24	108.08	105.74
76	S1	1710	MA6	C4-N9-C8	2.23	108.08	105.74
74	L5	2319	A2M	C4-N9-C8	2.22	108.07	105.74
74	L5	1472	A2M	C6-C5-C4	2.22	120.20	117.18
76	S1	686	PSU	C5-C6-N1	-2.22	119.06	122.14
74	L5	2274	A2M	C5-C4-N9	2.21	108.22	105.81
74	L5	2803	PSU	O4'-C1'-C2'	2.21	108.20	105.15
74	L5	657	1MA	C8-N7-C5	2.20	108.18	104.26
74	L5	1158	A2M	C4-N9-C8	2.19	108.04	105.74
76	S1	1116	B8N	O4-C4-C5	-2.19	118.80	122.58
76	S1	83	A2M	C4-C5-N7	-2.18	108.08	110.58
76	S1	1727	PSU	C6-N1-C2	-2.18	120.67	122.69
76	S1	899	A2M	C6-C5-C4	2.17	120.14	117.18
74	L5	2923	A2M	C6-C5-C4	2.17	120.14	117.18
74	L5	1472	A2M	C4-C5-N7	-2.17	108.10	110.58
76	S1	1112	PSU	C5-C6-N1	-2.17	119.13	122.14
74	L5	2724	A2M	C4-C5-N7	-2.17	108.10	110.58
74	L5	826	A2M	C4-C5-N7	-2.17	108.11	110.58
74	L5	2842	PSU	O4'-C1'-C2'	2.16	108.14	105.15
76	S1	547	OMU	O2-C2-N1	-2.16	119.98	122.80
74	L5	2921	PSU	C5-C6-N1	-2.15	119.15	122.14
74	L5	2923	A2M	C4-N9-C8	2.15	108.00	105.74
74	L5	826	A2M	C6-C5-C4	2.15	120.11	117.18
74	L5	2831	PSU	C5-C6-N1	-2.14	119.17	122.14
74	L5	917	OMG	C8-N7-C5	2.13	108.06	104.26
74	L5	945	A2M	C6-C5-C4	2.12	120.08	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S1	1678	A2M	C4-N9-C8	2.12	107.97	105.74
74	L5	2724	A2M	C6-C5-C4	2.12	120.07	117.18
74	L5	2857	PSU	O4'-C1'-C2'	2.11	108.08	105.15
76	S1	1710	MA6	C4-C5-N7	-2.11	108.17	110.58
74	L5	2897	PSU	C5-C6-N1	-2.10	119.23	122.14
76	S1	28	A2M	C4-N9-C8	2.10	107.94	105.74
74	L5	2901	PSU	O4'-C1'-C2'	2.09	108.05	105.15
74	L5	2932	PSU	C5-C6-N1	-2.08	119.25	122.14
74	L5	2803	PSU	C5-C6-N1	-2.08	119.25	122.14
76	S1	1701	4AC	C6-C5-C4	2.07	119.50	117.00
74	L5	658	A2M	C6-C5-C4	2.07	120.00	117.18
74	L5	658	A2M	C4-C5-N7	-2.06	108.22	110.58
74	L5	661	A2M	C4-C5-N7	-2.06	108.23	110.58
74	L5	2842	PSU	C5-C6-N1	-2.05	119.29	122.14
76	S1	1106	PSU	C5-C6-N1	-2.05	119.29	122.14
74	L5	2410	OMU	C5'-C4'-C3'	2.05	122.60	115.21
74	L5	2274	A2M	C4-N9-C8	2.05	107.89	105.74
74	L5	2901	PSU	C6-N1-C2	-2.04	120.80	122.69
76	S1	83	A2M	C5-C4-N9	2.04	108.04	105.81
74	L5	814	OMG	C8-N7-C5	2.04	107.90	104.26
74	L5	2319	A2M	C4-C5-N7	-2.04	108.25	110.58
76	S1	1215	PSU	C5-C6-N1	-2.04	119.31	122.14
76	S1	1116	B8N	O4'-C1'-C2'	2.04	107.97	105.15
76	S1	1215	PSU	C6-N1-C2	-2.04	120.80	122.69
74	L5	1472	A2M	C4-N9-C8	2.03	107.87	105.74
74	L5	2724	A2M	C2'-C1'-N9	-2.03	110.42	113.75
74	L5	2952	PSU	C5-C6-N1	-2.02	119.33	122.14
76	S1	1701	4AC	C5-C4-N3	-2.02	119.44	122.60
74	L5	2792	OMG	C8-N7-C5	2.02	107.85	104.26
74	L5	945	A2M	C3'-C2'-C1'	2.01	106.66	102.81
74	L5	945	A2M	C4-C5-N7	-2.01	108.28	110.58
76	S1	1322	PSU	O4'-C1'-C2'	2.01	107.94	105.15
76	S1	1322	PSU	C6-N1-C2	-2.01	120.83	122.69
76	S1	1322	PSU	C5-C6-N1	-2.01	119.35	122.14
74	L5	661	A2M	C6-C5-C4	2.00	119.91	117.18

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
72	SO	144	IAS	N-CA-CB-CG
72	SO	144	IAS	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
74	L5	2281	OMG	O4'-C4'-C5'-O5'
74	L5	2410	OMU	O4'-C4'-C5'-O5'
74	L5	2414	UY1	C1'-C2'-O2'-CM2
74	L5	2596	OMG	C1'-C2'-O2'-CM2
74	L5	2724	A2M	C1'-C2'-O2'-CM'
74	L5	2898	UY1	O4'-C1'-C5-C4
74	L5	2898	UY1	O4'-C1'-C5-C6
74	L5	2898	UY1	O4'-C4'-C5'-O5'
74	L5	2923	A2M	O4'-C4'-C5'-O5'
76	S1	1156	OMU	O4'-C4'-C5'-O5'
76	S1	1196	OMG	C1'-C2'-O2'-CM2
76	S1	1309	OMU	O4'-C1'-N1-C2
76	S1	1309	OMU	O4'-C1'-N1-C6
74	L5	658	A2M	O4'-C4'-C5'-O5'
74	L5	2923	A2M	C3'-C4'-C5'-O5'
74	L5	2932	PSU	C3'-C4'-C5'-O5'
74	L5	2932	PSU	O4'-C4'-C5'-O5'
76	S1	1156	OMU	C3'-C4'-C5'-O5'
74	L5	2410	OMU	C3'-C4'-C5'-O5'
74	L5	2900	PSU	O4'-C4'-C5'-O5'
76	S1	83	A2M	O4'-C4'-C5'-O5'
76	S1	1116	B8N	N34-C33-C34-O36
74	L5	2724	A2M	C3'-C2'-O2'-CM'
74	L5	2281	OMG	C3'-C4'-C5'-O5'
74	L5	2900	PSU	C3'-C4'-C5'-O5'
74	L5	2898	UY1	C3'-C4'-C5'-O5'
74	L5	2274	A2M	O4'-C4'-C5'-O5'
76	S1	1322	PSU	O4'-C4'-C5'-O5'
76	S1	1710	MA6	C5-C6-N6-C10
74	L5	658	A2M	C3'-C4'-C5'-O5'
74	L5	2274	A2M	C3'-C4'-C5'-O5'
76	S1	1322	PSU	C3'-C4'-C5'-O5'
74	L5	2596	OMG	O4'-C4'-C5'-O5'
76	S1	1116	B8N	N34-C33-C34-O35
73	L4	43	OMG	C3'-C4'-C5'-O5'
74	L5	2596	OMG	C3'-C4'-C5'-O5'
74	L5	661	A2M	C3'-C4'-C5'-O5'
74	L5	2897	PSU	C3'-C4'-C5'-O5'
74	L5	826	A2M	C4'-C5'-O5'-P
74	L5	2899	OMG	C3'-C2'-O2'-CM2
74	L5	661	A2M	C4'-C5'-O5'-P
74	L5	2900	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
74	L5	2897	PSU	O4'-C4'-C5'-O5'
74	L5	2847	5MC	O4'-C1'-N1-C6
76	S1	1710	MA6	C4'-C5'-O5'-P
74	L5	657	1MA	C2'-C1'-N9-C8
74	L5	917	OMG	C4'-C5'-O5'-P
74	L5	2847	5MC	C2'-C1'-N1-C6
74	L5	657	1MA	C2'-C1'-N9-C4
76	S1	1361	OMG	C4'-C5'-O5'-P
76	S1	1116	B8N	C32-C33-C34-O36
76	S1	83	A2M	C3'-C4'-C5'-O5'
76	S1	1727	PSU	C3'-C4'-C5'-O5'
76	S1	1727	PSU	O4'-C4'-C5'-O5'
74	L5	2847	5MC	O4'-C1'-N1-C2
76	S1	1116	B8N	C32-C33-C34-O35

There are no ring outliers.

23 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L5	657	1MA	1	0
74	L5	661	A2M	1	0
74	L5	2921	PSU	1	0
76	S1	1701	4AC	1	0
74	L5	2936	OMC	1	0
74	L5	2792	OMG	1	0
74	L5	2856	OMC	1	0
76	S1	899	A2M	1	0
76	S1	1507	7MG	1	0
76	S1	1196	OMG	1	0
72	SO	144	IAS	1	0
74	L5	814	OMG	1	0
73	L4	43	OMG	1	0
74	L5	1158	A2M	1	0
76	S1	1709	MA6	1	0
76	S1	1560	PSU	1	0
74	L5	2857	PSU	1	0
74	L5	2847	5MC	2	0
74	L5	2274	A2M	3	0
74	L5	826	A2M	1	0
74	L5	1472	A2M	1	0
76	S1	1322	PSU	1	0
74	L5	2724	A2M	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 167 ligands modelled in this entry, 167 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

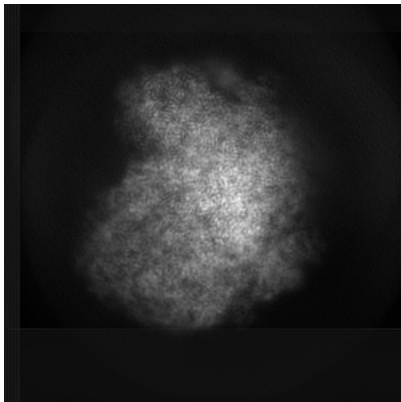
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72933. These allow visual inspection of the internal detail of the map and identification of artifacts.

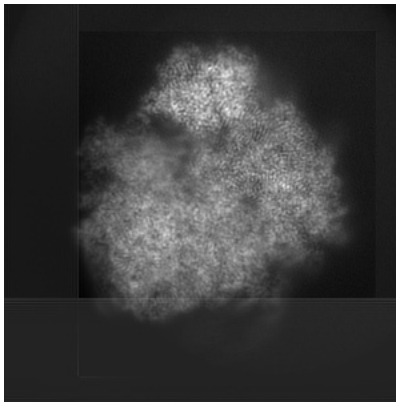
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

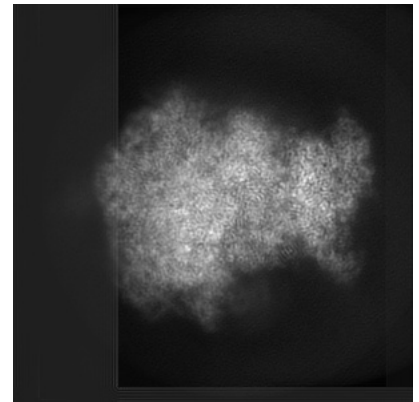
#### 6.1.1 Primary map



X



Y

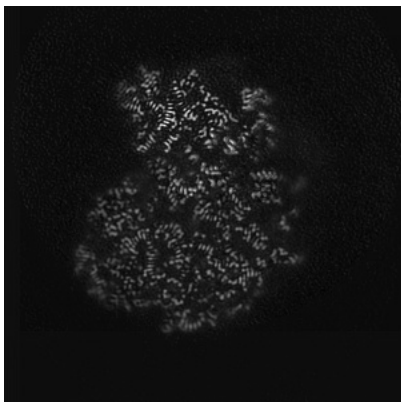


Z

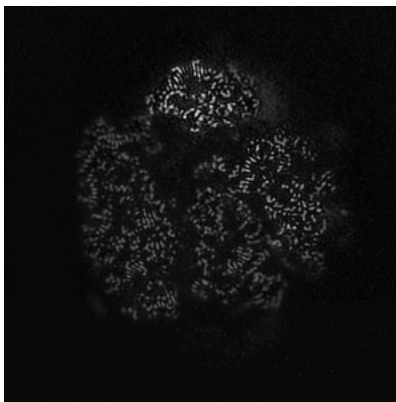
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

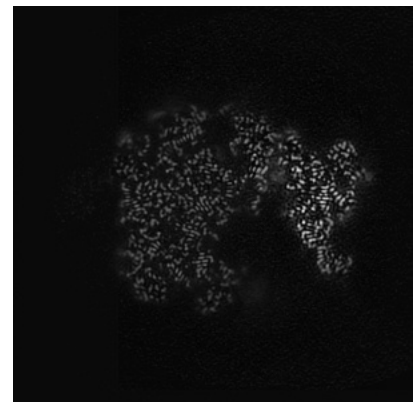
#### 6.2.1 Primary map



X Index: 224



Y Index: 224

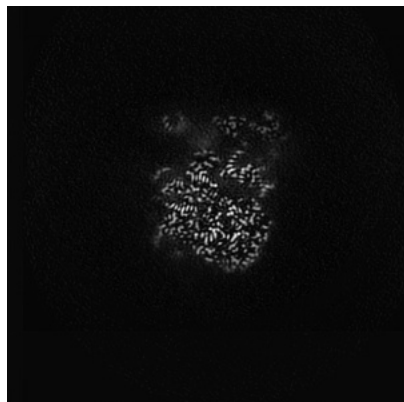


Z Index: 224

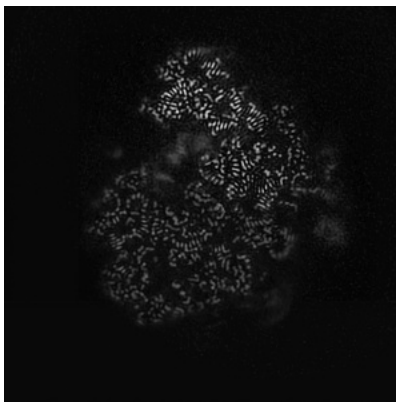
The images above show central slices of the map in three orthogonal directions.

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

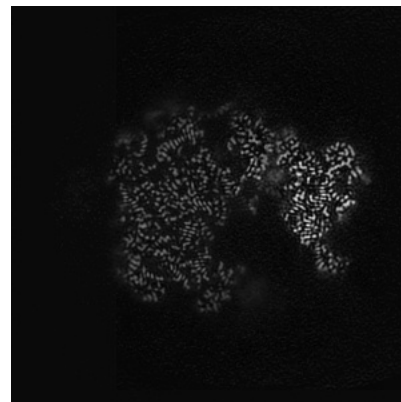
### 6.3.1 Primary map



X Index: 333



Y Index: 254

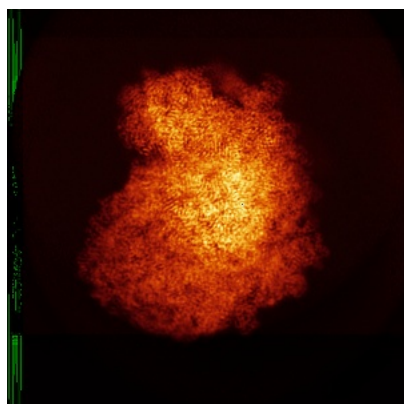


Z Index: 222

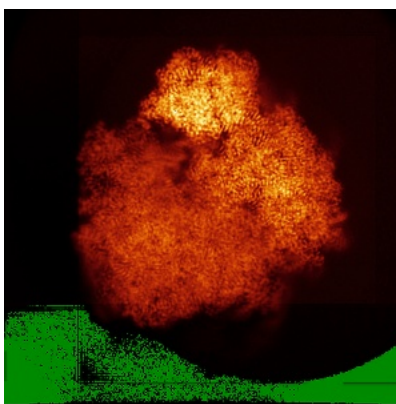
The images above show the largest variance slices of the map in three orthogonal directions.

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

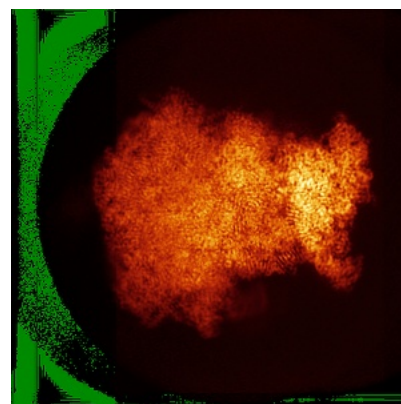
### 6.4.1 Primary map



X



Y

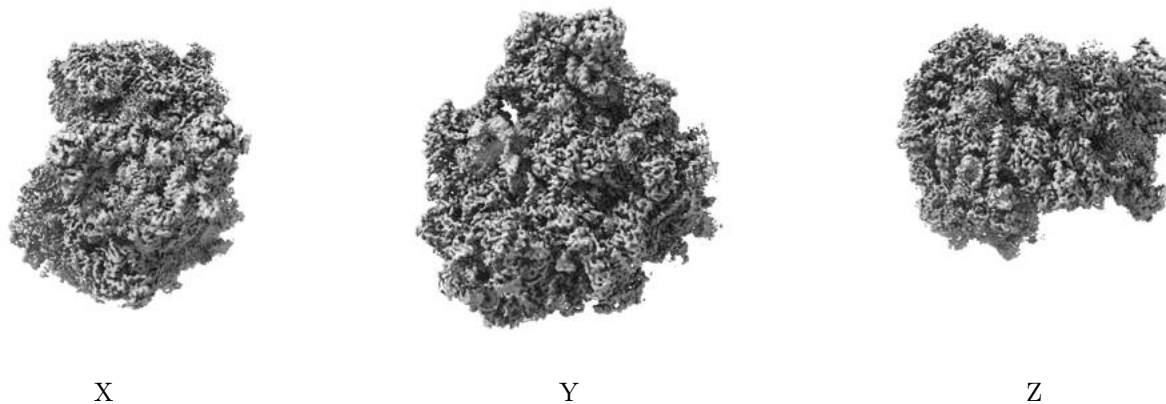


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

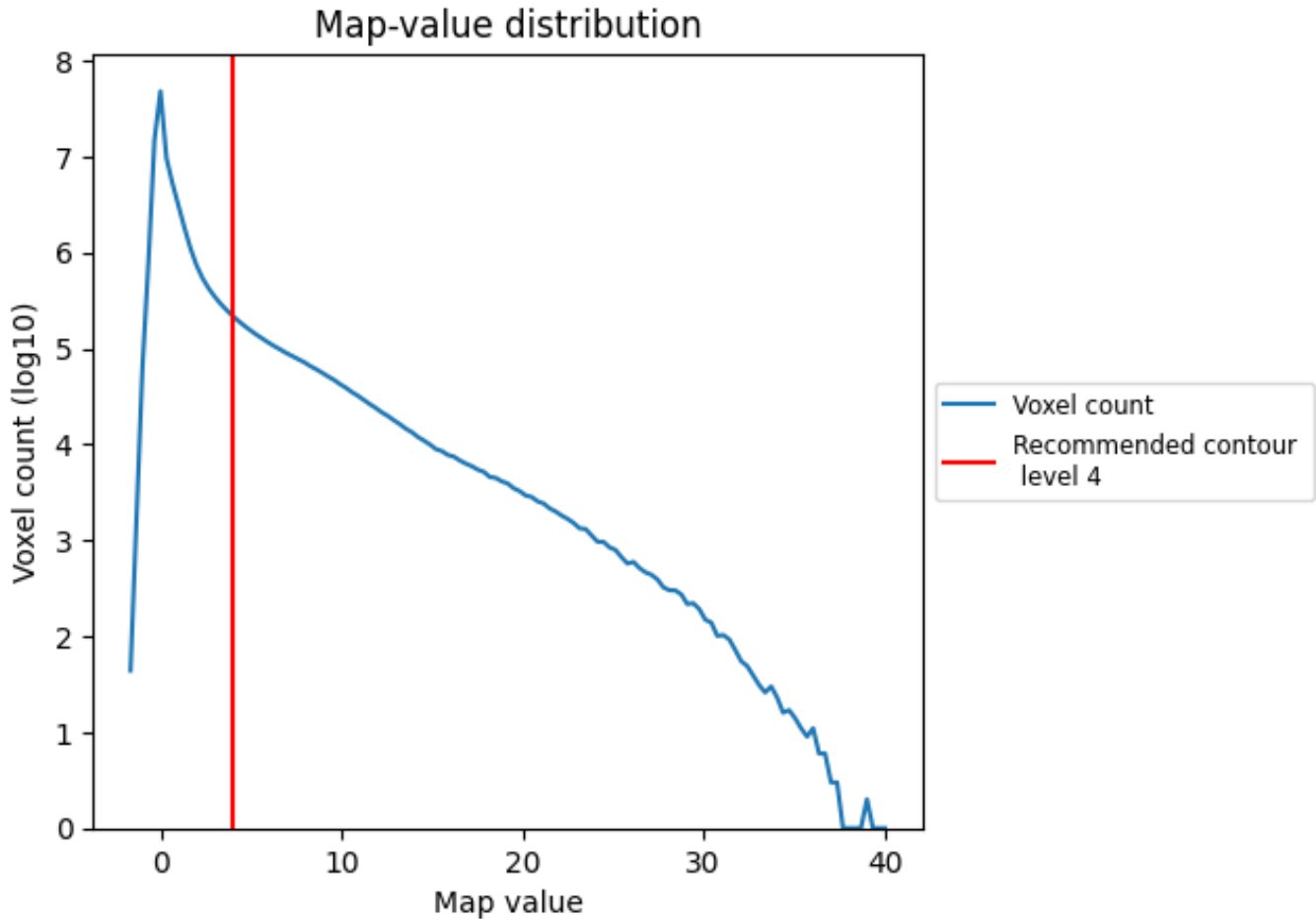
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

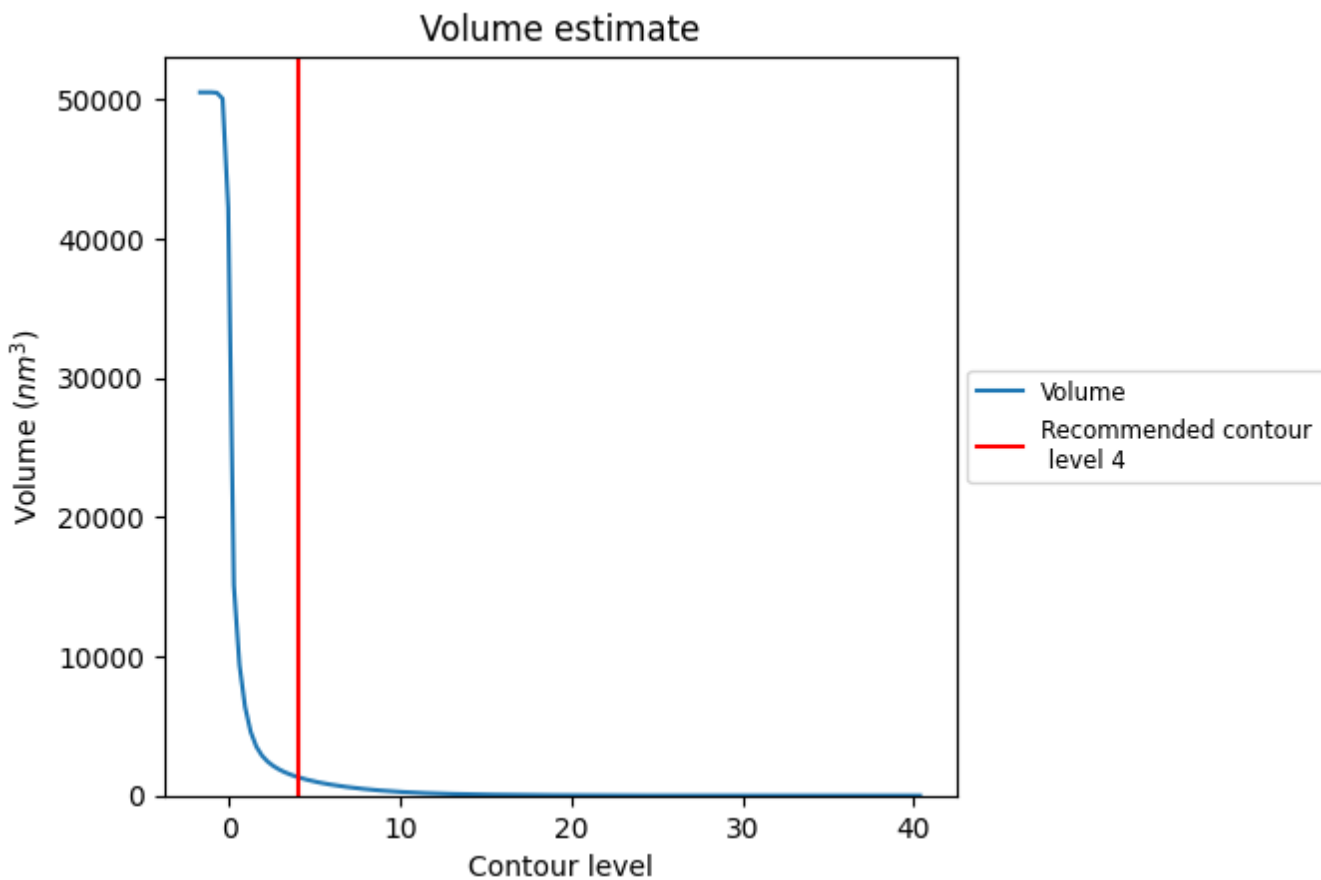
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

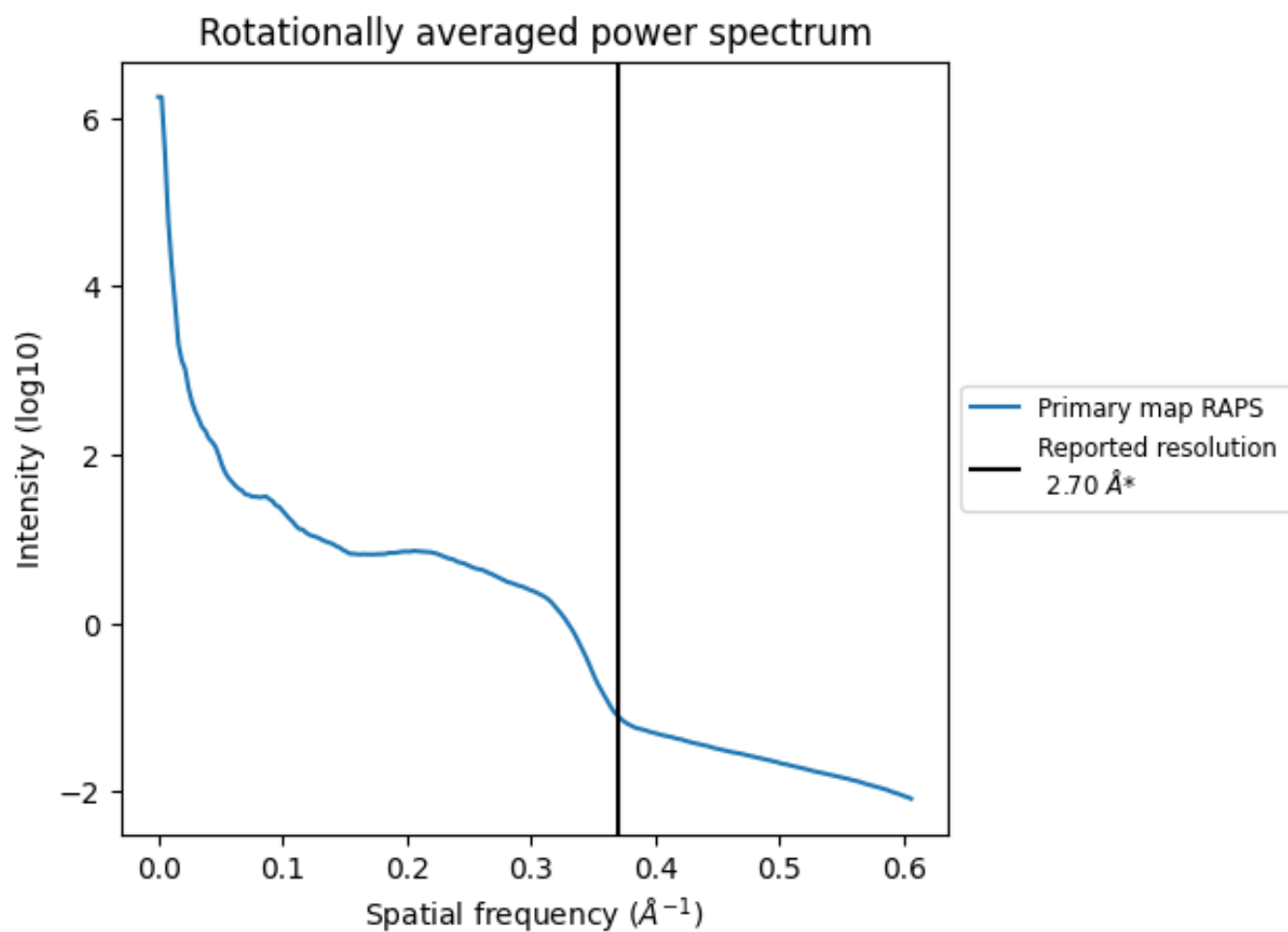
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1334  $\text{nm}^3$ ; this corresponds to an approximate mass of 1205 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



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

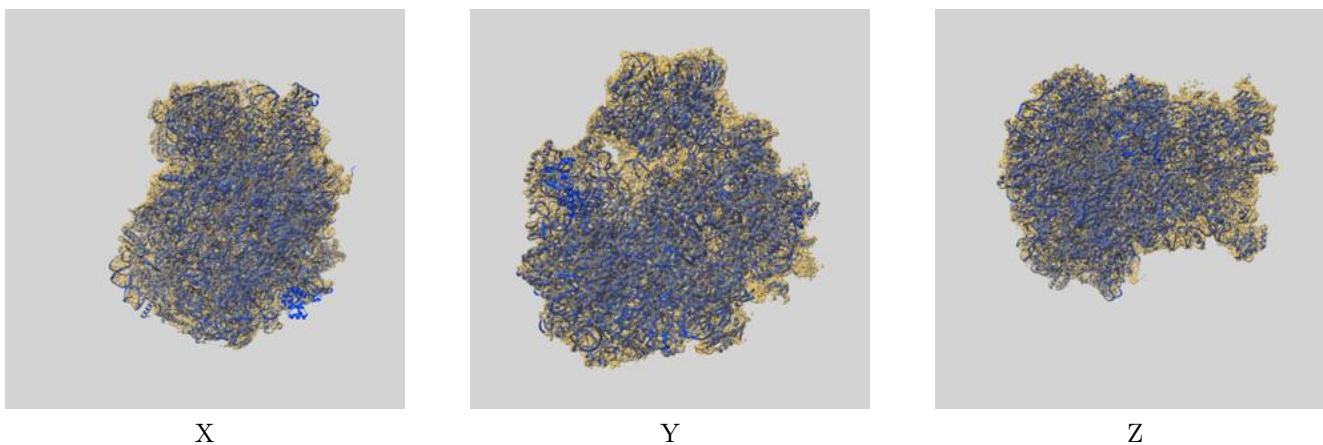
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

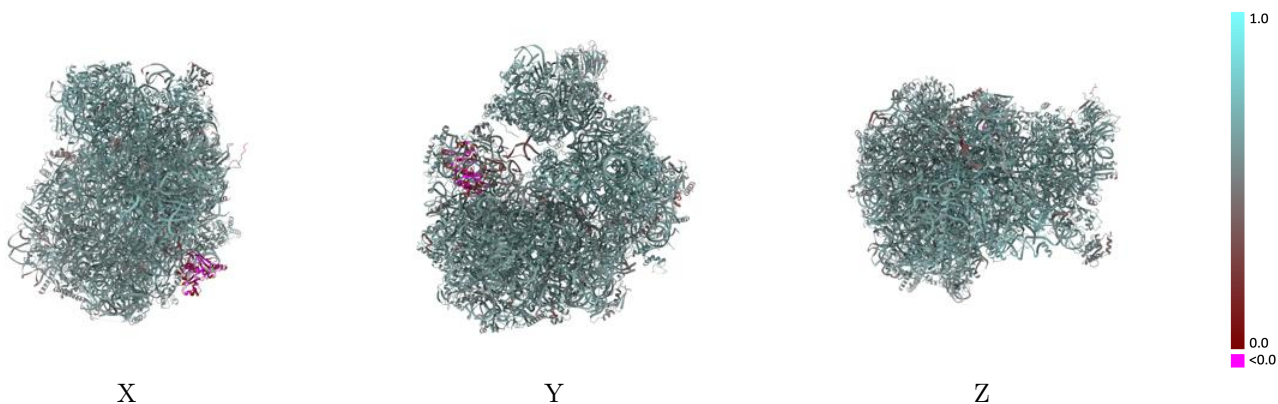
This section contains information regarding the fit between EMDB map EMD-72933 and PDB model 9YGM. Per-residue inclusion information can be found in section [3](#) on page [23](#).

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



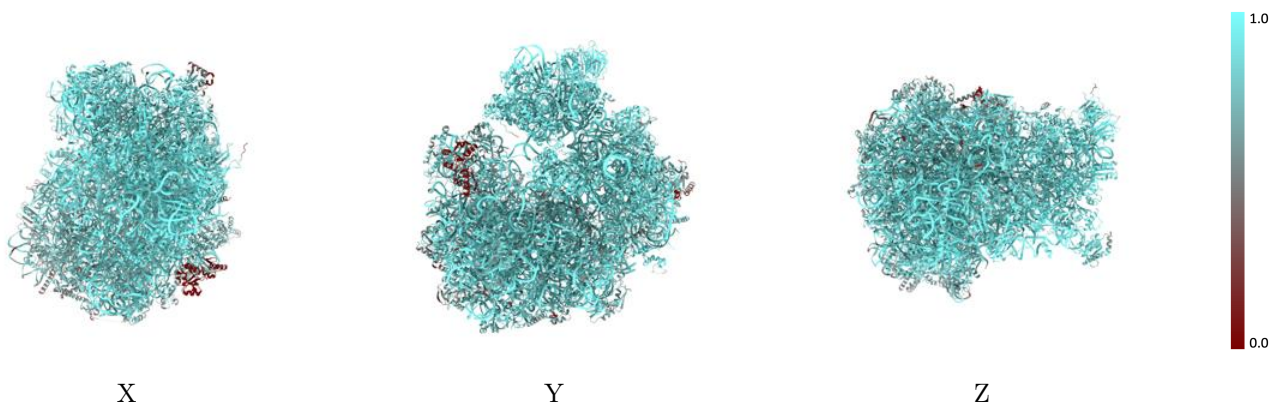
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



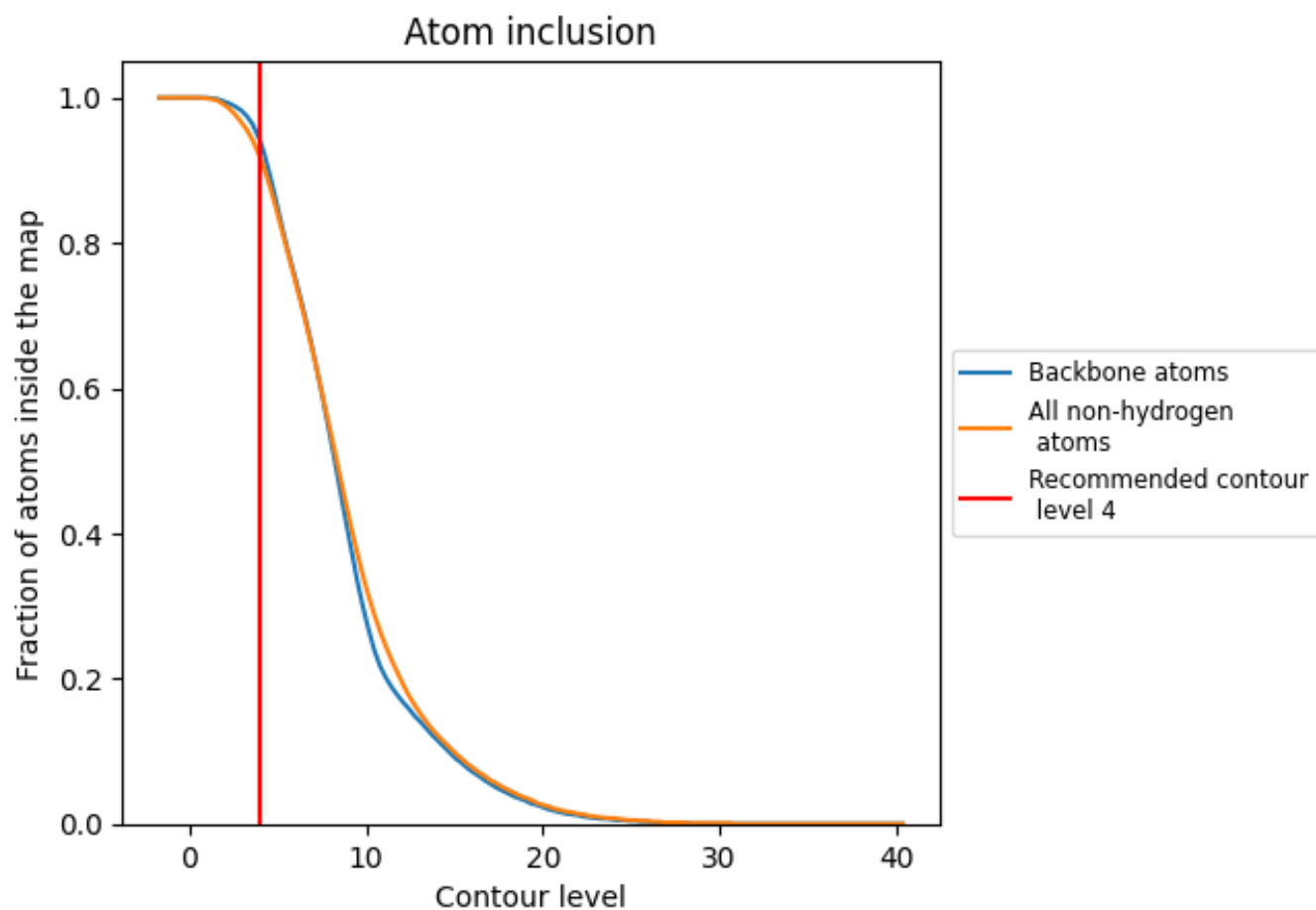
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.6000
L3	 0.9730	 0.6000
L4	 0.9410	 0.5990
L5	 0.9620	 0.6070
LA	 0.2130	 0.0540
LB	 0.9220	 0.6230
LC	 0.9070	 0.6200
LD	 0.7160	 0.5860
LE	 0.7710	 0.5430
LF	 0.7510	 0.5740
LG	 0.6490	 0.5500
LH	 0.7570	 0.5770
LI	 0.8460	 0.6020
LJ	 0.8360	 0.6030
LK	 0.8990	 0.5960
LL	 0.7250	 0.5830
LM	 0.8820	 0.6250
LN	 0.9280	 0.6310
LO	 0.7530	 0.5810
LP	 0.7740	 0.5710
LQ	 0.8480	 0.6090
LR	 0.8550	 0.5740
LS	 0.7780	 0.5890
LT	 0.7870	 0.5950
LU	 0.8960	 0.6190
LV	 0.7250	 0.5400
LW	 0.7930	 0.5840
LX	 0.8400	 0.5910
LY	 0.8720	 0.5790
LZ	 0.7280	 0.5630
La	 0.7610	 0.5640
Lb	 0.8440	 0.5950
Lc	 0.8320	 0.5950
Ld	 0.8530	 0.5680
Le	 0.8470	 0.6010











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Chain	Atom inclusion	Q-score
Lf	0.8560	0.6150
Lg	0.9140	0.6290
Lh	0.8970	0.6200
Li	0.8430	0.5910
Lj	0.9330	0.6360
Lk	0.7340	0.5650
Ll	0.8880	0.6260
Lm	0.7850	0.5860
Ln	0.9600	0.6440
Lo	0.9200	0.6090
Lp	0.8900	0.5800
S1	0.9900	0.6280
S7	0.9920	0.3800
SA	0.9290	0.6150
SB	0.8740	0.5850
SC	0.9590	0.5690
SD	0.9320	0.6280
SE	0.9430	0.6360
SF	0.9640	0.6340
SG	0.8870	0.6000
SH	0.9910	0.6140
SI	0.7150	0.5590
SJ	0.9680	0.6390
SK	0.9600	0.6260
SL	0.9870	0.6280
SM	0.9570	0.5780
SN	0.9860	0.5980
SO	0.9680	0.6150
SP	0.9410	0.6330
SQ	0.8110	0.4850
SR	0.9820	0.6070
SS	0.9950	0.6260
ST	0.9470	0.6290
SU	0.9660	0.6520
SV	0.9580	0.5790
SW	0.9720	0.5960
SX	0.9750	0.6170
SY	0.8900	0.6150
SZ	0.9290	0.6260
Sa	0.9410	0.5890
Sb	0.9620	0.6280
Sc	0.8850	0.6220

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Chain	Atom inclusion	Q-score
Sd	 0.9660	 0.5790
Se	 0.9220	 0.6180
Sf	 0.8960	 0.5500
Sg	 0.9200	 0.5620