



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:11 PM UTC

PDB ID : 7OLC / pdb_00007olc
EMDB ID : EMD-12976
Title : Thermophilic eukaryotic 80S ribosome at idle POST state
Authors : Kisonaite, M.; Wild, K.; Sinning, I.
Deposited on : 2021-05-19
Resolution : 2.90 Å(reported)
Based on initial model : 4V88

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

We welcome your comments at 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>.

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

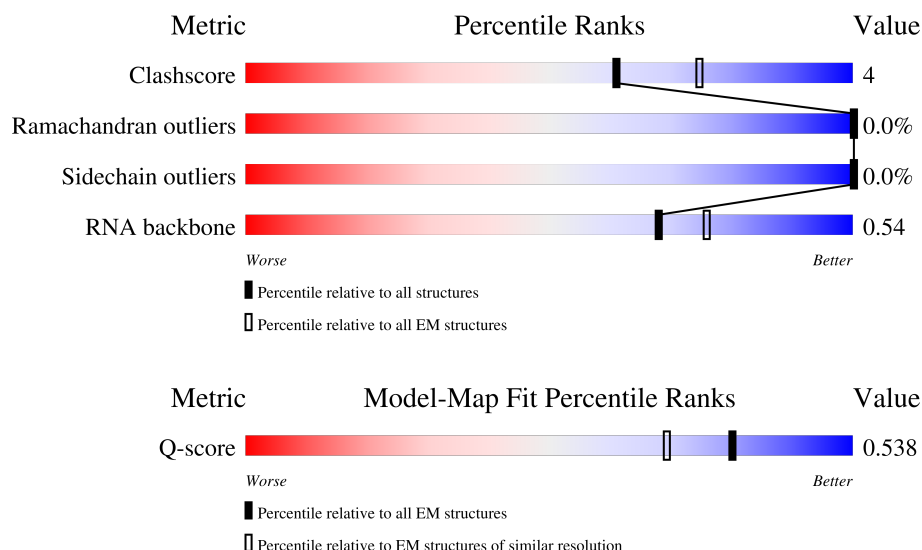
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 2.90 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.



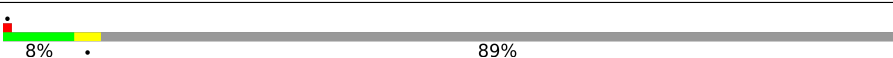
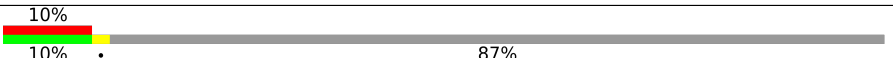
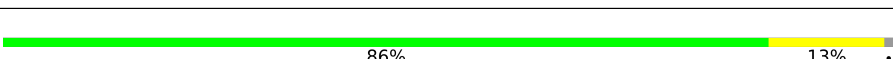
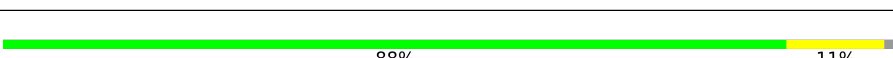
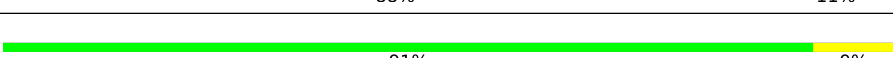
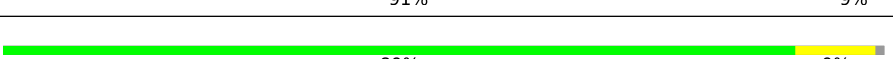
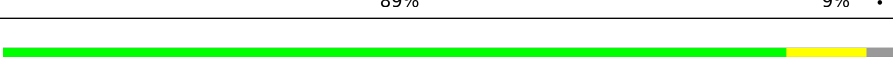
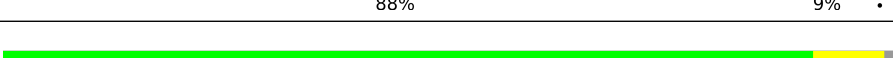
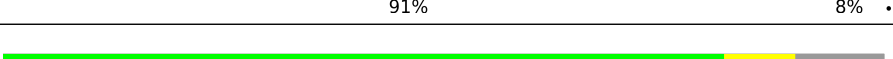
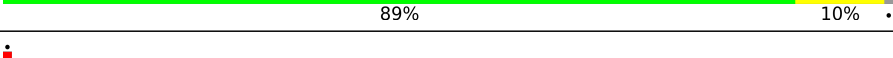
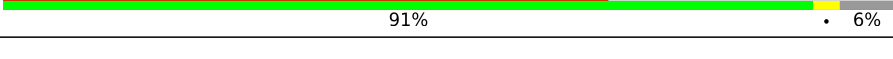
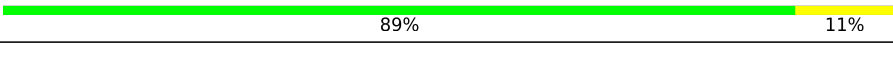
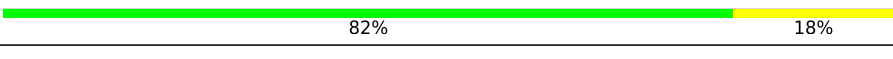
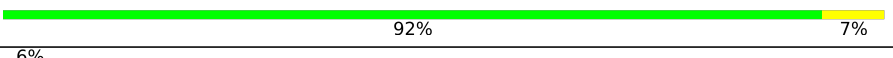
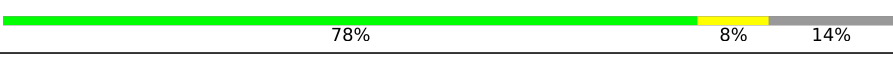
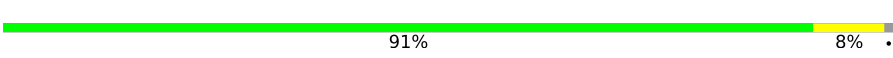
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	3337	
2	2	1796	
3	3	120	

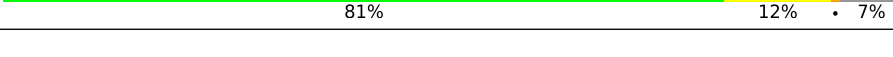
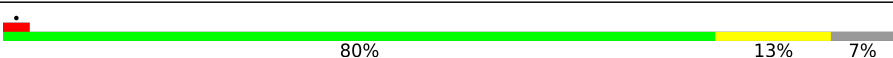
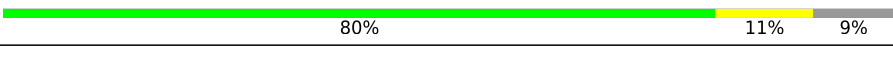
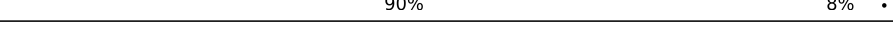
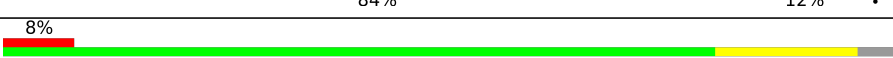
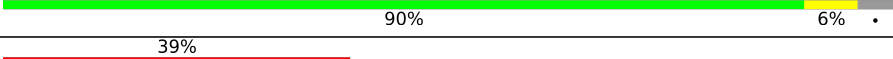
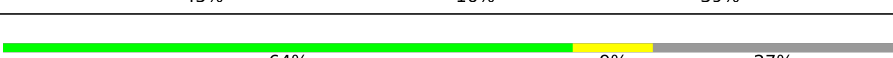
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Mol	Chain	Length	Quality of chain
4	4	156	
5	A	316	
6	B	302	
7	C	614	
8	LA	254	
9	LB	392	
10	LC	365	
11	LD	304	
12	LE	200	
13	LF	249	
14	LG	262	
15	LH	192	
16	LI	219	
17	LJ	173	
18	LK	165	
19	LL	213	
20	LM	142	
21	LN	203	
22	LO	204	
23	LP	187	
24	LQ	213	
25	LR	192	
26	LS	174	
27	LT	160	
28	LU	127	

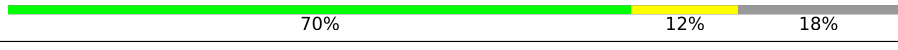
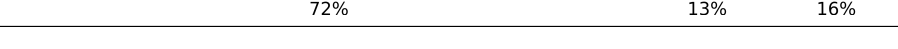
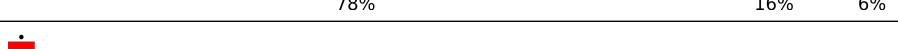
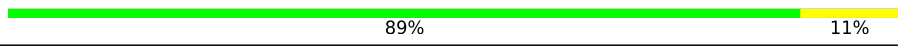
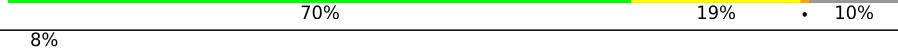
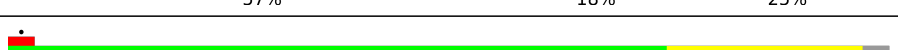
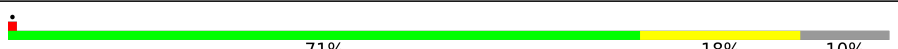
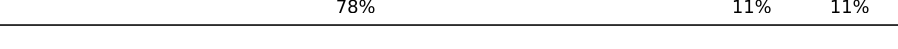
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Mol	Chain	Length	Quality of chain
29	LV	139	
30	LW	161	
31	LX	156	
32	LY	138	
33	LZ	135	
34	La	149	
35	Lb	65	
36	Lc	108	
37	Ld	120	
38	Le	131	
39	Lf	109	
40	Lg	119	
41	Lh	126	
42	Li	110	
43	Lj	95	
44	Lk	81	
45	Ll	51	
46	Lm	128	
47	Ln	25	
47	Lr	25	
48	Lo	106	
49	Lp	92	
50	Lq	147	
51	Ls	312	
52	SA	285	

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Mol	Chain	Length	Quality of chain
53	SB	255	
54	SC	263	
55	SD	254	
56	SE	264	
57	SF	212	
58	SG	239	
59	SH	203	
60	SI	202	
61	SJ	190	
62	SK	159	
63	SL	161	
64	SM	144	
65	SN	151	
66	SO	150	
67	SP	153	
68	SQ	143	
69	SR	143	
70	SS	156	
71	ST	153	
72	SU	116	
73	SV	98	
74	SW	130	
75	SX	145	
76	SY	136	
77	SZ	99	

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Mol	Chain	Length	Quality of chain
78	Sa	119	
79	Sb	82	
80	Sc	68	
81	Sd	56	
82	Se	62	
83	Sf	154	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 207344 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 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3191	Total	C	N	O	P	0	0
			68242	30465	12334	22252	3191		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1765	Total	C	N	O	P	0	0
			37645	16822	6706	12352	1765		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	119	Total	C	N	O	P	0	0
			2535	1132	453	831	119		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	156	Total	C	N	O	P	0	0
			3319	1484	589	1090	156		

- Molecule 5 is a protein called Putative guanine nucleotide-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	312	Total	C	N	O	S	0	0
			2438	1534	424	468	12		

- Molecule 6 is a protein called HABP4_PA1-RBP1 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	32	Total	C	N	O	0	0
			244	145	49	50		

- Molecule 7 is a protein called Ribosome-associated molecular chaperone SSB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	78	Total	C	N	O	S	0	0
			619	388	106	123	2		

- Molecule 8 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LA	252	Total	C	N	O	S	0	0
			1925	1203	385	334	3		

- Molecule 9 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	387	Total	C	N	O	S	0	0
			3088	1964	576	535	13		

- Molecule 10 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	363	Total	C	N	O	S	0	0
			2758	1741	527	481	9		

- Molecule 11 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	300	Total	C	N	O	S	0	0
			2440	1545	431	461	3		

- Molecule 12 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	194	Total	C	N	O	S	0	0
			1518	974	274	267	3		

- Molecule 13 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	235	Total	C	N	O	S	0	0
			1900	1218	351	326	5		

- Molecule 15 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	191	Total	C	N	O	S	0	0
			1505	955	269	275	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 16 is a protein called 60S ribosomal protein L10-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	217	Total	C	N	O	S	0	0
			1760	1109	343	299	9		

- Molecule 17 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	167	Total	C	N	O	S	0	0
			1367	854	268	239	6		

- Molecule 18 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LK	155	Total	C	N	O		0	0
			762	452	155	155			

- Molecule 19 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LL	209	Total	C	N	O	S	0	0
			1666	1037	340	287	2		

- Molecule 20 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LM	141	Total	C	N	O	S	0	0
			1125	714	216	194	1		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LN	202	Total	C	N	O	S	0	0
			1703	1062	360	277	4		

- Molecule 22 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LO	203	Total	C	N	O	S	0	0
			1613	1036	305	267	5		

- Molecule 23 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LP	186	Total	C	N	O	S	0	0
			1472	912	295	262	3		

- Molecule 24 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LQ	183	Total	C	N	O	S	0	0
			1481	935	306	238	2		

- Molecule 25 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LR	184	Total	C	N	O	S	0	0
			1506	928	324	249	5		

- Molecule 26 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	173	Total	C	N	O	S	0	0
			1425	917	266	238	4		

- Molecule 27 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	158	Total	C	N	O	S	0	0
			1266	803	246	215	2		

- Molecule 28 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LU	101	Total	C	N	O	S	0	0
			819	532	142	144	1		

- Molecule 29 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LV	135	Total	C	N	O	S	0	0
			994	633	185	169	7		

- Molecule 30 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LW	133	Total	C	N	O	S	0	0
			1075	667	221	185	2		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	VAL	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	PHE	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	HIS	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ASP	deletion	UNP G0S1P9
LW	?	-	ASN	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ASP	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	HIS	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	GLY	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	ILE	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9
LW	?	-	PRO	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	GLN	deletion	UNP G0S1P9
LW	?	-	LEU	deletion	UNP G0S1P9
LW	?	-	ARG	deletion	UNP G0S1P9
LW	?	-	ALA	deletion	UNP G0S1P9
LW	?	-	GLU	deletion	UNP G0S1P9
LW	?	-	VAL	deletion	UNP G0S1P9
LW	?	-	GLN	deletion	UNP G0S1P9
LW	?	-	LYS	deletion	UNP G0S1P9
LW	?	-	THR	deletion	UNP G0S1P9
LW	?	-	SER	deletion	UNP G0S1P9
LW	?	-	MET	deletion	UNP G0S1P9

- Molecule 31 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	LX	121	Total	C	N	O	0	0
			965	620	175	170		

- Molecule 32 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LZ	135	Total	C	N	O	S	0	0
			1111	713	207	187	4		

- Molecule 34 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	La	148	Total	C	N	O	S	0	0
			1180	745	239	194	2		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
La	1	MET	TYR	conflict	UNP G0SGT6
La	3	THR	-	insertion	UNP G0SGT6
La	4	ARG	VAL	conflict	UNP G0SGT6
La	6	SER	GLN	conflict	UNP G0SGT6
La	7	LYS	ASP	conflict	UNP G0SGT6
La	8	THR	LYS	conflict	UNP G0SGT6
La	9	ARG	LYS	conflict	UNP G0SGT6
La	10	LYS	ALA	conflict	UNP G0SGT6
La	11	HIS	PRO	conflict	UNP G0SGT6
La	13	GLY	PRO	conflict	UNP G0SGT6
La	14	HIS	ARG	conflict	UNP G0SGT6
La	16	SER	-	insertion	UNP G0SGT6
La	17	ALA	-	insertion	UNP G0SGT6
La	18	GLY	-	insertion	UNP G0SGT6
La	19	LYS	ARG	conflict	UNP G0SGT6
La	20	GLY	ARG	conflict	UNP G0SGT6

- Molecule 35 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lb	62	Total	C	N	O		0	0
			508	310	112	86			

- Molecule 36 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lc	97	Total	C	N	O	S	0	0
			722	458	125	134	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ld	112	Total	C	N	O	S	0	0
			911	575	178	157	1		

- Molecule 38 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Le	124	Total	C	N	O	S	0	0
			1001	629	205	161	6		

- Molecule 39 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lf	107	Total	C	N	O	S	0	0
			853	540	170	142	1		

- Molecule 40 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lg	112	Total	C	N	O	S	0	0
			891	554	181	152	4		

- Molecule 41 is a protein called Dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lh	122	Total	C	N	O	S	0	0
			1003	637	198	168			

- Molecule 42 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Li	102	Total	C	N	O	S	0	0
			836	515	184	136	1		

- Molecule 43 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lj	86	Total	C	N	O	S	0	0
			684	418	152	109	5		

- Molecule 44 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89

- Molecule 45 is a protein called eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Ll	50	Total	C	N	O	0	0
			435	275	97	63		

- Molecule 46 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lm	52	Total	C	N	O	S	0	0
			418	261	86	65	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lm	1	MET	SER	conflict	UNP G0S8G4
Lm	2	GLN	ARG	conflict	UNP G0S8G4

- Molecule 47 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ln	24	Total	C	N	O	S	0	0
			224	136	61	26	1		
47	Lr	24	Total	C	N	O	S	0	0
			224	136	61	26	1		

- Molecule 48 is a protein called 60S ribosomal protein L44-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lo	104	Total	C	N	O	S	0	0
			822	520	161	136	5		

- Molecule 49 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lp	91	Total	C	N	O	S	0	0
			697	430	138	123	6		

- Molecule 50 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lq	141	Total	C	N	O	S	0	0
			1083	678	215	190			

- Molecule 51 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ls	189	Total	C	N	O	S	0	0
			1449	927	250	265	7		

- Molecule 52 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SA	208	Total	C	N	O	S	0	0
			1641	1051	289	295	6		

- Molecule 53 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SB	232	Total	C	N	O	S	0	0
			1871	1190	351	325	5		

- Molecule 54 is a protein called 40S ribosomal protein S2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SC	216	Total	C	N	O	S	0	0
			1672	1074	294	301	3		

- Molecule 55 is a protein called 40S ribosomal protein S3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SD	214	Total	C	N	O	S	0	0
			1688	1068	307	305	8		

- Molecule 56 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SE	261	Total	C	N	O	S	0	0
			2072	1314	389	362	7		

- Molecule 57 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SF	199	Total	C	N	O	S	0	0
			1557	971	294	285	7		

- Molecule 58 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SG	232	Total	C	N	O	S	0	0
			1875	1171	376	323	5		

- Molecule 59 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SH	195	Total	C	N	O	S	0	0
			1562	983	300	279			

- Molecule 60 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SI	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 61 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SJ	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 62 is a protein called 40S ribosomal protein s10-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SK	89	Total	C	N	O	S	0	0
			742	487	124	129	2		

- Molecule 63 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SL	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 64 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SM	118	Total	C	N	O	S	0	0
			923	577	167	171	8		

- Molecule 65 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SN	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 66 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SO	135	Total	C	N	O	S	0	0
			1002	614	199	184	5		

- Molecule 67 is a protein called 40S ribosomal protein s15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SP	115	Total	C	N	O	S	0	0
			917	583	172	159	3		

- Molecule 68 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SQ	138	Total	C	N	O	S	0	0
			1081	693	202	184	2		

- Molecule 69 is a protein called 40S ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SR	128	Total	C	N	O	S	0	0
			1045	657	190	195	3		

- Molecule 70 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	137	Total	C	N	O	S	0	0
			1118	699	222	196	1		

- Molecule 71 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	ST	142	Total	C	N	O	S	0	0
			1117	694	221	201	1		

- Molecule 72 is a protein called 40S ribosomal protein S20-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SU	103	Total	C	N	O	S	0	0
			819	517	150	148	4		

- Molecule 73 is a protein called 40S ribosomal protein S21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SV	86	Total	C	N	O	S	0	0
			664	408	124	128	4		

- Molecule 74 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SW	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 75 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SX	142	Total	C	N	O	S	0	0
			1099	694	215	188	2		

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SY	132	Total	C	N	O	S	0	0
			1061	668	209	182	2		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SZ	69	Total	C	N	O	S	0	0
			546	345	101	98	2		

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sa	104	Total	C	N	O	S	0	0
			839	518	177	137	7		

- Molecule 79 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sb	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 80 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sc	61	Total	C	N	O	S	0	0
			484	298	97	88	1		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sd	52	Total	C	N	O	S	0	0
			419	261	84	70	4		

- Molecule 82 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Se	40	Total	C	N	O	0	0
			322	202	67	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sf	73	Total	C	N	O	S	0	0
			604	382	115	101	6		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	1	415	Total	Mg	0
			415	415	
84	2	121	Total	Mg	0
			121	121	
84	3	8	Total	Mg	0
			8	8	
84	4	11	Total	Mg	0
			11	11	
84	LA	1	Total	Mg	0
			1	1	
84	LB	1	Total	Mg	0
			1	1	
84	LI	1	Total	Mg	0
			1	1	
84	LN	3	Total	Mg	0
			3	3	
84	LP	1	Total	Mg	0
			1	1	
84	LT	2	Total	Mg	0
			2	2	
84	LV	1	Total	Mg	0
			1	1	
84	Lb	1	Total	Mg	0
			1	1	
84	Lo	1	Total	Mg	0
			1	1	
84	SN	1	Total	Mg	0
			1	1	
84	SO	1	Total	Mg	0
			1	1	
84	SQ	1	Total	Mg	0
			1	1	
84	SX	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Lg	1	Total 1	Zn 1	0
85	Lj	1	Total 1	Zn 1	0
85	Lm	1	Total 1	Zn 1	0
85	Lo	1	Total 1	Zn 1	0
85	Lp	1	Total 1	Zn 1	0
85	Sa	1	Total 1	Zn 1	0
85	Sb	1	Total 1	Zn 1	0
85	Sd	1	Total 1	Zn 1	0

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	1	748	Total 748	O 748	0
86	2	136	Total 136	O 136	0
86	4	20	Total 20	O 20	0
86	LB	3	Total 3	O 3	0
86	LC	3	Total 3	O 3	0
86	LD	1	Total 1	O 1	0
86	LN	6	Total 6	O 6	0
86	LO	5	Total 5	O 5	0
86	LP	2	Total 2	O 2	0
86	LQ	1	Total 1	O 1	0
86	LT	4	Total 4	O 4	0
86	LW	4	Total 4	O 4	0

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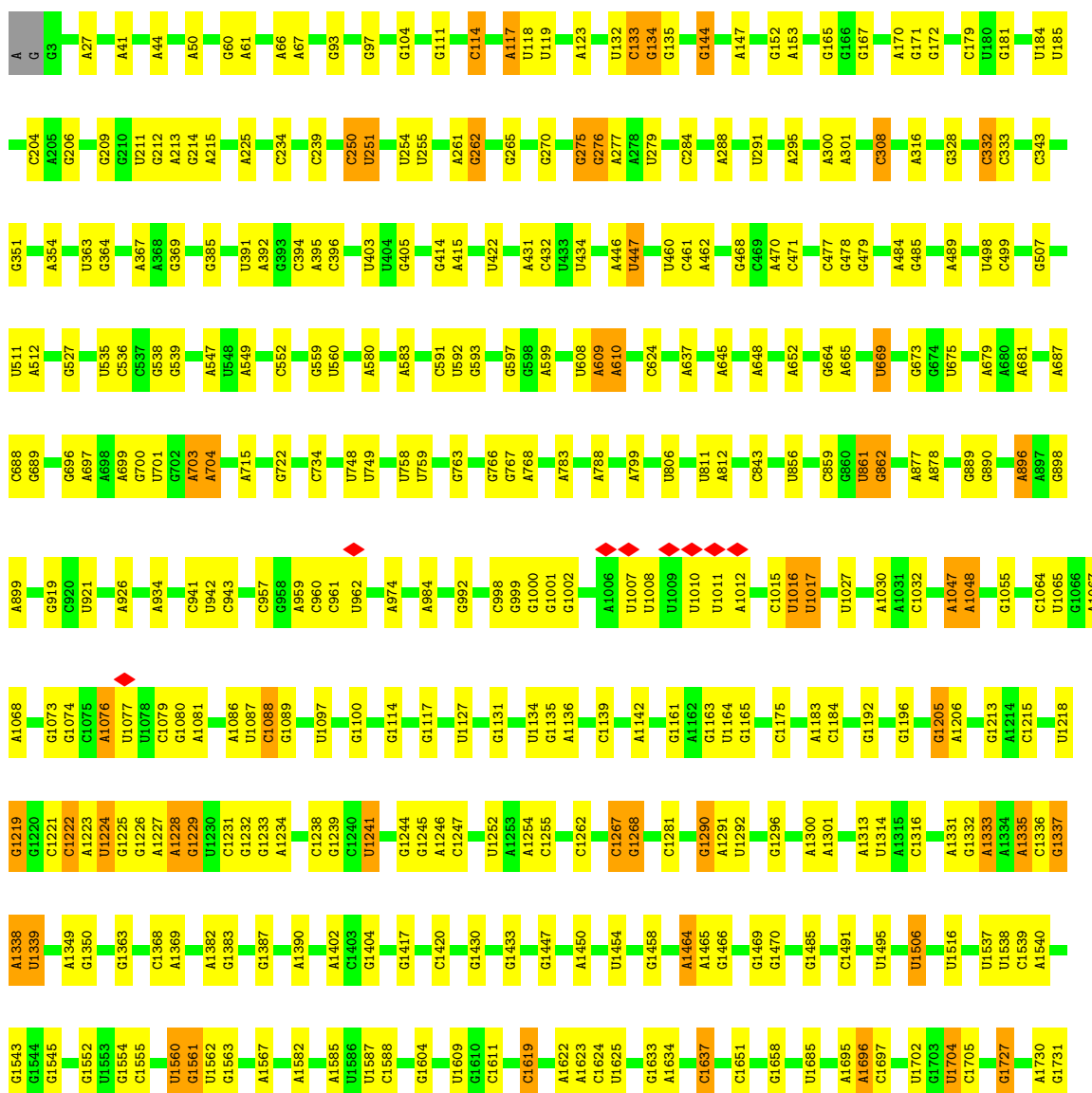
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86	Lb	1	Total 1	O 1	0
86	Ld	1	Total 1	O 1	0
86	Le	4	Total 4	O 4	0
86	Lj	1	Total 1	O 1	0
86	SL	2	Total 2	O 2	0
86	SN	2	Total 2	O 2	0
86	Sa	1	Total 1	O 1	0

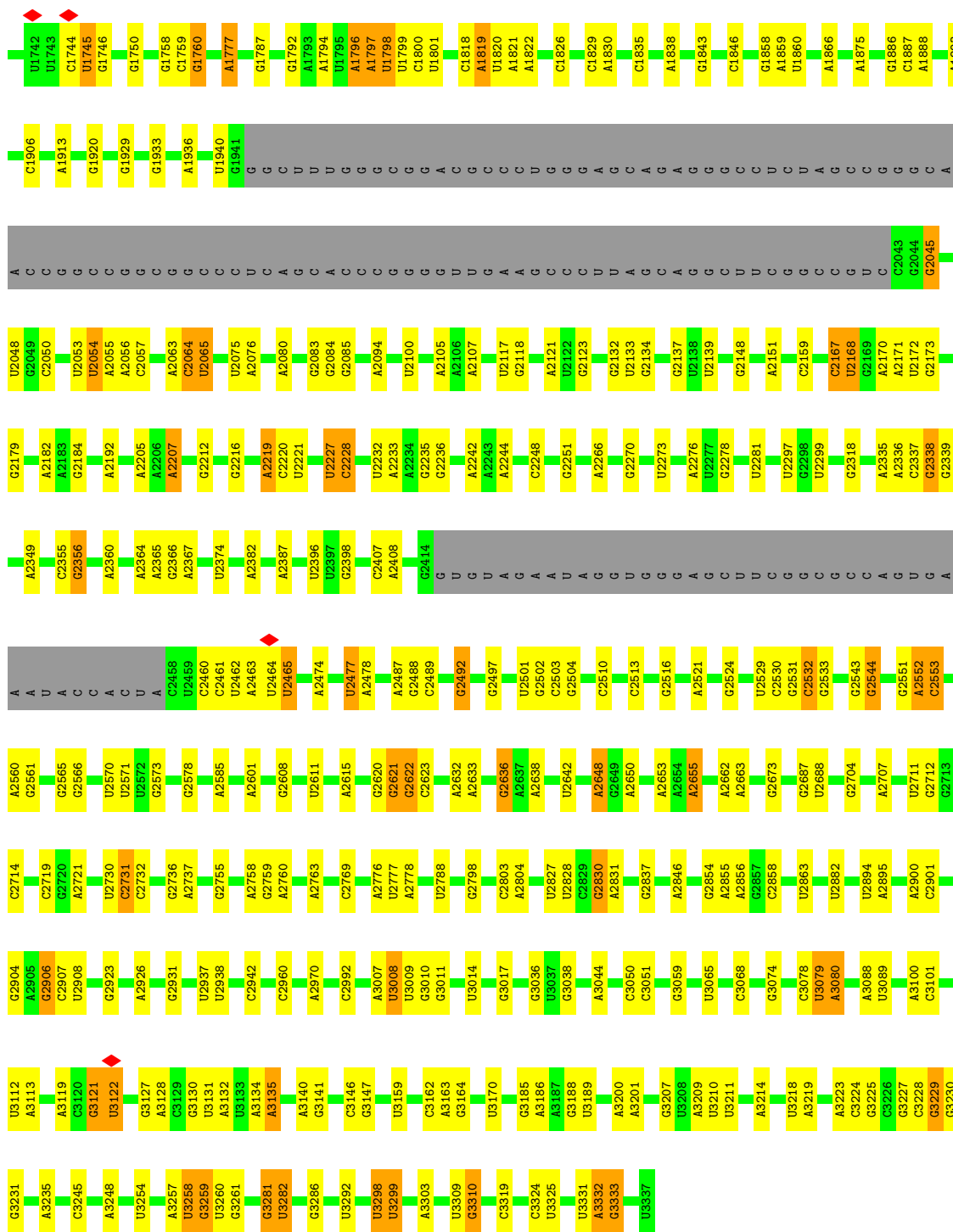
3 Residue-property plots

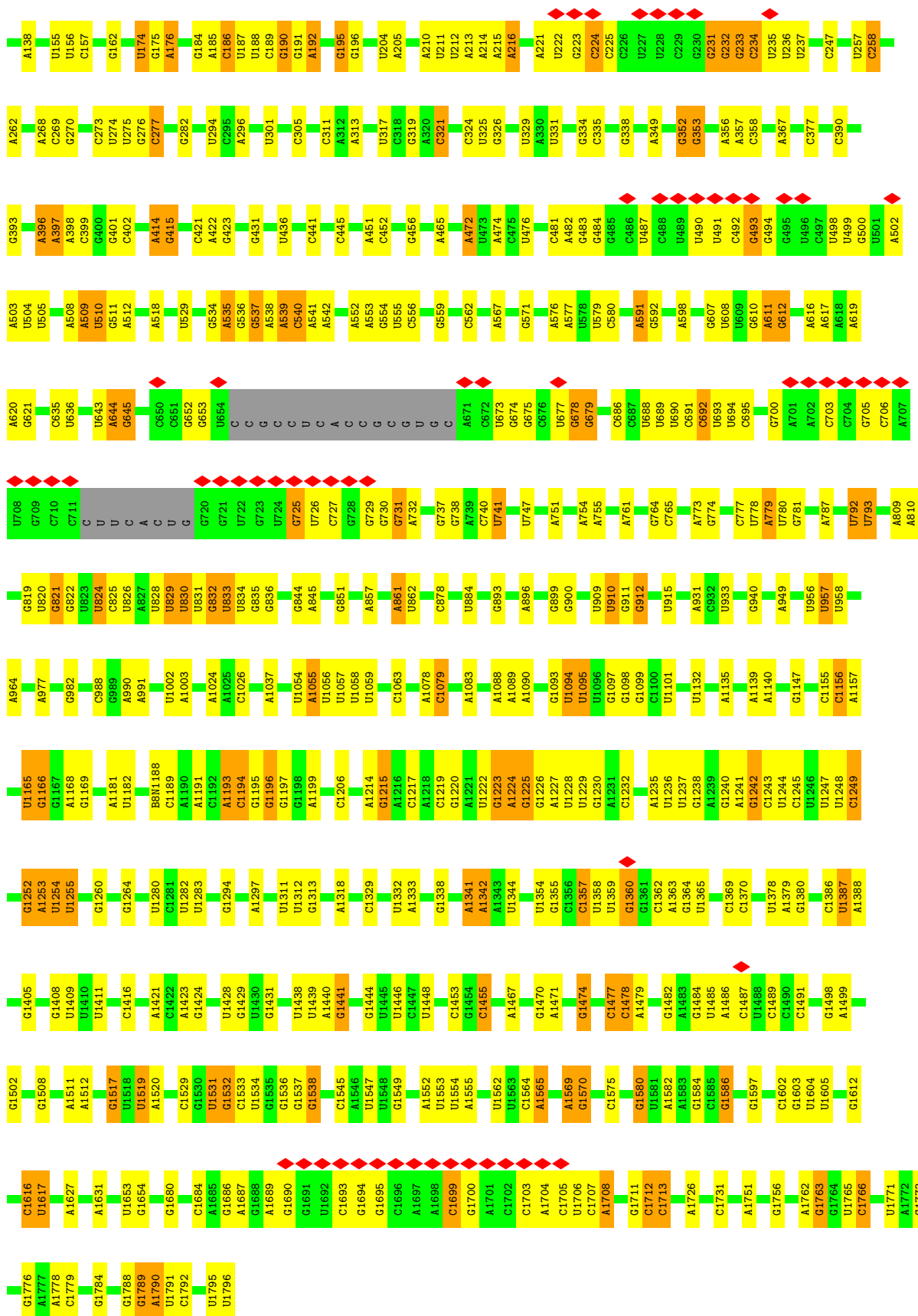
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 26S rRNA

Chain 1:  74% 18%

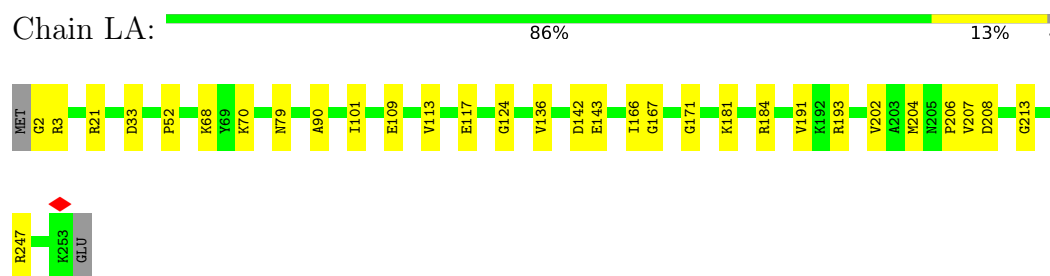




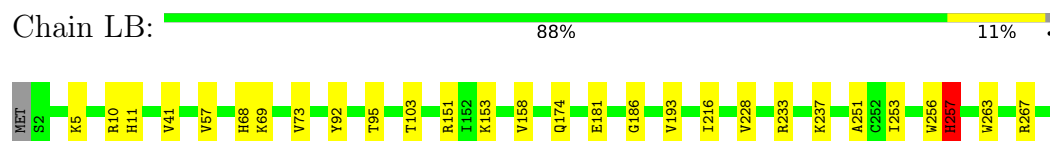


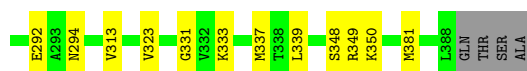
• Molecule 3: 5S rRNA

- Molecule 8: 60S ribosomal protein L2-like protein



- Molecule 9: 60S ribosomal protein L3-like protein





- Molecule 10: 60S ribosomal protein L4-like protein

Chain LC: 91% 9%



- Molecule 11: 60S ribosomal protein l5-like protein

Chain LD: 89% 9%



GLU

- Molecule 12: 60S ribosomal protein L6

Chain LE: 88% 9%



- Molecule 13: 60S ribosomal protein l7-like protein

Chain LF: 91% 8%



- Molecule 14: 60S ribosomal protein L8

Chain LG: 81% 8% 10%



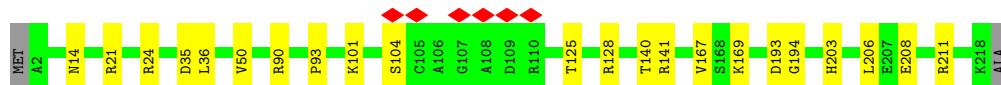
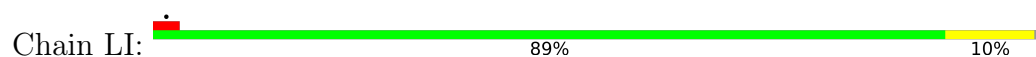
G237, E249, R252, K253, E257, THR, ALA, ILE, LYS, VAL

- Molecule 15: 60S ribosomal protein l9-like protein

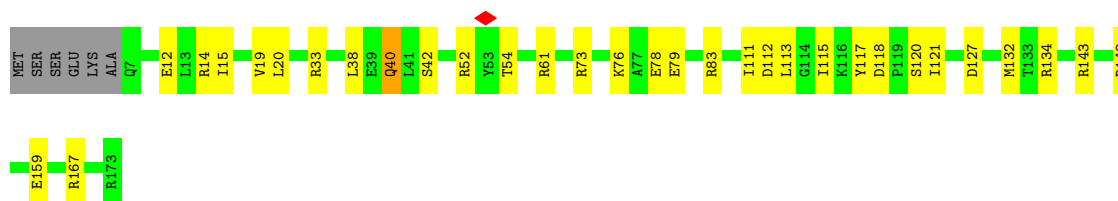
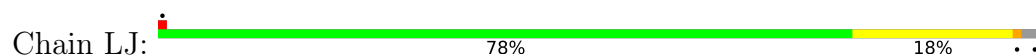
Chain LH: 83% 16%



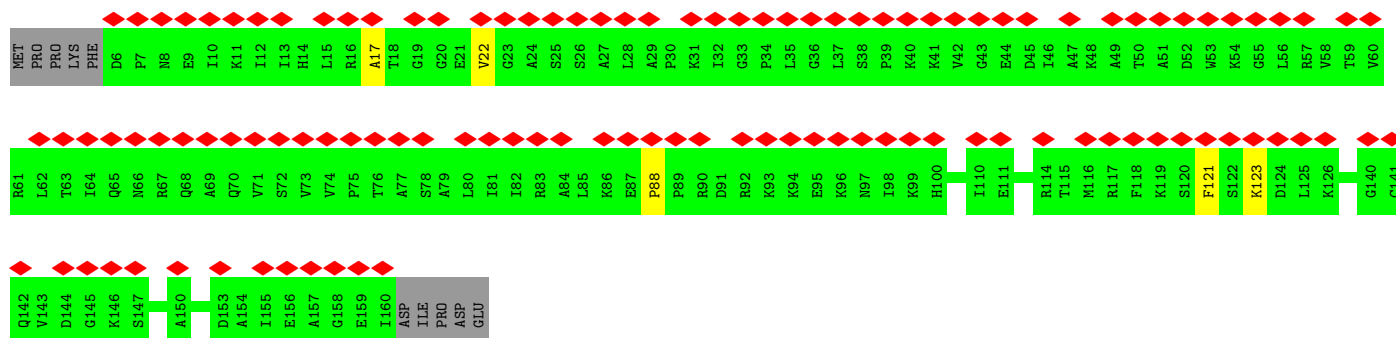
- Molecule 16: 60S ribosomal protein L10-like protein



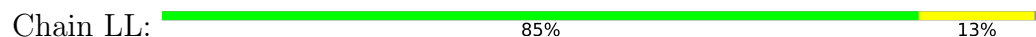
- Molecule 17: Putative ribosomal protein



- Molecule 18: 60S ribosomal protein L12-like protein



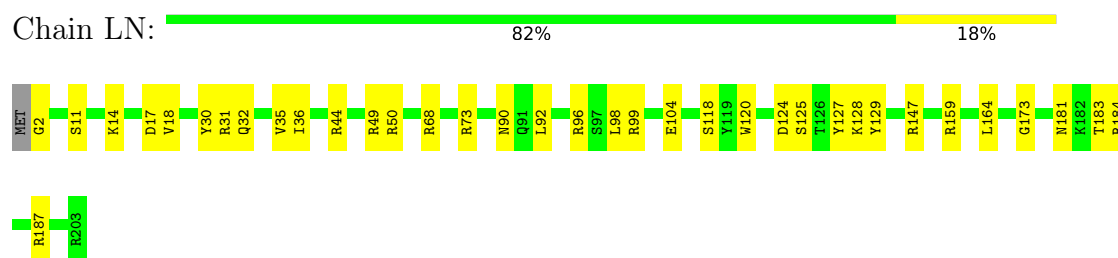
- Molecule 19: 60S ribosomal protein L13



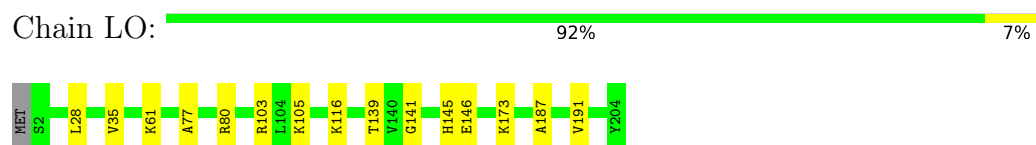
- Molecule 20: 60S ribosomal protein L14-like protein



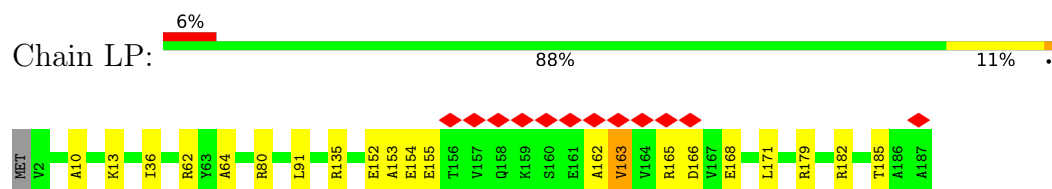
- Molecule 21: Ribosomal protein L15



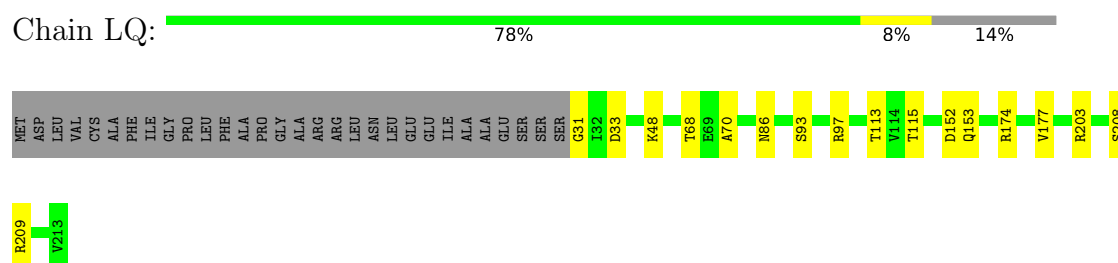
- Molecule 22: 60S ribosomal protein L16-like protein



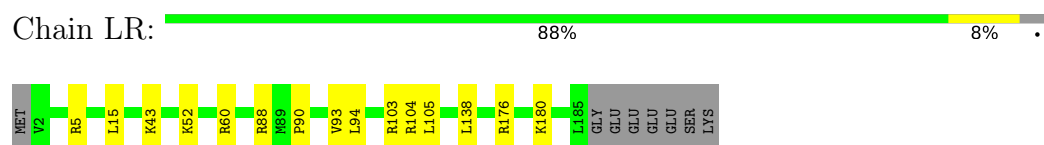
- Molecule 23: 60S ribosomal protein l17-like protein



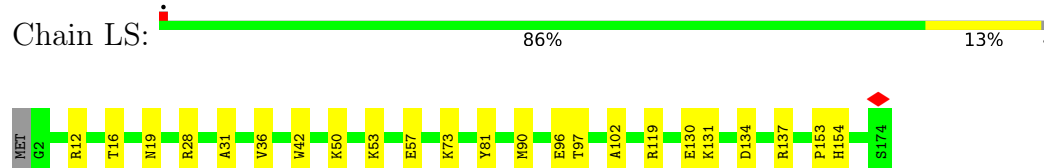
- Molecule 24: Ribosomal protein L18-like protein



- Molecule 25: Ribosomal protein L19

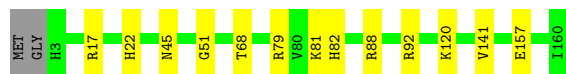


- Molecule 26: 60S ribosomal protein L20



- Molecule 27: 60S ribosomal protein l21-like protein

Chain LT:  91% 8% .



- Molecule 28: 60S ribosomal protein L22-like protein

Chain LU:  70% 9% 20%



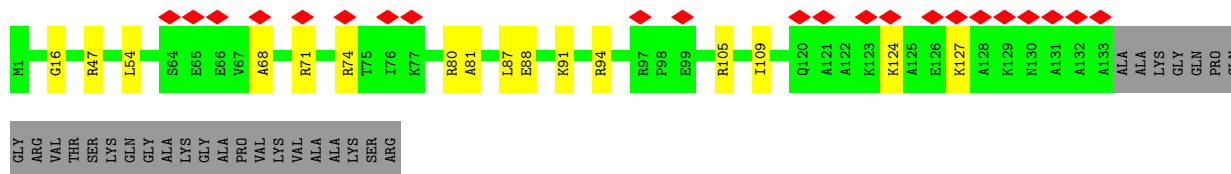
- Molecule 29: 60S ribosomal protein l23-like protein

Chain LV:  89% 8% .



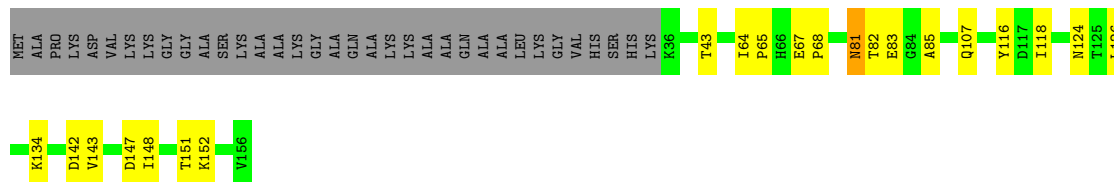
- Molecule 30: 60S ribosomal protein L24-like protein

Chain LW:  14% 73% 10% 17%



- Molecule 31: 60S ribosomal protein L25-like protein

Chain LX:  64% 13% 22%



- Molecule 32: 60S ribosomal protein L26-like protein

Chain LY:  83% 14% .



- Molecule 33: 60S ribosomal protein L27

Chain LZ:  87% 13%



- Molecule 34: 60S ribosomal protein L28-like protein

Chain La:  86% 13%



- Molecule 35: 60S ribosomal protein L29

Chain Lb:  86% 9% 5%



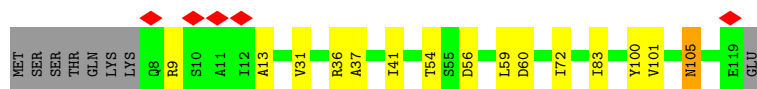
- Molecule 36: 60S ribosomal protein l30-like protein

Chain Lc:  80% 10% 10%



- Molecule 37: Putative 60S ribosomal protein

Chain Ld:  81% 12% 7%



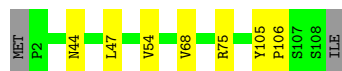
- Molecule 38: 60S ribosomal protein L32-like protein

Chain Le:  88% 7% 5%



- Molecule 39: 60S ribosomal protein l33-like protein

Chain Lf:  92% 6%



- Molecule 40: Ribosomal protein l34-like protein

Chain Lg:  86% 8% 6%



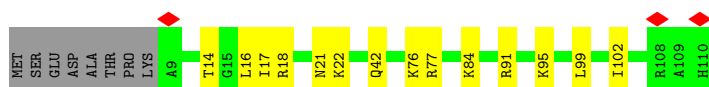
- Molecule 41: Dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:  84% 13% .



- Molecule 42: 60S ribosomal protein L36

Chain Li:  80% 13% 7%



- Molecule 43: Ribosomal protein L37

Chain Lj:  80% 11% 9%



- Molecule 44: 60S ribosomal protein L38-like protein

Chain Lk:  79% 15% 6%



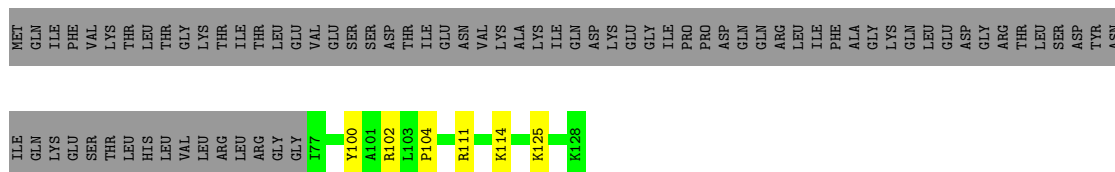
- Molecule 45: eL39

Chain Ll:  90% 8% .



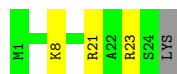
- Molecule 46: Ubiquitin

Chain Lm:  36% 5% 59%



- Molecule 47: 60S ribosomal protein L41-A

Chain Ln:  84% 12%



- Molecule 47: 60S ribosomal protein L41-A

Chain Lr:  8% 80% 16%



- Molecule 48: 60S ribosomal protein L44-like protein

Chain Lo:  90% 8%



- Molecule 49: 60S ribosomal protein L43-like protein

Chain Lp:  86% 13%

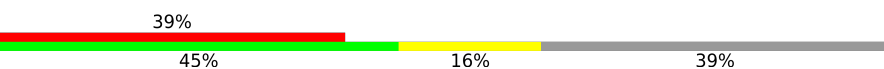


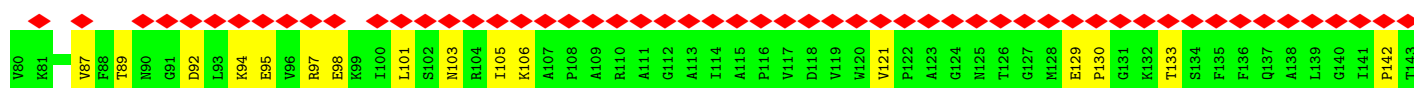
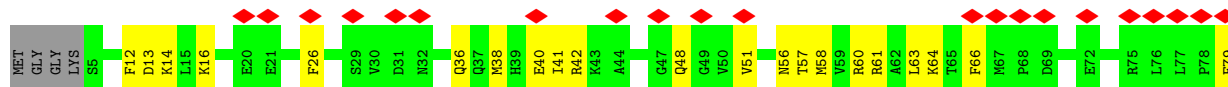
- Molecule 50: Putative 60S ribosomal protein

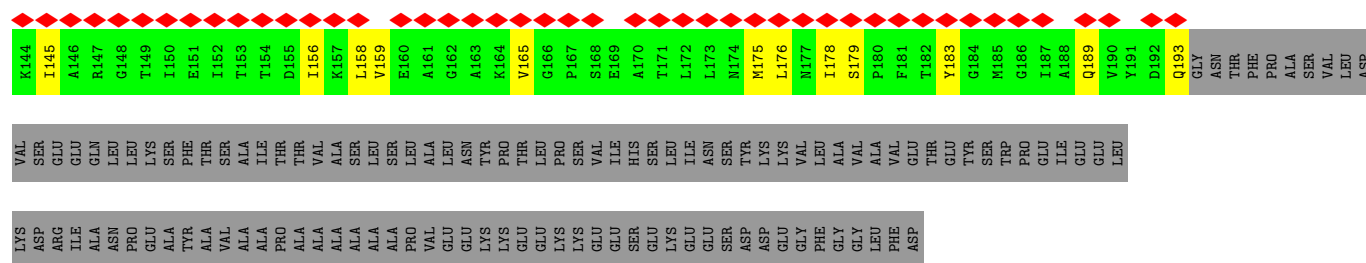
Chain Lq:  90% 6%



- Molecule 51: 60S acidic ribosomal protein P0

Chain Ls:  39% 45% 16% 39%





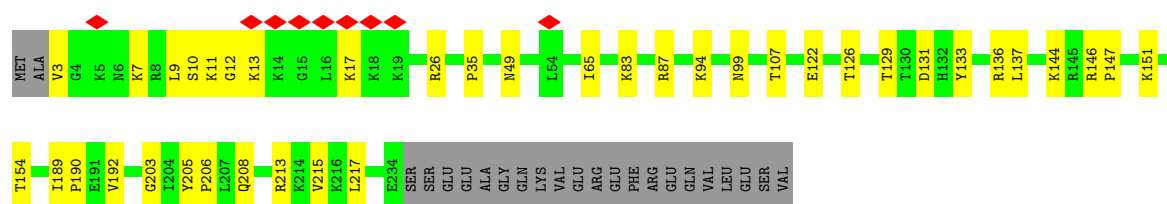
• Molecule 52: 40S ribosomal protein S0

Chain SA: 64% 9% 27%



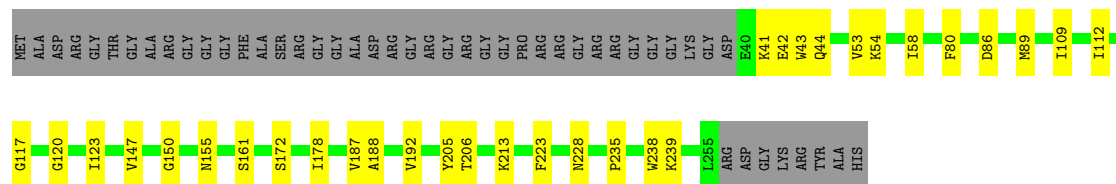
• Molecule 53: 40S ribosomal protein S1

Chain SB: 76% 15% 9%



• Molecule 54: 40S ribosomal protein S2-like protein

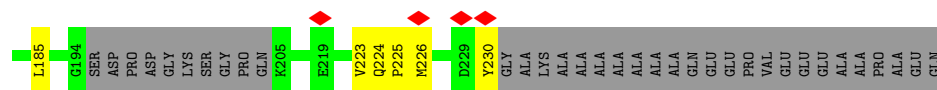
Chain SC: 70% 12% 18%



• Molecule 55: 40S ribosomal protein S3-like protein

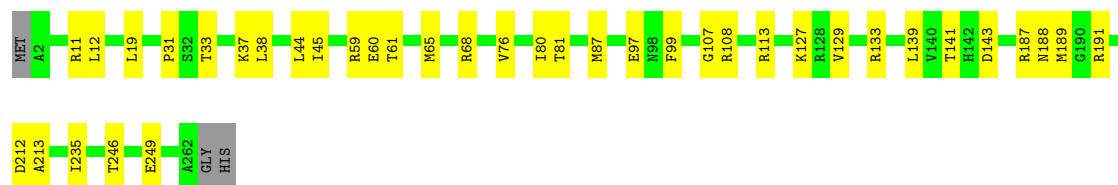
Chain SD: 72% 13% 16%





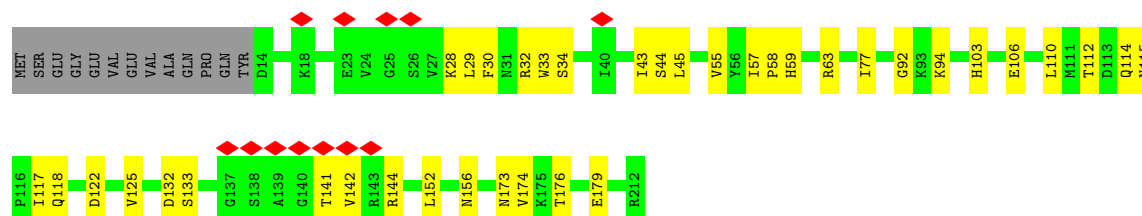
- Molecule 56: 40S ribosomal protein S4

Chain SE: 84% 14%



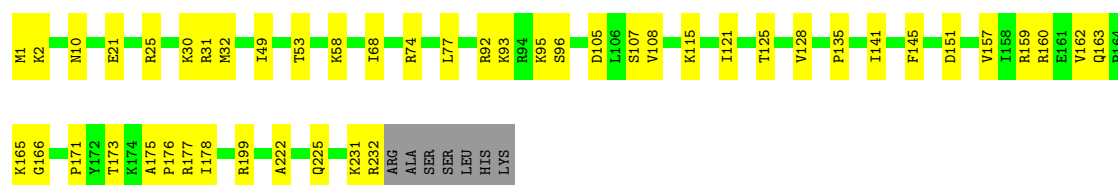
- Molecule 57: 40S ribosomal protein s5-like protein

Chain SF: 6% 76% 18% 6%



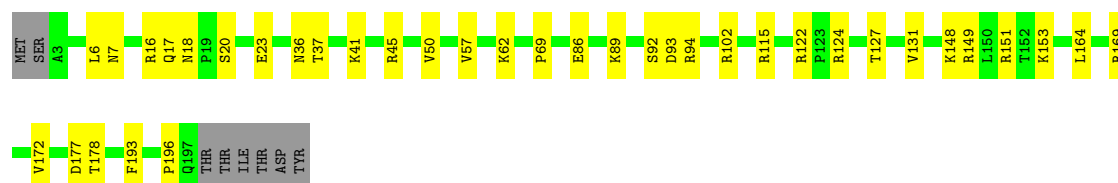
- Molecule 58: 40S ribosomal protein S6

Chain SG: 77% 20%



- Molecule 59: 40S ribosomal protein S7

Chain SH: 78% 18%

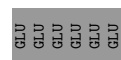
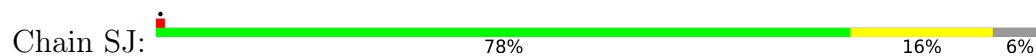


- Molecule 60: 40S ribosomal protein S8

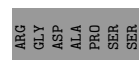
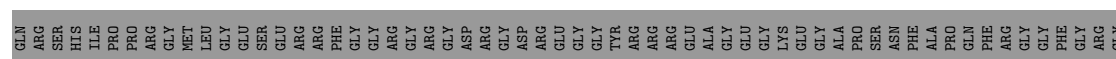
Chain SI: 84% 15%



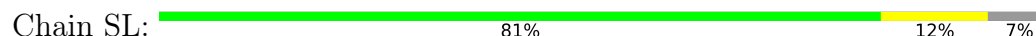
- Molecule 61: 40S ribosomal protein s9-like protein



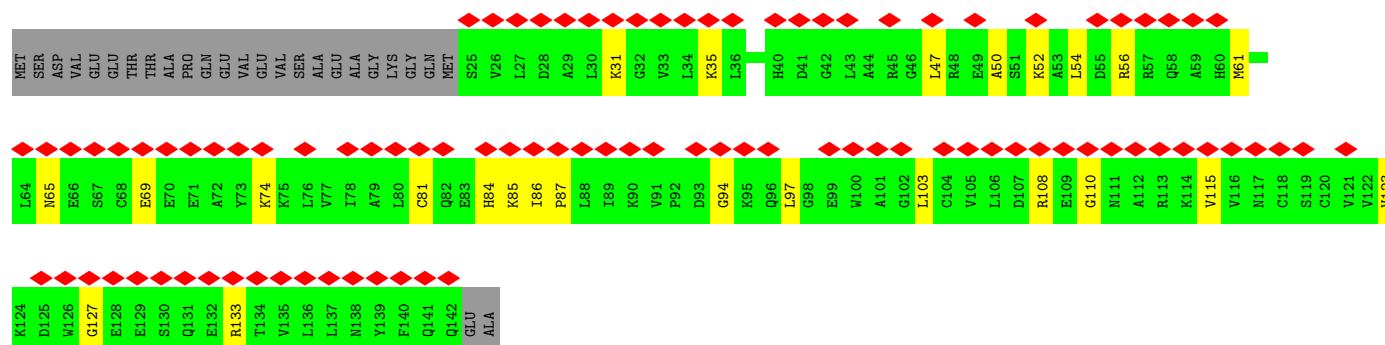
- Molecule 62: 40S ribosomal protein s10-like protein



- Molecule 63: 40S ribosomal protein S11-like protein



- Molecule 64: 40S ribosomal protein S12



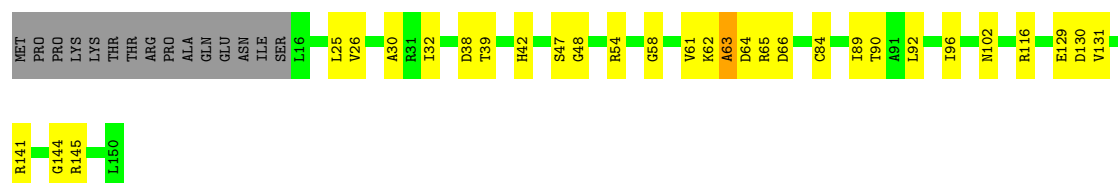
- Molecule 65: 40S ribosomal protein S13-like protein

Chain SN:  89% 11% .



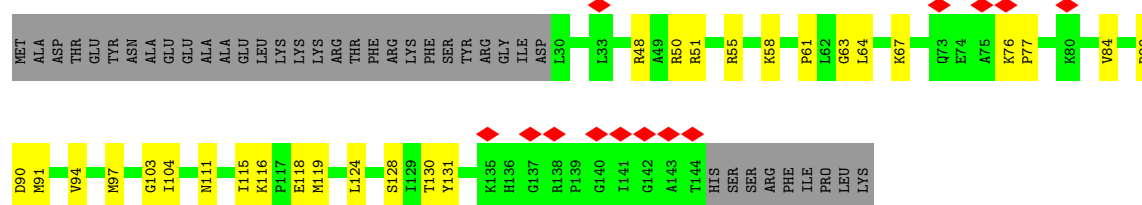
- Molecule 66: 40S ribosomal protein S14-like protein

Chain SO:  70% 19% . 10%



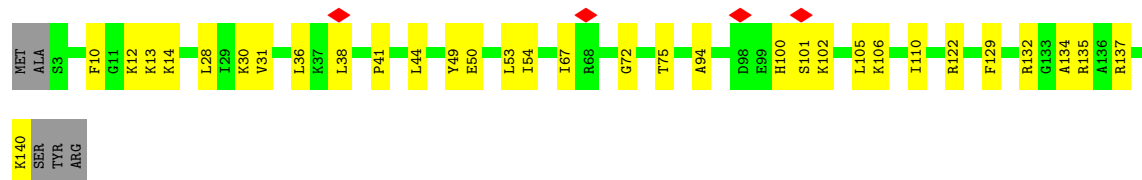
- Molecule 67: 40S ribosomal protein s15-like protein

Chain SP:  8% 57% 18% 25%



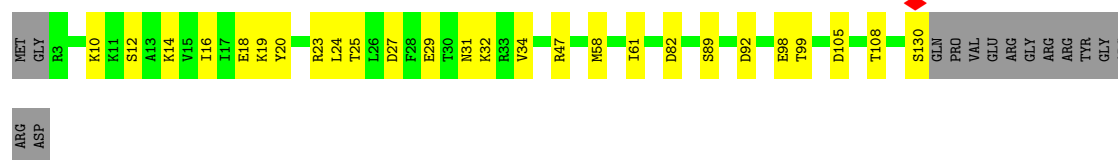
- Molecule 68: 40S ribosomal protein S16-like protein

Chain SQ:  74% 22% .



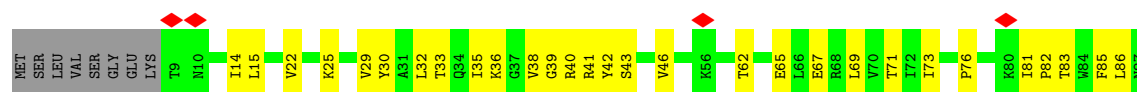
- Molecule 69: 40S ribosomal protein S17-like protein

Chain SR:  71% 18% 10%

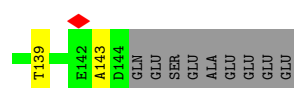


- Molecule 70: Putative ribosomal protein

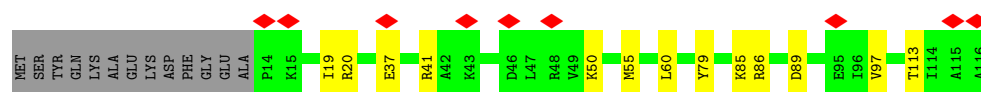
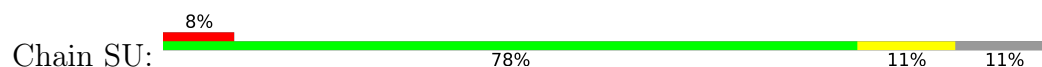
Chain SS:  52% 36% 12%



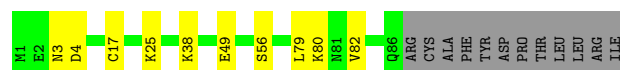
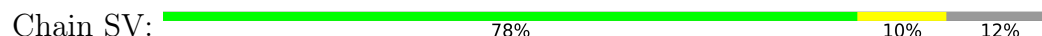
- Molecule 71: 40S ribosomal protein S19-like protein



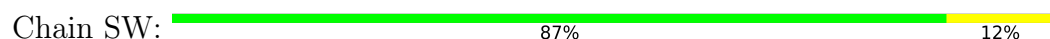
- Molecule 72: 40S ribosomal protein S20-like protein



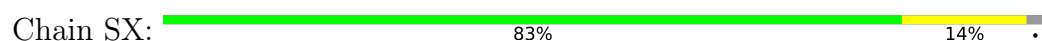
- Molecule 73: 40S ribosomal protein S21-like protein



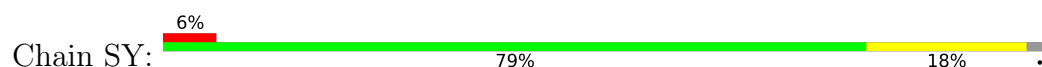
- Molecule 74: 40S ribosomal protein S22-like protein



- Molecule 75: 40S ribosomal protein s23-like protein

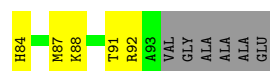


- Molecule 76: 40S ribosomal protein S24





- Molecule 77: 40S ribosomal protein S25



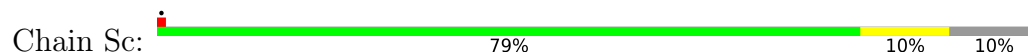
- Molecule 78: 40S ribosomal protein S26



- Molecule 79: Ribosomal protein s27-like protein



- Molecule 80: 40S ribosomal protein S28-like protein



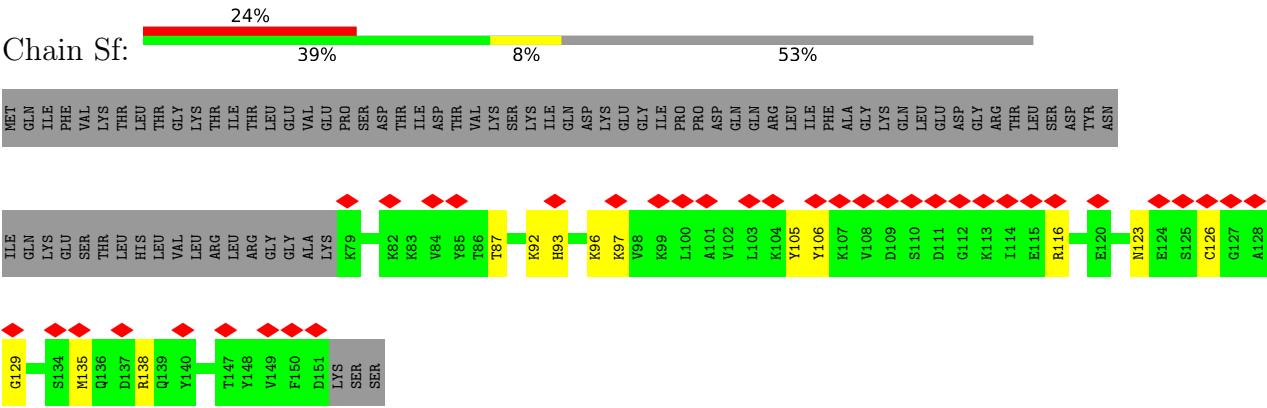
- Molecule 81: uS14



- Molecule 82: 40S ribosomal protein S30



● Molecule 83: 40S ribosomal protein S27a-like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	18.276	Depositor
Minimum map value	-8.430	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.534	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	534.60004, 534.60004, 534.60004	wwPDB
Map dimensions	486, 486, 486	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, B8N, SAC, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.17	0/76339	0.21	0/119028
2	2	0.13	0/42072	0.20	0/65562
3	3	0.15	0/2833	0.18	0/4413
4	4	0.15	0/3710	0.17	0/5778
5	A	0.09	0/2495	0.28	0/3390
6	B	0.15	0/243	0.36	0/316
7	C	0.09	0/622	0.25	0/827
8	LA	0.18	0/1964	0.32	0/2641
9	LB	0.17	0/3156	0.33	0/4238
10	LC	0.15	0/2815	0.28	0/3795
11	LD	0.14	0/2487	0.28	0/3341
12	LE	0.12	0/1547	0.29	0/2081
13	LF	0.15	0/2055	0.28	0/2758
14	LG	0.13	0/1929	0.25	0/2579
15	LH	0.15	0/1525	0.31	0/2050
16	LI	0.15	0/1797	0.28	0/2413
17	LJ	0.12	0/1389	0.31	0/1856
18	LK	0.08	0/761	0.30	0/1056
19	LL	0.14	0/1695	0.30	0/2276
20	LM	0.14	0/1144	0.28	0/1539
21	LN	0.17	0/1740	0.29	0/2332
22	LO	0.15	0/1638	0.27	0/2197
23	LP	0.15	0/1495	0.31	0/2014
24	LQ	0.15	0/1507	0.29	0/2017
25	LR	0.14	0/1525	0.22	0/2028
26	LS	0.16	0/1460	0.29	0/1965
27	LT	0.15	0/1292	0.25	0/1738
28	LU	0.10	0/832	0.27	0/1112
29	LV	0.16	0/1012	0.32	0/1361
30	LW	0.13	0/1088	0.26	0/1443
31	LX	0.15	0/981	0.35	0/1324
32	LY	0.14	0/1079	0.26	0/1443

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LZ	0.13	0/1134	0.26	0/1519
34	La	0.17	0/1212	0.30	0/1627
35	Lb	0.13	0/518	0.33	0/684
36	Lc	0.14	0/731	0.25	0/983
37	Ld	0.18	0/925	0.33	0/1238
38	Le	0.15	0/1019	0.26	0/1358
39	Lf	0.17	0/874	0.28	0/1176
40	Lg	0.16	0/904	0.33	0/1210
41	Lh	0.14	0/1014	0.25	0/1349
42	Li	0.13	0/844	0.25	0/1115
43	Lj	0.16	0/697	0.30	0/922
44	Lk	0.16	0/640	0.28	0/850
45	Ll	0.16	0/445	0.32	0/593
46	Lm	0.14	0/424	0.25	0/561
47	Ln	0.17	0/225	0.26	0/289
47	Lr	0.10	0/225	0.23	0/289
48	Lo	0.15	0/835	0.27	0/1105
49	Lp	0.16	0/705	0.31	0/940
50	Lq	0.13	0/1101	0.27	0/1482
51	Ls	0.10	0/1477	0.30	0/1995
52	SA	0.13	0/1683	0.30	0/2299
53	SB	0.14	0/1900	0.32	0/2551
54	SC	0.12	0/1703	0.26	0/2303
55	SD	0.10	0/1712	0.27	0/2299
56	SE	0.11	0/2112	0.29	0/2842
57	SF	0.10	0/1578	0.29	0/2130
58	SG	0.10	0/1906	0.26	0/2547
59	SH	0.11	0/1587	0.30	0/2140
60	SI	0.13	0/1654	0.28	0/2213
61	SJ	0.12	0/1489	0.27	0/1993
62	SK	0.12	0/764	0.32	0/1038
63	SL	0.13	0/1249	0.26	0/1678
64	SM	0.10	0/934	0.33	0/1255
65	SN	0.16	0/1205	0.28	0/1627
66	SO	0.16	0/1014	0.39	2/1361 (0.1%)
67	SP	0.09	0/932	0.28	0/1248
68	SQ	0.10	0/1098	0.31	0/1472
69	SR	0.11	0/1060	0.30	0/1424
70	SS	0.10	0/1133	0.30	0/1520
71	ST	0.12	0/1137	0.31	0/1533
72	SU	0.10	0/828	0.30	0/1112
73	SV	0.13	0/671	0.28	0/900
74	SW	0.13	0/1055	0.31	0/1416

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SX	0.14	0/1116	0.29	0/1489
76	SY	0.10	0/1075	0.23	0/1431
77	SZ	0.08	0/550	0.25	0/736
78	Sa	0.16	0/852	0.28	0/1136
79	Sb	0.12	0/623	0.34	0/843
80	Sc	0.12	0/487	0.34	0/653
81	Sd	0.08	0/427	0.24	0/570
82	Se	0.10	0/325	0.28	0/427
83	Sf	0.08	0/614	0.28	0/813
All	All	0.15	0/220649	0.24	2/323195 (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
9	LB	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	SO	63	ALA	CA-C-N	5.46	131.96	121.54
66	SO	63	ALA	C-N-CA	5.46	131.96	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	LB	257	HIS	Peptide

5.2 Too-close contacts

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	1	68242	0	34375	266	0
2	2	37645	0	18955	279	0
3	3	2535	0	1284	12	0
4	4	3319	0	1678	16	0
5	A	2438	0	2385	63	0
6	B	244	0	233	6	0
7	C	619	0	654	11	0
8	LA	1925	0	1999	22	0
9	LB	3088	0	3206	33	0
10	LC	2758	0	2883	21	0
11	LD	2440	0	2431	22	0
12	LE	1518	0	1619	13	0
13	LF	2017	0	2130	15	0
14	LG	1900	0	2066	15	0
15	LH	1505	0	1581	20	0
16	LI	1760	0	1798	13	0
17	LJ	1367	0	1405	22	0
18	LK	762	0	362	3	0
19	LL	1666	0	1756	21	0
20	LM	1125	0	1198	10	0
21	LN	1703	0	1767	29	0
22	LO	1613	0	1706	9	0
23	LP	1472	0	1518	15	0
24	LQ	1481	0	1596	15	0
25	LR	1506	0	1603	12	0
26	LS	1425	0	1484	17	0
27	LT	1266	0	1328	11	0
28	LU	819	0	864	8	0
29	LV	994	0	1054	7	0
30	LW	1075	0	1146	12	0
31	LX	965	0	1050	15	0
32	LY	1065	0	1156	17	0
33	LZ	1111	0	1181	14	0
34	La	1180	0	1203	16	0
35	Lb	508	0	526	6	0
36	Lc	722	0	766	7	0
37	Ld	911	0	965	12	0
38	Le	1001	0	1070	6	0
39	Lf	853	0	880	4	0
40	Lg	891	0	958	8	0
41	Lh	1003	0	1116	12	0
42	Li	836	0	915	12	0
43	Lj	684	0	712	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lk	632	0	693	7	0
45	Ll	435	0	473	3	0
46	Lm	418	0	459	6	0
47	Ln	224	0	271	3	0
47	Lr	224	0	271	2	0
48	Lo	822	0	891	7	0
49	Lp	697	0	737	9	0
50	Lq	1083	0	1140	8	0
51	Ls	1449	0	1488	36	0
52	SA	1641	0	1650	17	0
53	SB	1871	0	1989	28	0
54	SC	1672	0	1777	23	0
55	SD	1688	0	1750	27	0
56	SE	2072	0	2155	23	0
57	SF	1557	0	1608	29	0
58	SG	1875	0	1983	31	0
59	SH	1562	0	1641	23	0
60	SI	1621	0	1645	23	0
61	SJ	1466	0	1582	22	0
62	SK	742	0	738	26	0
63	SL	1222	0	1289	16	0
64	SM	923	0	946	16	0
65	SN	1182	0	1264	11	0
66	SO	1002	0	1034	22	0
67	SP	917	0	978	22	0
68	SQ	1081	0	1151	24	0
69	SR	1045	0	1083	15	0
70	SS	1118	0	1172	39	0
71	ST	1117	0	1133	30	0
72	SU	819	0	895	10	0
73	SV	664	0	662	8	0
74	SW	1037	0	1076	10	0
75	SX	1099	0	1169	16	0
76	SY	1061	0	1150	17	0
77	SZ	546	0	591	18	0
78	Sa	839	0	891	15	0
79	Sb	611	0	633	3	0
80	Sc	484	0	513	4	0
81	Sd	419	0	418	11	0
82	Se	322	0	365	3	0
83	Sf	604	0	640	13	0
84	1	415	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	2	121	0	0	0	0
84	3	8	0	0	0	0
84	4	11	0	0	0	0
84	LA	1	0	0	0	0
84	LB	1	0	0	0	0
84	LI	1	0	0	0	0
84	LN	3	0	0	0	0
84	LP	1	0	0	0	0
84	LT	2	0	0	0	0
84	LV	1	0	0	0	0
84	Lb	1	0	0	0	0
84	Lo	1	0	0	0	0
84	SN	1	0	0	0	0
84	SO	1	0	0	0	0
84	SQ	1	0	0	0	0
84	SX	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	1	0	0	0	0
85	Lm	1	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sb	1	0	0	0	0
85	Sd	1	0	0	0	0
86	1	748	0	0	30	0
86	2	136	0	0	3	0
86	4	20	0	0	3	0
86	LB	3	0	0	0	0
86	LC	3	0	0	0	0
86	LD	1	0	0	0	0
86	LN	6	0	0	0	0
86	LO	5	0	0	0	0
86	LP	2	0	0	0	0
86	LQ	1	0	0	0	0
86	LT	4	0	0	0	0
86	LW	4	0	0	0	0
86	Lb	1	0	0	0	0
86	Ld	1	0	0	0	0
86	Le	4	0	0	0	0
86	Lj	1	0	0	0	0
86	SL	2	0	0	1	0
86	SN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Sa	1	0	0	0	0
All	All	207344	0	154556	1509	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 4.

All (1509) 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)
2:2:191:G:HO2'	2:2:192:A:H8	1.05	1.02
60:SI:87:ASN:HB3	60:SI:90:LEU:HD23	1.60	0.83
2:2:1474:G:OP1	71:ST:44:LYS:NZ	2.13	0.81
2:2:691:C:H4'	2:2:692:C:H5'	1.63	0.80
68:SQ:28:LEU:HD21	68:SQ:30:LYS:HE2	1.63	0.80
2:2:78:C:H5'	58:SG:175:ALA:HB3	1.63	0.79
1:1:1000:G:H1	1:1:1017:U:H3	1.27	0.79
59:SH:62:LYS:HE2	59:SH:94:ARG:HE	1.48	0.78
1:1:673:G:OP1	19:LL:39:ARG:NH2	2.17	0.78
10:LC:149:VAL:HG13	10:LC:150:PRO:HD3	1.65	0.77
51:Ls:57:THR:HB	51:Ls:60:ARG:HB2	1.66	0.77
2:2:103:A:OP2	2:2:305:C:N4	2.18	0.77
17:LJ:111:ILE:HG12	17:LJ:117:TYR:HB2	1.67	0.77
73:SV:79:LEU:HD23	73:SV:82:VAL:HG11	1.67	0.76
51:Ls:159:VAL:HG11	51:Ls:165:VAL:HG22	1.68	0.76
1:1:2477:U:OP1	14:LG:71:ARG:NH1	2.19	0.75
64:SM:108:ARG:HG2	64:SM:110:GLY:H	1.51	0.75
2:2:1441:G:N2	83:Sf:87:THR:O	2.20	0.75
2:2:1357:C:HO2'	71:ST:3:GLY:N	1.85	0.75
62:SK:31:HIS:CE1	62:SK:37:ASN:H	2.04	0.75
2:2:878:C:OP1	65:SN:107:LYS:NZ	2.20	0.75
37:Ld:105:ASN:O	37:Ld:105:ASN:ND2	2.19	0.74
1:1:1337:G:N2	1:1:1339:U:O2'	2.19	0.74
16:LI:14:ASN:O	16:LI:128:ARG:NH2	2.22	0.73
10:LC:284:GLN:HE22	10:LC:286:ASP:HB3	1.53	0.73
61:SJ:155:ASP:OD2	61:SJ:156:PHE:N	2.22	0.73
57:SF:133:SER:HB2	57:SF:144:ARG:HB3	1.72	0.72
7:C:569:ARG:NH2	17:LJ:52:ARG:O	2.23	0.72
2:2:487:U:H3	2:2:494:G:H1	1.38	0.72
67:SP:51:ARG:HH21	67:SP:55:ARG:HH21	1.36	0.72
62:SK:37:ASN:HA	62:SK:40:VAL:HG22	1.72	0.72
14:LG:74:VAL:HB	14:LG:237:GLY:HA3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lk:8:ILE:HD11	44:Lk:49:LEU:HD21	1.70	0.72
1:1:2900:A:N7	9:LB:257:HIS:NE2	2.32	0.72
12:LE:139:GLU:HG2	12:LE:152:LYS:HE2	1.71	0.71
2:2:483:G:H1	2:2:498:U:H3	1.39	0.71
2:2:1554:U:H3	67:SP:130:THR:HG1	1.35	0.71
2:2:1687:A:H2	2:2:1706:U:H3	1.37	0.71
2:2:824:U:H3	2:2:844:G:H1	1.38	0.70
2:2:706:C:H42	2:2:725:G:H1	1.36	0.70
58:SG:157:VAL:HG11	58:SG:178:ILE:HD11	1.73	0.70
21:LN:68:ARG:NH1	21:LN:124:ASP:O	2.25	0.70
26:LS:96:GLU:OE2	26:LS:102:ALA:N	2.25	0.70
12:LE:19:ALA:HB3	12:LE:23:LYS:HG2	1.73	0.70
30:LW:81:ALA:HB2	30:LW:87:LEU:HG	1.73	0.70
67:SP:94:VAL:H	67:SP:97:MET:HE2	1.55	0.69
23:LP:64:ALA:O	23:LP:80:ARG:NH1	2.26	0.69
2:2:1363:A:O2'	71:ST:8:ARG:NH1	2.25	0.69
34:La:93:GLY:O	34:La:96:LYS:NZ	2.24	0.69
34:La:133:GLU:OE2	34:La:136:ARG:NH2	2.25	0.69
4:4:95:G:OP2	43:Lj:72:ARG:NH1	2.25	0.69
1:1:2830:G:N7	86:1:3956:HOH:O	2.26	0.69
55:SD:67:ARG:NH1	62:SK:87:ALA:O	2.26	0.69
2:2:1547:U:O4	67:SP:48:ARG:NH1	2.26	0.68
26:LS:130:GLU:HG3	26:LS:131:LYS:HG2	1.74	0.68
76:SY:123:GLY:O	76:SY:128:LYS:NZ	2.26	0.68
1:1:2355:C:O2'	9:LB:267:ARG:NH2	2.25	0.68
62:SK:48:GLN:HE22	62:SK:55:THR:HG22	1.58	0.68
1:1:2632:A:O2'	17:LJ:127:ASP:OD1	2.11	0.68
4:4:140:G:O6	86:4:301:HOH:O	2.10	0.68
2:2:6:G:N7	54:SC:213:LYS:NZ	2.40	0.67
1:1:144:G:H3'	21:LN:49:ARG:HH22	1.59	0.67
2:2:1538:G:N2	2:2:1565:A:OP2	2.26	0.67
1:1:675:U:OP2	19:LL:36:ARG:NH2	2.28	0.67
1:1:2908:U:OP1	86:1:3903:HOH:O	2.13	0.67
1:1:2908:U:OP1	86:1:3904:HOH:O	2.13	0.67
1:1:405:G:OP1	23:LP:62:ARG:NH1	2.27	0.66
2:2:747:U:OP1	74:SW:82:ARG:NH1	2.28	0.66
2:2:1455:C:OP2	70:SS:138:THR:OG1	2.11	0.66
44:Lk:6:SER:OG	44:Lk:10:LYS:NZ	2.27	0.66
49:Lp:33:GLN:OE1	49:Lp:49:ARG:NH1	2.28	0.66
70:SS:100:ILE:HD13	70:SS:108:LYS:HG3	1.77	0.66
2:2:1517:G:O2'	2:2:1519:U:OP2	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LG:36:ASN:ND2	14:LG:41:GLN:OE1	2.29	0.66
82:Se:20:LYS:NZ	82:Se:22:GLU:OE2	2.27	0.66
11:LD:295:ILE:HG13	16:LI:206:LEU:HD21	1.78	0.66
70:SS:25:LYS:HZ2	77:SZ:29:VAL:H	1.42	0.66
58:SG:74:ARG:HD2	58:SG:96:SER:HB3	1.77	0.66
2:2:1498:G:N7	71:ST:102:ARG:NH2	2.39	0.66
66:SO:61:VAL:HG11	66:SO:66:ASP:HB2	1.78	0.66
10:LC:365:ALA:HB3	26:LS:28:ARG:HD2	1.78	0.66
64:SM:65:ASN:O	64:SM:74:LYS:NZ	2.29	0.66
1:1:1244:G:N2	1:1:1244:G:OP2	2.29	0.66
1:1:275:G:O2'	1:1:276:G:OP2	2.12	0.66
2:2:78:C:H1'	58:SG:177:ARG:HG3	1.78	0.65
58:SG:231:LYS:HD2	58:SG:232:ARG:HG2	1.78	0.65
71:ST:136:ILE:O	71:ST:139:THR:OG1	2.14	0.65
62:SK:85:VAL:HG22	62:SK:87:ALA:H	1.60	0.65
1:1:1929:G:OP1	25:LR:104:ARG:NH1	2.29	0.65
5:A:57:ARG:HH22	5:A:94:THR:HA	1.61	0.65
1:1:2338:G:OP2	86:1:3902:HOH:O	2.13	0.65
38:Le:68:MET:HE2	38:Le:72:HIS:HB2	1.79	0.65
68:SQ:38:LEU:HD11	71:ST:11:ASP:HA	1.78	0.65
1:1:921:U:OP1	86:1:3905:HOH:O	2.15	0.65
37:Ld:105:ASN:C	37:Ld:105:ASN:HD22	2.03	0.65
5:A:30:MET:HE1	5:A:71:ILE:HD13	1.79	0.65
5:A:36:ARG:HA	5:A:65:ILE:HG13	1.78	0.65
5:A:66:VAL:HA	5:A:82:SER:HA	1.79	0.65
1:1:295:A:N6	86:1:3989:HOH:O	2.30	0.64
15:LH:14:GLU:OE2	20:LM:2:ALA:N	2.30	0.64
2:2:398:A:OP2	86:2:2001:HOH:O	2.15	0.64
1:1:2100:U:OP2	1:1:2105:A:N6	2.31	0.64
4:4:111:A:N1	86:4:303:HOH:O	2.29	0.64
1:1:261:A:OP1	21:LN:50:ARG:NH1	2.30	0.64
77:SZ:26:GLN:O	77:SZ:59:LYS:NZ	2.30	0.64
2:2:188:U:OP2	2:2:189:C:N4	2.28	0.64
2:2:1199:A:N6	2:2:1453:C:OP1	2.31	0.64
7:C:607:VAL:HG22	7:C:611:MET:HE2	1.80	0.64
1:1:681:A:H5''	10:LC:43:MET:HE3	1.80	0.64
4:4:55:U:H3	4:4:62:A:H2	1.43	0.64
55:SD:45:THR:OG1	55:SD:48:VAL:O	2.12	0.64
70:SS:90:ARG:HA	70:SS:95:GLY:HA3	1.80	0.64
75:SX:69:ARG:HG3	75:SX:117:ILE:HG12	1.79	0.64
5:A:43:TRP:HA	5:A:55:PRO:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LX:81:ASN:O	31:LX:81:ASN:ND2	2.26	0.63
2:2:1294:G:N2	2:2:1297:A:OP2	2.27	0.63
23:LP:10:ALA:H	23:LP:13:LYS:HE2	1.63	0.63
27:LT:81:LYS:O	27:LT:82:HIS:ND1	2.31	0.63
31:LX:67:GLU:OE2	31:LX:68:PRO:HD2	1.97	0.63
33:LZ:32:THR:OG1	33:LZ:34:SER:O	2.15	0.63
53:SB:122:GLU:OE2	53:SB:213:ARG:NH1	2.32	0.63
60:SI:36:THR:HG21	60:SI:177:PRO:HB2	1.80	0.63
1:1:2338:G:OP2	86:1:3906:HOH:O	2.16	0.63
1:1:3135:A:OP2	22:LO:173:LYS:NZ	2.29	0.63
4:4:82:U:OP1	4:4:85:G:N2	2.32	0.63
5:A:79:LEU:HD23	5:A:113:PHE:HZ	1.62	0.63
76:SY:24:LYS:HB2	76:SY:78:ILE:HB	1.81	0.63
78:Sa:100:ARG:O	78:Sa:102:ARG:NH1	2.31	0.63
2:2:398:A:OP2	86:2:2002:HOH:O	2.15	0.63
2:2:1083:A:H5'	54:SC:172:SER:HB2	1.80	0.63
68:SQ:129:PHE:HB3	68:SQ:134:ALA:HA	1.80	0.63
72:SU:79:TYR:HB3	81:Sd:52:PHE:HB3	1.79	0.63
75:SX:70:LYS:HB3	75:SX:93:LEU:HD11	1.79	0.63
2:2:1101:U:OP1	75:SX:14:LYS:NZ	2.32	0.63
17:LJ:15:ILE:HG12	17:LJ:132:MET:HE1	1.79	0.63
34:La:59:ARG:NH2	48:Lo:38:GLN:OE1	2.31	0.63
37:Ld:9:ARG:O	37:Ld:13:ALA:N	2.27	0.63
60:SI:110:ARG:NH2	60:SI:122:GLY:O	2.32	0.63
1:1:167:G:H1	1:1:239:C:H42	1.47	0.62
1:1:1469:G:H21	40:Lg:7:THR:HG22	1.64	0.62
56:SE:188:ASN:HB3	56:SE:191:ARG:HD3	1.80	0.62
67:SP:116:LYS:H	67:SP:119:MET:HE2	1.64	0.62
14:LG:166:VAL:HA	14:LG:169:LEU:HD23	1.81	0.62
70:SS:83:THR:OG1	70:SS:97:ASP:OD2	2.15	0.62
2:2:1446:U:O2'	81:Sd:7:TRP:O	2.17	0.62
2:2:1549:G:N7	67:SP:55:ARG:NH2	2.47	0.62
62:SK:32:GLU:HG2	62:SK:33:ILE:HG12	1.81	0.62
75:SX:37:ALA:O	75:SX:41:SER:OG	2.18	0.62
2:2:321:C:OP1	63:SL:138:LYS:NZ	2.28	0.62
2:2:1479:A:H4'	68:SQ:72:GLY:H	1.63	0.62
59:SH:6:LEU:O	59:SH:16:ARG:NH2	2.31	0.62
1:1:117:A:OP2	21:LN:2:GLY:N	2.33	0.62
19:LL:3:ILE:HD11	34:La:34:MET:SD	2.40	0.62
34:La:149:ALA:HB2	42:Li:16:LEU:HA	1.82	0.62
66:SO:30:ALA:HB2	66:SO:92:LEU:HD23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LV:81:VAL:HB	29:LV:120:VAL:HG23	1.82	0.62
57:SF:132:ASP:OD1	57:SF:133:SER:N	2.32	0.62
2:2:1689:A:H2'	2:2:1690:G:H8	1.64	0.62
31:LX:148:ILE:HA	31:LX:151:THR:HG22	1.82	0.62
5:A:193:GLY:N	5:A:213:ASP:OD1	2.33	0.62
8:LA:117:GLU:HG2	8:LA:124:GLY:H	1.65	0.62
76:SY:44:ARG:HD2	76:SY:58:VAL:HG23	1.81	0.62
21:LN:183:THR:HG22	21:LN:187:ARG:HB2	1.82	0.62
8:LA:2:GLY:HA2	8:LA:207:VAL:HG23	1.80	0.61
60:SI:36:THR:OG1	60:SI:96:LEU:O	2.18	0.61
6:B:129:GLU:HA	6:B:132:LEU:HD13	1.81	0.61
32:LY:50:ARG:HB2	32:LY:114:ARG:HH12	1.65	0.61
26:LS:73:LYS:NZ	26:LS:97:THR:O	2.34	0.61
2:2:598:A:OP2	75:SY:110:LYS:NZ	2.32	0.61
2:2:643:U:H2'	2:2:644:A:H8	1.64	0.61
54:SC:178:ILE:HB	54:SC:205:TYR:HB2	1.80	0.61
59:SH:164:LEU:HD11	59:SH:193:PHE:HD2	1.64	0.61
2:2:331:U:O4	60:SI:5:ARG:NH2	2.33	0.61
2:2:402:C:O2'	58:SG:92:ARG:O	2.17	0.61
37:Ld:9:ARG:HB3	37:Ld:13:ALA:HB2	1.81	0.61
39:Lf:44:ASN:HA	39:Lf:47:LEU:HD23	1.81	0.61
3:3:76:G:N2	3:3:101:A:OP2	2.28	0.61
9:LB:153:LYS:HG2	9:LB:193:VAL:HG11	1.82	0.61
2:2:277:C:H5''	30:LW:109:ILE:HD11	1.81	0.61
2:2:393:G:N2	2:2:396:A:OP2	2.34	0.61
2:2:1491:C:H42	2:2:1508:G:H1	1.49	0.61
59:SH:7:ASN:HA	59:SH:16:ARG:HH12	1.66	0.61
75:SY:107:PHE:HE1	75:SY:123:LYS:HB3	1.64	0.61
1:1:766:G:N2	24:LQ:97:ARG:HE	1.98	0.60
1:1:2608:G:OP1	7:C:605:ARG:NH1	2.34	0.60
5:A:236:ILE:HG22	5:A:252:THR:HG22	1.82	0.60
1:1:1221:C:H3'	1:1:1222:C:H5''	1.83	0.60
1:1:1252:U:N3	1:1:1255:C:OP2	2.30	0.60
1:1:2356:G:N7	86:1:3996:HOH:O	2.31	0.60
2:2:1264:G:H1	2:2:1438:U:H3	1.48	0.60
4:4:78:G:O2'	41:Lh:47:ASN:OD1	2.18	0.60
12:LE:116:GLN:HA	12:LE:119:ILE:HD12	1.82	0.60
34:La:82:VAL:O	34:La:87:ARG:NH1	2.34	0.60
2:2:1680:G:H1	2:2:1713:C:H42	1.49	0.60
10:LC:140:GLY:O	10:LC:184:LYS:NZ	2.35	0.60
53:SB:190:PRO:HG2	53:SB:192:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SP:89:ARG:NH2	67:SP:128:SER:O	2.34	0.60
1:1:1619:C:OP2	40:Lg:75:ARG:NH2	2.34	0.60
1:1:3209:A:OP1	12:LE:64:ARG:NH2	2.28	0.60
64:SM:61:MET:HA	64:SM:87:PRO:HB2	1.82	0.60
1:1:308:C:OP1	19:LL:102:LYS:NZ	2.34	0.60
2:2:65:A:H2	2:2:83:A:H62	1.50	0.60
2:2:1215:G:N2	2:2:1440:A:OP2	2.34	0.60
11:LD:91:GLY:O	11:LD:94:ASN:ND2	2.33	0.60
64:SM:47:LEU:HA	64:SM:50:ALA:HB3	1.82	0.60
2:2:1354:U:O3'	71:ST:127:GLN:NE2	2.30	0.60
38:Le:82:ASP:OD1	50:Lq:30:ARG:NH2	2.34	0.60
2:2:67:A:O2'	2:2:69:G:OP1	2.19	0.60
2:2:1431:G:N7	62:SK:25:LYS:NZ	2.49	0.60
4:4:23:U:OP1	32:LY:15:ARG:NH1	2.34	0.60
20:LM:12:ARG:HB3	20:LM:18:ARG:HH12	1.67	0.60
24:LQ:152:ASP:OD1	24:LQ:153:GLN:N	2.35	0.60
59:SH:36:ASN:OD1	59:SH:37:THR:N	2.35	0.60
67:SP:115:ILE:HD12	67:SP:119:MET:HE3	1.82	0.60
1:1:209:G:OP1	32:LY:11:ARG:NH1	2.35	0.59
1:1:2856:A:H5''	46:Lm:125:LYS:HG3	1.83	0.59
28:LU:40:GLU:O	28:LU:44:ASN:ND2	2.34	0.59
51:Ls:121:VAL:HG23	51:Ls:158:LEU:HD11	1.84	0.59
1:1:351:G:N2	1:1:354:A:OP2	2.31	0.59
17:LJ:42:SER:O	17:LJ:76:LYS:NZ	2.32	0.59
2:2:1545:C:OP1	67:SP:50:ARG:NH2	2.36	0.59
51:Ls:42:ARG:NH2	51:Ls:51:VAL:O	2.35	0.59
1:1:333:C:OP1	86:1:3907:HOH:O	2.17	0.59
1:1:1139:C:OP2	13:LF:100:LYS:NZ	2.36	0.59
1:1:2960:C:O2'	9:LB:181:GLU:OE2	2.21	0.59
62:SK:86:PRO:HA	62:SK:89:HIS:HB3	1.84	0.59
25:LR:15:LEU:HD13	25:LR:52:LYS:HB2	1.85	0.59
53:SB:11:LYS:HZ2	53:SB:17:LYS:HE2	1.66	0.59
57:SF:33:TRP:HB3	57:SF:115:ASN:HD21	1.67	0.59
2:2:456:G:OP1	76:SY:112:LYS:NZ	2.29	0.59
50:Lq:31:ASP:HB3	50:Lq:34:ASN:HB2	1.84	0.59
29:LV:89:ARG:HH12	29:LV:139:MET:HG3	1.67	0.59
5:A:64:HIS:ND1	5:A:65:ILE:HG22	2.18	0.59
1:1:768:A:N6	24:LQ:115:THR:HG21	2.18	0.59
1:1:1229:G:N2	1:1:1247:C:O2'	2.36	0.58
2:2:195:G:H2'	2:2:196:G:H8	1.68	0.58
1:1:1241:U:H3	1:1:1244:G:H22	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1506:U:O2'	31:LX:124:ASN:ND2	2.36	0.58
28:LU:18:THR:HG22	28:LU:75:HIS:HD1	1.68	0.58
1:1:2623:C:OP2	17:LJ:143:ARG:NH1	2.37	0.58
2:2:1132:U:OP2	75:SX:121:ARG:NH2	2.36	0.58
32:LY:69:VAL:HG12	32:LY:81:VAL:HG12	1.85	0.58
51:Ls:57:THR:HA	51:Ls:60:ARG:HE	1.68	0.58
55:SD:141:VAL:HG13	55:SD:185:LEU:HD21	1.85	0.58
59:SH:20:SER:N	59:SH:23:GLU:OE2	2.36	0.58
66:SO:84:CYS:HB3	66:SO:89:ILE:HD11	1.84	0.58
2:2:1217:C:H42	2:2:1260:G:H1	1.50	0.58
56:SE:246:THR:OG1	56:SE:249:GLU:OE1	2.21	0.58
57:SF:45:LEU:HG	57:SF:125:VAL:HG23	1.85	0.58
1:1:3074:G:OP1	1:1:3074:G:N2	2.35	0.58
2:2:1195:G:OP1	2:2:1196:G:O2'	2.20	0.58
5:A:140:TYR:HE2	5:A:182:CYS:HB3	1.69	0.58
57:SF:110:LEU:HD11	77:SZ:48:LEU:HB3	1.84	0.58
1:1:270:G:OP1	86:1:3908:HOH:O	2.17	0.58
19:LL:140:LYS:HA	19:LL:143:GLN:HG3	1.86	0.58
28:LU:20:LYS:HE2	28:LU:22:ILE:HD11	1.85	0.58
53:SB:3:VAL:N	66:SO:58:GLY:O	2.37	0.58
1:1:1447:G:N2	1:1:1450:A:OP2	2.36	0.58
66:SO:26:VAL:HG23	66:SO:89:ILE:HA	1.85	0.58
1:1:332:C:OP1	1:1:1363:G:O2'	2.22	0.58
1:1:2854:G:O2'	46:Lm:100:TYR:O	2.21	0.58
62:SK:11:ILE:HG21	62:SK:40:VAL:HG12	1.86	0.58
63:SL:107:LYS:O	75:SX:13:ARG:NH2	2.37	0.58
74:SW:15:ASN:HD21	74:SW:71:LYS:HG3	1.67	0.58
1:1:1349:A:OP1	86:1:3909:HOH:O	2.17	0.58
2:2:1708:A:H4'	2:2:1708:A:OP1	2.02	0.58
71:ST:45:GLU:HG2	71:ST:46:LEU:HG	1.86	0.58
2:2:1549:G:N1	2:2:1552:A:OP2	2.37	0.57
2:2:1708:A:N1	30:LW:74:ARG:NH2	2.52	0.57
5:A:79:LEU:HD23	5:A:113:PHE:CZ	2.38	0.57
51:Ls:105:ILE:HG22	51:Ls:183:TYR:HB2	1.86	0.57
62:SK:14:TYR:HD1	62:SK:21:MET:HE1	1.69	0.57
1:1:2080:A:HO2'	1:1:3038:G:HO2'	1.52	0.57
2:2:909:U:O2	53:SB:7:LYS:NZ	2.37	0.57
2:2:1169:G:OP1	70:SS:144:ARG:NE	2.36	0.57
10:LC:149:VAL:CG1	10:LC:150:PRO:HD3	2.33	0.57
11:LD:95:TRP:CD1	11:LD:161:ARG:HA	2.39	0.57
39:Lf:105:TYR:HB2	39:Lf:106:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SG:49:ILE:HG12	58:SG:115:LYS:HB3	1.86	0.57
2:2:611:A:OP2	75:SX:5:LYS:NZ	2.38	0.57
2:2:1605:U:H5''	68:SQ:75:THR:HG22	1.86	0.57
34:La:112:LEU:HD22	34:La:125:VAL:HG11	1.87	0.57
57:SF:110:LEU:O	77:SZ:47:ARG:NH1	2.38	0.57
67:SP:104:ILE:N	67:SP:111:ASN:O	2.33	0.57
41:Lh:37:GLN:HE22	41:Lh:45:LYS:HD2	1.68	0.57
4:4:75:G:OP2	32:LY:73:TYR:OH	2.21	0.57
51:Ls:133:THR:HG21	51:Ls:145:ILE:HD11	1.86	0.57
26:LS:31:ALA:HB1	26:LS:36:VAL:HG23	1.86	0.57
41:Lh:24:LEU:HD11	41:Lh:28:LYS:HE3	1.87	0.57
60:SI:176:ARG:HE	60:SI:179:GLN:HG3	1.70	0.57
2:2:352:G:H2'	2:2:353:G:H8	1.70	0.56
10:LC:159:ALA:HB3	10:LC:162:ALA:HB2	1.87	0.56
66:SO:38:ASP:OD1	66:SO:39:THR:N	2.37	0.56
76:SY:57:GLN:NE2	76:SY:79:TYR:O	2.37	0.56
19:LL:115:ARG:NH2	19:LL:155:PHE:O	2.30	0.56
70:SS:46:VAL:HG21	70:SS:73:ILE:HD11	1.86	0.56
78:Sa:23:CYS:HB3	78:Sa:28:ARG:H	1.71	0.56
2:2:1703:C:H2'	2:2:1704:A:C8	2.41	0.56
51:Ls:94:LYS:HG3	51:Ls:97:ARG:HH21	1.70	0.56
58:SG:121:ILE:H	58:SG:125:THR:HG22	1.71	0.56
58:SG:159:ARG:HD3	58:SG:173:THR:HG21	1.86	0.56
72:SU:37:GLU:OE1	72:SU:41:ARG:NH2	2.38	0.56
73:SV:38:LYS:HD3	73:SV:49:GLU:HB3	1.85	0.56
1:1:114:C:OP1	21:LN:147:ARG:NE	2.28	0.56
7:C:547:LEU:HD22	7:C:586:LEU:HD11	1.88	0.56
15:LH:31:ARG:NH1	15:LH:151:ASN:OD1	2.38	0.56
17:LJ:134:ARG:NH2	17:LJ:159:GLU:OE1	2.39	0.56
55:SD:67:ARG:HD2	62:SK:88:THR:HG22	1.87	0.56
1:1:276:G:OP1	48:Lo:45:ARG:NH1	2.38	0.56
3:3:79:C:H42	3:3:99:G:H1	1.53	0.56
5:A:32:LEU:HD12	5:A:71:ILE:HG12	1.86	0.56
13:LF:91:PHE:HB2	13:LF:145:PRO:HG3	1.86	0.56
17:LJ:112:ASP:OD1	17:LJ:113:LEU:N	2.37	0.56
2:2:1354:U:H2'	2:2:1355:G:C8	2.40	0.56
2:2:1484:G:H3'	2:2:1511:A:H61	1.70	0.56
2:2:1485:U:OP2	2:2:1511:A:N6	2.39	0.56
5:A:20:SER:OG	5:A:67:SER:O	2.20	0.56
11:LD:53:VAL:HG12	11:LD:62:THR:HG22	1.87	0.56
67:SP:76:LYS:HG2	67:SP:77:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1117:G:O2'	1:1:2601:A:N3	2.37	0.56
2:2:1189:C:O2'	68:SQ:137:ARG:NH2	2.39	0.56
3:3:16:U:OP1	17:LJ:148:ARG:NH1	2.39	0.56
21:LN:181:ASN:OD1	21:LN:184:ARG:NH2	2.38	0.56
5:A:54:TYR:CD2	5:A:55:PRO:HD2	2.40	0.56
17:LJ:79:GLU:OE2	17:LJ:83:ARG:NH1	2.38	0.56
5:A:199:THR:HG21	5:A:240:VAL:HA	1.87	0.55
21:LN:44:ARG:NH1	21:LN:120:TRP:O	2.39	0.55
42:Li:17:ILE:HA	42:Li:22:LYS:HB2	1.89	0.55
55:SD:75:LEU:HD22	62:SK:63:TYR:HD1	1.71	0.55
55:SD:157:ASP:OD1	55:SD:158:GLY:N	2.39	0.55
2:2:1477:C:O2'	2:2:1478:C:O5'	2.23	0.55
17:LJ:54:THR:HG23	17:LJ:61:ARG:HA	1.88	0.55
52:SA:193:ASN:HB3	52:SA:196:THR:HG22	1.89	0.55
1:1:333:C:OP1	86:1:3913:HOH:O	2.18	0.55
1:1:687:A:H4'	19:LL:68:ARG:HH12	1.71	0.55
1:1:934:A:N3	1:1:1097:U:O2'	2.35	0.55
2:2:1232:C:N3	83:Sf:138:ARG:NH1	2.53	0.55
2:2:1586:G:OP1	71:ST:91:SER:OG	2.24	0.55
7:C:595:GLU:OE1	48:Lo:89:LYS:NZ	2.39	0.55
24:LQ:203:ARG:O	34:La:51:GLY:HA2	2.05	0.55
32:LY:30:MET:HB3	32:LY:100:PRO:HG2	1.88	0.55
72:SU:55:MET:HB2	72:SU:85:LYS:HB2	1.89	0.55
21:LN:124:ASP:OD1	21:LN:125:SER:N	2.38	0.55
70:SS:120:ARG:HG2	70:SS:125:LEU:HD11	1.88	0.55
74:SW:80:ASN:OD1	74:SW:124:LYS:NZ	2.36	0.55
1:1:1196:G:OP1	26:LS:137:ARG:NH1	2.38	0.55
1:1:1281:C:OP2	86:1:3911:HOH:O	2.17	0.55
1:1:2830:G:OP2	86:1:3914:HOH:O	2.18	0.55
2:2:1519:U:O5'	71:ST:78:LYS:NZ	2.39	0.55
9:LB:41:VAL:HG12	9:LB:186:GLY:HA3	1.89	0.55
1:1:2730:U:O2'	1:1:2731:C:O4'	2.25	0.55
55:SD:145:LEU:HD12	55:SD:151:LYS:HG3	1.87	0.55
68:SQ:129:PHE:HA	68:SQ:135:ARG:HH22	1.71	0.55
1:1:1792:G:O6	33:LZ:63:LYS:NZ	2.38	0.55
2:2:1054:U:H2'	2:2:1055:A:C8	2.41	0.55
5:A:212:LYS:HD3	5:A:235:GLU:HG3	1.89	0.55
24:LQ:68:THR:HG22	24:LQ:70:ALA:H	1.70	0.55
56:SE:80:ILE:HG13	56:SE:81:THR:HG23	1.88	0.55
56:SE:87:MET:HE1	56:SE:235:ILE:HD13	1.88	0.55
5:A:79:LEU:HD12	5:A:87:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LJ:61:ARG:NH1	48:Lo:105:VAL:O	2.40	0.55
1:1:1067:A:H4'	11:LD:44:TYR:CE2	2.42	0.55
2:2:282:G:OP1	58:SG:199:ARG:NH2	2.39	0.55
37:Ld:54:THR:HG23	37:Ld:56:ASP:H	1.72	0.55
53:SB:83:LYS:NZ	66:SO:129:GLU:OE2	2.40	0.55
1:1:478:G:H2'	1:1:479:G:H8	1.72	0.54
1:1:2719:C:N3	48:Lo:63:LYS:NZ	2.54	0.54
1:1:3298:U:O2'	1:1:3299:U:OP1	2.24	0.54
13:LF:124:LYS:HD3	13:LF:197:VAL:HG11	1.89	0.54
23:LP:168:GLU:OE1	23:LP:179:ARG:NH1	2.39	0.54
2:2:1098:G:H5''	74:SW:76:SER:HB3	1.88	0.54
2:2:1405:G:N2	2:2:1408:G:OP2	2.38	0.54
2:2:1790:A:N3	78:Sa:79:ILE:HD11	2.22	0.54
50:Lq:54:ILE:HG12	50:Lq:63:VAL:HG22	1.89	0.54
51:Ls:106:LYS:NZ	51:Ls:179:SER:O	2.39	0.54
2:2:529:U:OP1	61:SJ:130:ARG:NH2	2.41	0.54
55:SD:51:ILE:HB	55:SD:89:LEU:HD23	1.88	0.54
2:2:1448:U:OP1	81:Sd:10:ARG:NH1	2.41	0.54
5:A:29:ASN:HA	5:A:45:LEU:HB2	1.90	0.54
1:1:957:C:H5'	24:LQ:86:ASN:HD22	1.73	0.54
2:2:257:U:H3'	2:2:258:C:H5'	1.90	0.54
10:LC:29:ALA:O	50:Lq:3:ASN:ND2	2.41	0.54
23:LP:154:GLU:HG2	23:LP:155:GLU:H	1.73	0.54
53:SB:13:LYS:HD2	53:SB:13:LYS:H	1.72	0.54
71:ST:117:ASP:OD1	71:ST:124:ARG:NH1	2.41	0.54
1:1:3332:A:O2'	1:1:3333:G:OP1	2.25	0.54
2:2:1416:C:OP1	81:Sd:54:LYS:NZ	2.41	0.54
5:A:248:LEU:O	5:A:259:PHE:N	2.33	0.54
8:LA:79:ASN:ND2	8:LA:166:ILE:O	2.40	0.54
13:LF:98:ILE:HD12	24:LQ:33:ASP:HB2	1.88	0.54
60:SI:82:VAL:HG22	60:SI:200:LEU:HD11	1.88	0.54
62:SK:26:ASP:O	62:SK:37:ASN:ND2	2.40	0.54
1:1:921:U:OP1	86:1:3912:HOH:O	2.18	0.54
1:1:1940:U:O2	1:1:2045:G:N1	2.41	0.54
2:2:231:G:H2'	2:2:232:G:C8	2.43	0.54
31:LX:82:THR:H	31:LX:85:ALA:HB3	1.72	0.54
56:SE:141:THR:OG1	56:SE:143:ASP:OD1	2.25	0.54
72:SU:19:ILE:HD13	72:SU:97:VAL:HG11	1.90	0.54
8:LA:68:LYS:HD3	8:LA:70:LYS:HE2	1.89	0.54
27:LT:79:ARG:HG2	27:LT:79:ARG:HH11	1.73	0.54
40:Lg:79:GLY:O	40:Lg:80:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:3:PRO:HD3	73:SV:80:LYS:HE3	1.89	0.54
56:SE:129:VAL:HG12	56:SE:139:LEU:HB3	1.90	0.54
1:1:1454:U:OP1	25:LR:5:ARG:NH1	2.41	0.54
2:2:851:G:OP1	25:LR:176:ARG:NH1	2.41	0.54
3:3:7:G:OP1	11:LD:33:ARG:NH1	2.40	0.54
56:SE:99:PHE:HE1	56:SE:113:ARG:HD3	1.72	0.54
68:SQ:101:SER:O	68:SQ:105:LEU:N	2.30	0.54
70:SS:76:PRO:HB2	70:SS:81:ILE:HD11	1.90	0.54
1:1:2900:A:OP2	9:LB:257:HIS:HD2	1.91	0.53
4:4:97:A:OP1	41:Lh:68:ARG:NH2	2.41	0.53
32:LY:52:GLY:H	32:LY:69:VAL:HG23	1.72	0.53
1:1:2387:A:OP1	21:LN:90:ASN:ND2	2.40	0.53
27:LT:51:GLY:HA3	27:LT:92:ARG:HG3	1.90	0.53
35:Lb:60:GLY:H	35:Lb:62:ARG:NH1	2.04	0.53
46:Lm:104:PRO:HD3	46:Lm:111:ARG:HH21	1.73	0.53
53:SB:35:PRO:HG3	53:SB:99:ASN:HA	1.90	0.53
55:SD:165:GLN:N	55:SD:166:PRO:HD2	2.22	0.53
71:ST:131:ARG:NH1	71:ST:132:ASP:OD1	2.41	0.53
76:SY:125:ALA:HA	76:SY:128:LYS:HE2	1.90	0.53
1:1:1205:G:N7	51:Ls:58:MET:HE3	2.24	0.53
1:1:2064:C:O2'	1:1:2065:U:OP1	2.26	0.53
2:2:539:A:N1	82:Se:28:LYS:NZ	2.41	0.53
5:A:28:PRO:O	5:A:47:ARG:NH2	2.42	0.53
32:LY:50:ARG:HG2	32:LY:51:LYS:H	1.73	0.53
53:SB:146:ARG:HD3	53:SB:147:PRO:HD2	1.90	0.53
60:SI:59:ARG:O	60:SI:60:LEU:HD23	2.09	0.53
70:SS:86:LEU:HD12	70:SS:97:ASP:HB3	1.89	0.53
2:2:216:A:H5''	2:2:831:U:H1'	1.90	0.53
2:2:231:G:H2'	2:2:232:G:H8	1.73	0.53
2:2:301:U:OP1	63:SL:141:ARG:NH1	2.41	0.53
2:2:644:A:H2'	2:2:645:G:C8	2.44	0.53
2:2:977:A:N3	2:2:1771:U:O2'	2.41	0.53
2:2:1357:C:O2'	71:ST:3:GLY:N	2.40	0.53
15:LH:107:ALA:O	15:LH:108:GLU:HG3	2.08	0.53
32:LY:50:ARG:HG2	32:LY:51:LYS:N	2.24	0.53
53:SB:144:LYS:HB2	53:SB:208:GLN:HB3	1.89	0.53
1:1:291:U:OP2	42:Li:42:GLN:NE2	2.42	0.53
1:1:1695:A:H4'	1:1:1696:A:H5'	1.89	0.53
2:2:508:A:OP2	61:SJ:174:LYS:NZ	2.36	0.53
53:SB:129:THR:OG1	53:SB:131:ASP:O	2.24	0.53
53:SB:154:THR:OG1	53:SB:205:TYR:OH	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2349:A:OP1	86:1:3915:HOH:O	2.19	0.53
2:2:700:G:N2	2:2:731:G:O2'	2.42	0.53
12:LE:76:LEU:HB2	12:LE:80:VAL:HG23	1.90	0.53
51:Ls:57:THR:HA	51:Ls:60:ARG:HH21	1.73	0.53
70:SS:38:VAL:HG23	70:SS:42:TYR:HB3	1.89	0.53
71:ST:45:GLU:OE1	71:ST:45:GLU:N	2.41	0.53
1:1:1213:G:H1	1:1:1262:C:H42	1.54	0.53
2:2:956:U:OP2	79:Sb:20:LYS:NZ	2.38	0.53
2:2:607:G:O2'	2:2:610:G:O2'	2.16	0.53
5:A:170:TRP:HA	5:A:194:TYR:HB2	1.90	0.53
24:LQ:208:SER:OG	24:LQ:209:ARG:NH1	2.42	0.53
37:Ld:105:ASN:ND2	37:Ld:105:ASN:C	2.64	0.53
41:Lh:18:GLU:CD	41:Lh:18:GLU:H	2.17	0.53
49:Lp:29:GLN:HE21	49:Lp:69:TYR:HD1	1.56	0.53
52:SA:87:ARG:NH2	69:SR:82:ASP:O	2.41	0.53
56:SE:31:PRO:HG2	56:SE:38:LEU:HG	1.91	0.53
61:SJ:62:GLU:O	61:SJ:63:LYS:HG3	2.09	0.53
1:1:1940:U:H1'	1:1:2045:G:H22	1.73	0.53
1:1:3008:U:O2'	30:LW:16:GLY:O	2.27	0.53
3:3:40:C:O2	17:LJ:73:ARG:NH1	2.41	0.53
37:Ld:37:ALA:H	37:Ld:72:ILE:HG23	1.73	0.53
1:1:1843:G:N1	1:1:1846:C:OP2	2.41	0.53
37:Ld:83:ILE:HG12	37:Ld:101:VAL:HG12	1.90	0.53
38:Le:68:MET:HB2	38:Le:69:PRO:HD2	1.91	0.53
77:SZ:84:HIS:H	77:SZ:88:LYS:HD3	1.73	0.53
81:Sd:26:HIS:ND1	81:Sd:39:CYS:SG	2.76	0.53
1:1:1239:G:O2'	18:LK:121:PHE:O	2.27	0.52
1:1:3159:U:H1'	12:LE:190:ARG:NH1	2.25	0.52
43:Lj:29:ASN:O	43:Lj:32:LYS:NZ	2.30	0.52
72:SU:20:ARG:O	72:SU:113:THR:OG1	2.26	0.52
1:1:3185:G:O6	9:LB:151:ARG:NH1	2.41	0.52
35:Lb:60:GLY:H	35:Lb:62:ARG:HH12	1.57	0.52
58:SG:31:ARG:HH12	58:SG:68:ILE:HG23	1.75	0.52
70:SS:127:HIS:CE1	70:SS:133:VAL:HG11	2.44	0.52
5:A:292:SER:OG	5:A:294:ASP:OD1	2.27	0.52
54:SC:155:ASN:ND2	73:SV:3:ASN:O	2.43	0.52
59:SH:169:ARG:NH2	59:SH:196:PRO:O	2.43	0.52
70:SS:91:ASP:OD1	70:SS:92:ILE:N	2.42	0.52
80:Sc:11:VAL:HG12	80:Sc:33:PHE:HA	1.91	0.52
6:B:135:GLU:OE1	6:B:138:ALA:N	2.42	0.52
70:SS:92:ILE:HG13	70:SS:93:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:162:G:O2'	30:LW:80:ARG:NH2	2.43	0.52
2:2:472:A:OP1	61:SJ:128:ARG:HG3	2.09	0.52
4:4:71:A:OP2	32:LY:50:ARG:NH1	2.42	0.52
78:Sa:68:TYR:O	78:Sa:69:LEU:HD23	2.10	0.52
2:2:1249:C:OP2	83:Sf:105:TYR:OH	2.16	0.52
62:SK:20:VAL:O	62:SK:21:MET:HE2	2.10	0.52
81:Sd:10:ARG:HE	81:Sd:11:PRO:HD2	1.75	0.52
1:1:1196:G:H5''	26:LS:137:ARG:HH12	1.74	0.52
1:1:2266:A:OP1	47:Ln:23:ARG:NH1	2.36	0.52
21:LN:159:ARG:HB2	21:LN:164:LEU:HB2	1.91	0.52
24:LQ:174:ARG:HB3	24:LQ:177:VAL:HG23	1.92	0.52
34:La:82:VAL:HG13	34:La:87:ARG:HB2	1.92	0.52
56:SE:212:ASP:OD1	56:SE:213:ALA:N	2.42	0.52
57:SF:112:THR:HG22	57:SF:114:GLN:H	1.74	0.52
67:SP:91:MET:HE3	67:SP:124:LEU:HD11	1.92	0.52
2:2:1582:A:OP1	68:SQ:132:ARG:N	2.43	0.52
20:LM:72:LEU:HD12	20:LM:73:PRO:HD2	1.92	0.52
59:SH:57:VAL:HG21	59:SH:178:THR:HA	1.92	0.52
65:SN:87:ASP:OD1	65:SN:88:LEU:N	2.41	0.52
70:SS:41:ARG:NH2	71:ST:37:THR:O	2.43	0.52
1:1:265:G:H1'	42:Li:91:ARG:HH12	1.74	0.52
1:1:3186:A:H4'	9:LB:95:THR:HG22	1.92	0.52
2:2:1703:C:H2'	2:2:1704:A:H8	1.75	0.52
33:LZ:75:ASN:OD1	33:LZ:76:TYR:N	2.43	0.52
63:SL:61:LYS:NZ	86:SL:201:HOH:O	2.39	0.52
74:SW:28:ARG:HB3	74:SW:29:PRO:HD3	1.91	0.52
1:1:1818:C:H5''	1:1:1819:A:H5'	1.92	0.52
26:LS:134:ASP:OD2	26:LS:134:ASP:N	2.43	0.52
40:Lg:46:GLY:N	40:Lg:80:SER:O	2.39	0.52
70:SS:42:TYR:HD1	70:SS:85:PHE:HE2	1.58	0.52
2:2:1790:A:OP2	78:Sa:4:LYS:NZ	2.38	0.51
61:SJ:81:ILE:HD11	61:SJ:145:MET:HG3	1.91	0.51
1:1:2904:G:O2'	1:1:2907:C:OP2	2.22	0.51
36:Lc:101:SER:OG	36:Lc:102:ASP:N	2.42	0.51
77:SZ:71:ASP:OD1	77:SZ:72:LEU:N	2.43	0.51
1:1:1267:C:O2'	1:1:1268:G:OP1	2.24	0.51
11:LD:245:GLU:OE1	11:LD:249:GLN:NE2	2.44	0.51
64:SM:127:GLY:O	64:SM:133:ARG:NH2	2.44	0.51
1:1:1704:U:H1'	1:1:1705:C:C6	2.46	0.51
5:A:195:ILE:HA	5:A:211:GLY:HA3	1.92	0.51
8:LA:113:VAL:HG12	8:LA:166:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LT:88:ARG:NH1	35:Lb:33:LYS:O	2.43	0.51
35:Lb:58:LYS:O	35:Lb:62:ARG:NH2	2.44	0.51
63:SL:137:SER:OG	63:SL:138:LYS:N	2.44	0.51
67:SP:84:VAL:O	67:SP:103:GLY:N	2.33	0.51
76:SY:39:SER:HB2	76:SY:42:GLU:OE1	2.10	0.51
1:1:1073:G:H2'	1:1:1074:G:H8	1.75	0.51
1:1:1227:A:H5''	1:1:1254:A:H4'	1.93	0.51
1:1:2855:A:OP1	46:Lm:102:ARG:NE	2.33	0.51
67:SP:131:TYR:OH	70:SS:126:ARG:NH1	2.39	0.51
70:SS:32:LEU:O	70:SS:35:ILE:HG22	2.10	0.51
77:SZ:31:LEU:HB2	77:SZ:64:LEU:HD21	1.92	0.51
1:1:2621:G:O2'	1:1:2622:G:OP1	2.28	0.51
53:SB:189:ILE:HG13	53:SB:190:PRO:HD3	1.92	0.51
58:SG:135:PRO:HG2	58:SG:141:ILE:HD13	1.93	0.51
64:SM:56:ARG:NH2	83:Sf:126:CYS:SG	2.84	0.51
1:1:806:U:H5''	8:LA:21:ARG:HD3	1.93	0.51
1:1:2184:G:N7	42:Li:76:LYS:NZ	2.55	0.51
2:2:1354:U:H2'	2:2:1355:G:H8	1.76	0.51
33:LZ:51:LYS:O	33:LZ:64:ARG:NH1	2.43	0.51
1:1:2492:G:N7	86:1:4011:HOH:O	2.34	0.51
1:1:2532:C:H5''	33:LZ:56:MET:HG2	1.92	0.51
5:A:109:LEU:N	5:A:123:GLY:O	2.40	0.51
30:LW:88:GLU:HA	30:LW:91:LYS:NZ	2.25	0.51
65:SN:83:ASP:OD1	65:SN:84:ILE:N	2.44	0.51
1:1:701:U:P	42:Li:18:ARG:HH22	2.34	0.51
1:1:768:A:H62	24:LQ:115:THR:HG21	1.74	0.51
23:LP:154:GLU:N	23:LP:154:GLU:OE1	2.44	0.51
51:Ls:26:PHE:O	51:Ls:87:VAL:N	2.37	0.51
2:2:537:G:N2	2:2:539:A:N7	2.59	0.51
5:A:236:ILE:HD12	5:A:239:LEU:HD11	1.92	0.51
11:LD:39:GLN:NE2	11:LD:46:ALA:O	2.23	0.51
11:LD:59:ASP:OD2	11:LD:81:HIS:NE2	2.43	0.51
62:SK:21:MET:HB2	62:SK:64:TYR:HB2	1.92	0.51
66:SO:131:VAL:HG12	66:SO:131:VAL:O	2.11	0.51
1:1:896:A:N1	8:LA:204:MET:HE2	2.26	0.50
2:2:1531:U:O2'	2:2:1532:G:OP2	2.28	0.50
45:Ll:27:ILE:O	45:Ll:33:ASN:ND2	2.43	0.50
52:SA:55:LYS:HD3	73:SV:82:VAL:HG23	1.93	0.50
1:1:206:G:OP2	32:LY:1:MET:N	2.44	0.50
1:1:507:G:N7	86:1:4015:HOH:O	2.34	0.50
1:1:696:G:N2	1:1:699:A:OP2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2407:C:H2'	1:1:2408:A:C8	2.46	0.50
56:SE:44:LEU:HB3	56:SE:65:MET:HE1	1.93	0.50
76:SY:63:LEU:HD23	76:SY:74:GLY:HA3	1.92	0.50
1:1:1333:A:H2'	1:1:1335:A:H5''	1.93	0.50
1:1:2396:U:H1'	21:LN:125:SER:HB2	1.93	0.50
19:LL:47:ALA:HB3	19:LL:48:PRO:HD3	1.92	0.50
61:SJ:133:ARG:NH1	61:SJ:135:GLY:O	2.44	0.50
81:Sd:30:LEU:HD21	81:Sd:37:ASN:HA	1.93	0.50
2:2:673:U:H2'	2:2:674:G:C8	2.46	0.50
2:2:1364:G:O3'	71:ST:69:LYS:NZ	2.38	0.50
5:A:226:HIS:CG	55:SD:224:GLN:HE22	2.29	0.50
65:SN:49:GLN:HA	65:SN:52:VAL:HG12	1.93	0.50
1:1:1464:A:O2'	1:1:1838:A:H1'	2.11	0.50
2:2:792:U:H1'	2:2:793:U:OP2	2.11	0.50
2:2:910:U:H1'	2:2:912:G:C2	2.47	0.50
9:LB:228:VAL:HG21	9:LB:271:MET:HE3	1.93	0.50
62:SK:42:LYS:HA	62:SK:45:GLN:HG3	1.92	0.50
2:2:120:U:H1'	56:SE:33:THR:HG23	1.93	0.50
2:2:1223:G:O2'	2:2:1253:A:N6	2.34	0.50
32:LY:30:MET:HE1	32:LY:74:ARG:HG2	1.92	0.50
57:SF:29:LEU:HD12	57:SF:30:PHE:O	2.12	0.50
64:SM:61:MET:HE3	64:SM:123:VAL:HB	1.93	0.50
68:SQ:94:ALA:HB2	68:SQ:102:LYS:HD2	1.93	0.50
1:1:1651:C:O3'	25:LR:60:ARG:NH1	2.44	0.50
2:2:607:G:C8	2:2:611:A:H1'	2.47	0.50
12:LE:142:PHE:HD2	12:LE:150:GLN:HE22	1.59	0.50
68:SQ:49:TYR:O	68:SQ:53:LEU:HD12	2.12	0.50
76:SY:91:ARG:HE	76:SY:103:VAL:HG23	1.76	0.50
77:SZ:67:LYS:HA	77:SZ:70:LYS:NZ	2.26	0.50
1:1:1893:A:N3	1:1:2083:G:H2'	2.27	0.50
2:2:1386:C:H2'	2:2:1387:U:H4'	1.94	0.50
16:LI:101:LYS:HB3	16:LI:104:SER:HB3	1.93	0.50
25:LR:105:LEU:HD23	25:LR:138:LEU:HD23	1.93	0.50
70:SS:67:GLU:O	70:SS:71:THR:HG23	2.12	0.50
1:1:2621:G:H2'	1:1:2622:G:C8	2.47	0.50
1:1:3159:U:H1'	12:LE:190:ARG:HH12	1.77	0.50
10:LC:10:PHE:CZ	10:LC:147:PRO:HB2	2.47	0.50
17:LJ:12:GLU:OE2	17:LJ:14:ARG:NH2	2.32	0.50
55:SD:175:THR:O	55:SD:176:ARG:NH1	2.35	0.50
64:SM:31:LYS:O	64:SM:35:LYS:HG2	2.12	0.50
66:SO:116:ARG:HH12	80:Sc:63:GLU:CD	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1569:A:H4'	2:2:1570:G:OP2	2.12	0.49
33:LZ:83:ARG:NH1	40:Lg:98:GLU:OE1	2.44	0.49
70:SS:36:LYS:HB3	70:SS:102:ALA:HA	1.94	0.49
1:1:1470:G:O6	86:1:3917:HOH:O	2.19	0.49
2:2:1616:C:O2'	2:2:1617:U:OP1	2.26	0.49
51:Ls:48:GLN:NE2	51:Ls:89:THR:OG1	2.30	0.49
55:SD:30:ARG:O	62:SK:56:GLN:NE2	2.45	0.49
59:SH:17:GLN:OE1	59:SH:18:ASN:ND2	2.45	0.49
1:1:1316:C:O2	13:LF:215:ASN:ND2	2.45	0.49
1:1:3079:U:H1'	1:1:3080:A:H5''	1.94	0.49
5:A:35:SER:OG	5:A:36:ARG:N	2.43	0.49
8:LA:167:GLY:HA2	49:Lp:79:MET:HE2	1.95	0.49
17:LJ:78:GLU:OE2	17:LJ:167:ARG:NH1	2.45	0.49
69:SR:24:LEU:HB3	69:SR:34:VAL:HG11	1.94	0.49
70:SS:82:PRO:HG2	70:SS:85:PHE:HB2	1.94	0.49
1:1:2356:G:H4'	9:LB:253:ILE:HD13	1.95	0.49
2:2:66:U:O2	58:SG:160:ARG:HD3	2.11	0.49
5:A:66:VAL:HG12	5:A:82:SER:HB2	1.95	0.49
26:LS:16:THR:HG23	26:LS:19:ASN:H	1.77	0.49
59:SH:92:SER:OG	59:SH:93:ASP:N	2.45	0.49
64:SM:94:GLY:HA2	64:SM:97:LEU:HB2	1.93	0.49
65:SN:53:ILE:O	65:SN:57:SER:OG	2.18	0.49
70:SS:120:ARG:HD2	70:SS:120:ARG:O	2.13	0.49
1:1:1225:G:OP1	1:1:1225:G:N2	2.33	0.49
1:1:3281:G:O2'	1:1:3282:U:OP1	2.29	0.49
26:LS:81:TYR:CE1	26:LS:90:MET:HE3	2.47	0.49
66:SO:42:HIS:HD1	66:SO:54:ARG:HD3	1.77	0.49
2:2:204:U:H2'	2:2:205:A:H8	1.78	0.49
21:LN:147:ARG:HG3	41:Lh:106:LEU:HD21	1.94	0.49
30:LW:105:ARG:NH1	58:SG:151:ASP:OD1	2.45	0.49
1:1:3207:G:OP2	12:LE:88:LYS:NZ	2.46	0.49
2:2:1531:U:H4'	2:2:1532:G:O5'	2.13	0.49
59:SH:151:ARG:HH21	59:SH:153:LYS:HD3	1.78	0.49
71:ST:77:ARG:NH1	71:ST:95:ASP:OD2	2.46	0.49
75:SX:53:VAL:HG12	75:SX:100:ASP:H	1.78	0.49
1:1:766:G:C8	24:LQ:93:SER:HB3	2.48	0.49
2:2:204:U:H2'	2:2:205:A:C8	2.48	0.49
2:2:893:G:H1	2:2:915:U:H3	1.61	0.49
2:2:1225:G:O6	64:SM:69:GLU:N	2.34	0.49
26:LS:12:ARG:NH2	26:LS:57:GLU:OE2	2.41	0.49
44:Lk:5:VAL:HG11	44:Lk:11:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SC:117:GLY:HA2	54:SC:147:VAL:HG22	1.94	0.49
1:1:2123:G:O6	86:1:3910:HOH:O	2.17	0.49
2:2:643:U:H2'	2:2:644:A:C8	2.47	0.49
5:A:23:THR:HG21	5:A:292:SER:HA	1.95	0.49
19:LL:76:THR:HG22	19:LL:101:ARG:HB3	1.95	0.49
59:SH:50:VAL:HG23	59:SH:69:PRO:HD3	1.95	0.49
60:SI:36:THR:HG22	60:SI:57:ALA:O	2.11	0.49
1:1:1744:C:OP1	25:LR:43:LYS:NZ	2.37	0.49
1:1:1796:A:H2'	1:1:1797:A:C8	2.48	0.49
2:2:1252:G:O2'	2:2:1253:A:O5'	2.26	0.49
56:SE:97:GLU:N	56:SE:97:GLU:OE2	2.46	0.49
61:SJ:107:LEU:HB2	61:SJ:144:PHE:HB3	1.95	0.49
62:SK:31:HIS:CE1	62:SK:36:ARG:HA	2.47	0.49
76:SY:121:LEU:HD13	76:SY:128:LYS:HG3	1.94	0.49
1:1:2167:C:O2'	1:1:2168:U:OP1	2.31	0.48
2:2:233:G:O2'	2:2:234:C:OP1	2.28	0.48
33:LZ:30:GLN:CD	33:LZ:30:GLN:H	2.21	0.48
51:Ls:129:GLU:CD	51:Ls:130:PRO:HD2	2.38	0.48
51:Ls:189:GLN:OE1	51:Ls:193:GLN:N	2.45	0.48
1:1:1744:C:H3'	1:1:1745:U:H5''	1.94	0.48
2:2:1329:C:C2'	55:SD:165:GLN:HE22	2.26	0.48
3:3:69:G:H1	3:3:108:C:H42	1.60	0.48
51:Ls:12:PHE:HE1	51:Ls:60:ARG:HH11	1.60	0.48
57:SF:59:HIS:CD2	57:SF:94:LYS:HD3	2.48	0.48
1:1:652:A:H5'	10:LC:108:ARG:HA	1.94	0.48
1:1:1205:G:OP2	1:1:1205:G:H8	1.97	0.48
21:LN:127:TYR:HB3	21:LN:129:TYR:HE1	1.78	0.48
33:LZ:91:LEU:O	33:LZ:91:LEU:HD12	2.13	0.48
54:SC:42:GLU:OE2	54:SC:44:GLN:NE2	2.43	0.48
77:SZ:54:LEU:HD23	77:SZ:60:ILE:HD11	1.95	0.48
1:1:861:U:O2'	23:LP:135:ARG:NH2	2.43	0.48
2:2:329:U:P	60:SI:56:ARG:HH22	2.36	0.48
2:2:1224:A:O2'	2:2:1225:G:OP2	2.27	0.48
8:LA:52:PRO:HB2	8:LA:191:VAL:HG21	1.94	0.48
16:LI:93:PRO:HB2	16:LI:125:THR:HG22	1.94	0.48
60:SI:137:LYS:HG2	60:SI:143:GLU:OE2	2.13	0.48
62:SK:15:LEU:HA	62:SK:21:MET:HE3	1.95	0.48
77:SZ:57:ARG:HG3	77:SZ:58:LEU:HD22	1.95	0.48
1:1:535:U:H2'	1:1:536:C:H5''	1.96	0.48
1:1:1604:G:N7	86:1:4020:HOH:O	2.35	0.48
2:2:273:C:O2	2:2:276:G:N2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:476:U:O2'	61:SJ:118:LYS:NZ	2.36	0.48
2:2:1254:U:O4'	62:SK:8:ARG:NH1	2.38	0.48
2:2:1790:A:H1'	78:Sa:79:ILE:HD11	1.95	0.48
5:A:91:GLU:OE1	5:A:93:SER:OG	2.23	0.48
10:LC:155:SER:HG	10:LC:259:SER:HG	1.59	0.48
16:LI:208:GLU:HA	16:LI:211:ARG:HG2	1.96	0.48
57:SF:152:LEU:O	57:SF:156:ASN:ND2	2.46	0.48
59:SH:41:LYS:O	59:SH:45:ARG:HG3	2.12	0.48
67:SP:90:ASP:OD1	67:SP:90:ASP:N	2.45	0.48
1:1:859:C:HO2'	1:1:862:G:HO2'	1.59	0.48
1:1:2053:U:H4'	1:1:2054:U:H5''	1.95	0.48
2:2:820:U:H2'	2:2:821:G:H5''	1.95	0.48
15:LH:18:VAL:HG11	15:LH:53:ILE:HD11	1.95	0.48
31:LX:126:LEU:HD21	31:LX:134:LYS:HE3	1.95	0.48
63:SL:7:VAL:HG13	63:SL:8:GLN:HG2	1.95	0.48
65:SN:88:LEU:HD13	65:SN:125:LEU:HD22	1.95	0.48
68:SQ:50:GLU:O	68:SQ:54:ILE:HG12	2.14	0.48
1:1:2552:A:H4'	1:1:2553:C:O5'	2.13	0.48
9:LB:10:ARG:NH1	9:LB:11:HIS:O	2.47	0.48
11:LD:194:ASP:O	11:LD:195:THR:OG1	2.26	0.48
61:SJ:94:VAL:HA	61:SJ:97:LEU:HD13	1.96	0.48
78:Sa:101:VAL:HG12	78:Sa:104:ASN:H	1.78	0.48
1:1:1745:U:H4'	1:1:1745:U:OP1	2.14	0.48
2:2:1602:C:H2'	2:2:1603:G:C8	2.48	0.48
3:3:70:G:H1	3:3:107:C:H42	1.62	0.48
21:LN:35:VAL:HG12	21:LN:36:ILE:HG13	1.94	0.48
53:SB:137:LEU:HG	53:SB:215:VAL:HG22	1.94	0.48
58:SG:163:GLN:HB3	58:SG:171:PRO:HB3	1.96	0.48
59:SH:177:ASP:OD1	59:SH:178:THR:N	2.47	0.48
63:SL:140:VAL:C	63:SL:141:ARG:HD2	2.39	0.48
64:SM:52:LYS:HD3	83:Sf:129:GLY:HA3	1.95	0.48
1:1:403:U:O4	86:1:3916:HOH:O	2.19	0.48
1:1:701:U:OP1	42:Li:18:ARG:NH2	2.46	0.48
1:1:1223:A:N1	1:1:1227:A:O2'	2.41	0.48
1:1:2992:C:O2	15:LH:124:ILE:HG12	2.14	0.48
13:LF:80:SER:OG	27:LT:141:VAL:O	2.25	0.48
15:LH:103:VAL:HG13	15:LH:103:VAL:O	2.14	0.48
19:LL:85:ILE:HD12	19:LL:116:LEU:HD21	1.96	0.48
74:SW:10:ALA:HB1	74:SW:27:ILE:HD13	1.96	0.48
78:Sa:44:MET:HG2	78:Sa:65:PRO:O	2.14	0.48
1:1:328:G:OP2	32:LY:13:LYS:NZ	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:364:G:N1	1:1:367:A:OP2	2.44	0.48
11:LD:194:ASP:OD2	11:LD:197:VAL:HG23	2.14	0.48
49:Lp:32:THR:O	49:Lp:37:TYR:OH	2.29	0.48
64:SM:84:HIS:ND1	64:SM:85:LYS:HG2	2.28	0.48
1:1:1658:G:OP2	28:LU:84:LYS:NZ	2.47	0.47
2:2:777:C:H2'	2:2:778:U:H2'	1.96	0.47
2:2:1689:A:H2'	2:2:1690:G:C8	2.47	0.47
5:A:17:TRP:HB2	5:A:36:ARG:HG3	1.95	0.47
1:1:2655:A:OP1	7:C:605:ARG:NE	2.46	0.47
2:2:644:A:O2'	2:2:645:G:OP1	2.29	0.47
51:Ls:16:LYS:HE3	51:Ls:64:LYS:HZ1	1.79	0.47
57:SF:43:ILE:HG13	57:SF:44:SER:H	1.79	0.47
70:SS:30:TYR:HE1	70:SS:40:ARG:HD3	1.80	0.47
2:2:483:G:H2'	2:2:484:G:C8	2.49	0.47
2:2:1763:G:OP1	2:2:1766:C:H4'	2.14	0.47
5:A:185:GLN:HB2	55:SD:230:TYR:HB2	1.94	0.47
5:A:191:HIS:ND1	5:A:213:ASP:OD2	2.34	0.47
37:Ld:60:ASP:OD1	37:Ld:100:TYR:OH	2.26	0.47
53:SB:3:VAL:HG13	66:SO:62:LYS:HA	1.97	0.47
56:SE:11:ARG:O	56:SE:12:LEU:HB2	2.14	0.47
1:1:2837:G:H5''	9:LB:5:LYS:HE3	1.95	0.47
9:LB:331:GLY:HA3	9:LB:337:MET:HE1	1.97	0.47
55:SD:83:PRO:O	55:SD:86:SER:OG	2.24	0.47
57:SF:32:ARG:NH1	57:SF:106:GLU:OE2	2.46	0.47
1:1:1027:U:OP1	16:LI:90:ARG:NH2	2.34	0.47
1:1:1076:A:O5'	27:LT:120:LYS:NZ	2.48	0.47
5:A:210:GLY:HA3	5:A:236:ILE:HD11	1.97	0.47
30:LW:88:GLU:HA	30:LW:91:LYS:HZ3	1.80	0.47
54:SC:53:VAL:HG22	54:SC:58:ILE:HD11	1.96	0.47
60:SI:36:THR:O	60:SI:95:THR:OG1	2.28	0.47
62:SK:67:THR:HG22	62:SK:69:ALA:H	1.80	0.47
63:SL:29:SER:O	63:SL:37:ARG:NH1	2.47	0.47
70:SS:62:THR:OG1	70:SS:65:GLU:OE1	2.32	0.47
72:SU:20:ARG:HA	72:SU:89:ASP:HA	1.97	0.47
1:1:2551:G:N7	86:1:4018:HOH:O	2.35	0.47
2:2:1219:C:H2'	2:2:1220:G:H8	1.80	0.47
2:2:1254:U:O2'	2:2:1255:U:O4'	2.32	0.47
2:2:1784:G:C8	66:SO:145:ARG:NH1	2.83	0.47
16:LI:50:VAL:HG12	16:LI:167:VAL:HG22	1.96	0.47
54:SC:239:LYS:HE3	54:SC:239:LYS:HB2	1.73	0.47
60:SI:201:HIS:O	60:SI:201:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1238:C:H2'	1:1:1239:G:H8	1.78	0.47
2:2:188:U:O2'	2:2:190:G:O6	2.27	0.47
2:2:324:C:H2'	2:2:325:U:C6	2.50	0.47
2:2:644:A:H2'	2:2:645:G:H8	1.79	0.47
2:2:862:U:O2	79:Sb:21:LEU:HB3	2.15	0.47
2:2:1329:C:H2'	55:SD:165:GLN:HE22	1.80	0.47
2:2:1380:G:P	72:SU:86:ARG:HH22	2.38	0.47
2:2:1575:C:H5''	68:SQ:140:LYS:HE3	1.95	0.47
10:LC:37:LYS:O	10:LC:41:THR:HG23	2.14	0.47
13:LF:169:LEU:O	13:LF:169:LEU:HD12	2.14	0.47
13:LF:217:ASN:H	13:LF:247:ALA:HB1	1.78	0.47
17:LJ:20:LEU:HD11	17:LJ:38:LEU:HD11	1.96	0.47
22:LO:187:ALA:O	22:LO:191:VAL:HG22	2.15	0.47
53:SB:126:THR:HG22	53:SB:136:ARG:HE	1.78	0.47
58:SG:165:LYS:HG3	58:SG:166:GLY:H	1.79	0.47
65:SN:92:ILE:HD13	65:SN:122:ILE:HD13	1.97	0.47
68:SQ:10:PHE:CE2	68:SQ:12:LYS:HE3	2.49	0.47
70:SS:30:TYR:O	70:SS:33:THR:OG1	2.28	0.47
1:1:211:U:H4'	32:LY:99:HIS:CD2	2.50	0.47
1:1:1016:U:H2'	1:1:1017:U:C6	2.50	0.47
1:1:1047:A:H4'	1:1:1048:A:O5'	2.14	0.47
1:1:1088:C:H2'	1:1:1089:G:C8	2.50	0.47
1:1:2137:G:OP2	8:LA:193:ARG:NH1	2.47	0.47
2:2:414:A:H4'	2:2:415:G:O5'	2.14	0.47
5:A:242:SER:OG	5:A:245:ARG:O	2.31	0.47
7:C:571:GLN:O	7:C:575:ILE:HG13	2.15	0.47
49:Lp:85:ARG:O	49:Lp:89:ILE:HG12	2.15	0.47
1:1:1920:G:H21	1:1:3303:A:H8	1.63	0.47
2:2:472:A:OP2	61:SJ:124:ARG:NH1	2.48	0.47
2:2:1529:C:OP2	77:SZ:66:ARG:NH2	2.46	0.47
52:SA:134:GLN:NE2	52:SA:138:GLU:OE2	2.35	0.47
53:SB:26:ARG:NH1	53:SB:49:ASN:OD1	2.43	0.47
61:SJ:131:HIS:HD2	61:SJ:160:SER:HB2	1.80	0.47
1:1:1215:C:O2'	51:Ls:36:GLN:OE1	2.21	0.47
1:1:3310:G:N1	9:LB:381:MET:O	2.46	0.47
2:2:778:U:O2'	2:2:779:A:O4'	2.33	0.47
5:A:226:HIS:CD2	55:SD:224:GLN:HE22	2.32	0.47
21:LN:31:ARG:NH1	21:LN:124:ASP:OD2	2.47	0.47
37:Ld:31:VAL:HG23	37:Ld:36:ARG:HG2	1.97	0.47
52:SA:12:PRO:O	52:SA:13:THR:OG1	2.30	0.47
1:1:974:A:N6	86:1:4001:HOH:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:174:U:O2'	2:2:176:A:OP2	2.33	0.46
2:2:1369:C:H4'	2:2:1370:C:H5''	1.97	0.46
9:LB:233:ARG:HA	9:LB:271:MET:HE2	1.97	0.46
34:La:75:ILE:HG22	34:La:115:LYS:H	1.80	0.46
51:Ls:175:MET:SD	51:Ls:175:MET:N	2.87	0.46
51:Ls:189:GLN:NE2	51:Ls:193:GLN:O	2.48	0.46
71:ST:128:GLN:HA	71:ST:131:ARG:HG2	1.96	0.46
2:2:234:C:H2'	2:2:832:G:H1'	1.97	0.46
2:2:833:U:H2'	2:2:834:U:C6	2.50	0.46
8:LA:181:LYS:HB2	8:LA:184:ARG:HG3	1.96	0.46
11:LD:95:TRP:HD1	11:LD:161:ARG:HA	1.79	0.46
21:LN:99:ARG:NH2	21:LN:118:SER:O	2.48	0.46
56:SE:68:ARG:HB3	56:SE:76:VAL:HG21	1.97	0.46
61:SJ:84:LEU:HD12	61:SJ:97:LEU:HD11	1.97	0.46
1:1:2923:G:N2	1:1:2926:A:OP2	2.37	0.46
2:2:1359:U:H4'	2:2:1360:G:C2	2.50	0.46
2:2:1387:U:HO2'	2:2:1388:A:H8	1.64	0.46
2:2:1428:U:H4'	2:2:1429:G:H5''	1.97	0.46
2:2:1731:C:OP1	29:LV:34:ARG:NH2	2.49	0.46
14:LG:53:VAL:HG12	31:LX:43:THR:HA	1.97	0.46
19:LL:64:LYS:HD2	34:La:69:TRP:CD1	2.51	0.46
20:LM:112:LEU:HD22	20:LM:116:ASP:OD2	2.15	0.46
54:SC:188:ALA:HB1	54:SC:192:VAL:HG23	1.97	0.46
65:SN:3:ARG:HB2	65:SN:6:SER:HB3	1.97	0.46
67:SP:91:MET:HE1	67:SP:97:MET:HE1	1.98	0.46
1:1:2179:G:OP1	42:Li:84:LYS:NZ	2.48	0.46
2:2:652:G:H2'	2:2:653:G:C8	2.51	0.46
12:LE:23:LYS:HD2	13:LF:6:VAL:HG21	1.96	0.46
13:LF:94:ARG:NH2	13:LF:97:GLY:O	2.44	0.46
21:LN:11:SER:O	21:LN:14:LYS:NZ	2.43	0.46
34:La:15:VAL:O	34:La:16:SER:OG	2.29	0.46
36:Lc:51:THR:HG23	36:Lc:56:LYS:HE2	1.97	0.46
57:SF:141:THR:HG22	57:SF:142:VAL:H	1.81	0.46
69:SR:18:GLU:OE2	69:SR:19:LYS:HG3	2.16	0.46
71:ST:65:VAL:HG22	71:ST:71:VAL:HG11	1.98	0.46
2:2:678:G:O2'	2:2:679:G:OP1	2.29	0.46
2:2:703:C:H42	2:2:730:G:H21	1.64	0.46
2:2:1280:U:OP1	86:2:2003:HOH:O	2.20	0.46
2:2:1531:U:C4	57:SF:174:VAL:HA	2.51	0.46
5:A:5:LEU:HB3	5:A:310:TRP:HB3	1.97	0.46
14:LG:210:ASP:OD1	14:LG:210:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LX:152:LYS:HA	31:LX:152:LYS:HD3	1.81	0.46
49:Lp:49:ARG:HH21	49:Lp:52:VAL:HA	1.80	0.46
64:SM:86:ILE:HG22	64:SM:86:ILE:O	2.14	0.46
67:SP:64:LEU:HD11	67:SP:91:MET:HE2	1.96	0.46
67:SP:76:LYS:HD2	67:SP:77:PRO:O	2.16	0.46
74:SW:102:VAL:HB	74:SW:113:HIS:HB3	1.98	0.46
3:3:46:C:OP1	11:LD:161:ARG:HG3	2.15	0.46
17:LJ:115:ILE:O	17:LJ:115:ILE:HG22	2.16	0.46
55:SD:224:GLN:HB3	55:SD:225:PRO:HD3	1.98	0.46
83:Sf:123:ASN:HB3	83:Sf:126:CYS:C	2.40	0.46
1:1:669:U:O4	10:LC:119:LYS:NZ	2.47	0.46
1:1:1290:G:H5'	22:LO:61:LYS:HE3	1.97	0.46
2:2:559:G:H1	2:2:580:C:H42	1.63	0.46
2:2:834:U:H2'	2:2:835:G:C8	2.51	0.46
8:LA:109:GLU:HA	8:LA:136:VAL:HG23	1.96	0.46
29:LV:29:ASP:OD2	29:LV:31:SER:OG	2.31	0.46
43:Lj:84:LYS:HG3	43:Lj:85:GLY:N	2.31	0.46
59:SH:164:LEU:HD11	59:SH:193:PHE:CD2	2.49	0.46
77:SZ:54:LEU:HB3	77:SZ:60:ILE:HD11	1.97	0.46
1:1:1338:A:H4'	1:1:1339:U:O5'	2.16	0.46
1:1:2570:U:H2'	1:1:2571:U:C6	2.51	0.46
1:1:2827:U:O4	86:1:3919:HOH:O	2.20	0.46
5:A:42:ILE:HG23	5:A:56:LYS:HG2	1.98	0.46
44:Lk:54:LYS:HA	44:Lk:57:LYS:HE2	1.97	0.46
60:SI:26:ALA:O	60:SI:29:LEU:HD23	2.16	0.46
71:ST:64:HIS:CE1	71:ST:76:LEU:HD21	2.50	0.46
1:1:3332:A:HO2'	1:1:3333:G:P	2.38	0.46
14:LG:252:ARG:HH21	14:LG:253:LYS:NZ	2.14	0.46
16:LI:21:ARG:O	16:LI:24:ARG:NH1	2.49	0.46
33:LZ:8:ARG:HA	33:LZ:8:ARG:HD3	1.70	0.46
56:SE:59:ARG:HE	56:SE:60:GLU:HG3	1.81	0.46
70:SS:29:VAL:O	70:SS:43:SER:OG	2.26	0.46
1:1:446:A:H1'	1:1:447:U:H5'	1.97	0.46
2:2:1359:U:H1'	2:2:1360:G:H2'	1.98	0.46
5:A:185:GLN:HG2	5:A:186:THR:N	2.31	0.46
19:LL:89:LEU:O	19:LL:92:THR:HG22	2.16	0.46
22:LO:77:ALA:HB3	22:LO:80:ARG:HG2	1.97	0.46
52:SA:36:MET:HE2	52:SA:156:LEU:HD11	1.96	0.46
52:SA:46:ASP:OD2	69:SR:130:SER:N	2.49	0.46
60:SI:61:ASP:OD1	60:SI:61:ASP:N	2.49	0.46
62:SK:26:ASP:OD1	62:SK:26:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SR:25:THR:HG23	69:SR:27:ASP:H	1.80	0.46
78:Sa:79:ILE:HG22	78:Sa:84:VAL:HG23	1.97	0.46
1:1:1702:U:OP2	25:LR:103:ARG:NH1	2.48	0.45
8:LA:245:LEU:HD23	8:LA:247:ARG:HE	1.81	0.45
19:LL:7:GLN:O	34:La:49:HIS:NE2	2.48	0.45
51:Ls:56:ASN:O	51:Ls:60:ARG:NH2	2.47	0.45
63:SL:40:TYR:HB3	63:SL:66:THR:HG22	1.97	0.45
63:SL:64:PRO:HB3	63:SL:71:ILE:HD11	1.98	0.45
66:SO:144:GLY:O	78:Sa:22:ARG:NH2	2.49	0.45
76:SY:58:VAL:HG12	76:SY:78:ILE:HD13	1.96	0.45
2:2:1362:C:H2'	2:2:1363:A:C8	2.51	0.45
6:B:93:PHE:CG	6:B:94:ARG:N	2.85	0.45
9:LB:57:VAL:HG22	9:LB:73:VAL:HG22	1.97	0.45
16:LI:35:ASP:C	16:LI:36:LEU:HD12	2.41	0.45
21:LN:17:ASP:OD2	21:LN:18:VAL:N	2.48	0.45
32:LY:26:ARG:HG2	32:LY:77:TYR:CE1	2.51	0.45
56:SE:45:ILE:HG13	56:SE:61:THR:HG21	1.98	0.45
57:SF:77:ILE:H	57:SF:77:ILE:HD12	1.81	0.45
1:1:2056:A:O2'	1:1:2057:C:OP2	2.32	0.45
1:1:2636:G:O2'	1:1:2638:A:N7	2.47	0.45
2:2:66:U:C5	58:SG:176:PRO:HB3	2.51	0.45
8:LA:33:ASP:OD1	8:LA:33:ASP:N	2.49	0.45
53:SB:217:LEU:HD23	53:SB:217:LEU:H	1.81	0.45
58:SG:2:LYS:HB2	58:SG:108:VAL:HG22	1.98	0.45
62:SK:75:ARG:HH11	62:SK:81:PRO:HA	1.81	0.45
66:SO:63:ALA:O	66:SO:64:ASP:OD1	2.33	0.45
1:1:2182:A:P	42:Li:77:ARG:HH21	2.40	0.45
2:2:235:U:OP2	2:2:832:G:O2'	2.33	0.45
2:2:542:A:H2'	82:Se:31:LYS:NZ	2.31	0.45
4:4:72:A:N3	4:4:88:A:O2'	2.49	0.45
14:LG:102:PRO:HG3	14:LG:193:VAL:HG23	1.99	0.45
60:SI:57:ALA:HB2	60:SI:181:GLY:HA2	1.97	0.45
61:SJ:88:ARG:HB3	61:SJ:93:TYR:CD2	2.51	0.45
1:1:704:A:OP1	1:1:734:C:O2'	2.34	0.45
19:LL:60:CYS:HB2	19:LL:65:TYR:O	2.16	0.45
21:LN:68:ARG:HA	21:LN:98:LEU:HD21	1.99	0.45
28:LU:24:ASN:HB3	28:LU:111:GLU:HB3	1.98	0.45
57:SF:29:LEU:HB2	57:SF:34:SER:HA	1.99	0.45
57:SF:57:ILE:HG13	57:SF:58:PRO:HD2	1.98	0.45
58:SG:21:GLU:OE1	58:SG:25:ARG:NE	2.49	0.45
71:ST:19:TYR:HD1	71:ST:136:ILE:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:104:G:O3'	19:LL:68:ARG:NH2	2.50	0.45
1:1:2219:A:N1	2:2:1751:A:O2'	2.43	0.45
2:2:674:G:H2'	2:2:675:G:C8	2.52	0.45
2:2:1215:G:H1	2:2:1440:A:H2'	1.82	0.45
2:2:1693:C:H2'	2:2:1694:G:H8	1.81	0.45
11:LD:246:ALA:O	11:LD:250:ILE:HG12	2.17	0.45
37:Ld:41:ILE:HG23	37:Ld:59:LEU:HD11	1.98	0.45
39:Lf:54:VAL:HG12	39:Lf:68:VAL:HG22	1.99	0.45
51:Ls:142:PRO:HD2	51:Ls:156:ILE:HG13	1.98	0.45
52:SA:124:ILE:HG12	52:SA:144:ILE:HG21	1.98	0.45
72:SU:60:LEU:HD12	81:Sd:34:TYR:CZ	2.51	0.45
2:2:635:C:N3	59:SH:124:ARG:NH2	2.65	0.45
5:A:165:ILE:HG13	5:A:177:TRP:HB2	1.99	0.45
11:LD:17:GLN:NE2	27:LT:22:HIS:O	2.48	0.45
52:SA:142:VAL:HG23	52:SA:144:ILE:CD1	2.46	0.45
80:Sc:35:ASP:OD1	80:Sc:36:ASP:N	2.50	0.45
1:1:250:C:O2'	1:1:251:U:OP1	2.28	0.45
1:1:2227:U:O2'	1:1:2228:C:OP1	2.30	0.45
2:2:1054:U:O2	2:2:1055:A:N6	2.49	0.45
2:2:1707:C:H3'	2:2:1708:A:H5''	1.99	0.45
5:A:212:LYS:HA	5:A:235:GLU:HG2	1.98	0.45
26:LS:137:ARG:HA	26:LS:137:ARG:HD3	1.67	0.45
28:LU:100:LEU:HD23	28:LU:112:LEU:HD23	1.99	0.45
70:SS:129:TRP:HB3	70:SS:131:LEU:HD13	1.99	0.45
1:1:1582:A:N6	31:LX:83:GLU:OE2	2.50	0.45
2:2:195:G:H2'	2:2:196:G:C8	2.48	0.45
9:LB:237:LYS:HE2	9:LB:237:LYS:HB2	1.70	0.45
19:LL:32:LYS:O	19:LL:36:ARG:HG3	2.17	0.45
27:LT:17:ARG:NH1	27:LT:45:ASN:OD1	2.50	0.45
1:1:1300:A:O2'	1:1:1301:A:H3'	2.17	0.45
1:1:2387:A:H5''	21:LN:90:ASN:ND2	2.32	0.45
2:2:1181:A:HO2'	2:2:1206:C:HO2'	1.58	0.45
5:A:44:ASN:ND2	5:A:56:LYS:HB3	2.31	0.45
29:LV:19:LEU:HD12	29:LV:19:LEU:O	2.16	0.45
31:LX:147:ASP:OD1	31:LX:148:ILE:N	2.50	0.45
51:Ls:63:LEU:HA	51:Ls:66:PHE:CD2	2.52	0.45
52:SA:95:HIS:ND1	52:SA:205:TYR:OH	2.38	0.45
71:ST:11:ASP:OD1	71:ST:12:ALA:N	2.49	0.45
1:1:2148:G:OP1	8:LA:202:VAL:HG23	2.17	0.44
1:1:3068:C:HO2'	15:LH:157:SER:HG	1.57	0.44
2:2:66:U:H5	58:SG:176:PRO:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:166:VAL:HG12	5:A:176:VAL:HG22	1.99	0.44
9:LB:313:VAL:O	9:LB:333:LYS:NZ	2.45	0.44
10:LC:34:ASP:OD1	10:LC:35:ILE:N	2.50	0.44
66:SO:25:LEU:HB2	66:SO:90:THR:OG1	2.17	0.44
1:1:1205:G:C8	51:Ls:58:MET:HE3	2.53	0.44
5:A:85:LYS:HE3	5:A:105:THR:C	2.43	0.44
5:A:87:LEU:HB3	5:A:101:PHE:HB2	1.99	0.44
6:B:139:GLU:N	6:B:139:GLU:OE2	2.50	0.44
8:LA:207:VAL:HG13	8:LA:208:ASP:OD2	2.16	0.44
11:LD:116:ASP:N	11:LD:116:ASP:OD1	2.47	0.44
14:LG:249:GLU:OE1	14:LG:252:ARG:NH2	2.50	0.44
52:SA:151:ASP:OD1	52:SA:152:THR:N	2.40	0.44
53:SB:7:LYS:HE3	53:SB:10:SER:HA	1.99	0.44
59:SH:148:LYS:C	59:SH:149:ARG:HD2	2.42	0.44
59:SH:172:VAL:HG23	59:SH:172:VAL:O	2.17	0.44
61:SJ:61:ASP:OD1	61:SJ:62:GLU:N	2.50	0.44
69:SR:25:THR:O	69:SR:31:ASN:ND2	2.43	0.44
69:SR:98:GLU:OE1	69:SR:99:THR:HG23	2.18	0.44
77:SZ:91:THR:OG1	77:SZ:92:ARG:N	2.48	0.44
1:1:1758:G:O2'	1:1:1760:G:OP2	2.32	0.44
3:3:75:A:N3	26:LS:50:LYS:NZ	2.65	0.44
5:A:235:GLU:OE1	5:A:237:HIS:NE2	2.51	0.44
9:LB:285:ARG:NH1	9:LB:294:ASN:O	2.50	0.44
13:LF:52:LYS:HB2	13:LF:52:LYS:HE2	1.76	0.44
17:LJ:40:GLN:NE2	17:LJ:40:GLN:H	2.14	0.44
31:LX:116:TYR:O	31:LX:118:ILE:HG23	2.17	0.44
55:SD:146:ARG:O	55:SD:146:ARG:HG3	2.17	0.44
55:SD:179:LEU:H	55:SD:179:LEU:HD23	1.82	0.44
78:Sa:18:VAL:HG11	78:Sa:33:ASP:OD2	2.17	0.44
1:1:2463:A:O2'	1:1:2465:U:O4'	2.36	0.44
2:2:1165:U:HO2'	2:2:1166:G:P	2.41	0.44
5:A:33:SER:OG	5:A:43:TRP:NE1	2.43	0.44
12:LE:84:THR:HB	12:LE:94:LEU:HA	2.00	0.44
51:Ls:57:THR:O	51:Ls:61:ARG:NH1	2.29	0.44
64:SM:54:LEU:HD21	64:SM:81:CYS:HA	1.99	0.44
1:1:147:A:P	21:LN:147:ARG:HH22	2.41	0.44
1:1:1787:G:O6	86:1:3918:HOH:O	2.20	0.44
2:2:481:C:H2'	2:2:482:A:C8	2.53	0.44
2:2:1139:A:H5''	78:Sa:2:VAL:CG1	2.48	0.44
2:2:1341:A:H4'	2:2:1342:A:OP1	2.18	0.44
15:LH:22:SER:O	15:LH:22:SER:OG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LJ:33:ARG:NH1	17:LJ:121:ILE:O	2.48	0.44
20:LM:12:ARG:HB3	20:LM:18:ARG:NH1	2.31	0.44
27:LT:79:ARG:HG2	27:LT:79:ARG:NH1	2.33	0.44
70:SS:114:GLU:HA	70:SS:117:LYS:HB3	1.98	0.44
1:1:171:G:H2'	1:1:172:G:H8	1.83	0.44
1:1:811:U:H3	1:1:877:A:N6	2.16	0.44
2:2:1193:A:H4'	2:2:1194:C:O5'	2.15	0.44
2:2:1247:U:O2'	83:Sf:135:MET:SD	2.72	0.44
5:A:192:THR:OG1	5:A:213:ASP:OD1	2.22	0.44
12:LE:72:LEU:HA	12:LE:83:VAL:HG12	2.00	0.44
38:Le:33:TRP:CH2	38:Le:53:MET:HG2	2.53	0.44
51:Ls:51:VAL:HG12	51:Ls:87:VAL:HG22	2.00	0.44
56:SE:19:LEU:HD11	56:SE:108:ARG:HD2	1.99	0.44
57:SF:63:ARG:NH1	68:SQ:122:ARG:HE	2.15	0.44
57:SF:141:THR:HG22	57:SF:142:VAL:N	2.33	0.44
69:SR:20:TYR:HD2	69:SR:23:ARG:HD2	1.83	0.44
1:1:284:C:OP1	21:LN:68:ARG:HG3	2.17	0.44
1:1:1135:G:N2	1:1:1183:A:H61	2.16	0.44
1:1:1239:G:H4'	18:LK:123:LYS:HA	2.00	0.44
2:2:1094:U:H4'	2:2:1095:U:O5'	2.16	0.44
2:2:1686:G:N2	2:2:1708:A:N7	2.66	0.44
2:2:1694:G:H2'	2:2:1695:G:C8	2.53	0.44
6:B:93:PHE:CD1	6:B:94:ARG:HG2	2.52	0.44
9:LB:292:GLU:OE1	9:LB:292:GLU:N	2.49	0.44
15:LH:57:ILE:HG13	15:LH:68:LEU:HD13	1.99	0.44
21:LN:96:ARG:NH2	21:LN:104:GLU:OE1	2.50	0.44
31:LX:142:ASP:OD1	31:LX:143:VAL:HG23	2.18	0.44
40:Lg:21:THR:HB	40:Lg:33:VAL:HG13	1.99	0.44
48:Lo:25:VAL:HG22	48:Lo:72:LEU:HD22	2.00	0.44
58:SG:222:ALA:O	58:SG:225:GLN:NE2	2.50	0.44
59:SH:102:ARG:HD2	59:SH:131:VAL:HG23	1.99	0.44
63:SL:104:ARG:HG3	75:SX:12:ALA:HB2	1.99	0.44
67:SP:58:LYS:C	67:SP:61:PRO:HD2	2.43	0.44
68:SQ:31:VAL:HG12	68:SQ:67:ILE:HD12	1.99	0.44
1:1:2407:C:H2'	1:1:2408:A:H8	1.83	0.44
1:1:2704:G:N2	1:1:2707:A:OP2	2.49	0.44
2:2:1242:G:H21	83:Sf:93:HIS:CE1	2.35	0.44
3:3:86:C:O2'	26:LS:119:ARG:NH1	2.51	0.44
9:LB:228:VAL:HG21	9:LB:271:MET:CE	2.48	0.44
21:LN:73:ARG:HH21	21:LN:92:LEU:HD21	1.82	0.44
21:LN:173:GLY:HA3	21:LN:183:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ls:176:LEU:HB3	51:Ls:178:ILE:HG22	1.99	0.44
54:SC:228:ASN:OD1	73:SV:25:LYS:NZ	2.33	0.44
56:SE:107:GLY:HA2	56:SE:189:MET:HG2	2.00	0.44
66:SO:63:ALA:C	66:SO:65:ARG:H	2.26	0.44
1:1:1913:A:OP2	86:1:3921:HOH:O	2.21	0.44
2:2:591:A:OP1	61:SJ:35:ARG:NH1	2.51	0.44
2:2:1332:U:H2'	2:2:1333:A:H8	1.83	0.44
23:LP:165:ARG:NH2	23:LP:166:ASP:OD2	2.50	0.44
36:Lc:65:MET:HE3	36:Lc:65:MET:HB3	1.78	0.44
1:1:1727:G:N2	44:Lk:2:PRO:HG2	2.32	0.43
1:1:2461:C:H2'	1:1:2462:U:C6	2.53	0.43
2:2:509:A:H2'	2:2:510:U:C6	2.53	0.43
2:2:1244:U:H5''	83:Sf:92:LYS:HA	2.00	0.43
2:2:1245:C:OP2	83:Sf:93:HIS:ND1	2.51	0.43
19:LL:147:THR:HA	41:Lh:124:LYS:HA	1.99	0.43
24:LQ:48:LYS:HE2	24:LQ:48:LYS:HB2	1.91	0.43
54:SC:120:GLY:HA2	54:SC:223:PHE:CE1	2.52	0.43
2:2:1470:G:H2'	2:2:1471:A:C8	2.53	0.43
5:A:127:LYS:HG2	5:A:149:GLU:HA	1.98	0.43
5:A:131:LEU:HD12	5:A:140:TYR:HB3	1.98	0.43
9:LB:348:SER:C	9:LB:350:LYS:H	2.26	0.43
11:LD:41:LYS:HB2	27:LT:68:THR:O	2.17	0.43
14:LG:223:GLU:HA	14:LG:227:GLU:HG3	2.00	0.43
20:LM:19:VAL:HG23	20:LM:65:THR:OG1	2.18	0.43
23:LP:182:ARG:HA	23:LP:185:THR:HG22	2.00	0.43
31:LX:64:ILE:HG13	31:LX:65:PRO:HD2	1.99	0.43
38:Le:114:LYS:HE3	38:Le:114:LYS:HB2	1.78	0.43
49:Lp:89:ILE:HG13	49:Lp:90:THR:N	2.33	0.43
51:Ls:38:MET:HA	51:Ls:41:ILE:HG22	2.00	0.43
62:SK:5:LYS:HE2	62:SK:5:LYS:HB2	1.87	0.43
64:SM:65:ASN:HD21	64:SM:94:GLY:HA3	1.83	0.43
70:SS:76:PRO:HG3	70:SS:99:GLN:HB3	1.99	0.43
70:SS:107:SER:HA	70:SS:110:ARG:HH21	1.83	0.43
83:Sf:106:TYR:HB3	83:Sf:116:ARG:HH21	1.83	0.43
1:1:1796:A:O2'	1:1:1797:A:OP1	2.33	0.43
2:2:124:U:O2'	56:SE:133:ARG:NH2	2.51	0.43
17:LJ:118:ASP:OD2	17:LJ:120:SER:OG	2.24	0.43
22:LO:139:THR:HG22	22:LO:141:GLY:H	1.84	0.43
47:Lr:14:LYS:HE2	47:Lr:18:ARG:NH2	2.33	0.43
51:Ls:79:PHE:HZ	51:Ls:189:GLN:HB3	1.83	0.43
58:SG:10:ASN:HB3	58:SG:128:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SL:104:ARG:HB2	75:SX:9:LEU:O	2.18	0.43
70:SS:126:ARG:HB2	70:SS:133:VAL:HG12	2.01	0.43
74:SW:94:LEU:HD23	74:SW:94:LEU:HA	1.88	0.43
1:1:270:G:OP1	86:1:3920:HOH:O	2.21	0.43
1:1:3254:U:O5'	9:LB:174:GLN:NE2	2.51	0.43
2:2:899:G:C6	2:2:900:G:C6	3.07	0.43
10:LC:303:PRO:O	10:LC:304:LYS:HG2	2.18	0.43
16:LI:169:LYS:HE2	27:LT:157:GLU:OE2	2.17	0.43
19:LL:203:LYS:HB3	19:LL:203:LYS:HE3	1.86	0.43
26:LS:42:TRP:CD1	26:LS:53:LYS:HD2	2.54	0.43
30:LW:94:ARG:HG2	58:SG:145:PHE:HA	2.00	0.43
32:LY:60:GLY:O	32:LY:63:LYS:HG3	2.18	0.43
55:SD:226:MET:SD	55:SD:226:MET:N	2.92	0.43
58:SG:30:LYS:HD3	58:SG:30:LYS:HA	1.81	0.43
74:SW:89:TRP:O	74:SW:93:LEU:HD23	2.18	0.43
1:1:1223:A:N6	1:1:1228:A:OP1	2.51	0.43
11:LD:182:ARG:HD2	11:LD:182:ARG:HA	1.86	0.43
13:LF:104:LYS:HB3	13:LF:105:PRO:HD3	2.00	0.43
15:LH:31:ARG:HB2	15:LH:82:VAL:O	2.19	0.43
47:Ln:21:ARG:HG3	47:Ln:21:ARG:HH11	1.83	0.43
51:Ls:16:LYS:HE3	51:Ls:16:LYS:HB2	1.85	0.43
51:Ls:40:GLU:CD	51:Ls:103:ASN:HD22	2.26	0.43
51:Ls:98:GLU:HA	51:Ls:101:LEU:HD23	1.99	0.43
59:SH:86:GLU:HA	59:SH:89:LYS:HG2	2.00	0.43
66:SO:145:ARG:HG3	78:Sa:29:CYS:HB2	2.00	0.43
68:SQ:106:LYS:O	68:SQ:110:ILE:HG12	2.19	0.43
1:1:447:U:O2'	1:1:468:G:N1	2.47	0.43
1:1:2167:C:H2'	1:1:2168:U:C6	2.54	0.43
2:2:825:C:H2'	2:2:826:U:C6	2.53	0.43
2:2:899:G:OP2	2:2:899:G:N2	2.37	0.43
3:3:107:C:OP2	16:LI:203:HIS:NE2	2.37	0.43
5:A:252:THR:OG1	5:A:255:SER:O	2.26	0.43
8:LA:3:ARG:HG2	8:LA:207:VAL:HG22	1.99	0.43
8:LA:171:GLY:O	49:Lp:68:ALA:HB2	2.18	0.43
15:LH:61:SER:OG	15:LH:62:ARG:N	2.52	0.43
51:Ls:13:ASP:OD2	51:Ls:14:LYS:N	2.52	0.43
68:SQ:41:PRO:HG2	68:SQ:44:LEU:HD12	2.01	0.43
73:SV:4:ASP:OD1	73:SV:4:ASP:N	2.45	0.43
14:LG:95:LYS:HE2	14:LG:95:LYS:HB2	1.80	0.43
1:1:462:A:OP1	50:Lq:92:LYS:NZ	2.41	0.43
1:1:609:A:H4'	1:1:610:A:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:664:G:O6	24:LQ:113:THR:HG21	2.18	0.43
1:1:1759:C:N4	25:LR:88:ARG:O	2.51	0.43
2:2:352:G:O2'	2:2:353:G:OP1	2.34	0.43
2:2:390:C:OP2	60:SI:2:GLY:N	2.52	0.43
2:2:539:A:O2'	2:2:540:C:H3'	2.19	0.43
9:LB:216:ILE:HD12	9:LB:339:LEU:HD22	1.99	0.43
44:Lk:39:ARG:HH11	44:Lk:44:LEU:HB2	1.84	0.43
55:SD:38:SER:O	55:SD:54:ARG:HB2	2.18	0.43
70:SS:42:TYR:HD1	70:SS:85:PHE:CE2	2.37	0.43
70:SS:107:SER:HA	70:SS:110:ARG:HE	1.84	0.43
76:SY:10:LEU:HD21	76:SY:47:LEU:HD13	2.00	0.43
1:1:133:C:H5''	1:1:134:G:C4	2.54	0.43
2:2:1341:A:H2'	2:2:1342:A:C8	2.53	0.43
7:C:547:LEU:HA	7:C:600:GLU:OE1	2.19	0.43
21:LN:68:ARG:HD2	21:LN:128:LYS:HG3	2.00	0.43
36:Lc:16:LYS:HB3	36:Lc:103:ILE:HG12	2.00	0.43
38:Le:35:LYS:HD2	38:Le:36:PRO:HD2	2.01	0.43
43:Lj:31:LYS:HB3	43:Lj:33:VAL:HG22	2.01	0.43
53:SB:94:LYS:HD3	53:SB:94:LYS:HA	1.75	0.43
55:SD:223:VAL:O	55:SD:226:MET:HE1	2.19	0.43
58:SG:1:MET:HG2	58:SG:107:SER:O	2.18	0.43
69:SR:10:LYS:O	69:SR:14:LYS:HG2	2.18	0.43
71:ST:23:LEU:HD11	71:ST:55:TYR:HB3	1.99	0.43
1:1:859:C:O2'	1:1:862:G:O2'	2.27	0.43
1:1:1223:A:H61	1:1:1228:A:P	2.41	0.43
1:1:2544:G:N3	1:1:2544:G:H2'	2.34	0.43
47:Lr:13:LEU:HD11	47:Lr:17:ARG:NH2	2.34	0.43
51:Ls:16:LYS:HE3	51:Ls:64:LYS:NZ	2.33	0.43
54:SC:235:PRO:HA	54:SC:238:TRP:NE1	2.33	0.43
55:SD:123:TYR:HD2	55:SD:127:ARG:HH12	1.67	0.43
68:SQ:13:LYS:HG3	68:SQ:14:LYS:H	1.83	0.43
81:Sd:20:ALA:HB1	81:Sd:25:THR:HA	2.01	0.43
1:1:498:U:H2'	1:1:499:C:C6	2.54	0.42
1:1:1073:G:H2'	1:1:1074:G:C8	2.53	0.42
1:1:1835:C:N4	86:1:3901:HOH:O	2.44	0.42
1:1:1875:A:O2'	1:1:3011:G:H4'	2.19	0.42
1:1:2620:G:H2'	1:1:2621:G:H8	1.84	0.42
1:1:3134:A:C4	22:LO:116:LYS:HA	2.54	0.42
2:2:294:U:H5''	56:SE:37:LYS:HD2	2.01	0.42
2:2:737:G:H2'	2:2:738:G:H8	1.84	0.42
2:2:1254:U:C5	62:SK:5:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:133:C:OP1	31:LX:107:GLN:NE2	2.52	0.42
7:C:573:ASP:HA	7:C:576:GLU:HG2	2.00	0.42
9:LB:68:HIS:CD2	9:LB:69:LYS:HG3	2.54	0.42
11:LD:41:LYS:HA	11:LD:41:LYS:HD3	1.86	0.42
15:LH:88:TYR:CZ	15:LH:186:LYS:HG2	2.54	0.42
34:La:85:ASP:OD1	34:La:85:ASP:N	2.51	0.42
52:SA:149:LEU:HD23	52:SA:165:THR:HG21	2.01	0.42
55:SD:89:LEU:HD23	55:SD:89:LEU:HA	1.93	0.42
58:SG:77:LEU:HD12	58:SG:95:LYS:HB2	2.01	0.42
1:1:2460:C:H2'	1:1:2461:C:C6	2.54	0.42
2:2:352:G:H2'	2:2:353:G:C8	2.53	0.42
2:2:957:U:H5''	65:SN:15:ALA:O	2.20	0.42
4:4:141:C:N4	86:4:307:HOH:O	2.51	0.42
9:LB:286:ILE:HG12	9:LB:323:VAL:HG12	2.00	0.42
10:LC:319:PRO:O	10:LC:320:LEU:HB2	2.19	0.42
13:LF:142:TYR:CZ	13:LF:236:ASN:HB2	2.54	0.42
15:LH:83:THR:HG23	15:LH:84:LYS:HG3	2.01	0.42
19:LL:3:ILE:HD12	19:LL:3:ILE:H	1.84	0.42
23:LP:36:ILE:HD11	23:LP:91:LEU:HD13	1.99	0.42
28:LU:20:LYS:HE3	28:LU:20:LYS:HB2	1.69	0.42
35:Lb:33:LYS:HB3	35:Lb:33:LYS:HE3	1.78	0.42
37:Ld:37:ALA:HB2	37:Ld:72:ILE:HA	2.01	0.42
52:SA:78:VAL:HG12	52:SA:125:VAL:HB	2.00	0.42
53:SB:131:ASP:O	53:SB:133:TYR:N	2.52	0.42
69:SR:58:MET:HA	69:SR:61:ILE:HB	2.00	0.42
73:SV:17:CYS:HB2	73:SV:56:SER:HB3	2.01	0.42
1:1:1637:C:O2'	1:1:1777:A:OP2	2.27	0.42
2:2:57:G:OP2	76:SY:119:LYS:NZ	2.47	0.42
2:2:612:G:O4'	2:2:612:G:OP1	2.38	0.42
2:2:761:A:OP1	61:SJ:77:ARG:NH2	2.50	0.42
2:2:824:U:H2'	2:2:825:C:C6	2.54	0.42
20:LM:32:GLU:HB3	20:LM:40:LEU:HB3	2.01	0.42
48:Lo:82:GLN:O	48:Lo:83:LEU:HD23	2.19	0.42
1:1:688:C:H2'	1:1:689:G:H8	1.84	0.42
2:2:64:U:H2'	2:2:65:A:H5''	1.99	0.42
2:2:835:G:H2'	2:2:836:G:H8	1.84	0.42
2:2:1063:C:OP1	53:SB:151:LYS:NZ	2.43	0.42
2:2:1078:A:N3	2:2:1079:C:N4	2.66	0.42
53:SB:205:TYR:CD1	53:SB:206:PRO:HD2	2.55	0.42
67:SP:116:LYS:HB3	67:SP:118:GLU:OE1	2.19	0.42
1:1:300:A:H2'	1:1:301:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:85:A:H2'	2:2:86:C:C6	2.54	0.42
2:2:1355:G:H4'	71:ST:131:ARG:HB3	2.01	0.42
10:LC:280:ASN:OD1	10:LC:281:ILE:N	2.52	0.42
39:Lf:47:LEU:HD11	39:Lf:75:ARG:HA	2.00	0.42
54:SC:150:GLY:N	54:SC:161:SER:O	2.46	0.42
54:SC:172:SER:O	54:SC:172:SER:OG	2.29	0.42
54:SC:187:VAL:O	54:SC:206:THR:OG1	2.30	0.42
60:SI:106:ALA:HB2	60:SI:169:LEU:HG	2.00	0.42
66:SO:42:HIS:ND1	66:SO:54:ARG:HD3	2.34	0.42
76:SY:131:LYS:HE2	76:SY:131:LYS:HB2	1.88	0.42
79:Sb:67:THR:OG1	79:Sb:68:GLY:N	2.52	0.42
81:Sd:38:ILE:HD11	81:Sd:43:PHE:HD1	1.83	0.42
1:1:2560:A:H2'	1:1:2561:G:C8	2.55	0.42
2:2:1055:A:H2	53:SB:203:GLY:HA2	1.85	0.42
9:LB:349:ARG:O	9:LB:349:ARG:HG2	2.19	0.42
53:SB:107:THR:HG21	66:SO:130:ASP:O	2.19	0.42
61:SJ:84:LEU:HD21	61:SJ:88:ARG:O	2.19	0.42
63:SL:91:ILE:HD11	63:SL:112:LEU:HD23	2.01	0.42
65:SN:83:ASP:OD1	65:SN:84:ILE:HG12	2.20	0.42
70:SS:14:ILE:C	70:SS:15:LEU:HD12	2.45	0.42
77:SZ:39:LEU:O	77:SZ:43:VAL:HG22	2.20	0.42
1:1:1368:C:O3'	50:Lq:30:ARG:NH1	2.52	0.42
1:1:1430:G:O2'	1:1:2318:G:O6	2.28	0.42
1:1:3140:A:OP1	26:LS:154:HIS:HD2	2.03	0.42
2:2:510:U:OP1	61:SJ:131:HIS:NE2	2.53	0.42
2:2:694:U:H2'	2:2:695:C:C6	2.55	0.42
2:2:861:A:O2'	2:2:862:U:H5'	2.19	0.42
2:2:1605:U:O2'	57:SF:92:GLY:O	2.30	0.42
5:A:236:ILE:HA	5:A:252:THR:HA	2.01	0.42
15:LH:163:ILE:O	15:LH:166:ILE:HG22	2.19	0.42
69:SR:105:ASP:OD1	69:SR:108:THR:OG1	2.31	0.42
71:ST:119:GLU:OE2	71:ST:120:ARG:NE	2.51	0.42
78:Sa:36:ILE:HD11	78:Sa:75:VAL:HG12	2.02	0.42
1:1:1232:G:H2'	1:1:1233:G:H8	1.84	0.42
1:1:1233:G:H2'	1:1:1234:A:C8	2.55	0.42
5:A:30:MET:HG2	5:A:42:ILE:HD11	2.02	0.42
23:LP:152:GLU:HG3	23:LP:153:ALA:N	2.35	0.42
44:Lk:75:ASN:OD1	44:Lk:75:ASN:N	2.53	0.42
52:SA:194:ARG:HE	52:SA:194:ARG:HB2	1.71	0.42
57:SF:115:ASN:O	57:SF:118:GLN:HB3	2.18	0.42
57:SF:122:ASP:HA	57:SF:125:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SP:63:GLY:O	67:SP:67:LYS:HG2	2.20	0.42
69:SR:12:SER:O	69:SR:16:ILE:HG12	2.19	0.42
71:ST:53:TRP:HA	71:ST:56:ILE:HG22	2.00	0.42
83:Sf:97:LYS:HA	83:Sf:97:LYS:HD3	1.84	0.42
2:2:1229:U:H2'	2:2:1230:G:H8	1.85	0.42
2:2:1705:C:H2'	2:2:1706:U:C6	2.55	0.42
14:LG:159:ASP:N	14:LG:159:ASP:OD1	2.51	0.42
22:LO:28:LEU:O	22:LO:103:ARG:NH1	2.53	0.42
57:SF:176:THR:OG1	57:SF:179:GLU:OE2	2.36	0.42
58:SG:93:LYS:HE3	58:SG:93:LYS:HB2	1.75	0.42
66:SO:47:SER:OG	66:SO:48:GLY:N	2.53	0.42
74:SW:76:SER:OG	74:SW:77:PRO:HD3	2.19	0.42
76:SY:130:ALA:O	76:SY:133:LYS:NZ	2.49	0.42
1:1:2207:A:O4'	8:LA:243:THR:HG21	2.20	0.42
1:1:3065:U:OP1	46:Lm:114:LYS:NZ	2.48	0.42
2:2:157:C:O2'	58:SG:95:LYS:NZ	2.50	0.42
15:LH:40:HIS:CD2	15:LH:40:HIS:H	2.38	0.42
29:LV:83:GLN:HG3	29:LV:85:LYS:H	1.85	0.42
41:Lh:60:LEU:HD23	41:Lh:60:LEU:HA	1.85	0.42
54:SC:188:ALA:HB2	54:SC:206:THR:HG21	2.01	0.42
61:SJ:2:ALA:HB3	61:SJ:3:PRO:HD3	2.02	0.42
61:SJ:56:ILE:O	61:SJ:59:THR:HG22	2.20	0.42
77:SZ:37:ASP:O	77:SZ:41:LYS:HG2	2.20	0.42
1:1:703:A:H3'	34:La:115:LYS:HG3	2.02	0.41
2:2:483:G:H2'	2:2:484:G:H8	1.85	0.41
2:2:1712:C:O2'	2:2:1713:C:H5''	2.19	0.41
5:A:54:TYR:CE1	68:SQ:100:HIS:HB2	2.54	0.41
7:C:583:MET:HE2	7:C:583:MET:HA	2.02	0.41
17:LJ:20:LEU:CD1	17:LJ:38:LEU:HD11	2.50	0.41
36:Lc:56:LYS:O	36:Lc:60:GLU:HG3	2.19	0.41
57:SF:29:LEU:HD22	57:SF:34:SER:HB3	2.02	0.41
1:1:1001:G:H2'	1:1:1002:G:H8	1.85	0.41
1:1:1797:A:O2'	1:1:1798:U:H5'	2.20	0.41
2:2:68:A:H5''	58:SG:162:VAL:HG21	2.01	0.41
2:2:493:G:H2'	2:2:494:G:C8	2.55	0.41
2:2:844:G:H2'	2:2:845:A:H8	1.84	0.41
4:4:51:G:O3'	45:Ll:21:ARG:NH2	2.53	0.41
9:LB:256:TRP:CD1	9:LB:256:TRP:C	2.98	0.41
10:LC:317:LYS:HD3	10:LC:322:ASN:HD22	1.85	0.41
13:LF:105:PRO:HB3	13:LF:136:VAL:HG12	2.02	0.41
21:LN:30:TYR:C	21:LN:32:GLN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SQ:10:PHE:HE2	68:SQ:12:LYS:HE3	1.85	0.41
72:SU:20:ARG:HG3	72:SU:89:ASP:HB3	2.01	0.41
1:1:2906:G:C2	9:LB:251:ALA:HB1	2.54	0.41
1:1:3258:U:H1'	1:1:3259:G:OP2	2.20	0.41
2:2:190:G:N2	2:2:191:G:N7	2.68	0.41
2:2:535:A:H5'	2:2:540:C:C5	2.55	0.41
9:LB:103:THR:HG21	9:LB:151:ARG:HD2	2.01	0.41
15:LH:16:LEU:H	15:LH:16:LEU:HD23	1.85	0.41
15:LH:87:LYS:N	15:LH:187:GLY:O	2.53	0.41
22:LO:35:VAL:HG22	22:LO:105:LYS:HB2	2.01	0.41
36:Lc:63:SER:O	36:Lc:67:LYS:N	2.54	0.41
54:SC:86:ASP:HA	54:SC:112:ILE:HG22	2.01	0.41
59:SH:122:ARG:NH1	59:SH:127:THR:HG22	2.36	0.41
75:SX:107:PHE:CE1	75:SX:123:LYS:HB3	2.50	0.41
1:1:2117:U:H2'	1:1:2118:G:H8	1.85	0.41
1:1:2524:G:OP2	33:LZ:54:ARG:NH1	2.51	0.41
1:1:3078:C:H3'	46:Lm:111:ARG:NH1	2.35	0.41
2:2:821:G:H2'	2:2:822:G:O4'	2.20	0.41
2:2:1789:G:O6	78:Sa:34:LYS:NZ	2.52	0.41
6:B:141:ILE:HD11	54:SC:89:MET:SD	2.60	0.41
10:LC:311:ARG:HH21	10:LC:314:VAL:HB	1.85	0.41
13:LF:116:GLN:HG3	24:LQ:31:GLY:O	2.20	0.41
14:LG:56:PRO:HG2	14:LG:59:ILE:HD12	2.03	0.41
30:LW:124:LYS:HA	30:LW:127:LYS:HE2	2.01	0.41
33:LZ:92:LYS:HE2	33:LZ:92:LYS:HB3	1.92	0.41
35:Lb:47:LEU:HA	35:Lb:50:THR:HG22	2.01	0.41
42:Li:99:LEU:O	42:Li:102:ILE:HG22	2.20	0.41
52:SA:86:GLN:OE1	52:SA:102:ALA:HB1	2.20	0.41
1:1:250:C:HO2'	1:1:251:U:P	2.43	0.41
1:1:254:U:H2'	1:1:255:U:O4'	2.20	0.41
1:1:3121:G:HO2'	1:1:3122:U:P	2.43	0.41
2:2:844:G:H2'	2:2:845:A:C8	2.55	0.41
2:2:1219:C:H2'	2:2:1220:G:C8	2.55	0.41
2:2:1229:U:H2'	2:2:1230:G:C8	2.55	0.41
5:A:81:ALA:HB1	5:A:108:VAL:HG23	2.01	0.41
7:C:551:ILE:HD13	7:C:583:MET:HE3	2.02	0.41
16:LI:193:ASP:OD1	16:LI:194:GLY:N	2.44	0.41
33:LZ:13:THR:HB	40:Lg:87:ARG:HG3	2.01	0.41
51:Ls:92:ASP:O	51:Ls:95:GLU:HG3	2.20	0.41
66:SO:102:ASN:HB3	66:SO:141:ARG:HG3	2.02	0.41
2:2:1156:C:O3'	68:SQ:140:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1222:U:H3'	2:2:1223:G:C8	2.56	0.41
5:A:235:GLU:O	5:A:253:ALA:N	2.54	0.41
10:LC:284:GLN:NE2	10:LC:286:ASP:HB3	2.26	0.41
12:LE:163:LYS:HB3	12:LE:163:LYS:HE3	1.84	0.41
22:LO:145:HIS:HB3	22:LO:146:GLU:OE1	2.19	0.41
23:LP:162:ALA:O	23:LP:163:VAL:HG12	2.20	0.41
36:Lc:34:LEU:HD23	36:Lc:34:LEU:HA	1.91	0.41
50:Lq:58:GLU:H	50:Lq:58:GLU:CD	2.27	0.41
53:SB:9:LEU:HG	53:SB:12:GLY:HA2	2.03	0.41
53:SB:65:ILE:HG22	53:SB:87:ARG:HB2	2.03	0.41
54:SC:109:ILE:HG12	54:SC:123:ILE:HG12	2.02	0.41
55:SD:160:MET:HE2	55:SD:160:MET:HB2	1.92	0.41
57:SF:28:LYS:HZ1	57:SF:55:VAL:C	2.28	0.41
69:SR:89:SER:HB3	69:SR:92:ASP:HB2	2.03	0.41
75:SX:126:LYS:HE2	75:SX:129:GLY:HA2	2.03	0.41
1:1:957:C:H5'	24:LQ:86:ASN:ND2	2.36	0.41
1:1:2159:C:H2'	1:1:2205:A:H61	1.86	0.41
1:1:2937:U:O2'	1:1:2938:U:H5'	2.21	0.41
2:2:829:U:O2'	2:2:830:U:H5'	2.20	0.41
2:2:1193:A:H4'	2:2:1194:C:C5'	2.50	0.41
2:2:1536:G:C6	2:2:1537:G:C4	3.08	0.41
8:LA:142:ASP:O	8:LA:143:GLU:HG3	2.21	0.41
23:LP:168:GLU:HB3	23:LP:171:LEU:HD11	2.02	0.41
41:Lh:49:ILE:HG13	41:Lh:50:HIS:N	2.35	0.41
49:Lp:29:GLN:NE2	49:Lp:69:TYR:HD1	2.18	0.41
51:Ls:12:PHE:O	51:Ls:16:LYS:HG2	2.20	0.41
54:SC:43:TRP:O	54:SC:54:LYS:NZ	2.52	0.41
58:SG:32:MET:HE3	58:SG:53:THR:O	2.20	0.41
1:1:477:C:H2'	1:1:478:G:C8	2.56	0.41
1:1:2642:U:H5'	17:LJ:19:VAL:HG11	2.03	0.41
2:2:224:C:H2'	2:2:225:C:C6	2.55	0.41
2:2:518:A:H4'	76:SY:39:SER:OG	2.21	0.41
2:2:1168:A:H2'	2:2:1169:G:C8	2.55	0.41
2:2:1477:C:H4'	2:2:1478:C:OP1	2.20	0.41
2:2:1520:A:N3	2:2:1586:G:O2'	2.50	0.41
2:2:1686:G:H2'	2:2:1687:A:C8	2.56	0.41
5:A:91:GLU:OE2	5:A:95:GLY:N	2.54	0.41
5:A:244:ASN:HD21	5:A:245:ARG:NH1	2.19	0.41
10:LC:148:GLU:HG2	50:Lq:73:LYS:HG2	2.03	0.41
41:Lh:90:THR:HG22	41:Lh:92:ALA:H	1.85	0.41
52:SA:81:SER:O	52:SA:86:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SE:127:LYS:HD3	56:SE:127:LYS:HA	1.75	0.41
57:SF:115:ASN:OD1	57:SF:117:ILE:HG12	2.20	0.41
69:SR:29:GLU:HA	69:SR:29:GLU:OE1	2.21	0.41
71:ST:128:GLN:H	71:ST:128:GLN:HG3	1.73	0.41
71:ST:139:THR:O	71:ST:143:ALA:HB2	2.20	0.41
1:1:1001:G:H2'	1:1:1002:G:C8	2.55	0.41
1:1:1633:G:H2'	1:1:1634:A:H8	1.86	0.41
1:1:2064:C:H2'	1:1:2065:U:C6	2.55	0.41
1:1:2117:U:H2'	1:1:2118:G:C8	2.55	0.41
1:1:3009:U:H2'	1:1:3010:G:H8	1.86	0.41
2:2:499:U:H2'	2:2:500:G:C8	2.56	0.41
2:2:509:A:O2'	2:2:510:U:OP1	2.38	0.41
2:2:534:G:N7	61:SJ:169:ARG:HD2	2.35	0.41
2:2:741:U:O2	59:SH:115:ARG:NH1	2.54	0.41
2:2:832:G:O2'	2:2:833:U:OP1	2.39	0.41
2:2:857:A:C6	65:SN:73:ARG:HD3	2.56	0.41
2:2:1099:G:OP2	75:SX:7:ARG:HD2	2.21	0.41
2:2:1235:A:H2'	2:2:1236:U:O4'	2.20	0.41
2:2:1699:C:H2'	2:2:1700:G:C8	2.56	0.41
2:2:1773:G:O6	47:Ln:8:LYS:NZ	2.54	0.41
5:A:46:THR:HG22	5:A:48:ASP:HB2	2.03	0.41
5:A:99:ARG:HA	5:A:99:ARG:HD3	1.82	0.41
5:A:107:ASP:OD1	5:A:107:ASP:N	2.53	0.41
5:A:175:LYS:HB3	5:A:184:LEU:HD13	2.03	0.41
8:LA:206:PRO:HG3	8:LA:213:GLY:H	1.85	0.41
16:LI:140:THR:OG1	16:LI:141:ARG:N	2.54	0.41
19:LL:170:LYS:HE3	19:LL:170:LYS:HB2	1.82	0.41
23:LP:91:LEU:HD23	23:LP:91:LEU:HA	1.93	0.41
25:LR:90:PRO:HG2	25:LR:93:VAL:HG12	2.03	0.41
28:LU:56:LEU:HD23	28:LU:56:LEU:H	1.86	0.41
30:LW:68:ALA:HA	30:LW:71:ARG:HH11	1.85	0.41
34:La:7:LYS:HA	34:La:7:LYS:HD3	1.84	0.41
42:Li:95:LYS:HA	42:Li:95:LYS:HD3	1.93	0.41
43:Lj:14:LYS:NZ	45:Ll:51:LEU:HD21	2.35	0.41
54:SC:58:ILE:HG13	54:SC:80:PHE:HZ	1.86	0.41
57:SF:173:ASN:OD1	57:SF:174:VAL:N	2.53	0.41
59:SH:6:LEU:C	59:SH:16:ARG:HH22	2.25	0.41
69:SR:32:LYS:HD2	69:SR:47:ARG:NH2	2.36	0.41
70:SS:15:LEU:HB2	70:SS:22:VAL:HG22	2.03	0.41
70:SS:69:LEU:HD23	70:SS:69:LEU:HA	1.96	0.41
72:SU:50:LYS:HB3	72:SU:89:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75: SX:126: LYS: HG2	75: SX:131: GLY: HA2	2.02	0.41
80: Sc:12: LYS: O	80: Sc:32: GLU: N	2.51	0.41
1:1:2648: A: N3	1:1:2648: A: H2'	2.36	0.41
2:2:1616: C: HO2'	2:2:1617: U: P	2.42	0.41
4:4:36: G: C5	41: Lh:91: ARG: HD3	2.55	0.41
8: LA:90: ALA: HA	8: LA:101: ILE: O	2.21	0.41
14: LG:67: ILE: O	14: LG:71: ARG: HG2	2.21	0.41
23: LP:10: ALA: HB3	23: LP:13: LYS: HG2	2.02	0.41
60: SI:25: ARG: HD3	60: SI:25: ARG: HA	1.84	0.41
1:1:552: C: OP2	20: LM:77: ARG: NH1	2.55	0.40
1:1:1350: G: OP2	86: 1:3922: HOH: O	2.22	0.40
1:1:1560: U: O2'	1:1:1561: G: H5''	2.21	0.40
1:1:2227: U: HO2'	1:1:2228: C: P	2.44	0.40
1:1:2662: A: N6	11: LD:28: THR: O	2.52	0.40
2:2:102: A: H4'	2:2:103: A: O5'	2.20	0.40
2:2:186: C: OP2	60: SI:138: LYS: HG3	2.21	0.40
2:2:535: A: H5'	2:2:540: C: H5	1.86	0.40
2:2:751: A: P	56: SE:187: ARG: HE	2.44	0.40
2:2:1355: G: O2'	71: ST:134: ASP: OD2	2.37	0.40
3:3:62: U: O3'	11: LD:290: ARG: NH1	2.54	0.40
15: LH:107: ALA: C	15: LH:109: THR: H	2.29	0.40
15: LH:149: SER: HB2	15: LH:189: ILE: HD11	2.03	0.40
19: LL:141: ASP: HB2	19: LL:142: GLN: OE1	2.22	0.40
56: SE:59: ARG: NH2	76: SY:90: PRO: HG3	2.35	0.40
57: SF:103: HIS: ND1	77: SZ:87: MET: SD	2.94	0.40
2:2:115: U: H2'	2:2:116: U: C6	2.56	0.40
2:2:324: C: H2'	2:2:325: U: H6	1.86	0.40
2:2:1562: U: H5''	70: SS:39: GLY: H	1.86	0.40
2:2:1580: G: C8	68: SQ:122: ARG: HD3	2.56	0.40
14: LG:109: LYS: HA	14: LG:109: LYS: HD3	1.72	0.40
20: LM:82: LYS: O	20: LM:86: GLU: HG2	2.21	0.40
29: LV:16: THR: HG21	29: LV:85: LYS: HE3	2.02	0.40
54: SC:41: LYS: HD2	54: SC:42: GLU: O	2.21	0.40
63: SL:127: MET: HE3	63: SL:127: MET: HB3	1.95	0.40
70: SS:111: GLU: HG2	70: SS:112: ASP: N	2.36	0.40
1:1:262: G: H5''	21: LN:14: LYS: HE2	2.04	0.40
1:1:1224: U: O2'	1:1:1226: G: OP2	2.32	0.40
1:1:3298: U: H2'	1:1:3299: U: C6	2.56	0.40
2:2:503: A: H2'	2:2:504: U: C6	2.57	0.40
2:2:910: U: H5'	53: SB:11: LYS: O	2.20	0.40
4:4:97: A: OP1	41: Lh:72: ARG: NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:263:TRP:H	9:LB:263:TRP:CD1	2.39	0.40
11:LD:99:TYR:OH	11:LD:171:ASP:OD2	2.35	0.40
25:LR:94:LEU:HD23	25:LR:94:LEU:HA	1.93	0.40
25:LR:180:LYS:HE2	25:LR:180:LYS:HB2	1.72	0.40
40:Lg:99:GLN:HA	40:Lg:99:GLN:OE1	2.22	0.40
43:Lj:39:TYR:CD1	43:Lj:40:PRO:HA	2.56	0.40
55:SD:75:LEU:HG	62:SK:20:VAL:HB	2.02	0.40
58:SG:58:LYS:HG3	58:SG:105:ASP:O	2.22	0.40
64:SM:103:LEU:O	64:SM:115:VAL:HG11	2.21	0.40
68:SQ:36:LEU:HD23	68:SQ:36:LEU:HA	1.96	0.40
77:SZ:40:TYR:O	77:SZ:44:GLN:NE2	2.49	0.40
83:Sf:96:LYS:HE3	83:Sf:96:LYS:HB3	1.91	0.40
1:1:1215:C:H41	1:1:1244:G:H3'	1.87	0.40
1:1:1387:G:N2	1:1:1390:A:OP2	2.54	0.40
2:2:17:C:H2'	2:2:18:C:C6	2.56	0.40
2:2:397:A:H5''	60:SI:25:ARG:HA	2.03	0.40
2:2:1224:A:H4'	2:2:1225:G:H5'	2.03	0.40
2:2:1584:G:H1	2:2:1604:U:H3	1.70	0.40
5:A:289:LEU:HD23	5:A:289:LEU:HA	1.85	0.40
15:LH:94:TYR:HA	15:LH:179:ASP:OD2	2.21	0.40
20:LM:11:TRP:CZ2	26:LS:153:PRO:HB3	2.55	0.40
30:LW:47:ARG:CZ	30:LW:54:LEU:HD21	2.52	0.40
31:LX:82:THR:O	31:LX:85:ALA:N	2.53	0.40
32:LY:66:GLU:OE2	32:LY:66:GLU:N	2.55	0.40
33:LZ:127:ARG:HD2	33:LZ:127:ARG:HA	1.88	0.40
54:SC:43:TRP:H	54:SC:43:TRP:CD1	2.38	0.40
60:SI:11:ARG:O	63:SL:138:LYS:NZ	2.54	0.40
63:SL:80:VAL:HG22	63:SL:126:ASP:H	1.86	0.40
67:SP:116:LYS:N	67:SP:119:MET:HE2	2.34	0.40
70:SS:88:ARG:HB3	70:SS:98:SER:HB2	2.04	0.40
1:1:1219:G:C6	18:LK:17:ALA:HB3	2.56	0.40
1:1:2219:A:N6	2:2:1751:A:H8	2.19	0.40
1:1:3228:C:N4	1:1:3229:G:O6	2.55	0.40
2:2:1365:U:P	71:ST:69:LYS:HZ1	2.45	0.40
2:2:1429:G:N2	81:Sd:45:GLU:OE1	2.53	0.40
9:LB:92:TYR:HB2	9:LB:158:VAL:HG22	2.03	0.40
9:LB:151:ARG:HE	9:LB:151:ARG:HB2	1.62	0.40
33:LZ:41:LEU:HD22	33:LZ:73:VAL:HG12	2.04	0.40
42:Li:14:THR:HG23	42:Li:21:ASN:HB3	2.04	0.40
57:SF:110:LEU:HD11	77:SZ:48:LEU:HD23	2.04	0.40
60:SI:175:SER:OG	60:SI:176:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SO:32:ILE:HB	66:SO:96:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	310/316 (98%)	293 (94%)	17 (6%)	0	100	100
6	B	28/302 (9%)	19 (68%)	9 (32%)	0	100	100
7	C	76/614 (12%)	76 (100%)	0	0	100	100
8	LA	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
9	LB	385/392 (98%)	366 (95%)	18 (5%)	1 (0%)	36	65
10	LC	361/365 (99%)	343 (95%)	18 (5%)	0	100	100
11	LD	298/304 (98%)	291 (98%)	7 (2%)	0	100	100
12	LE	192/200 (96%)	174 (91%)	18 (9%)	0	100	100
13	LF	245/249 (98%)	237 (97%)	8 (3%)	0	100	100
14	LG	233/262 (89%)	229 (98%)	4 (2%)	0	100	100
15	LH	189/192 (98%)	183 (97%)	6 (3%)	0	100	100
16	LI	215/219 (98%)	201 (94%)	14 (6%)	0	100	100
17	LJ	165/173 (95%)	160 (97%)	5 (3%)	0	100	100
18	LK	153/165 (93%)	133 (87%)	18 (12%)	2 (1%)	9	32
19	LL	207/213 (97%)	201 (97%)	6 (3%)	0	100	100
20	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
21	LN	200/203 (98%)	192 (96%)	8 (4%)	0	100	100
22	LO	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
23	LP	184/187 (98%)	173 (94%)	10 (5%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	LQ	181/213 (85%)	174 (96%)	7 (4%)	0	100	100
25	LR	182/192 (95%)	178 (98%)	4 (2%)	0	100	100
26	LS	171/174 (98%)	167 (98%)	4 (2%)	0	100	100
27	LT	156/160 (98%)	151 (97%)	5 (3%)	0	100	100
28	LU	99/127 (78%)	94 (95%)	5 (5%)	0	100	100
29	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
30	LW	131/161 (81%)	126 (96%)	5 (4%)	0	100	100
31	LX	119/156 (76%)	113 (95%)	6 (5%)	0	100	100
32	LY	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
33	LZ	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
34	La	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
35	Lb	60/65 (92%)	59 (98%)	1 (2%)	0	100	100
36	Lc	95/108 (88%)	94 (99%)	1 (1%)	0	100	100
37	Ld	110/120 (92%)	108 (98%)	2 (2%)	0	100	100
38	Le	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
39	Lf	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
40	Lg	110/119 (92%)	104 (94%)	6 (6%)	0	100	100
41	Lh	120/126 (95%)	117 (98%)	3 (2%)	0	100	100
42	Li	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
43	Lj	84/95 (88%)	79 (94%)	5 (6%)	0	100	100
44	Lk	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
45	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
46	Lm	50/128 (39%)	50 (100%)	0	0	100	100
47	Ln	22/25 (88%)	22 (100%)	0	0	100	100
47	Lr	22/25 (88%)	22 (100%)	0	0	100	100
48	Lo	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
49	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
50	Lq	139/147 (95%)	134 (96%)	5 (4%)	0	100	100
51	Ls	187/312 (60%)	183 (98%)	4 (2%)	0	100	100
52	SA	206/285 (72%)	193 (94%)	13 (6%)	0	100	100
53	SB	230/255 (90%)	216 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	SC	214/263 (81%)	206 (96%)	8 (4%)	0	100	100
55	SD	210/254 (83%)	199 (95%)	11 (5%)	0	100	100
56	SE	259/264 (98%)	246 (95%)	13 (5%)	0	100	100
57	SF	197/212 (93%)	181 (92%)	16 (8%)	0	100	100
58	SG	230/239 (96%)	220 (96%)	10 (4%)	0	100	100
59	SH	193/203 (95%)	185 (96%)	8 (4%)	0	100	100
60	SI	199/202 (98%)	192 (96%)	7 (4%)	0	100	100
61	SJ	177/190 (93%)	169 (96%)	8 (4%)	0	100	100
62	SK	87/159 (55%)	87 (100%)	0	0	100	100
63	SL	148/161 (92%)	146 (99%)	2 (1%)	0	100	100
64	SM	116/144 (81%)	105 (90%)	11 (10%)	0	100	100
65	SN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
66	SO	133/150 (89%)	127 (96%)	6 (4%)	0	100	100
67	SP	113/153 (74%)	109 (96%)	4 (4%)	0	100	100
68	SQ	136/143 (95%)	129 (95%)	7 (5%)	0	100	100
69	SR	126/143 (88%)	123 (98%)	3 (2%)	0	100	100
70	SS	135/156 (86%)	123 (91%)	12 (9%)	0	100	100
71	ST	140/153 (92%)	134 (96%)	6 (4%)	0	100	100
72	SU	101/116 (87%)	94 (93%)	7 (7%)	0	100	100
73	SV	84/98 (86%)	82 (98%)	2 (2%)	0	100	100
74	SW	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
75	SX	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
76	SY	130/136 (96%)	128 (98%)	2 (2%)	0	100	100
77	SZ	67/99 (68%)	66 (98%)	1 (2%)	0	100	100
78	Sa	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
79	Sb	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
80	Sc	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
81	Sd	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
82	Se	38/62 (61%)	37 (97%)	1 (3%)	0	100	100
83	Sf	71/154 (46%)	62 (87%)	9 (13%)	0	100	100
All	All	11698/13795 (85%)	11185 (96%)	509 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	LK	88	PRO
18	LK	22	VAL
23	LP	163	VAL
9	LB	257	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	271/274 (99%)	271 (100%)	0	100	100
6	B	21/224 (9%)	21 (100%)	0	100	100
7	C	68/511 (13%)	68 (100%)	0	100	100
8	LA	196/198 (99%)	196 (100%)	0	100	100
9	LB	327/331 (99%)	327 (100%)	0	100	100
10	LC	284/285 (100%)	284 (100%)	0	100	100
11	LD	250/253 (99%)	250 (100%)	0	100	100
12	LE	162/166 (98%)	162 (100%)	0	100	100
13	LF	213/215 (99%)	213 (100%)	0	100	100
14	LG	203/222 (91%)	203 (100%)	0	100	100
15	LH	168/169 (99%)	168 (100%)	0	100	100
16	LI	182/183 (100%)	182 (100%)	0	100	100
17	LJ	145/150 (97%)	144 (99%)	1 (1%)	76	92
19	LL	172/176 (98%)	172 (100%)	0	100	100
20	LM	116/117 (99%)	116 (100%)	0	100	100
21	LN	179/180 (99%)	179 (100%)	0	100	100
22	LO	161/162 (99%)	161 (100%)	0	100	100
23	LP	151/152 (99%)	151 (100%)	0	100	100
24	LQ	155/178 (87%)	155 (100%)	0	100	100
25	LR	153/160 (96%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LS	153/154 (99%)	153 (100%)	0	100	100
27	LT	134/135 (99%)	134 (100%)	0	100	100
28	LU	89/108 (82%)	89 (100%)	0	100	100
29	LV	99/102 (97%)	99 (100%)	0	100	100
30	LW	107/125 (86%)	107 (100%)	0	100	100
31	LX	108/129 (84%)	107 (99%)	1 (1%)	70	90
32	LY	117/119 (98%)	117 (100%)	0	100	100
33	LZ	121/121 (100%)	121 (100%)	0	100	100
34	La	121/122 (99%)	121 (100%)	0	100	100
35	Lb	53/55 (96%)	53 (100%)	0	100	100
36	Lc	78/88 (89%)	78 (100%)	0	100	100
37	Ld	97/105 (92%)	96 (99%)	1 (1%)	68	89
38	Le	107/114 (94%)	107 (100%)	0	100	100
39	Lf	88/90 (98%)	88 (100%)	0	100	100
40	Lg	97/102 (95%)	97 (100%)	0	100	100
41	Lh	109/112 (97%)	109 (100%)	0	100	100
42	Li	86/93 (92%)	86 (100%)	0	100	100
43	Lj	70/78 (90%)	70 (100%)	0	100	100
44	Lk	73/77 (95%)	73 (100%)	0	100	100
45	Ll	45/46 (98%)	45 (100%)	0	100	100
46	Lm	47/115 (41%)	47 (100%)	0	100	100
47	Ln	22/23 (96%)	22 (100%)	0	100	100
47	Lr	22/23 (96%)	22 (100%)	0	100	100
48	Lo	88/90 (98%)	88 (100%)	0	100	100
49	Lp	73/74 (99%)	73 (100%)	0	100	100
50	Lq	109/112 (97%)	109 (100%)	0	100	100
51	Ls	155/255 (61%)	155 (100%)	0	100	100
52	SA	178/225 (79%)	178 (100%)	0	100	100
53	SB	203/223 (91%)	203 (100%)	0	100	100
54	SC	181/206 (88%)	181 (100%)	0	100	100
55	SD	182/206 (88%)	181 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	SE	219/221 (99%)	219 (100%)	0	100	100
57	SF	167/178 (94%)	167 (100%)	0	100	100
58	SG	198/204 (97%)	198 (100%)	0	100	100
59	SH	169/177 (96%)	169 (100%)	0	100	100
60	SI	163/164 (99%)	163 (100%)	0	100	100
61	SJ	154/162 (95%)	154 (100%)	0	100	100
62	SK	77/126 (61%)	77 (100%)	0	100	100
63	SL	133/143 (93%)	133 (100%)	0	100	100
64	SM	101/121 (84%)	101 (100%)	0	100	100
65	SN	129/130 (99%)	129 (100%)	0	100	100
66	SO	102/117 (87%)	102 (100%)	0	100	100
67	SP	99/132 (75%)	99 (100%)	0	100	100
68	SQ	111/115 (96%)	111 (100%)	0	100	100
69	SR	119/131 (91%)	119 (100%)	0	100	100
70	SS	120/135 (89%)	120 (100%)	0	100	100
71	ST	114/124 (92%)	114 (100%)	0	100	100
72	SU	93/103 (90%)	93 (100%)	0	100	100
73	SV	69/80 (86%)	69 (100%)	0	100	100
74	SW	112/113 (99%)	112 (100%)	0	100	100
75	SX	113/116 (97%)	113 (100%)	0	100	100
76	SY	112/115 (97%)	112 (100%)	0	100	100
77	SZ	60/80 (75%)	60 (100%)	0	100	100
78	Sa	91/103 (88%)	91 (100%)	0	100	100
79	Sb	70/71 (99%)	70 (100%)	0	100	100
80	Sc	54/61 (88%)	54 (100%)	0	100	100
81	Sd	43/46 (94%)	43 (100%)	0	100	100
82	Se	34/51 (67%)	34 (100%)	0	100	100
83	Sf	66/139 (48%)	66 (100%)	0	100	100
All	All	9881/11391 (87%)	9877 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	LJ	40	GLN
31	LX	81	ASN
37	Ld	105	ASN
55	SD	177	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	14	HIS
5	A	60	HIS
7	C	577	GLN
8	LA	19	HIS
9	LB	166	GLN
9	LB	225	HIS
9	LB	260	HIS
10	LC	203	HIS
10	LC	284	GLN
10	LC	322	ASN
11	LD	4	HIS
11	LD	57	ASN
12	LE	116	GLN
13	LF	99	ASN
13	LF	178	ASN
13	LF	200	ASN
14	LG	36	ASN
14	LG	41	GLN
14	LG	246	GLN
15	LH	15	ASN
15	LH	35	GLN
17	LJ	40	GLN
21	LN	123	GLN
21	LN	158	HIS
22	LO	132	GLN
23	LP	97	ASN
23	LP	116	HIS
24	LQ	43	HIS
24	LQ	153	GLN
24	LQ	179	HIS
25	LR	91	GLN
26	LS	88	HIS
27	LT	22	HIS
27	LT	127	GLN
29	LV	100	ASN

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Mol	Chain	Res	Type
31	LX	107	GLN
32	LY	109	HIS
33	LZ	126	ASN
35	Lb	17	HIS
37	Ld	64	ASN
38	Le	21	HIS
38	Le	72	HIS
39	Lf	79	ASN
41	Lh	37	GLN
41	Lh	64	ASN
42	Li	100	GLN
44	Lk	41	GLN
48	Lo	90	HIS
49	Lp	29	GLN
49	Lp	45	ASN
51	Ls	103	ASN
52	SA	52	ASN
53	SB	202	GLN
53	SB	209	ASN
54	SC	95	GLN
54	SC	155	ASN
55	SD	7	GLN
55	SD	59	GLN
55	SD	85	ASN
55	SD	224	GLN
56	SE	9	GLN
56	SE	57	ASN
56	SE	98	ASN
57	SF	82	ASN
57	SF	90	ASN
57	SF	145	GLN
58	SG	13	GLN
58	SG	119	GLN
59	SH	18	ASN
60	SI	53	HIS
62	SK	31	HIS
62	SK	48	GLN
65	SN	36	GLN
65	SN	62	GLN
67	SP	111	ASN
68	SQ	5	GLN
69	SR	94	HIS

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Mol	Chain	Res	Type
70	SS	34	GLN
70	SS	74	GLN
70	SS	99	GLN
72	SU	29	GLN
73	SV	33	GLN
74	SW	15	ASN
75	SX	18	ASN
79	Sb	57	GLN
79	Sb	61	ASN
81	Sd	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3188/3337 (95%)	476 (14%)	39 (1%)
2	2	1761/1796 (98%)	311 (17%)	34 (1%)
3	3	118/120 (98%)	9 (7%)	1 (0%)
4	4	155/156 (99%)	20 (12%)	0
All	All	5222/5409 (96%)	816 (15%)	74 (1%)

All (816) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	A
1	1	41	A
1	1	44	A
1	1	50	A
1	1	60	G
1	1	61	A
1	1	66	A
1	1	67	A
1	1	93	G
1	1	97	G
1	1	111	G
1	1	114	C
1	1	117	A
1	1	118	U
1	1	119	U
1	1	123	A
1	1	132	U
1	1	133	C

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Mol	Chain	Res	Type
1	1	134	G
1	1	135	G
1	1	144	G
1	1	152	G
1	1	153	A
1	1	165	G
1	1	170	A
1	1	179	C
1	1	181	G
1	1	184	U
1	1	185	U
1	1	204	C
1	1	212	G
1	1	213	A
1	1	214	G
1	1	215	A
1	1	225	A
1	1	234	C
1	1	251	U
1	1	262	G
1	1	276	G
1	1	277	A
1	1	279	U
1	1	288	A
1	1	308	C
1	1	316	A
1	1	332	C
1	1	343	C
1	1	363	U
1	1	369	G
1	1	385	G
1	1	391	U
1	1	392	A
1	1	394	C
1	1	395	A
1	1	396	C
1	1	414	G
1	1	415	A
1	1	422	U
1	1	432	C
1	1	434	U
1	1	447	U

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Mol	Chain	Res	Type
1	1	460	U
1	1	461	C
1	1	470	A
1	1	471	C
1	1	485	G
1	1	489	A
1	1	511	U
1	1	512	A
1	1	527	G
1	1	538	G
1	1	539	G
1	1	547	A
1	1	549	A
1	1	559	G
1	1	560	U
1	1	580	A
1	1	583	A
1	1	591	C
1	1	592	U
1	1	593	G
1	1	597	G
1	1	599	A
1	1	608	U
1	1	609	A
1	1	610	A
1	1	624	C
1	1	637	A
1	1	645	A
1	1	648	A
1	1	665	A
1	1	669	U
1	1	679	A
1	1	697	A
1	1	700	G
1	1	703	A
1	1	704	A
1	1	715	A
1	1	722	G
1	1	748	U
1	1	749	U
1	1	758	U
1	1	759	U

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Mol	Chain	Res	Type
1	1	763	G
1	1	767	G
1	1	783	A
1	1	788	A
1	1	799	A
1	1	812	A
1	1	843	C
1	1	856	U
1	1	861	U
1	1	862	G
1	1	878	A
1	1	889	G
1	1	890	G
1	1	896	A
1	1	898	G
1	1	899	A
1	1	919	G
1	1	926	A
1	1	941	C
1	1	942	U
1	1	943	C
1	1	959	A
1	1	960	C
1	1	961	C
1	1	962	U
1	1	984	A
1	1	992	G
1	1	998	C
1	1	999	G
1	1	1007	U
1	1	1008	U
1	1	1010	U
1	1	1011	U
1	1	1012	A
1	1	1015	C
1	1	1017	U
1	1	1030	A
1	1	1032	C
1	1	1047	A
1	1	1048	A
1	1	1055	G
1	1	1064	C

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Mol	Chain	Res	Type
1	1	1065	U
1	1	1068	A
1	1	1076	A
1	1	1077	U
1	1	1079	C
1	1	1080	G
1	1	1081	A
1	1	1086	A
1	1	1087	U
1	1	1088	C
1	1	1100	G
1	1	1114	G
1	1	1127	U
1	1	1131	G
1	1	1134	U
1	1	1136	A
1	1	1142	A
1	1	1161	G
1	1	1163	G
1	1	1164	U
1	1	1165	G
1	1	1175	C
1	1	1184	C
1	1	1192	G
1	1	1205	G
1	1	1206	A
1	1	1218	U
1	1	1219	G
1	1	1222	C
1	1	1224	U
1	1	1228	A
1	1	1229	G
1	1	1231	C
1	1	1241	U
1	1	1245	G
1	1	1246	A
1	1	1268	G
1	1	1290	G
1	1	1291	A
1	1	1292	U
1	1	1296	G
1	1	1313	A

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Mol	Chain	Res	Type
1	1	1314	U
1	1	1331	A
1	1	1332	G
1	1	1333	A
1	1	1335	A
1	1	1336	C
1	1	1337	G
1	1	1339	U
1	1	1369	A
1	1	1382	A
1	1	1383	G
1	1	1402	A
1	1	1404	G
1	1	1417	G
1	1	1420	C
1	1	1433	G
1	1	1458	G
1	1	1464	A
1	1	1465	A
1	1	1466	G
1	1	1485	G
1	1	1491	C
1	1	1495	U
1	1	1506	U
1	1	1516	U
1	1	1537	U
1	1	1538	U
1	1	1539	C
1	1	1540	A
1	1	1543	G
1	1	1545	G
1	1	1552	G
1	1	1554	G
1	1	1555	C
1	1	1560	U
1	1	1561	G
1	1	1562	U
1	1	1563	G
1	1	1567	A
1	1	1585	A
1	1	1587	U
1	1	1588	C

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Mol	Chain	Res	Type
1	1	1609	U
1	1	1611	C
1	1	1619	C
1	1	1622	A
1	1	1623	A
1	1	1624	C
1	1	1625	U
1	1	1637	C
1	1	1685	U
1	1	1696	A
1	1	1697	C
1	1	1704	U
1	1	1727	G
1	1	1730	A
1	1	1731	G
1	1	1745	U
1	1	1746	G
1	1	1750	G
1	1	1760	G
1	1	1777	A
1	1	1794	A
1	1	1796	A
1	1	1797	A
1	1	1798	U
1	1	1799	U
1	1	1800	C
1	1	1801	U
1	1	1819	A
1	1	1820	U
1	1	1821	A
1	1	1822	A
1	1	1826	C
1	1	1829	C
1	1	1830	A
1	1	1858	G
1	1	1859	A
1	1	1860	U
1	1	1866	A
1	1	1886	G
1	1	1887	C
1	1	1888	A
1	1	1906	C

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Mol	Chain	Res	Type
1	1	1933	G
1	1	1936	A
1	1	2045	G
1	1	2048	U
1	1	2050	C
1	1	2054	U
1	1	2055	A
1	1	2063	A
1	1	2065	U
1	1	2076	A
1	1	2084	G
1	1	2085	G
1	1	2094	A
1	1	2107	A
1	1	2121	A
1	1	2132	G
1	1	2133	U
1	1	2134	G
1	1	2139	U
1	1	2151	A
1	1	2168	U
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	G
1	1	2192	A
1	1	2207	A
1	1	2212	G
1	1	2216	G
1	1	2219	A
1	1	2220	C
1	1	2221	U
1	1	2228	C
1	1	2233	A
1	1	2235	G
1	1	2236	G
1	1	2242	A
1	1	2244	A
1	1	2248	C
1	1	2251	G
1	1	2270	G
1	1	2273	U

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Mol	Chain	Res	Type
1	1	2276	A
1	1	2278	G
1	1	2281	U
1	1	2297	U
1	1	2299	U
1	1	2335	A
1	1	2336	A
1	1	2337	C
1	1	2338	G
1	1	2339	G
1	1	2356	G
1	1	2360	A
1	1	2364	A
1	1	2365	A
1	1	2366	G
1	1	2367	A
1	1	2374	U
1	1	2382	A
1	1	2398	G
1	1	2464	U
1	1	2465	U
1	1	2474	A
1	1	2477	U
1	1	2478	A
1	1	2487	A
1	1	2488	G
1	1	2489	C
1	1	2492	G
1	1	2497	G
1	1	2501	U
1	1	2502	G
1	1	2503	C
1	1	2504	G
1	1	2510	C
1	1	2513	C
1	1	2516	G
1	1	2521	A
1	1	2529	U
1	1	2530	C
1	1	2531	G
1	1	2532	C
1	1	2533	G

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Mol	Chain	Res	Type
1	1	2543	G
1	1	2544	G
1	1	2552	A
1	1	2553	C
1	1	2565	G
1	1	2566	G
1	1	2573	G
1	1	2578	OMG
1	1	2585	A
1	1	2611	U
1	1	2615	A
1	1	2622	G
1	1	2633	A
1	1	2636	G
1	1	2648	A
1	1	2650	A
1	1	2653	A
1	1	2655	A
1	1	2663	A
1	1	2673	G
1	1	2687	G
1	1	2688	U
1	1	2711	U
1	1	2712	G
1	1	2714	C
1	1	2721	A
1	1	2731	C
1	1	2732	C
1	1	2736	G
1	1	2737	A
1	1	2755	G
1	1	2758	A
1	1	2759	G
1	1	2760	A
1	1	2763	A
1	1	2769	C
1	1	2776	A
1	1	2777	U
1	1	2778	A
1	1	2788	U
1	1	2798	G
1	1	2803	C

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Mol	Chain	Res	Type
1	1	2804	A
1	1	2828	U
1	1	2830	G
1	1	2831	A
1	1	2846	A
1	1	2858	C
1	1	2863	U
1	1	2882	U
1	1	2894	U
1	1	2895	A
1	1	2901	C
1	1	2906	G
1	1	2931	G
1	1	2942	C
1	1	2970	A
1	1	3007	A
1	1	3008	U
1	1	3014	U
1	1	3017	G
1	1	3036	G
1	1	3044	A
1	1	3050	C
1	1	3051	C
1	1	3059	G
1	1	3080	A
1	1	3088	A
1	1	3089	U
1	1	3100	A
1	1	3101	C
1	1	3112	U
1	1	3113	A
1	1	3119	A
1	1	3122	U
1	1	3127	G
1	1	3128	A
1	1	3130	G
1	1	3131	U
1	1	3132	A
1	1	3135	A
1	1	3141	G
1	1	3146	C
1	1	3147	G

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Mol	Chain	Res	Type
1	1	3162	C
1	1	3163	A
1	1	3164	G
1	1	3170	U
1	1	3188	G
1	1	3189	U
1	1	3200	A
1	1	3201	A
1	1	3211	U
1	1	3214	A
1	1	3218	U
1	1	3219	A
1	1	3223	A
1	1	3225	G
1	1	3227	G
1	1	3229	G
1	1	3230	G
1	1	3231	G
1	1	3235	A
1	1	3245	C
1	1	3248	A
1	1	3257	A
1	1	3258	U
1	1	3259	G
1	1	3260	U
1	1	3261	G
1	1	3282	U
1	1	3286	G
1	1	3292	U
1	1	3299	U
1	1	3309	U
1	1	3310	G
1	1	3319	C
1	1	3324	C
1	1	3325	U
1	1	3331	U
1	1	3332	A
1	1	3333	G
2	2	17	C
2	2	25	C
2	2	26	A
2	2	27	U

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Mol	Chain	Res	Type
2	2	34	G
2	2	42	G
2	2	47	A
2	2	57	G
2	2	68	A
2	2	69	G
2	2	73	U
2	2	74	U
2	2	75	A
2	2	76	U
2	2	77	A
2	2	103	A
2	2	113	C
2	2	115	U
2	2	126	G
2	2	127	U
2	2	138	A
2	2	155	U
2	2	156	U
2	2	174	U
2	2	175	G
2	2	176	A
2	2	184	G
2	2	185	A
2	2	186	C
2	2	187	U
2	2	190	G
2	2	192	A
2	2	195	G
2	2	210	A
2	2	212	U
2	2	213	A
2	2	214	A
2	2	215	A
2	2	216	A
2	2	221	A
2	2	222	U
2	2	223	G
2	2	224	C
2	2	231	G
2	2	232	G
2	2	234	C

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Mol	Chain	Res	Type
2	2	236	U
2	2	237	U
2	2	247	C
2	2	258	C
2	2	262	A
2	2	268	A
2	2	269	C
2	2	270	G
2	2	274	U
2	2	275	U
2	2	277	C
2	2	296	A
2	2	311	C
2	2	313	A
2	2	317	U
2	2	319	G
2	2	321	C
2	2	326	G
2	2	334	G
2	2	335	C
2	2	338	G
2	2	349	A
2	2	353	G
2	2	356	A
2	2	357	A
2	2	358	C
2	2	367	A
2	2	377	C
2	2	396	A
2	2	397	A
2	2	399	C
2	2	401	G
2	2	414	A
2	2	415	G
2	2	421	C
2	2	422	A
2	2	423	G
2	2	431	G
2	2	436	U
2	2	441	C
2	2	445	C
2	2	451	A

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Mol	Chain	Res	Type
2	2	452	C
2	2	465	A
2	2	472	A
2	2	474	A
2	2	490	U
2	2	491	U
2	2	492	C
2	2	493	G
2	2	502	A
2	2	505	U
2	2	510	U
2	2	511	G
2	2	512	A
2	2	535	A
2	2	536	G
2	2	537	G
2	2	538	A
2	2	539	A
2	2	540	C
2	2	541	A
2	2	552	A
2	2	553	A
2	2	554	G
2	2	555	U
2	2	556	C
2	2	562	C
2	2	567	A
2	2	571	G
2	2	576	A
2	2	577	A
2	2	579	U
2	2	591	A
2	2	592	G
2	2	608	U
2	2	611	A
2	2	612	G
2	2	616	A
2	2	617	A
2	2	619	A
2	2	620	A
2	2	621	G
2	2	636	U

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Mol	Chain	Res	Type
2	2	645	G
2	2	677	U
2	2	679	G
2	2	686	C
2	2	688	U
2	2	689	U
2	2	690	U
2	2	692	C
2	2	693	U
2	2	705	G
2	2	725	G
2	2	726	U
2	2	727	C
2	2	729	G
2	2	731	G
2	2	732	A
2	2	741	U
2	2	754	A
2	2	755	A
2	2	764	G
2	2	765	C
2	2	773	A
2	2	774	G
2	2	779	A
2	2	780	U
2	2	781	G
2	2	787	A
2	2	792	U
2	2	793	U
2	2	809	A
2	2	810	A
2	2	819	G
2	2	821	G
2	2	824	U
2	2	828	U
2	2	829	U
2	2	830	U
2	2	832	G
2	2	833	U
2	2	861	A
2	2	884	U
2	2	896	A

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Mol	Chain	Res	Type
2	2	910	U
2	2	911	G
2	2	912	G
2	2	931	A
2	2	933	U
2	2	940	G
2	2	949	A
2	2	957	U
2	2	958	U
2	2	964	A
2	2	982	G
2	2	988	C
2	2	990	A
2	2	991	A
2	2	1002	U
2	2	1003	A
2	2	1024	A
2	2	1026	C
2	2	1037	A
2	2	1055	A
2	2	1056	U
2	2	1057	U
2	2	1058	U
2	2	1059	U
2	2	1079	C
2	2	1088	A
2	2	1089	A
2	2	1090	A
2	2	1093	G
2	2	1094	U
2	2	1095	U
2	2	1097	G
2	2	1135	A
2	2	1140	A
2	2	1147	G
2	2	1155	C
2	2	1156	C
2	2	1157	A
2	2	1166	G
2	2	1182	U
2	2	1191	A
2	2	1193	A

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Mol	Chain	Res	Type
2	2	1194	C
2	2	1196	G
2	2	1197	G
2	2	1214	A
2	2	1215	G
2	2	1223	G
2	2	1225	G
2	2	1226	G
2	2	1227	A
2	2	1228	U
2	2	1237	U
2	2	1238	G
2	2	1240	G
2	2	1241	A
2	2	1242	G
2	2	1243	C
2	2	1248	U
2	2	1249	C
2	2	1252	G
2	2	1253	A
2	2	1254	U
2	2	1255	U
2	2	1282	U
2	2	1283	U
2	2	1311	U
2	2	1312	U
2	2	1313	G
2	2	1318	A
2	2	1338	G
2	2	1341	A
2	2	1342	A
2	2	1344	U
2	2	1357	C
2	2	1358	U
2	2	1360	G
2	2	1379	A
2	2	1387	U
2	2	1409	U
2	2	1411	U
2	2	1421	A
2	2	1423	A
2	2	1424	G

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Mol	Chain	Res	Type
2	2	1439	U
2	2	1441	G
2	2	1444	G
2	2	1455	C
2	2	1467	A
2	2	1474	G
2	2	1478	C
2	2	1482	G
2	2	1486	A
2	2	1487	C
2	2	1489	C
2	2	1499	A
2	2	1502	G
2	2	1512	A
2	2	1517	G
2	2	1519	U
2	2	1532	G
2	2	1533	C
2	2	1534	U
2	2	1538	G
2	2	1553	U
2	2	1555	A
2	2	1565	A
2	2	1570	G
2	2	1580	G
2	2	1586	G
2	2	1597	G
2	2	1612	G
2	2	1617	U
2	2	1627	A
2	2	1631	A
2	2	1653	U
2	2	1654	G
2	2	1684	C
2	2	1699	C
2	2	1708	A
2	2	1711	G
2	2	1712	C
2	2	1713	C
2	2	1726	A
2	2	1756	G
2	2	1762	A

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Mol	Chain	Res	Type
2	2	1763	G
2	2	1765	U
2	2	1766	C
2	2	1776	G
2	2	1778	A
2	2	1779	C
2	2	1788	G
2	2	1789	G
2	2	1790	A
2	2	1791	U
2	2	1792	C
2	2	1795	U
2	2	1796	U
3	3	7	G
3	3	54	U
3	3	55	A
3	3	65	G
3	3	73	U
3	3	90	G
3	3	92	C
3	3	101	A
3	3	111	G
4	4	23	U
4	4	34	U
4	4	35	C
4	4	48	A
4	4	59	A
4	4	62	A
4	4	63	G
4	4	79	A
4	4	81	U
4	4	82	U
4	4	83	C
4	4	87	G
4	4	88	A
4	4	95	G
4	4	104	A
4	4	106	C
4	4	111	A
4	4	113	U
4	4	125	U
4	4	138	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	133	C
1	1	250	C
1	1	275	G
1	1	431	A
1	1	484	A
1	1	609	A
1	1	703	A
1	1	898	G
1	1	960	C
1	1	1016	U
1	1	1047	A
1	1	1064	C
1	1	1267	C
1	1	1290	G
1	1	1338	A
1	1	1587	U
1	1	1796	A
1	1	2064	C
1	1	2075	U
1	1	2167	C
1	1	2172	U
1	1	2220	C
1	1	2227	U
1	1	2232	U
1	1	2503	C
1	1	2532	C
1	1	2552	A
1	1	2621	G
1	1	2731	C
1	1	3079	U
1	1	3121	G
1	1	3163	A
1	1	3210	U
1	1	3224	C
1	1	3230	G
1	1	3258	U
1	1	3281	G
1	1	3298	U
1	1	3332	A
2	2	102	A
2	2	184	G
2	2	211	U

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Mol	Chain	Res	Type
2	2	231	G
2	2	233	G
2	2	269	C
2	2	352	G
2	2	414	A
2	2	509	A
2	2	539	A
2	2	552	A
2	2	555	U
2	2	644	A
2	2	678	G
2	2	726	U
2	2	740	C
2	2	754	A
2	2	792	U
2	2	832	G
2	2	1094	U
2	2	1165	U
2	2	1193	A
2	2	1224	A
2	2	1241	A
2	2	1252	G
2	2	1282	U
2	2	1341	A
2	2	1378	U
2	2	1477	C
2	2	1531	U
2	2	1564	C
2	2	1569	A
2	2	1616	C
2	2	1653	U
3	3	72	G

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B8N	2	1188	2	25,29,30	2.58	5 (20%)	28,42,45	1.32	4 (14%)
1	OMG	1	2578	1	23,26,27	0.50	0	32,38,41	0.44	0
22	SAC	LO	2	22	7,8,9	1.03	0	7,9,11	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8N	2	1188	2	-	1/16/34/35	0/2/2/2
1	OMG	1	2578	1	-	2/9/27/28	0/3/3/3
22	SAC	LO	2	22	-	2/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1188	B8N	O4-C4	9.58	1.42	1.23
2	2	1188	B8N	C2-N3	-3.87	1.32	1.38
2	2	1188	B8N	C4-N3	-3.80	1.33	1.40
2	2	1188	B8N	C4-C5	-3.51	1.39	1.47
2	2	1188	B8N	C6-C5	3.14	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1188	B8N	N3-C2-N1	3.42	120.90	116.72
2	2	1188	B8N	C4-N3-C2	-3.26	121.61	125.62
2	2	1188	B8N	O4'-C1'-C2'	2.09	108.04	105.15
2	2	1188	B8N	C1'-C5-C4	2.02	120.68	117.61

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	LO	2	SAC	N-CA-CB-OG
22	LO	2	SAC	C-CA-CB-OG
1	1	2578	OMG	O4'-C4'-C5'-O5'
2	2	1188	B8N	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
1	1	2578	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 579 ligands modelled in this entry, 579 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.

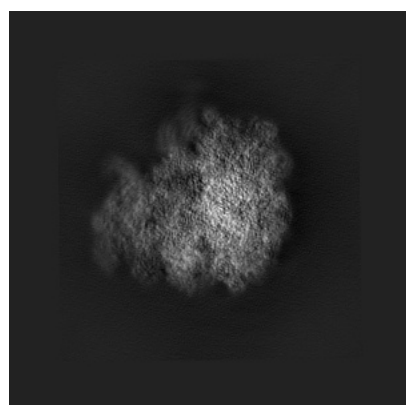
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12976. These allow visual inspection of the internal detail of the map and identification of artifacts.

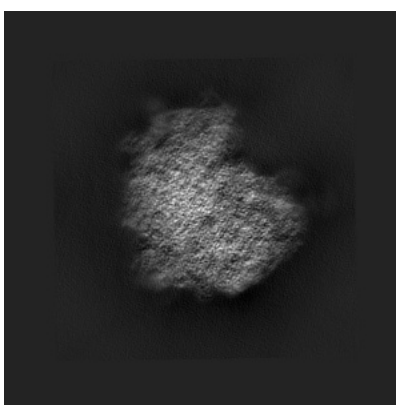
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

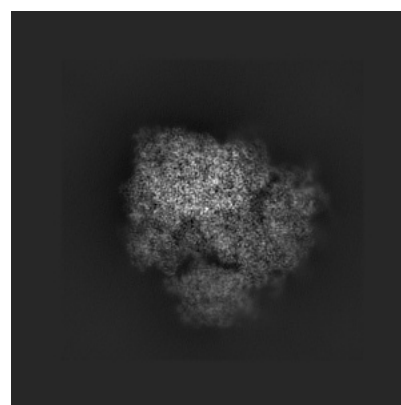
6.1.1 Primary map



X



Y

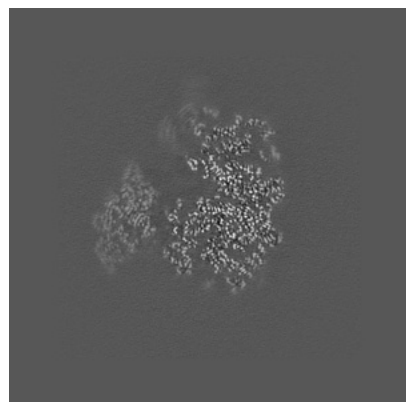


Z

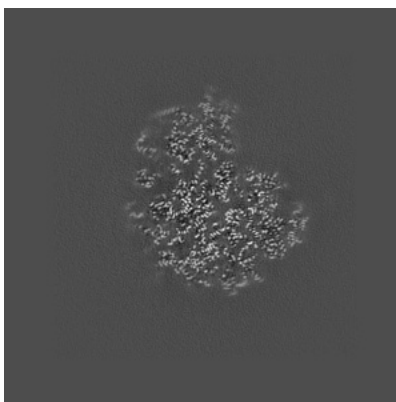
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

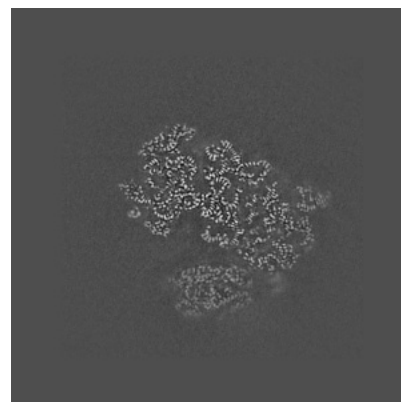
6.2.1 Primary map



X Index: 243



Y Index: 243

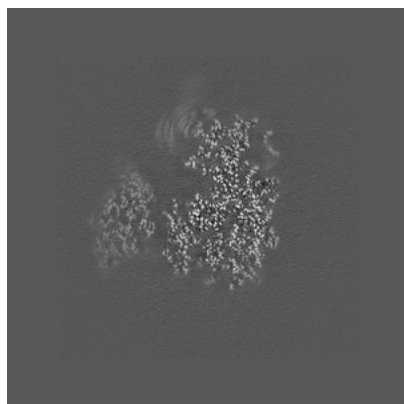


Z Index: 243

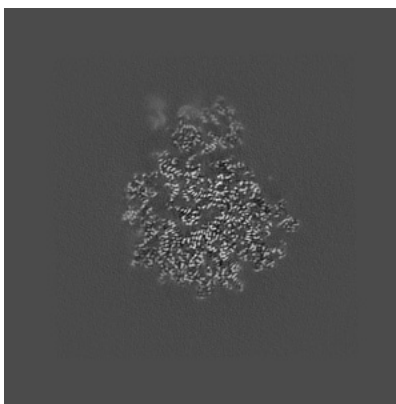
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

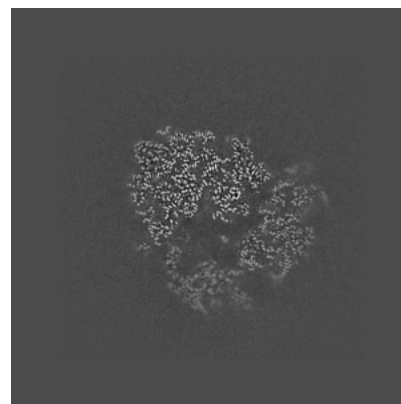
6.3.1 Primary map



X Index: 247



Y Index: 267

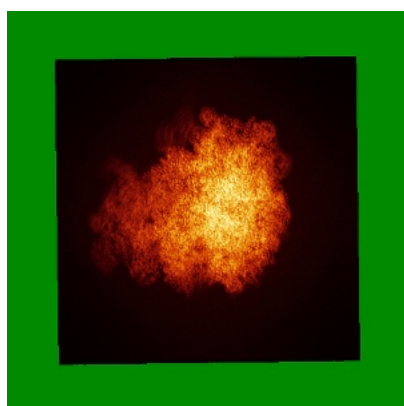


Z Index: 258

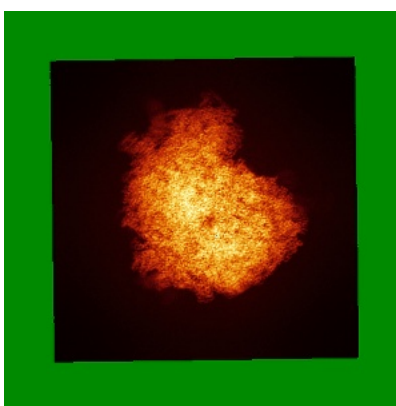
The images above show the largest variance slices of the map in three orthogonal directions.

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

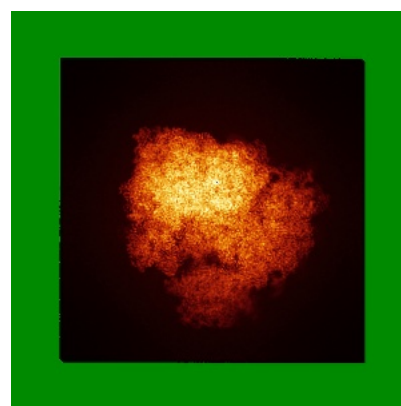
6.4.1 Primary map



X



Y

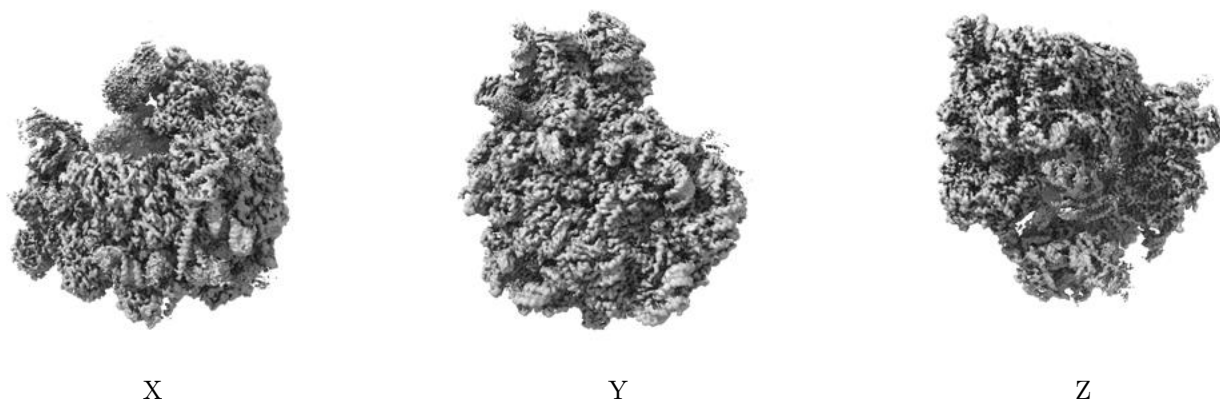


Z

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 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

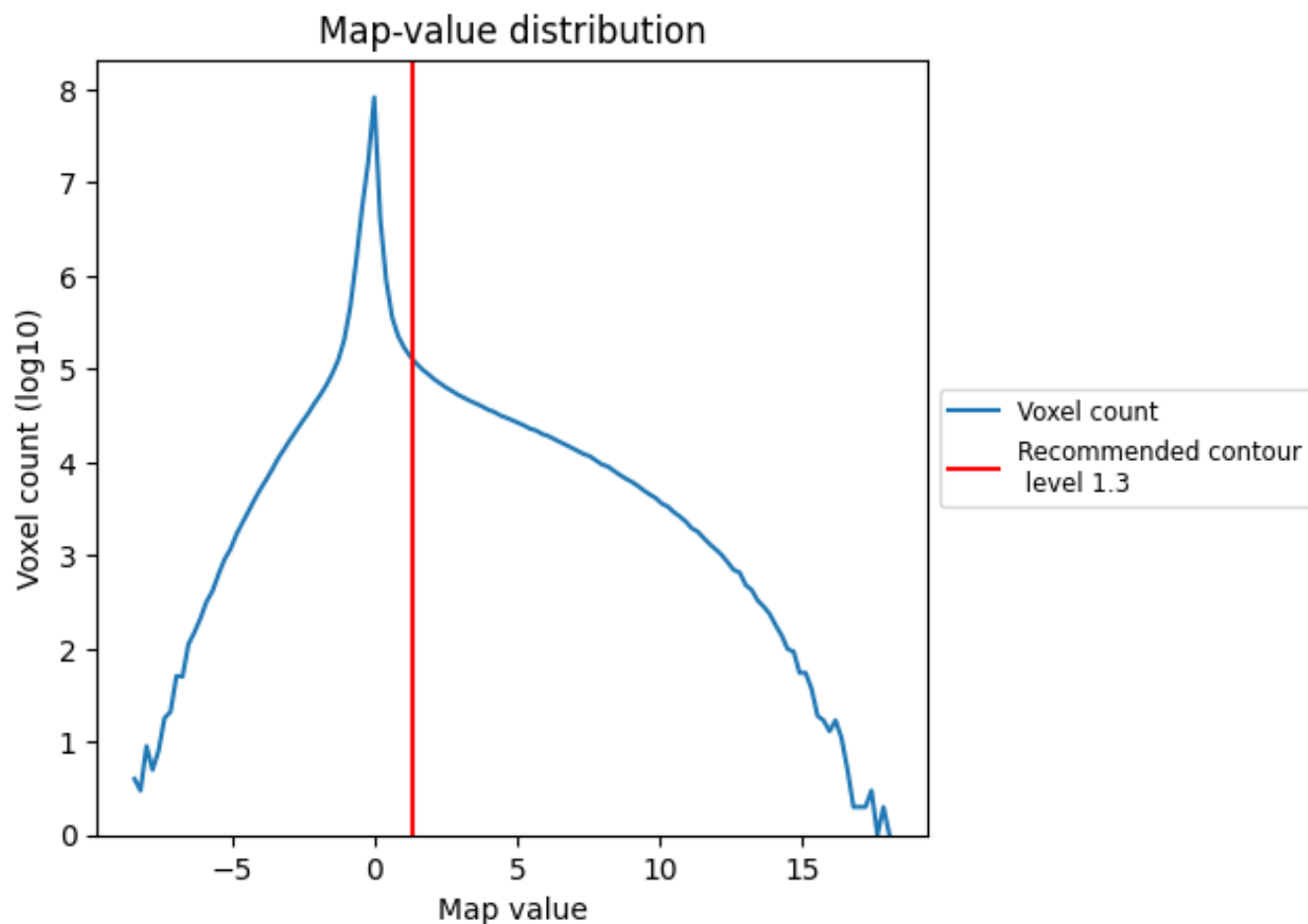
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

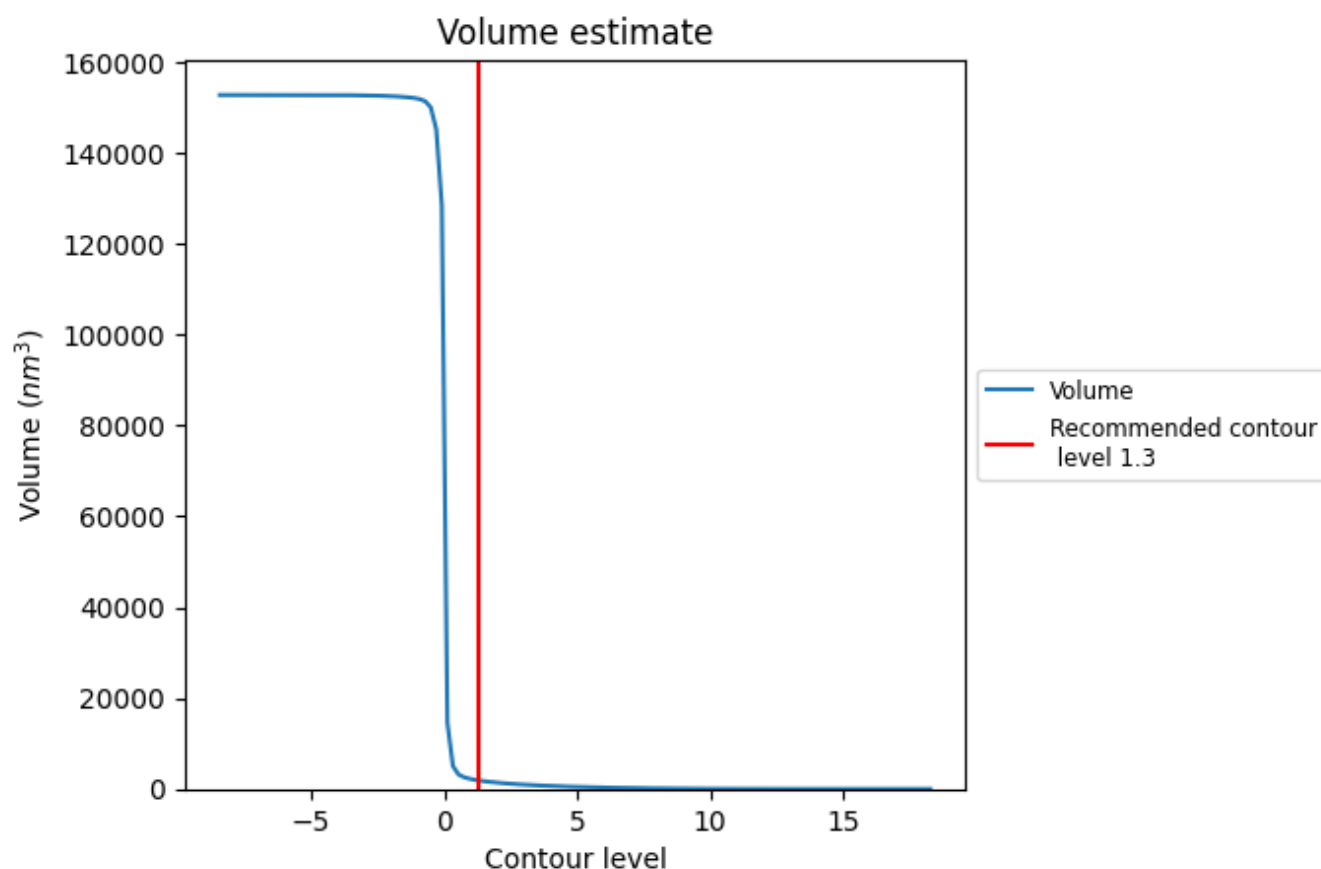
This section contains the results of statistical analysis of the map.

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.

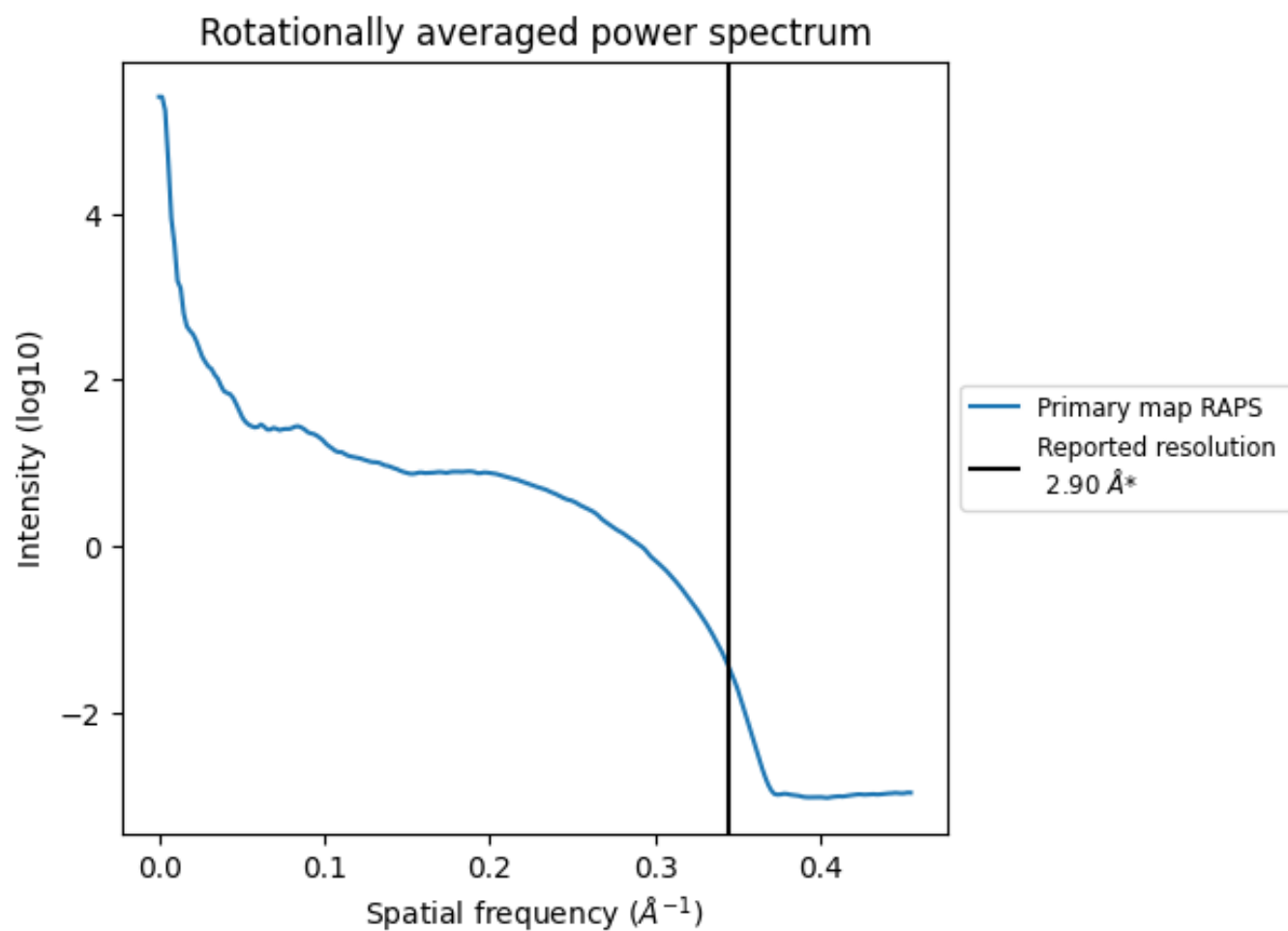
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1875 nm³; this corresponds to an approximate mass of 1694 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

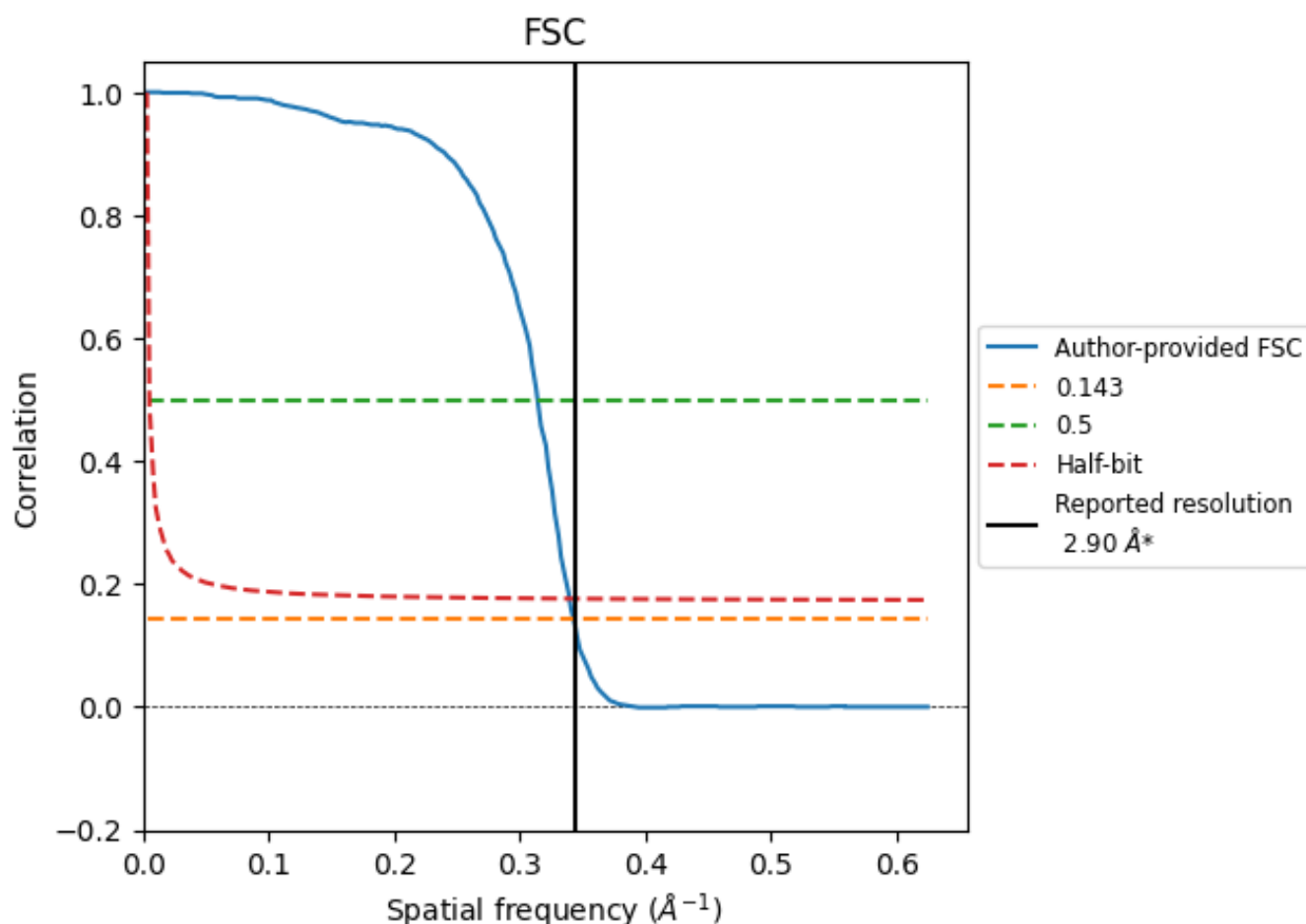


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

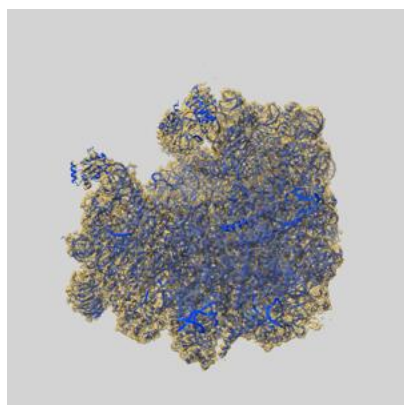
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.18	2.94
Unmasked-calculated*	-	-	-

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

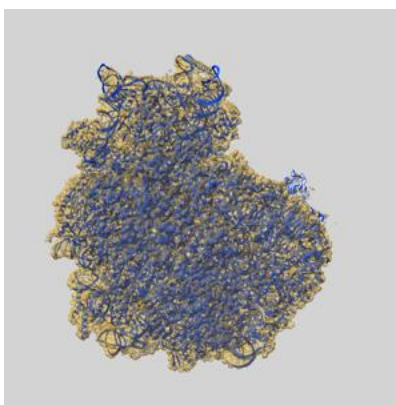
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12976 and PDB model 7OLC. Per-residue inclusion information can be found in section 3 on page 25.

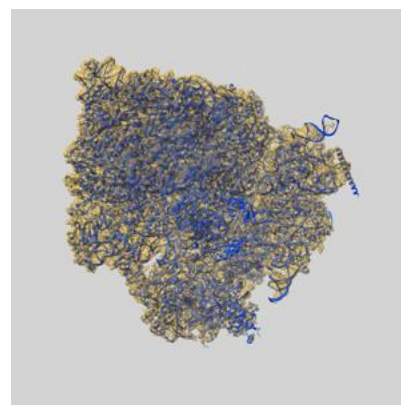
9.1 Map-model overlay [i](#)



X



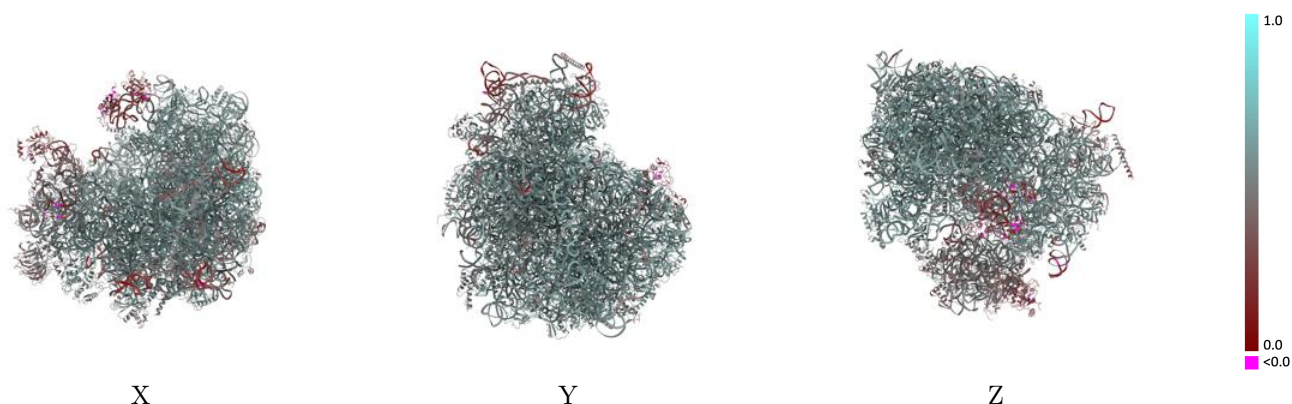
Y



Z

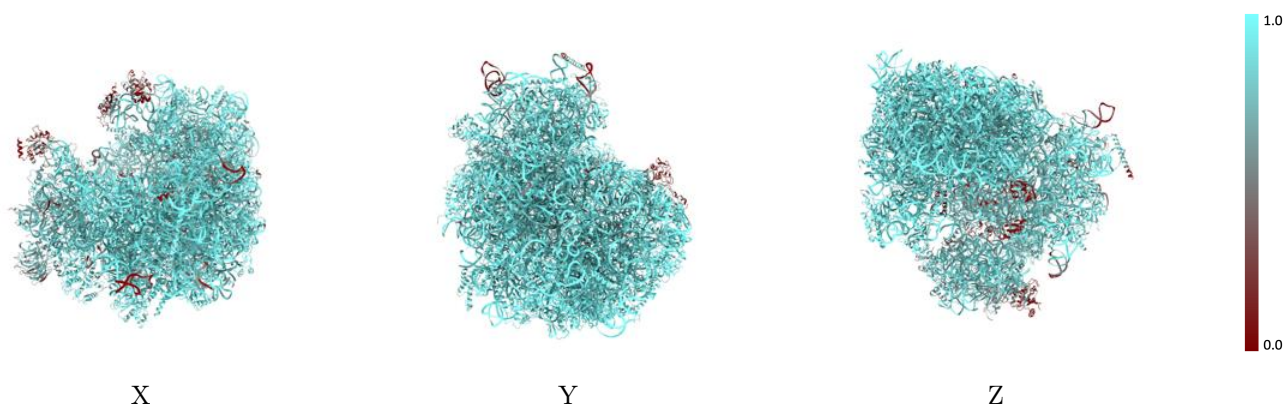
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



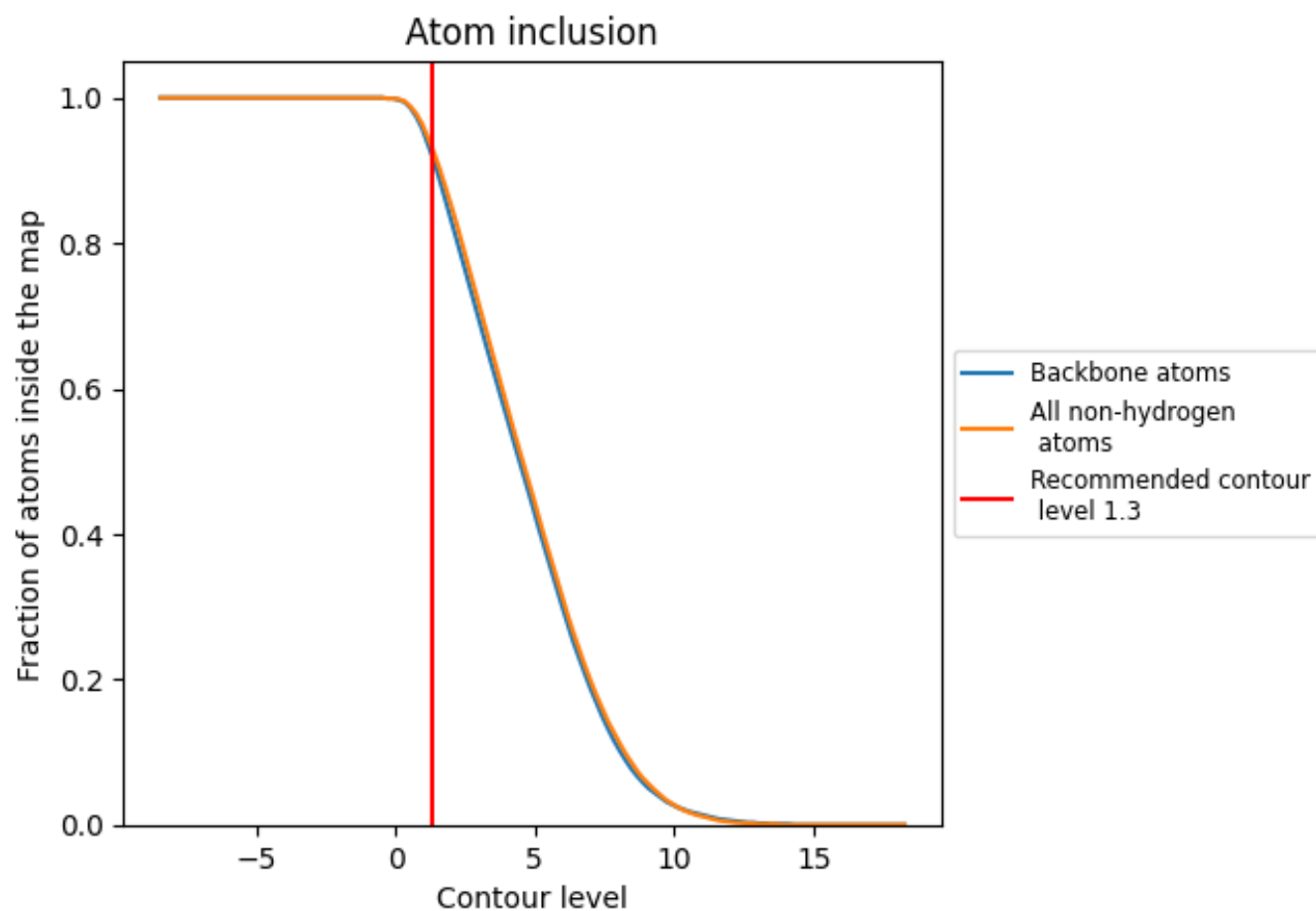
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.5380
1	 0.9860	 0.5640
2	 0.9410	 0.5140
3	 0.9990	 0.5860
4	 0.9910	 0.5580
A	 0.6780	 0.4190
B	 0.7500	 0.4500
C	 0.2640	 0.4510
LA	 0.9710	 0.5830
LB	 0.9790	 0.5870
LC	 0.9680	 0.5750
LD	 0.9350	 0.5470
LE	 0.9280	 0.5400
LF	 0.9610	 0.5790
LG	 0.9440	 0.5460
LH	 0.9570	 0.5650
LI	 0.9530	 0.5750
LJ	 0.9030	 0.5140
LK	 0.3070	 0.2010
LL	 0.9560	 0.5590
LM	 0.9540	 0.5730
LN	 0.9830	 0.5860
LO	 0.9740	 0.5830
LP	 0.9130	 0.5560
LQ	 0.9740	 0.5870
LR	 0.9560	 0.5620
LS	 0.9780	 0.5850
LT	 0.9740	 0.5730
LU	 0.9180	 0.5080
LV	 0.9740	 0.5820
LW	 0.7460	 0.4870
LX	 0.9370	 0.5450
LY	 0.9560	 0.5620
LZ	 0.9560	 0.5570
La	 0.9770	 0.5810



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Chain	Atom inclusion	Q-score
Lb	 0.9350	 0.5320
Lc	 0.9630	 0.5620
Ld	 0.9200	 0.5550
Le	 0.9750	 0.5880
Lf	 0.9730	 0.5950
Lg	 0.9660	 0.5640
Lh	 0.9250	 0.5330
Li	 0.9110	 0.5270
Lj	 0.9850	 0.5870
Lk	 0.8960	 0.5050
Ll	 0.9610	 0.5500
Lm	 0.9780	 0.5780
Ln	 0.9700	 0.5840
Lo	 0.9540	 0.5770
Lp	 0.9600	 0.5640
Lq	 0.9590	 0.5720
Lr	 0.8280	 0.5060
Ls	 0.3000	 0.2350
SA	 0.9430	 0.5430
SB	 0.9050	 0.5320
SC	 0.9430	 0.5600
SD	 0.7710	 0.4710
SE	 0.9380	 0.5540
SF	 0.8020	 0.4640
SG	 0.9130	 0.5210
SH	 0.9010	 0.5030
SI	 0.9060	 0.5450
SJ	 0.9450	 0.5490
SK	 0.7880	 0.3950
SL	 0.9460	 0.5720
SM	 0.1950	 0.2690
SN	 0.9450	 0.5560
SO	 0.9420	 0.5420
SP	 0.7610	 0.3860
SQ	 0.7880	 0.4660
SR	 0.8680	 0.5010
SS	 0.8110	 0.4280
ST	 0.7920	 0.4260
SU	 0.7150	 0.4540
SV	 0.9470	 0.5470
SW	 0.9480	 0.5640
SX	 0.9470	 0.5690

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Chain	Atom inclusion	Q-score
SY	 0.8730	 0.5330
SZ	 0.7920	 0.4180
Sa	 0.9270	 0.5450
Sb	 0.9470	 0.5290
Sc	 0.9010	 0.5120
Sd	 0.9180	 0.5090
Se	 0.9290	 0.5320
Sf	 0.4260	 0.2630