



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 12:28 pm BST

PDB ID : 6QZP / pdb_00006qzp
EMDB ID : EMD-3883
Title : High-resolution cryo-EM structure of the human 80S ribosome
Authors : Natchiar, S.K.; Myasnikov, A.G.; Kratzat, H.; Hazemann, I.; Klaholz, B.P.
Deposited on : 2019-03-12
Resolution : 2.90 Å(reported)

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:

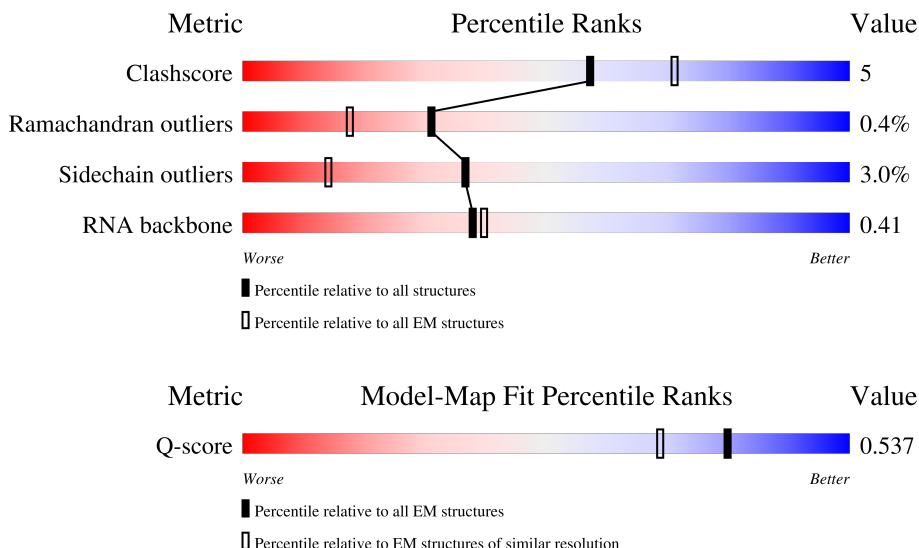
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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.



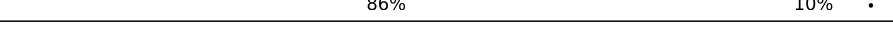
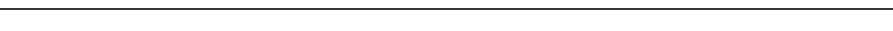
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	L5	3773	
2	L7	120	
3	L8	156	

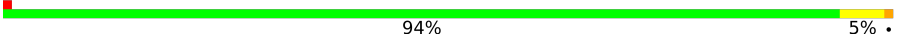
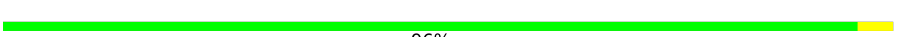
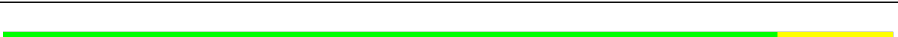
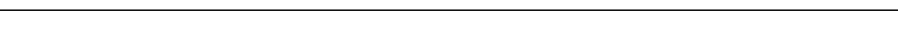
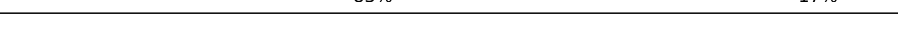
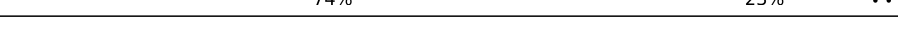
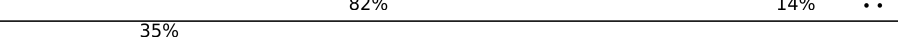
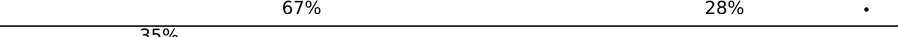
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Mol	Chain	Length	Quality of chain
4	LA	248	 82% 16% .
5	LB	402	 79% 19% .
6	LC	368	 86% 12% .
7	LD	293	 80% 18% .
8	LE	236	 85% 13% .
9	LF	225	 85% 12% .
10	LG	241	 83% 15% .
11	LH	190	 85% 15% .
12	LI	213	 85% 14% .
13	LJ	176	 78% 18% .
14	LL	210	 86% 13% .
15	LM	139	 88% 12%
16	LN	203	 83% 16%
17	LO	201	 86% 10% .
18	LP	153	 76% 22% .
19	LQ	187	 87% 12% .
20	LR	187	 89% 10% ..
21	LS	175	 91% 8% .
22	LT	159	 86% 13% .
23	LU	101	 82% 15% .
24	LV	131	 83% 12% . .
25	LW	124	 86% 11% .
26	LX	120	 89% 9% ..
27	LY	134	 82% 16% ..
28	LZ	135	 85% 15%

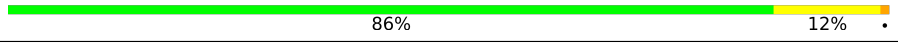
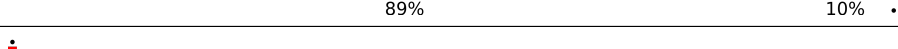
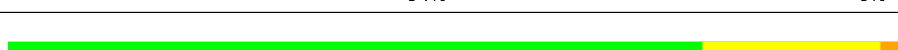
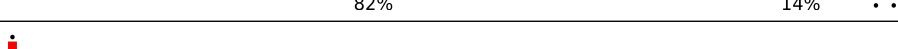
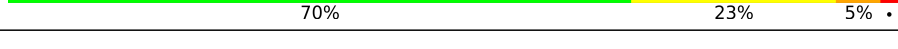
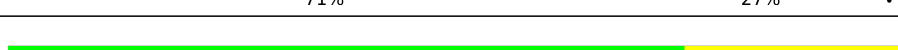
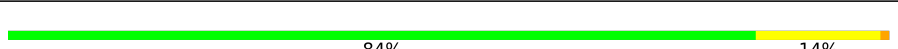
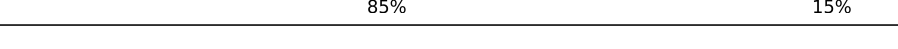
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Mol	Chain	Length	Quality of chain
29	La	147	
30	Lb	109	
31	Lc	98	
32	Ld	107	
33	Le	128	
34	Lf	109	
35	Lg	114	
36	Lh	122	
37	Li	102	
38	Lj	86	
39	Lk	69	
40	Ll	50	
41	Lm	52	
42	Ln	24	
43	Lo	105	
44	Lp	91	
45	Lr	125	
46	Lz	217	
47	S2	1740	
48	S6	75	
49	SA	221	
50	SB	214	
51	SD	227	
52	SE	262	
53	SF	189	

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Mol	Chain	Length	Quality of chain
54	SH	186	
55	SI	206	
56	SK	98	
57	SL	153	
58	SP	127	
59	SQ	141	
60	SR	135	
61	SS	145	
62	ST	143	
63	SU	103	
64	SV	83	
65	SX	141	
66	Sa	102	
67	Sc	64	
68	Sd	55	
69	Sg	313	
70	SC	222	
71	SG	237	
72	SJ	185	
73	SM	122	
74	SN	150	
75	SO	140	
76	SW	129	
77	SY	131	
78	SZ	75	

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Mol	Chain	Length	Quality of chain
79	Sb	83	78% 19%
80	Se	58	100%
81	Sf	67	93% 7%

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 219527 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 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3773	Total	C	N	O	P	0	0
			80201	35717	14590	26122	3772		

- Molecule 2 is a RNA chain called 5S rRNA (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2928	1841	583	489	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	SER	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	VAL	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

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

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLU	deletion	UNP P47914
Lb	?	-	VAL	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	ILE	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLY	deletion	UNP P47914

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Chain	Residue	Modelled	Actual	Comment	Reference
Lb	89	ALA	VAL	conflict	UNP P47914

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	86	Total	C	N	O	S	1	0
			713	439	158	111	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	1	0
			870	547	178	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1740	Total	C	N	O	P	0	0
			36938	16494	6600	12105	1739		

- Molecule 48 is a RNA chain called E site tRNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S6	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SH	?	-	SER	deletion	UNP P62081
SH	?	-	ARG	deletion	UNP P62081
SH	?	-	THR	deletion	UNP P62081

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 56 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 57 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 60 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 61 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 62 is a protein called 40S ribosomal protein S19.

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

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 64 is a protein called 40S ribosomal protein S21.

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

- Molecule 65 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 66 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sa	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 67 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 68 is a protein called 40S ribosomal protein S29.

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

- Molecule 69 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 70 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SC	222	Total	C	N	O	S	1	0
			1733	1120	301	302	10		

- Molecule 71 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 72 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 73 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 78 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 79 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 80 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

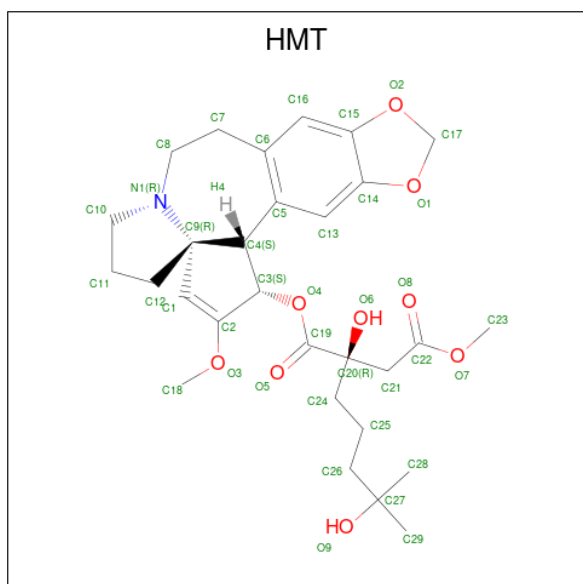
Mol	Chain	Residues	Atoms		AltConf
82	L5	279	Total	Mg	0
			279	279	
82	L7	3	Total	Mg	0
			3	3	
82	L8	6	Total	Mg	0
			6	6	
82	LA	1	Total	Mg	0
			1	1	
82	LI	1	Total	Mg	0
			1	1	
82	LN	1	Total	Mg	0
			1	1	
82	LP	1	Total	Mg	0
			1	1	
82	LS	1	Total	Mg	0
			1	1	
82	LV	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
82	Le	2	Total	Mg	0
			2	2	
82	Lf	1	Total	Mg	0
			1	1	
82	S2	140	Total	Mg	0
			140	140	
82	SF	1	Total	Mg	0
			1	1	

- Molecule 83 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano yl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉).



Mol	Chain	Residues	Atoms				AltConf
83	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

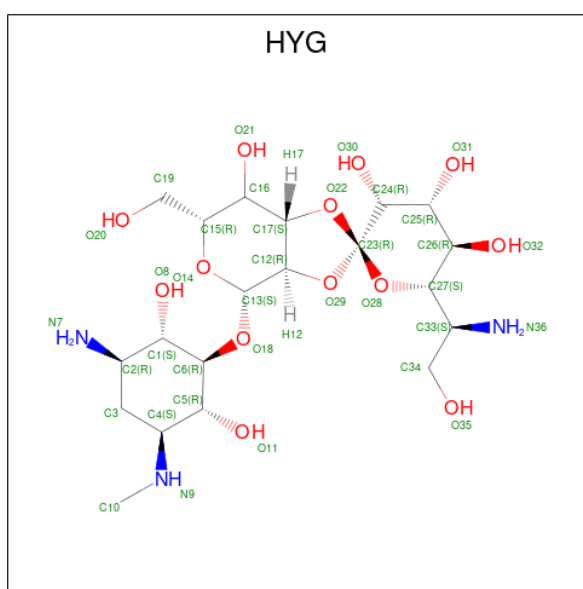
Mol	Chain	Residues	Atoms		AltConf
84	Lg	1	Total	Zn	0
			1	1	
84	Lj	1	Total	Zn	0
			1	1	
84	Lm	1	Total	Zn	0
			1	1	
84	Lo	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
84	Lp	1	Total	Zn	0
			1	1	
84	Sa	1	Total	Zn	0
			1	1	
84	Sd	1	Total	Zn	0
			1	1	
84	Sf	1	Total	Zn	0
			1	1	

- Molecule 85 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms				AltConf
85	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	L5	11	Total	O	0
			11	11	
86	LA	1	Total	O	0
			1	1	
86	LB	1	Total	O	0
			1	1	
86	LC	1	Total	O	0
			1	1	

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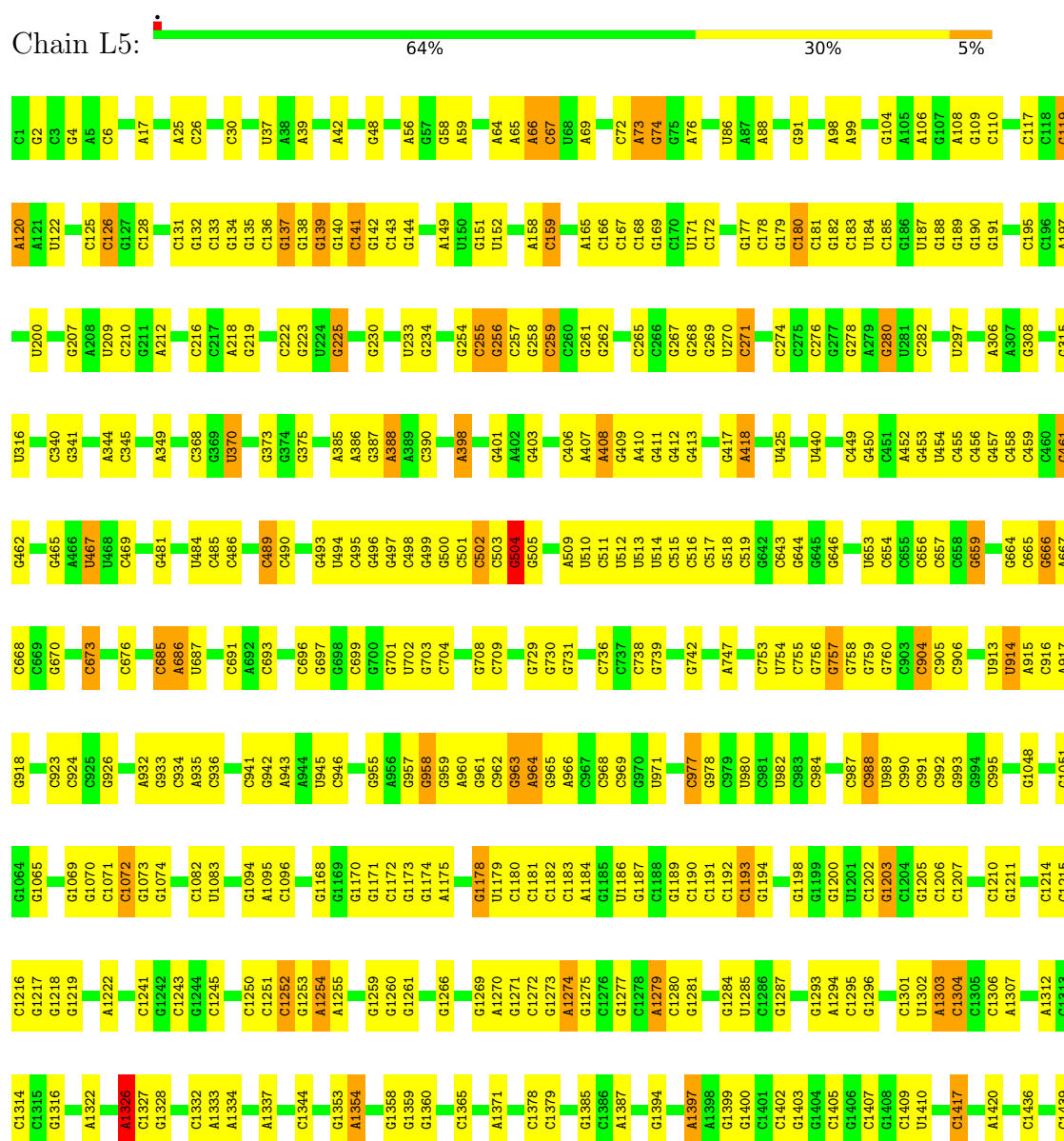
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Mol	Chain	Residues	Atoms		AltConf
86	LF	1	Total 1	O 1	0
86	LG	1	Total 1	O 1	0
86	LH	1	Total 1	O 1	0
86	LI	1	Total 1	O 1	0
86	LY	1	Total 1	O 1	0
86	La	2	Total 2	O 2	0
86	Lb	1	Total 1	O 1	0
86	Lf	1	Total 1	O 1	0
86	Lm	1	Total 1	O 1	0
86	S2	12	Total 12	O 12	0
86	SF	1	Total 1	O 1	0
86	SL	1	Total 1	O 1	0
86	SR	1	Total 1	O 1	0
86	SS	1	Total 1	O 1	0
86	SV	1	Total 1	O 1	0
86	SC	1	Total 1	O 1	0
86	SG	1	Total 1	O 1	0
86	SN	1	Total 1	O 1	0

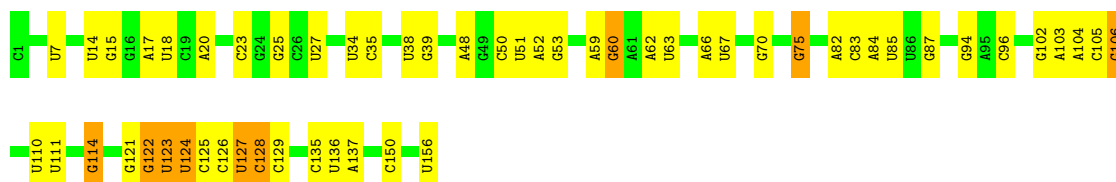
3 Residue-property plots

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: 28S rRNA (3773-MER)

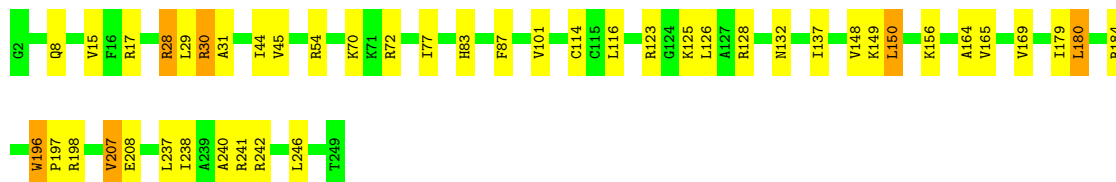


C3782	A3663	G2902	G2754	G2618	G2506	A2396	C2016	G1946	C1820	C1703	G1581	U1440
A3785	C3667	G2903	A2755	U2626	A2507	A2396	A2017	U1947	G1821	C1704	G1581	C1441
U3786	G3672	U2904	G2756	C2627	U2508	G2397	C2019	G1948	U1822	G1705	U1582	C1442
G3787	G3673	G2906	G2760	U2637	A2511	A2401	C2019	G1951	G1823	A1706	A1443	U1443
C3788	G3674	G2907	U2761	G2652	A2512	G2406	G2021	G1952	G1824	C1707	G1586	U1444
C3789	U3677	U2908	G2762	C2654	A2513	U2407	G2024	U1953	U1834	G1716	C1590	U1445
G3792	U3680	G2910	U2763	C2654	U2519	A2408	A2025	U1959	G1835	A1719	U1591	C1446
A3799	G3681	C3584	A2764	G2662	A2527	U2409	A2026	A1960	A1837	U1726	U1596	C1447
A3800	A3682	G3585	C2770	C2669	A2528	A2417	G2033	G1961	G1842	U1726	G1453	G1448
U3801	U3688	C3586	G2773	C2670	A2529	A2418	C2035	A1962	G1855	A1729	A1600	C1456
U3802	U3688	G3587	U2768	C2670	C2533	G2421	U2038	G1966	U1852	G1734	A1601	G1457
C3810	A3692	C3588	A2769	G2673	A2537	C2422	G2039	A1967	G1855	G1739	G1618	C1472
C3811	U3709	G3589	U2790	C2675	A2543	A2423	G2301	G1968	U1860	C1740	G1624	G1482
C3812	C3708	G3591	U2801	A2676	U2545	G2424	U2044	G1969	G1741	G1741	G1625	C1483
A3813	U3709	C3592	C2804	U2687	G2544	U2425	G2046	A1970	U1866	A1742	G1628	C1486
U3814	C3708	C3593	A2812	U2688	U2546	G2434	G2049	G1971	G1869	G1750	A1631	C1493
A3817	U3710	C3594	G2813	C2688	G2547	G2434	G2050	G1976	G1870	G1753	A1632	G1493
U3818	A3711	A3596	C2814	U2688	G2547	U2440	G2051	G1977	A1871	U1754	A1633	A1497
G3819	G3714	G3597	A2815	A2696	U2554	C2441	G2052	C1977	G1872	C1755	A1634	G1498
A3825	U3715	G3602	G2816	A2696	G2555	G2441	G2055	U1980	U1876	U1756	A1638	C1502
C3837	A3718	A3604	C2820	G2703	G2556	G2450	G2056	G1981	U1889	U1757	G1639	G1502
U3838	U3718	C3605	G2821	C2704	G2557	G2450	G2056	G1982	G1882	G1758	C1640	A1503
G3839	A3723	U3606	U2826	G2705	G2558	A2453	C2062	A1983	G1883	G1759	G1641	G1504
U3840	G3726	G3614	G2827	G2706	G2559	G2453	G2062	A1984	U1888	G1760	A1642	U1513
A3726	A3727	G3615	G2838	U2707	G2560	C2464	G2068	U1985	A1888	G1761	A1646	U1514
C3727	U3728	G3616	U2708	U2708	C2561	C2465	A2069	U1986	U1889	C1762	A1646	U1515
U3729	G3729	C3617	C2710	G2711	G2562	C2469	C2084	G1987	G1890	C1763	G1654	G1516
U3734	A3735	G3618	G2712	G2712	G2563	C2470	G2085	G1988	A1892	A1765	G1661	A1517
A3736	G3736	U3626	C2713	G2713	G2564	G2471	G2089	G1989	U1897	A1766	G1661	A1518
C3737	A3737	A3630	G2714	G2714	G2565	G2471	U2090	A1990	A1897	A1767	C1676	C1521
A3738	U3738	C3635	G2715	G2715	G2566	G2475	U2091	A1991	U1917	G1768	U1677	G1522
C3739	G3739	A3636	U2718	G2718	A2573	G2475	G2092	U1982	U1918	A1770	A1523	A1524
U3740	A3740	U3641	G2721	G2721	G2578	C2478	A2093	G1996	G1919	U1771	G1680	A1525
A3741	C3741	C3642	G2724	G2724	A2581	C2482	G2094	U1997	C1921	A1775	U1683	A1594
C3742	U3742	A3643	A2725	G2725	A2582	G2483	G2096	A1998	G1922	C1778	U1684	A1547
A3743	A2743	U3644	G2726	G2726	C2583	G2484	G2099	A1999	G1925	A1787	G1685	G1548
U3744	U3744	U3645	G2732	G2732	A2587	C2487	A2100	G1999	G1925	G1797	C1686	G1549
C3745	C3745	A3646	C2738	C2738	C2588	C2488	C2101	A2002	U1930	G1797	G1691	G1559
A3746	A3746	C3647	C2739	C2739	C2589	C2489	G2106	G2003	C1931	G1797	C1692	G1566
U3747	U3747	U3648	G2742	G2742	A2601	C2491	C2107	G2006	A1802	A1802	U1693	C1566
A3748	A3748	C3649	A2743	A2743	G2602	C2492	G2111	U2008	G1803	A1804	C1694	U1567
C3749	C3749	G3650	G2749	G2749	A2611	C2493	G2112	U2009	C1935	A1804	U1695	C1568
U3750	U3750	A3656	C2750	C2750	C2616	G2493	G2252	U2008	G1940	G1810	G1697	U1569
A3751	A3751	C3657	G2901	G2901	G2617	G2502	A2253	U2009	A1943	G1811	C1698	G1570
C3752	C3752	U3659	U2900	U2900	C2617	C2503	A2253	A2010	A1943	C1812	A1699	G1571
A3753	A3753	G3660	G2901	G2901	G2617	C2505	A2253	C2011	A1943	G1819	G1700	U1578
U3754	U3754	A3662	U2901	U2901	G2617	C2505	A2253	A2013	G1945			



• Molecule 4: 60S ribosomal protein L8

Chain LA: 82% 16%



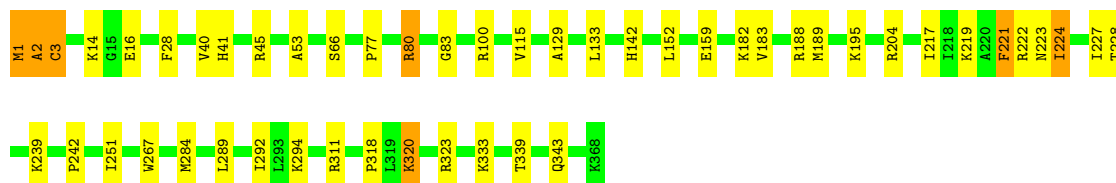
• Molecule 5: 60S ribosomal protein L3

Chain LB: 79% 19%



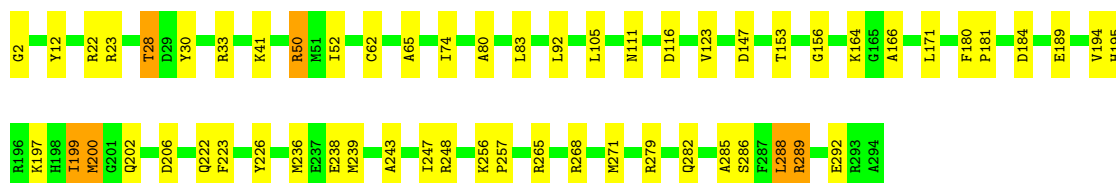
• Molecule 6: 60S ribosomal protein L4

Chain LC: 86% 12%

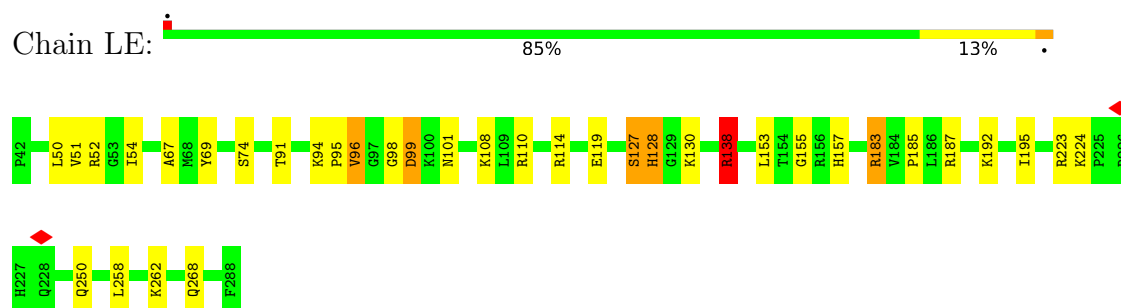


• Molecule 7: 60S ribosomal protein L5

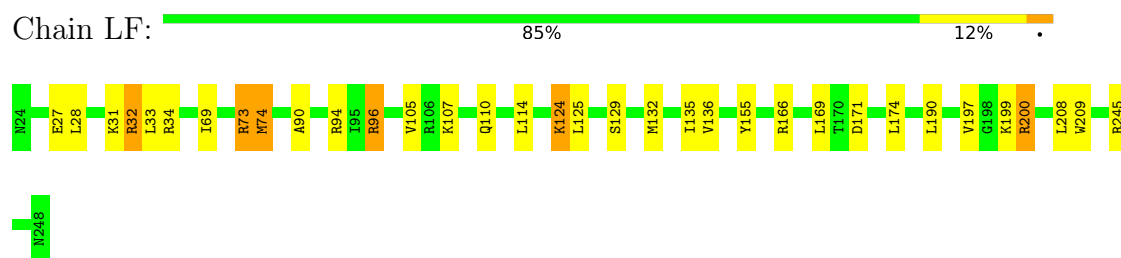
Chain LD: 80% 18%



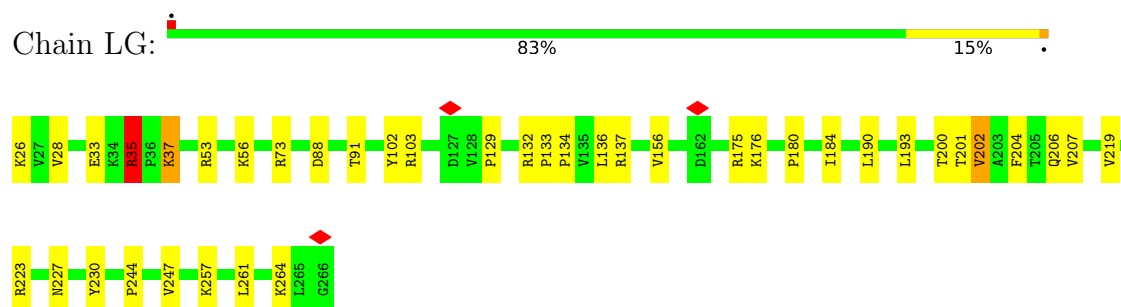
- Molecule 8: 60S ribosomal protein L6



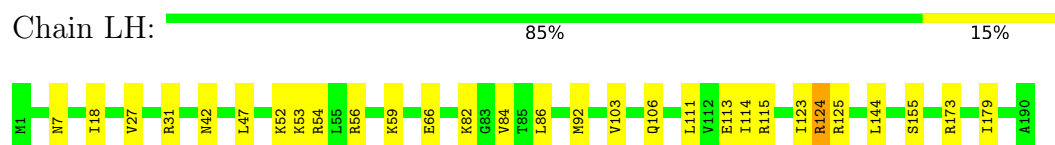
- Molecule 9: 60S ribosomal protein L7



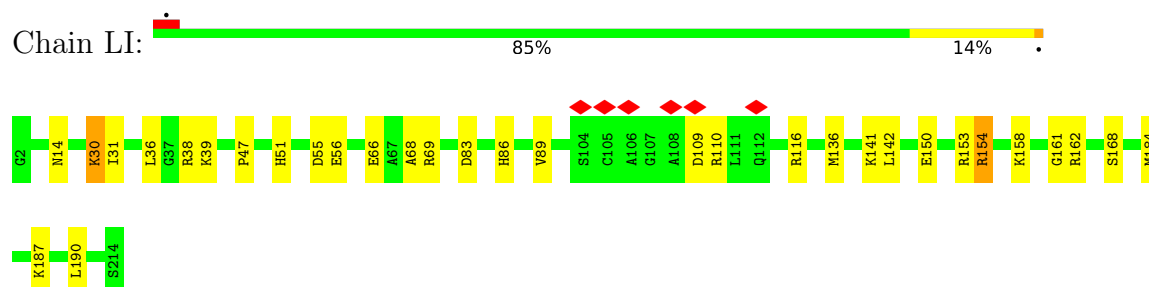
- Molecule 10: 60S ribosomal protein L7a



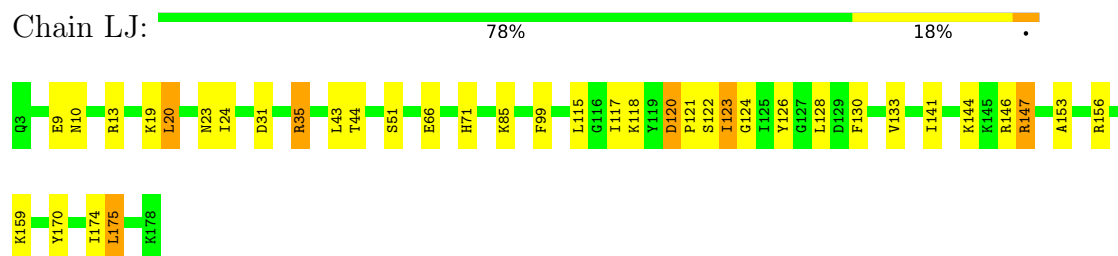
- Molecule 11: 60S ribosomal protein L9



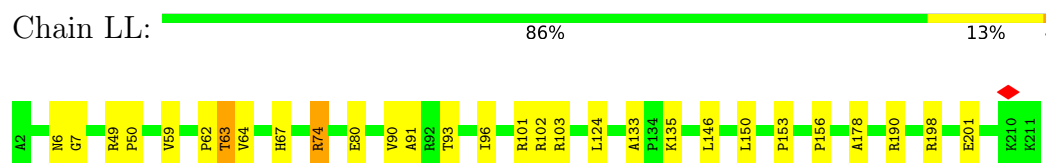
- Molecule 12: 60S ribosomal protein L10-like



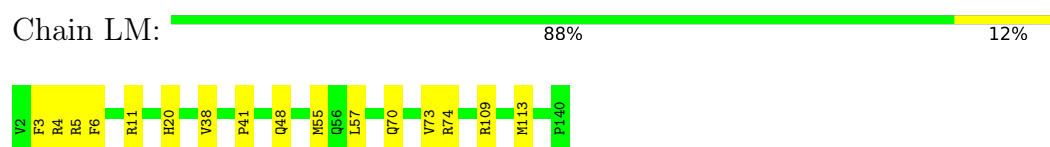
- Molecule 13: 60S ribosomal protein L11



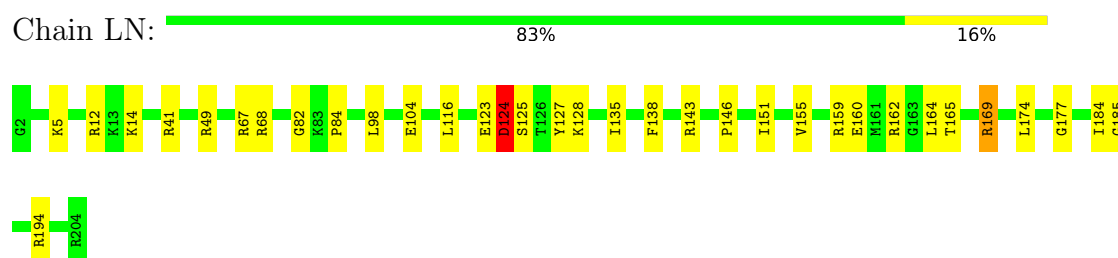
- Molecule 14: 60S ribosomal protein L13



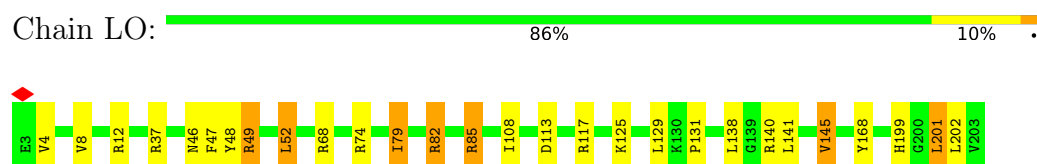
- Molecule 15: 60S ribosomal protein L14



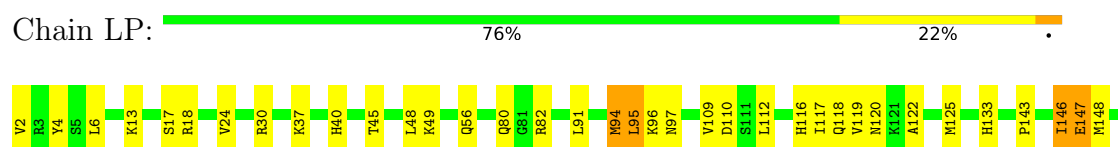
- Molecule 16: 60S ribosomal protein L15



- Molecule 17: 60S ribosomal protein L13a



- Molecule 18: 60S ribosomal protein L17





- Molecule 19: 60S ribosomal protein L18

Chain LQ: 87% 12% .



- Molecule 20: 60S ribosomal protein L19

Chain LR: 89% 10% ..



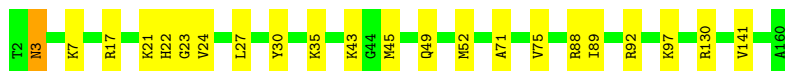
- Molecule 21: 60S ribosomal protein L18a

Chain LS: 91% 8% .



- Molecule 22: 60S ribosomal protein L21

Chain LT: 86% 13% .



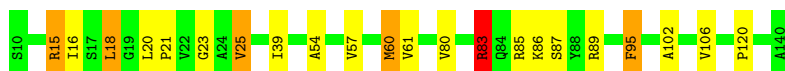
- Molecule 23: 60S ribosomal protein L22

Chain LU: 82% 15% .



- Molecule 24: 60S ribosomal protein L23

Chain LV: 83% 12% ..



- Molecule 25: 60S ribosomal protein L24

Chain LW: 86% 11% .



- Molecule 26: 60S ribosomal protein L23a

Chain LX: 89% 9% ..



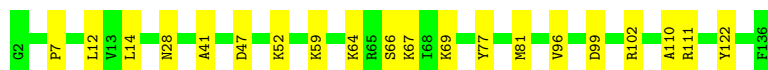
- Molecule 27: 60S ribosomal protein L26

Chain LY: 82% 16% ..



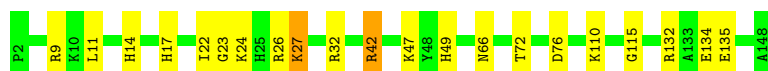
- Molecule 28: 60S ribosomal protein L27

Chain LZ: 85% 15%



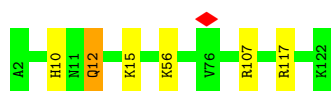
- Molecule 29: 60S ribosomal protein L27a

Chain La: 86% 13%



- Molecule 30: 60S ribosomal protein L29

Chain Lb: 94% 5%



- Molecule 31: 60S ribosomal protein L30

Chain Lc: 82% 15% ..



- Molecule 32: 60S ribosomal protein L31

Chain Ld: 87% 13%



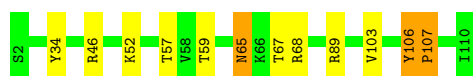
- Molecule 33: 60S ribosomal protein L32

Chain Le: 78% 20% .



- Molecule 34: 60S ribosomal protein L35a

Chain Lf: 89% 8% .



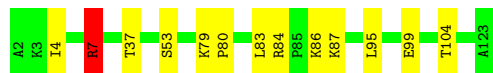
- Molecule 35: 60S ribosomal protein L34

Chain Lg: 96% .



- Molecule 36: 60S ribosomal protein L35

Chain Lh: 89% 10% .



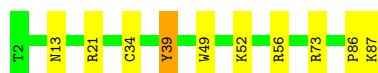
- Molecule 37: 60S ribosomal protein L36

Chain Li: 90% 10% .



- Molecule 38: 60S ribosomal protein L37

Chain Lj: 88% 10% .

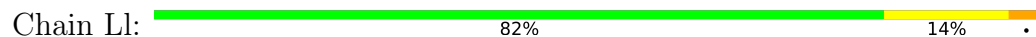


- Molecule 39: 60S ribosomal protein L38

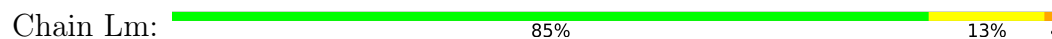
Chain Lk: 87% 13% .



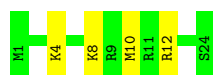
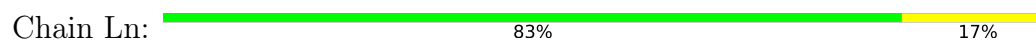
- Molecule 40: 60S ribosomal protein L39



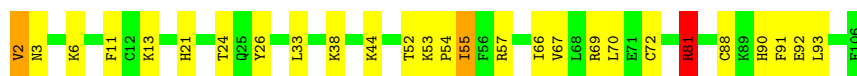
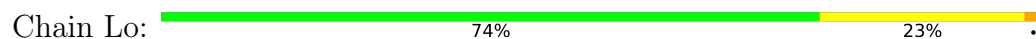
- Molecule 41: Ubiquitin-60S ribosomal protein L40



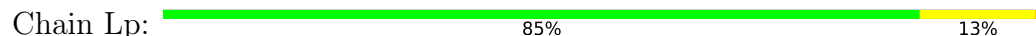
- Molecule 42: 60S ribosomal protein L41



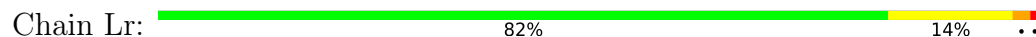
- Molecule 43: 60S ribosomal protein L36a



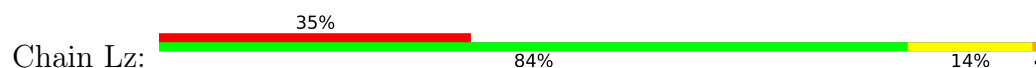
- Molecule 44: 60S ribosomal protein L37a

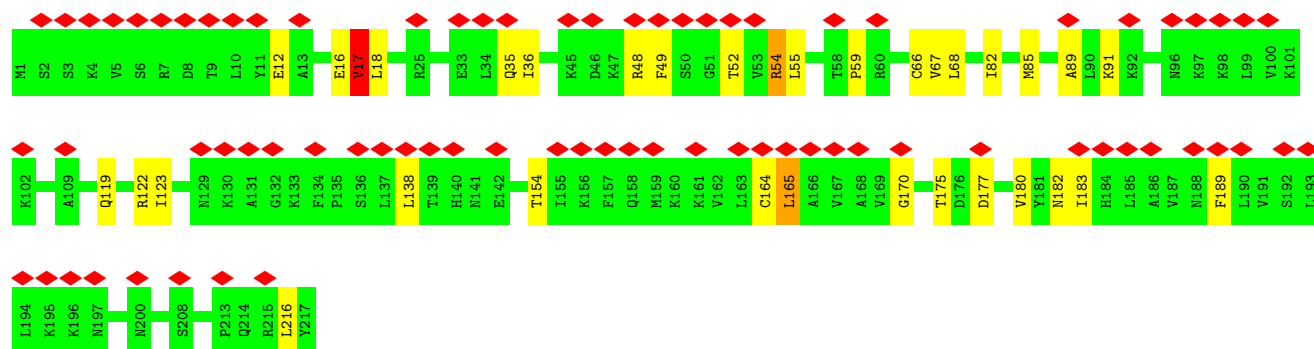


- Molecule 45: 60S ribosomal protein L28



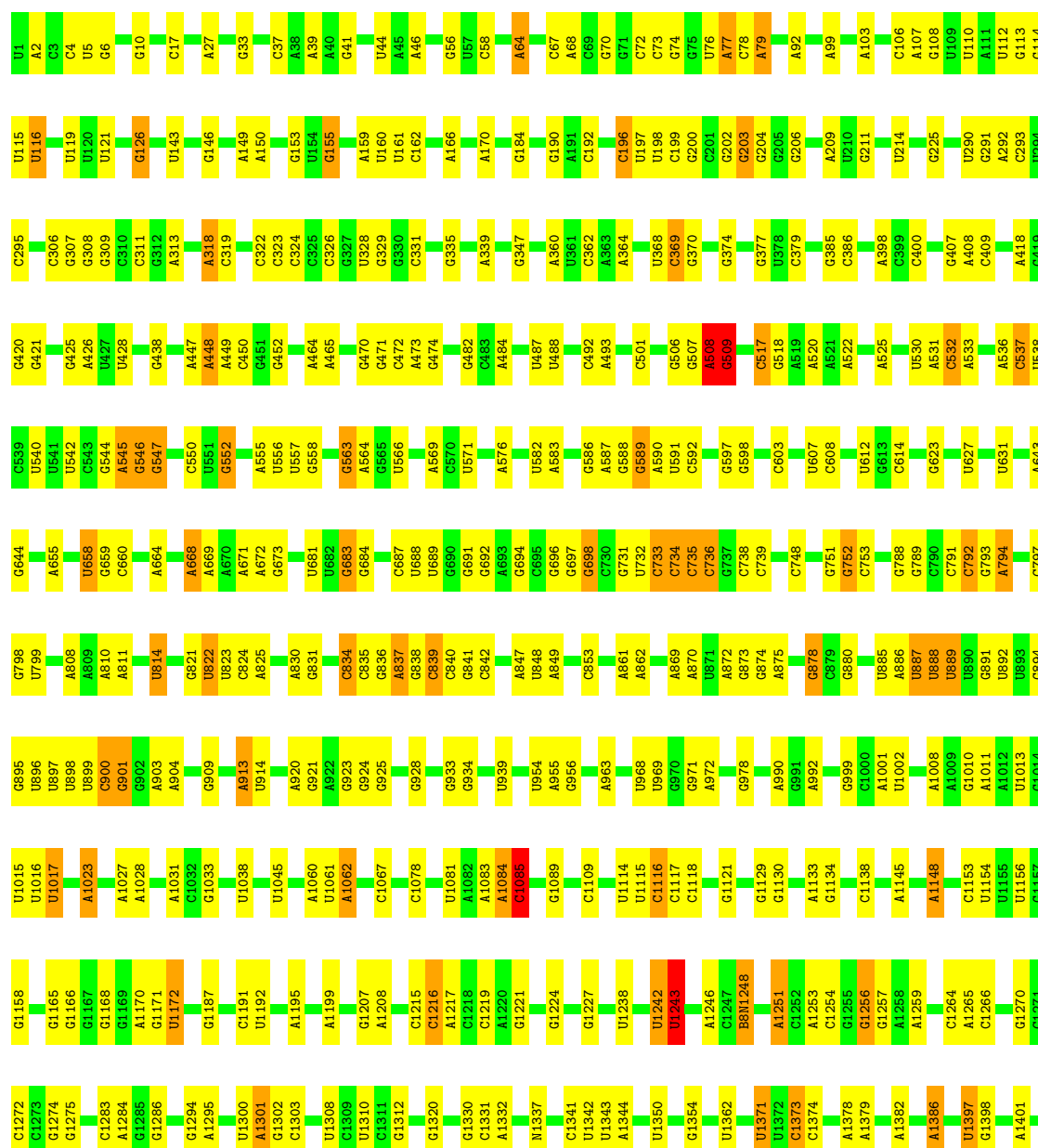
- Molecule 46: 60S ribosomal protein L10a

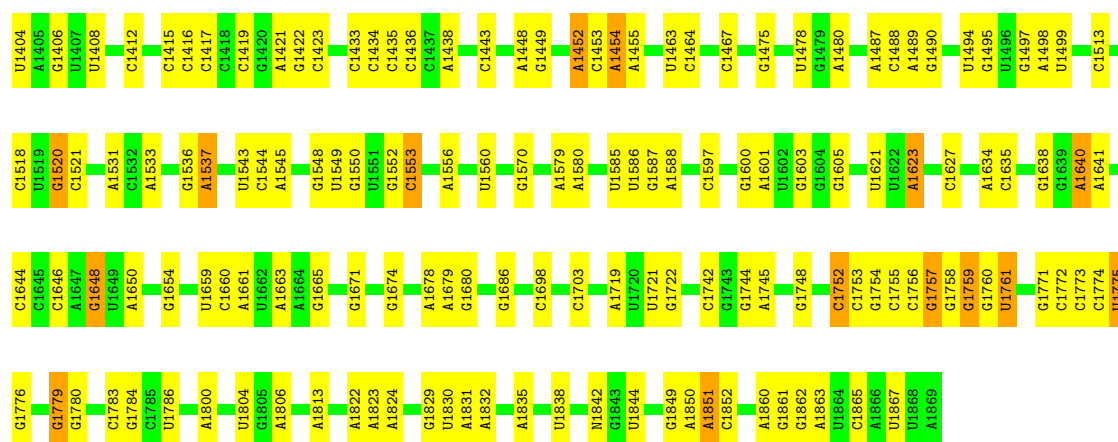




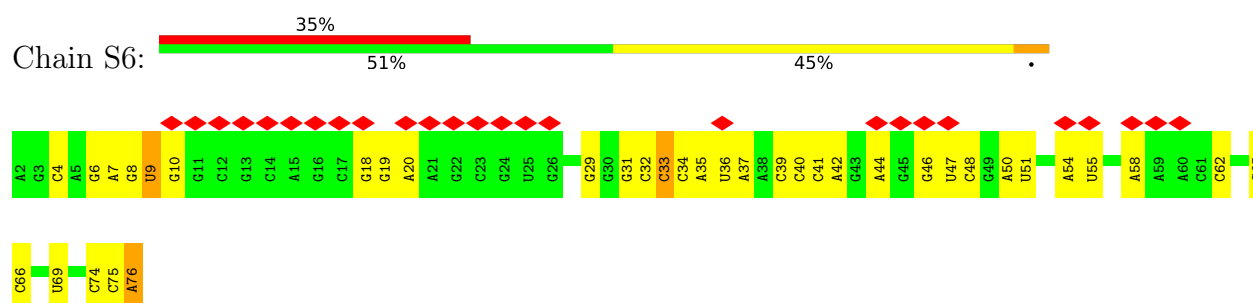
• Molecule 47: 18S rRNA (1740-MER)

Chain S2: 67% 28% .

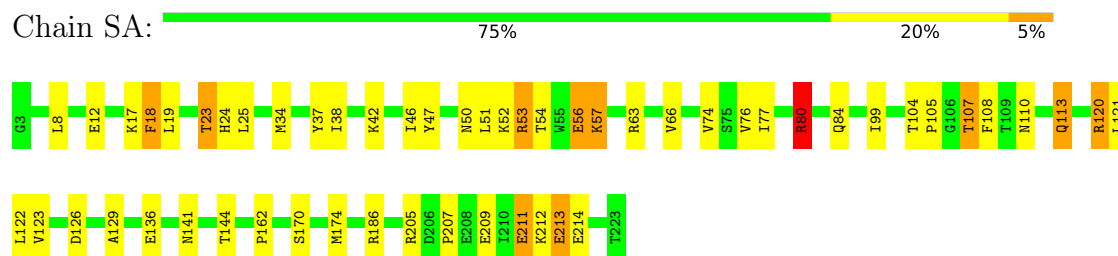




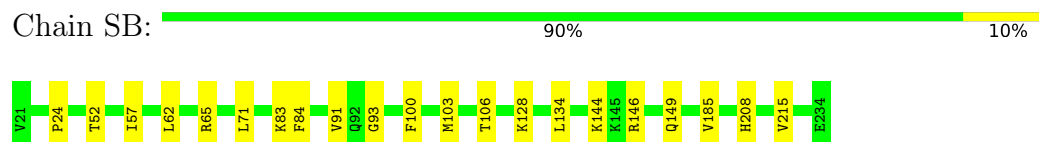
• Molecule 48: E site tRNA (75-MER)



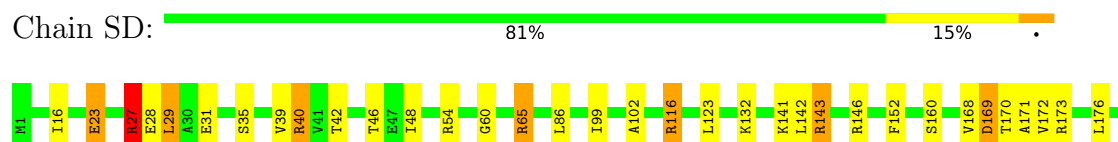
• Molecule 49: 40S ribosomal protein SA



• Molecule 50: 40S ribosomal protein S3a



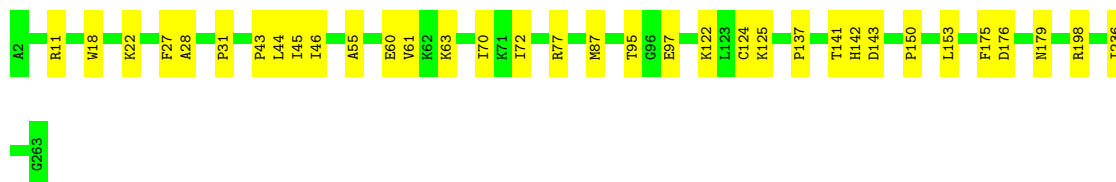
• Molecule 51: 40S ribosomal protein S3





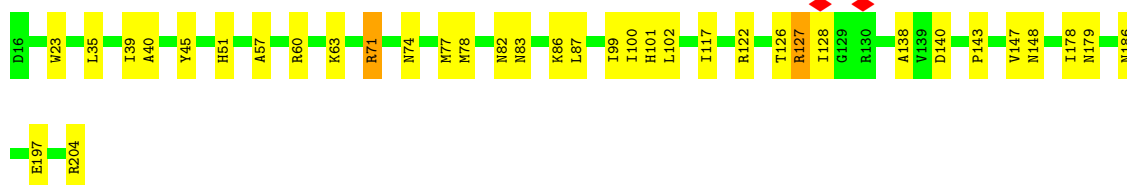
- Molecule 52: 40S ribosomal protein S4, X isoform

Chain SE: 87% 13%



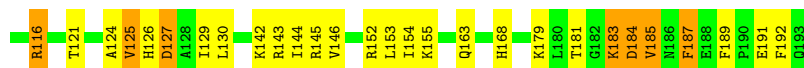
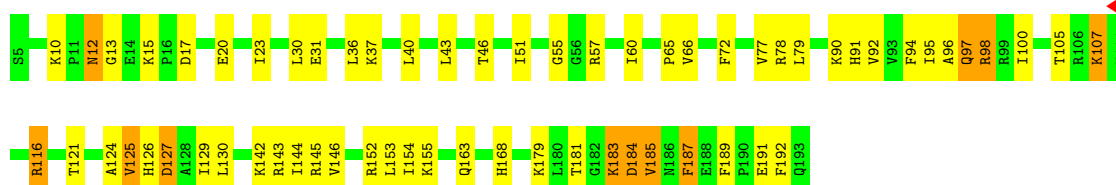
- Molecule 53: 40S ribosomal protein S5

Chain SF: 81% 18%



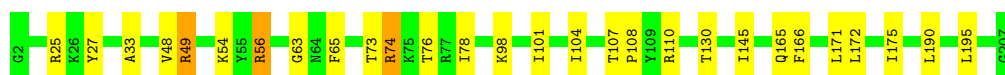
- Molecule 54: 40S ribosomal protein S7

Chain SH: 66% 28% 6%



- Molecule 55: 40S ribosomal protein S8

Chain SI: 86% 12%

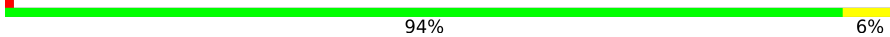


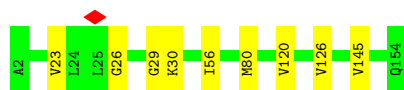
- Molecule 56: 40S ribosomal protein S10

Chain SK: 89% 10%



- Molecule 57: 40S ribosomal protein S11

Chain SL:  94% 6%



- Molecule 58: 40S ribosomal protein S15

Chain SP:  78% 20%



- Molecule 59: 40S ribosomal protein S16

Chain SQ:  81% 16%



- Molecule 60: 40S ribosomal protein S17

Chain SR:  86% 13%



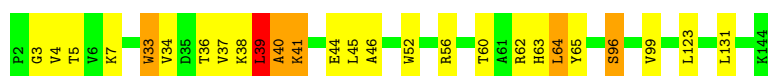
- Molecule 61: 40S ribosomal protein S18

Chain SS:  82% 14%



- Molecule 62: 40S ribosomal protein S19

Chain ST:  82% 14%



- Molecule 63: 40S ribosomal protein S20

Chain SU:  88% 10%



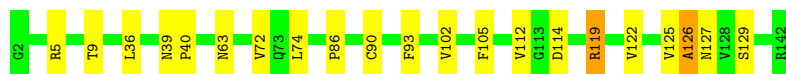
- Molecule 64: 40S ribosomal protein S21

Chain SV:  83% 13% .



- Molecule 65: 40S ribosomal protein S23

Chain SX:  85% 13% .



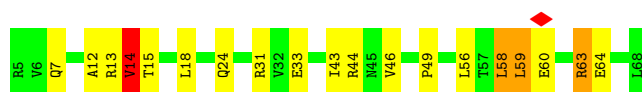
- Molecule 66: 40S ribosomal protein S26

Chain Sa:  86% 11% ..



- Molecule 67: 40S ribosomal protein S28

Chain Sc:  70% 23% 5% .



- Molecule 68: 40S ribosomal protein S29

Chain Sd:  71% 27% .



- Molecule 69: Receptor of activated protein C kinase 1

Chain Sg:  76% 24% .



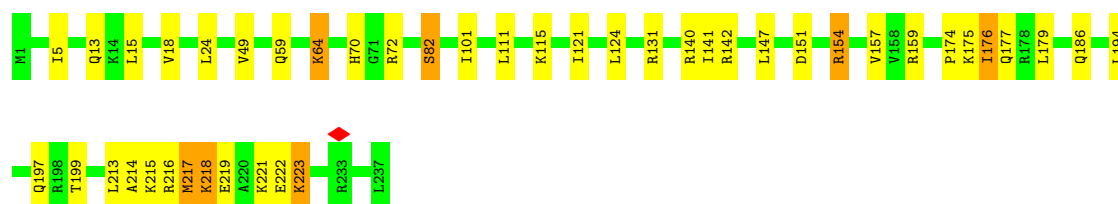
- Molecule 70: 40S ribosomal protein S2

Chain SC:  84% 14% .



- Molecule 71: 40S ribosomal protein S6

Chain SG:  81% 16% .



- Molecule 72: 40S ribosomal protein S9

Chain SJ:  87% 12% .



- Molecule 73: 40S ribosomal protein S12

Chain SM:  85% 15% .



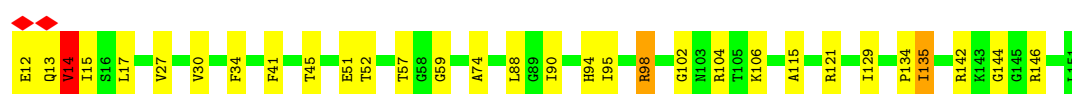
- Molecule 74: 40S ribosomal protein S13

Chain SN:  89% 9% .



- Molecule 75: 40S ribosomal protein S14

Chain SO:  78% 20% ..



- Molecule 76: 40S ribosomal protein S15a

Chain SW:  83% 17%



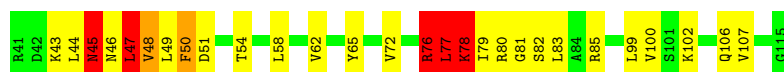
- Molecule 77: 40S ribosomal protein S24

Chain SY:  87% 13%



- Molecule 78: 40S ribosomal protein S25

Chain SZ:  63% 28% 7%



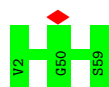
- Molecule 79: 40S ribosomal protein S27

Chain Sb:  78% 19% 3%



- Molecule 80: 40S ribosomal protein S30

Chain Se:  100%



- Molecule 81: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	544.0, 544.0, 544.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 4AC, 2MG, B8H, MLZ, PSU, HYG, M7A, 5MC, 5MU, A2M, 1MA, JMH, 6MZ, B8T, MA6, OMU, OMG, B8N, HMT, OMC, MG, 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	L5	0.27	1/87760 (0.0%)	0.40	11/136810 (0.0%)
2	L7	0.22	0/2858	0.33	1/4455 (0.0%)
3	L8	0.25	0/3679	0.39	1/5732 (0.0%)
4	LA	0.36	0/1936	0.69	2/2596 (0.1%)
5	LB	0.32	0/3306	0.69	3/4424 (0.1%)
6	LC	0.30	0/2971	0.62	3/3988 (0.1%)
7	LD	0.24	0/2428	0.57	0/3252
8	LE	0.27	0/1942	0.68	2/2606 (0.1%)
9	LF	0.28	0/1916	0.59	0/2553
10	LG	0.27	0/1971	0.62	2/2651 (0.1%)
11	LH	0.29	1/1537 (0.1%)	0.55	0/2066
12	LI	0.21	0/1751	0.52	0/2340
13	LJ	0.25	0/1433	0.66	2/1915 (0.1%)
14	LL	0.27	0/1732	0.59	1/2315 (0.0%)
15	LM	0.26	0/1161	0.56	0/1554
16	LN	0.27	0/1746	0.59	0/2338
17	LO	0.35	0/1682	0.61	2/2250 (0.1%)
18	LP	0.32	0/1268	0.56	0/1701
19	LQ	0.25	0/1537	0.59	0/2052
20	LR	0.27	0/1582	0.56	0/2091
21	LS	0.23	0/1493	0.47	0/2003
22	LT	0.31	0/1326	0.57	0/1770
23	LU	0.24	0/839	0.66	0/1126
24	LV	0.30	0/993	0.64	0/1332
25	LW	0.25	0/1030	0.61	0/1364
26	LX	0.22	0/1002	0.49	1/1345 (0.1%)
27	LY	0.23	0/1132	0.57	0/1504
28	LZ	0.20	0/1130	0.53	0/1507
29	La	0.28	0/1191	0.52	0/1591
30	Lb	0.21	0/895	0.62	2/1182 (0.2%)
31	Lc	0.28	0/774	0.58	1/1038 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.21	0/903	0.52	0/1216
33	Le	0.34	0/1071	0.61	0/1429
34	Lf	0.25	0/895	0.54	0/1198
35	Lg	0.21	0/916	0.49	0/1220
36	Lh	0.18	0/1023	0.49	0/1351
37	Li	0.18	0/843	0.50	0/1115
38	Lj	0.25	0/731	0.62	2/966 (0.2%)
39	Lk	0.19	0/575	0.49	0/761
40	Ll	0.34	0/454	0.68	1/599 (0.2%)
41	Lm	0.26	0/425	0.59	0/561
42	Ln	0.41	0/231	0.62	0/294
43	Lo	0.30	0/887	0.61	0/1170
44	Lp	0.26	0/718	0.62	1/953 (0.1%)
45	Lr	0.25	0/1017	0.56	0/1364
46	Lz	0.22	0/1769	0.63	0/2371
47	S2	0.25	0/40466	0.36	3/63037 (0.0%)
48	S6	0.15	0/1795	0.34	0/2798
49	SA	0.30	0/1778	0.64	1/2416 (0.0%)
50	SB	0.20	0/1765	0.47	0/2362
51	SD	0.26	0/1793	0.61	0/2414
52	SE	0.24	0/2118	0.53	1/2849 (0.0%)
53	SF	0.26	0/1516	0.63	1/2037 (0.0%)
54	SH	0.28	0/1519	0.69	2/2033 (0.1%)
55	SI	0.31	0/1715	0.60	0/2287
56	SK	0.22	0/851	0.56	0/1147
57	SL	0.24	0/1268	0.58	0/1696
58	SP	0.25	0/1065	0.65	2/1423 (0.1%)
59	SQ	0.28	0/1142	0.68	2/1528 (0.1%)
60	SR	0.23	0/1105	0.60	0/1484
61	SS	0.25	0/1216	0.58	1/1628 (0.1%)
62	ST	0.30	0/1131	0.62	1/1515 (0.1%)
63	SU	0.22	0/827	0.59	0/1110
64	SV	0.29	0/643	0.59	0/860
65	SX	0.27	0/1116	0.68	1/1490 (0.1%)
66	Sa	0.31	0/847	0.64	0/1135
67	Sc	0.38	0/508	0.88	1/680 (0.1%)
68	Sd	0.29	0/470	0.64	0/623
69	Sg	0.22	0/2493	0.62	2/3394 (0.1%)
70	SC	0.42	4/1773 (0.2%)	0.72	4/2395 (0.2%)
71	SG	0.25	0/1946	0.67	3/2590 (0.1%)
72	SJ	0.24	0/1561	0.63	0/2083
73	SM	0.17	0/950	0.50	0/1275
74	SN	0.22	0/1232	0.45	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.30	0/1062	0.72	2/1425 (0.1%)
76	SW	0.25	0/1051	0.56	0/1406
77	SY	0.23	0/1094	0.52	0/1452
78	SZ	0.32	0/604	0.73	1/810 (0.1%)
79	Sb	0.23	0/665	0.59	0/891
80	Se	0.20	0/465	0.51	0/612
81	Sf	0.23	0/560	0.71	0/745
All	All	0.26	6/232569 (0.0%)	0.48	66/341305 (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
4	LA	0	1
5	LB	0	4
6	LC	0	2
8	LE	0	1
9	LF	0	1
10	LG	0	2
12	LI	0	3
13	LJ	0	3
14	LL	0	2
15	LM	0	1
16	LN	0	2
19	LQ	0	2
20	LR	0	1
23	LU	0	1
24	LV	0	1
25	LW	0	1
27	LY	0	1
29	La	0	3
32	Ld	0	1
33	Le	0	1
34	Lf	0	2
36	Lh	0	2
38	Lj	0	1
39	Lk	0	1
40	Ll	0	1
41	Lm	0	1
43	Lo	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	Lp	0	1
45	Lr	0	5
46	Lz	0	2
49	SA	0	4
51	SD	0	6
53	SF	0	5
54	SH	0	1
55	SI	0	3
56	SK	0	1
58	SP	0	2
59	SQ	0	2
60	SR	0	2
61	SS	0	1
62	ST	0	1
63	SU	0	1
65	SX	0	5
66	Sa	0	1
69	Sg	0	1
70	SC	0	3
72	SJ	0	3
74	SN	0	1
75	SO	0	1
77	SY	0	1
All	All	0	97

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	SC	200[A]	ARG	C-O	7.48	1.32	1.24
70	SC	200[B]	ARG	C-O	7.48	1.32	1.24
70	SC	200[A]	ARG	CA-C	5.70	1.60	1.52
70	SC	200[B]	ARG	CA-C	5.70	1.60	1.52
11	LH	173	ARG	N-CA	5.31	1.52	1.46
1	L5	3785	A2M	O3'-P	5.03	1.61	1.56

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3884	U	C3'-C2'-O2'	14.04	131.77	110.70
47	S2	508	A	C1'-C2'-O2'	11.78	126.07	108.40
1	L5	504	G	C2'-C3'-O3'	10.24	124.86	109.50
1	L5	914	U	C2'-C3'-O3'	9.79	124.19	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2416	G	C2'-C3'-O3'	9.50	123.75	109.50
47	S2	1085	C	C1'-C2'-O2'	-8.45	99.13	111.80
5	LB	16	PHE	CA-C-N	-8.20	113.00	122.52
5	LB	16	PHE	C-N-CA	-8.20	113.00	122.52
44	Lp	90	LYS	N-CA-C	-8.12	102.51	111.36
71	SG	214	ALA	N-CA-C	-7.96	103.16	113.12
71	SG	219	GLU	N-CA-C	-7.87	102.69	111.82
70	SC	200[A]	ARG	N-CA-C	7.84	121.72	109.96
70	SC	200[B]	ARG	N-CA-C	7.84	121.72	109.96
8	LE	127	SER	N-CA-C	7.62	122.65	113.12
75	SO	14	VAL	CA-C-N	7.60	135.38	121.70
75	SO	14	VAL	C-N-CA	7.60	135.38	121.70
62	ST	39	LEU	N-CA-C	7.29	121.72	111.52
70	SC	200[A]	ARG	CA-C-O	7.13	128.85	120.58
70	SC	200[B]	ARG	CA-C-O	7.13	128.85	120.58
67	Sc	14	VAL	N-CA-C	7.06	118.06	107.75
53	SF	147	VAL	N-CA-C	-6.88	106.08	112.96
38	Lj	21	ARG	CA-C-N	6.52	133.99	121.54
38	Lj	21	ARG	C-N-CA	6.52	133.99	121.54
5	LB	389	MET	N-CA-C	-6.45	100.11	109.59
78	SZ	47	LEU	N-CA-C	6.39	124.41	110.80
17	LO	79	ILE	N-CA-C	-6.27	104.17	111.00
1	L5	2084	C	C4'-C3'-O3'	6.26	118.80	109.40
2	L7	109	U	C4'-C3'-O3'	-6.25	103.63	113.00
4	LA	238	ILE	N-CA-C	6.24	116.49	108.12
8	LE	183	ARG	N-CA-C	6.20	120.16	112.47
40	LI	42	ARG	N-CA-C	6.12	119.38	109.40
49	SA	23	THR	N-CA-C	6.07	123.73	110.80
69	Sg	143	GLN	CA-C-N	5.90	132.81	121.54
69	Sg	143	GLN	C-N-CA	5.90	132.81	121.54
31	Lc	81	LEU	N-CA-C	-5.88	104.86	112.68
1	L5	2280	G	C4'-C3'-O3'	-5.82	104.27	113.00
1	L5	2019	C	O4'-C1'-C2'	-5.81	101.79	107.60
4	LA	196	TRP	N-CA-C	5.78	122.58	109.81
6	LC	142	HIS	N-CA-C	5.71	119.94	112.92
71	SG	215	LYS	N-CA-C	-5.55	104.92	110.97
65	SX	74	LEU	N-CA-C	5.53	118.25	110.23
6	LC	183	VAL	N-CA-C	-5.43	105.56	110.82
58	SP	127	LYS	CA-C-N	5.41	131.88	121.54
58	SP	127	LYS	C-N-CA	5.41	131.88	121.54
59	SQ	16	LYS	CA-C-N	5.38	131.82	121.54
59	SQ	16	LYS	C-N-CA	5.38	131.82	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	LJ	170	TYR	CA-C-N	5.38	131.81	121.54
13	LJ	170	TYR	C-N-CA	5.38	131.81	121.54
6	LC	223	ASN	N-CA-C	5.36	118.61	111.75
3	L8	7	U	C1'-C2'-O2'	-5.35	100.37	108.40
14	LL	62	PRO	CA-C-O	-5.33	117.27	121.38
1	L5	2019	C	C2'-C3'-O3'	5.33	121.69	113.70
30	Lb	10	HIS	CA-C-N	5.32	131.71	121.54
30	Lb	10	HIS	C-N-CA	5.32	131.71	121.54
26	LX	134	LYS	N-CA-C	5.29	117.36	108.73
54	SH	65	PRO	CA-C-N	5.27	123.56	120.24
54	SH	65	PRO	C-N-CA	5.27	123.56	120.24
1	L5	408	A	C4'-C3'-O3'	-5.21	105.19	113.00
52	SE	27	PHE	N-CA-C	5.16	118.48	110.17
1	L5	2760	G	P-O3'-C3'	5.14	127.91	120.20
17	LO	202	LEU	N-CA-C	5.11	117.41	111.02
47	S2	501	C	C2-N1-C1'	5.08	134.03	118.80
1	L5	3966	A	O4'-C4'-C3'	-5.07	98.93	104.00
10	LG	129	PRO	CA-C-N	5.07	131.22	121.54
10	LG	129	PRO	C-N-CA	5.07	131.22	121.54
61	SS	84	LEU	N-CA-C	5.03	116.42	110.19

There are no chirality outliers.

All (97) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	30	ARG	Sidechain
5	LB	17	LEU	Peptide
5	LB	174	ARG	Sidechain
5	LB	19	ARG	Sidechain
5	LB	258	HIS	Peptide
6	LC	188	ARG	Sidechain
6	LC	2	ALA	Peptide
8	LE	138	ARG	Sidechain
9	LF	73	ARG	Sidechain
10	LG	35	ARG	Sidechain
10	LG	73	ARG	Sidechain
12	LI	14	ASN	Peptide
12	LI	153	ARG	Sidechain
12	LI	154	ARG	Sidechain
13	LJ	147	ARG	Sidechain
13	LJ	175	LEU	Peptide
13	LJ	35	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	LL	190	ARG	Sidechain
14	LL	74	ARG	Sidechain
15	LM	109	ARG	Sidechain
16	LN	124	ASP	Peptide
16	LN	41	ARG	Sidechain
19	LQ	143	ARG	Sidechain
19	LQ	15	ARG	Sidechain
20	LR	172	ARG	Sidechain
23	LU	101	ARG	Sidechain
24	LV	83	ARG	Sidechain
25	LW	80	ARG	Sidechain
27	LY	27	ARG	Sidechain
29	La	22	ILE	Peptide
29	La	26	ARG	Sidechain
29	La	9	ARG	Sidechain
32	Ld	30	HIS	Peptide
33	Le	48	ARG	Sidechain
34	Lf	103	VAL	Peptide
34	Lf	106	TYR	Peptide
36	Lh	7	ARG	Sidechain
36	Lh	86	LYS	Peptide
38	Lj	39	TYR	Peptide
39	Lk	17	ARG	Sidechain
40	Ll	21	ARG	Sidechain
41	Lm	111	ARG	Sidechain
43	Lo	57	ARG	Sidechain
43	Lo	81	ARG	Sidechain
44	Lp	85	ARG	Sidechain
45	Lr	103	ARG	Sidechain
45	Lr	66	ARG	Sidechain
45	Lr	67	ARG	Sidechain
45	Lr	79	ARG	Sidechain
45	Lr	87	ARG	Sidechain
46	Lz	17	VAL	Peptide
46	Lz	54	ARG	Sidechain
49	SA	120	ARG	Sidechain
49	SA	186	ARG	Sidechain
49	SA	53	ARG	Sidechain
49	SA	80	ARG	Sidechain
70	SC	200[A]	ARG	Sidechain
70	SC	200[B]	ARG	Sidechain
70	SC	76	LYS	Peptide

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Mol	Chain	Res	Type	Group
51	SD	142	LEU	Peptide
51	SD	143	ARG	Sidechain
51	SD	27	ARG	Sidechain
51	SD	40	ARG	Sidechain
51	SD	54	ARG	Sidechain
51	SD	65	ARG	Sidechain
53	SF	126	THR	Peptide
53	SF	127	ARG	Peptide
53	SF	39	ILE	Peptide
53	SF	71	ARG	Sidechain
53	SF	78	MET	Peptide
54	SH	15	LYS	Peptide
55	SI	130	THR	Peptide
55	SI	49	ARG	Sidechain
55	SI	56	ARG	Sidechain
72	SJ	2	PRO	Peptide
72	SJ	65	GLU	Peptide
72	SJ	70	ARG	Sidechain
56	SK	65	ARG	Sidechain
74	SN	99	ARG	Sidechain
75	SO	104	ARG	Sidechain
58	SP	127	LYS	Peptide
58	SP	18	ARG	Sidechain
59	SQ	37	ARG	Sidechain
59	SQ	43	GLU	Peptide
60	SR	47	ARG	Sidechain
60	SR	67	ARG	Sidechain
61	SS	55	ARG	Sidechain
62	ST	46	ALA	Peptide
63	SU	66	ARG	Sidechain
65	SX	119	ARG	Sidechain
65	SX	125	VAL	Peptide
65	SX	126	ALA	Peptide
65	SX	5	ARG	Sidechain
65	SX	86	PRO	Peptide
77	SY	94	HIS	Peptide
66	Sa	6	ARG	Sidechain
69	Sg	60	ARG	Sidechain

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	L5	80201	0	40426	436	0
2	L7	2558	0	1296	11	0
3	L8	3315	0	1685	23	0
4	LA	1898	0	1993	30	0
5	LB	3238	0	3376	60	0
6	LC	2928	0	3105	33	0
7	LD	2382	0	2410	45	0
8	LE	1904	0	2055	35	0
9	LF	1878	0	2009	29	0
10	LG	1935	0	2087	26	0
11	LH	1518	0	1601	26	0
12	LI	1711	0	1749	22	0
13	LJ	1410	0	1441	27	0
14	LL	1701	0	1818	19	0
15	LM	1138	0	1204	11	0
16	LN	1701	0	1749	24	0
17	LO	1650	0	1794	28	0
18	LP	1242	0	1269	32	0
19	LQ	1513	0	1628	14	0
20	LR	1566	0	1729	13	0
21	LS	1453	0	1490	12	0
22	LT	1298	0	1366	17	0
23	LU	825	0	850	12	0
24	LV	979	0	1039	19	0
25	LW	1015	0	1079	13	0
26	LX	985	0	1066	8	0
27	LY	1115	0	1205	15	0
28	LZ	1107	0	1182	13	0
29	La	1162	0	1213	15	0
30	Lb	882	0	962	5	0
31	Lc	764	0	804	20	0
32	Ld	888	0	930	7	0
33	Le	1053	0	1147	18	0
34	Lf	876	0	912	9	0
35	Lg	906	0	1002	2	0
36	Lh	1015	0	1148	10	0
37	Li	832	0	917	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lj	713	0	751	8	0
39	Lk	569	0	637	6	0
40	Ll	444	0	483	5	0
41	Lm	430	0	466	8	0
42	Ln	230	0	276	7	0
43	Lo	870	0	945	15	0
44	Lp	708	0	756	17	0
45	Lr	1002	0	1068	16	0
46	Lz	1741	0	1854	17	0
47	S2	36938	0	18623	172	0
48	S6	1604	0	816	13	0
49	SA	1741	0	1746	43	0
50	SB	1738	0	1809	14	0
51	SD	1765	0	1865	42	0
52	SE	2076	0	2177	19	0
53	SF	1495	0	1549	35	0
54	SH	1497	0	1590	52	0
55	SI	1686	0	1772	18	0
56	SK	827	0	854	7	0
57	SL	1247	0	1323	5	0
58	SP	1045	0	1095	20	0
59	SQ	1124	0	1193	20	0
60	SR	1090	0	1149	13	0
61	SS	1198	0	1261	22	0
62	ST	1112	0	1146	23	0
63	SU	817	0	882	10	0
64	SV	636	0	637	15	0
65	SX	1098	0	1167	7	0
66	Sa	829	0	883	13	0
67	Sc	506	0	536	26	0
68	Sd	459	0	448	14	0
69	Sg	2436	0	2393	50	0
70	SC	1733	0	1826	22	0
71	SG	1923	0	2089	28	0
72	SJ	1533	0	1653	20	0
73	SM	940	0	965	10	0
74	SN	1208	0	1294	12	0
75	SO	1049	0	1073	22	0
76	SW	1034	0	1080	15	0
77	SY	1073	0	1155	12	0
78	SZ	598	0	656	40	0
79	Sb	651	0	672	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Se	459	0	503	0	0
81	Sf	548	0	551	3	0
82	L5	279	0	0	0	0
82	L7	3	0	0	0	0
82	L8	6	0	0	0	0
82	LA	1	0	0	0	0
82	LI	1	0	0	0	0
82	LN	1	0	0	0	0
82	LP	1	0	0	0	0
82	LS	1	0	0	0	0
82	LV	1	0	0	0	0
82	Le	2	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	140	0	0	0	0
82	SF	1	0	0	0	0
83	L5	39	0	39	4	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sd	1	0	0	0	0
84	Sf	1	0	0	0	0
85	S2	36	0	37	0	0
86	L5	11	0	0	0	0
86	LA	1	0	0	0	0
86	LB	1	0	0	0	0
86	LC	1	0	0	0	0
86	LF	1	0	0	0	0
86	LG	1	0	0	0	0
86	LH	1	0	0	0	0
86	LI	1	0	0	0	0
86	LY	1	0	0	0	0
86	La	2	0	0	0	0
86	Lb	1	0	0	0	0
86	Lf	1	0	0	0	0
86	Lm	1	0	0	0	0
86	S2	12	0	0	0	0
86	SC	1	0	0	0	0
86	SF	1	0	0	0	0
86	SG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	SL	1	0	0	0	0
86	SN	1	0	0	0	0
86	SR	1	0	0	0	0
86	SS	1	0	0	0	0
86	SV	1	0	0	0	0
All	All	219527	0	162479	1793	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 5.

All (1793) 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)
11:LH:115:ARG:NH1	11:LH:123:ILE:HG12	1.47	1.30
31:Lc:20:LEU:CD1	31:Lc:101:ASP:HB3	1.71	1.20
1:L5:3946:G:O2'	1:L5:3947:A:H5''	1.42	1.19
31:Lc:20:LEU:HD12	31:Lc:101:ASP:CB	1.72	1.17
67:Sc:44:ARG:NH2	67:Sc:63:ARG:HB2	1.62	1.12
53:SF:51:HIS:O	59:SQ:50:LYS:HE2	1.53	1.09
54:SH:185:VAL:CG2	54:SH:187:PHE:HE1	1.68	1.06
67:Sc:44:ARG:HH12	67:Sc:63:ARG:HG3	1.15	1.05
54:SH:185:VAL:CG2	54:SH:187:PHE:CE1	2.42	1.02
31:Lc:22:MET:HE2	31:Lc:85:CYS:HB2	1.38	1.02
54:SH:185:VAL:HG21	54:SH:187:PHE:CE1	1.95	1.02
10:LG:35:ARG:HH22	28:LZ:52:LYS:HD2	1.25	1.01
67:Sc:44:ARG:HH22	67:Sc:63:ARG:HB2	0.87	1.01
54:SH:98:ARG:HG3	54:SH:125:VAL:HG22	1.42	1.00
31:Lc:20:LEU:HD12	31:Lc:101:ASP:HB3	1.36	0.99
31:Lc:20:LEU:HD12	31:Lc:101:ASP:HB2	1.41	0.99
31:Lc:20:LEU:HD13	31:Lc:101:ASP:HB3	1.46	0.98
45:Lr:30:ASN:HD22	45:Lr:30:ASN:H	1.00	0.97
61:SS:98:VAL:HG23	61:SS:103:LEU:HB2	1.47	0.96
1:L5:3946:G:O2'	1:L5:3947:A:C5'	2.13	0.96
5:LB:160:ILE:HD11	5:LB:193:LYS:HG3	1.48	0.96
62:ST:38:LYS:HE2	62:ST:44:GLU:HA	1.47	0.96
49:SA:209:GLU:O	49:SA:213:GLU:HB2	1.66	0.95
51:SD:99:ILE:HG23	51:SD:173:ARG:NH2	1.82	0.95
11:LH:115:ARG:HH11	11:LH:123:ILE:HG12	1.31	0.95
1:L5:1968:G:H5''	1:L5:1968:G:H8	1.31	0.94
55:SI:74:ARG:HG2	55:SI:74:ARG:HH11	1.31	0.93
9:LF:200:ARG:HG2	9:LF:200:ARG:HH11	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LG:134:PRO:HB3	10:LG:206:GLN:HG2	1.50	0.93
44:Lp:85:ARG:HH22	47:S2:939:U:H4'	1.33	0.92
11:LH:115:ARG:HH12	11:LH:123:ILE:HG12	1.28	0.92
1:L5:3946:G:O2'	1:L5:3947:A:N3	2.03	0.91
7:LD:195:HIS:CE1	7:LD:199:ILE:HD11	2.05	0.91
34:Lf:65:ASN:OD1	34:Lf:67:THR:HG23	1.69	0.90
1:L5:1175:A:H5''	7:LD:268:ARG:HH21	1.36	0.90
44:Lp:85:ARG:NH2	47:S2:939:U:H4'	1.87	0.89
1:L5:1252:C:H6	1:L5:1252:C:H5''	1.36	0.88
49:SA:50:ASN:HB3	49:SA:53:ARG:HG3	1.54	0.88
30:Lb:12:GLN:NE2	30:Lb:15:LYS:HD3	1.89	0.88
47:S2:1641:A:H5''	47:S2:1641:A:H8	1.38	0.88
8:LE:128:HIS:ND1	8:LE:128:HIS:O	2.08	0.87
54:SH:10:LYS:HE3	54:SH:17:ASP:OD1	1.73	0.87
26:LX:100:VAL:CG2	26:LX:134:LYS:HG2	2.05	0.87
75:SO:98:ARG:HD3	75:SO:98:ARG:C	2.00	0.86
24:LV:83:ARG:HG3	24:LV:102:ALA:HB3	1.56	0.86
78:SZ:43:LYS:HB3	78:SZ:45:ASN:HD21	1.40	0.85
45:Lr:30:ASN:HD22	45:Lr:30:ASN:N	1.74	0.85
26:LX:100:VAL:HG23	26:LX:134:LYS:HG2	1.58	0.85
49:SA:207:PRO:O	49:SA:211:GLU:HG3	1.76	0.85
1:L5:1767:A:H2'	1:L5:1769:G:H5'	1.56	0.85
12:LI:56:GLU:OE1	12:LI:161:GLY:CA	2.25	0.85
67:Sc:44:ARG:HH22	67:Sc:63:ARG:CB	1.83	0.85
12:LI:56:GLU:OE1	12:LI:161:GLY:HA3	1.76	0.84
1:L5:2906:G:H2'	1:L5:2908:U:H1'	1.57	0.84
48:S6:33:C:C5	48:S6:35:A:H5''	2.13	0.84
51:SD:172:VAL:O	51:SD:173:ARG:HD3	1.77	0.83
7:LD:23:ARG:HD2	7:LD:23:ARG:O	1.78	0.83
48:S6:76:A:H8	48:S6:76:A:H5'	1.44	0.83
51:SD:146:ARG:HB3	51:SD:146:ARG:NH1	1.93	0.83
78:SZ:48:VAL:HA	78:SZ:83:LEU:HD11	1.57	0.83
75:SO:98:ARG:HG2	75:SO:98:ARG:HH11	1.43	0.83
47:S2:1755:C:C5	47:S2:1757:G:O6	2.32	0.83
49:SA:120:ARG:HD2	70:SC:266:TYR:HB3	1.59	0.82
54:SH:185:VAL:HG23	54:SH:187:PHE:CE1	2.13	0.82
10:LG:134:PRO:HB3	10:LG:206:GLN:CG	2.09	0.82
31:Lc:22:MET:CE	31:Lc:85:CYS:HB2	2.10	0.82
1:L5:4212:A:N1	22:LT:3:ASN:ND2	2.29	0.81
70:SC:74:LYS:HD2	70:SC:269:PHE:CD1	2.16	0.81
75:SO:98:ARG:HD3	75:SO:98:ARG:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Sc:44:ARG:HH12	67:Sc:63:ARG:CG	1.93	0.81
51:SD:99:ILE:HG23	51:SD:173:ARG:HH22	1.40	0.80
49:SA:56:GLU:OE1	64:SV:79:VAL:HB	1.82	0.80
13:LJ:120:ASP:HB3	13:LJ:121:PRO:HD2	1.63	0.80
11:LH:124:ARG:HG2	11:LH:124:ARG:HH11	1.47	0.79
49:SA:50:ASN:HB3	49:SA:53:ARG:CG	2.11	0.79
61:SS:86:ARG:HG3	61:SS:106:LYS:HD2	1.63	0.79
48:S6:76:A:H5'	48:S6:76:A:C8	2.16	0.79
45:Lr:30:ASN:H	45:Lr:30:ASN:ND2	1.77	0.79
47:S2:1755:C:H5	47:S2:1757:G:O6	1.66	0.78
6:LC:339:THR:O	6:LC:343:GLN:HG3	1.84	0.78
5:LB:170:LEU:HB3	5:LB:328:ASN:HD21	1.45	0.78
49:SA:110:ASN:OD1	49:SA:113:GLN:HG2	1.83	0.78
28:LZ:7:PRO:HD3	28:LZ:28:ASN:ND2	1.98	0.78
71:SG:217:MET:O	71:SG:217:MET:HE3	1.84	0.78
16:LN:174:LEU:HD12	16:LN:174:LEU:O	1.84	0.77
47:S2:1641:A:H5''	47:S2:1641:A:C8	2.19	0.77
1:L5:1178:G:H2'	1:L5:1178:G:N3	1.98	0.77
1:L5:1968:G:H5''	1:L5:1968:G:C8	2.19	0.77
5:LB:44:THR:HG21	5:LB:186:ASN:ND2	1.99	0.77
1:L5:1940:G:H22	1:L5:4434:C:H5''	1.50	0.76
13:LJ:120:ASP:HB2	13:LJ:123:ILE:HB	1.68	0.76
78:SZ:43:LYS:HE3	78:SZ:45:ASN:ND2	2.00	0.76
1:L5:182:G:N2	1:L5:255:C:HO2'	1.84	0.76
1:L5:3596:A:OP1	1:L5:3596:A:H3'	1.84	0.76
51:SD:29:LEU:N	51:SD:29:LEU:HD23	2.01	0.76
54:SH:181:THR:CG2	54:SH:183:LYS:HG3	2.16	0.76
51:SD:172:VAL:C	51:SD:173:ARG:HD3	2.12	0.75
67:Sc:44:ARG:NH1	67:Sc:63:ARG:HG3	1.99	0.75
78:SZ:65:TYR:CZ	78:SZ:76:ARG:NH1	2.54	0.75
62:ST:33:TRP:O	62:ST:37:VAL:HG13	1.86	0.75
4:LA:180:LEU:HD22	44:Lp:18:TYR:HB3	1.69	0.75
1:L5:1968:G:H8	1:L5:1968:G:C5'	2.00	0.75
55:SI:74:ARG:HG2	55:SI:74:ARG:NH1	2.02	0.74
1:L5:3946:G:H1'	1:L5:3947:A:C2	2.21	0.74
44:Lp:64:VAL:HG11	44:Lp:71:TYR:CE1	2.22	0.74
7:LD:289:ARG:HG2	7:LD:289:ARG:HH11	1.52	0.74
7:LD:289:ARG:HG2	7:LD:289:ARG:NH1	2.03	0.74
17:LO:201:LEU:HD12	17:LO:201:LEU:N	2.02	0.74
56:SK:65:ARG:HD3	68:Sd:25:SER:HB2	1.69	0.73
1:L5:3946:G:H1'	1:L5:3947:A:N1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:315:ASN:HD21	5:LB:326:VAL:H	1.36	0.73
17:LO:47:PHE:CE1	17:LO:140:ARG:HG2	2.23	0.73
39:Lk:3:ARG:HB2	39:Lk:43:TYR:HD1	1.53	0.73
47:S2:1373:C:O2'	60:SR:10:LYS:HE3	1.89	0.73
60:SR:89:SER:HB3	60:SR:92:ASP:OD2	1.89	0.73
69:Sg:14:HIS:CD2	69:Sg:41:ILE:HG13	2.22	0.73
51:SD:27:ARG:HG2	51:SD:27:ARG:HH11	1.52	0.73
69:Sg:14:HIS:HD2	69:Sg:41:ILE:CG1	2.01	0.73
69:Sg:62:HIS:CE1	69:Sg:88:ARG:HG3	2.22	0.73
8:LE:114:ARG:HB3	45:Lr:87:ARG:HH12	1.54	0.73
28:LZ:7:PRO:HD3	28:LZ:28:ASN:HD21	1.54	0.73
41:Lm:111:ARG:HH21	41:Lm:111:ARG:HB3	1.54	0.73
18:LP:117:ILE:HD12	18:LP:148:MET:HE2	1.70	0.72
42:Ln:10:MET:SD	47:S2:1172:U:H5''	2.29	0.72
1:L5:1762:C:H3'	1:L5:1763:C:H6	1.54	0.72
1:L5:3946:G:C2'	1:L5:3947:A:H5''	2.19	0.72
9:LF:200:ARG:HG2	9:LF:200:ARG:NH1	2.00	0.72
53:SF:71:ARG:HH12	53:SF:148:ASN:ND2	1.87	0.72
69:Sg:241:PHE:CE1	69:Sg:248:LEU:HD12	2.24	0.72
75:SO:98:ARG:HG2	75:SO:98:ARG:NH1	2.02	0.71
1:L5:169:G:N2	1:L5:171:U:H3	1.87	0.71
6:LC:189:MET:HE2	6:LC:195:LYS:HD3	1.72	0.71
1:L5:1254:A:H2'	1:L5:1254:A:N3	2.05	0.71
44:Lp:85:ARG:HH22	47:S2:939:U:C4'	2.03	0.71
64:SV:70:LEU:HD21	64:SV:83:PHE:CZ	2.25	0.71
67:Sc:7:GLN:HB3	67:Sc:60:GLU:HA	1.71	0.71
1:L5:3946:G:O2'	1:L5:3947:A:C2	2.41	0.71
47:S2:1397:U:H6	47:S2:1397:U:H5'	1.55	0.71
1:L5:1970:A:H5''	1:L5:1970:A:H8	1.55	0.71
31:Lc:18:LEU:HD12	31:Lc:18:LEU:O	1.91	0.70
59:SQ:37:ARG:HD2	62:ST:7:LYS:HD2	1.71	0.70
54:SH:181:THR:HG21	54:SH:183:LYS:HG3	1.73	0.70
62:ST:33:TRP:CE3	62:ST:37:VAL:HG11	2.27	0.70
76:SW:3:ARG:HH22	76:SW:28:ARG:HH21	1.37	0.70
55:SI:172:LEU:HD11	55:SI:195:LEU:CD1	2.22	0.70
13:LJ:24:ILE:HG13	13:LJ:128:LEU:HB3	1.74	0.70
47:S2:1553:C:N4	68:Sd:22:ARG:HH21	1.89	0.70
48:S6:75:C:H2'	48:S6:76:A:H4'	1.73	0.70
7:LD:22:ARG:HB3	7:LD:28:THR:HG23	1.73	0.70
75:SO:106:LYS:HD2	75:SO:135:ILE:CD1	2.22	0.70
10:LG:35:ARG:NH2	28:LZ:52:LYS:HD2	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L8:127:U:H3'	3:L8:127:U:H6	1.55	0.69
47:S2:925:G:H1	47:S2:1017:U:H3	1.36	0.69
5:LB:160:ILE:CD1	5:LB:193:LYS:HG3	2.21	0.69
1:L5:1767:A:H62	58:SP:10:ARG:HH11	1.38	0.69
78:SZ:76:ARG:HG2	78:SZ:76:ARG:HH11	1.57	0.69
78:SZ:79:ILE:HG23	78:SZ:83:LEU:HB2	1.73	0.69
78:SZ:43:LYS:HE3	78:SZ:45:ASN:HD21	1.56	0.69
78:SZ:76:ARG:NH1	78:SZ:76:ARG:HG2	2.06	0.69
78:SZ:77:LEU:HD12	78:SZ:79:ILE:CD1	2.23	0.69
10:LG:134:PRO:CB	10:LG:206:GLN:HG2	2.23	0.68
61:SS:98:VAL:CG2	61:SS:103:LEU:HB2	2.22	0.68
72:SJ:120:ALA:HB1	72:SJ:125:HIS:HD2	1.58	0.68
51:SD:116:ARG:CG	51:SD:116:ARG:HH11	2.07	0.68
67:Sc:44:ARG:NH2	67:Sc:63:ARG:CB	2.50	0.68
71:SG:213:LEU:HG	71:SG:213:LEU:O	1.92	0.68
41:Lm:111:ARG:HH21	41:Lm:111:ARG:CB	2.06	0.68
1:L5:1252:C:H6	1:L5:1252:C:C5'	2.07	0.68
1:L5:2362:U:H2'	1:L5:2363:A2M:H8	1.75	0.68
15:LM:70:GLN:HE21	15:LM:74:ARG:NH2	1.92	0.68
59:SQ:37:ARG:HH11	59:SQ:37:ARG:CG	2.07	0.68
51:SD:146:ARG:HB3	51:SD:146:ARG:CZ	2.24	0.68
64:SV:53:TYR:CD1	64:SV:72:LEU:HD23	2.29	0.67
75:SO:102:GLY:N	75:SO:134:PRO:O	2.22	0.67
1:L5:3946:G:C2'	1:L5:3947:A:C5'	2.71	0.67
40:Ll:51:LEU:HD12	40:Ll:51:LEU:C	2.20	0.67
61:SS:25:LYS:HG3	61:SS:55:ARG:NH2	2.09	0.67
1:L5:2096:G:H2'	1:L5:2096:G:N3	2.08	0.67
8:LE:99:ASP:OD1	8:LE:99:ASP:N	2.27	0.67
1:L5:166:C:O5'	1:L5:166:C:H6	1.78	0.67
8:LE:119:GLU:HG3	33:Le:7:LEU:HG	1.77	0.67
78:SZ:77:LEU:HD12	78:SZ:79:ILE:HD13	1.74	0.67
10:LG:136:LEU:HD22	10:LG:202:VAL:HG13	1.77	0.67
49:SA:66:VAL:HG12	64:SV:46:PHE:CD2	2.29	0.66
1:L5:1930:U:OP2	17:LO:49:ARG:HG3	1.95	0.66
43:Lo:2:VAL:N	43:Lo:88:CYS:HG	1.94	0.66
72:SJ:120:ALA:HB1	72:SJ:125:HIS:CD2	2.31	0.66
1:L5:455:C:H6	1:L5:455:C:O5'	1.77	0.66
54:SH:184:ASP:OD1	54:SH:184:ASP:N	2.28	0.66
1:L5:3789:C:O5'	1:L5:3789:C:H6	1.78	0.66
1:L5:1304:C:C5'	1:L5:1304:C:H6	2.09	0.66
11:LH:113:GLU:HG2	11:LH:125:ARG:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SD:27:ARG:HH11	51:SD:27:ARG:CG	2.08	0.66
1:L5:1304:C:H6	1:L5:1304:C:H5''	1.59	0.66
12:LI:56:GLU:OE1	12:LI:161:GLY:HA2	1.96	0.66
33:Le:37:LYS:HE3	33:Le:55:MET:HE1	1.77	0.66
58:SP:34:MET:O	58:SP:42:ARG:HG3	1.94	0.66
64:SV:16:LYS:HG2	64:SV:23:ILE:HD13	1.76	0.66
48:S6:76:A:H8	48:S6:76:A:C5'	2.08	0.66
71:SG:64:LYS:HZ1	71:SG:82:SER:HB2	1.61	0.66
1:L5:73:A:H8	1:L5:73:A:H5''	1.60	0.66
7:LD:292:GLU:O	7:LD:292:GLU:HG3	1.96	0.66
64:SV:70:LEU:HD21	64:SV:83:PHE:HZ	1.60	0.66
1:L5:3943:A:H8	1:L5:3943:A:O5'	1.79	0.65
61:SS:23:ARG:O	61:SS:55:ARG:HD3	1.97	0.65
78:SZ:50:PHE:HE1	78:SZ:79:ILE:HD11	1.58	0.65
1:L5:4922:C:H6	1:L5:4922:C:O5'	1.79	0.65
7:LD:23:ARG:HD2	7:LD:23:ARG:C	2.18	0.65
47:S2:681:U:H4'	65:SX:9:THR:HG22	1.76	0.65
71:SG:64:LYS:NZ	71:SG:82:SER:HB2	2.11	0.65
50:SB:62:LEU:HA	50:SB:65:ARG:HD2	1.79	0.65
9:LF:96:ARG:HG2	9:LF:96:ARG:NH1	2.12	0.65
47:S2:1397:U:H5'	47:S2:1397:U:C6	2.32	0.65
1:L5:1279:A:H5''	1:L5:1279:A:H8	1.61	0.65
1:L5:1446:C:H6	1:L5:1446:C:C5'	2.10	0.65
25:LW:105:ARG:HH22	71:SG:151:ASP:HA	1.61	0.65
18:LP:4:TYR:HE1	18:LP:18:ARG:HD2	1.61	0.64
47:S2:533:A:H61	47:S2:550:C:H42	1.45	0.64
9:LF:32:ARG:C	9:LF:34:ARG:H	2.04	0.64
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.78	0.64
47:S2:532:C:H6	47:S2:532:C:H5''	1.62	0.64
47:S2:1238:U:O2	47:S2:1242:U:H5	1.80	0.64
1:L5:256:G:O5'	1:L5:256:G:H8	1.79	0.64
1:L5:73:A:N6	14:LL:103:ARG:HH22	1.95	0.64
1:L5:4620:OMU:H6	1:L5:4620:OMU:O5'	1.97	0.64
51:SD:116:ARG:HH11	51:SD:116:ARG:HG2	1.63	0.64
53:SF:122:ARG:HE	67:Sc:59:LEU:HD22	1.60	0.64
1:L5:4416:G:H5''	1:L5:4416:G:H8	1.63	0.64
24:LV:18:LEU:HD23	24:LV:54:ALA:HB3	1.80	0.64
49:SA:205:ARG:HH12	60:SR:84:TYR:HB3	1.63	0.64
69:Sg:14:HIS:HD2	69:Sg:41:ILE:HG13	1.61	0.64
71:SG:223:LYS:N	71:SG:223:LYS:HD3	2.12	0.64
17:LO:74:ARG:HH11	17:LO:74:ARG:HG3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LP:109:VAL:HA	18:LP:112:LEU:HD13	1.80	0.63
71:SG:222:GLU:HB3	71:SG:223:LYS:HZ3	1.63	0.63
6:LC:221:PHE:HD2	6:LC:227:ILE:HG21	1.64	0.63
9:LF:32:ARG:O	9:LF:34:ARG:N	2.32	0.63
14:LL:133:ALA:HB1	14:LL:135:LYS:HE3	1.80	0.63
70:SC:68:ARG:HH21	70:SC:71:LYS:HD2	1.63	0.63
1:L5:182:G:N1	1:L5:255:C:O2'	2.32	0.63
1:L5:1697:G:OP1	1:L5:1697:G:H4'	1.95	0.63
1:L5:2416:G:H8	1:L5:2416:G:OP2	1.81	0.63
3:L8:66:A:OP1	36:Lh:7:ARG:HG2	1.99	0.63
1:L5:4910:G:H4'	5:LB:95:THR:HG22	1.79	0.63
67:Sc:12:ALA:HB1	67:Sc:33:GLU:O	1.99	0.63
1:L5:375:G:OP2	38:Lj:52:LYS:NZ	2.32	0.63
1:L5:3672:G:H4'	16:LN:67:ARG:HH12	1.63	0.63
47:S2:659:G:H2'	47:S2:659:G:N3	2.13	0.63
31:Lc:74:TYR:CD2	31:Lc:81:LEU:HD22	2.34	0.63
1:L5:2003:G:H1	1:L5:2016:C:H42	1.45	0.63
47:S2:734:C:H3'	47:S2:736:C:N4	2.14	0.63
1:L5:182:G:N2	1:L5:255:C:O2'	2.32	0.62
1:L5:1279:A:H5''	1:L5:1279:A:C8	2.33	0.62
8:LE:67:ALA:HA	8:LE:69:TYR:CE1	2.34	0.62
72:SJ:47:LYS:HB3	72:SJ:102:ILE:HD12	1.81	0.62
54:SH:185:VAL:HG21	54:SH:187:PHE:HE1	1.38	0.62
16:LN:124:ASP:HB3	16:LN:127:TYR:H	1.63	0.62
1:L5:1767:A:H62	58:SP:10:ARG:NH1	1.97	0.62
1:L5:4452:U:H5'	83:L5:5374:HMT:H16	1.82	0.62
1:L5:4523:A2M:H5''	1:L5:4524:G:H5'	1.82	0.62
53:SF:138:ALA:HB3	53:SF:204:ARG:O	2.00	0.62
77:SY:10:ARG:HD2	77:SY:11:LYS:HG3	1.81	0.62
3:L8:127:U:H3'	3:L8:127:U:C6	2.35	0.62
1:L5:368:C:O4'	6:LC:83:GLY:HA3	1.99	0.62
9:LF:124:LYS:HG3	9:LF:197:VAL:HG11	1.79	0.62
54:SH:126:HIS:CE1	54:SH:181:THR:HG23	2.35	0.62
1:L5:151:G:C2'	16:LN:49:ARG:HH12	2.13	0.61
1:L5:1252:C:H5''	1:L5:1252:C:C6	2.27	0.61
59:SQ:37:ARG:HH11	59:SQ:37:ARG:HG2	1.64	0.61
1:L5:2490:U:OP1	1:L5:2490:U:H2'	2.00	0.61
1:L5:3949:A:N3	1:L5:3949:A:H5''	2.15	0.61
47:S2:928:G:H1	47:S2:1013:U:H3	1.48	0.61
8:LE:114:ARG:HB3	45:Lr:87:ARG:NH1	2.15	0.61
61:SS:45:LEU:HD22	61:SS:50:ILE:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SZ:76:ARG:HH11	78:SZ:76:ARG:CG	2.13	0.61
7:LD:200:MET:HA	7:LD:200:MET:HE3	1.82	0.61
18:LP:4:TYR:HE1	18:LP:18:ARG:CD	2.12	0.61
49:SA:56:GLU:OE1	64:SV:79:VAL:CB	2.49	0.61
69:Sg:14:HIS:CD2	69:Sg:41:ILE:CG1	2.83	0.61
78:SZ:65:TYR:CE2	78:SZ:76:ARG:NH2	2.68	0.61
11:LH:106:GLN:NE2	11:LH:106:GLN:HA	2.16	0.61
49:SA:42:LYS:HD3	49:SA:46:ILE:HB	1.82	0.61
58:SP:33:LEU:CD1	58:SP:37:TYR:CE2	2.82	0.61
30:Lb:12:GLN:NE2	30:Lb:15:LYS:CD	2.63	0.61
62:ST:39:LEU:O	62:ST:40:ALA:HB3	1.99	0.61
1:L5:180:C:H3'	1:L5:180:C:H6	1.64	0.61
34:Lf:57:THR:HG21	34:Lf:68:ARG:HD3	1.82	0.61
49:SA:38:ILE:HD11	49:SA:47:TYR:HB3	1.83	0.61
77:SY:99:LYS:HD3	77:SY:101:LYS:HE2	1.82	0.61
1:L5:3956:G:O4'	1:L5:3964:U:H6	1.84	0.60
13:LJ:31:ASP:HB2	13:LJ:35:ARG:HH11	1.65	0.60
23:LU:47:ILE:HG21	23:LU:56:LEU:HD23	1.83	0.60
31:Lc:20:LEU:CD1	31:Lc:101:ASP:CB	2.43	0.60
47:S2:1148:A:OP2	66:Sa:6:ARG:NH1	2.34	0.60
1:L5:2337:C:H4'	45:Lr:19:LYS:HB2	1.83	0.60
1:L5:4146:G:H2'	1:L5:4147:G:H8	1.66	0.60
51:SD:16:ILE:HD13	68:Sd:22:ARG:HH11	1.65	0.60
75:SO:57:THR:HG22	75:SO:59:GLY:H	1.66	0.60
17:LO:46:ASN:OD1	17:LO:49:ARG:HB2	2.00	0.60
67:Sc:31:ARG:HA	67:Sc:43:ILE:HA	1.83	0.60
1:L5:4942:C:H5''	8:LE:155:GLY:HA2	1.83	0.60
9:LF:96:ARG:HH11	9:LF:96:ARG:CG	2.13	0.60
13:LJ:141:ILE:HA	13:LJ:144:LYS:HE3	1.84	0.60
48:S6:33:C:H5	48:S6:35:A:H5''	1.67	0.60
53:SF:122:ARG:CB	67:Sc:59:LEU:HD21	2.32	0.60
69:Sg:14:HIS:HD2	69:Sg:41:ILE:HG12	1.66	0.60
76:SW:27:ILE:HB	76:SW:61:ILE:HB	1.83	0.60
1:L5:2563:C:O5'	1:L5:2563:C:H6	1.84	0.60
1:L5:3682:A:H5''	4:LA:132:ASN:ND2	2.16	0.60
14:LL:50:PRO:HB3	14:LL:150:LEU:HB3	1.83	0.60
47:S2:1640:A:OP2	47:S2:1640:A:H8	1.85	0.60
29:La:76:ASP:HB3	29:La:115:GLY:HA3	1.83	0.60
39:Lk:26:LYS:HB2	39:Lk:69:LEU:HD12	1.84	0.60
41:Lm:94:MET:HG2	41:Lm:105:PRO:HA	1.84	0.60
51:SD:195:THR:H	51:SD:201:LYS:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:51:HIS:HD2	53:SF:86:LYS:HG2	1.67	0.60
62:ST:33:TRP:HE3	62:ST:33:TRP:C	2.10	0.60
4:LA:83:HIS:HB3	44:Lp:64:VAL:HG23	1.84	0.60
27:LY:8:THR:HG21	27:LY:17:ARG:NH1	2.17	0.60
1:L5:1762:C:H2'	1:L5:1763:C:C5	2.37	0.60
1:L5:1769:G:H21	58:SP:10:ARG:HH22	1.48	0.60
1:L5:1812:C:H5''	30:Lb:56:LYS:HE3	1.82	0.60
51:SD:99:ILE:CG2	51:SD:173:ARG:NH2	2.62	0.60
55:SI:101:ILE:HD12	55:SI:190:LEU:HD11	1.84	0.60
66:Sa:45:VAL:O	66:Sa:46:GLU:HB3	2.01	0.60
69:Sg:17:TRP:HB2	69:Sg:36:ARG:HD3	1.82	0.60
1:L5:4277:G:H5''	22:LT:17:ARG:HG2	1.84	0.59
8:LE:157:HIS:HD2	8:LE:187:ARG:HH11	1.50	0.59
27:LY:34:LEU:HD23	27:LY:38:LEU:HB3	1.84	0.59
46:Lz:16:GLU:HG3	46:Lz:18:LEU:HB2	1.84	0.59
9:LF:96:ARG:HG2	9:LF:96:ARG:HH11	1.66	0.59
18:LP:4:TYR:CE1	18:LP:18:ARG:HD2	2.37	0.59
25:LW:11:TYR:HD2	25:LW:32:LEU:HD22	1.66	0.59
1:L5:168:C:O5'	1:L5:168:C:H6	1.83	0.59
3:L8:127:U:C6	3:L8:127:U:C3'	2.85	0.59
18:LP:118:GLN:NE2	18:LP:120:ASN:HD21	2.00	0.59
69:Sg:220:ASP:HB3	69:Sg:224:GLY:H	1.67	0.59
5:LB:4:ARG:O	5:LB:5:LYS:HB3	2.01	0.59
47:S2:1771:G:H5''	47:S2:1771:G:N3	2.18	0.59
1:L5:1726:U:H5'	9:LF:135:ILE:HD11	1.84	0.59
1:L5:3956:G:O4'	1:L5:3964:U:C6	2.55	0.59
1:L5:4141:G:H4'	1:L5:4141:G:OP1	2.01	0.59
53:SF:122:ARG:HE	67:Sc:59:LEU:CD2	2.16	0.59
78:SZ:50:PHE:CE1	78:SZ:79:ILE:CG1	2.85	0.59
3:L8:70:G:H5''	27:LY:27:ARG:NH2	2.17	0.59
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	1.85	0.59
58:SP:33:LEU:HD13	58:SP:37:TYR:CE2	2.38	0.59
4:LA:180:LEU:HD22	44:Lp:18:TYR:CB	2.33	0.58
49:SA:76:VAL:HG12	49:SA:123:VAL:HB	1.85	0.58
58:SP:33:LEU:CD1	58:SP:37:TYR:HE2	2.16	0.58
1:L5:2492:C:O5'	1:L5:2492:C:H6	1.86	0.58
79:Sb:34:ASP:HB2	79:Sb:80:ARG:HB2	1.84	0.58
1:L5:3956:G:H4'	1:L5:3964:U:H1'	1.85	0.58
6:LC:320:LYS:HB2	6:LC:320:LYS:HZ3	1.68	0.58
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.84	0.58
1:L5:1175:A:C5'	7:LD:268:ARG:HH21	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2487:G:H22	1:L5:2492:C:H1'	1.69	0.58
18:LP:2:VAL:HB	18:LP:18:ARG:NH1	2.19	0.58
53:SF:63:LYS:HE2	53:SF:71:ARG:NH1	2.19	0.58
54:SH:55:GLY:H	54:SH:57:ARG:HE	1.50	0.58
73:SM:126:GLU:HG3	73:SM:129:LYS:HE3	1.86	0.58
47:S2:37:C:H6	47:S2:37:C:H5''	1.68	0.58
47:S2:1156:U:O4	70:SC:194:ARG:NH1	2.36	0.58
1:L5:1252:C:C5'	1:L5:1252:C:C6	2.86	0.58
1:L5:1762:C:H3'	1:L5:1763:C:C6	2.38	0.58
8:LE:119:GLU:OE1	33:Le:93:LYS:HG2	2.03	0.58
13:LJ:24:ILE:HD11	13:LJ:128:LEU:HD22	1.85	0.58
47:S2:1134:G:P	66:Sa:6:ARG:HH21	2.27	0.58
70:SC:74:LYS:HD2	70:SC:269:PHE:CE1	2.39	0.58
70:SC:199:PRO:HG3	72:SJ:58:ARG:HE	1.69	0.58
16:LN:146:PRO:HB2	36:Lh:104:THR:HG23	1.86	0.58
62:ST:33:TRP:O	62:ST:33:TRP:HE3	1.87	0.58
69:Sg:62:HIS:HE1	69:Sg:88:ARG:HG3	1.69	0.58
1:L5:3641:U:OP2	1:L5:3646:A:N6	2.36	0.58
33:Le:7:LEU:HD13	33:Le:8:VAL:HG23	1.85	0.57
47:S2:1272:C:HO2'	68:Sd:2:GLY:N	2.01	0.57
51:SD:132:LYS:HE3	51:SD:191:PRO:HA	1.85	0.57
53:SF:140:ASP:OD2	67:Sc:58:LEU:HD11	2.04	0.57
13:LJ:120:ASP:HB3	13:LJ:121:PRO:CD	2.32	0.57
13:LJ:120:ASP:CB	13:LJ:121:PRO:HD2	2.31	0.57
49:SA:74:VAL:HG12	49:SA:121:LEU:HB3	1.86	0.57
12:LI:38:ARG:HD3	12:LI:83:ASP:HB2	1.86	0.57
17:LO:49:ARG:HH21	17:LO:49:ARG:CG	2.18	0.57
1:L5:987:C:H2'	1:L5:988:C:H6	1.69	0.57
1:L5:2738:C:H5''	4:LA:184:ARG:HH12	1.69	0.57
78:SZ:47:LEU:HD23	78:SZ:78:LYS:HB3	1.87	0.57
72:SJ:79:ARG:HH12	72:SJ:83:ARG:HH21	1.51	0.57
1:L5:1436:C:H42	1:L5:1448:G:H1	1.52	0.57
9:LF:28:LEU:O	9:LF:32:ARG:HD3	2.05	0.57
24:LV:60:MET:CE	24:LV:80:VAL:HG22	2.35	0.57
52:SE:87:MET:HE1	52:SE:236:ILE:HD13	1.86	0.57
1:L5:3594:C:H5''	1:L5:3595:U:H5	1.70	0.57
19:LQ:39:THR:HG22	19:LQ:41:SER:H	1.70	0.57
49:SA:107:THR:HG22	49:SA:108:PHE:CD1	2.39	0.57
51:SD:219:PRO:HB2	69:Sg:192:THR:HG22	1.87	0.57
61:SS:90:VAL:O	61:SS:90:VAL:HG13	2.04	0.57
69:Sg:241:PHE:HE1	69:Sg:248:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SC:275:LYS:HG3	70:SC:276:THR:HG23	1.85	0.57
1:L5:2469:C:H5	1:L5:2471:G:H1	1.53	0.57
5:LB:381:THR:OG1	5:LB:384:GLU:HG3	2.05	0.57
51:SD:23:GLU:HG3	68:Sd:46:TYR:OH	2.05	0.57
55:SI:27:TYR:HB3	55:SI:49:ARG:NH1	2.20	0.57
6:LC:14:LYS:HE2	6:LC:16:GLU:HB2	1.87	0.57
70:SC:64:THR:HG23	70:SC:66:LEU:H	1.69	0.57
77:SY:129:LYS:HA	77:SY:132:LYS:HB3	1.87	0.57
49:SA:77:ILE:HG12	49:SA:99:ILE:HB	1.86	0.56
54:SH:181:THR:HG22	54:SH:183:LYS:CG	2.34	0.56
1:L5:3688:U:OP2	4:LA:198:ARG:NH1	2.39	0.56
1:L5:3937:C:H1'	16:LN:125:SER:HB3	1.87	0.56
7:LD:282:GLN:HA	7:LD:285:ALA:HB3	1.85	0.56
7:LD:289:ARG:HG2	7:LD:289:ARG:O	2.03	0.56
54:SH:46:THR:HG21	54:SH:97:GLN:OE1	2.05	0.56
79:Sb:36:LYS:HB3	79:Sb:78:SER:HB3	1.86	0.56
1:L5:3606:U:O2'	20:LR:89:MET:HE2	2.05	0.56
6:LC:152:LEU:HD23	6:LC:251:ILE:HG12	1.86	0.56
47:S2:508:A:H8	47:S2:508:A:H5''	1.69	0.56
75:SO:74:ALA:HB1	75:SO:115:ALA:HB2	1.87	0.56
11:LH:124:ARG:HG2	11:LH:124:ARG:NH1	2.20	0.56
18:LP:45:THR:HG22	18:LP:49:LYS:HE2	1.87	0.56
24:LV:20:LEU:N	24:LV:21:PRO:HD3	2.20	0.56
48:S6:50:A:H61	48:S6:62:C:H42	1.53	0.56
69:Sg:201:SER:HA	69:Sg:241:PHE:CD2	2.39	0.56
69:Sg:238:ALA:H	69:Sg:251:ALA:HB3	1.69	0.56
78:SZ:99:LEU:HD11	78:SZ:102:LYS:HB2	1.87	0.56
47:S2:1650:A:H5''	59:SQ:139:ALA:HB2	1.85	0.56
49:SA:52:LYS:HB2	60:SR:109:LEU:HD13	1.86	0.56
76:SW:49:GLU:HB2	76:SW:64:ASN:HD22	1.71	0.56
1:L5:1303:A:H2'	1:L5:1304:C:H5''	1.88	0.56
23:LU:105:ASN:HB2	23:LU:111:GLU:OE2	2.05	0.56
54:SH:181:THR:HG22	54:SH:183:LYS:HG3	1.85	0.56
1:L5:1970:A:H5''	1:L5:1970:A:C8	2.39	0.56
1:L5:3946:G:H21	1:L5:3947:A:H62	1.53	0.56
24:LV:25:VAL:O	24:LV:25:VAL:HG22	2.05	0.56
29:La:72:THR:HG22	29:La:110:LYS:HB3	1.86	0.56
1:L5:1175:A:H5''	7:LD:268:ARG:NH2	2.16	0.56
6:LC:189:MET:HE2	6:LC:195:LYS:CD	2.36	0.56
14:LL:80:GLU:OE2	14:LL:102:ARG:NH1	2.38	0.56
52:SE:55:ALA:HB1	52:SE:60:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SR:60:ARG:HE	60:SR:66:VAL:HG11	1.71	0.56
1:L5:3967:G:N2	1:L5:4055:U:H3	2.03	0.56
1:L5:4564:A:H5'	17:LO:68:ARG:HH12	1.70	0.56
11:LH:115:ARG:HH11	11:LH:115:ARG:HG2	1.71	0.56
16:LN:123:GLU:HG2	16:LN:128:LYS:HG3	1.87	0.56
48:S6:76:A:C8	48:S6:76:A:C5'	2.85	0.56
58:SP:93:MET:HE1	58:SP:104:GLN:NE2	2.20	0.56
1:L5:968:C:H5'	8:LE:110:ARG:HD3	1.88	0.56
1:L5:4508:C:N3	1:L5:4512:U:H5	2.03	0.56
5:LB:4:ARG:O	5:LB:5:LYS:CB	2.54	0.56
17:LO:49:ARG:HG3	17:LO:49:ARG:HH21	1.72	0.56
47:S2:913:A:C5	54:SH:98:ARG:O	2.59	0.56
61:SS:15:VAL:HG12	61:SS:16:LEU:HD12	1.88	0.56
66:Sa:10:ARG:NH2	66:Sa:12:LYS:HE2	2.21	0.56
1:L5:1763:C:H2'	1:L5:1764:G:H5'	1.88	0.55
1:L5:4194:U:O2'	12:LI:116:ARG:NH1	2.39	0.55
39:Lk:3:ARG:HB2	39:Lk:43:TYR:CD1	2.37	0.55
44:Lp:38:THR:HA	44:Lp:45:THR:HA	1.87	0.55
47:S2:834:C:H42	47:S2:839:C:H42	1.51	0.55
1:L5:1521:C:OP1	6:LC:100:ARG:NH2	2.39	0.55
2:L7:6:C:H4'	7:LD:52:ILE:HD13	1.88	0.55
65:SX:72:VAL:HG11	65:SX:102:VAL:HG11	1.88	0.55
1:L5:1353:G:N7	19:LQ:104:ARG:NH1	2.53	0.55
1:L5:4489:G:N2	1:L5:4592:C:OP1	2.40	0.55
3:L8:18:U:O5'	3:L8:18:U:H6	1.88	0.55
9:LF:69:ILE:CG2	9:LF:73:ARG:HH21	2.19	0.55
24:LV:60:MET:CE	24:LV:106:VAL:HG21	2.37	0.55
27:LY:27:ARG:NH1	27:LY:48:PRO:HG2	2.21	0.55
75:SO:106:LYS:HD2	75:SO:135:ILE:HD11	1.87	0.55
1:L5:2020:U:O5'	1:L5:2020:U:H6	1.88	0.55
11:LH:7:ASN:HD22	11:LH:56:ARG:HH21	1.53	0.55
54:SH:100:ILE:CG1	54:SH:125:VAL:HG11	2.37	0.55
11:LH:106:GLN:HB2	11:LH:111:LEU:HB3	1.88	0.55
47:S2:582:U:OP1	72:SJ:162:ARG:NH1	2.40	0.55
70:SC:115:GLN:HE22	70:SC:120:GLN:HE21	1.53	0.55
1:L5:1764:G:H2'	1:L5:1766:A:P	2.46	0.55
1:L5:3961:G:H3'	1:L5:3962:A:H4'	1.87	0.55
4:LA:83:HIS:HB3	44:Lp:64:VAL:CG2	2.37	0.55
11:LH:82:LYS:HG3	11:LH:86:LEU:HD12	1.88	0.55
25:LW:80:ARG:HG2	71:SG:131:ARG:HH11	1.72	0.55
62:ST:33:TRP:O	62:ST:37:VAL:CG1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LD:33:ARG:HH21	22:LT:27:LEU:HD23	1.71	0.55
28:LZ:12:LEU:HB2	28:LZ:81:MET:HB3	1.89	0.55
78:SZ:50:PHE:CE1	78:SZ:79:ILE:HD11	2.41	0.55
32:Ld:57:MET:HG2	32:Ld:88:LEU:HD23	1.88	0.55
1:L5:736:C:OP1	15:LM:74:ARG:NH1	2.40	0.55
53:SF:51:HIS:CD2	53:SF:86:LYS:HG2	2.42	0.55
1:L5:489:C:H42	1:L5:664:G:H1	1.53	0.55
4:LA:246:LEU:O	4:LA:246:LEU:HG	2.07	0.55
5:LB:37:PRO:HA	5:LB:188:GLY:H	1.71	0.55
5:LB:173:LEU:HD21	5:LB:342:LYS:HB3	1.88	0.55
22:LT:49:GLN:HA	22:LT:52:MET:HE3	1.89	0.55
39:Lk:33:LYS:HG2	39:Lk:46:VAL:HG22	1.89	0.55
1:L5:730:G:C2	9:LF:73:ARG:NH1	2.73	0.54
4:LA:207:VAL:HG23	4:LA:208:GLU:HG3	1.88	0.54
44:Lp:85:ARG:NH2	47:S2:939:U:C4'	2.66	0.54
46:Lz:175:THR:HG23	46:Lz:177:ASP:H	1.72	0.54
47:S2:1553:C:H41	68:Sd:22:ARG:HH21	1.55	0.54
57:SL:120:VAL:HG22	57:SL:145:VAL:HG11	1.89	0.54
5:LB:286:LYS:HE2	5:LB:365:LEU:HD12	1.88	0.54
31:Lc:55:LEU:HD21	35:Lg:92:LYS:HG3	1.88	0.54
47:S2:1644:C:H4'	59:SQ:140:ARG:HB2	1.89	0.54
59:SQ:13:PHE:CD1	59:SQ:13:PHE:C	2.85	0.54
1:L5:4870:OMG:OP2	15:LM:5:ARG:NH1	2.37	0.54
1:L5:258:G:H2'	1:L5:259:C:C6	2.43	0.54
1:L5:699:C:O2'	1:L5:968:C:O2	2.24	0.54
1:L5:759:G:H22	1:L5:904:C:H2'	1.71	0.54
1:L5:3636:C:O5'	1:L5:3636:C:H6	1.90	0.54
4:LA:180:LEU:CD2	44:Lp:18:TYR:HB3	2.38	0.54
28:LZ:99:ASP:HB2	28:LZ:102:ARG:HE	1.72	0.54
45:Lr:49:VAL:HG12	45:Lr:64:ILE:HG22	1.88	0.54
78:SZ:78:LYS:HB2	78:SZ:78:LYS:NZ	2.22	0.54
1:L5:3956:G:H5'	1:L5:3966:A:C5	2.42	0.54
9:LF:94:ARG:HB2	9:LF:114:LEU:HD23	1.89	0.54
22:LT:71:ALA:HA	22:LT:92:ARG:HA	1.90	0.54
69:Sg:199:THR:HG21	69:Sg:240:CYS:HA	1.89	0.54
1:L5:1270:A:OP1	30:Lb:107:ARG:NH1	2.41	0.54
23:LU:107:LYS:O	23:LU:108:GLU:HG3	2.07	0.54
53:SF:71:ARG:HH12	53:SF:148:ASN:HD21	1.53	0.54
62:ST:33:TRP:CE3	62:ST:33:TRP:C	2.85	0.54
64:SV:83:PHE:C	64:SV:83:PHE:CD1	2.86	0.54
69:Sg:14:HIS:HB2	69:Sg:37:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:246:ARG:HG2	5:LB:246:ARG:HH11	1.73	0.54
23:LU:20:LYS:H	23:LU:73:THR:HA	1.72	0.54
55:SI:48:VAL:HG11	55:SI:54:LYS:HE3	1.89	0.54
75:SO:30:VAL:HG12	75:SO:94:HIS:HB2	1.90	0.54
1:L5:3594:C:H2'	1:L5:3595:U:H5'	1.90	0.54
29:La:11:LEU:HD23	29:La:17:HIS:C	2.33	0.54
33:Le:91:CYS:HB3	33:Le:95:TYR:HB2	1.88	0.54
60:SR:61:ILE:HG22	60:SR:66:VAL:HB	1.90	0.54
78:SZ:50:PHE:CE1	78:SZ:79:ILE:HG13	2.43	0.54
1:L5:99:A:H5''	16:LN:184:ILE:HD13	1.89	0.54
1:L5:375:G:N7	38:Lj:56:ARG:NH1	2.56	0.54
1:L5:469:C:H42	8:LE:101:ASN:HD21	1.56	0.54
5:LB:220:ILE:HD11	5:LB:348:ARG:HE	1.73	0.54
5:LB:223:THR:HB	5:LB:275:HIS:H	1.72	0.54
9:LF:69:ILE:HG21	9:LF:73:ARG:HH21	1.72	0.54
12:LI:47:PRO:HD2	12:LI:141:LYS:HA	1.90	0.54
1:L5:1762:C:H2'	1:L5:1763:C:C6	2.43	0.54
1:L5:1870:C:H2'	1:L5:1871:A2M:H8	1.90	0.54
1:L5:3968:U:O2	1:L5:3968:U:H2'	2.08	0.54
4:LA:114:CYS:HB2	4:LA:169:VAL:HG13	1.90	0.54
5:LB:79:VAL:CG2	5:LB:331:VAL:HB	2.38	0.54
11:LH:115:ARG:HH11	11:LH:123:ILE:CG1	2.12	0.54
47:S2:70:G:H21	47:S2:79:A:H62	1.54	0.54
47:S2:733:C:H4'	47:S2:733:C:OP2	2.07	0.54
54:SH:116:ARG:NH1	54:SH:121:THR:HA	2.23	0.54
62:ST:65:TYR:CD1	62:ST:65:TYR:C	2.85	0.54
69:Sg:10:THR:HG21	69:Sg:306:LEU:HD13	1.90	0.54
36:Lh:80:PRO:HD2	36:Lh:83:LEU:HD12	1.91	0.53
1:L5:1072:C:H2'	1:L5:1073:G:C8	2.44	0.53
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.89	0.53
17:LO:201:LEU:HD12	17:LO:201:LEU:H	1.70	0.53
18:LP:13:LYS:HB3	18:LP:152:GLU:HB3	1.90	0.53
1:L5:1762:C:H5'	1:L5:1763:C:C5	2.43	0.53
14:LL:198:ARG:HA	14:LL:201:GLU:HG2	1.91	0.53
47:S2:1199:A:H5''	66:Sa:2:THR:HB	1.89	0.53
53:SF:138:ALA:CB	53:SF:204:ARG:O	2.57	0.53
58:SP:108:LYS:HZ1	61:SS:116:LYS:HD3	1.73	0.53
1:L5:2303:C:H5''	33:Le:104:SER:HB3	1.91	0.53
50:SB:71:LEU:HD21	50:SB:84:PHE:CE1	2.44	0.53
5:LB:103:LYS:HD3	5:LB:104:THR:N	2.23	0.53
47:S2:537:C:O2	47:S2:537:C:H2'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4041:C:H5'	1:L5:4042:G:H5''	1.90	0.53
1:L5:4146:G:H2'	1:L5:4147:G:C8	2.44	0.53
1:L5:4618:G:H5''	24:LV:15:ARG:HB3	1.89	0.53
15:LM:70:GLN:NE2	15:LM:74:ARG:HH22	2.06	0.53
33:Le:8:VAL:HG12	33:Le:10:PRO:HD3	1.90	0.53
59:SQ:25:CYS:HB3	59:SQ:68:ILE:HD13	1.90	0.53
78:SZ:79:ILE:CD1	78:SZ:79:ILE:H	2.21	0.53
78:SZ:79:ILE:N	78:SZ:79:ILE:HD12	2.24	0.53
1:L5:388:A:H1'	1:L5:403:G:N2	2.24	0.53
1:L5:1251:C:H2'	1:L5:1252:C:H5''	1.90	0.53
1:L5:1445:U:O2	1:L5:1445:U:H2'	2.07	0.53
47:S2:517:OMC:HM22	47:S2:518:G:H5'	1.91	0.53
54:SH:66:VAL:HG22	54:SH:96:ALA:HB1	1.90	0.53
55:SI:107:THR:N	55:SI:108:PRO:CD	2.72	0.53
61:SS:98:VAL:CG2	61:SS:103:LEU:HD13	2.39	0.53
1:L5:230:G:OP1	27:LY:15:ARG:NH1	2.41	0.53
1:L5:3946:G:H21	1:L5:3947:A:N6	2.07	0.53
11:LH:52:LYS:HB2	11:LH:54:ARG:HH11	1.74	0.53
17:LO:79:ILE:HG21	17:LO:138:LEU:HD11	1.91	0.53
33:Le:92:ASN:OD1	33:Le:119:ALA:HB3	2.09	0.53
51:SD:23:GLU:O	51:SD:27:ARG:HD2	2.09	0.53
54:SH:144:ILE:HA	54:SH:154:ILE:HA	1.90	0.53
54:SH:144:ILE:HG23	76:SW:52:ILE:HB	1.89	0.53
71:SG:70:HIS:HB3	71:SG:101:ILE:HB	1.91	0.53
1:L5:180:C:H3'	1:L5:180:C:C6	2.43	0.53
1:L5:2674:A:N6	44:Lp:41:PHE:O	2.39	0.53
1:L5:4934:A:H2'	1:L5:4935:C:C6	2.44	0.53
47:S2:369:C:H3'	47:S2:369:C:OP2	2.09	0.53
17:LO:108:ILE:HG21	17:LO:113:ASP:HA	1.92	0.52
63:SU:67:LYS:HB2	63:SU:78:ASP:HB2	1.90	0.52
69:Sg:11:LEU:HB2	69:Sg:307:VAL:HB	1.90	0.52
1:L5:2626:U:O4	23:LU:97:ARG:NH1	2.42	0.52
1:L5:4416:G:H5''	1:L5:4416:G:C8	2.44	0.52
47:S2:153:G:H21	71:SG:13:GLN:HE22	1.56	0.52
9:LF:199:LYS:O	9:LF:200:ARG:HD3	2.09	0.52
64:SV:53:TYR:CD1	64:SV:72:LEU:CD2	2.92	0.52
76:SW:55:ASP:HB3	79:Sb:25:VAL:HG23	1.90	0.52
78:SZ:44:LEU:O	78:SZ:45:ASN:C	2.52	0.52
1:L5:1250:C:H2'	1:L5:1251:C:C6	2.45	0.52
1:L5:4112:C:H5''	1:L5:4113:U:H5	1.73	0.52
24:LV:39:ILE:HG12	24:LV:61:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:520:A:O2'	47:S2:825:A:N3	2.42	0.52
1:L5:2905:C:H5''	1:L5:2905:C:H6	1.73	0.52
5:LB:323:TYR:HD1	5:LB:342:LYS:HG2	1.74	0.52
51:SD:170:THR:HG22	51:SD:171:ALA:N	2.24	0.52
70:SC:187:ARG:HH21	70:SC:192:LEU:HB3	1.73	0.52
1:L5:180:C:C6	1:L5:180:C:C3'	2.93	0.52
1:L5:2033:A:OP1	12:LI:162:ARG:NH1	2.43	0.52
1:L5:4213:A:H5''	1:L5:4214:A:H5'	1.92	0.52
73:SM:49:LEU:HA	73:SM:74:ILE:HG23	1.92	0.52
1:L5:702:U:O5'	1:L5:702:U:H6	1.93	0.52
6:LC:66:SER:HA	6:LC:77:PRO:HA	1.92	0.52
8:LE:130:LYS:CD	8:LE:130:LYS:N	2.73	0.52
52:SE:60:GLU:HA	52:SE:63:LYS:HG2	1.91	0.52
56:SK:3:MET:HE1	56:SK:48:ALA:HB2	1.91	0.52
1:L5:2847:G:OP1	24:LV:85:ARG:HD3	2.10	0.52
1:L5:4070:U:H2'	1:L5:4071:U:C6	2.45	0.52
1:L5:4148:C:O2	1:L5:4148:C:H2'	2.09	0.52
12:LI:89:VAL:HG12	12:LI:136:MET:HG2	1.91	0.52
17:LO:125:LYS:HG2	17:LO:129:LEU:HD12	1.92	0.52
33:Le:98:GLU:HG3	33:Le:123:THR:HB	1.90	0.52
47:S2:1312:G:O6	73:SM:36:ARG:HG2	2.09	0.52
47:S2:1452:A:O2'	47:S2:1475:G:N2	2.43	0.52
47:S2:1860:A:OP2	66:Sa:10:ARG:HD2	2.10	0.52
51:SD:27:ARG:HG2	51:SD:27:ARG:NH1	2.22	0.52
54:SH:79:LEU:HD22	54:SH:94:PHE:HZ	1.74	0.52
1:L5:942:G:OP1	9:LF:245:ARG:NH1	2.42	0.52
1:L5:2096:G:N3	1:L5:2096:G:C2'	2.72	0.52
1:L5:2611:A:H5'	1:L5:2688:G:H4'	1.91	0.52
1:L5:3946:G:HO2'	1:L5:3947:A:N3	1.46	0.52
49:SA:80:ARG:O	49:SA:84:GLN:HG3	2.10	0.52
69:Sg:174:VAL:HB	69:Sg:188:HIS:HB2	1.92	0.52
77:SY:117:VAL:HG21	77:SY:125:VAL:HG21	1.92	0.52
1:L5:1968:G:C8	1:L5:1968:G:C5'	2.86	0.52
18:LP:94:MET:HE3	18:LP:146:ILE:HB	1.92	0.52
47:S2:1771:G:N3	47:S2:1771:G:C5'	2.73	0.52
70:SC:272:HIS:CD2	70:SC:272:HIS:O	2.63	0.52
71:SG:154:ARG:HD3	71:SG:179:LEU:HD21	1.92	0.52
1:L5:3641:U:H5	1:L5:3646:A:N7	2.07	0.51
47:S2:146:G:N7	71:SG:140:ARG:NH2	2.59	0.51
47:S2:536:A:H8	47:S2:536:A:O5'	1.92	0.51
52:SE:137:PRO:HG2	52:SE:150:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SH:51:ILE:HG21	54:SH:179:LYS:HE3	1.92	0.51
54:SH:77:VAL:HG23	54:SH:78:ARG:HD3	1.92	0.51
79:Sb:48:SER:OG	79:Sb:49:HIS:HD2	1.93	0.51
24:LV:60:MET:HE2	24:LV:80:VAL:CG2	2.40	0.51
28:LZ:66:SER:HB2	28:LZ:122:TYR:HE2	1.75	0.51
47:S2:1679:A:N6	53:SF:57:ALA:O	2.43	0.51
49:SA:34:MET:HE1	49:SA:162:PRO:HB3	1.90	0.51
2:L7:12:U:O3'	2:L7:109:U:O2'	2.24	0.51
5:LB:57:VAL:HB	5:LB:367:PHE:HB3	1.92	0.51
27:LY:4:ASN:HD22	27:LY:5:PRO:HD2	1.76	0.51
31:Lc:74:TYR:CG	31:Lc:81:LEU:HD22	2.45	0.51
40:Ll:51:LEU:HG	40:Ll:51:LEU:O	2.09	0.51
54:SH:127:ASP:OD2	54:SH:127:ASP:C	2.53	0.51
75:SO:17:LEU:HD13	75:SO:88:LEU:HD12	1.92	0.51
1:L5:1503:A:H4'	1:L5:1504:G:H5'	1.92	0.51
8:LE:130:LYS:N	8:LE:130:LYS:HD2	2.24	0.51
1:L5:1448:G:H8	1:L5:1448:G:O5'	1.93	0.51
1:L5:1763:C:H41	1:L5:1764:G:H21	1.58	0.51
1:L5:3964:U:H3'	1:L5:3964:U:O2	2.11	0.51
6:LC:2:ALA:HA	6:LC:3:CYS:HB3	1.90	0.51
32:Ld:50:ARG:HG2	32:Ld:54:MET:HE2	1.92	0.51
46:Lz:85:MET:HG3	46:Lz:89:ALA:HB3	1.92	0.51
53:SF:40:ALA:HB1	53:SF:45:TYR:HE2	1.76	0.51
77:SY:20:ARG:NH2	77:SY:74:MET:SD	2.83	0.51
1:L5:3594:C:H5''	1:L5:3595:U:C5	2.46	0.51
1:L5:4746:C:H42	1:L5:4954:G:H1	1.59	0.51
12:LI:66:GLU:HG3	12:LI:69:ARG:HH11	1.75	0.51
31:Lc:47:ILE:HD12	31:Lc:94:LEU:HD11	1.93	0.51
47:S2:1116:C:H2'	47:S2:1117:C:C6	2.45	0.51
47:S2:1379:A:O2'	49:SA:105:PRO:HG2	2.11	0.51
47:S2:1443:C:H5'	59:SQ:13:PHE:CD2	2.45	0.51
76:SW:69:LEU:HD21	76:SW:72:CYS:HB3	1.92	0.51
20:LR:21:LYS:HE3	20:LR:55:VAL:HG12	1.93	0.51
51:SD:170:THR:HG22	51:SD:171:ALA:H	1.76	0.51
61:SS:25:LYS:HG3	61:SS:55:ARG:HH22	1.74	0.51
81:Sf:95:ARG:NH1	81:Sf:96:LYS:O	2.44	0.51
7:LD:166:ALA:HB1	7:LD:171:LEU:HD12	1.92	0.51
11:LH:124:ARG:HH11	11:LH:124:ARG:CG	2.17	0.51
19:LQ:12:LYS:HB2	19:LQ:14:ARG:HH11	1.75	0.51
27:LY:54:GLU:HA	27:LY:69:LYS:HA	1.92	0.51
43:Lo:33:LEU:HA	43:Lo:38:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:10:G:H21	70:SC:114:LYS:HA	1.74	0.51
69:Sg:191:HIS:CD2	69:Sg:195:LEU:HD21	2.46	0.51
1:L5:5064:G:O2'	18:LP:56:GLN:NE2	2.44	0.51
11:LH:31:ARG:HB2	11:LH:84:VAL:O	2.11	0.51
13:LJ:9:GLU:HB2	13:LJ:13:ARG:HB2	1.92	0.51
17:LO:8:VAL:HG12	17:LO:117:ARG:HG3	1.93	0.51
36:Lh:95:LEU:HD23	36:Lh:99:GLU:HG3	1.92	0.51
61:SS:132:ARG:HB2	61:SS:134:GLN:HE22	1.75	0.51
66:Sa:52:ASP:OD2	75:SO:121:ARG:HG3	2.10	0.51
1:L5:73:A:H62	14:LL:103:ARG:NH2	2.09	0.51
1:L5:138:G:H2'	1:L5:139:G:H8	1.76	0.51
10:LG:223:ARG:HB2	10:LG:227:ASN:HB2	1.92	0.51
47:S2:1013:U:OP1	47:S2:1129:G:O2'	2.29	0.51
47:S2:1543:U:O5'	47:S2:1543:U:H6	1.94	0.51
1:L5:2297:G:H4'	6:LC:242:PRO:HB2	1.92	0.50
18:LP:2:VAL:HB	18:LP:18:ARG:HH12	1.76	0.50
41:Lm:111:ARG:HB3	41:Lm:111:ARG:NH2	2.24	0.50
47:S2:190:G:H5''	55:SI:145:ILE:HG12	1.92	0.50
47:S2:508:A:H3'	47:S2:509:OMG:H8	1.76	0.50
49:SA:18:PHE:HE1	49:SA:174:MET:SD	2.34	0.50
49:SA:63:ARG:HD3	64:SV:37:ALA:O	2.11	0.50
62:ST:38:LYS:O	62:ST:38:LYS:HG2	2.10	0.50
64:SV:53:TYR:CE1	64:SV:72:LEU:HD23	2.45	0.50
69:Sg:106:LYS:HB2	69:Sg:126:ASP:HB3	1.91	0.50
1:L5:308:G:O6	16:LN:12:ARG:NH1	2.44	0.50
3:L8:75:G:OP2	27:LY:74:TYR:OH	2.26	0.50
47:S2:1084:A:OP2	47:S2:1085:C:H2'	2.11	0.50
64:SV:81:LYS:HG3	64:SV:81:LYS:O	2.12	0.50
1:L5:1072:C:H2'	1:L5:1073:G:H8	1.75	0.50
1:L5:1646:A:O2'	38:Lj:49:TRP:O	2.26	0.50
1:L5:3812:C:H3'	1:L5:3813:A:H2'	1.92	0.50
8:LE:157:HIS:HD2	8:LE:187:ARG:NH1	2.10	0.50
9:LF:190:LEU:HD21	9:LF:208:LEU:HD21	1.94	0.50
11:LH:124:ARG:NH1	11:LH:124:ARG:CG	2.74	0.50
16:LN:5:LYS:HG3	37:Li:40:VAL:HG11	1.92	0.50
17:LO:49:ARG:CG	17:LO:49:ARG:NH2	2.73	0.50
34:Lf:65:ASN:OD1	34:Lf:67:THR:CG2	2.52	0.50
42:Ln:8:LYS:HE3	42:Ln:12:ARG:HH21	1.75	0.50
45:Lr:51:VAL:HG12	45:Lr:62:VAL:HG22	1.92	0.50
47:S2:814:5MU:OP1	52:SE:22:LYS:NZ	2.44	0.50
47:S2:1755:C:C5	47:S2:1757:G:C6	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2909:C:H2'	1:L5:2909:C:O2	2.10	0.50
5:LB:91:GLY:HA2	5:LB:160:ILE:HA	1.92	0.50
20:LR:78:ILE:O	20:LR:78:ILE:HG13	2.10	0.50
47:S2:190:G:O2'	47:S2:209:A:N6	2.44	0.50
47:S2:588:G:H4'	47:S2:589:G:H5'	1.93	0.50
49:SA:213:GLU:OE1	49:SA:213:GLU:HA	2.12	0.50
54:SH:144:ILE:HD11	54:SH:152:ARG:HB3	1.93	0.50
72:SJ:133:ARG:HH22	77:SY:65:GLY:HA2	1.77	0.50
24:LV:60:MET:CE	24:LV:80:VAL:CG2	2.89	0.50
52:SE:11:ARG:HA	52:SE:28:ALA:HB2	1.94	0.50
53:SF:122:ARG:HB2	67:Sc:59:LEU:HD21	1.94	0.50
53:SF:122:ARG:HB3	67:Sc:59:LEU:HD21	1.93	0.50
1:L5:2896:G:H5''	20:LR:134:ASN:HD22	1.75	0.50
1:L5:4043:G:H8	1:L5:4045:G:O2'	1.95	0.50
4:LA:116:LEU:HD11	4:LA:148:VAL:HG21	1.94	0.50
7:LD:289:ARG:HH11	7:LD:289:ARG:CG	2.22	0.50
12:LI:150:GLU:O	12:LI:154:ARG:HG3	2.11	0.50
18:LP:4:TYR:CE1	18:LP:18:ARG:CD	2.94	0.50
44:Lp:7:LYS:O	44:Lp:27:LYS:NZ	2.42	0.50
68:Sd:22:ARG:CG	68:Sd:38:MET:HG2	2.42	0.50
72:SJ:83:ARG:HE	72:SJ:150:ARG:HD3	1.77	0.50
1:L5:4986:G:C1'	5:LB:174:ARG:NH1	2.75	0.50
25:LW:6:CYS:HB3	25:LW:11:TYR:H	1.76	0.50
46:Lz:48:ARG:HD2	46:Lz:49:PHE:HB2	1.94	0.50
47:S2:1597:C:OP2	78:SZ:85:ARG:NH2	2.41	0.50
59:SQ:38:PRO:HD2	59:SQ:41:MET:HB2	1.92	0.50
1:L5:125:C:H2'	1:L5:126:C:C6	2.47	0.50
1:L5:1203:G:N3	1:L5:1203:G:H2'	2.26	0.50
3:L8:127:U:H6	3:L8:127:U:C3'	2.21	0.50
12:LI:31:ILE:HD11	12:LI:89:VAL:HG21	1.93	0.50
28:LZ:47:ASP:OD2	28:LZ:69:LYS:NZ	2.38	0.50
47:S2:1531:A:H4'	47:S2:1605:G:H4'	1.94	0.50
49:SA:108:PHE:HB2	49:SA:136:GLU:HG2	1.93	0.50
52:SE:44:LEU:HD13	52:SE:72:ILE:HD11	1.93	0.50
52:SE:95:THR:HG23	52:SE:97:GLU:HG2	1.94	0.50
54:SH:142:LYS:HD3	54:SH:154:ILE:HD11	1.93	0.50
81:Sf:107:LYS:HG3	81:Sf:117:LEU:HD11	1.94	0.50
1:L5:270:U:H2'	1:L5:271:C:C6	2.46	0.50
1:L5:461:G:H2'	1:L5:462:G:H8	1.77	0.50
1:L5:1628:C:H5''	4:LA:15:VAL:HG21	1.93	0.50
1:L5:4274:A:H2'	1:L5:4275:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4452:U:H5'	83:L5:5374:HMT:H7	1.93	0.50
7:LD:195:HIS:CE1	7:LD:199:ILE:CD1	2.88	0.50
10:LG:180:PRO:HG3	10:LG:219:VAL:HG13	1.94	0.50
25:LW:34:ALA:HA	25:LW:37:GLU:HG3	1.94	0.50
25:LW:105:ARG:NH2	71:SG:151:ASP:HA	2.25	0.50
54:SH:163:GLN:HG3	54:SH:189:PHE:CE2	2.47	0.50
70:SC:79:GLU:HA	70:SC:82:TYR:HB2	1.94	0.50
75:SO:98:ARG:HH11	75:SO:98:ARG:CG	2.15	0.50
1:L5:425:U:OP1	18:LP:37:LYS:NZ	2.41	0.49
1:L5:4986:G:H1'	5:LB:174:ARG:NH1	2.27	0.49
47:S2:583:A:OP1	72:SJ:169:ARG:NH2	2.44	0.49
67:Sc:15:THR:HB	67:Sc:31:ARG:HG3	1.94	0.49
78:SZ:45:ASN:ND2	78:SZ:45:ASN:N	2.60	0.49
1:L5:1354:A:N1	1:L5:1385:G:O2'	2.45	0.49
1:L5:1581:G:H2'	1:L5:1582:PSU:H5'	1.93	0.49
1:L5:3948:C:H3'	1:L5:3949:A:C2	2.47	0.49
13:LJ:124:GLY:HA3	13:LJ:126:TYR:CE2	2.47	0.49
16:LN:68:ARG:HA	16:LN:98:LEU:HD21	1.93	0.49
22:LT:17:ARG:HB2	22:LT:22:HIS:CE1	2.47	0.49
78:SZ:72:VAL:O	78:SZ:76:ARG:HB2	2.12	0.49
1:L5:1872:G:O2'	1:L5:4219:A:N3	2.43	0.49
1:L5:3681:G:H2'	4:LA:128:ARG:HG3	1.94	0.49
1:L5:4140:C:H3'	1:L5:4141:G:H4'	1.95	0.49
47:S2:1362:U:H4'	47:S2:1371:U:O2	2.12	0.49
47:S2:1756:C:H42	47:S2:1775:U:H3	1.59	0.49
54:SH:20:GLU:HG3	54:SH:23:ILE:HB	1.94	0.49
1:L5:88:A:N7	19:LQ:173:LYS:NZ	2.60	0.49
12:LI:30:LYS:HE2	12:LI:66:GLU:OE1	2.12	0.49
27:LY:4:ASN:HB3	27:LY:7:VAL:HG22	1.94	0.49
47:S2:64:A:OP1	71:SG:177:GLN:NE2	2.45	0.49
47:S2:508:A:H5''	47:S2:508:A:C8	2.46	0.49
62:ST:39:LEU:O	62:ST:40:ALA:CB	2.61	0.49
1:L5:980:U:H3	1:L5:1274:A:H61	1.59	0.49
1:L5:2714:G:H2'	1:L5:2715:G:H8	1.78	0.49
3:L8:127:U:H2'	3:L8:128:C:H5''	1.95	0.49
5:LB:14:LEU:HD23	5:LB:17:LEU:HD21	1.93	0.49
15:LM:38:VAL:HG21	15:LM:55:MET:HE1	1.94	0.49
26:LX:37:LYS:HB3	26:LX:38:LYS:HE2	1.94	0.49
47:S2:78:C:O5'	47:S2:78:C:H6	1.95	0.49
55:SI:165:GLN:HE21	55:SI:171:LEU:HA	1.77	0.49
56:SK:14:LEU:HA	56:SK:17:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Sg:152:SER:H	69:Sg:169:GLY:HA2	1.78	0.49
1:L5:73:A:H62	14:LL:103:ARG:HH22	1.59	0.49
1:L5:3946:G:C1'	1:L5:3947:A:C2	2.93	0.49
39:Lk:3:ARG:HG3	39:Lk:43:TYR:HE1	1.77	0.49
52:SE:18:TRP:HH2	52:SE:31:PRO:HD3	1.77	0.49
1:L5:1446:C:H6	1:L5:1446:C:H5''	1.78	0.49
1:L5:2017:A:H5''	1:L5:2018:C:H5	1.78	0.49
1:L5:3960:A:N6	1:L5:4043:G:N7	2.60	0.49
10:LG:200:THR:HG22	10:LG:201:THR:HG23	1.94	0.49
47:S2:1023:A:H5''	74:SN:4:MET:HE2	1.94	0.49
62:ST:62:ARG:O	62:ST:62:ARG:HG2	2.12	0.49
63:SU:22:ILE:HG12	63:SU:114:VAL:HG22	1.95	0.49
69:Sg:73:SER:H	69:Sg:117:ASN:HD21	1.61	0.49
5:LB:103:LYS:HD3	5:LB:104:THR:H	1.76	0.49
46:Lz:119:GLN:HA	46:Lz:122:ARG:HH21	1.77	0.49
47:S2:1116:C:H5'	47:S2:1116:C:H6	1.76	0.49
52:SE:175:PHE:HE2	52:SE:198:ARG:HG3	1.78	0.49
78:SZ:48:VAL:HA	78:SZ:83:LEU:CD1	2.37	0.49
1:L5:1178:G:N3	1:L5:1178:G:C2'	2.72	0.49
1:L5:1207:C:O2	1:L5:1207:C:H2'	2.12	0.49
1:L5:1802:A:N3	22:LT:130:ARG:NH1	2.60	0.49
5:LB:46:PHE:HE2	5:LB:81:THR:HB	1.78	0.49
5:LB:160:ILE:CG1	5:LB:193:LYS:HG3	2.43	0.49
5:LB:323:TYR:CD1	5:LB:342:LYS:HG2	2.48	0.49
13:LJ:43:LEU:HD12	13:LJ:44:THR:HG23	1.95	0.49
47:S2:1549:U:OP1	68:Sd:34:TYR:OH	2.31	0.49
1:L5:4265:U:OP1	7:LD:12:TYR:OH	2.30	0.49
5:LB:37:PRO:HA	5:LB:188:GLY:N	2.28	0.49
5:LB:85:VAL:HG22	5:LB:204:GLN:HG2	1.94	0.49
7:LD:223:PHE:HB3	7:LD:226:TYR:HB2	1.94	0.49
51:SD:169:ASP:OD2	51:SD:190:LEU:HD21	2.13	0.49
69:Sg:124:SER:OG	69:Sg:126:ASP:OD1	2.28	0.49
69:Sg:178:ASN:HB3	69:Sg:185:LYS:HD2	1.93	0.49
69:Sg:191:HIS:CG	69:Sg:195:LEU:HD21	2.47	0.49
75:SO:95:ILE:HB	75:SO:129:ILE:HA	1.93	0.49
77:SY:104:ARG:O	77:SY:108:LYS:HG3	2.12	0.49
1:L5:504:G:H2'	1:L5:504:G:N3	2.27	0.48
1:L5:2561:C:H2'	1:L5:2562:G:C8	2.48	0.48
6:LC:318:PRO:HG2	9:LF:155:TYR:HB3	1.95	0.48
7:LD:50:ARG:HG3	7:LD:147:ASP:HB2	1.95	0.48
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LL:91:ALA:HB1	14:LL:96:ILE:HB	1.94	0.48
18:LP:122:ALA:HB3	18:LP:143:PRO:HG2	1.94	0.48
47:S2:733:C:C5	47:S2:734:C:H1'	2.48	0.48
47:S2:1627:C:H5''	62:ST:41:LYS:HD3	1.94	0.48
54:SH:12:ASN:HD22	54:SH:13:GLY:H	1.61	0.48
69:Sg:120:ILE:HB	69:Sg:132:TRP:HB2	1.95	0.48
71:SG:5:ILE:HG13	71:SG:111:LEU:HB2	1.94	0.48
1:L5:1600:A:H5'	18:LP:133:HIS:HA	1.95	0.48
1:L5:2847:G:O2'	24:LV:21:PRO:HD2	2.13	0.48
1:L5:4940:C:H5'	8:LE:187:ARG:HH21	1.79	0.48
10:LG:257:LYS:HE2	10:LG:261:LEU:HG	1.95	0.48
58:SP:38:SER:O	58:SP:42:ARG:HB2	2.13	0.48
1:L5:73:A:H8	1:L5:73:A:C5'	2.23	0.48
1:L5:1763:C:N4	1:L5:1764:G:H21	2.12	0.48
3:L8:53:G:H4'	40:Ll:40:LYS:HD2	1.96	0.48
15:LM:70:GLN:HE21	15:LM:74:ARG:HH22	1.58	0.48
28:LZ:41:ALA:HB2	28:LZ:77:TYR:HE1	1.78	0.48
45:Lr:87:ARG:HB2	45:Lr:87:ARG:CZ	2.43	0.48
70:SC:196:ILE:HB	70:SC:223:TYR:HB2	1.94	0.48
71:SG:194:LEU:HD13	71:SG:197:GLN:HE21	1.77	0.48
74:SN:40:LEU:HB3	74:SN:45:LEU:HD12	1.95	0.48
5:LB:168:MET:HE2	5:LB:175:GLN:HE21	1.78	0.48
43:Lo:44:LYS:HE3	43:Lo:52:THR:HB	1.94	0.48
1:L5:1966:C:H42	1:L5:2021:G:H1	1.61	0.48
20:LR:172:ARG:HG2	20:LR:173:ARG:N	2.27	0.48
23:LU:101:ARG:HB3	23:LU:113:ARG:HB2	1.96	0.48
47:S2:1310:U:H5''	81:Sf:130:VAL:HB	1.96	0.48
53:SF:138:ALA:HB2	53:SF:204:ARG:HA	1.95	0.48
1:L5:139:G:H2'	1:L5:140:G:C8	2.48	0.48
3:L8:114:G:H1	3:L8:136:U:H3	1.60	0.48
5:LB:115:LYS:HA	5:LB:118:PHE:HD2	1.79	0.48
5:LB:117:ARG:HA	5:LB:177:LYS:HD2	1.95	0.48
16:LN:135:ILE:HD12	16:LN:151:ILE:HD13	1.95	0.48
47:S2:878:G:C2	47:S2:909:G:N2	2.81	0.48
49:SA:50:ASN:HB3	49:SA:53:ARG:HG2	1.92	0.48
50:SB:103:MET:HE2	50:SB:215:VAL:HG23	1.96	0.48
51:SD:39:VAL:HG13	51:SD:48:ILE:HG12	1.94	0.48
58:SP:96:VAL:HG11	58:SP:116:LEU:HB3	1.96	0.48
67:Sc:18:LEU:HD11	67:Sc:31:ARG:HD2	1.95	0.48
71:SG:121:ILE:HD12	71:SG:124:LEU:HD22	1.95	0.48
7:LD:111:ASN:HB3	7:LD:116:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LQ:159:PRO:HA	19:LQ:160:HIS:HA	1.62	0.48
34:Lf:46:ARG:HD3	34:Lf:106:TYR:HD2	1.79	0.48
52:SE:45:ILE:HA	52:SE:61:VAL:HG11	1.96	0.48
53:SF:23:TRP:HH2	53:SF:101:HIS:CG	2.30	0.48
75:SO:34:PHE:HB3	75:SO:41:PHE:HB2	1.96	0.48
1:L5:458:C:H2'	1:L5:459:C:C6	2.48	0.48
1:L5:1692:C:H4'	19:LQ:143:ARG:HH12	1.78	0.48
1:L5:2838:G:H5'	5:LB:247:GLY:HA2	1.95	0.48
1:L5:3956:G:C4'	1:L5:3964:U:C6	2.96	0.48
3:L8:121:G:C2'	3:L8:122:G:H5'	2.44	0.48
19:LQ:27:LEU:HD11	45:Lr:4:HIS:HB3	1.95	0.48
26:LX:71:LEU:HD22	26:LX:103:LYS:HD2	1.96	0.48
47:S2:1344:A:N6	47:S2:1386:A:H5'	2.29	0.48
47:S2:1755:C:C6	47:S2:1757:G:O6	2.65	0.48
1:L5:179:G:O5'	1:L5:179:G:H8	1.97	0.48
1:L5:4139:G:H2'	1:L5:4140:C:H5''	1.96	0.48
5:LB:219:VAL:HG11	5:LB:337:VAL:HG13	1.95	0.48
5:LB:262:VAL:HG11	5:LB:268:ARG:HH11	1.78	0.48
5:LB:378:ARG:HD2	25:LW:32:LEU:HD21	1.95	0.48
6:LC:182:LYS:HG2	6:LC:204:ARG:HD2	1.96	0.48
49:SA:122:LEU:HB3	49:SA:144:THR:HG22	1.95	0.48
53:SF:60:ARG:HH21	67:Sc:49:PRO:HA	1.79	0.48
78:SZ:79:ILE:H	78:SZ:79:ILE:HD12	1.78	0.48
1:L5:1400:G:H1	1:L5:1417:C:H42	1.62	0.48
47:S2:1171:G:O2'	47:S2:1187:G:O6	2.32	0.48
69:Sg:79:LEU:HD11	69:Sg:87:LEU:HD23	1.95	0.48
1:L5:2850:A:N3	1:L5:2850:A:H2'	2.29	0.47
1:L5:4650:G:H8	1:L5:4650:G:O5'	1.97	0.47
47:S2:522:A:H5''	72:SJ:145:PRO:HD2	1.96	0.47
47:S2:1145:A:O3'	66:Sa:89:ARG:NH1	2.47	0.47
47:S2:1284:A:HO2'	73:SM:106:CYS:HG	1.59	0.47
79:Sb:19:HIS:CD2	79:Sb:21:LYS:H	2.32	0.47
1:L5:4464:A:H2'	1:L5:4464:A:N3	2.29	0.47
6:LC:1:MET:HB2	6:LC:2:ALA:H	1.56	0.47
7:LD:80:ALA:HA	7:LD:83:LEU:HD13	1.95	0.47
8:LE:119:GLU:CG	33:Le:7:LEU:HG	2.43	0.47
12:LI:109:ASP:HA	12:LI:110:ARG:HA	1.67	0.47
33:Le:43:ASN:O	33:Le:47:ARG:HG3	2.14	0.47
49:SA:77:ILE:HD12	49:SA:122:LEU:HD11	1.95	0.47
54:SH:60:ILE:HG23	54:SH:90:LYS:HD2	1.96	0.47
55:SI:63:GLY:HA3	55:SI:65:PHE:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SQ:97:GLN:OE1	69:Sg:60:ARG:NH1	2.47	0.47
73:SM:51:VAL:HG23	73:SM:77:ILE:HB	1.96	0.47
1:L5:963:G:N7	1:L5:964:A:N6	2.62	0.47
1:L5:1695:U:H2'	1:L5:1696:C:C6	2.49	0.47
1:L5:2406:G:N7	40:L1:2:SER:N	2.63	0.47
17:LO:201:LEU:N	17:LO:201:LEU:CD1	2.73	0.47
52:SE:43:PRO:HG2	52:SE:46:ILE:HG12	1.97	0.47
58:SP:81:ARG:NH2	58:SP:117:GLY:O	2.47	0.47
78:SZ:77:LEU:HD12	78:SZ:79:ILE:HD11	1.96	0.47
1:L5:1762:C:H3'	1:L5:1763:C:H5''	1.97	0.47
1:L5:2847:G:H1'	24:LV:21:PRO:HD2	1.97	0.47
19:LQ:122:THR:OG1	19:LQ:124:ASP:OD1	2.28	0.47
31:Lc:23:LYS:O	31:Lc:23:LYS:HD3	2.14	0.47
47:S2:956:G:H5''	47:S2:956:G:H8	1.79	0.47
47:S2:1254:C:H4'	63:SU:75:LYS:HE2	1.96	0.47
51:SD:141:LYS:HD3	51:SD:180:GLY:HA3	1.95	0.47
62:ST:3:GLY:HA3	62:ST:4:VAL:HA	1.67	0.47
69:Sg:40:ILE:HB	69:Sg:59:LEU:HB2	1.96	0.47
1:L5:2019:C:O2	1:L5:2019:C:H2'	2.14	0.47
1:L5:2025:A:N3	1:L5:2026:A:H1'	2.29	0.47
1:L5:2424:OMG:H2'	1:L5:2426:U:C5	2.50	0.47
8:LE:128:HIS:ND1	8:LE:128:HIS:C	2.73	0.47
8:LE:157:HIS:CD2	8:LE:187:ARG:HH11	2.31	0.47
47:S2:1550:G:H3'	47:S2:1579:A:H61	1.79	0.47
49:SA:37:TYR:HE1	49:SA:57:LYS:HD3	1.78	0.47
58:SP:33:LEU:HD11	58:SP:37:TYR:CE2	2.48	0.47
66:Sa:10:ARG:NH2	66:Sa:12:LYS:CE	2.77	0.47
1:L5:418:A:C2	3:L8:17:A:H1'	2.50	0.47
23:LU:61:VAL:HG23	23:LU:74:SER:HB3	1.96	0.47
28:LZ:64:LYS:HA	28:LZ:67:LYS:HE3	1.97	0.47
47:S2:545:A:H2'	47:S2:546:G:C8	2.50	0.47
49:SA:18:PHE:CE1	49:SA:174:MET:SD	3.07	0.47
51:SD:28:GLU:C	51:SD:29:LEU:HD23	2.40	0.47
63:SU:81:GLN:HE21	68:Sd:55:LEU:HB2	1.80	0.47
72:SJ:120:ALA:HB2	72:SJ:129:LEU:HD12	1.96	0.47
1:L5:3892:U:H4'	18:LP:80:GLN:HE22	1.80	0.47
4:LA:179:ILE:O	4:LA:179:ILE:HG22	2.15	0.47
7:LD:164:LYS:HD3	7:LD:180:PHE:CZ	2.49	0.47
8:LE:262:LYS:HG3	8:LE:268:GLN:HE21	1.80	0.47
10:LG:261:LEU:HD13	10:LG:264:LYS:HD3	1.97	0.47
16:LN:116:LEU:HD22	16:LN:135:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lz:91:LYS:HZ1	46:Lz:123:ILE:HG22	1.79	0.47
47:S2:197:U:H5'	47:S2:203:G:H22	1.80	0.47
53:SF:179:ASN:HD21	53:SF:186:ASN:HB3	1.80	0.47
70:SC:272:HIS:HA	70:SC:275:LYS:HE2	1.95	0.47
71:SG:142:ARG:HB2	71:SG:147:LEU:HB2	1.97	0.47
1:L5:1762:C:H5'	1:L5:1763:C:H5	1.78	0.47
1:L5:2253:A:H61	9:LF:27:GLU:HB3	1.80	0.47
1:L5:2637:U:HO2'	1:L5:2718:U:HO2'	1.59	0.47
1:L5:3656:A:H2'	1:L5:3657:U:C6	2.50	0.47
2:L7:73:U:H6	2:L7:73:U:O5'	1.98	0.47
5:LB:29:VAL:HG13	5:LB:348:ARG:HD3	1.96	0.47
9:LF:32:ARG:C	9:LF:34:ARG:N	2.67	0.47
22:LT:3:ASN:OD1	22:LT:3:ASN:N	2.44	0.47
27:LY:10:ASP:HB2	27:LY:13:LYS:HB2	1.96	0.47
40:Ll:16:LYS:HG2	40:Ll:19:GLN:HE21	1.79	0.47
43:Lo:66:ILE:HD13	43:Lo:91:PHE:HB2	1.96	0.47
46:Lz:17:VAL:HG21	46:Lz:180:VAL:HG23	1.97	0.47
47:S2:698:G:H3'	47:S2:698:G:OP2	2.15	0.47
47:S2:1256:G:H8	63:SU:66:ARG:HB2	1.80	0.47
73:SM:31:LEU:HD22	73:SM:112:LYS:H	1.79	0.47
1:L5:1193:C:H2'	1:L5:1194:G:H8	1.80	0.47
11:LH:106:GLN:HA	11:LH:106:GLN:HE21	1.78	0.47
12:LI:184:MET:HB3	12:LI:190:LEU:HD13	1.95	0.47
24:LV:60:MET:HE1	24:LV:106:VAL:HG21	1.96	0.47
31:Lc:81:LEU:O	31:Lc:81:LEU:HD12	2.15	0.47
41:Lm:98:MLZ:HD3	41:Lm:118:THR:HG21	1.96	0.47
47:S2:1254:C:H4'	63:SU:75:LYS:CE	2.44	0.47
53:SF:71:ARG:NH1	53:SF:148:ASN:ND2	2.57	0.47
54:SH:124:ALA:HA	54:SH:127:ASP:OD1	2.14	0.47
55:SI:110:ARG:NH2	55:SI:166:PHE:O	2.48	0.47
1:L5:2907:G:O5'	1:L5:2907:G:H8	1.97	0.47
1:L5:3963:A:H8	1:L5:3965:A:H5''	1.80	0.47
9:LF:124:LYS:HB3	9:LF:124:LYS:HE2	1.60	0.47
31:Lc:15:ASN:HA	31:Lc:18:LEU:HB3	1.97	0.47
47:S2:1243:PSU:OP2	47:S2:1518:C:H1'	2.15	0.47
53:SF:102:LEU:HD11	78:SZ:100:VAL:HG21	1.97	0.47
1:L5:2100:A:H2'	1:L5:2100:A:N3	2.29	0.46
1:L5:4868:G:O2'	1:L5:4872:2MG:OP1	2.31	0.46
1:L5:5026:U:H4'	1:L5:5027:C:H5'	1.97	0.46
49:SA:57:LYS:HE2	49:SA:57:LYS:HB3	1.49	0.46
1:L5:167:C:O5'	1:L5:167:C:H6	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1824:G:H5''	22:LT:35:LYS:HE3	1.97	0.46
1:L5:3658:C:H4'	4:LA:240:ALA:HB2	1.96	0.46
1:L5:3658:C:H2'	1:L5:3659:G:C8	2.50	0.46
1:L5:4472:G:H5''	41:Lm:102:ARG:NH2	2.30	0.46
4:LA:116:LEU:HB2	4:LA:126:LEU:HB2	1.97	0.46
9:LF:171:ASP:HB3	9:LF:174:LEU:HD13	1.95	0.46
47:S2:448:A:H5''	55:SI:25:ARG:HA	1.97	0.46
47:S2:1117:C:H2'	47:S2:1118:C:C6	2.51	0.46
51:SD:146:ARG:NH1	51:SD:146:ARG:CB	2.73	0.46
1:L5:158:A:H5''	1:L5:159:C:H2'	1.98	0.46
1:L5:467:U:H5	1:L5:686:A:H61	1.63	0.46
1:L5:1447:C:N3	1:L5:2099:G:N1	2.63	0.46
1:L5:3946:G:O2'	1:L5:3947:A:C4	2.61	0.46
1:L5:4379:A:C8	43:Lo:54:PRO:HB3	2.51	0.46
1:L5:4426:C:C2'	1:L5:4427:G:H5'	2.45	0.46
1:L5:4699:U:H1'	1:L5:4700:A:H5''	1.98	0.46
1:L5:4921:C:O2	1:L5:4921:C:H2'	2.15	0.46
1:L5:5006:U:H4'	1:L5:5007:A:H5'	1.98	0.46
6:LC:320:LYS:HZ3	6:LC:320:LYS:CB	2.28	0.46
42:Lm:8:LYS:HE3	42:Lm:12:ARG:NH2	2.31	0.46
50:SB:83:LYS:HE3	50:SB:106:THR:HG22	1.97	0.46
53:SF:99:ILE:HD11	78:SZ:106:GLN:HE22	1.80	0.46
67:Sc:44:ARG:CZ	67:Sc:63:ARG:HB2	2.38	0.46
70:SC:144:SER:HB3	70:SC:150:ALA:HB2	1.98	0.46
1:L5:709:C:OP1	34:Lf:89:ARG:NH1	2.48	0.46
1:L5:1739:G:N3	1:L5:1742:A:N6	2.63	0.46
10:LG:102:TYR:CE2	10:LG:207:VAL:HG13	2.51	0.46
16:LN:104:GLU:HA	16:LN:160:GLU:HG3	1.97	0.46
21:LS:85:ASP:HB3	21:LS:90:THR:HB	1.97	0.46
24:LV:60:MET:HE2	24:LV:80:VAL:HG22	1.96	0.46
31:Lc:90:ARG:NH1	44:Lp:44:LYS:HG2	2.29	0.46
55:SI:63:GLY:HA3	55:SI:65:PHE:CE1	2.50	0.46
65:SX:102:VAL:HG12	65:SX:122:VAL:HG22	1.97	0.46
73:SM:48:HIS:HB2	73:SM:111:VAL:HG23	1.98	0.46
1:L5:2418:A:H5'	18:LP:125:MET:HE1	1.98	0.46
15:LM:41:PRO:HG3	15:LM:73:VAL:HG23	1.97	0.46
47:S2:107:A:H2'	47:S2:108:G:C8	2.51	0.46
47:S2:1742:C:H6	47:S2:1742:C:H5''	1.81	0.46
71:SG:141:ILE:HD11	71:SG:157:VAL:HA	1.98	0.46
78:SZ:77:LEU:HD23	78:SZ:77:LEU:N	2.30	0.46
1:L5:3954:A:N6	1:L5:4056:A:N1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LJ:35:ARG:HD2	13:LJ:122:SER:O	2.16	0.46
25:LW:5:LEU:HD13	25:LW:11:TYR:O	2.15	0.46
29:La:42:ARG:HG3	29:La:42:ARG:NH2	2.30	0.46
36:Lh:7:ARG:HH11	38:Lj:87:LYS:NZ	2.14	0.46
37:Li:79:THR:HG22	37:Li:81:ILE:H	1.81	0.46
74:SN:3:ARG:HB3	74:SN:6:ALA:O	2.15	0.46
1:L5:2561:C:O5'	1:L5:2561:C:H6	1.99	0.46
6:LC:1:MET:HA	6:LC:267:TRP:HB2	1.96	0.46
6:LC:133:LEU:HD13	45:Lr:6:GLN:HE21	1.81	0.46
17:LO:12:ARG:HB2	17:LO:37:ARG:HD2	1.97	0.46
27:LY:56:GLN:HB3	27:LY:67:ILE:HD13	1.96	0.46
43:Lo:11:PHE:CE2	43:Lo:13:LYS:HA	2.51	0.46
46:Lz:55:LEU:HD22	46:Lz:183:ILE:HG12	1.97	0.46
47:S2:1752:C:N3	47:S2:1779:G:N1	2.59	0.46
52:SE:125:LYS:H	52:SE:142:HIS:HD2	1.63	0.46
74:SN:46:THR:H	74:SN:49:GLN:HE21	1.64	0.46
75:SO:14:VAL:HG23	75:SO:15:ILE:HA	1.97	0.46
1:L5:3948:C:H3'	1:L5:3949:A:N3	2.31	0.46
10:LG:103:ARG:HE	10:LG:193:LEU:HA	1.80	0.46
31:Lc:36:LYS:O	31:Lc:40:GLN:NE2	2.48	0.46
33:Le:70:LEU:HD21	33:Le:76:LYS:HB2	1.98	0.46
47:S2:1115:U:O2	47:S2:1115:U:O2'	2.21	0.46
48:S6:6:G:H2'	48:S6:7:A:H8	1.80	0.46
1:L5:1304:C:C5'	1:L5:1304:C:C6	2.96	0.46
1:L5:4935:C:H2'	1:L5:4936:G:H8	1.81	0.46
7:LD:256:LYS:HD2	7:LD:257:PRO:HD2	1.97	0.46
8:LE:128:HIS:O	8:LE:128:HIS:CG	2.69	0.46
13:LJ:10:ASN:OD1	13:LJ:10:ASN:N	2.48	0.46
47:S2:824:C:H1'	72:SJ:144:ILE:HG21	1.97	0.46
71:SG:59:GLN:OE1	71:SG:72:ARG:NH2	2.49	0.46
1:L5:1778:C:H1'	7:LD:2:GLY:HA2	1.98	0.46
1:L5:3658:C:H4'	4:LA:240:ALA:CB	2.45	0.46
1:L5:4139:G:C2'	1:L5:4140:C:H5''	2.46	0.46
1:L5:4645:C:OP2	20:LR:62:ARG:NH1	2.47	0.46
8:LE:138:ARG:N	8:LE:138:ARG:HD3	2.31	0.46
32:Ld:62:VAL:HG12	32:Ld:104:THR:HB	1.98	0.46
51:SD:146:ARG:HB3	51:SD:146:ARG:HH11	1.77	0.46
63:SU:24:LEU:HB3	63:SU:32:LEU:HD11	1.97	0.46
69:Sg:39:THR:HG22	69:Sg:60:ARG:HG2	1.98	0.46
10:LG:176:LYS:HD2	37:Li:39:PHE:HE1	1.81	0.45
12:LI:184:MET:HA	12:LI:187:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:140:ASP:HB3	67:Sc:46:VAL:HG12	1.98	0.45
59:SQ:13:PHE:HA	59:SQ:22:VAL:HA	1.98	0.45
79:Sb:36:LYS:HE2	79:Sb:43:ILE:HD11	1.99	0.45
1:L5:178:C:H6	1:L5:178:C:H5''	1.80	0.45
2:L7:102:U:H2'	2:L7:103:A:H8	1.81	0.45
5:LB:245:HIS:ND1	5:LB:245:HIS:C	2.73	0.45
10:LG:156:VAL:HG13	10:LG:184:ILE:HG13	1.98	0.45
13:LJ:85:LYS:HB3	13:LJ:115:LEU:HB3	1.98	0.45
13:LJ:120:ASP:CB	13:LJ:121:PRO:CD	2.91	0.45
18:LP:48:LEU:HD21	18:LP:91:LEU:HB3	1.98	0.45
18:LP:147:GLU:O	18:LP:147:GLU:HG2	2.16	0.45
47:S2:77:A:H1'	71:SG:176:ILE:HG13	1.98	0.45
47:S2:508:A:H3'	47:S2:509:OMG:C8	2.50	0.45
47:S2:923:G:OP1	74:SN:2:GLY:HA2	2.16	0.45
49:SA:56:GLU:OE2	49:SA:56:GLU:HA	2.16	0.45
50:SB:91:VAL:HG12	50:SB:93:GLY:H	1.81	0.45
53:SF:143:PRO:HD3	67:Sc:56:LEU:HD23	1.97	0.45
68:Sd:22:ARG:HG2	68:Sd:38:MET:HG2	1.97	0.45
76:SW:37:PHE:HE1	76:SW:41:MET:HE3	1.81	0.45
1:L5:180:C:H6	1:L5:180:C:C3'	2.29	0.45
1:L5:3667:C:H4'	4:LA:8:GLN:HA	1.98	0.45
4:LA:28:ARG:HG3	4:LA:123:ARG:HH11	1.81	0.45
5:LB:224:LYS:HG3	5:LB:340:THR:HG22	1.99	0.45
8:LE:74:SER:HA	30:Lb:117:ARG:HB3	1.98	0.45
39:Lk:22:SER:HA	39:Lk:65:ALA:HB3	1.99	0.45
44:Lp:64:VAL:CG1	44:Lp:71:TYR:CE1	2.97	0.45
54:SH:40:LEU:HD12	54:SH:43:LEU:HD11	1.97	0.45
54:SH:43:LEU:HB2	54:SH:72:PHE:HE1	1.80	0.45
54:SH:107:LYS:HE3	54:SH:107:LYS:HB2	1.78	0.45
78:SZ:50:PHE:HE1	78:SZ:79:ILE:CD1	2.26	0.45
1:L5:1332:C:H2'	1:L5:1333:A:C8	2.51	0.45
1:L5:2325:C:H2'	1:L5:2326:G:H8	1.81	0.45
13:LJ:120:ASP:HB2	13:LJ:123:ILE:HD13	1.97	0.45
18:LP:40:HIS:NE2	18:LP:110:ASP:O	2.48	0.45
21:LS:88:SER:OG	21:LS:89:GLY:N	2.49	0.45
23:LU:107:LYS:HE2	23:LU:107:LYS:HB2	1.53	0.45
27:LY:131:GLU:HA	27:LY:134:LYS:HE3	1.97	0.45
46:Lz:49:PHE:HE2	46:Lz:189:PHE:HB3	1.81	0.45
46:Lz:59:PRO:HB3	46:Lz:170:GLY:HA3	1.98	0.45
47:S2:1543:U:H4'	59:SQ:43:GLU:HG3	1.98	0.45
49:SA:17:LYS:HB3	60:SR:91:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SD:42:THR:H	51:SD:46:THR:HG22	1.80	0.45
78:SZ:65:TYR:OH	78:SZ:76:ARG:NH1	2.48	0.45
1:L5:190:G:H2'	1:L5:191:G:H8	1.80	0.45
1:L5:2583:C:OP2	35:Lg:76:ARG:NH1	2.43	0.45
1:L5:4147:G:H2'	1:L5:4148:C:H6	1.81	0.45
1:L5:4752:U:H4'	17:LO:4:VAL:HG11	1.98	0.45
10:LG:136:LEU:HD21	10:LG:204:PHE:CE1	2.52	0.45
17:LO:199:HIS:C	17:LO:201:LEU:HD12	2.41	0.45
28:LZ:96:VAL:HG12	28:LZ:110:ALA:HB1	1.99	0.45
47:S2:1158:G:H5''	76:SW:76:SER:HB3	1.99	0.45
59:SQ:19:ALA:HB2	59:SQ:75:GLY:HA3	1.99	0.45
62:ST:5:THR:HG23	62:ST:7:LYS:H	1.82	0.45
1:L5:74:G:H5'	14:LL:59:VAL:HG13	1.98	0.45
8:LE:185:PRO:HA	8:LE:250:GLN:HE22	1.82	0.45
9:LF:200:ARG:HH11	9:LF:200:ARG:CG	2.13	0.45
11:LH:115:ARG:NH1	11:LH:123:ILE:CG1	2.43	0.45
16:LN:138:PHE:HA	16:LN:143:ARG:HD2	1.98	0.45
43:Lo:92:GLU:HG3	43:Lo:93:LEU:N	2.30	0.45
46:Lz:67:VAL:HA	46:Lz:68:LEU:HA	1.60	0.45
50:SB:146:ARG:HB2	50:SB:149:GLN:HB2	1.98	0.45
51:SD:102:ALA:HB1	51:SD:173:ARG:HG2	1.99	0.45
54:SH:187:PHE:N	54:SH:187:PHE:CD1	2.85	0.45
61:SS:38:ARG:O	61:SS:42:HIS:ND1	2.35	0.45
64:SV:50:PHE:C	64:SV:50:PHE:HD1	2.25	0.45
1:L5:2581:A:N3	1:L5:2654:C:O2'	2.48	0.45
1:L5:4389:C:H2'	1:L5:4390:A:C8	2.50	0.45
1:L5:4491:G:H5''	5:LB:9:PRO:HG3	1.99	0.45
1:L5:4957:C:H2'	1:L5:4958:C:C6	2.51	0.45
6:LC:159:GLU:HA	6:LC:217:ILE:HB	1.98	0.45
8:LE:130:LYS:HD2	8:LE:130:LYS:H	1.82	0.45
24:LV:83:ARG:HD3	24:LV:120:PRO:O	2.17	0.45
55:SI:74:ARG:NH1	55:SI:74:ARG:CG	2.73	0.45
58:SP:44:ARG:NH1	58:SP:82:ASP:O	2.47	0.45
68:Sd:3:HIS:CE1	68:Sd:5:GLN:HB2	2.52	0.45
1:L5:1559:G:OP1	20:LR:126:LYS:NZ	2.50	0.45
1:L5:2487:G:N1	1:L5:2491:C:N3	2.64	0.45
1:L5:4775:C:C3'	1:L5:4775:C:C6	3.00	0.45
1:L5:4986:G:H5''	5:LB:176:LYS:HG3	1.98	0.45
83:L5:5374:HMT:O8	83:L5:5374:HMT:O6	2.35	0.45
8:LE:91:THR:HG22	8:LE:108:LYS:HB3	1.98	0.45
47:S2:1191:C:H2'	47:S2:1192:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SD:172:VAL:O	51:SD:173:ARG:CD	2.58	0.45
61:SS:38:ARG:HB3	62:ST:45:LEU:HD21	1.99	0.45
1:L5:1754:U:O5'	1:L5:1754:U:C6	2.70	0.45
1:L5:2434:G:O2'	1:L5:2527:A:N1	2.48	0.45
1:L5:4279:A:H5'	1:L5:4281:A:H1'	1.98	0.45
1:L5:4996:C:H4'	32:Ld:26:THR:HG23	1.99	0.45
7:LD:194:VAL:HA	7:LD:197:LYS:HD3	1.98	0.45
29:La:132:ARG:HA	29:La:135:GLU:HG2	1.98	0.45
52:SE:45:ILE:HG23	52:SE:46:ILE:HG23	1.99	0.45
54:SH:185:VAL:HG23	54:SH:187:PHE:CD1	2.52	0.45
56:SK:1:MET:HG3	56:SK:3:MET:HB2	1.98	0.45
58:SP:76:VAL:O	58:SP:95:GLY:N	2.46	0.45
58:SP:123:TYR:CG	58:SP:123:TYR:O	2.70	0.45
69:Sg:119:GLN:HE22	69:Sg:179:LEU:HD12	1.82	0.45
1:L5:128:C:O5'	1:L5:128:C:H6	2.00	0.45
1:L5:390:C:H42	1:L5:401:G:H1	1.63	0.45
1:L5:2062:C:O2'	21:LS:111:ARG:NH1	2.50	0.45
1:L5:2417:A:OP2	1:L5:2417:A:C8	2.70	0.45
1:L5:4133:C:H42	1:L5:4151:G:H1	1.65	0.45
17:LO:85:ARG:HE	17:LO:85:ARG:HB3	1.61	0.45
18:LP:118:GLN:HE21	18:LP:120:ASN:ND2	2.15	0.45
47:S2:1623:A:N1	61:SS:132:ARG:NH1	2.65	0.45
49:SA:50:ASN:CB	49:SA:53:ARG:HG3	2.36	0.45
54:SH:95:ILE:HD11	54:SH:129:ILE:HG12	1.99	0.45
74:SN:20:ARG:HH21	76:SW:56:HIS:HB3	1.82	0.45
1:L5:370:U:O5'	1:L5:370:U:H6	2.00	0.44
1:L5:2047:A:N3	1:L5:2050:OMG:H5''	2.32	0.44
1:L5:2563:C:OP1	1:L5:2563:C:C5	2.70	0.44
5:LB:160:ILE:HG21	5:LB:194:LEU:HD12	1.98	0.44
7:LD:202:GLN:O	7:LD:206:ASP:CG	2.60	0.44
10:LG:102:TYR:HE2	10:LG:207:VAL:HG13	1.82	0.44
12:LI:68:ALA:HB2	12:LI:158:LYS:HB2	1.99	0.44
18:LP:94:MET:SD	18:LP:148:MET:HE3	2.58	0.44
26:LX:82:THR:HG21	36:Lh:37:THR:HG22	1.99	0.44
46:Lz:35:GLN:OE1	46:Lz:164:CYS:HB3	2.17	0.44
47:S2:748:C:H42	47:S2:794:A:H61	1.65	0.44
47:S2:1453:C:H4'	60:SR:49:LYS:HA	2.00	0.44
1:L5:3715:PSU:OP1	48:S6:4:C:O2'	2.34	0.44
15:LM:20:HIS:CD2	15:LM:48:GLN:HE22	2.35	0.44
55:SI:165:GLN:NE2	55:SI:172:LEU:H	2.15	0.44
57:SL:126:VAL:HG22	57:SL:145:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SW:102:ILE:HB	76:SW:113:HIS:HB3	1.99	0.44
1:L5:2096:G:C8	1:L5:2096:G:O5'	2.70	0.44
1:L5:4966:A:H5'	5:LB:128:LYS:HG3	1.98	0.44
2:L7:28:C:OP1	13:LJ:144:LYS:NZ	2.44	0.44
6:LC:40:VAL:HG22	6:LC:115:VAL:HG11	2.00	0.44
21:LS:95:ARG:HE	21:LS:95:ARG:HB3	1.58	0.44
33:Le:7:LEU:HB2	33:Le:93:LYS:HG3	1.99	0.44
43:Lo:21:HIS:HA	43:Lo:72:CYS:HA	1.99	0.44
47:S2:1499:U:H4'	51:SD:176:LEU:HD13	2.00	0.44
54:SH:191:GLU:HG3	54:SH:192:PHE:H	1.83	0.44
73:SM:91:LEU:HD13	73:SM:104:VAL:HG13	1.98	0.44
77:SY:10:ARG:HG2	77:SY:10:ARG:HH11	1.80	0.44
1:L5:1333:A:H2'	1:L5:1334:A:C8	2.52	0.44
8:LE:258:LEU:HD23	8:LE:262:LYS:HE2	2.00	0.44
11:LH:59:LYS:HE3	11:LH:66:GLU:HB3	1.99	0.44
25:LW:11:TYR:CD2	25:LW:32:LEU:HD22	2.51	0.44
47:S2:1779:G:H2'	47:S2:1780:G:H8	1.83	0.44
51:SD:60:GLY:HA3	51:SD:65:ARG:H	1.83	0.44
62:ST:96:SER:OG	62:ST:99:VAL:HG12	2.18	0.44
63:SU:55:ARG:HG2	63:SU:87:ARG:HG2	1.99	0.44
64:SV:50:PHE:C	64:SV:50:PHE:CD1	2.95	0.44
1:L5:254:G:H2'	1:L5:255:C:O5'	2.17	0.44
1:L5:256:G:C8	1:L5:256:G:OP2	2.70	0.44
1:L5:977:C:H4'	6:LC:333:MLZ:HCM1	1.99	0.44
1:L5:1581:G:C2'	1:L5:1582:PSU:H5'	2.46	0.44
1:L5:3946:G:C2'	1:L5:3947:A:H5'	2.45	0.44
1:L5:4323:A:C8	7:LD:153:THR:HG21	2.53	0.44
3:L8:102:G:OP2	3:L8:104:A:O2'	2.33	0.44
3:L8:106:G:H4'	3:L8:137:A:H5'	1.98	0.44
5:LB:115:LYS:HA	5:LB:118:PHE:CD2	2.52	0.44
10:LG:26:LYS:HG3	10:LG:28:VAL:HG13	1.98	0.44
16:LN:159:ARG:HH21	16:LN:165:THR:HA	1.81	0.44
51:SD:48:ILE:HB	51:SD:86:LEU:HD23	2.00	0.44
53:SF:127:ARG:HB3	53:SF:128:ILE:H	1.66	0.44
1:L5:1446:C:C5'	1:L5:1446:C:C6	2.95	0.44
9:LF:74:MET:HE3	9:LF:74:MET:HB3	1.64	0.44
11:LH:47:LEU:HD12	11:LH:53:LYS:HE3	1.98	0.44
12:LI:47:PRO:HG2	12:LI:142:LEU:HG	1.98	0.44
32:Ld:22:THR:HG23	32:Ld:122:VAL:HB	2.00	0.44
46:Lz:66:CYS:HB3	46:Lz:82:ILE:HD13	1.99	0.44
47:S2:37:C:H5''	47:S2:37:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:155:G:H4'	71:SG:15:LEU:HD13	2.00	0.44
54:SH:146:VAL:HG22	54:SH:152:ARG:HG2	2.00	0.44
60:SR:28:PHE:HA	60:SR:55:THR:HG21	1.99	0.44
68:Sd:6:LEU:HA	68:Sd:9:SER:HB3	2.00	0.44
75:SO:45:THR:HG22	75:SO:52:THR:HA	2.00	0.44
1:L5:169:G:H21	1:L5:171:U:H3	1.64	0.44
1:L5:685:C:H4'	1:L5:686:A:C4	2.53	0.44
1:L5:1618:G:H5''	38:Lj:13:ASN:HD21	1.82	0.44
1:L5:2503:G:O2'	1:L5:2505:C:O2	2.34	0.44
5:LB:49:TYR:N	5:LB:49:TYR:CD1	2.85	0.44
7:LD:123:VAL:HA	7:LD:248:ARG:HH12	1.82	0.44
20:LR:169:ALA:HA	20:LR:172:ARG:HD2	1.98	0.44
29:La:14:HIS:ND1	29:La:14:HIS:N	2.63	0.44
44:Lp:85:ARG:NH2	47:S2:939:U:C5'	2.80	0.44
47:S2:954:U:OP1	50:SB:24:PRO:HG3	2.18	0.44
49:SA:50:ASN:CB	49:SA:53:ARG:CG	2.90	0.44
59:SQ:51:LEU:HB2	59:SQ:81:ILE:HG23	1.99	0.44
62:ST:65:TYR:HB2	62:ST:123:LEU:HD11	2.00	0.44
66:Sa:28:ARG:HG3	66:Sa:29:CYS:N	2.32	0.44
1:L5:1448:G:O5'	1:L5:1448:G:C8	2.71	0.44
1:L5:4530:UR3:H2'	1:L5:4531:PSU:C6	2.53	0.44
1:L5:4875:G:H2'	21:LS:169:THR:HG22	1.99	0.44
1:L5:4921:C:H3'	1:L5:4922:C:C5	2.53	0.44
6:LC:221:PHE:CD2	6:LC:227:ILE:HG21	2.48	0.44
41:Lm:93:LYS:HD3	41:Lm:102:ARG:HG2	1.99	0.44
45:Lr:119:ARG:HG2	45:Lr:122:LYS:HE2	1.99	0.44
47:S2:888:U:H4'	47:S2:889:U:H5'	2.00	0.44
47:S2:1060:A:O2'	47:S2:1062:A:N7	2.46	0.44
50:SB:128:LYS:HA	50:SB:134:LEU:HA	1.99	0.44
61:SS:95:TYR:HD1	61:SS:95:TYR:H	1.64	0.44
79:Sb:49:HIS:ND1	79:Sb:69:GLY:O	2.51	0.44
1:L5:957:G:C2'	1:L5:958:G:H5'	2.47	0.44
1:L5:2528:G:N3	1:L5:2528:G:C2'	2.81	0.44
1:L5:3677:U:H5'	4:LA:17:ARG:HA	2.00	0.44
3:L8:121:G:H2'	3:L8:122:G:H5'	2.00	0.44
6:LC:80:ARG:H	6:LC:80:ARG:HG2	1.52	0.44
17:LO:141:LEU:O	17:LO:145:VAL:HB	2.18	0.44
22:LT:45:MET:HE2	22:LT:45:MET:HB3	1.85	0.44
24:LV:16:ILE:HD11	24:LV:57:VAL:H	1.82	0.44
26:LX:88:LYS:HD2	26:LX:88:LYS:HA	1.32	0.44
47:S2:921:G:H1'	74:SN:11:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:100:PHE:CD2	50:SB:185:VAL:HG21	2.53	0.44
57:SL:29:GLY:HA3	57:SL:30:LYS:HA	1.68	0.44
60:SR:67:ARG:HA	60:SR:68:GLY:HA3	1.57	0.44
1:L5:2050:OMG:CM2	1:L5:3885:G:H5'	2.48	0.43
1:L5:2820:C:H5''	20:LR:56:THR:HG23	2.00	0.43
1:L5:2864:A:H2'	1:L5:2865:U:C6	2.53	0.43
1:L5:3886:G:H5''	17:LO:82:ARG:HH22	1.83	0.43
2:L7:87:G:OP1	21:LS:87:ARG:NH2	2.51	0.43
4:LA:28:ARG:HG3	4:LA:123:ARG:HB3	2.00	0.43
6:LC:320:LYS:HB2	6:LC:320:LYS:NZ	2.27	0.43
21:LS:45:TRP:HA	21:LS:48:VAL:HG12	1.99	0.43
47:S2:1015:U:O2'	74:SN:55:ARG:NH1	2.51	0.43
49:SA:19:LEU:HD23	49:SA:24:HIS:CE1	2.53	0.43
54:SH:31:GLU:HA	54:SH:37:LYS:HZ2	1.83	0.43
59:SQ:97:GLN:HB3	59:SQ:105:LYS:HD3	2.00	0.43
69:Sg:69:VAL:HG23	69:Sg:80:SER:HB3	2.00	0.43
73:SM:13:ASP:HA	73:SM:16:THR:HB	2.00	0.43
1:L5:1281:G:OP2	8:LE:128:HIS:HE1	2.01	0.43
5:LB:379:PHE:CD1	5:LB:379:PHE:N	2.86	0.43
7:LD:288:LEU:HD22	7:LD:288:LEU:HA	1.83	0.43
22:LT:17:ARG:HA	22:LT:17:ARG:HD2	1.88	0.43
31:Lc:34:THR:HG21	31:Lc:93:THR:HG22	2.00	0.43
41:Lm:110:CYS:SG	41:Lm:111:ARG:N	2.91	0.43
45:Lr:28:GLU:HB2	45:Lr:31:ASN:HB2	2.00	0.43
46:Lz:52:THR:OG1	46:Lz:138:LEU:O	2.33	0.43
47:S2:106:C:O5'	47:S2:106:C:H6	2.01	0.43
47:S2:831:G:N7	77:SY:11:LYS:NZ	2.66	0.43
51:SD:169:ASP:OD2	51:SD:190:LEU:CD2	2.66	0.43
71:SG:18:VAL:HG11	71:SG:24:LEU:HD21	2.00	0.43
1:L5:1446:C:H5''	1:L5:1446:C:C6	2.53	0.43
1:L5:1590:C:H4'	1:L5:2857:A:H5'	2.00	0.43
1:L5:1966:C:C2	1:L5:1967:A:H1'	2.53	0.43
1:L5:4426:C:H2'	1:L5:4427:G:H5'	2.00	0.43
1:L5:4768:G:OP1	17:LO:168:TYR:OH	2.33	0.43
3:L8:15:G:H8	3:L8:15:G:O5'	2.01	0.43
7:LD:195:HIS:O	7:LD:199:ILE:HD12	2.19	0.43
18:LP:118:GLN:HE21	18:LP:120:ASN:HD21	1.67	0.43
23:LU:107:LYS:C	23:LU:108:GLU:HG3	2.43	0.43
45:Lr:52:GLU:N	45:Lr:61:VAL:O	2.50	0.43
47:S2:886:A:H3'	47:S2:887:U:C6	2.54	0.43
47:S2:1759:G:N7	47:S2:1761:U:H1'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SD:146:ARG:CB	51:SD:146:ARG:HH11	2.32	0.43
59:SQ:32:ILE:HG12	59:SQ:39:LEU:HD13	1.99	0.43
61:SS:95:TYR:N	61:SS:95:TYR:CD1	2.86	0.43
63:SU:26:SER:HB3	63:SU:32:LEU:HD22	1.99	0.43
70:SC:68:ARG:HH21	70:SC:71:LYS:CD	2.30	0.43
75:SO:27:VAL:HG13	75:SO:90:ILE:HA	1.99	0.43
1:L5:1254:A:N3	1:L5:1254:A:C2'	2.79	0.43
1:L5:1306:C:H2'	1:L5:1307:A:C8	2.53	0.43
1:L5:2380:G:N2	1:L5:2424:OMG:H5'	2.34	0.43
1:L5:4045:G:C6	1:L5:4048:A:H8	2.37	0.43
11:LH:18:ILE:HG22	11:LH:27:VAL:HA	2.00	0.43
23:LU:80:LYS:HE3	23:LU:108:GLU:HA	1.99	0.43
43:Lo:70:LEU:HD12	43:Lo:81:ARG:HH21	1.83	0.43
51:SD:123:LEU:HD22	51:SD:152:PHE:HB3	2.00	0.43
62:ST:64:LEU:HD23	62:ST:64:LEU:HA	1.75	0.43
1:L5:195:C:H4'	27:LY:122:LYS:HG2	2.01	0.43
1:L5:280:G:H5''	16:LN:14:LYS:HE2	2.00	0.43
1:L5:2812:A:OP1	20:LR:88:ARG:NH1	2.51	0.43
1:L5:3886:G:H5''	17:LO:82:ARG:NH2	2.33	0.43
2:L7:102:U:H2'	2:L7:103:A:C8	2.54	0.43
5:LB:73:VAL:O	24:LV:89:ARG:NH1	2.50	0.43
5:LB:289:GLN:HB3	5:LB:301:ASN:HB3	2.01	0.43
7:LD:41:LYS:NZ	22:LT:30:TYR:O	2.42	0.43
11:LH:59:LYS:HA	11:LH:59:LYS:HD2	1.86	0.43
29:La:27:LYS:HE2	29:La:27:LYS:HB3	1.80	0.43
33:Le:90:MET:HG3	45:Lr:33:LYS:HA	2.01	0.43
33:Le:91:CYS:O	33:Le:93:LYS:N	2.51	0.43
69:Sg:256:ILE:HB	69:Sg:270:LEU:HB2	2.00	0.43
1:L5:66:A:H61	1:L5:282:C:HO2'	1.67	0.43
1:L5:958:G:H5''	6:LC:311:ARG:NH1	2.33	0.43
1:L5:1754:U:O5'	1:L5:1754:U:H6	2.01	0.43
22:LT:22:HIS:HB3	22:LT:23:GLY:H	1.70	0.43
43:Lo:11:PHE:CD2	43:Lo:11:PHE:C	2.96	0.43
47:S2:1130:G:H4'	74:SN:10:GLY:HA2	2.00	0.43
56:SK:32:HIS:HD2	56:SK:45:VAL:HG11	1.83	0.43
57:SL:80:MET:HE3	57:SL:80:MET:HB2	1.90	0.43
78:SZ:102:LYS:HA	78:SZ:107:VAL:HG12	2.01	0.43
1:L5:685:C:OP2	1:L5:685:C:C6	2.70	0.43
1:L5:757:G:H1	1:L5:906:C:H42	1.66	0.43
6:LC:224:ILE:HB	6:LC:227:ILE:HD12	2.00	0.43
13:LJ:20:LEU:CD1	13:LJ:130:PHE:HD1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:108:ILE:CG2	17:LO:113:ASP:HA	2.48	0.43
20:LR:95:TRP:HE3	20:LR:98:ARG:HH21	1.66	0.43
25:LW:85:ALA:HB1	25:LW:89:ASP:HB3	2.01	0.43
33:Le:38:PRO:O	33:Le:46:ARG:HD3	2.18	0.43
42:Ln:10:MET:O	42:Ln:10:MET:HG3	2.19	0.43
47:S2:428:U:H4'	72:SJ:2:PRO:HD2	2.00	0.43
47:S2:837:A:H61	77:SY:9:THR:H	1.67	0.43
47:S2:1454:A:H5''	60:SR:3:ARG:HD3	2.01	0.43
52:SE:72:ILE:HD12	52:SE:77:ARG:HG3	2.01	0.43
62:ST:34:VAL:O	62:ST:52:TRP:NE1	2.47	0.43
71:SG:222:GLU:HB3	71:SG:223:LYS:NZ	2.31	0.43
1:L5:197:A:N3	1:L5:222:C:O2'	2.48	0.43
1:L5:254:G:C6	1:L5:255:C:C2	3.07	0.43
1:L5:1866:UR3:H3U2	1:L5:4405:G:C8	2.54	0.43
1:L5:2910:G:H8	1:L5:2910:G:O5'	2.01	0.43
1:L5:4196:OMG:HM23	1:L5:4196:OMG:H1'	1.84	0.43
1:L5:4775:C:C6	1:L5:4775:C:H3'	2.54	0.43
3:L8:129:C:O5'	3:L8:129:C:H6	2.02	0.43
7:LD:271:MET:HE1	7:LD:279:ARG:HD2	2.01	0.43
15:LM:6:PHE:O	15:LM:11:ARG:NE	2.50	0.43
33:Le:12:ILE:HG22	33:Le:14:LYS:HD3	2.00	0.43
42:Ln:4:LYS:HE2	47:S2:1844:U:O4	2.18	0.43
47:S2:878:G:N2	47:S2:909:G:N2	2.67	0.43
47:S2:1216:C:O5'	47:S2:1216:C:H6	2.01	0.43
72:SJ:78:LEU:HD23	72:SJ:92:MET:HB2	2.00	0.43
78:SZ:79:ILE:CD1	78:SZ:79:ILE:N	2.81	0.43
1:L5:1684:A:OP1	29:La:47:LYS:NZ	2.51	0.43
1:L5:1883:OMG:HM23	1:L5:1883:OMG:H1'	1.69	0.43
1:L5:4629:U:H1'	24:LV:95:PHE:CE2	2.54	0.43
5:LB:173:LEU:CD2	5:LB:342:LYS:HB3	2.48	0.43
11:LH:103:VAL:HG22	11:LH:114:ILE:HG12	2.00	0.43
12:LI:39:LYS:HA	12:LI:86:HIS:CD2	2.54	0.43
12:LI:55:ASP:O	12:LI:56:GLU:HG3	2.19	0.43
18:LP:118:GLN:NE2	18:LP:120:ASN:ND2	2.65	0.43
33:Le:37:LYS:HE3	33:Le:55:MET:CE	2.46	0.43
47:S2:5:U:H2'	47:S2:6:G:H8	1.84	0.43
47:S2:126:G:H2'	71:SG:199:THR:HG21	2.00	0.43
47:S2:913:A:N7	54:SH:98:ARG:O	2.52	0.43
47:S2:1330:G:H4'	47:S2:1331:C:H3'	1.99	0.43
47:S2:1373:C:H6	47:S2:1373:C:C5'	2.32	0.43
53:SF:122:ARG:NH2	53:SF:197:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SH:125:VAL:O	54:SH:129:ILE:HG13	2.18	0.43
54:SH:181:THR:HG22	54:SH:183:LYS:HG2	2.01	0.43
56:SK:65:ARG:HH22	68:Sd:20:SER:CB	2.32	0.43
69:Sg:87:LEU:HB2	69:Sg:101:PHE:HB2	1.99	0.43
1:L5:1820:C:N4	1:L5:1822:U:O2'	2.52	0.43
4:LA:196:TRP:HB3	4:LA:197:PRO:HD3	2.00	0.43
18:LP:117:ILE:CD1	18:LP:148:MET:HE2	2.44	0.43
20:LR:179:ALA:HA	20:LR:182:GLU:HB2	2.00	0.43
21:LS:85:ASP:HA	21:LS:90:THR:HA	2.01	0.43
47:S2:658:U:H4'	47:S2:659:G:O5'	2.19	0.43
79:Sb:56:CYS:HB3	79:Sb:59:CYS:O	2.18	0.43
1:L5:131:C:O2	1:L5:138:G:N2	2.52	0.42
1:L5:2566:G:H8	1:L5:2566:G:O5'	2.02	0.42
1:L5:4863:G:H8	1:L5:4863:G:O5'	2.02	0.42
5:LB:35:ASP:HB2	5:LB:186:ASN:CG	2.44	0.42
36:Lh:79:LYS:O	36:Lh:84:ARG:NH2	2.40	0.42
37:Li:52:PRO:HB3	37:Li:55:ARG:HH21	1.84	0.42
47:S2:583:A:H5'	72:SJ:169:ARG:HH12	1.84	0.42
47:S2:848:U:H2'	47:S2:849:A:H8	1.84	0.42
69:Sg:64:HIS:ND1	69:Sg:65:PHE:N	2.65	0.42
1:L5:37:U:H4'	29:La:32:ARG:HD2	2.01	0.42
1:L5:3710:G:H4'	1:L5:3711:A:H5'	2.01	0.42
1:L5:4127:A:C4	10:LG:37:LYS:HE2	2.53	0.42
8:LE:98:GLY:HA3	8:LE:99:ASP:HA	1.83	0.42
14:LL:153:PRO:HB2	14:LL:156:PRO:HB3	2.01	0.42
25:LW:17:HIS:ND1	25:LW:17:HIS:N	2.67	0.42
34:Lf:46:ARG:HB3	34:Lf:106:TYR:HB2	2.01	0.42
38:Lj:34:CYS:HB3	38:Lj:39:TYR:H	1.84	0.42
47:S2:563:G:N7	47:S2:586:G:N2	2.67	0.42
47:S2:1513:C:OP1	68:Sd:12:ARG:NH1	2.51	0.42
52:SE:44:LEU:HD21	52:SE:70:ILE:HG21	2.00	0.42
60:SR:28:PHE:HZ	60:SR:48:ASN:HB2	1.84	0.42
67:Sc:44:ARG:HH12	67:Sc:63:ARG:CB	2.32	0.42
69:Sg:199:THR:OG1	69:Sg:239:LEU:O	2.32	0.42
73:SM:31:LEU:HD13	73:SM:111:VAL:HG12	2.01	0.42
76:SW:32:LYS:HA	76:SW:35:VAL:HG22	2.00	0.42
1:L5:1327:C:H2'	1:L5:1328:G:C8	2.54	0.42
1:L5:4141:G:N3	1:L5:4141:G:H2'	2.34	0.42
83:L5:5374:HMT:H29A	83:L5:5374:HMT:H25A	1.88	0.42
5:LB:79:VAL:HG23	5:LB:79:VAL:O	2.19	0.42
7:LD:65:ALA:HB2	7:LD:74:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LM:11:ARG:HG2	15:LM:57:LEU:HD22	2.01	0.42
18:LP:30:ARG:HA	18:LP:119:VAL:HG21	2.01	0.42
49:SA:66:VAL:CG1	64:SV:46:PHE:CD2	2.99	0.42
50:SB:52:THR:HG23	50:SB:57:ILE:HA	2.02	0.42
50:SB:144:LYS:HD2	50:SB:208:HIS:HB3	2.01	0.42
53:SF:100:ILE:HG23	53:SF:178:ILE:HD11	2.01	0.42
62:ST:39:LEU:HD21	62:ST:56:ARG:NH1	2.34	0.42
2:L7:1:G:O3'	7:LD:265:ARG:NH1	2.53	0.42
7:LD:236:MET:HG3	7:LD:239:MET:HE3	2.02	0.42
43:Lo:26:TYR:HB3	43:Lo:67:VAL:HB	2.01	0.42
46:Lz:36:ILE:HD11	46:Lz:165:LEU:HD12	2.01	0.42
47:S2:921:G:C5	76:SW:28:ARG:HD2	2.54	0.42
62:ST:33:TRP:O	62:ST:33:TRP:CE3	2.70	0.42
76:SW:57:ARG:H	76:SW:57:ARG:HD2	1.84	0.42
1:L5:119:G:H5''	1:L5:119:G:H8	1.85	0.42
1:L5:1601:A:OP2	1:L5:3643:A:N6	2.52	0.42
1:L5:2705:G:H22	1:L5:2710:C:H5	1.66	0.42
1:L5:4077:A:N1	1:L5:4171:C:N4	2.66	0.42
5:LB:79:VAL:HG22	5:LB:331:VAL:O	2.20	0.42
6:LC:284:MET:HB2	19:LQ:28:LEU:HD23	2.00	0.42
7:LD:243:ALA:O	7:LD:247:ILE:HG12	2.19	0.42
13:LJ:99:PHE:HB2	13:LJ:159:LYS:HE3	2.01	0.42
47:S2:532:C:O2	47:S2:552:G:N2	2.53	0.42
53:SF:122:ARG:NE	67:Sc:59:LEU:CD2	2.82	0.42
53:SF:204:ARG:O	53:SF:204:ARG:HG3	2.19	0.42
3:L8:67:U:H5''	38:Lj:86:PRO:HA	2.01	0.42
9:LF:90:ALA:HB2	9:LF:125:LEU:HD11	2.01	0.42
10:LG:175:ARG:HH11	10:LG:230:TYR:HD2	1.68	0.42
10:LG:244:PRO:HA	10:LG:247:VAL:HG12	2.01	0.42
14:LL:6:ASN:HD22	14:LL:7:GLY:H	1.66	0.42
32:Ld:21:VAL:HG12	32:Ld:90:ARG:HE	1.85	0.42
47:S2:196:C:H42	47:S2:203:G:H2'	1.84	0.42
47:S2:1016:U:OP1	79:Sb:30:SER:OG	2.32	0.42
47:S2:1467:C:H5''	60:SR:1:MET:HG3	2.01	0.42
49:SA:18:PHE:HD1	49:SA:18:PHE:HA	1.71	0.42
61:SS:12:ILE:HD12	61:SS:19:ASN:HB2	2.02	0.42
69:Sg:59:LEU:HD23	69:Sg:90:TRP:CD2	2.55	0.42
69:Sg:65:PHE:O	69:Sg:83:TRP:N	2.48	0.42
71:SG:217:MET:HE2	71:SG:217:MET:HB3	1.62	0.42
78:SZ:54:THR:O	78:SZ:58:LEU:N	2.52	0.42
1:L5:755:C:H2'	1:L5:756:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1189:G:H2'	1:L5:1190:C:C6	2.55	0.42
1:L5:1961:G:H2'	1:L5:2024:G:N2	2.34	0.42
1:L5:4220:6MZ:H8	1:L5:4220:6MZ:OP1	2.19	0.42
5:LB:251:VAL:HG21	5:LB:267:ALA:HB3	2.02	0.42
10:LG:132:ARG:HA	10:LG:133:PRO:HD3	1.86	0.42
13:LJ:20:LEU:HD13	13:LJ:130:PHE:HD1	1.85	0.42
13:LJ:23:ASN:O	13:LJ:128:LEU:HB2	2.20	0.42
14:LL:90:VAL:O	14:LL:93:THR:OG1	2.36	0.42
47:S2:377:G:H5'	55:SI:98:LYS:HB3	2.02	0.42
47:S2:752:G:OP1	47:S2:792:C:O2'	2.34	0.42
69:Sg:166:VAL:HG12	69:Sg:176:VAL:HG22	2.01	0.42
1:L5:2528:G:N3	1:L5:2528:G:H3'	2.35	0.42
1:L5:4085:A:H5''	10:LG:56:LYS:HB2	2.02	0.42
1:L5:5010:U:H2'	1:L5:5011:A:C8	2.55	0.42
8:LE:192:LYS:HE2	34:Lf:107:PRO:HB3	2.02	0.42
9:LF:129:SER:HA	9:LF:132:MET:HG2	2.02	0.42
10:LG:156:VAL:HG12	10:LG:190:LEU:HD21	2.02	0.42
13:LJ:174:ILE:HG22	13:LJ:175:LEU:H	1.85	0.42
18:LP:95:LEU:HA	18:LP:95:LEU:HD12	1.89	0.42
34:Lf:52:LYS:HG2	34:Lf:67:THR:HG22	2.02	0.42
43:Lo:24:THR:HG21	43:Lo:69:ARG:HH21	1.83	0.42
47:S2:900:C:H5'	47:S2:901:G:C8	2.55	0.42
47:S2:1679:A:H2'	53:SF:60:ARG:HD2	2.01	0.42
54:SH:98:ARG:HD3	54:SH:98:ARG:HA	1.36	0.42
54:SH:145:ARG:O	54:SH:153:LEU:N	2.52	0.42
57:SL:23:VAL:HG23	57:SL:26:GLY:H	1.84	0.42
75:SO:12:GLU:HA	75:SO:13:GLN:HA	1.82	0.42
5:LB:175:GLN:NE2	5:LB:177:LYS:O	2.53	0.42
8:LE:223:ARG:HA	8:LE:224:LYS:HA	1.76	0.42
19:LQ:79:THR:HB	19:LQ:136:THR:HG22	2.01	0.42
44:Lp:56:HIS:HD2	44:Lp:63:THR:HB	1.85	0.42
47:S2:1010:G:H2'	47:S2:1011:A:C8	2.55	0.42
61:SS:84:LEU:HD23	61:SS:95:TYR:HB3	2.02	0.42
66:Sa:87:ARG:HE	66:Sa:92:ARG:HA	1.84	0.42
69:Sg:66:VAL:HA	69:Sg:82:SER:HA	2.01	0.42
69:Sg:282:GLU:HA	69:Sg:283:PRO:HD3	1.91	0.42
1:L5:139:G:H2'	1:L5:140:G:H8	1.85	0.42
1:L5:481:G:H1	1:L5:673:C:H42	1.67	0.42
1:L5:2558:C:H42	1:L5:2569:G:H1	1.68	0.42
1:L5:3786:U:OP1	1:L5:4550:G:O2'	2.36	0.42
1:L5:4212:A:C2	22:LT:3:ASN:ND2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LF:166:ARG:HD2	9:LF:209:TRP:CE2	2.55	0.42
29:La:132:ARG:H	29:La:132:ARG:HD2	1.84	0.42
43:Lo:2:VAL:N	43:Lo:90:HIS:O	2.53	0.42
1:L5:4906:C:H2'	1:L5:4907:G:H8	1.85	0.41
6:LC:41:HIS:NE2	6:LC:45:ARG:HD3	2.34	0.41
12:LI:51:HIS:CD2	12:LI:168:SER:HB2	2.55	0.41
32:Ld:105:LEU:HG	32:Ld:107:THR:HG23	2.01	0.41
47:S2:532:C:C2	47:S2:533:A:C8	3.08	0.41
47:S2:735:C:OP2	47:S2:736:C:C5	2.73	0.41
47:S2:894:G:H8	47:S2:895:G:C8	2.38	0.41
51:SD:35:SER:HA	51:SD:99:ILE:HB	2.02	0.41
69:Sg:64:HIS:CG	69:Sg:65:PHE:H	2.37	0.41
72:SJ:125:HIS:NE2	72:SJ:129:LEU:HD11	2.35	0.41
1:L5:1174:G:N2	1:L5:1175:A:H1'	2.35	0.41
1:L5:2035:C:H5'	21:LS:118:ARG:HE	1.85	0.41
1:L5:4147:G:H2'	1:L5:4148:C:C6	2.55	0.41
13:LJ:51:SER:HB3	13:LJ:71:HIS:CD2	2.55	0.41
61:SS:67:VAL:HG12	61:SS:71:MET:HE2	2.01	0.41
69:Sg:243:PRO:HG3	69:Sg:293:ALA:HA	2.02	0.41
75:SO:34:PHE:HA	75:SO:98:ARG:HD2	2.02	0.41
77:SY:10:ARG:HG2	77:SY:10:ARG:NH1	2.35	0.41
78:SZ:77:LEU:HB2	78:SZ:78:LYS:H	1.58	0.41
79:Sb:19:HIS:HD2	79:Sb:21:LYS:H	1.67	0.41
1:L5:151:G:H2'	16:LN:49:ARG:HH12	1.84	0.41
1:L5:502:C:OP2	1:L5:502:C:H4'	2.18	0.41
1:L5:988:C:O2	1:L5:988:C:H2'	2.20	0.41
1:L5:1186:U:H2'	1:L5:1187:G:N3	2.34	0.41
1:L5:1326:A2M:H2'	1:L5:1327:C:C6	2.55	0.41
1:L5:1354:A:OP1	19:LQ:108:ARG:NH1	2.53	0.41
1:L5:2673:G:H5''	1:L5:2674:A:H3'	2.02	0.41
4:LA:31:ALA:HB2	4:LA:123:ARG:HH21	1.86	0.41
5:LB:45:ALA:HA	5:LB:348:ARG:HA	2.03	0.41
9:LF:107:LYS:HD2	9:LF:110:GLN:HE21	1.85	0.41
16:LN:185:GLY:HA3	16:LN:194:ARG:HH22	1.85	0.41
23:LU:100:LEU:HD23	23:LU:112:LEU:HD12	2.02	0.41
47:S2:1256:G:C8	63:SU:66:ARG:HB2	2.55	0.41
47:S2:1648:G:O2'	47:S2:1674:G:O6	2.38	0.41
49:SA:126:ASP:HB3	49:SA:129:ALA:HB3	2.01	0.41
53:SF:74:ASN:HA	53:SF:77:MET:HE2	2.03	0.41
66:Sa:22:ARG:HD2	66:Sa:22:ARG:HA	1.72	0.41
69:Sg:83:TRP:HA	69:Sg:107:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SZ:46:ASN:CG	78:SZ:78:LYS:HG2	2.45	0.41
1:L5:1397:A:N1	1:L5:1498:G:O2'	2.53	0.41
4:LA:70:LYS:HD2	4:LA:72:ARG:HE	1.85	0.41
11:LH:92:MET:HE2	11:LH:179:ILE:HG22	2.01	0.41
20:LR:109:TYR:HB3	20:LR:115:ILE:HG12	2.02	0.41
37:Li:74:LYS:HE2	37:Li:80:HIS:HB2	2.02	0.41
49:SA:38:ILE:HD12	49:SA:38:ILE:HA	1.96	0.41
49:SA:53:ARG:HG2	49:SA:53:ARG:H	1.67	0.41
51:SD:116:ARG:CG	51:SD:116:ARG:NH1	2.72	0.41
52:SE:122:LYS:NZ	52:SE:143:ASP:OD2	2.53	0.41
66:Sa:10:ARG:HH22	66:Sa:12:LYS:HE2	1.84	0.41
76:SW:46:TYR:HD2	76:SW:69:LEU:HD13	1.85	0.41
1:L5:490:C:H1'	1:L5:666:G:H1	1.84	0.41
1:L5:1281:G:N1	8:LE:128:HIS:HB2	2.35	0.41
1:L5:2094:G:H3'	1:L5:2095:A:H5''	2.02	0.41
1:L5:2474:G:N2	1:L5:2502:G:O2'	2.53	0.41
1:L5:2905:C:H5''	1:L5:2905:C:C6	2.54	0.41
1:L5:4208:U:H4'	1:L5:4274:A:H2	1.85	0.41
2:L7:8:G:OP2	7:LD:30:TYR:OH	2.31	0.41
18:LP:17:SER:HB2	18:LP:97:ASN:ND2	2.35	0.41
21:LS:27:LEU:HD21	22:LT:141:VAL:HG11	2.03	0.41
43:Lo:6:LYS:HG2	43:Lo:93:LEU:HD23	2.02	0.41
47:S2:1246:A:N3	47:S2:1251:A:O2'	2.49	0.41
49:SA:50:ASN:CG	49:SA:53:ARG:HG2	2.46	0.41
49:SA:50:ASN:C	49:SA:50:ASN:HD22	2.28	0.41
50:SB:62:LEU:O	50:SB:65:ARG:HG3	2.21	0.41
51:SD:222:PRO:HB3	69:Sg:219:TRP:HH2	1.84	0.41
53:SF:82:ASN:OD1	53:SF:82:ASN:N	2.52	0.41
54:SH:189:PHE:N	54:SH:189:PHE:CD1	2.89	0.41
70:SC:64:THR:HG23	70:SC:67:GLY:H	1.86	0.41
76:SW:42:MET:HE2	76:SW:42:MET:HB3	1.96	0.41
1:L5:1763:C:H41	1:L5:1764:G:N2	2.18	0.41
1:L5:1943:A:N6	1:L5:2039:G:O2'	2.53	0.41
1:L5:1966:C:N3	1:L5:1967:A:H1'	2.34	0.41
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.56	0.41
5:LB:153:MET:HG3	5:LB:157:CYS:SG	2.61	0.41
5:LB:231:VAL:HG21	5:LB:251:VAL:HG23	2.02	0.41
12:LI:36:LEU:HD22	12:LI:69:ARG:HH21	1.84	0.41
13:LJ:153:ALA:HA	13:LJ:156:ARG:HE	1.86	0.41
18:LP:4:TYR:OH	18:LP:18:ARG:HG3	2.20	0.41
21:LS:164:LYS:HE3	34:Lf:34:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LW:96:GLN:H	25:LW:96:GLN:HG2	1.66	0.41
37:Li:44:ILE:HA	37:Li:47:VAL:HG12	2.03	0.41
47:S2:1640:A:OP2	47:S2:1640:A:C8	2.70	0.41
70:SC:210:PRO:HD3	70:SC:236:PHE:CE2	2.56	0.41
1:L5:73:A:C5'	1:L5:73:A:C8	3.02	0.41
1:L5:4187:G:H4'	16:LN:82:GLY:HA2	2.02	0.41
1:L5:4471:U:H2'	1:L5:4472:G:H8	1.86	0.41
7:LD:80:ALA:HB1	7:LD:92:LEU:HD12	2.02	0.41
16:LN:155:VAL:O	16:LN:162:ARG:NH2	2.54	0.41
26:LX:148:ASP:HA	26:LX:151:ASN:HD22	1.86	0.41
42:Ln:4:LYS:CE	47:S2:1844:U:O4	2.69	0.41
48:S6:33:C:H3'	48:S6:33:C:H6	1.86	0.41
51:SD:27:ARG:CG	51:SD:27:ARG:NH1	2.73	0.41
56:SK:90:VAL:HB	56:SK:94:LEU:HD12	2.02	0.41
58:SP:57:LEU:HD11	58:SP:83:MET:HE2	2.03	0.41
1:L5:1174:G:H22	1:L5:1186:U:H3	1.69	0.41
1:L5:3946:G:H2'	1:L5:3947:A:H5'	2.03	0.41
1:L5:4537:C:H2'	1:L5:4538:G:C8	2.56	0.41
1:L5:4881:U:C4	15:LM:113:MET:HG2	2.56	0.41
4:LA:44:ILE:HD12	4:LA:87:PHE:HE1	1.85	0.41
5:LB:168:MET:HE3	5:LB:168:MET:HB3	1.90	0.41
13:LJ:120:ASP:CB	13:LJ:123:ILE:HD13	2.51	0.41
17:LO:74:ARG:HH11	17:LO:74:ARG:CG	2.29	0.41
23:LU:28:PRO:HB2	23:LU:34:MET:HG2	2.03	0.41
50:SB:100:PHE:CD1	50:SB:100:PHE:C	2.98	0.41
59:SQ:76:GLY:O	59:SQ:80:GLN:HG3	2.21	0.41
65:SX:39:ASN:HA	65:SX:40:PRO:HD3	1.90	0.41
78:SZ:76:ARG:HD3	78:SZ:76:ARG:HA	1.85	0.41
1:L5:86:U:OP1	19:LQ:169:SER:OG	2.38	0.41
1:L5:223:G:H4'	1:L5:225:G:N7	2.36	0.41
1:L5:267:G:H2'	1:L5:268:G:H8	1.86	0.41
1:L5:1071:C:C5	8:LE:67:ALA:HB2	2.55	0.41
1:L5:2019:C:C6	1:L5:2019:C:C5'	3.04	0.41
1:L5:2319:C:O5'	1:L5:2319:C:H6	2.03	0.41
1:L5:2528:G:N3	1:L5:2528:G:H2'	2.36	0.41
1:L5:2578:G:OP2	28:LZ:111:ARG:NH2	2.54	0.41
1:L5:2908:U:H6	1:L5:2908:U:H5''	1.85	0.41
1:L5:4736:C:H2'	1:L5:4737:G:C8	2.56	0.41
1:L5:4741:C:H4'	1:L5:4742:G:H5'	2.02	0.41
3:L8:60:G:O6	3:L8:96:C:O2'	2.33	0.41
6:LC:228:THR:HG21	6:LC:239:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LD:156:GLY:HA2	7:LD:181:PRO:HG3	2.02	0.41
11:LH:103:VAL:HG11	11:LH:144:LEU:HD21	2.02	0.41
12:LI:56:GLU:CD	12:LI:162:ARG:H	2.28	0.41
14:LL:49:ARG:HA	14:LL:50:PRO:HD3	1.92	0.41
16:LN:169:ARG:HH21	16:LN:174:LEU:HD11	1.86	0.41
19:LQ:46:VAL:HA	19:LQ:49:LYS:HE3	2.02	0.41
19:LQ:72:LEU:HA	19:LQ:73:PRO:HD3	1.95	0.41
26:LX:89:LYS:HE3	26:LX:93:ASN:HD22	1.86	0.41
46:Lz:54:ARG:HA	46:Lz:154:THR:HG21	2.02	0.41
47:S2:39:A:H5'	72:SJ:7:TRP:HE1	1.86	0.41
47:S2:532:C:N3	47:S2:533:A:N7	2.69	0.41
47:S2:924:G:OP2	74:SN:3:ARG:NH1	2.54	0.41
47:S2:1350:U:O2	49:SA:110:ASN:ND2	2.54	0.41
48:S6:75:C:C2'	48:S6:76:A:H4'	2.47	0.41
52:SE:124:CYS:HB3	52:SE:141:THR:HB	2.02	0.41
53:SF:87:LEU:HD11	59:SQ:47:LEU:HD11	2.03	0.41
54:SH:91:HIS:HE1	54:SH:168:HIS:HD2	1.69	0.41
54:SH:97:GLN:HE21	54:SH:97:GLN:HB3	1.69	0.41
55:SI:65:PHE:CD1	55:SI:65:PHE:N	2.88	0.41
61:SS:95:TYR:HD1	61:SS:95:TYR:N	2.19	0.41
65:SX:63:ASN:ND2	65:SX:114:ASP:OD2	2.53	0.41
67:Sc:63:ARG:HB3	67:Sc:64:GLU:H	1.61	0.41
69:Sg:14:HIS:HE1	69:Sg:18:VAL:HG22	1.86	0.41
69:Sg:15:ASN:ND2	69:Sg:15:ASN:H	2.19	0.41
71:SG:49:VAL:HG22	71:SG:115:LYS:HB3	2.03	0.41
72:SJ:169:ARG:HH11	72:SJ:175:ARG:HH12	1.68	0.41
75:SO:106:LYS:CE	75:SO:135:ILE:HD12	2.51	0.41
1:L5:67:C:O3'	16:LN:177:GLY:HA2	2.21	0.41
1:L5:4975:G:O2'	1:L5:4977:A:N6	2.50	0.41
4:LA:126:LEU:HD13	4:LA:150:LEU:HD11	2.03	0.41
5:LB:82:PRO:HG3	5:LB:171:LEU:HD21	2.01	0.41
5:LB:220:ILE:HB	5:LB:346:THR:HB	2.03	0.41
6:LC:333:MLZ:HE3	8:LE:54:ILE:HG12	2.02	0.41
7:LD:200:MET:HE2	7:LD:200:MET:HB3	1.92	0.41
10:LG:88:ASP:HB2	10:LG:91:THR:HG22	2.03	0.41
25:LW:44:ARG:HD3	25:LW:49:ILE:HD11	2.02	0.41
29:La:23:GLY:HA3	29:La:24:LYS:HA	1.76	0.41
31:Lc:81:LEU:HD12	31:Lc:81:LEU:C	2.45	0.41
47:S2:536:A:H3'	47:S2:537:C:C5'	2.51	0.41
47:S2:1017:U:H5'	74:SN:55:ARG:HD3	2.03	0.41
47:S2:1536:G:H2'	47:S2:1537:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S6:9:U:H4'	48:S6:48:C:H4'	2.03	0.41
52:SE:176:ASP:H	52:SE:179:ASN:HD22	1.69	0.41
65:SX:90:CYS:HA	65:SX:93:PHE:HD2	1.86	0.41
70:SC:74:LYS:CD	70:SC:269:PHE:CE1	3.03	0.41
74:SN:22:VAL:HA	74:SN:23:PRO:HD3	1.97	0.41
1:L5:76:A:N7	14:LL:74:ARG:NH2	2.68	0.40
1:L5:76:A:H5'	14:LL:101:ARG:HH21	1.86	0.40
1:L5:1206:C:H2'	1:L5:1207:C:O4'	2.21	0.40
1:L5:2362:U:OP1	18:LP:82:ARG:NH2	2.53	0.40
4:LA:116:LEU:HD23	4:LA:164:ALA:HB2	2.03	0.40
13:LJ:19:LYS:HE3	13:LJ:133:VAL:HG21	2.02	0.40
13:LJ:146:ARG:HE	13:LJ:147:ARG:HH21	1.68	0.40
16:LN:143:ARG:HH21	36:Lh:95:LEU:HA	1.86	0.40
22:LT:75:VAL:HG22	22:LT:88:ARG:HG2	2.03	0.40
27:LY:23:SER:HA	27:LY:26:ARG:HB2	2.03	0.40
28:LZ:14:LEU:HD11	28:LZ:81:MET:HB2	2.03	0.40
42:Ln:10:MET:HE2	42:Ln:10:MET:HB2	1.75	0.40
45:Lr:26:SER:OG	45:Lr:28:GLU:OE1	2.29	0.40
47:S2:546:G:H1'	47:S2:547:G:N7	2.36	0.40
47:S2:571:U:H5''	77:SY:37:LYS:HG3	2.02	0.40
47:S2:1270:G:O2'	47:S2:1301:A:N7	2.51	0.40
47:S2:1520:G:H21	58:SP:126:VAL:HG11	1.86	0.40
70:SC:78:LEU:HD23	70:SC:81:ILE:HD12	2.03	0.40
78:SZ:82:SER:O	78:SZ:83:LEU:C	2.63	0.40
1:L5:495:C:O2	1:L5:659:G:N1	2.55	0.40
1:L5:2019:C:O2	1:L5:2019:C:C2'	2.69	0.40
1:L5:2293:U:H2'	1:L5:2294:G:C8	2.56	0.40
1:L5:2409:U:O2	1:L5:2409:U:C2'	2.69	0.40
1:L5:2492:C:O5'	1:L5:2492:C:C6	2.72	0.40
1:L5:3946:G:O2'	1:L5:3947:A:H5'	2.10	0.40
1:L5:4300:U:H4'	22:LT:89:ILE:HG22	2.03	0.40
11:LH:42:ASN:HD21	17:LO:131:PRO:HB2	1.86	0.40
14:LL:7:GLY:O	29:La:49:HIS:NE2	2.41	0.40
36:Lh:4:ILE:HD11	36:Lh:53:SER:HB3	2.04	0.40
47:S2:379:C:H5'	55:SI:33:ALA:HA	2.03	0.40
47:S2:1659:U:H5	47:S2:1660:C:N3	2.18	0.40
50:SB:65:ARG:NH2	75:SO:51:GLU:HG2	2.35	0.40
51:SD:222:PRO:HG2	69:Sg:226:HIS:CE1	2.56	0.40
53:SF:35:LEU:HD22	53:SF:117:ILE:HD13	2.04	0.40
69:Sg:236:ILE:HG12	69:Sg:252:THR:HG22	2.04	0.40
2:L7:47:G:H21	7:LD:222:GLN:HE22	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LE:94:LYS:HA	8:LE:95:PRO:HD3	1.91	0.40
17:LO:47:PHE:HE1	17:LO:140:ARG:HG2	1.81	0.40
18:LP:6:LEU:HD12	18:LP:116:HIS:CD2	2.56	0.40
36:Lh:87:LYS:HA	38:Lj:73:ARG:HH22	1.86	0.40
43:Lo:2:VAL:HB	43:Lo:3:ASN:H	1.66	0.40
47:S2:318:A:N6	71:SG:186:GLN:HE22	2.18	0.40
51:SD:214:LYS:HG3	51:SD:215:ASP:H	1.86	0.40
58:SP:25:LEU:HD13	58:SP:112:ILE:HD13	2.03	0.40
59:SQ:85:ARG:NH1	59:SQ:116:ASP:OD2	2.45	0.40
65:SX:105:PHE:HB3	65:SX:112:VAL:HG21	2.02	0.40
67:Sc:14:VAL:HG23	67:Sc:15:THR:O	2.21	0.40
1:L5:120:A:H2'	1:L5:149:A:H61	1.85	0.40
1:L5:141:C:O2	1:L5:141:C:C2'	2.70	0.40
2:L7:94:C:H4'	21:LS:122:HIS:HB2	2.03	0.40
6:LC:28:PHE:HA	6:LC:129:ALA:HA	2.03	0.40
6:LC:320:LYS:CB	6:LC:320:LYS:NZ	2.79	0.40
7:LD:184:ASP:HB3	7:LD:189:GLU:HB3	2.03	0.40
14:LL:63:THR:HG21	29:La:66:ASN:HB3	2.03	0.40
17:LO:48:TYR:CE2	17:LO:52:LEU:HD11	2.56	0.40
27:LY:31:SER:HA	27:LY:48:PRO:HA	2.02	0.40
46:Lz:12:GLU:HG3	46:Lz:216:LEU:HA	2.04	0.40
54:SH:100:ILE:HG13	54:SH:125:VAL:HG11	2.04	0.40
54:SH:143:ARG:HB2	54:SH:155:LYS:HB2	2.03	0.40
58:SP:77:LYS:HB3	58:SP:102:PHE:CE1	2.57	0.40
61:SS:28:PHE:HE1	61:SS:38:ARG:HE	1.70	0.40
79:Sb:63:LEU:HD12	79:Sb:63:LEU:HA	1.77	0.40
1:L5:137:G:H2'	1:L5:138:G:C8	2.57	0.40
1:L5:256:G:H8	1:L5:256:G:P	2.44	0.40
1:L5:1568:C:H2'	1:L5:1569:U:C6	2.57	0.40
1:L5:2749:C:H2'	1:L5:2750:G:C8	2.56	0.40
1:L5:3837:C:H2'	1:L5:3838:U:C6	2.57	0.40
1:L5:3964:U:O2	1:L5:3964:U:C2'	2.70	0.40
1:L5:4935:C:H2'	1:L5:4936:G:C8	2.56	0.40
3:L8:27:U:H4'	6:LC:53:ALA:HB3	2.03	0.40
3:L8:123:U:H5''	3:L8:124:U:C4	2.57	0.40
3:L8:150:C:N4	10:LG:53:ARG:HA	2.37	0.40
14:LL:64:VAL:HA	14:LL:67:HIS:CD2	2.57	0.40
14:LL:178:ALA:HB3	29:La:134:GLU:HG3	2.04	0.40
29:La:27:LYS:HA	29:La:27:LYS:HE3	2.02	0.40
54:SH:181:THR:CG2	54:SH:183:LYS:CG	2.92	0.40
70:SC:128:VAL:HG11	70:SC:155:ILE:HG13	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	
4	LA	246/248 (99%)	223 (91%)	22 (9%)	1 (0%)	30	59
5	LB	400/402 (100%)	373 (93%)	26 (6%)	1 (0%)	36	65
6	LC	365/368 (99%)	337 (92%)	25 (7%)	3 (1%)	16	44
7	LD	291/293 (99%)	268 (92%)	23 (8%)	0	100	100
8	LE	232/236 (98%)	205 (88%)	26 (11%)	1 (0%)	30	59
9	LF	224/225 (100%)	215 (96%)	8 (4%)	1 (0%)	30	59
10	LG	240/241 (100%)	218 (91%)	22 (9%)	0	100	100
11	LH	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
12	LI	211/213 (99%)	183 (87%)	28 (13%)	0	100	100
13	LJ	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
14	LL	208/210 (99%)	187 (90%)	21 (10%)	0	100	100
15	LM	137/139 (99%)	125 (91%)	11 (8%)	1 (1%)	18	48
16	LN	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	12	39
17	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
18	LP	151/153 (99%)	139 (92%)	12 (8%)	0	100	100
19	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
20	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
23	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
24	LV	129/131 (98%)	117 (91%)	10 (8%)	2 (2%)	7	27
25	LW	122/124 (98%)	104 (85%)	17 (14%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LX	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
27	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
29	La	145/147 (99%)	133 (92%)	12 (8%)	0	100	100
30	Lb	105/109 (96%)	91 (87%)	14 (13%)	0	100	100
31	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
32	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
33	Le	126/128 (98%)	116 (92%)	8 (6%)	2 (2%)	7	27
34	Lf	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	41
35	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
38	Lj	85/86 (99%)	78 (92%)	7 (8%)	0	100	100
39	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
40	Ll	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	Lm	49/52 (94%)	48 (98%)	1 (2%)	0	100	100
42	Ln	22/24 (92%)	22 (100%)	0	0	100	100
43	Lo	104/105 (99%)	100 (96%)	3 (3%)	1 (1%)	12	39
44	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
46	Lz	215/217 (99%)	156 (73%)	59 (27%)	0	100	100
49	SA	219/221 (99%)	194 (89%)	21 (10%)	4 (2%)	6	25
50	SB	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
51	SD	225/227 (99%)	201 (89%)	24 (11%)	0	100	100
52	SE	260/262 (99%)	243 (94%)	17 (6%)	0	100	100
53	SF	187/189 (99%)	165 (88%)	22 (12%)	0	100	100
54	SH	182/186 (98%)	158 (87%)	24 (13%)	0	100	100
55	SI	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
56	SK	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
57	SL	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
58	SP	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	SQ	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	30
60	SR	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
61	SS	143/145 (99%)	128 (90%)	14 (10%)	1 (1%)	18	48
62	ST	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	9	30
63	SU	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
64	SV	81/83 (98%)	74 (91%)	5 (6%)	2 (2%)	4	17
65	SX	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	30
66	Sa	101/102 (99%)	91 (90%)	10 (10%)	0	100	100
67	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
68	Sd	53/55 (96%)	50 (94%)	2 (4%)	1 (2%)	6	23
69	Sg	311/313 (99%)	268 (86%)	40 (13%)	3 (1%)	12	39
70	SC	221/222 (100%)	202 (91%)	17 (8%)	2 (1%)	14	41
71	SG	235/237 (99%)	217 (92%)	16 (7%)	2 (1%)	14	41
72	SJ	184/185 (100%)	167 (91%)	16 (9%)	1 (0%)	24	54
73	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
74	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
75	SO	138/140 (99%)	120 (87%)	17 (12%)	1 (1%)	18	48
76	SW	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
77	SY	130/131 (99%)	123 (95%)	7 (5%)	0	100	100
78	SZ	73/75 (97%)	58 (80%)	7 (10%)	8 (11%)	0	1
79	Sb	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	10	34
80	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
81	Sf	65/67 (97%)	51 (78%)	14 (22%)	0	100	100
All	All	11561/11713 (99%)	10531 (91%)	980 (8%)	50 (0%)	31	59

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LC	3	CYS
16	LN	124	ASP
33	Le	92	ASN
65	SX	127	ASN
70	SC	173	LYS
78	SZ	50	PHE

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Mol	Chain	Res	Type
4	LA	180	LEU
6	LC	222	ARG
9	LF	33	LEU
15	LM	3	PHE
24	LV	23	GLY
49	SA	211	GLU
62	ST	40	ALA
62	ST	41	LYS
64	SV	82	ASN
70	SC	78	LEU
78	SZ	45	ASN
78	SZ	47	LEU
49	SA	141	ASN
59	SQ	44	PRO
65	SX	126	ALA
68	Sd	14	PHE
71	SG	218	LYS
75	SO	144	GLY
33	Le	94	SER
34	Lf	107	PRO
43	Lo	55	ILE
64	SV	80	SER
6	LC	221	PHE
24	LV	18	LEU
25	LW	11	TYR
49	SA	12	GLU
49	SA	23	THR
58	SP	128	HIS
59	SQ	43	GLU
69	Sg	13	GLY
69	Sg	144	ASP
69	Sg	246	TYR
71	SG	174	PRO
78	SZ	76	ARG
78	SZ	77	LEU
78	SZ	80	ARG
8	LE	96	VAL
78	SZ	78	LYS
5	LB	187	GLY
16	LN	84	PRO
78	SZ	81	GLY
61	SS	90	VAL

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Mol	Chain	Res	Type
72	SJ	123	ILE
79	Sb	57	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/190 (100%)	177 (93%)	13 (7%)	14	42
5	LB	348/348 (100%)	338 (97%)	10 (3%)	37	71
6	LC	305/305 (100%)	296 (97%)	9 (3%)	36	70
7	LD	246/247 (100%)	238 (97%)	8 (3%)	33	67
8	LE	209/209 (100%)	200 (96%)	9 (4%)	26	60
9	LF	195/194 (100%)	188 (96%)	7 (4%)	31	65
10	LG	204/205 (100%)	198 (97%)	6 (3%)	37	71
11	LH	169/169 (100%)	167 (99%)	2 (1%)	63	86
12	LI	180/180 (100%)	179 (99%)	1 (1%)	78	93
13	LJ	148/148 (100%)	142 (96%)	6 (4%)	27	61
14	LL	176/176 (100%)	173 (98%)	3 (2%)	53	82
15	LM	118/118 (100%)	117 (99%)	1 (1%)	73	90
16	LN	171/171 (100%)	169 (99%)	2 (1%)	63	86
17	LO	173/173 (100%)	167 (96%)	6 (4%)	32	66
18	LP	134/134 (100%)	128 (96%)	6 (4%)	24	58
19	LQ	164/164 (100%)	161 (98%)	3 (2%)	51	80
20	LR	166/166 (100%)	161 (97%)	5 (3%)	36	70
21	LS	156/156 (100%)	152 (97%)	4 (3%)	40	73
22	LT	139/139 (100%)	133 (96%)	6 (4%)	26	60
23	LU	91/91 (100%)	89 (98%)	2 (2%)	45	77
24	LV	101/101 (100%)	94 (93%)	7 (7%)	14	41
25	LW	103/103 (100%)	99 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LX	108/108 (100%)	105 (97%)	3 (3%)	38	72
27	LY	124/124 (100%)	121 (98%)	3 (2%)	43	75
28	LZ	117/117 (100%)	116 (99%)	1 (1%)	70	90
29	La	120/120 (100%)	118 (98%)	2 (2%)	53	82
30	Lb	89/89 (100%)	88 (99%)	1 (1%)	65	88
31	Lc	83/83 (100%)	79 (95%)	4 (5%)	23	55
32	Ld	98/98 (100%)	98 (100%)	0	100	100
33	Le	114/114 (100%)	109 (96%)	5 (4%)	25	59
34	Lf	88/88 (100%)	86 (98%)	2 (2%)	44	76
35	Lg	98/98 (100%)	96 (98%)	2 (2%)	48	78
36	Lh	109/109 (100%)	108 (99%)	1 (1%)	70	90
37	Li	86/86 (100%)	86 (100%)	0	100	100
38	Lj	74/73 (101%)	74 (100%)	0	100	100
39	Lk	64/64 (100%)	64 (100%)	0	100	100
40	Ll	47/47 (100%)	43 (92%)	4 (8%)	10	31
41	Lm	47/47 (100%)	47 (100%)	0	100	100
42	Ln	23/23 (100%)	23 (100%)	0	100	100
43	Lo	94/93 (101%)	90 (96%)	4 (4%)	26	60
44	Lp	74/74 (100%)	71 (96%)	3 (4%)	27	61
45	Lr	109/109 (100%)	104 (95%)	5 (5%)	24	57
46	Lz	195/196 (100%)	192 (98%)	3 (2%)	57	84
49	SA	183/183 (100%)	168 (92%)	15 (8%)	10	32
50	SB	195/195 (100%)	195 (100%)	0	100	100
51	SD	190/190 (100%)	179 (94%)	11 (6%)	18	49
52	SE	224/224 (100%)	223 (100%)	1 (0%)	84	94
53	SF	159/159 (100%)	158 (99%)	1 (1%)	78	93
54	SH	166/166 (100%)	150 (90%)	16 (10%)	8	26
55	SI	178/178 (100%)	171 (96%)	7 (4%)	28	63
56	SK	89/89 (100%)	88 (99%)	1 (1%)	65	88
57	SL	137/137 (100%)	136 (99%)	1 (1%)	76	92
58	SP	113/113 (100%)	112 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	SQ	117/117 (100%)	113 (97%)	4 (3%)	32	66
60	SR	122/122 (100%)	121 (99%)	1 (1%)	73	90
61	SS	126/126 (100%)	120 (95%)	6 (5%)	23	55
62	ST	113/113 (100%)	105 (93%)	8 (7%)	13	40
63	SU	94/94 (100%)	93 (99%)	1 (1%)	65	88
64	SV	67/67 (100%)	63 (94%)	4 (6%)	17	47
65	SX	113/113 (100%)	110 (97%)	3 (3%)	39	73
66	Sa	90/89 (101%)	85 (94%)	5 (6%)	19	50
67	Sc	57/57 (100%)	51 (90%)	6 (10%)	6	22
68	Sd	48/48 (100%)	45 (94%)	3 (6%)	16	45
69	Sg	272/272 (100%)	268 (98%)	4 (2%)	57	84
70	SC	189/188 (100%)	186 (98%)	3 (2%)	55	83
71	SG	207/207 (100%)	196 (95%)	11 (5%)	20	52
72	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	86
73	SM	102/104 (98%)	100 (98%)	2 (2%)	48	78
74	SN	130/130 (100%)	127 (98%)	3 (2%)	44	76
75	SO	110/110 (100%)	105 (96%)	5 (4%)	24	58
76	SW	112/112 (100%)	111 (99%)	1 (1%)	70	90
77	SY	114/113 (101%)	113 (99%)	1 (1%)	70	90
78	SZ	66/66 (100%)	57 (86%)	9 (14%)	3	12
79	Sb	75/75 (100%)	71 (95%)	4 (5%)	20	52
80	Se	47/47 (100%)	47 (100%)	0	100	100
81	Sf	60/60 (100%)	60 (100%)	0	100	100
All	All	10074/10072 (100%)	9771 (97%)	303 (3%)	37	70

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	28	ARG
4	LA	29	LEU
4	LA	30	ARG
4	LA	45	VAL
4	LA	54	ARG
4	LA	77	ILE

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Mol	Chain	Res	Type
4	LA	125	LYS
4	LA	150	LEU
4	LA	156	LYS
4	LA	207	VAL
4	LA	237	LEU
4	LA	241	ARG
4	LA	242	ARG
5	LB	34	LYS
5	LB	35	ASP
5	LB	65	SER
5	LB	103	LYS
5	LB	120	LYS
5	LB	174	ARG
5	LB	189	THR
5	LB	193	LYS
5	LB	245	HIS
5	LB	386	LYS
6	LC	1	MET
6	LC	80	ARG
6	LC	219	LYS
6	LC	224	ILE
6	LC	289	LEU
6	LC	292	ILE
6	LC	294	LYS
6	LC	320	LYS
6	LC	323	ARG
7	LD	28	THR
7	LD	50	ARG
7	LD	199	ILE
7	LD	200	MET
7	LD	238	GLU
7	LD	286	SER
7	LD	288	LEU
7	LD	289	ARG
8	LE	50	LEU
8	LE	51	VAL
8	LE	52	ARG
8	LE	96	VAL
8	LE	99	ASP
8	LE	127	SER
8	LE	128	HIS
8	LE	138	ARG

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Mol	Chain	Res	Type
8	LE	183	ARG
9	LF	31	LYS
9	LF	32	ARG
9	LF	74	MET
9	LF	96	ARG
9	LF	124	LYS
9	LF	169	LEU
9	LF	200	ARG
10	LG	33	GLU
10	LG	35	ARG
10	LG	37	LYS
10	LG	137[A]	ARG
10	LG	137[B]	ARG
10	LG	202	VAL
11	LH	124	ARG
11	LH	155	SER
12	LI	30	LYS
13	LJ	20	LEU
13	LJ	66	GLU
13	LJ	117	ILE
13	LJ	118	LYS
13	LJ	120	ASP
13	LJ	123	ILE
14	LL	63	THR
14	LL	124	LEU
14	LL	146	LEU
15	LM	4	ARG
16	LN	164	LEU
16	LN	169	ARG
17	LO	49	ARG
17	LO	52	LEU
17	LO	82	ARG
17	LO	85	ARG
17	LO	145	VAL
17	LO	201	LEU
18	LP	24	VAL
18	LP	94	MET
18	LP	95	LEU
18	LP	96	LYS
18	LP	146	ILE
18	LP	147	GLU
19	LQ	21	GLN

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Mol	Chain	Res	Type
19	LQ	83	VAL
19	LQ	143	ARG
20	LR	28	GLU
20	LR	78	ILE
20	LR	114	LYS
20	LR	139	MET
20	LR	172	ARG
21	LS	52	LYS
21	LS	90	THR
21	LS	95	ARG
21	LS	126	ILE
22	LT	3	ASN
22	LT	7	LYS
22	LT	21	LYS
22	LT	24	VAL
22	LT	43	LYS
22	LT	97	LYS
23	LU	105	ASN
23	LU	107	LYS
24	LV	15	ARG
24	LV	25	VAL
24	LV	60	MET
24	LV	83	ARG
24	LV	86	LYS
24	LV	87	SER
24	LV	95	PHE
25	LW	19	ARG
25	LW	43	LYS
25	LW	53	VAL
25	LW	96	GLN
26	LX	88	LYS
26	LX	134	LYS
26	LX	138	VAL
27	LY	13	LYS
27	LY	27	ARG
27	LY	79	VAL
28	LZ	59	LYS
29	La	27	LYS
29	La	42	ARG
30	Lb	12	GLN
31	Lc	20	LEU
31	Lc	23	LYS

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Mol	Chain	Res	Type
31	Lc	81	LEU
31	Lc	83	THR
33	Le	19	LYS
33	Le	26	ASP
33	Le	67	LYS
33	Le	69	MET
33	Le	93	LYS
34	Lf	59	THR
34	Lf	65	ASN
35	Lg	40	LYS
35	Lg	71	LYS
36	Lh	7	ARG
40	Li	5	LYS
40	Li	9	ILE
40	Li	42	ARG
40	Li	51	LEU
43	Lo	2	VAL
43	Lo	53	LYS
43	Lo	55	ILE
43	Lo	81	ARG
44	Lp	25	MET
44	Lp	64	VAL
44	Lp	85	ARG
45	Lr	30	ASN
45	Lr	48	THR
45	Lr	67	ARG
45	Lr	79	ARG
45	Lr	87	ARG
46	Lz	17	VAL
46	Lz	165	LEU
46	Lz	182	ASN
49	SA	8	LEU
49	SA	18	PHE
49	SA	25	LEU
49	SA	51	LEU
49	SA	54	THR
49	SA	56	GLU
49	SA	57	LYS
49	SA	80	ARG
49	SA	104	THR
49	SA	107	THR
49	SA	113	GLN

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Mol	Chain	Res	Type
49	SA	170	SER
49	SA	212	LYS
49	SA	213	GLU
49	SA	214	GLU
51	SD	23	GLU
51	SD	27	ARG
51	SD	29	LEU
51	SD	31	GLU
51	SD	40	ARG
51	SD	116	ARG
51	SD	143	ARG
51	SD	160	SER
51	SD	168	VAL
51	SD	169	ASP
51	SD	190	LEU
52	SE	153	LEU
53	SF	83	ASN
54	SH	12	ASN
54	SH	30	LEU
54	SH	36	LEU
54	SH	92	VAL
54	SH	97	GLN
54	SH	98	ARG
54	SH	105	THR
54	SH	107	LYS
54	SH	116	ARG
54	SH	125	VAL
54	SH	127	ASP
54	SH	130	LEU
54	SH	183	LYS
54	SH	184	ASP
54	SH	185	VAL
54	SH	187	PHE
55	SI	56	ARG
55	SI	73	THR
55	SI	74	ARG
55	SI	76	THR
55	SI	78	ILE
55	SI	104	ILE
55	SI	175	ILE
56	SK	40	VAL
57	SL	56	ILE

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Mol	Chain	Res	Type
58	SP	104	GLN
59	SQ	15	ARG
59	SQ	22	VAL
59	SQ	37	ARG
59	SQ	50	LYS
60	SR	4	VAL
61	SS	51	ASP
61	SS	84	LEU
61	SS	90	VAL
61	SS	94	LYS
61	SS	95	TYR
61	SS	98	VAL
62	ST	33	TRP
62	ST	36	THR
62	ST	39	LEU
62	ST	60	THR
62	ST	63	HIS
62	ST	64	LEU
62	ST	96	SER
62	ST	131	LEU
63	SU	75	LYS
64	SV	50	PHE
64	SV	71	ARG
64	SV	72	LEU
64	SV	83	PHE
65	SX	36	LEU
65	SX	119	ARG
65	SX	129	SER
66	Sa	6	ARG
66	Sa	29	CYS
66	Sa	52	ASP
66	Sa	85[A]	ARG
66	Sa	85[B]	ARG
67	Sc	13	ARG
67	Sc	14	VAL
67	Sc	24	GLN
67	Sc	58	LEU
67	Sc	59	LEU
67	Sc	63	ARG
68	Sd	22	ARG
68	Sd	26	ASN
68	Sd	32	ARG

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Mol	Chain	Res	Type
69	Sg	12	LYS
69	Sg	15	ASN
69	Sg	135	LEU
69	Sg	197	THR
70	SC	71	LYS
70	SC	72	ASP
70	SC	176	LYS
71	SG	64	LYS
71	SG	82	SER
71	SG	154	ARG
71	SG	159	ARG
71	SG	175	LYS
71	SG	176	ILE
71	SG	216	ARG
71	SG	217	MET
71	SG	218	LYS
71	SG	221	LYS
71	SG	223	LYS
72	SJ	138[A]	ARG
72	SJ	138[B]	ARG
73	SM	109	VAL
73	SM	121	LYS
74	SN	3	ARG
74	SN	4	MET
74	SN	64	ARG
75	SO	14	VAL
75	SO	98	ARG
75	SO	135	ILE
75	SO	142	ARG
75	SO	146	ARG
76	SW	103	VAL
77	SY	72	PHE
78	SZ	45	ASN
78	SZ	47	LEU
78	SZ	48	VAL
78	SZ	49	LEU
78	SZ	51	ASP
78	SZ	62	VAL
78	SZ	76	ARG
78	SZ	77	LEU
78	SZ	78	LYS
79	Sb	17	ARG

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Mol	Chain	Res	Type
79	Sb	55	LEU
79	Sb	56	CYS
79	Sb	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	97	ASN
4	LA	132	ASN
4	LA	205	ASN
4	LA	215	ASN
4	LA	216	HIS
5	LB	121	ASN
5	LB	175	GLN
5	LB	184	GLN
5	LB	213	GLN
5	LB	328	ASN
6	LC	47	ASN
6	LC	50	GLN
6	LC	317	ASN
7	LD	195	HIS
7	LD	202	GLN
8	LE	268	GLN
9	LF	235	ASN
10	LG	46	GLN
10	LG	208	ASN
10	LG	236	HIS
11	LH	42	ASN
11	LH	106	GLN
11	LH	116	ASN
11	LH	156	ASN
12	LI	73	ASN
12	LI	147	HIS
13	LJ	71	HIS
14	LL	6	ASN
14	LL	175	ASN
14	LL	188	ASN
15	LM	20	HIS
15	LM	34	ASN
15	LM	48	GLN
15	LM	69	HIS
15	LM	70	GLN

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Mol	Chain	Res	Type
16	LN	15	GLN
16	LN	37	HIS
16	LN	139	HIS
16	LN	149	GLN
17	LO	173	GLN
17	LO	180	GLN
17	LO	184	ASN
18	LP	56	GLN
18	LP	80	GLN
18	LP	97	ASN
18	LP	116	HIS
18	LP	118	GLN
20	LR	7	GLN
20	LR	130	ASN
21	LS	77	ASN
21	LS	125	GLN
22	LT	22	HIS
22	LT	127	GLN
23	LU	44	GLN
23	LU	50	ASN
23	LU	94	ASN
23	LU	105	ASN
25	LW	48	GLN
26	LX	93	ASN
26	LX	125	ASN
27	LY	4	ASN
27	LY	56	GLN
27	LY	86	GLN
27	LY	96	HIS
27	LY	127	GLN
28	LZ	28	ASN
28	LZ	78	ASN
29	La	60	HIS
29	La	85	GLN
29	La	93	ASN
30	Lb	6	ASN
30	Lb	12	GLN
30	Lb	19	ASN
30	Lb	60	ASN
31	Lc	33	GLN
32	Ld	79	ASN
33	Le	43	ASN

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Mol	Chain	Res	Type
33	Le	107	ASN
34	Lf	80	ASN
34	Lf	99	HIS
35	Lg	3	GLN
35	Lg	18	ASN
35	Lg	114	GLN
36	Lh	107	GLN
38	Lj	13	ASN
40	Ll	19	GLN
40	Ll	20	ASN
40	Ll	33	ASN
43	Lo	105	GLN
45	Lr	4	HIS
45	Lr	6	GLN
45	Lr	21	ASN
45	Lr	30	ASN
45	Lr	41	ASN
45	Lr	100	ASN
46	Lz	22	GLN
46	Lz	40	ASN
46	Lz	72	GLN
46	Lz	96	ASN
49	SA	9	GLN
49	SA	50	ASN
49	SA	215	GLN
50	SB	43	ASN
50	SB	160	GLN
50	SB	186	ASN
52	SE	98	ASN
52	SE	112	HIS
52	SE	142	HIS
52	SE	214	ASN
53	SF	29	GLN
53	SF	83	ASN
53	SF	148	ASN
54	SH	12	ASN
54	SH	25	GLN
54	SH	33	ASN
54	SH	76	GLN
54	SH	91	HIS
54	SH	97	GLN
54	SH	114	GLN

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Mol	Chain	Res	Type
54	SH	162	GLN
54	SH	165	ASN
54	SH	186	ASN
55	SI	52	ASN
55	SI	165	GLN
55	SI	181	GLN
56	SK	50	GLN
56	SK	61	GLN
57	SL	11	GLN
57	SL	65	ASN
58	SP	41	GLN
58	SP	53	GLN
58	SP	104	GLN
59	SQ	86	GLN
60	SR	118	GLN
61	SS	17	ASN
62	ST	63	HIS
63	SU	18	HIS
63	SU	81	GLN
64	SV	2	GLN
64	SV	29	HIS
64	SV	82	ASN
65	SX	23	HIS
65	SX	61	GLN
67	Sc	24	GLN
68	Sd	26	ASN
69	Sg	14	HIS
69	Sg	15	ASN
69	Sg	26	GLN
69	Sg	62	HIS
69	Sg	117	ASN
69	Sg	162	ASN
69	Sg	222	ASN
69	Sg	311	GLN
70	SC	115	GLN
70	SC	272	HIS
71	SG	13	GLN
71	SG	70	HIS
71	SG	186	GLN
71	SG	197	GLN
72	SJ	156	HIS
72	SJ	177	ASN

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Mol	Chain	Res	Type
73	SM	55	ASN
73	SM	119	GLN
74	SN	36	GLN
74	SN	58	HIS
74	SN	105	ASN
75	SO	13	GLN
75	SO	32	HIS
76	SW	90	GLN
77	SY	112	ASN
78	SZ	45	ASN
79	Sb	9	HIS
80	Se	15	GLN
80	Se	44	ASN
80	Se	58	ASN
81	Sf	91	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3705/3773 (98%)	1016 (27%)	35 (0%)
2	L7	119/120 (99%)	15 (12%)	0
3	L8	155/156 (99%)	37 (23%)	1 (0%)
47	S2	1715/1740 (98%)	431 (25%)	11 (0%)
48	S6	74/75 (98%)	29 (39%)	1 (1%)
All	All	5768/5864 (98%)	1528 (26%)	48 (0%)

All (1528) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	4	G
1	L5	6	C
1	L5	17	A
1	L5	25	A
1	L5	26	C
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	58	G

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Mol	Chain	Res	Type
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	66	A
1	L5	67	C
1	L5	69	A
1	L5	72	C
1	L5	73	A
1	L5	74	G
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	106	A
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	117	C
1	L5	119	G
1	L5	120	A
1	L5	122	U
1	L5	126	C
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	136	C
1	L5	137	G
1	L5	139	G
1	L5	141	C
1	L5	142	G
1	L5	143	C
1	L5	144	G
1	L5	152	U
1	L5	159	C
1	L5	165	A
1	L5	172	C
1	L5	177	G
1	L5	180	C
1	L5	181	C
1	L5	183	C
1	L5	184	U
1	L5	185	C

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Mol	Chain	Res	Type
1	L5	187	U
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	207	G
1	L5	209	U
1	L5	210	C
1	L5	212	A
1	L5	216	C
1	L5	218	A
1	L5	219	G
1	L5	225	G
1	L5	233	U
1	L5	234	G
1	L5	255	C
1	L5	256	G
1	L5	257	C
1	L5	259	C
1	L5	261	G
1	L5	262	G
1	L5	265	C
1	L5	269	G
1	L5	271	C
1	L5	274	C
1	L5	276	C
1	L5	278	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	341	G
1	L5	344	A
1	L5	345	C
1	L5	349	A
1	L5	370	U
1	L5	386	A
1	L5	387	G
1	L5	388	A
1	L5	398	A2M
1	L5	407	A

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Mol	Chain	Res	Type
1	L5	408	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	417	G
1	L5	418	A
1	L5	440	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	461	G
1	L5	465	G
1	L5	467	U
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	496	G
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	501	C
1	L5	502	C
1	L5	503	C
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	511	C
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	516	C

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Mol	Chain	Res	Type
1	L5	517	C
1	L5	518	G
1	L5	519	C
1	L5	643	C
1	L5	644	G
1	L5	646	G
1	L5	653	U
1	L5	654	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	670	G
1	L5	673	C
1	L5	676	C
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	691	C
1	L5	693	C
1	L5	696	C
1	L5	697	G
1	L5	701	G
1	L5	703	G
1	L5	704	C
1	L5	708	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	742	G
1	L5	747	A
1	L5	753	C
1	L5	754	U
1	L5	757	G
1	L5	758	G
1	L5	760	G
1	L5	904	C
1	L5	905	C
1	L5	913	U

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Mol	Chain	Res	Type
1	L5	914	U
1	L5	915	A
1	L5	916	C
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	934	C
1	L5	935	A
1	L5	936	C
1	L5	941	C
1	L5	943	A
1	L5	945	U
1	L5	946	C
1	L5	955	G
1	L5	958	G
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	963	G
1	L5	964	A
1	L5	965	G
1	L5	966	A
1	L5	969	C
1	L5	971	U
1	L5	977	C
1	L5	982	U
1	L5	984	C
1	L5	988	C
1	L5	989	U
1	L5	990	C
1	L5	991	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	1048	G
1	L5	1051	G
1	L5	1065	G

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Mol	Chain	Res	Type
1	L5	1069	G
1	L5	1070	G
1	L5	1072	C
1	L5	1074	G
1	L5	1083	U
1	L5	1094	G
1	L5	1095	A
1	L5	1096	C
1	L5	1168	G
1	L5	1170	G
1	L5	1171	G
1	L5	1172	C
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1184	A
1	L5	1191	C
1	L5	1192	C
1	L5	1193	C
1	L5	1198	G
1	L5	1200	G
1	L5	1202	C
1	L5	1203	G
1	L5	1205	G
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1216	C
1	L5	1217	G
1	L5	1218	G
1	L5	1219	G
1	L5	1222	A
1	L5	1241	C
1	L5	1243	C
1	L5	1245	C
1	L5	1252	C
1	L5	1253	G

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Mol	Chain	Res	Type
1	L5	1254	A
1	L5	1255	A
1	L5	1259	G
1	L5	1260	G
1	L5	1261	G
1	L5	1266	G
1	L5	1269	G
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1277	G
1	L5	1279	A
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1293	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1302	U
1	L5	1303	A
1	L5	1304	C
1	L5	1312	A
1	L5	1314	C
1	L5	1326	A2M
1	L5	1337	A
1	L5	1344	C
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1360	G
1	L5	1365	C
1	L5	1371	A
1	L5	1378	C
1	L5	1379	C
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A

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Mol	Chain	Res	Type
1	L5	1399	G
1	L5	1402	C
1	L5	1403	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1417	C
1	L5	1420	A
1	L5	1439	C
1	L5	1440	U
1	L5	1441	C
1	L5	1442	C
1	L5	1444	G
1	L5	1446	C
1	L5	1447	C
1	L5	1453	G
1	L5	1457	G
1	L5	1472	C
1	L5	1482	G
1	L5	1483	C
1	L5	1486	C
1	L5	1493	G
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1513	U
1	L5	1515	A
1	L5	1518	A
1	L5	1525	A
1	L5	1534	A2M
1	L5	1547	A
1	L5	1549	G
1	L5	1566	C
1	L5	1571	G
1	L5	1578	U
1	L5	1582	PSU
1	L5	1586	G
1	L5	1591	U
1	L5	1596	U
1	L5	1624	G
1	L5	1625	OMG

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Mol	Chain	Res	Type
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	PSU
1	L5	1680	G
1	L5	1681	G
1	L5	1686	C
1	L5	1691	G
1	L5	1694	C
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1707	C
1	L5	1716	G
1	L5	1719	A
1	L5	1726	U
1	L5	1729	A
1	L5	1734	G
1	L5	1740	C
1	L5	1741	G
1	L5	1742	A
1	L5	1750	G
1	L5	1753	G
1	L5	1755	C
1	L5	1756	U
1	L5	1757	U
1	L5	1758	G
1	L5	1760	G
1	L5	1761	G
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G

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Mol	Chain	Res	Type
1	L5	1765	A
1	L5	1766	A
1	L5	1768	C
1	L5	1769	G
1	L5	1770	A
1	L5	1771	U
1	L5	1775	A
1	L5	1787	A
1	L5	1797	G
1	L5	1803	G
1	L5	1804	A
1	L5	1810	G
1	L5	1819	G
1	L5	1821	G
1	L5	1822	U
1	L5	1823	G
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1852	U
1	L5	1855	G
1	L5	1866	UR3
1	L5	1869	G
1	L5	1876	U
1	L5	1882	U
1	L5	1888	A
1	L5	1889	U
1	L5	1890	G
1	L5	1892	A
1	L5	1897	A
1	L5	1917	A
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1935	C
1	L5	1936	C

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Mol	Chain	Res	Type
1	L5	1940	G
1	L5	1945	G
1	L5	1947	U
1	L5	1948	G
1	L5	1951	G
1	L5	1953	U
1	L5	1959	U
1	L5	1960	A
1	L5	1961	G
1	L5	1962	A
1	L5	1965	G
1	L5	1966	C
1	L5	1967	A
1	L5	1969	G
1	L5	1971	C
1	L5	1974	U
1	L5	1975	G
1	L5	1976	G
1	L5	1977	C
1	L5	1980	U
1	L5	1981	G
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1987	C
1	L5	1988	G
1	L5	1989	G
1	L5	1991	A
1	L5	1995	G
1	L5	1996	C
1	L5	1998	A
1	L5	1999	A
1	L5	2002	A
1	L5	2003	G
1	L5	2006	U
1	L5	2007	G
1	L5	2009	A
1	L5	2010	A
1	L5	2011	C
1	L5	2012	A
1	L5	2013	A

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Mol	Chain	Res	Type
1	L5	2015	U
1	L5	2016	C
1	L5	2018	C
1	L5	2020	U
1	L5	2025	A
1	L5	2026	A
1	L5	2033	A
1	L5	2038	U
1	L5	2044	U
1	L5	2046	G
1	L5	2048	U
1	L5	2050	OMG
1	L5	2055	G
1	L5	2056	G
1	L5	2062	C
1	L5	2068	C
1	L5	2069	A
1	L5	2084	C
1	L5	2085	G
1	L5	2089	G
1	L5	2090	U
1	L5	2092	G
1	L5	2093	A
1	L5	2094	G
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2106	G
1	L5	2107	C
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2252	G
1	L5	2253	A
1	L5	2256	C
1	L5	2258	C
1	L5	2259	G
1	L5	2260	C
1	L5	2289	C
1	L5	2300	A

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Mol	Chain	Res	Type
1	L5	2301	G
1	L5	2306	G
1	L5	2313	A
1	L5	2316	G
1	L5	2332	A
1	L5	2333	G
1	L5	2337	C
1	L5	2338	C
1	L5	2346	C
1	L5	2348	G
1	L5	2351	C
1	L5	2357	G
1	L5	2360	A
1	L5	2370	A
1	L5	2382	A
1	L5	2389	A
1	L5	2395	A
1	L5	2396	A
1	L5	2397	G
1	L5	2408	U
1	L5	2416	G
1	L5	2417	A
1	L5	2421	G
1	L5	2422	OMC
1	L5	2424	OMG
1	L5	2425	U
1	L5	2426	U
1	L5	2440	U
1	L5	2441	C
1	L5	2450	G
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2482	C
1	L5	2483	G
1	L5	2485	U
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U

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Mol	Chain	Res	Type
1	L5	2491	C
1	L5	2493	G
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2511	A
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2529	A
1	L5	2533	C
1	L5	2537	A
1	L5	2543	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2556	G
1	L5	2559	G
1	L5	2565	A
1	L5	2566	G
1	L5	2573	A
1	L5	2583	C
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2602	G
1	L5	2611	A
1	L5	2616	C
1	L5	2618	G
1	L5	2627	C
1	L5	2637	U
1	L5	2652	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2673	G
1	L5	2676	A
1	L5	2687	U
1	L5	2695	A

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Mol	Chain	Res	Type
1	L5	2696	A
1	L5	2703	G
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2712	G
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2732	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2754	G
1	L5	2756	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2770	C
1	L5	2788	U
1	L5	2790	U
1	L5	2801	U
1	L5	2814	C
1	L5	2815	A
1	L5	2826	U
1	L5	2827	G
1	L5	2838	G
1	L5	2842	G
1	L5	2848	G
1	L5	2855	G
1	L5	2856	C
1	L5	2867	C
1	L5	2877	G
1	L5	2892	C
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U
1	L5	2905	C
1	L5	2906	G

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Mol	Chain	Res	Type
1	L5	2907	G
1	L5	2908	U
1	L5	2910	G
1	L5	3585	G
1	L5	3586	G
1	L5	3587	C
1	L5	3588	C
1	L5	3589	G
1	L5	3590	G
1	L5	3591	C
1	L5	3593	C
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3602	C
1	L5	3604	A
1	L5	3605	C
1	L5	3606	U
1	L5	3615	G
1	L5	3616	U
1	L5	3618	C
1	L5	3626	G
1	L5	3630	A
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3648	A
1	L5	3650	C
1	L5	3662	A
1	L5	3663	A
1	L5	3673	C
1	L5	3674	G
1	L5	3680	U
1	L5	3681	G
1	L5	3692	A
1	L5	3710	G
1	L5	3711	A
1	L5	3713	U
1	L5	3714	G
1	L5	3726	A
1	L5	3727	A

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Mol	Chain	Res	Type
1	L5	3729	PSU
1	L5	3734	U
1	L5	3735	G
1	L5	3736	A
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3762	B8H
1	L5	3764	PSU
1	L5	3771	C
1	L5	3775	A
1	L5	3776	G
1	L5	3777	G
1	L5	3785	A2M
1	L5	3786	U
1	L5	3787	G
1	L5	3799	A
1	L5	3801	U
1	L5	3802	U
1	L5	3810	C
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3851	U
1	L5	3867	A2M
1	L5	3868	G
1	L5	3870	C
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3890	A
1	L5	3892	U

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Mol	Chain	Res	Type
1	L5	3897	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3916	G
1	L5	3922	G
1	L5	3926	C
1	L5	3942	A
1	L5	3943	A
1	L5	3947	A
1	L5	3948	C
1	L5	3949	A
1	L5	3950	U
1	L5	3951	G
1	L5	3953	G
1	L5	3955	G
1	L5	3956	G
1	L5	3957	U
1	L5	3958	G
1	L5	3959	U
1	L5	3960	A
1	L5	3961	G
1	L5	3962	A
1	L5	3963	A
1	L5	3964	U
1	L5	3965	A
1	L5	3966	A
1	L5	3967	G
1	L5	3968	U
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3972	A
1	L5	3973	G
1	L5	3974	G
1	L5	3975	C
1	L5	3977	C
1	L5	4035	G
1	L5	4036	G
1	L5	4039	G

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Mol	Chain	Res	Type
1	L5	4041	C
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4045	G
1	L5	4046	A
1	L5	4047	A
1	L5	4048	A
1	L5	4049	U
1	L5	4051	C
1	L5	4052	C
1	L5	4053	A
1	L5	4054	C
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4059	C
1	L5	4061	G
1	L5	4062	A
1	L5	4064	C
1	L5	4067	U
1	L5	4068	U
1	L5	4069	U
1	L5	4076	G
1	L5	4086	G
1	L5	4091	G
1	L5	4099	G
1	L5	4100	C
1	L5	4102	C
1	L5	4104	G
1	L5	4107	G
1	L5	4108	G
1	L5	4110	C
1	L5	4113	U
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4121	G
1	L5	4127	A
1	L5	4133	C
1	L5	4135	G

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Mol	Chain	Res	Type
1	L5	4138	C
1	L5	4139	G
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4145	C
1	L5	4146	G
1	L5	4150	G
1	L5	4162	C
1	L5	4163	U
1	L5	4168	G
1	L5	4170	A
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4201	G
1	L5	4203	A
1	L5	4212	A
1	L5	4213	A
1	L5	4220	6MZ
1	L5	4222	G
1	L5	4224	A
1	L5	4225	G
1	L5	4229	U
1	L5	4233	A
1	L5	4249	G
1	L5	4251	A
1	L5	4254	G
1	L5	4257	A
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A
1	L5	4280	A
1	L5	4295	U
1	L5	4304	A
1	L5	4305	G
1	L5	4306	OMU
1	L5	4314	C
1	L5	4326	G
1	L5	4329	G

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Mol	Chain	Res	Type
1	L5	4330	G
1	L5	4332	C
1	L5	4349	C
1	L5	4351	U
1	L5	4354	U
1	L5	4373	G
1	L5	4374	U
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4380	A
1	L5	4381	A
1	L5	4385	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4400	G
1	L5	4415	1MA
1	L5	4416	G
1	L5	4420	U
1	L5	4422	A
1	L5	4426	C
1	L5	4427	G
1	L5	4437	U
1	L5	4444	C
1	L5	4448	G
1	L5	4449	A
1	L5	4463	U
1	L5	4464	A
1	L5	4466	C
1	L5	4475	G
1	L5	4476	C
1	L5	4488	A
1	L5	4494	OMG
1	L5	4500	PSU
1	L5	4510	A
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4523	A2M

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Mol	Chain	Res	Type
1	L5	4524	G
1	L5	4531	PSU
1	L5	4532	U
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4554	G
1	L5	4556	U
1	L5	4560	C
1	L5	4567	G
1	L5	4570	G
1	L5	4573	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A
1	L5	4600	G
1	L5	4601	U
1	L5	4606	G
1	L5	4617	G
1	L5	4633	G
1	L5	4635	A
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4652	G
1	L5	4656	A
1	L5	4657	U
1	L5	4658	G
1	L5	4670	C
1	L5	4672	A
1	L5	4679	G
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4732	G
1	L5	4734	A
1	L5	4735	G
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G

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Mol	Chain	Res	Type
1	L5	4747	C
1	L5	4751	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4772	C
1	L5	4776	G
1	L5	4859	C
1	L5	4860	G
1	L5	4862	G
1	L5	4870	OMG
1	L5	4871	C
1	L5	4875	G
1	L5	4876	U
1	L5	4881	U
1	L5	4882	U
1	L5	4883	C
1	L5	4885	U
1	L5	4888	U
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4899	G
1	L5	4900	C
1	L5	4901	G
1	L5	4903	G
1	L5	4910	G
1	L5	4912	G
1	L5	4913	G
1	L5	4914	C
1	L5	4916	G
1	L5	4923	C
1	L5	4925	U
1	L5	4926	C
1	L5	4928	C
1	L5	4931	G
1	L5	4934	A
1	L5	4937	C
1	L5	4938	A
1	L5	4940	C

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Mol	Chain	Res	Type
1	L5	4941	G
1	L5	4942	C
1	L5	4943	A
1	L5	4947	U
1	L5	4949	G
1	L5	4950	U
1	L5	4951	G
1	L5	4955	A
1	L5	4960	G
1	L5	4966	A
1	L5	4967	A
1	L5	4975	G
1	L5	4976	U
1	L5	4985	U
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C
1	L5	4991	U
1	L5	5014	A
1	L5	5016	A
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5028	G
1	L5	5029	C
1	L5	5030	U
1	L5	5034	A
1	L5	5038	A
1	L5	5041	G
1	L5	5047	C
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5058	A
1	L5	5061	A
1	L5	5069	U
2	L7	7	G
2	L7	22	A
2	L7	31	G
2	L7	33	U

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Mol	Chain	Res	Type
2	L7	38	U
2	L7	52	C
2	L7	53	U
2	L7	54	A
2	L7	62	U
2	L7	63	C
2	L7	64	G
2	L7	71	G
2	L7	100	A
2	L7	103	A
2	L7	110	G
3	L8	20	A
3	L8	23	C
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	38	U
3	L8	39	G
3	L8	48	A
3	L8	50	C
3	L8	51	U
3	L8	52	A
3	L8	59	A
3	L8	60	G
3	L8	62	A
3	L8	63	U
3	L8	75	G
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	106	G
3	L8	110	U
3	L8	111	U
3	L8	114	G
3	L8	122	G
3	L8	123	U
3	L8	124	U

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Mol	Chain	Res	Type
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	128	C
3	L8	135	C
3	L8	156	U
47	S2	2	A
47	S2	4	C
47	S2	17	C
47	S2	33	G
47	S2	41	G
47	S2	44	U
47	S2	46	A
47	S2	56	G
47	S2	58	C
47	S2	64	A
47	S2	67	C
47	S2	68	A
47	S2	72	C
47	S2	73	C
47	S2	74	G
47	S2	76	U
47	S2	77	A
47	S2	79	A
47	S2	92	A
47	S2	99	A
47	S2	103	A
47	S2	110	U
47	S2	113	G
47	S2	114	G
47	S2	115	U
47	S2	116	OMU
47	S2	126	G
47	S2	143	U
47	S2	149	A
47	S2	150	A
47	S2	155	G
47	S2	160	U
47	S2	161	U
47	S2	162	C
47	S2	170	A
47	S2	184	G

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Mol	Chain	Res	Type
47	S2	192	C
47	S2	196	C
47	S2	198	U
47	S2	199	C
47	S2	200	G
47	S2	202	G
47	S2	203	G
47	S2	204	G
47	S2	206	G
47	S2	211	G
47	S2	214	U
47	S2	225	G
47	S2	290	U
47	S2	291	G
47	S2	292	A
47	S2	293	C
47	S2	295	C
47	S2	306	C
47	S2	307	G
47	S2	308	G
47	S2	309	G
47	S2	311	C
47	S2	313	A
47	S2	318	A
47	S2	319	C
47	S2	322	C
47	S2	323	C
47	S2	324	C
47	S2	326	C
47	S2	328	U
47	S2	329	G
47	S2	331	C
47	S2	335	G
47	S2	339	A
47	S2	347	G
47	S2	360	A
47	S2	362	C
47	S2	364	A
47	S2	368	U
47	S2	369	C
47	S2	370	G
47	S2	374	G

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Mol	Chain	Res	Type
47	S2	385	G
47	S2	386	C
47	S2	398	A
47	S2	400	C
47	S2	407	G
47	S2	408	A
47	S2	409	C
47	S2	418	A
47	S2	421	G
47	S2	425	G
47	S2	426	A
47	S2	438	G
47	S2	447	A
47	S2	448	A
47	S2	449	A
47	S2	450	C
47	S2	452	G
47	S2	464	A
47	S2	465	A
47	S2	470	G
47	S2	471	G
47	S2	472	C
47	S2	473	A
47	S2	474	G
47	S2	482	G
47	S2	487	U
47	S2	488	U
47	S2	492	C
47	S2	493	A
47	S2	506	G
47	S2	507	G
47	S2	508	A
47	S2	509	OMG
47	S2	525	A
47	S2	530	U
47	S2	531	A
47	S2	532	C
47	S2	537	C
47	S2	538	U
47	S2	540	U
47	S2	542	U
47	S2	544	G

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Mol	Chain	Res	Type
47	S2	545	A
47	S2	546	G
47	S2	547	G
47	S2	552	G
47	S2	555	A
47	S2	556	U
47	S2	557	U
47	S2	558	G
47	S2	563	G
47	S2	564	A
47	S2	566	U
47	S2	569	A
47	S2	576	A
47	S2	587	A
47	S2	589	G
47	S2	590	A
47	S2	591	U
47	S2	592	C
47	S2	597	G
47	S2	598	G
47	S2	603	C
47	S2	607	U
47	S2	608	C
47	S2	614	C
47	S2	623	G
47	S2	627	U
47	S2	631	U
47	S2	643	A
47	S2	655	A
47	S2	658	U
47	S2	660	C
47	S2	664	A
47	S2	668	A2M
47	S2	669	A
47	S2	671	A
47	S2	672	A
47	S2	673	G
47	S2	683	OMG
47	S2	684	G
47	S2	687	C
47	S2	688	U
47	S2	689	U

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Mol	Chain	Res	Type
47	S2	691	G
47	S2	692	G
47	S2	694	G
47	S2	696	G
47	S2	697	G
47	S2	698	G
47	S2	731	G
47	S2	732	U
47	S2	733	C
47	S2	734	C
47	S2	735	C
47	S2	736	C
47	S2	738	C
47	S2	739	C
47	S2	751	G
47	S2	752	G
47	S2	753	C
47	S2	788	G
47	S2	789	G
47	S2	791	C
47	S2	792	C
47	S2	793	G
47	S2	794	A
47	S2	797	C
47	S2	798	G
47	S2	799	U
47	S2	808	A
47	S2	810	A
47	S2	811	A
47	S2	821	G
47	S2	822	PSU
47	S2	830	A
47	S2	834	C
47	S2	835	C
47	S2	836	G
47	S2	837	A
47	S2	838	G
47	S2	839	C
47	S2	840	C
47	S2	841	G
47	S2	842	C
47	S2	847	A

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Mol	Chain	Res	Type
47	S2	853	C
47	S2	861	A
47	S2	862	A
47	S2	869	A
47	S2	870	A
47	S2	872	A
47	S2	873	G
47	S2	874	G
47	S2	875	A
47	S2	878	G
47	S2	880	G
47	S2	885	U
47	S2	887	U
47	S2	888	U
47	S2	889	U
47	S2	891	G
47	S2	892	U
47	S2	896	U
47	S2	897	U
47	S2	898	U
47	S2	899	U
47	S2	900	C
47	S2	901	G
47	S2	903	A
47	S2	904	A
47	S2	913	A
47	S2	914	U
47	S2	920	A
47	S2	933	G
47	S2	934	G
47	S2	955	A
47	S2	963	A
47	S2	968	U
47	S2	969	U
47	S2	971	G
47	S2	972	A
47	S2	978	G
47	S2	990	A
47	S2	992	A
47	S2	999	G
47	S2	1001	A
47	S2	1002	U

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Mol	Chain	Res	Type
47	S2	1008	A
47	S2	1017	U
47	S2	1023	A
47	S2	1027	A
47	S2	1028	A
47	S2	1033	G
47	S2	1038	U
47	S2	1045	U
47	S2	1061	U
47	S2	1062	A
47	S2	1067	C
47	S2	1078	C
47	S2	1083	A
47	S2	1084	A
47	S2	1085	C
47	S2	1089	G
47	S2	1109	C
47	S2	1114	U
47	S2	1116	C
47	S2	1121	G
47	S2	1133	A
47	S2	1138	C
47	S2	1148	A
47	S2	1153	C
47	S2	1154	U
47	S2	1165	G
47	S2	1166	G
47	S2	1168	G
47	S2	1170	A
47	S2	1172	U
47	S2	1195	A
47	S2	1207	G
47	S2	1208	A
47	S2	1215	C
47	S2	1216	C
47	S2	1217	A
47	S2	1221	G
47	S2	1224	G
47	S2	1227	G
47	S2	1242	U
47	S2	1243	PSU
47	S2	1248	B8N

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Mol	Chain	Res	Type
47	S2	1251	A
47	S2	1253	A
47	S2	1256	G
47	S2	1257	G
47	S2	1259	A
47	S2	1264	C
47	S2	1265	A
47	S2	1266	C
47	S2	1274	G
47	S2	1275	G
47	S2	1283	C
47	S2	1286	G
47	S2	1294	G
47	S2	1295	A
47	S2	1300	U
47	S2	1301	A
47	S2	1302	G
47	S2	1303	C
47	S2	1308	U
47	S2	1320	G
47	S2	1332	A
47	S2	1341	C
47	S2	1342	U
47	S2	1343	U
47	S2	1354	G
47	S2	1371	U
47	S2	1373	C
47	S2	1378	A
47	S2	1382	A
47	S2	1386	A
47	S2	1397	U
47	S2	1398	G
47	S2	1401	A
47	S2	1404	U
47	S2	1406	G
47	S2	1408	U
47	S2	1412	C
47	S2	1415	C
47	S2	1416	C
47	S2	1417	C
47	S2	1419	C
47	S2	1421	A

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Mol	Chain	Res	Type
47	S2	1422	G
47	S2	1423	C
47	S2	1433	C
47	S2	1434	C
47	S2	1435	C
47	S2	1436	C
47	S2	1438	A
47	S2	1448	A
47	S2	1449	G
47	S2	1452	A
47	S2	1454	A
47	S2	1455	A
47	S2	1463	U
47	S2	1464	C
47	S2	1478	U
47	S2	1480	A
47	S2	1487	A
47	S2	1488	C
47	S2	1489	A
47	S2	1490	G
47	S2	1494	U
47	S2	1495	G
47	S2	1497	G
47	S2	1498	A
47	S2	1520	G
47	S2	1521	C
47	S2	1533	A
47	S2	1537	A
47	S2	1544	C
47	S2	1545	A
47	S2	1548	G
47	S2	1552	G
47	S2	1553	C
47	S2	1556	A
47	S2	1560	U
47	S2	1570	G
47	S2	1580	A
47	S2	1585	U
47	S2	1586	U
47	S2	1587	G
47	S2	1588	A
47	S2	1600	G

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Mol	Chain	Res	Type
47	S2	1601	A
47	S2	1603	G
47	S2	1621	U
47	S2	1623	A
47	S2	1634	A
47	S2	1635	C
47	S2	1638	G
47	S2	1640	A
47	S2	1646	C
47	S2	1648	G
47	S2	1654	G
47	S2	1661	A
47	S2	1663	A
47	S2	1665	G
47	S2	1671	G
47	S2	1680	G
47	S2	1686	G
47	S2	1698	C
47	S2	1719	A
47	S2	1721	U
47	S2	1722	G
47	S2	1744	G
47	S2	1745	A
47	S2	1748	G
47	S2	1752	C
47	S2	1753	C
47	S2	1754	G
47	S2	1757	G
47	S2	1758	G
47	S2	1759	G
47	S2	1760	G
47	S2	1761	U
47	S2	1772	C
47	S2	1773	C
47	S2	1774	C
47	S2	1775	U
47	S2	1776	G
47	S2	1779	G
47	S2	1783	C
47	S2	1784	G
47	S2	1786	U
47	S2	1800	A

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Mol	Chain	Res	Type
47	S2	1804	U
47	S2	1813	A
47	S2	1822	A
47	S2	1823	A
47	S2	1824	A
47	S2	1829	G
47	S2	1831	A
47	S2	1835	A
47	S2	1838	U
47	S2	1849	G
47	S2	1851	MA6
47	S2	1852	C
47	S2	1861	G
47	S2	1862	G
47	S2	1863	A
47	S2	1865	C
47	S2	1867	U
48	S6	8	G
48	S6	9	U
48	S6	10	G
48	S6	18	G
48	S6	19	G
48	S6	20	A
48	S6	29	G
48	S6	31	G
48	S6	32	C
48	S6	33	C
48	S6	34	C
48	S6	36	U
48	S6	37	A
48	S6	39	C
48	S6	40	C
48	S6	41	C
48	S6	42	A
48	S6	44	A
48	S6	46	G
48	S6	47	U
48	S6	51	U
48	S6	54	A
48	S6	55	U
48	S6	58	A
48	S6	65	C

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Mol	Chain	Res	Type
48	S6	66	C
48	S6	69	U
48	S6	74	C
48	S6	76	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	58	G
1	L5	73	A
1	L5	385	A
1	L5	406	C
1	L5	417	G
1	L5	504	G
1	L5	913	U
1	L5	914	U
1	L5	935	A
1	L5	959	G
1	L5	961	G
1	L5	988	C
1	L5	989	U
1	L5	1082	C
1	L5	1279	A
1	L5	1654	G
1	L5	2019	C
1	L5	2084	C
1	L5	2096	G
1	L5	2396	A
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	2905	C
1	L5	3614	G
1	L5	3673	C
1	L5	3948	C
1	L5	3959	U
1	L5	3961	G
1	L5	4378	A
1	L5	4475	G
1	L5	4531	PSU
1	L5	4699	U
1	L5	4913	G

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Mol	Chain	Res	Type
1	L5	4949	G
3	L8	83	C
47	S2	112	U
47	S2	291	G
47	S2	420	G
47	S2	508	A
47	S2	563	G
47	S2	688	U
47	S2	797	C
47	S2	861	A
47	S2	1397	U
47	S2	1434	C
47	S2	1744	G
48	S6	54	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

113 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
1	PSU	L5	3729	1	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
1	OMG	L5	1883	1	23,26,27	1.36	4 (17%)	33,38,41	2.12	8 (24%)
1	UR3	L5	1866	1	19,22,23	1.06	2 (10%)	26,32,35	1.52	4 (15%)
1	UR3	L5	4530	1	19,22,23	1.10	1 (5%)	26,32,35	1.58	4 (15%)
47	A2M	S2	166	47	22,25,26	1.47	4 (18%)	31,36,39	2.21	8 (25%)
1	6MZ	L5	4220	1	22,25,26	1.40	4 (18%)	30,36,39	2.16	9 (30%)
47	A2M	S2	668	47,82	22,25,26	1.43	5 (22%)	31,36,39	2.09	9 (29%)
1	OMG	L5	4870	1	23,26,27	1.20	3 (13%)	33,38,41	1.89	6 (18%)
47	A2M	S2	484	47	22,25,26	1.45	4 (18%)	31,36,39	2.06	8 (25%)
1	A2M	L5	1524	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	8 (25%)
47	OMC	S2	1710	47	19,22,23	0.81	0	26,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	4500	1	18,21,22	1.08	1 (5%)	22,30,33	1.85	4 (18%)
47	A2M	S2	1031	47	22,25,26	1.44	5 (22%)	31,36,39	2.13	10 (32%)
1	5MC	L5	3782	1,82	18,22,23	0.97	2 (11%)	26,32,35	1.17	2 (7%)
1	A2M	L5	1534	1,82	22,25,26	1.47	5 (22%)	31,36,39	2.04	8 (25%)
47	PSU	S2	612	47	18,21,22	1.07	1 (5%)	22,30,33	1.85	5 (22%)
47	5MU	S2	814	47	19,22,23	1.40	6 (31%)	28,32,35	2.05	7 (25%)
1	OMG	L5	2364	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	2MG	L5	978	1	23,26,27	1.24	3 (13%)	32,38,41	2.18	6 (18%)
1	B8H	L5	3762	1	19,22,23	1.36	3 (15%)	22,32,35	2.00	3 (13%)
1	JMH	L5	1456	1	18,22,23	1.10	1 (5%)	21,32,35	0.95	1 (4%)
1	OMG	L5	4623	1	23,26,27	1.21	3 (13%)	33,38,41	1.97	7 (21%)
47	A2M	S2	159	47	22,25,26	1.46	4 (18%)	31,36,39	2.10	8 (25%)
47	OMC	S2	517	47	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	OMC	L5	3701	1,82	19,22,23	0.80	0	26,31,34	0.74	0
47	OMU	S2	121	47	19,22,23	1.22	3 (15%)	26,31,34	1.78	6 (23%)
1	OMG	L5	373	1	23,26,27	1.27	4 (17%)	33,38,41	2.14	8 (24%)
1	B8H	L5	1860	1	19,22,23	1.37	3 (15%)	22,32,35	1.97	4 (18%)
1	OMU	L5	4620	1	19,22,23	1.32	3 (15%)	26,31,34	1.86	6 (23%)
41	MLZ	Lm	98	41	8,9,10	0.77	0	4,9,11	0.62	0
1	OMG	L5	1316	1,82	23,26,27	1.36	4 (17%)	33,38,41	2.16	7 (21%)
1	A2M	L5	3825	1	22,25,26	1.45	5 (22%)	31,36,39	2.08	9 (29%)
1	OMC	L5	3869	1	19,22,23	0.82	0	26,31,34	0.96	1 (3%)
1	A2M	L5	2401	1	22,25,26	1.43	4 (18%)	31,36,39	2.08	9 (29%)
1	OMG	L5	3899	1	23,26,27	1.23	3 (13%)	33,38,41	2.00	5 (15%)
47	PSU	S2	822	47	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
6	MLZ	LC	333	6	8,9,10	0.75	0	4,9,11	0.67	0
1	OMC	L5	3909	1	19,22,23	0.81	0	26,31,34	0.94	1 (3%)
1	OMC	L5	3887	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
47	OMU	S2	116	47	19,22,23	1.25	4 (21%)	26,31,34	1.68	6 (23%)
47	OMG	S2	683	47	23,26,27	1.20	3 (13%)	33,38,41	2.02	6 (18%)
47	MA6	S2	1850	47	23,26,27	1.45	4 (17%)	34,38,41	2.18	10 (29%)
1	A2M	L5	1871	1,82	22,25,26	1.44	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	L5	4636	1	18,21,22	1.08	1 (5%)	22,30,33	1.88	5 (22%)
1	OMG	L5	2773	1	23,26,27	1.21	3 (13%)	33,38,41	1.88	6 (18%)
1	OMG	L5	1522	1	23,26,27	1.22	3 (13%)	33,38,41	1.97	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	L5	2365	1,82	19,22,23	0.80	0	26,31,34	0.76	0
1	OMU	L5	4306	1	19,22,23	1.29	4 (21%)	26,31,34	1.72	7 (26%)
1	PSU	L5	1683	1	18,21,22	1.11	1 (5%)	22,30,33	1.73	4 (18%)
47	UR3	S2	1830	47	19,22,23	1.03	2 (10%)	26,32,35	1.74	5 (19%)
1	PSU	L5	4531	1	18,21,22	1.37	2 (11%)	22,30,33	1.97	4 (18%)
47	PSU	S2	1243	47	18,21,22	1.53	5 (27%)	22,30,33	2.12	4 (18%)
47	MA6	S2	1851	47	23,26,27	1.45	4 (17%)	34,38,41	2.16	10 (29%)
1	A2M	L5	2363	1,82	22,25,26	1.43	3 (13%)	31,36,39	2.03	7 (22%)
47	PSU	S2	119	47	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
1	UR3	L5	4597	1	19,22,23	0.97	0	26,32,35	1.42	2 (7%)
1	A2M	L5	3785	1	22,25,26	1.38	4 (18%)	31,36,39	2.32	11 (35%)
1	OMG	L5	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.96	6 (18%)
1	1MA	L5	4415	1	21,25,26	1.36	4 (19%)	31,37,40	1.72	5 (16%)
1	A2M	L5	4523	1,82	22,25,26	1.38	4 (18%)	31,36,39	2.10	8 (25%)
1	B8T	L5	4671	1	19,22,23	0.84	0	26,31,34	1.09	2 (7%)
1	A2M	L5	3718	1	22,25,26	1.43	4 (18%)	31,36,39	2.06	9 (29%)
1	OMG	L5	4196	1	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
47	A2M	S2	1678	47	22,25,26	1.43	4 (18%)	31,36,39	2.14	10 (32%)
47	M7A	S2	1806	47	20,25,26	1.52	3 (15%)	28,37,40	2.17	6 (21%)
1	OMC	L5	2804	1	19,22,23	0.83	0	26,31,34	0.83	1 (3%)
1	OMG	L5	4637	1	23,26,27	1.23	3 (13%)	33,38,41	1.98	7 (21%)
1	PSU	L5	2508	1	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)
1	OMC	L5	2422	1,82	19,22,23	0.84	0	26,31,34	0.98	1 (3%)
47	4AC	S2	1337	47	21,24,25	1.09	2 (9%)	29,34,37	1.03	3 (10%)
47	OMC	S2	1703	47	19,22,23	0.83	0	26,31,34	0.87	1 (3%)
47	OMG	S2	644	47	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	5MC	L5	4447	1,82	18,22,23	1.04	2 (11%)	26,32,35	1.63	6 (23%)
47	OMC	S2	174	47,82	19,22,23	0.81	0	26,31,34	0.78	0
1	OMG	L5	1625	1	23,26,27	1.23	3 (13%)	33,38,41	1.97	6 (18%)
1	PSU	L5	4450	1,82	18,21,22	1.04	2 (11%)	22,30,33	1.80	5 (22%)
1	2MG	L5	729	1,82	23,26,27	1.24	3 (13%)	32,38,41	2.25	8 (25%)
1	PSU	L5	4442	1	18,21,22	1.04	1 (5%)	22,30,33	1.83	6 (27%)
1	OMC	L5	4536	1	19,22,23	0.83	0	26,31,34	0.93	1 (3%)
47	PSU	S2	823	47	18,21,22	1.14	1 (5%)	22,30,33	1.73	4 (18%)
1	A2M	L5	1326	1	22,25,26	1.35	4 (18%)	31,36,39	2.18	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L5	3867	1	22,25,26	1.42	4 (18%)	31,36,39	2.11	9 (29%)
1	2MG	L5	1517	1	23,26,27	1.22	3 (13%)	32,38,41	2.50	8 (25%)
47	4AC	S2	1842	47	21,24,25	0.96	1 (4%)	29,34,37	1.33	5 (17%)
1	PSU	L5	1677	1	18,21,22	1.55	5 (27%)	22,30,33	2.10	4 (18%)
1	B8H	L5	4296	1	19,22,23	1.36	3 (15%)	22,32,35	2.00	3 (13%)
1	B8T	L5	4483	1	19,22,23	0.77	0	26,31,34	0.88	1 (3%)
1	PSU	L5	4628	1	18,21,22	1.09	1 (5%)	22,30,33	1.81	4 (18%)
1	OMG	L5	2424	1	23,26,27	1.24	3 (13%)	33,38,41	1.88	6 (18%)
47	B8N	S2	1248	47	24,29,30	0.96	1 (4%)	29,42,45	1.47	4 (13%)
47	6MZ	S2	1832	47,82	22,25,26	1.43	3 (13%)	30,36,39	2.13	8 (26%)
1	1MA	L5	1322	1,82	21,25,26	1.38	3 (14%)	31,37,40	1.80	5 (16%)
1	2MG	L5	4872	1	23,26,27	1.22	4 (17%)	32,38,41	2.40	10 (31%)
47	PSU	S2	1081	47	18,21,22	0.97	1 (5%)	22,30,33	1.62	5 (22%)
1	PSU	L5	4293	1	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
1	PSU	L5	1582	1	18,21,22	1.50	4 (22%)	22,30,33	2.08	4 (18%)
1	PSU	L5	4403	1	18,21,22	1.01	1 (5%)	22,30,33	1.63	4 (18%)
1	OMC	L5	2861	1	19,22,23	0.80	0	26,31,34	0.78	1 (3%)
1	A2M	L5	3723	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	L5	3764	1	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
1	5MU	L5	4083	1	19,22,23	1.43	4 (21%)	28,32,35	2.30	7 (25%)
1	A2M	L5	4571	1	22,25,26	1.44	4 (18%)	31,36,39	2.03	9 (29%)
47	JMH	S2	1219	47,82	18,22,23	1.11	1 (5%)	21,32,35	1.00	2 (9%)
47	OMG	S2	509	47,82	23,26,27	1.38	4 (17%)	33,38,41	2.02	6 (18%)
1	5MC	L5	4335	1	18,22,23	0.95	2 (11%)	26,32,35	1.18	4 (15%)
1	OMG	L5	2050	1	23,26,27	1.35	4 (17%)	33,38,41	2.06	8 (24%)
47	A2M	S2	27	47,82	22,25,26	1.44	4 (18%)	31,36,39	2.21	9 (29%)
1	PSU	L5	3715	1,82	18,21,22	1.10	1 (5%)	22,30,33	1.64	4 (18%)
3	OMU	L8	14	1,3	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
1	A2M	L5	398	1	22,25,26	1.45	4 (18%)	31,36,39	2.10	10 (32%)
1	OMG	L5	4494	1	23,26,27	1.22	3 (13%)	33,38,41	1.92	5 (15%)
1	OMG	L5	4370	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	7 (21%)
47	5MC	S2	1374	47	18,22,23	0.92	2 (11%)	26,32,35	1.10	3 (11%)

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
1	PSU	L5	3729	1	-	2/7/25/26	0/2/2/2
1	OMG	L5	1883	1	-	3/9/27/28	0/3/3/3
1	UR3	L5	1866	1	-	2/7/25/26	0/2/2/2
1	UR3	L5	4530	1	-	2/7/25/26	0/2/2/2
47	A2M	S2	166	47	-	0/9/27/28	0/3/3/3
1	6MZ	L5	4220	1	-	2/9/27/28	0/3/3/3
47	A2M	S2	668	47,82	-	3/9/27/28	0/3/3/3
1	OMG	L5	4870	1	-	3/9/27/28	0/3/3/3
47	A2M	S2	484	47	-	0/9/27/28	0/3/3/3
1	A2M	L5	1524	1	-	1/9/27/28	0/3/3/3
47	OMC	S2	1710	47	-	0/9/27/28	0/2/2/2
1	PSU	L5	4500	1	-	3/7/25/26	0/2/2/2
47	A2M	S2	1031	47	-	0/9/27/28	0/3/3/3
1	5MC	L5	3782	1,82	-	0/7/25/26	0/2/2/2
1	A2M	L5	1534	1,82	-	2/9/27/28	0/3/3/3
47	PSU	S2	612	47	-	0/7/25/26	0/2/2/2
47	5MU	S2	814	47	-	0/7/25/26	0/2/2/2
1	OMG	L5	2364	1	-	1/9/27/28	0/3/3/3
1	2MG	L5	978	1	-	0/9/27/28	0/3/3/3
1	B8H	L5	3762	1	-	2/7/25/26	0/2/2/2
1	JMH	L5	1456	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
47	A2M	S2	159	47	-	0/9/27/28	0/3/3/3
47	OMC	S2	517	47	-	0/9/27/28	0/2/2/2
1	OMC	L5	3701	1,82	-	4/9/27/28	0/2/2/2
47	OMU	S2	121	47	-	0/9/27/28	0/2/2/2
1	OMG	L5	373	1	-	0/9/27/28	0/3/3/3
1	B8H	L5	1860	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
41	MLZ	Lm	98	41	-	0/7/8/10	-
1	OMG	L5	1316	1,82	-	0/9/27/28	0/3/3/3
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	2401	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	3899	1	-	4/9/27/28	0/3/3/3
47	PSU	S2	822	47	-	0/7/25/26	0/2/2/2
6	MLZ	LC	333	6	-	2/7/8/10	-
1	OMC	L5	3909	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
47	OMU	S2	116	47	-	3/9/27/28	0/2/2/2
47	OMG	S2	683	47	-	2/9/27/28	0/3/3/3
47	MA6	S2	1850	47	-	0/11/29/30	0/3/3/3
1	A2M	L5	1871	1,82	-	0/9/27/28	0/3/3/3
1	PSU	L5	4636	1	-	4/7/25/26	0/2/2/2
1	OMG	L5	2773	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	2365	1,82	-	0/9/27/28	0/2/2/2
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1683	1	-	0/7/25/26	0/2/2/2
47	UR3	S2	1830	47	-	2/7/25/26	0/2/2/2
1	PSU	L5	4531	1	-	2/7/25/26	0/2/2/2
47	PSU	S2	1243	47	-	2/7/25/26	0/2/2/2
47	MA6	S2	1851	47	-	5/11/29/30	0/3/3/3
1	A2M	L5	2363	1,82	-	0/9/27/28	0/3/3/3
47	PSU	S2	119	47	-	0/7/25/26	0/2/2/2
1	UR3	L5	4597	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3785	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	3792	1	-	0/9/27/28	0/3/3/3
1	1MA	L5	4415	1	-	2/7/25/26	0/3/3/3
1	A2M	L5	4523	1,82	-	2/9/27/28	0/3/3/3
1	B8T	L5	4671	1	-	0/7/27/28	0/2/2/2
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4196	1	-	0/9/27/28	0/3/3/3
47	A2M	S2	1678	47	-	0/9/27/28	0/3/3/3
47	M7A	S2	1806	47	-	0/7/37/38	0/3/3/3
1	OMC	L5	2804	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4637	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2422	1,82	-	1/9/27/28	0/2/2/2
47	4AC	S2	1337	47	-	2/11/29/30	0/2/2/2
47	OMC	S2	1703	47	-	2/9/27/28	0/2/2/2
47	OMG	S2	644	47	-	1/9/27/28	0/3/3/3
1	5MC	L5	4447	1,82	-	4/7/25/26	0/2/2/2
47	OMC	S2	174	47,82	-	0/9/27/28	0/2/2/2
1	OMG	L5	1625	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4450	1,82	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	L5	729	1,82	-	3/9/27/28	0/3/3/3
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
47	PSU	S2	823	47	-	0/7/25/26	0/2/2/2
1	A2M	L5	1326	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	3867	1	-	3/9/27/28	0/3/3/3
1	2MG	L5	1517	1	-	0/9/27/28	0/3/3/3
47	4AC	S2	1842	47	-	0/11/29/30	0/2/2/2
1	PSU	L5	1677	1	-	1/7/25/26	0/2/2/2
1	B8H	L5	4296	1	-	0/7/25/26	0/2/2/2
1	B8T	L5	4483	1	-	0/7/27/28	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2424	1	-	2/9/27/28	0/3/3/3
47	B8N	S2	1248	47	-	4/16/34/35	0/2/2/2
47	6MZ	S2	1832	47,82	-	2/9/27/28	0/3/3/3
1	1MA	L5	1322	1,82	-	4/7/25/26	0/3/3/3
1	2MG	L5	4872	1	-	2/9/27/28	0/3/3/3
47	PSU	S2	1081	47	-	1/7/25/26	0/2/2/2
1	PSU	L5	4293	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	1582	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	4403	1	-	2/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	3723	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3764	1	-	1/7/25/26	0/2/2/2
1	5MU	L5	4083	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
47	JMH	S2	1219	47,82	-	0/7/25/26	0/2/2/2
47	OMG	S2	509	47,82	-	2/9/27/28	0/3/3/3
1	5MC	L5	4335	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2050	1	-	0/9/27/28	0/3/3/3
47	A2M	S2	27	47,82	-	0/9/27/28	0/3/3/3
1	PSU	L5	3715	1,82	-	0/7/25/26	0/2/2/2
3	OMU	L8	14	1,3	-	1/9/27/28	0/2/2/2
1	A2M	L5	398	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4494	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
47	5MC	S2	1374	47	-	0/7/25/26	0/2/2/2

All (279) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1851	MA6	C5-C4	4.46	1.47	1.39
47	S2	1832	6MZ	C5-C4	4.44	1.47	1.39
1	L5	3723	A2M	C5-C4	4.44	1.47	1.39
47	S2	1806	M7A	C8-N9	-4.43	1.35	1.45
47	S2	159	A2M	C5-C4	4.41	1.47	1.39
47	S2	166	A2M	C5-C4	4.41	1.47	1.39
47	S2	1850	MA6	C5-C4	4.38	1.47	1.39
1	L5	398	A2M	C5-C4	4.31	1.47	1.39
1	L5	1524	A2M	C5-C4	4.31	1.47	1.39
47	S2	484	A2M	C5-C4	4.30	1.47	1.39
1	L5	3825	A2M	C5-C4	4.29	1.47	1.39
1	L5	1534	A2M	C5-C4	4.28	1.47	1.39
1	L5	4220	6MZ	C5-C4	4.25	1.46	1.39
1	L5	3718	A2M	C5-C4	4.24	1.46	1.39
1	L5	2401	A2M	C5-C4	4.24	1.46	1.39
1	L5	3867	A2M	C5-C4	4.23	1.46	1.39
47	S2	27	A2M	C5-C4	4.23	1.46	1.39
1	L5	2363	A2M	C5-C4	4.22	1.46	1.39
47	S2	1031	A2M	C5-C4	4.21	1.46	1.39
1	L5	4571	A2M	C5-C4	4.20	1.46	1.39
47	S2	1678	A2M	C5-C4	4.18	1.46	1.39
1	L5	1871	A2M	C5-C4	4.17	1.46	1.39
47	S2	668	A2M	C5-C4	4.15	1.46	1.39
1	L5	3785	A2M	C5-C4	4.01	1.46	1.39
1	L5	4523	A2M	C5-C4	4.00	1.46	1.39
47	S2	823	PSU	C6-C5	3.66	1.39	1.35
1	L5	3729	PSU	C6-C5	3.56	1.39	1.35
1	L5	1326	A2M	C5-C4	3.55	1.45	1.39
1	L5	3715	PSU	C6-C5	3.53	1.39	1.35
1	L5	1683	PSU	C6-C5	3.51	1.39	1.35
1	L5	3764	PSU	C6-C5	3.48	1.39	1.35
1	L5	4628	PSU	C6-C5	3.47	1.39	1.35
1	L5	1316	OMG	C6-N1	-3.43	1.32	1.38
1	L5	2508	PSU	C6-C5	3.37	1.39	1.35
1	L5	4403	PSU	C6-C5	3.33	1.39	1.35
1	L5	4500	PSU	C6-C5	3.33	1.39	1.35
47	S2	509	OMG	C6-N1	-3.32	1.32	1.38
47	S2	612	PSU	C6-C5	3.31	1.39	1.35
1	L5	2050	OMG	C6-N1	-3.29	1.32	1.38
1	L5	1582	PSU	C4-N3	-3.26	1.32	1.38
1	L5	4636	PSU	C6-C5	3.25	1.39	1.35
47	S2	119	PSU	C6-C5	3.23	1.39	1.35
1	L5	4083	5MU	C4-N3	-3.21	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4442	PSU	C6-C5	3.21	1.39	1.35
47	S2	822	PSU	C6-C5	3.20	1.39	1.35
1	L5	4293	PSU	C6-C5	3.19	1.39	1.35
47	S2	1248	B8N	C6-C5	3.18	1.39	1.34
1	L5	1860	B8H	C6-C5	3.15	1.39	1.34
47	S2	1081	PSU	C6-C5	3.11	1.38	1.35
1	L5	1883	OMG	C6-N1	-3.11	1.33	1.38
47	S2	1806	M7A	C5-C6	3.08	1.49	1.40
1	L5	4447	5MC	C6-C5	3.07	1.39	1.34
1	L5	1677	PSU	C4-N3	-3.07	1.33	1.38
47	S2	1243	PSU	C4-N3	-3.06	1.33	1.38
1	L5	4415	1MA	C5-C4	3.06	1.47	1.38
1	L5	4620	OMU	C4-N3	-3.05	1.33	1.38
1	L5	4415	1MA	C6-N6	3.03	1.35	1.28
1	L5	1625	OMG	C5-C4	3.01	1.47	1.38
1	L5	2424	OMG	C5-C4	2.99	1.47	1.38
1	L5	4196	OMG	C5-C4	2.98	1.47	1.38
1	L5	2773	OMG	C5-C4	2.98	1.47	1.38
1	L5	4870	OMG	C5-C4	2.98	1.47	1.38
1	L5	4450	PSU	C6-C5	2.97	1.38	1.35
1	L5	1517	2MG	C5-C4	2.97	1.47	1.38
1	L5	3762	B8H	C6-C5	2.96	1.39	1.34
1	L5	4531	PSU	C4-N3	-2.94	1.33	1.38
1	L5	3792	OMG	C5-C4	2.93	1.46	1.38
47	S2	1850	MA6	C5-C6	2.92	1.49	1.41
1	L5	1522	OMG	C6-N1	-2.91	1.33	1.38
1	L5	4370	OMG	C5-C4	2.90	1.46	1.38
47	S2	1851	MA6	C5-C6	2.90	1.49	1.41
1	L5	3762	B8H	C4-N3	-2.88	1.33	1.38
1	L5	4494	OMG	C5-C4	2.88	1.46	1.38
1	L5	4637	OMG	C5-C4	2.87	1.46	1.38
47	S2	683	OMG	C5-C4	2.86	1.46	1.38
47	S2	1337	4AC	C4-N4	-2.86	1.35	1.39
1	L5	1322	1MA	C5-N7	-2.86	1.33	1.39
1	L5	729	2MG	C5-C4	2.86	1.46	1.38
1	L5	3899	OMG	C5-C4	2.85	1.46	1.38
47	S2	814	5MU	C4-N3	-2.85	1.33	1.38
47	S2	644	OMG	C5-C4	2.84	1.46	1.38
1	L5	978	2MG	C5-C4	2.84	1.46	1.38
1	L5	2364	OMG	C5-C4	2.84	1.46	1.38
1	L5	1322	1MA	C6-N6	2.83	1.35	1.28
1	L5	373	OMG	C6-N1	-2.83	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4296	B8H	C6-C5	2.81	1.38	1.34
1	L5	2364	OMG	C6-N1	-2.81	1.33	1.38
1	L5	2050	OMG	C5-N7	-2.81	1.33	1.39
1	L5	4623	OMG	C6-N1	-2.80	1.33	1.38
1	L5	4296	B8H	C4-N3	-2.80	1.33	1.38
1	L5	1522	OMG	C5-C4	2.80	1.46	1.38
1	L5	4083	5MU	C6-N1	-2.80	1.33	1.38
47	S2	644	OMG	C6-N1	-2.77	1.33	1.38
1	L5	4637	OMG	C6-N1	-2.75	1.33	1.38
1	L5	4623	OMG	C5-C4	2.75	1.46	1.38
1	L5	3899	OMG	C6-N1	-2.75	1.33	1.38
1	L5	4306	OMU	C4-N3	-2.74	1.33	1.38
1	L5	4083	5MU	C2-N3	-2.74	1.33	1.38
1	L5	3792	OMG	C6-N1	-2.73	1.33	1.38
47	S2	121	OMU	C4-N3	-2.73	1.33	1.38
3	L8	14	OMU	C4-N3	-2.72	1.33	1.38
1	L5	4494	OMG	C6-N1	-2.70	1.33	1.38
1	L5	4370	OMG	C6-N1	-2.70	1.33	1.38
1	L5	2424	OMG	C6-N1	-2.68	1.33	1.38
1	L5	1860	B8H	C4-N3	-2.67	1.33	1.38
1	L5	1625	OMG	C6-N1	-2.67	1.33	1.38
1	L5	4620	OMU	C2-N3	-2.66	1.33	1.38
1	L5	1582	PSU	C6-C5	2.65	1.38	1.35
1	L5	4196	OMG	C6-N1	-2.64	1.33	1.38
47	S2	1243	PSU	C2-N1	-2.63	1.33	1.36
47	S2	166	A2M	C5-C6	2.61	1.48	1.41
1	L5	4530	UR3	C2-N1	2.61	1.42	1.38
1	L5	1517	2MG	C6-N1	-2.61	1.34	1.38
1	L5	3723	A2M	C5-C6	2.61	1.48	1.41
47	S2	1806	M7A	C4-N9	-2.61	1.33	1.38
47	S2	683	OMG	C6-N1	-2.60	1.34	1.38
47	S2	509	OMG	C5-N7	-2.60	1.34	1.39
1	L5	729	2MG	C6-N1	-2.60	1.34	1.38
1	L5	4872	2MG	C5-C4	2.59	1.45	1.38
1	L5	1677	PSU	C6-C5	2.59	1.38	1.35
1	L5	4531	PSU	C6-C5	2.59	1.38	1.35
1	L5	398	A2M	C5-C6	2.57	1.48	1.41
1	L5	1883	OMG	C5-N7	-2.57	1.34	1.39
47	S2	1832	6MZ	C5-C6	2.57	1.48	1.41
47	S2	159	A2M	C5-C6	2.57	1.48	1.41
1	L5	4571	A2M	C5-C6	2.56	1.48	1.41
47	S2	27	A2M	C5-C6	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2401	A2M	C5-C6	2.54	1.48	1.41
1	L5	3782	5MC	C6-N1	-2.54	1.33	1.38
47	S2	509	OMG	C5-C4	2.54	1.45	1.38
1	L5	3718	A2M	C5-C6	2.53	1.48	1.41
1	L5	3867	A2M	C5-C6	2.53	1.48	1.41
1	L5	1322	1MA	C5-C4	2.53	1.45	1.38
1	L5	3825	A2M	C5-C6	2.53	1.48	1.41
1	L5	4335	5MC	C6-C5	2.53	1.38	1.34
1	L5	1883	OMG	C5-C4	2.53	1.45	1.38
1	L5	1534	A2M	C5-N7	-2.52	1.34	1.39
1	L5	1534	A2M	C5-C6	2.52	1.48	1.41
1	L5	4870	OMG	C6-N1	-2.52	1.34	1.38
1	L5	1326	A2M	C5-N7	-2.51	1.34	1.39
1	L5	4220	6MZ	C5-N7	-2.51	1.34	1.39
47	S2	116	OMU	C4-N3	-2.51	1.34	1.38
1	L5	2424	OMG	C5-N7	-2.51	1.34	1.39
1	L5	2363	A2M	C5-N7	-2.50	1.34	1.39
1	L5	2773	OMG	C6-N1	-2.50	1.34	1.38
47	S2	1031	A2M	C5-C6	2.50	1.48	1.41
47	S2	668	A2M	C5-C6	2.49	1.48	1.41
47	S2	1678	A2M	C5-C6	2.48	1.48	1.41
47	S2	484	A2M	C5-C6	2.48	1.48	1.41
1	L5	1524	A2M	C5-N7	-2.48	1.34	1.39
1	L5	1316	OMG	C5-N7	-2.48	1.34	1.39
1	L5	1625	OMG	C5-N7	-2.47	1.34	1.39
1	L5	978	2MG	C6-N1	-2.47	1.34	1.38
1	L5	373	OMG	C5-C4	2.47	1.45	1.38
1	L5	373	OMG	C5-N7	-2.46	1.34	1.39
1	L5	4335	5MC	C6-N1	-2.46	1.33	1.38
47	S2	116	OMU	C5-C4	-2.46	1.38	1.43
1	L5	4523	A2M	C5-N7	-2.46	1.34	1.39
1	L5	1871	A2M	C5-C6	2.45	1.47	1.41
1	L5	2050	OMG	C5-C4	2.45	1.45	1.38
47	S2	1374	5MC	C6-C5	2.45	1.38	1.34
47	S2	484	A2M	C5-N7	-2.45	1.34	1.39
1	L5	3782	5MC	C6-C5	2.45	1.38	1.34
1	L5	3785	A2M	C5-N7	-2.44	1.34	1.39
47	S2	814	5MU	C6-C5	2.44	1.38	1.34
1	L5	3718	A2M	C5-N7	-2.44	1.34	1.39
1	L5	4370	OMG	C5-N7	-2.44	1.34	1.39
1	L5	1524	A2M	C5-C6	2.43	1.47	1.41
47	S2	159	A2M	C5-N7	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4872	2MG	C4-N9	-2.42	1.31	1.38
1	L5	1871	A2M	C5-N7	-2.42	1.34	1.39
1	L5	3762	B8H	C2-N3	-2.41	1.33	1.38
1	L5	2363	A2M	C5-C6	2.41	1.47	1.41
1	L5	3867	A2M	C5-N7	-2.40	1.34	1.39
1	L5	398	A2M	C5-N7	-2.40	1.34	1.39
1	L5	1582	PSU	C2-N3	-2.39	1.33	1.37
47	S2	683	OMG	C5-N7	-2.39	1.34	1.39
47	S2	27	A2M	C5-N7	-2.39	1.34	1.39
1	L5	1677	PSU	C2-N1	-2.39	1.33	1.36
47	S2	166	A2M	C5-N7	-2.38	1.34	1.39
1	L5	4571	A2M	C5-N7	-2.38	1.34	1.39
1	L5	1517	2MG	C5-N7	-2.37	1.34	1.39
47	S2	814	5MU	C6-N1	-2.36	1.34	1.38
1	L5	4623	OMG	C5-N7	-2.36	1.34	1.39
47	S2	1031	A2M	C5-N7	-2.35	1.34	1.39
1	L5	398	A2M	C8-N7	2.35	1.36	1.31
1	L5	4494	OMG	C5-N7	-2.35	1.34	1.39
3	L8	14	OMU	C2-N3	-2.34	1.33	1.38
1	L5	1866	UR3	C2-N1	2.34	1.41	1.38
47	S2	668	A2M	C5-N7	-2.34	1.34	1.39
1	L5	3785	A2M	C5-C6	2.33	1.47	1.41
1	L5	4523	A2M	C5-C6	2.33	1.47	1.41
1	L5	1316	OMG	C5-C4	2.33	1.45	1.38
47	S2	1243	PSU	C2-N3	-2.32	1.33	1.37
47	S2	1678	A2M	C5-N7	-2.32	1.34	1.39
1	L5	3792	OMG	C5-N7	-2.32	1.34	1.39
1	L5	4196	OMG	C5-N7	-2.31	1.34	1.39
47	S2	1832	6MZ	C5-N7	-2.31	1.34	1.39
47	S2	644	OMG	C5-N7	-2.30	1.34	1.39
1	L5	4296	B8H	C2-N3	-2.30	1.33	1.38
1	L5	4870	OMG	C5-N7	-2.30	1.34	1.39
47	S2	121	OMU	C2-N3	-2.30	1.33	1.38
1	L5	4220	6MZ	C5-C6	2.30	1.47	1.41
1	L5	1326	A2M	C4-N9	-2.30	1.32	1.37
1	L5	4306	OMU	C5-C4	-2.30	1.38	1.43
1	L5	4872	2MG	C6-N1	-2.30	1.34	1.38
1	L5	2401	A2M	C8-N7	2.29	1.35	1.31
1	L5	3723	A2M	C8-N7	2.29	1.35	1.31
1	L5	1582	PSU	C2'-C1'	-2.28	1.50	1.53
1	L5	1883	OMG	C4-N9	-2.28	1.32	1.38
1	L5	3825	A2M	C5-N7	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4306	OMU	C2-N1	2.28	1.42	1.38
47	S2	1830	UR3	C2-N1	2.28	1.41	1.38
1	L5	4637	OMG	C5-N7	-2.27	1.34	1.39
1	L5	4306	OMU	C2-N3	-2.27	1.33	1.38
3	L8	14	OMU	C5-C4	-2.27	1.38	1.43
47	S2	1374	5MC	C6-N1	-2.26	1.34	1.38
1	L5	3723	A2M	C5-N7	-2.26	1.34	1.39
47	S2	121	OMU	C5-C4	-2.26	1.38	1.43
1	L5	4447	5MC	C6-N1	-2.26	1.34	1.38
47	S2	27	A2M	C8-N7	2.26	1.35	1.31
1	L5	373	OMG	C4-N9	-2.26	1.32	1.38
1	L5	1871	A2M	C8-N7	2.25	1.35	1.31
1	L5	1326	A2M	C5-C6	2.25	1.47	1.41
47	S2	1678	A2M	C8-N7	2.24	1.35	1.31
1	L5	2364	OMG	C5-N7	-2.24	1.34	1.39
1	L5	1860	B8H	C2-N3	-2.24	1.34	1.38
1	L5	3825	A2M	C8-N7	2.24	1.35	1.31
47	S2	668	A2M	C8-N7	2.24	1.35	1.31
1	L5	2401	A2M	C5-N7	-2.24	1.34	1.39
1	L5	3899	OMG	C5-N7	-2.24	1.34	1.39
47	S2	1219	JMH	C2-N1	2.23	1.41	1.38
47	S2	159	A2M	C8-N7	2.22	1.35	1.31
1	L5	4571	A2M	C8-N7	2.22	1.35	1.31
1	L5	1316	OMG	C4-N9	-2.21	1.32	1.38
1	L5	978	2MG	C5-N7	-2.21	1.34	1.39
1	L5	4415	1MA	C5-N7	-2.21	1.34	1.39
47	S2	484	A2M	C8-N7	2.21	1.35	1.31
47	S2	1243	PSU	C6-C5	2.21	1.37	1.35
47	S2	509	OMG	C4-N9	-2.21	1.32	1.38
1	L5	1534	A2M	C8-N7	2.21	1.35	1.31
47	S2	814	5MU	C2-N3	-2.20	1.34	1.38
1	L5	729	2MG	C5-N7	-2.19	1.34	1.39
47	S2	814	5MU	C4-C5	2.19	1.48	1.44
1	L5	4415	1MA	C2-N3	2.19	1.34	1.30
47	S2	1851	MA6	C8-N7	2.19	1.35	1.31
1	L5	4620	OMU	C5-C4	-2.19	1.38	1.43
47	S2	166	A2M	C8-N7	2.18	1.35	1.31
47	S2	1031	A2M	C8-N7	2.18	1.35	1.31
1	L5	2773	OMG	C5-N7	-2.18	1.34	1.39
1	L5	3785	A2M	C8-N7	2.18	1.35	1.31
1	L5	1522	OMG	C5-N7	-2.17	1.34	1.39
1	L5	4083	5MU	C6-C5	2.17	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3718	A2M	C8-N7	2.16	1.35	1.31
1	L5	1677	PSU	C2-N3	-2.16	1.33	1.37
1	L5	1456	JMH	C2-N1	2.16	1.41	1.38
1	L5	3825	A2M	C4-N9	-2.15	1.32	1.37
47	S2	1337	4AC	C7-N4	-2.14	1.33	1.37
1	L5	1677	PSU	C2'-C1'	-2.14	1.51	1.53
47	S2	1851	MA6	C5-N7	-2.14	1.35	1.39
47	S2	116	OMU	C2-N1	2.13	1.41	1.38
47	S2	1842	4AC	C4-N4	-2.13	1.36	1.39
47	S2	814	5MU	C2-N1	2.12	1.41	1.38
1	L5	2050	OMG	C4-N9	-2.12	1.32	1.38
1	L5	3867	A2M	C8-N7	2.10	1.35	1.31
1	L5	4872	2MG	C5-N7	-2.10	1.35	1.39
1	L5	1524	A2M	C8-N7	2.09	1.35	1.31
47	S2	116	OMU	C2-N3	-2.08	1.34	1.38
47	S2	1850	MA6	C5-N7	-2.07	1.35	1.39
47	S2	1850	MA6	C4-N9	-2.07	1.33	1.37
47	S2	1243	PSU	C2'-C1'	-2.07	1.51	1.53
1	L5	1866	UR3	C5-C4	-2.07	1.38	1.43
47	S2	668	A2M	C4-N9	-2.06	1.33	1.37
1	L5	4450	PSU	C4-C5	-2.04	1.38	1.44
1	L5	1534	A2M	C8-N9	-2.03	1.33	1.37
47	S2	1031	A2M	C4-N9	-2.03	1.33	1.37
1	L5	4220	6MZ	C8-N7	2.01	1.35	1.31
47	S2	1830	UR3	C5-C4	-2.00	1.38	1.43
1	L5	4523	A2M	C4-N9	-2.00	1.33	1.37

All (601) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1517	2MG	C2-N3-C4	8.50	122.58	112.04
1	L5	4872	2MG	C2-N3-C4	7.91	121.85	112.04
1	L5	729	2MG	C2-N3-C4	7.62	121.48	112.04
1	L5	978	2MG	C2-N3-C4	7.22	120.99	112.04
1	L5	1517	2MG	C5-C4-N3	-7.04	117.03	128.46
47	S2	1806	M7A	N3-C4-N9	6.77	135.42	126.87
47	S2	166	A2M	C5-C4-N3	-6.55	118.20	126.75
1	L5	1677	PSU	N1-C2-N3	6.46	122.45	115.13
47	S2	1832	6MZ	C5-C4-N3	-6.44	118.34	126.75
47	S2	683	OMG	C5-C4-N3	-6.40	118.08	128.46
1	L5	3867	A2M	C5-C4-N3	-6.38	118.43	126.75
47	S2	1243	PSU	N1-C2-N3	6.38	122.36	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4196	OMG	C5-C4-N3	-6.36	118.15	128.46
47	S2	484	A2M	C5-C4-N3	-6.33	118.49	126.75
1	L5	1625	OMG	C5-C4-N3	-6.33	118.20	128.46
47	S2	159	A2M	C5-C4-N3	-6.32	118.50	126.75
1	L5	3785	A2M	C5-C4-N3	-6.31	118.51	126.75
1	L5	1534	A2M	C5-C4-N3	-6.30	118.52	126.75
1	L5	2363	A2M	C5-C4-N3	-6.30	118.53	126.75
1	L5	3899	OMG	C5-C4-N3	-6.28	118.27	128.46
1	L5	1524	A2M	C5-C4-N3	-6.27	118.57	126.75
1	L5	1582	PSU	N1-C2-N3	6.26	122.22	115.13
1	L5	3792	OMG	C5-C4-N3	-6.24	118.34	128.46
1	L5	4523	A2M	C5-C4-N3	-6.22	118.64	126.75
1	L5	4370	OMG	C5-C4-N3	-6.20	118.40	128.46
1	L5	2401	A2M	C5-C4-N3	-6.19	118.67	126.75
1	L5	729	2MG	C5-C4-N3	-6.18	118.44	128.46
47	S2	27	A2M	C5-C4-N3	-6.17	118.69	126.75
47	S2	1678	A2M	C5-C4-N3	-6.17	118.70	126.75
1	L5	3723	A2M	C5-C4-N3	-6.17	118.70	126.75
1	L5	2424	OMG	C5-C4-N3	-6.15	118.48	128.46
1	L5	4637	OMG	C5-C4-N3	-6.14	118.50	128.46
1	L5	4623	OMG	C5-C4-N3	-6.13	118.52	128.46
1	L5	398	A2M	C5-C4-N3	-6.13	118.76	126.75
47	S2	1806	M7A	N9-C8-N7	6.13	112.14	103.38
1	L5	4220	6MZ	C5-C4-N3	-6.12	118.77	126.75
1	L5	3762	B8H	N3-C2-N1	6.11	121.74	115.14
1	L5	1316	OMG	C5-C4-N3	-6.08	118.60	128.46
1	L5	2050	OMG	C5-C4-N3	-6.07	118.61	128.46
1	L5	1522	OMG	C5-C4-N3	-6.06	118.63	128.46
1	L5	1326	A2M	C5-C4-N3	-6.05	118.86	126.75
1	L5	4494	OMG	C5-C4-N3	-6.04	118.65	128.46
1	L5	2364	OMG	C5-C4-N3	-6.04	118.66	128.46
47	S2	644	OMG	C5-C4-N3	-6.02	118.69	128.46
47	S2	509	OMG	C5-C4-N3	-5.99	118.74	128.46
1	L5	4571	A2M	C5-C4-N3	-5.97	118.96	126.75
1	L5	4870	OMG	C5-C4-N3	-5.96	118.79	128.46
1	L5	3718	A2M	C5-C4-N3	-5.92	119.02	126.75
47	S2	668	A2M	C5-C4-N3	-5.92	119.02	126.75
1	L5	4531	PSU	N1-C2-N3	5.89	121.81	115.13
1	L5	4296	B8H	N3-C2-N1	5.88	121.50	115.14
1	L5	1883	OMG	C5-C4-N3	-5.88	118.92	128.46
1	L5	1871	A2M	C5-C4-N3	-5.88	119.08	126.75
47	S2	1031	A2M	C5-C4-N3	-5.82	119.16	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1851	MA6	C5-C4-N3	-5.80	119.18	126.75
1	L5	978	2MG	C5-C4-N3	-5.80	119.06	128.46
1	L5	373	OMG	C5-C4-N3	-5.78	119.08	128.46
1	L5	3825	A2M	C5-C4-N3	-5.76	119.23	126.75
1	L5	1860	B8H	N3-C2-N1	5.70	121.30	115.14
1	L5	4415	1MA	C5-C4-N3	-5.64	118.85	127.26
1	L5	4872	2MG	C5-C4-N3	-5.61	119.36	128.46
47	S2	1850	MA6	C5-C4-N3	-5.58	119.47	126.75
1	L5	2773	OMG	C5-C4-N3	-5.57	119.43	128.46
1	L5	1517	2MG	N9-C4-N3	5.50	136.98	125.94
1	L5	1322	1MA	C5-C4-N3	-5.48	119.08	127.26
1	L5	4597	UR3	C4-N3-C2	-5.45	119.43	124.56
1	L5	4083	5MU	C4-N3-C2	-5.43	120.32	127.35
1	L5	4296	B8H	C4-N3-C2	-5.32	120.46	127.35
1	L5	1316	OMG	C2-N3-C4	5.32	121.78	112.30
47	S2	814	5MU	N3-C2-N1	5.27	121.88	114.89
1	L5	3762	B8H	C4-N3-C2	-5.27	120.53	127.35
47	S2	683	OMG	C2-N3-C4	5.26	121.67	112.30
47	S2	166	A2M	N3-C4-N9	5.25	135.74	127.08
1	L5	4083	5MU	N3-C2-N1	5.20	121.79	114.89
47	S2	1830	UR3	C4-N3-C2	-5.13	119.74	124.56
1	L5	3899	OMG	C2-N3-C4	5.10	121.38	112.30
1	L5	3785	A2M	N3-C4-N9	5.09	135.47	127.08
1	L5	1322	1MA	C2-N3-C4	5.08	122.40	112.41
47	S2	814	5MU	C4-N3-C2	-5.07	120.78	127.35
1	L5	4196	OMG	C2-N3-C4	5.07	121.33	112.30
1	L5	1524	A2M	N3-C4-N9	5.06	135.41	127.08
1	L5	1860	B8H	C4-N3-C2	-5.05	120.81	127.35
1	L5	3792	OMG	C2-N3-C4	5.05	121.30	112.30
1	L5	4623	OMG	C2-N3-C4	5.05	121.30	112.30
47	S2	1832	6MZ	N3-C4-N9	5.01	135.34	127.08
47	S2	1248	B8N	C4-N3-C2	-4.98	119.17	125.46
1	L5	3867	A2M	N3-C4-N9	4.97	135.27	127.08
1	L5	373	OMG	C2-N3-C4	4.95	121.13	112.30
1	L5	4637	OMG	C2-N3-C4	4.94	121.11	112.30
1	L5	2363	A2M	N3-C4-N9	4.94	135.22	127.08
1	L5	4370	OMG	C2-N3-C4	4.93	121.09	112.30
1	L5	1866	UR3	C4-N3-C2	-4.92	119.93	124.56
47	S2	159	A2M	N3-C4-N9	4.92	135.19	127.08
1	L5	4523	A2M	N3-C4-N9	4.91	135.18	127.08
1	L5	4494	OMG	C2-N3-C4	4.91	121.05	112.30
1	L5	1625	OMG	N9-C4-N3	4.91	135.79	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2050	OMG	C2-N3-C4	4.90	121.03	112.30
47	S2	484	A2M	N3-C4-N9	4.90	135.15	127.08
1	L5	1522	OMG	C2-N3-C4	4.89	121.02	112.30
1	L5	4636	PSU	C4-N3-C2	-4.88	119.31	126.34
1	L5	4530	UR3	C4-N3-C2	-4.88	119.97	124.56
1	L5	2401	A2M	N3-C4-N9	4.86	135.09	127.08
47	S2	1678	A2M	N3-C4-N9	4.86	135.09	127.08
1	L5	1625	OMG	C2-N3-C4	4.86	120.95	112.30
1	L5	1883	OMG	C2-N3-C4	4.84	120.93	112.30
47	S2	683	OMG	N9-C4-N3	4.84	135.65	125.94
47	S2	1850	MA6	C2-N1-C6	4.83	123.16	111.75
1	L5	2424	OMG	C2-N3-C4	4.83	120.90	112.30
1	L5	4370	OMG	N9-C4-N3	4.82	135.61	125.94
1	L5	4220	6MZ	N3-C4-N9	4.79	134.98	127.08
1	L5	373	OMG	C2'-C1'-N9	-4.79	104.92	114.22
47	S2	644	OMG	C2-N3-C4	4.78	120.82	112.30
1	L5	4415	1MA	C2-N3-C4	4.78	121.80	112.41
1	L5	4870	OMG	C2-N3-C4	4.77	120.81	112.30
1	L5	4196	OMG	N9-C4-N3	4.77	135.52	125.94
1	L5	3723	A2M	N3-C4-N9	4.76	134.93	127.08
1	L5	2364	OMG	C2-N3-C4	4.76	120.78	112.30
1	L5	4442	PSU	C4-N3-C2	-4.76	119.48	126.34
1	L5	4447	5MC	C5-C6-N1	-4.72	118.48	123.34
47	S2	612	PSU	N1-C2-N3	4.72	120.48	115.13
1	L5	1534	A2M	N3-C4-N9	4.71	134.85	127.08
1	L5	4500	PSU	C4-N3-C2	-4.71	119.55	126.34
1	L5	4628	PSU	N1-C2-N3	4.70	120.46	115.13
1	L5	4571	A2M	N3-C4-N9	4.70	134.83	127.08
47	S2	612	PSU	C4-N3-C2	-4.70	119.57	126.34
47	S2	668	A2M	N3-C4-N9	4.70	134.82	127.08
1	L5	4083	5MU	C5-C4-N3	4.69	119.32	115.31
1	L5	4450	PSU	C4-N3-C2	-4.67	119.61	126.34
1	L5	3792	OMG	N9-C4-N3	4.66	135.30	125.94
47	S2	27	A2M	N3-C4-N9	4.66	134.76	127.08
1	L5	2773	OMG	C2-N3-C4	4.65	120.58	112.30
1	L5	4500	PSU	N1-C2-N3	4.64	120.39	115.13
1	L5	398	A2M	N3-C4-N9	4.63	134.72	127.08
47	S2	509	OMG	C2-N3-C4	4.63	120.55	112.30
47	S2	121	OMU	N3-C2-N1	4.63	121.04	114.89
1	L5	4620	OMU	N3-C2-N1	4.63	121.03	114.89
1	L5	4442	PSU	N1-C2-N3	4.62	120.37	115.13
47	S2	1850	MA6	C4-C5-N7	-4.62	104.99	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1851	MA6	C2-N1-C6	4.61	122.63	111.75
1	L5	4636	PSU	N1-C2-N3	4.59	120.33	115.13
47	S2	1830	UR3	C1'-N1-C2	4.58	124.73	116.99
1	L5	2050	OMG	N9-C4-N3	4.57	135.12	125.94
47	S2	822	PSU	N1-C2-N3	4.55	120.29	115.13
1	L5	1582	PSU	C4-N3-C2	-4.55	119.79	126.34
1	L5	1326	A2M	N3-C4-N9	4.54	134.57	127.08
1	L5	4628	PSU	C4-N3-C2	-4.54	119.80	126.34
1	L5	1683	PSU	N1-C2-N3	4.54	120.27	115.13
47	S2	823	PSU	C4-N3-C2	-4.52	119.83	126.34
1	L5	729	2MG	N9-C4-N3	4.52	135.01	125.94
1	L5	2424	OMG	N9-C4-N3	4.51	135.00	125.94
1	L5	3899	OMG	N9-C4-N3	4.51	135.00	125.94
1	L5	4870	OMG	N9-C4-N3	4.51	135.00	125.94
1	L5	4293	PSU	C4-N3-C2	-4.51	119.84	126.34
1	L5	4620	OMU	C4-N3-C2	-4.50	120.65	126.58
47	S2	119	PSU	C4-N3-C2	-4.50	119.86	126.34
1	L5	1871	A2M	N3-C4-N9	4.49	134.48	127.08
1	L5	2364	OMG	N9-C4-N3	4.48	134.94	125.94
1	L5	2508	PSU	N1-C2-N3	4.47	120.20	115.13
1	L5	4450	PSU	N1-C2-N3	4.47	120.19	115.13
1	L5	1883	OMG	N9-C4-N3	4.46	134.89	125.94
1	L5	3718	A2M	N3-C4-N9	4.45	134.42	127.08
1	L5	2508	PSU	C4-N3-C2	-4.45	119.92	126.34
1	L5	4637	OMG	N9-C4-N3	4.44	134.85	125.94
47	S2	119	PSU	N1-C2-N3	4.43	120.15	115.13
1	L5	4872	2MG	C6-C5-N7	4.42	138.46	130.25
1	L5	4623	OMG	N9-C4-N3	4.42	134.81	125.94
47	S2	1031	A2M	N3-C4-N9	4.41	134.35	127.08
47	S2	644	OMG	N9-C4-N3	4.41	134.79	125.94
47	S2	823	PSU	N1-C2-N3	4.40	120.12	115.13
47	S2	822	PSU	C4-N3-C2	-4.40	120.00	126.34
1	L5	4494	OMG	N9-C4-N3	4.39	134.76	125.94
47	S2	1851	MA6	C4-C5-N7	-4.39	105.28	110.62
1	L5	3825	A2M	N3-C4-N9	4.38	134.30	127.08
3	L8	14	OMU	C4-N3-C2	-4.37	120.81	126.58
1	L5	1683	PSU	C4-N3-C2	-4.37	120.05	126.34
1	L5	3764	PSU	N1-C2-N3	4.36	120.07	115.13
1	L5	4293	PSU	N1-C2-N3	4.34	120.04	115.13
47	S2	509	OMG	N9-C4-N3	4.33	134.64	125.94
1	L5	3729	PSU	N1-C2-N3	4.32	120.03	115.13
1	L5	1522	OMG	N9-C4-N3	4.31	134.60	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	121	OMU	C4-N3-C2	-4.29	120.92	126.58
47	S2	1243	PSU	C4-N3-C2	-4.28	120.18	126.34
1	L5	4403	PSU	N1-C2-N3	4.26	119.96	115.13
1	L5	3715	PSU	C4-N3-C2	-4.26	120.21	126.34
1	L5	1883	OMG	C2'-C1'-N9	-4.24	105.99	114.22
1	L5	3729	PSU	C4-N3-C2	-4.24	120.23	126.34
47	S2	1243	PSU	O2-C2-N1	-4.22	118.14	122.79
1	L5	3764	PSU	C4-N3-C2	-4.22	120.26	126.34
1	L5	3715	PSU	N1-C2-N3	4.21	119.91	115.13
1	L5	978	2MG	N9-C4-N3	4.18	134.34	125.94
3	L8	14	OMU	N3-C2-N1	4.16	120.41	114.89
1	L5	373	OMG	N9-C4-N3	4.15	134.27	125.94
47	S2	27	A2M	C2'-C1'-N9	-4.15	106.55	113.53
1	L5	4306	OMU	N3-C2-N1	4.10	120.33	114.89
1	L5	1316	OMG	N9-C4-N3	4.08	134.14	125.94
47	S2	1081	PSU	N1-C2-N3	4.08	119.75	115.13
47	S2	166	A2M	C2-N3-C4	4.07	121.37	111.75
1	L5	1677	PSU	C4-N3-C2	-4.07	120.48	126.34
1	L5	2773	OMG	N9-C4-N3	4.07	134.10	125.94
47	S2	814	5MU	C5-C4-N3	4.05	118.77	115.31
1	L5	4083	5MU	O4-C4-C5	-4.05	120.21	124.90
1	L5	1316	OMG	C6-C5-N7	4.04	137.76	130.25
1	L5	4523	A2M	C2-N3-C4	4.03	121.26	111.75
1	L5	1534	A2M	C2-N3-C4	4.00	121.21	111.75
1	L5	1677	PSU	O2-C2-N1	-3.99	118.39	122.79
1	L5	4531	PSU	O2-C2-N1	-3.99	118.39	122.79
1	L5	4403	PSU	C4-N3-C2	-3.99	120.60	126.34
47	S2	1081	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L5	2401	A2M	C2-N3-C4	3.97	121.12	111.75
1	L5	4531	PSU	C4-N3-C2	-3.97	120.62	126.34
47	S2	1851	MA6	N3-C4-N9	3.95	133.60	127.08
1	L5	4083	5MU	C5-C6-N1	-3.95	119.27	123.34
1	L5	1326	A2M	C2-N3-C4	3.95	121.09	111.75
47	S2	1678	A2M	C2-N3-C4	3.95	121.08	111.75
47	S2	1832	6MZ	C2-N3-C4	3.94	121.06	111.75
1	L5	3785	A2M	C2-N3-C4	3.94	121.05	111.75
47	S2	27	A2M	C2-N3-C4	3.93	121.03	111.75
1	L5	398	A2M	C2-N3-C4	3.92	121.00	111.75
1	L5	1871	A2M	C2'-C1'-N9	-3.91	106.95	113.53
1	L5	3825	A2M	C2-N3-C4	3.90	120.97	111.75
1	L5	3867	A2M	C2-N3-C4	3.89	120.93	111.75
1	L5	4306	OMU	C4-N3-C2	-3.88	121.46	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1851	MA6	C2-N3-C4	3.88	120.92	111.75
47	S2	1850	MA6	C2-N3-C4	3.88	120.91	111.75
1	L5	2363	A2M	C2-N3-C4	3.87	120.90	111.75
47	S2	484	A2M	C2-N3-C4	3.86	120.86	111.75
1	L5	4571	A2M	C2-N3-C4	3.85	120.85	111.75
47	S2	668	A2M	C2-N3-C4	3.83	120.81	111.75
1	L5	4220	6MZ	C2-N3-C4	3.83	120.80	111.75
1	L5	1524	A2M	C2-N3-C4	3.83	120.80	111.75
47	S2	116	OMU	N3-C2-N1	3.83	119.97	114.89
1	L5	3785	A2M	O4'-C1'-N9	3.82	115.58	108.06
1	L5	1871	A2M	C2-N3-C4	3.82	120.76	111.75
1	L5	4220	6MZ	C9-N6-C6	-3.80	119.59	122.87
47	S2	1850	MA6	N3-C4-N9	3.80	133.34	127.08
1	L5	3723	A2M	C2-N3-C4	3.80	120.72	111.75
47	S2	1031	A2M	C2-N3-C4	3.77	120.67	111.75
47	S2	159	A2M	C2-N3-C4	3.75	120.61	111.75
47	S2	1031	A2M	C2'-C1'-N9	-3.71	107.29	113.53
1	L5	3718	A2M	C2-N3-C4	3.69	120.47	111.75
3	L8	14	OMU	C5-C4-N3	3.69	120.36	114.84
47	S2	116	OMU	C4-N3-C2	-3.68	121.72	126.58
47	S2	1806	M7A	C2-N3-C4	3.67	120.42	111.75
1	L5	373	OMG	C6-C5-N7	3.65	137.03	130.25
1	L5	2050	OMG	C2'-C1'-N9	-3.64	107.16	114.22
47	S2	814	5MU	O4-C4-C5	-3.58	120.75	124.90
47	S2	1850	MA6	C5-N7-C8	3.58	108.60	103.51
1	L5	4530	UR3	C1'-N1-C2	3.54	122.97	116.99
1	L5	4620	OMU	C5-C4-N3	3.54	120.14	114.84
1	L5	1322	1MA	N9-C4-N3	3.52	135.15	126.94
1	L5	3785	A2M	C2'-C1'-N9	-3.52	107.60	113.53
47	S2	1850	MA6	N1-C2-N3	-3.51	123.11	128.60
1	L5	4306	OMU	C5-C4-N3	3.50	120.08	114.84
1	L5	1522	OMG	C6-C5-N7	3.49	136.74	130.25
1	L5	2773	OMG	C6-C5-N7	3.49	136.74	130.25
1	L5	4415	1MA	N9-C4-N3	3.47	135.03	126.94
1	L5	4872	2MG	C4-C5-N7	-3.46	105.24	110.72
1	L5	1326	A2M	C4-C5-N7	-3.45	106.41	110.62
1	L5	3825	A2M	N3-C2-N1	-3.44	123.23	128.60
47	S2	121	OMU	C5-C4-N3	3.41	119.95	114.84
47	S2	1851	MA6	C5-N7-C8	3.41	108.35	103.51
47	S2	116	OMU	C5-C4-N3	3.41	119.94	114.84
47	S2	1806	M7A	C5-C4-N3	-3.40	118.65	126.62
47	S2	1842	4AC	O7-C7-N4	3.40	127.32	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3825	A2M	C2'-C1'-N9	-3.39	107.81	113.53
47	S2	1031	A2M	N3-C2-N1	-3.39	123.29	128.60
1	L5	4530	UR3	C6-N1-C2	-3.38	118.76	121.79
1	L5	1534	A2M	C4-C5-N7	-3.38	106.50	110.62
1	L5	4523	A2M	N3-C2-N1	-3.38	123.31	128.60
1	L5	398	A2M	N3-C2-N1	-3.37	123.32	128.60
1	L5	4637	OMG	C6-C5-N7	3.37	136.52	130.25
1	L5	4335	5MC	C5-C6-N1	-3.36	119.88	123.34
47	S2	1851	MA6	N1-C2-N3	-3.36	123.35	128.60
1	L5	978	2MG	C6-C5-N7	3.36	136.49	130.25
47	S2	1678	A2M	N3-C2-N1	-3.35	123.36	128.60
47	S2	27	A2M	C4-C5-N7	-3.35	106.53	110.62
47	S2	1031	A2M	C4-C5-N7	-3.35	106.54	110.62
1	L5	3762	B8H	O2-C2-N1	-3.34	119.11	122.87
1	L5	1883	OMG	C6-C5-N7	3.34	136.46	130.25
1	L5	3723	A2M	C4-C5-N7	-3.33	106.57	110.62
1	L5	398	A2M	C4-C5-N7	-3.32	106.57	110.62
1	L5	1326	A2M	N3-C2-N1	-3.32	123.41	128.60
47	S2	27	A2M	N3-C2-N1	-3.30	123.44	128.60
47	S2	509	OMG	C6-C5-N7	3.29	136.37	130.25
1	L5	1534	A2M	N3-C2-N1	-3.29	123.45	128.60
47	S2	1832	6MZ	C4-C5-N7	-3.29	106.61	110.62
1	L5	4571	A2M	N3-C2-N1	-3.29	123.46	128.60
47	S2	159	A2M	C4-C5-N7	-3.28	106.62	110.62
1	L5	729	2MG	C6-C5-N7	3.28	136.36	130.25
47	S2	1678	A2M	C4-C5-N7	-3.28	106.62	110.62
47	S2	166	A2M	N3-C2-N1	-3.28	123.47	128.60
47	S2	116	OMU	O4-C4-C5	-3.28	119.39	125.16
1	L5	1582	PSU	O2-C2-N1	-3.27	119.19	122.79
1	L5	4623	OMG	C6-C5-N7	3.27	136.33	130.25
1	L5	2050	OMG	C6-C5-N7	3.26	136.31	130.25
1	L5	2401	A2M	C4-C5-N7	-3.25	106.66	110.62
1	L5	1871	A2M	N3-C2-N1	-3.25	123.52	128.60
1	L5	3899	OMG	C6-C5-N7	3.25	136.30	130.25
1	L5	2364	OMG	C6-C5-N7	3.25	136.29	130.25
1	L5	2401	A2M	N3-C2-N1	-3.25	123.53	128.60
1	L5	4083	5MU	C2'-C1'-N1	-3.24	104.04	113.22
1	L5	1871	A2M	C4-C5-N7	-3.23	106.68	110.62
1	L5	4447	5MC	O2-C2-N3	-3.23	117.08	122.33
1	L5	3718	A2M	C2'-C1'-N9	-3.23	108.10	113.53
1	L5	4296	B8H	O2-C2-N1	-3.22	119.24	122.87
47	S2	484	A2M	C4-C5-N7	-3.21	106.71	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1374	5MC	C5-C6-N1	-3.20	120.05	123.34
1	L5	4220	6MZ	C6-C5-N7	3.20	135.85	132.39
1	L5	3718	A2M	C4-C5-N7	-3.20	106.72	110.62
47	S2	668	A2M	N3-C2-N1	-3.20	123.60	128.60
47	S2	1832	6MZ	C6-C5-N7	3.20	135.85	132.39
47	S2	166	A2M	C2'-C1'-N9	-3.19	108.16	113.53
47	S2	814	5MU	C5-C6-N1	-3.19	120.06	123.34
1	L5	2363	A2M	N3-C2-N1	-3.18	123.62	128.60
1	L5	4494	OMG	C6-C5-N7	3.18	136.16	130.25
47	S2	509	OMG	C2'-C1'-N9	-3.18	108.06	114.22
1	L5	4872	2MG	N9-C4-N3	3.17	132.31	125.94
1	L5	1866	UR3	C6-N1-C2	-3.17	118.95	121.79
1	L5	3792	OMG	C6-C5-N7	3.15	136.11	130.25
47	S2	644	OMG	C6-C5-N7	3.15	136.10	130.25
1	L5	3723	A2M	C2'-C1'-N9	-3.14	108.24	113.53
1	L5	3867	A2M	C4-C5-N7	-3.14	106.80	110.62
3	L8	14	OMU	O4-C4-C5	-3.13	119.66	125.16
1	L5	3825	A2M	C4-C5-N7	-3.11	106.83	110.62
1	L5	4220	6MZ	N1-C2-N3	-3.11	123.74	128.60
1	L5	1524	A2M	C4-C5-N7	-3.11	106.83	110.62
47	S2	668	A2M	C4-C5-N7	-3.08	106.86	110.62
1	L5	4571	A2M	C4-C5-N7	-3.08	106.86	110.62
47	S2	166	A2M	C4-C5-N7	-3.08	106.87	110.62
47	S2	1832	6MZ	N1-C2-N3	-3.07	123.80	128.60
1	L5	1677	PSU	C3'-C2'-C1'	3.07	105.22	101.64
47	S2	683	OMG	C6-C5-N7	3.07	135.95	130.25
1	L5	2422	OMC	O2-C2-N3	-3.07	117.34	122.33
1	L5	4220	6MZ	C4-C5-N7	-3.06	106.89	110.62
47	S2	484	A2M	N3-C2-N1	-3.05	123.84	128.60
47	S2	1850	MA6	C6-C5-N7	3.04	138.39	133.28
47	S2	121	OMU	O4-C4-C5	-3.04	119.81	125.16
1	L5	3785	A2M	N3-C2-N1	-3.04	123.85	128.60
1	L5	3723	A2M	N3-C2-N1	-3.03	123.86	128.60
1	L5	4500	PSU	O2-C2-N1	-3.03	119.46	122.79
1	L5	2363	A2M	C4-C5-N7	-3.03	106.93	110.62
1	L5	1524	A2M	N3-C2-N1	-3.02	123.87	128.60
1	L5	4196	OMG	C6-C5-N7	3.02	135.86	130.25
1	L5	4870	OMG	C6-C5-N7	3.01	135.85	130.25
1	L5	1316	OMG	C4-C5-N7	-3.01	105.95	110.72
1	L5	4306	OMU	O4-C4-C5	-3.01	119.87	125.16
1	L5	4370	OMG	C6-C5-N7	3.00	135.82	130.25
1	L5	3867	A2M	N3-C2-N1	-2.98	123.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1806	M7A	N3-C2-N1	-2.98	123.95	128.60
1	L5	1316	OMG	C2'-C1'-N9	-2.96	108.48	114.22
1	L5	3785	A2M	C4-C5-N7	-2.96	107.02	110.62
1	L5	1866	UR3	C1'-N1-C2	2.95	121.97	116.99
1	L5	4872	2MG	CM2-N2-C2	-2.94	117.37	123.86
47	S2	1830	UR3	C6-N1-C2	-2.93	119.16	121.79
1	L5	1326	A2M	C5-N7-C8	2.93	107.67	103.51
1	L5	3718	A2M	N3-C2-N1	-2.90	124.07	128.60
1	L5	3782	5MC	C5-C4-N3	-2.89	118.55	121.67
1	L5	4628	PSU	O2-C2-N1	-2.89	119.61	122.79
1	L5	2424	OMG	C6-C5-N7	2.89	135.62	130.25
1	L5	4083	5MU	O2-C2-N1	-2.88	118.96	122.79
1	L5	1860	B8H	O2-C2-N1	-2.88	119.63	122.87
1	L5	3782	5MC	C5-C6-N1	-2.88	120.38	123.34
47	S2	1842	4AC	C5-C4-N3	-2.86	117.98	122.59
1	L5	398	A2M	C5-N7-C8	2.84	107.54	103.51
1	L5	3869	OMC	O2-C2-N3	-2.83	117.72	122.33
1	L5	4523	A2M	C4-C5-N7	-2.83	107.17	110.62
47	S2	116	OMU	C1'-N1-C2	2.82	122.68	117.57
47	S2	668	A2M	C4-N9-C8	2.82	108.78	105.73
1	L5	1522	OMG	C4-C5-N7	-2.81	106.28	110.72
47	S2	159	A2M	C5-N7-C8	2.80	107.49	103.51
47	S2	1248	B8N	N3-C2-N1	2.80	120.71	116.76
47	S2	1678	A2M	C5-N7-C8	2.80	107.49	103.51
47	S2	1851	MA6	C6-C5-N7	2.80	137.97	133.28
47	S2	1678	A2M	C4-N9-C8	2.79	108.75	105.73
1	L5	3909	OMC	O2-C2-N3	-2.78	117.82	122.33
1	L5	3785	A2M	C4-N9-C8	2.77	108.73	105.73
47	S2	27	A2M	C5-N7-C8	2.77	107.45	103.51
47	S2	159	A2M	N3-C2-N1	-2.77	124.27	128.60
1	L5	1625	OMG	C6-C5-N7	2.76	135.38	130.25
1	L5	2401	A2M	C5-N7-C8	2.75	107.42	103.51
47	S2	612	PSU	O2-C2-N1	-2.74	119.78	122.79
1	L5	1517	2MG	C6-C5-N7	2.73	135.33	130.25
47	S2	822	PSU	O2-C2-N1	-2.73	119.79	122.79
1	L5	1326	A2M	C4-N9-C8	2.72	108.68	105.73
1	L5	2401	A2M	C4-N9-C8	2.72	108.67	105.73
47	S2	509	OMG	C4-C5-N7	-2.71	106.43	110.72
1	L5	4637	OMG	C4-C5-N7	-2.71	106.43	110.72
1	L5	4620	OMU	C2'-C1'-N1	-2.70	108.97	114.22
47	S2	1337	4AC	N4-C4-N3	2.70	118.38	113.85
47	S2	1031	A2M	C5-N7-C8	2.70	107.34	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4597	UR3	C6-N1-C2	-2.70	119.37	121.79
47	S2	1832	6MZ	C5-N7-C8	2.70	107.34	103.51
1	L5	373	OMG	C4-C5-N7	-2.69	106.46	110.72
1	L5	3723	A2M	C5-N7-C8	2.69	107.34	103.51
1	L5	3899	OMG	C4-C5-N7	-2.69	106.46	110.72
1	L5	2364	OMG	C4-C5-N7	-2.69	106.47	110.72
47	S2	1842	4AC	C6-C5-C4	2.68	120.24	116.96
1	L5	2773	OMG	C4-C5-N7	-2.67	106.49	110.72
1	L5	4450	PSU	O2-C2-N1	-2.67	119.85	122.79
47	S2	166	A2M	C5-N7-C8	2.67	107.30	103.51
47	S2	121	OMU	O2-C2-N1	-2.66	119.25	122.79
1	L5	3867	A2M	C5-N7-C8	2.66	107.28	103.51
1	L5	3764	PSU	O2-C2-N1	-2.65	119.87	122.79
1	L5	3785	A2M	C5-N7-C8	2.64	107.26	103.51
1	L5	4447	5MC	O4'-C1'-N1	2.64	114.39	108.36
1	L5	978	2MG	C4-C5-N7	-2.63	106.55	110.72
1	L5	3729	PSU	O2-C2-N1	-2.63	119.90	122.79
1	L5	4636	PSU	O2-C2-N1	-2.63	119.90	122.79
1	L5	4571	A2M	C5-N7-C8	2.63	107.24	103.51
47	S2	484	A2M	C5-N7-C8	2.62	107.23	103.51
1	L5	1524	A2M	C4-N9-C8	2.62	108.56	105.73
47	S2	1850	MA6	C4-N9-C8	2.62	108.56	105.73
1	L5	3718	A2M	C5-N7-C8	2.61	107.22	103.51
1	L5	1524	A2M	C5-N7-C8	2.61	107.22	103.51
1	L5	1871	A2M	C5-N7-C8	2.60	107.21	103.51
47	S2	668	A2M	C5-N7-C8	2.60	107.21	103.51
1	L5	4571	A2M	C4-N9-C8	2.60	108.55	105.73
1	L5	729	2MG	C4-C5-N7	-2.60	106.61	110.72
1	L5	1322	1MA	N1-C2-N3	-2.60	122.91	126.00
1	L5	4623	OMG	C4-C5-N7	-2.60	106.61	110.72
47	S2	1678	A2M	C2'-C1'-N9	-2.59	109.17	113.53
1	L5	1683	PSU	C6-N1-C2	-2.59	120.03	122.68
47	S2	823	PSU	O2-C2-N1	-2.58	119.94	122.79
1	L5	4671	B8T	C6-C5-C4	2.58	120.12	116.96
1	L5	4620	OMU	O4-C4-C5	-2.58	120.63	125.16
1	L5	4447	5MC	C5-C4-N3	-2.57	118.90	121.67
1	L5	2508	PSU	O2-C2-N1	-2.56	119.97	122.79
1	L5	4628	PSU	C6-N1-C2	-2.56	120.07	122.68
47	S2	119	PSU	O2-C2-N1	-2.55	119.98	122.79
47	S2	683	OMG	C4-C5-N7	-2.55	106.68	110.72
47	S2	1219	JMH	C1'-N1-C2	2.55	121.30	116.99
1	L5	4620	OMU	O2-C2-N1	-2.55	119.39	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4494	OMG	C4-C5-N7	-2.55	106.68	110.72
1	L5	4450	PSU	C6-C5-C4	2.55	119.98	118.20
1	L5	1456	JMH	C6-N1-C2	-2.55	119.51	121.79
1	L5	4415	1MA	C4-C5-N7	-2.54	106.69	110.72
1	L5	1883	OMG	O6-C6-C5	-2.54	119.86	126.60
1	L5	4335	5MC	C5-C4-N3	-2.54	118.93	121.67
47	S2	1703	OMC	O2-C2-N3	-2.54	118.20	122.33
1	L5	1326	A2M	O2'-C2'-C1'	-2.54	104.13	109.08
1	L5	1866	UR3	O2-C2-N3	-2.54	117.76	121.34
1	L5	1683	PSU	O2-C2-N1	-2.53	120.00	122.79
1	L5	1326	A2M	C6-C5-N7	2.53	136.73	132.02
1	L5	3715	PSU	O2-C2-N1	-2.53	120.01	122.79
1	L5	4530	UR3	O2-C2-N3	-2.53	117.78	121.34
1	L5	3792	OMG	C4-C5-N7	-2.52	106.73	110.72
1	L5	1534	A2M	C5-N7-C8	2.52	107.08	103.51
1	L5	4196	OMG	C4-C5-N7	-2.51	106.74	110.72
47	S2	644	OMG	C4-C5-N7	-2.51	106.75	110.72
1	L5	4220	6MZ	C5-N7-C8	2.49	107.05	103.51
1	L5	1883	OMG	C4-C5-N7	-2.49	106.78	110.72
1	L5	4293	PSU	O2-C2-N1	-2.49	120.05	122.79
1	L5	3729	PSU	C6-N1-C2	-2.49	120.14	122.68
1	L5	4442	PSU	O2-C2-N1	-2.48	120.06	122.79
47	S2	1031	A2M	C4-N9-C8	2.48	108.41	105.73
1	L5	4872	2MG	C2-N1-C6	-2.47	121.64	124.48
47	S2	822	PSU	C6-N1-C2	-2.46	120.17	122.68
1	L5	4403	PSU	O2-C2-N1	-2.46	120.09	122.79
1	L5	1871	A2M	C4-N9-C8	2.45	108.38	105.73
1	L5	3723	A2M	C4-N9-C8	2.45	108.38	105.73
1	L5	3825	A2M	C5-N7-C8	2.45	106.99	103.51
1	L5	3825	A2M	C6-C5-N7	2.45	136.58	132.02
1	L5	3715	PSU	C6-N1-C2	-2.45	120.18	122.68
1	L5	3764	PSU	C6-N1-C2	-2.44	120.19	122.68
1	L5	4403	PSU	C6-N1-C2	-2.42	120.21	122.68
1	L5	1582	PSU	C5-C6-N1	-2.41	118.49	122.11
1	L5	1517	2MG	O6-C6-C5	-2.41	120.19	126.60
47	S2	116	OMU	C6-N1-C2	-2.41	117.90	120.99
1	L5	3825	A2M	C4-N9-C8	2.41	108.34	105.73
47	S2	166	A2M	C4-N9-C8	2.41	108.34	105.73
47	S2	1337	4AC	O2-C2-N3	-2.41	118.41	122.33
47	S2	1374	5MC	C5-C4-N3	-2.41	119.07	121.67
1	L5	4447	5MC	N1-C2-N3	2.41	123.19	118.81
1	L5	4523	A2M	C5-N7-C8	2.40	106.92	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	822	PSU	O4'-C1'-C2'	2.40	108.53	105.14
47	S2	159	A2M	C4-N9-C8	2.40	108.33	105.73
1	L5	4870	OMG	C4-C5-N7	-2.38	106.95	110.72
1	L5	2363	A2M	C5-N7-C8	2.38	106.89	103.51
47	S2	1850	MA6	N9-C8-N7	-2.38	110.66	113.91
47	S2	1031	A2M	C6-C5-N7	2.38	136.46	132.02
1	L5	2424	OMG	C4-C5-N7	-2.38	106.96	110.72
1	L5	4306	OMU	C1'-N1-C2	2.37	121.86	117.57
1	L5	2050	OMG	C4-C5-N7	-2.37	106.97	110.72
1	L5	1326	A2M	N9-C8-N7	-2.37	110.67	113.91
1	L5	1517	2MG	C2-N1-C6	-2.36	121.76	124.48
1	L5	4523	A2M	C4-N9-C8	2.36	108.28	105.73
1	L5	4370	OMG	C4-C5-N7	-2.35	107.00	110.72
1	L5	1871	A2M	C6-C5-N7	2.35	136.40	132.02
47	S2	1851	MA6	C4-N9-C8	2.35	108.28	105.73
1	L5	1524	A2M	C2'-C1'-N9	-2.34	109.58	113.53
1	L5	4536	OMC	O2-C2-N3	-2.34	118.53	122.33
1	L5	398	A2M	C4-N9-C8	2.34	108.26	105.73
1	L5	1625	OMG	C4-C5-N7	-2.33	107.04	110.72
1	L5	4306	OMU	C6-N1-C2	-2.32	118.02	120.99
47	S2	27	A2M	C4-N9-C8	2.32	108.24	105.73
1	L5	2050	OMG	O6-C6-C5	-2.32	120.44	126.60
47	S2	1248	B8N	C31-N3-C4	2.31	120.72	117.31
47	S2	612	PSU	C6-N1-C2	-2.31	120.32	122.68
1	L5	1517	2MG	C4-C5-N7	-2.31	107.06	110.72
47	S2	823	PSU	C6-N1-C2	-2.29	120.34	122.68
1	L5	398	A2M	C2'-C1'-N9	-2.28	109.68	113.53
1	L5	4500	PSU	C6-N1-C2	-2.28	120.35	122.68
1	L5	2861	OMC	O2-C2-N3	-2.28	118.62	122.33
1	L5	2508	PSU	C6-N1-C2	-2.28	120.36	122.68
1	L5	1534	A2M	C6-C5-N7	2.27	136.25	132.02
1	L5	2401	A2M	C6-C5-N7	2.27	136.25	132.02
1	L5	1625	OMG	O6-C6-C5	-2.27	120.59	126.60
1	L5	3867	A2M	C4-N9-C8	2.26	108.18	105.73
1	L5	398	A2M	C6-C5-N7	2.26	136.23	132.02
1	L5	4483	B8T	C6-C5-C4	2.26	119.72	116.96
47	S2	484	A2M	C4-N9-C8	2.26	108.17	105.73
1	L5	4636	PSU	C6-C5-C4	2.26	119.78	118.20
1	L5	1316	OMG	C5-C6-N1	2.25	118.92	113.19
47	S2	119	PSU	C6-N1-C2	-2.25	120.38	122.68
47	S2	1374	5MC	O2-C2-N3	-2.25	118.68	122.33
1	L5	4220	6MZ	C4-N9-C8	2.25	108.16	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1678	A2M	C6-C5-N7	2.24	136.19	132.02
1	L5	2804	OMC	O2-C2-N3	-2.24	118.69	122.33
47	S2	1081	PSU	O4-C4-N3	-2.24	115.83	120.12
47	S2	1851	MA6	N9-C8-N7	-2.23	110.87	113.91
1	L5	4370	OMG	O6-C6-C5	-2.22	120.71	126.60
1	L5	4523	A2M	C2'-C1'-N9	-2.22	109.79	113.53
47	S2	27	A2M	C6-C5-N7	2.22	136.15	132.02
1	L5	4636	PSU	O4'-C1'-C2'	2.21	108.26	105.14
47	S2	1830	UR3	O2-C2-N3	-2.21	118.23	121.34
47	S2	668	A2M	C6-C5-N7	2.21	136.13	132.02
47	S2	1219	JMH	C6-N1-C2	-2.20	119.81	121.79
1	L5	4447	5MC	C3'-C2'-C1'	2.20	105.60	101.43
1	L5	1322	1MA	C4-C5-N7	-2.19	107.26	110.72
1	L5	4196	OMG	O6-C6-C5	-2.19	120.79	126.60
1	L5	3723	A2M	C6-C5-N7	2.19	136.10	132.02
47	S2	1678	A2M	N9-C8-N7	-2.19	110.92	113.91
1	L5	729	2MG	O6-C6-C5	-2.19	120.80	126.60
47	S2	517	OMC	O2-C2-N3	-2.19	118.78	122.33
1	L5	3718	A2M	C4-N9-C8	2.18	108.09	105.73
1	L5	4872	2MG	O6-C6-C5	-2.18	120.81	126.60
1	L5	373	OMG	O6-C6-C5	-2.18	120.82	126.60
1	L5	2424	OMG	O6-C6-C5	-2.18	120.83	126.60
1	L5	4293	PSU	C6-N1-C2	-2.17	120.46	122.68
47	S2	1248	B8N	O36-C34-O35	-2.17	119.16	124.09
47	S2	1830	UR3	C1'-N1-C6	-2.17	116.11	120.84
1	L5	4571	A2M	C6-C5-N7	2.17	136.06	132.02
1	L5	978	2MG	O6-C6-C5	-2.17	120.84	126.60
47	S2	1806	M7A	C2-N1-C6	2.17	122.49	118.77
1	L5	3785	A2M	N9-C8-N7	-2.16	110.96	113.91
1	L5	2050	OMG	C5-C6-N1	2.16	118.67	113.19
1	L5	1860	B8H	CN1-N1-C2	2.16	120.64	117.94
47	S2	121	OMU	C6-N1-C2	-2.15	118.24	120.99
1	L5	2364	OMG	O6-C6-C5	-2.15	120.91	126.60
1	L5	4442	PSU	C6-C5-C4	2.14	119.70	118.20
1	L5	4335	5MC	CM5-C5-C6	-2.14	119.99	122.85
1	L5	3718	A2M	C6-C5-N7	2.14	136.01	132.02
1	L5	1883	OMG	C5-C6-N1	2.14	118.62	113.19
47	S2	1337	4AC	C6-C5-C4	2.14	119.58	116.96
47	S2	668	A2M	N9-C8-N7	-2.14	110.99	113.91
47	S2	1832	6MZ	C4-N9-C8	2.14	108.04	105.73
47	S2	683	OMG	O6-C6-C5	-2.13	120.94	126.60
1	L5	4623	OMG	O6-C6-C5	-2.13	120.94	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	2363	A2M	C4-N9-C8	2.13	108.04	105.73
1	L5	1517	2MG	C5-C6-N1	2.13	118.60	113.19
1	L5	4450	PSU	C6-N1-C2	-2.13	120.51	122.68
1	L5	4870	OMG	O6-C6-C5	-2.12	120.96	126.60
1	L5	2401	A2M	N9-C8-N7	-2.12	111.01	113.91
1	L5	1326	A2M	C2'-C1'-N9	-2.12	109.95	113.53
1	L5	3887	OMC	O2-C2-N3	-2.12	118.88	122.33
1	L5	4671	B8T	O2-C2-N3	-2.12	118.88	122.33
47	S2	1842	4AC	O2-C2-N3	-2.12	118.88	122.33
47	S2	159	A2M	C2'-C1'-N9	-2.12	109.97	113.53
1	L5	3792	OMG	O6-C6-C5	-2.12	120.99	126.60
1	L5	3785	A2M	C6-C5-N7	2.11	135.96	132.02
1	L5	4415	1MA	C6-C5-N7	2.11	136.04	132.20
47	S2	814	5MU	C5M-C5-C4	2.11	121.08	118.77
1	L5	4335	5MC	O2-C2-N3	-2.10	118.91	122.33
47	S2	1031	A2M	C2-N1-C6	2.10	122.37	118.77
47	S2	1081	PSU	C6-N1-C2	-2.09	120.55	122.68
47	S2	1243	PSU	C5-C6-N1	-2.09	118.98	122.11
47	S2	612	PSU	O4'-C1'-C2'	2.09	108.08	105.14
1	L5	3867	A2M	C2'-C1'-N9	-2.07	110.05	113.53
1	L5	4442	PSU	O4'-C1'-C2'	2.07	108.06	105.14
1	L5	4872	2MG	C5-C6-N1	2.06	118.43	113.19
1	L5	4370	OMG	C5-C6-N1	2.06	118.43	113.19
1	L5	4637	OMG	O6-C6-C5	-2.06	121.14	126.60
1	L5	373	OMG	C5-C6-N1	2.06	118.41	113.19
1	L5	4531	PSU	C5-C6-N1	-2.06	119.03	122.11
1	L5	398	A2M	N9-C8-N7	-2.05	111.10	113.91
47	S2	814	5MU	O2-C2-N1	-2.05	120.06	122.79
47	S2	644	OMG	O6-C6-C5	-2.05	121.16	126.60
1	L5	2773	OMG	O6-C6-C5	-2.05	121.17	126.60
1	L5	4306	OMU	O2-C2-N3	-2.05	117.69	121.50
1	L5	4623	OMG	C5-C6-N1	2.03	118.36	113.19
1	L5	4442	PSU	C6-N1-C2	-2.03	120.61	122.68
1	L5	4571	A2M	N9-C8-N7	-2.03	111.14	113.91
1	L5	729	2MG	C5-C6-N1	2.03	118.35	113.19
47	S2	484	A2M	C6-C5-N7	2.02	135.79	132.02
1	L5	4637	OMG	C5-C6-N1	2.02	118.33	113.19
47	S2	1081	PSU	O2-C2-N1	-2.02	120.56	122.79
1	L5	729	2MG	C2-N1-C6	-2.02	122.16	124.48
1	L5	4872	2MG	C8-N7-C5	2.02	107.89	104.24
47	S2	1842	4AC	O7-C7-CM7	-2.02	118.31	122.06
1	L5	3867	A2M	C6-C5-N7	2.02	135.78	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1534	A2M	C4-N9-C8	2.00	107.90	105.73

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L5	729	2MG	N1-C2-N2-CM2
1	L5	729	2MG	N3-C2-N2-CM2
1	L5	1883	OMG	C1'-C2'-O2'-CM2
1	L5	2424	OMG	O4'-C4'-C5'-O5'
1	L5	2424	OMG	C3'-C4'-C5'-O5'
1	L5	3729	PSU	O4'-C4'-C5'-O5'
1	L5	3762	B8H	O4'-C4'-C5'-O5'
1	L5	4403	PSU	O4'-C1'-C5-C4
1	L5	4403	PSU	O4'-C1'-C5-C6
1	L5	4415	1MA	O4'-C4'-C5'-O5'
1	L5	4415	1MA	C3'-C4'-C5'-O5'
1	L5	4500	PSU	C3'-C4'-C5'-O5'
1	L5	4500	PSU	O4'-C4'-C5'-O5'
1	L5	4523	A2M	O4'-C4'-C5'-O5'
1	L5	4531	PSU	O4'-C4'-C5'-O5'
1	L5	4636	PSU	C2'-C1'-C5-C6
1	L5	4636	PSU	C3'-C4'-C5'-O5'
1	L5	4636	PSU	O4'-C4'-C5'-O5'
1	L5	4637	OMG	O4'-C4'-C5'-O5'
1	L5	4870	OMG	O4'-C4'-C5'-O5'
1	L5	4870	OMG	C3'-C4'-C5'-O5'
47	S2	116	OMU	C3'-C4'-C5'-O5'
47	S2	116	OMU	O4'-C4'-C5'-O5'
47	S2	668	A2M	C3'-C4'-C5'-O5'
47	S2	683	OMG	O4'-C4'-C5'-O5'
47	S2	683	OMG	C3'-C4'-C5'-O5'
47	S2	1243	PSU	C3'-C4'-C5'-O5'
47	S2	1243	PSU	O4'-C4'-C5'-O5'
47	S2	1248	B8N	O4'-C4'-C5'-O5'
47	S2	1337	4AC	O7-C7-N4-C4
47	S2	1337	4AC	CM7-C7-N4-C4
47	S2	1832	6MZ	N1-C6-N6-C9
47	S2	1851	MA6	O4'-C4'-C5'-O5'
1	L5	3701	OMC	C2'-C1'-N1-C6
1	L5	1582	PSU	C3'-C4'-C5'-O5'
1	L5	1582	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L5	3729	PSU	C3'-C4'-C5'-O5'
1	L5	3762	B8H	C3'-C4'-C5'-O5'
1	L5	3785	A2M	O4'-C4'-C5'-O5'
1	L5	3785	A2M	C3'-C4'-C5'-O5'
1	L5	3867	A2M	C3'-C4'-C5'-O5'
1	L5	4523	A2M	C3'-C4'-C5'-O5'
1	L5	4531	PSU	C3'-C4'-C5'-O5'
1	L5	4637	OMG	C3'-C4'-C5'-O5'
47	S2	509	OMG	C3'-C4'-C5'-O5'
47	S2	1248	B8N	C3'-C4'-C5'-O5'
47	S2	1851	MA6	C3'-C4'-C5'-O5'
47	S2	1830	UR3	O4'-C1'-N1-C2
1	L5	398	A2M	O4'-C4'-C5'-O5'
1	L5	1866	UR3	O4'-C4'-C5'-O5'
1	L5	3867	A2M	O4'-C4'-C5'-O5'
1	L5	4220	6MZ	O4'-C4'-C5'-O5'
1	L5	4220	6MZ	C3'-C4'-C5'-O5'
1	L5	4494	OMG	O4'-C4'-C5'-O5'
1	L5	4494	OMG	C3'-C4'-C5'-O5'
47	S2	668	A2M	O4'-C4'-C5'-O5'
1	L5	3701	OMC	C2'-C1'-N1-C2
47	S2	1703	OMC	O4'-C4'-C5'-O5'
6	LC	333	MLZ	CD-CE-NZ-CM
47	S2	1830	UR3	O4'-C1'-N1-C6
1	L5	398	A2M	C3'-C4'-C5'-O5'
1	L5	3899	OMG	C3'-C4'-C5'-O5'
1	L5	4530	UR3	C3'-C4'-C5'-O5'
1	L5	4293	PSU	O4'-C4'-C5'-O5'
1	L5	1866	UR3	C3'-C4'-C5'-O5'
1	L5	1883	OMG	C3'-C4'-C5'-O5'
47	S2	1851	MA6	C5-C6-N6-C10
47	S2	116	OMU	C3'-C2'-O2'-CM2
47	S2	509	OMG	O4'-C4'-C5'-O5'
47	S2	1832	6MZ	C5-C6-N6-C9
1	L5	4447	5MC	C2'-C1'-N1-C6
1	L5	3899	OMG	O4'-C4'-C5'-O5'
1	L5	4293	PSU	C3'-C4'-C5'-O5'
1	L5	4872	2MG	O4'-C4'-C5'-O5'
3	L8	14	OMU	C1'-C2'-O2'-CM2
47	S2	1248	B8N	C31-C32-C33-N34
1	L5	1534	A2M	C4'-C5'-O5'-P
47	S2	644	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	L5	4450	PSU	O4'-C4'-C5'-O5'
1	L5	4530	UR3	O4'-C4'-C5'-O5'
1	L5	3701	OMC	O4'-C1'-N1-C6
1	L5	4447	5MC	O4'-C1'-N1-C6
1	L5	3764	PSU	C4'-C5'-O5'-P
47	S2	1248	B8N	N3-C31-C32-C33
6	LC	333	MLZ	CG-CD-CE-NZ
1	L5	3701	OMC	O4'-C1'-N1-C2
1	L5	4447	5MC	O4'-C1'-N1-C2
1	L5	3887	OMC	C4'-C5'-O5'-P
1	L5	1326	A2M	C4'-C5'-O5'-P
1	L5	4500	PSU	C4'-C5'-O5'-P
1	L5	4870	OMG	C4'-C5'-O5'-P
47	S2	668	A2M	C2'-C1'-N9-C8
1	L5	4450	PSU	O4'-C1'-C5-C4
47	S2	1703	OMC	C3'-C4'-C5'-O5'
1	L5	1322	1MA	O4'-C4'-C5'-O5'
1	L5	1322	1MA	C2'-C1'-N9-C8
1	L5	1883	OMG	O4'-C4'-C5'-O5'
1	L5	4872	2MG	C3'-C4'-C5'-O5'
1	L5	3899	OMG	C1'-C2'-O2'-CM2
47	S2	1851	MA6	C5-C6-N6-C9
1	L5	1524	A2M	O4'-C1'-N9-C8
1	L5	1625	OMG	C4'-C5'-O5'-P
1	L5	729	2MG	O4'-C4'-C5'-O5'
1	L5	2364	OMG	O4'-C4'-C5'-O5'
1	L5	1677	PSU	O4'-C1'-C5-C6
1	L5	4636	PSU	O4'-C1'-C5-C6
1	L5	4447	5MC	C2'-C1'-N1-C2
1	L5	1322	1MA	C2'-C1'-N9-C4
1	L5	3867	A2M	C4'-C5'-O5'-P
47	S2	1851	MA6	C4'-C5'-O5'-P
1	L5	2422	OMC	O4'-C4'-C5'-O5'
1	L5	4450	PSU	C3'-C4'-C5'-O5'
1	L5	2401	A2M	C3'-C2'-O2'-CM'
1	L5	3899	OMG	C3'-C2'-O2'-CM2
1	L5	1322	1MA	C3'-C4'-C5'-O5'
1	L5	1534	A2M	O4'-C4'-C5'-O5'
47	S2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

23 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	1883	OMG	1	0
1	L5	1866	UR3	1	0
1	L5	4530	UR3	1	0
1	L5	4220	6MZ	1	0
1	L5	4870	OMG	1	0
47	S2	814	5MU	1	0
47	S2	517	OMC	1	0
1	L5	4620	OMU	1	0
41	Lm	98	MLZ	1	0
6	LC	333	MLZ	2	0
1	L5	1871	A2M	1	0
1	L5	4531	PSU	1	0
47	S2	1243	PSU	1	0
1	L5	2363	A2M	1	0
1	L5	4523	A2M	1	0
1	L5	4196	OMG	1	0
1	L5	1326	A2M	1	0
1	L5	2424	OMG	2	0
1	L5	4872	2MG	1	0
1	L5	1582	PSU	2	0
47	S2	509	OMG	2	0
1	L5	2050	OMG	2	0
1	L5	3715	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 448 ligands modelled in this entry, 446 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	HYG	S2	2039	-	35,39,39	0.97	1 (2%)	43,60,60	1.37	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	HMT	L5	5374	-	40,43,43	1.89	7 (17%)	41,66,66	1.49	6 (14%)

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
85	HYG	S2	2039	-	-	3/12/87/87	0/4/4/4
83	HMT	L5	5374	-	-	6/27/74/74	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	L5	5374	HMT	C5-C4	-7.13	1.40	1.51
83	L5	5374	HMT	C7-C6	-5.88	1.38	1.51
85	S2	2039	HYG	O28-C23	3.83	1.45	1.40
83	L5	5374	HMT	C3-C2	-3.80	1.40	1.50
83	L5	5374	HMT	C13-C14	-2.81	1.33	1.38
83	L5	5374	HMT	C16-C15	-2.71	1.33	1.38
83	L5	5374	HMT	C12-C9	-2.37	1.50	1.54
83	L5	5374	HMT	C14-C15	-2.16	1.33	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	2039	HYG	O22-C17-C12	-4.70	96.07	103.58
83	L5	5374	HMT	C25-C24-C20	-3.88	109.71	115.65
83	L5	5374	HMT	C7-C6-C16	-3.71	111.24	119.42
85	S2	2039	HYG	O18-C6-C1	3.55	116.73	107.28
83	L5	5374	HMT	C6-C5-C4	3.30	132.61	121.06
85	S2	2039	HYG	C13-O18-C6	3.17	125.80	117.96
85	S2	2039	HYG	O8-C1-C2	-2.90	104.49	109.81
83	L5	5374	HMT	C7-C6-C5	2.34	130.25	122.61
83	L5	5374	HMT	C3-O4-C19	-2.26	113.68	117.24
83	L5	5374	HMT	C10-N1-C9	-2.14	101.57	107.71
85	S2	2039	HYG	O29-C12-C17	-2.05	100.31	103.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

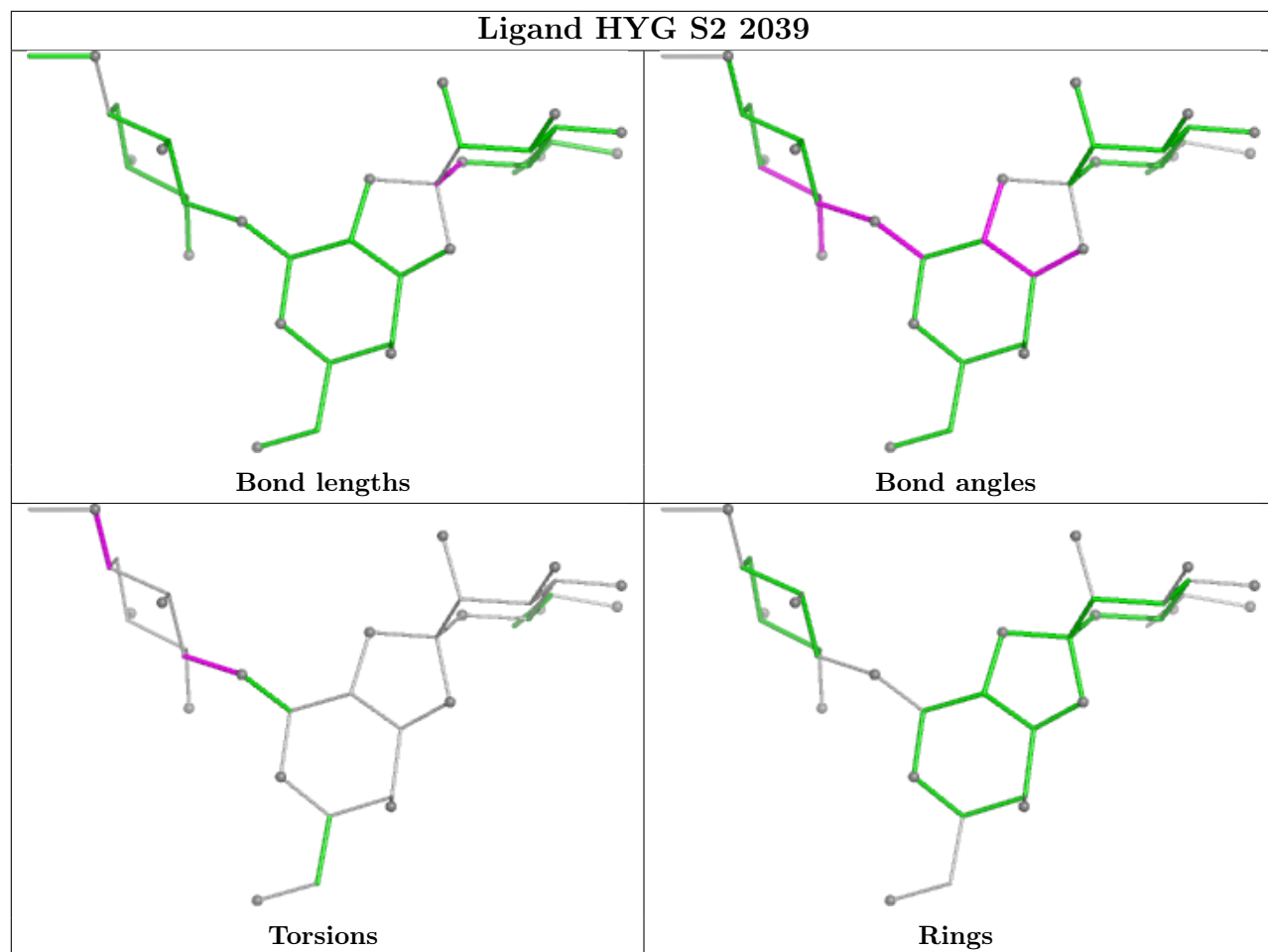
Mol	Chain	Res	Type	Atoms
83	L5	5374	HMT	C1-C2-O3-C18
83	L5	5374	HMT	C3-C2-O3-C18
83	L5	5374	HMT	C19-C20-C21-C22
83	L5	5374	HMT	O6-C20-C21-C22
85	S2	2039	HYG	C5-C4-N9-C10
85	S2	2039	HYG	C1-C6-O18-C13
83	L5	5374	HMT	C24-C20-C21-C22
85	S2	2039	HYG	C3-C4-N9-C10
83	L5	5374	HMT	O4-C19-C20-C24

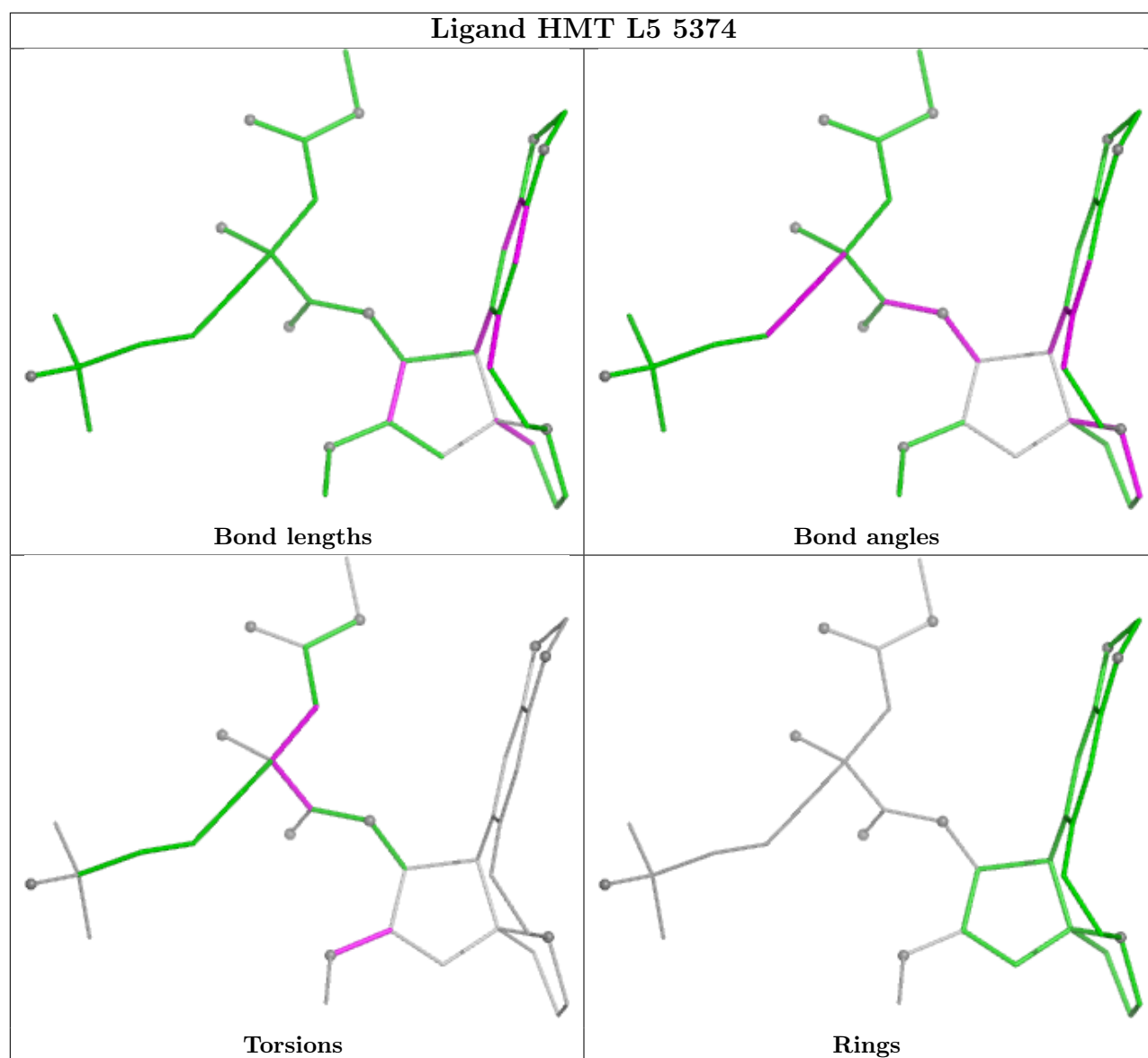
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5374	HMT	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L5	10
47	S2	4
30	Lb	1
8	LE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
54	SH	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:ALA	N	34.87
1	LE	76:ALA	C	88:VAL	N	26.61
1	S2	753:C	O3'	785:C	P	24.68
1	L5	2910:G	O3'	3584:C	P	22.67
1	S2	698:G	O3'	730:C	P	17.52
1	L5	519:C	O3'	642:G	P	17.50
1	L5	760:G	O3'	903:C	P	15.47
1	L5	4776:G	O3'	4858:C	P	15.05
1	S2	739:C	O3'	746:C	P	14.29
1	L5	2113:G	O3'	2249:C	P	13.33
1	L5	996:G	O3'	1047:C	P	12.79
1	L5	1222:A	O3'	1234:G	P	11.84
1	L5	1051:G	O3'	1064:G	P	11.72
1	SH	107:LYS	C	111:LYS	N	10.30
1	L5	1709:C	O3'	1714:C	P	8.37
1	L5	1100:U	O3'	1167:C	P	7.56
1	S2	225:G	O3'	287:U	P	7.18

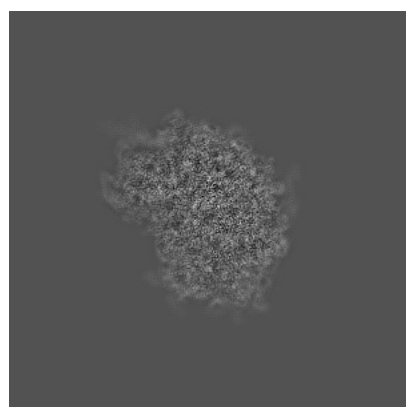
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3883. These allow visual inspection of the internal detail of the map and identification of artifacts.

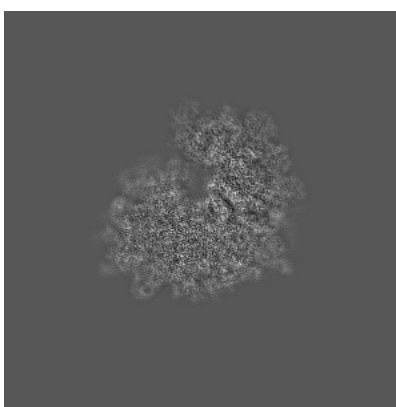
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

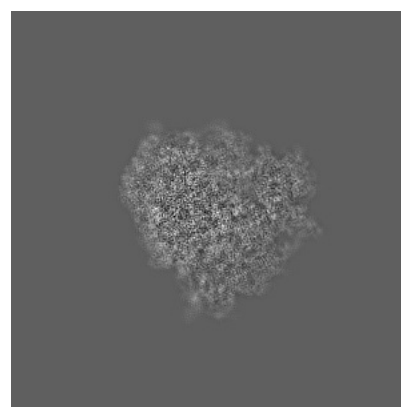
6.1.1 Primary map



X



Y

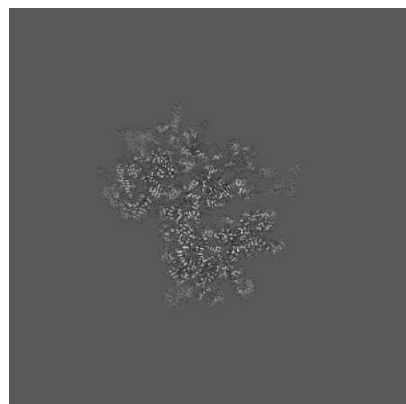


Z

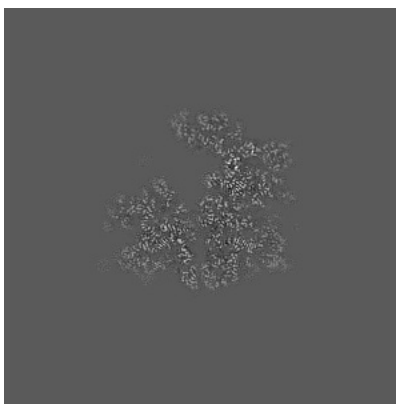
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

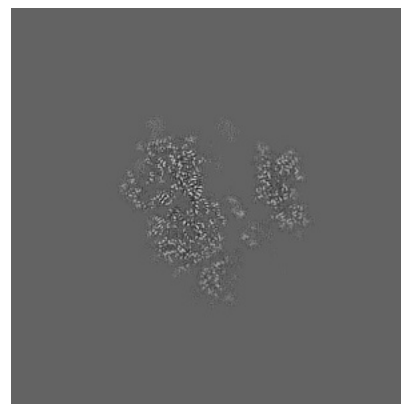
6.2.1 Primary map



X Index: 320



Y Index: 320

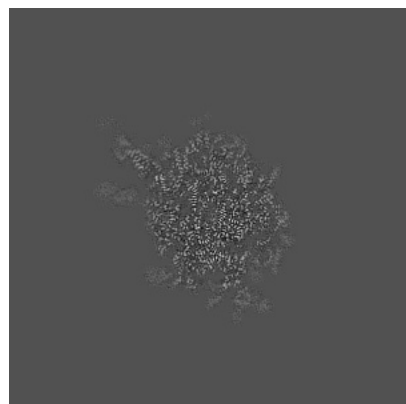


Z Index: 320

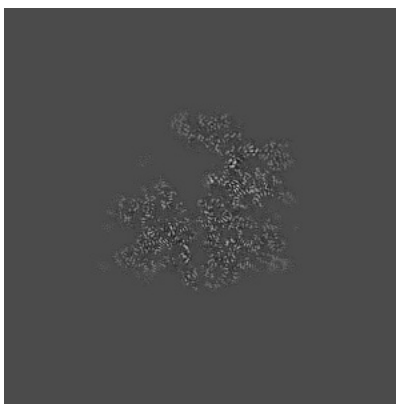
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

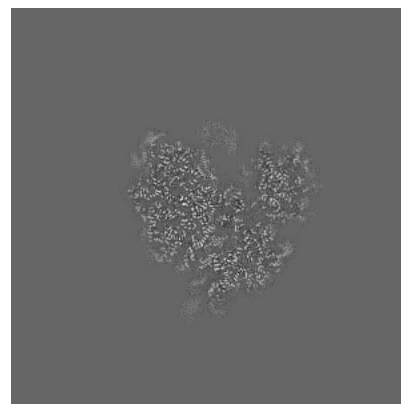
6.3.1 Primary map



X Index: 286



Y Index: 318

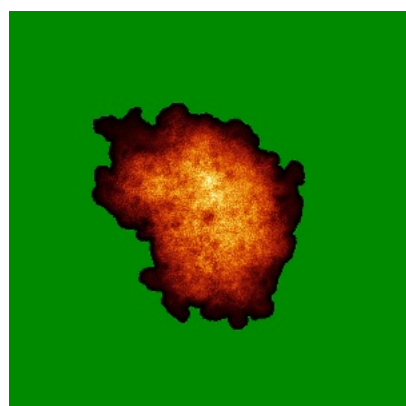


Z Index: 350

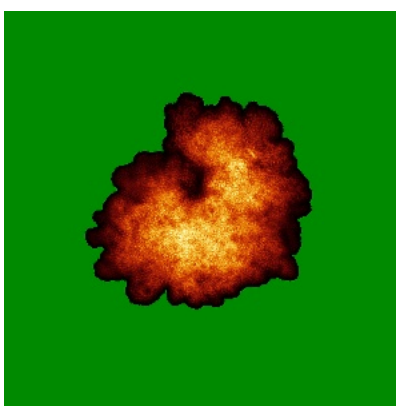
The images above show the largest variance slices of the map in three orthogonal directions.

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

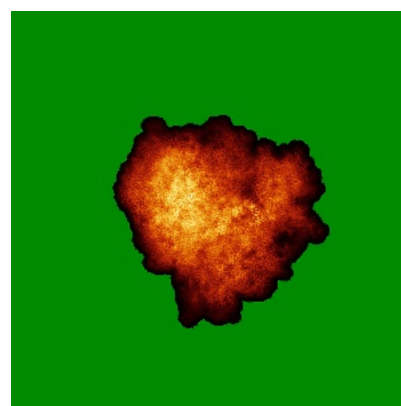
6.4.1 Primary map



X



Y

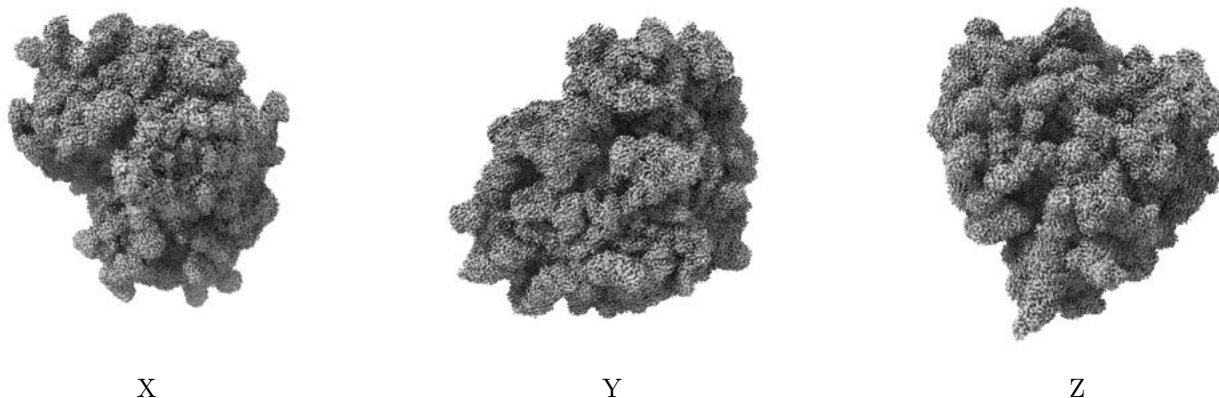


Z

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

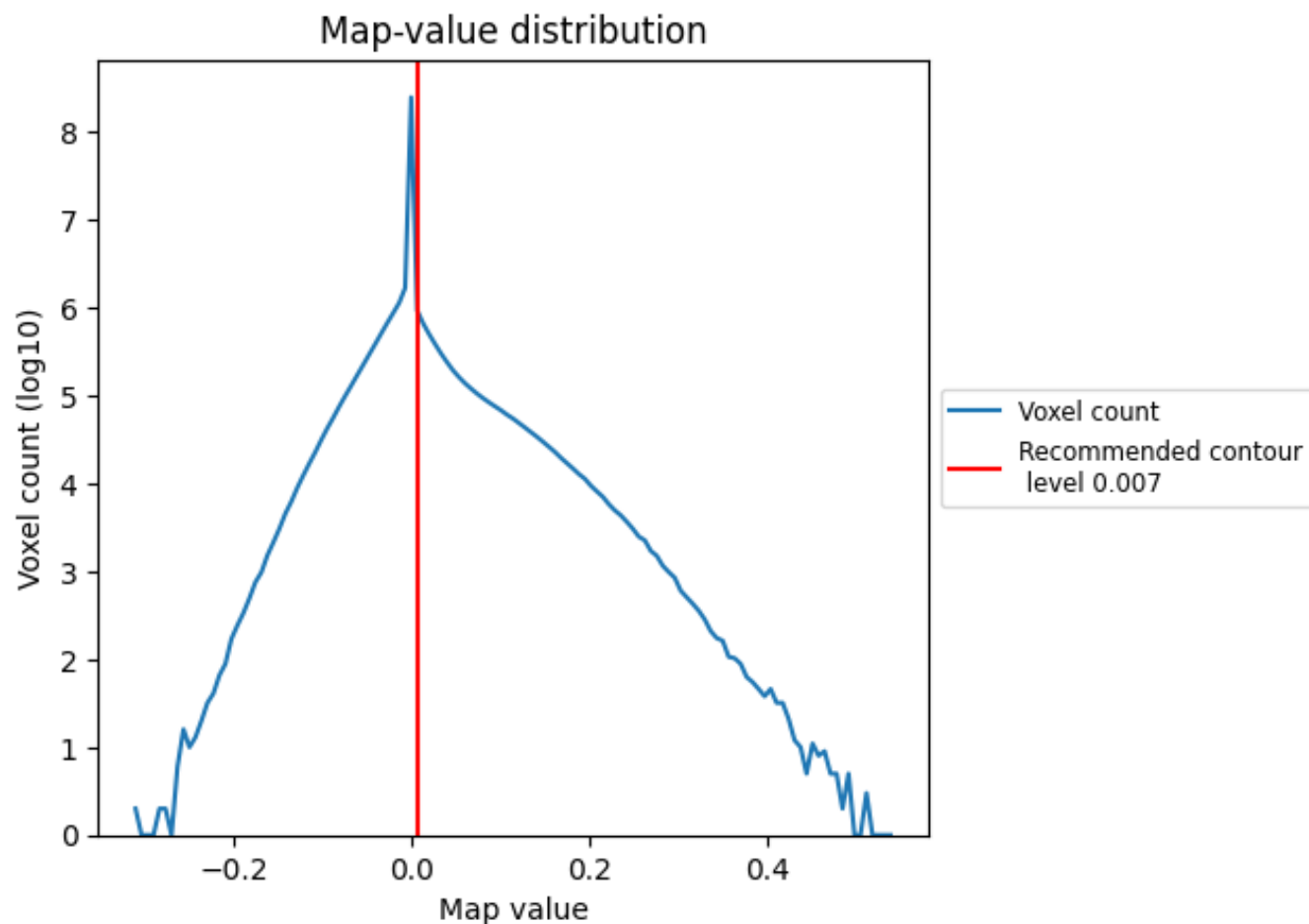
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

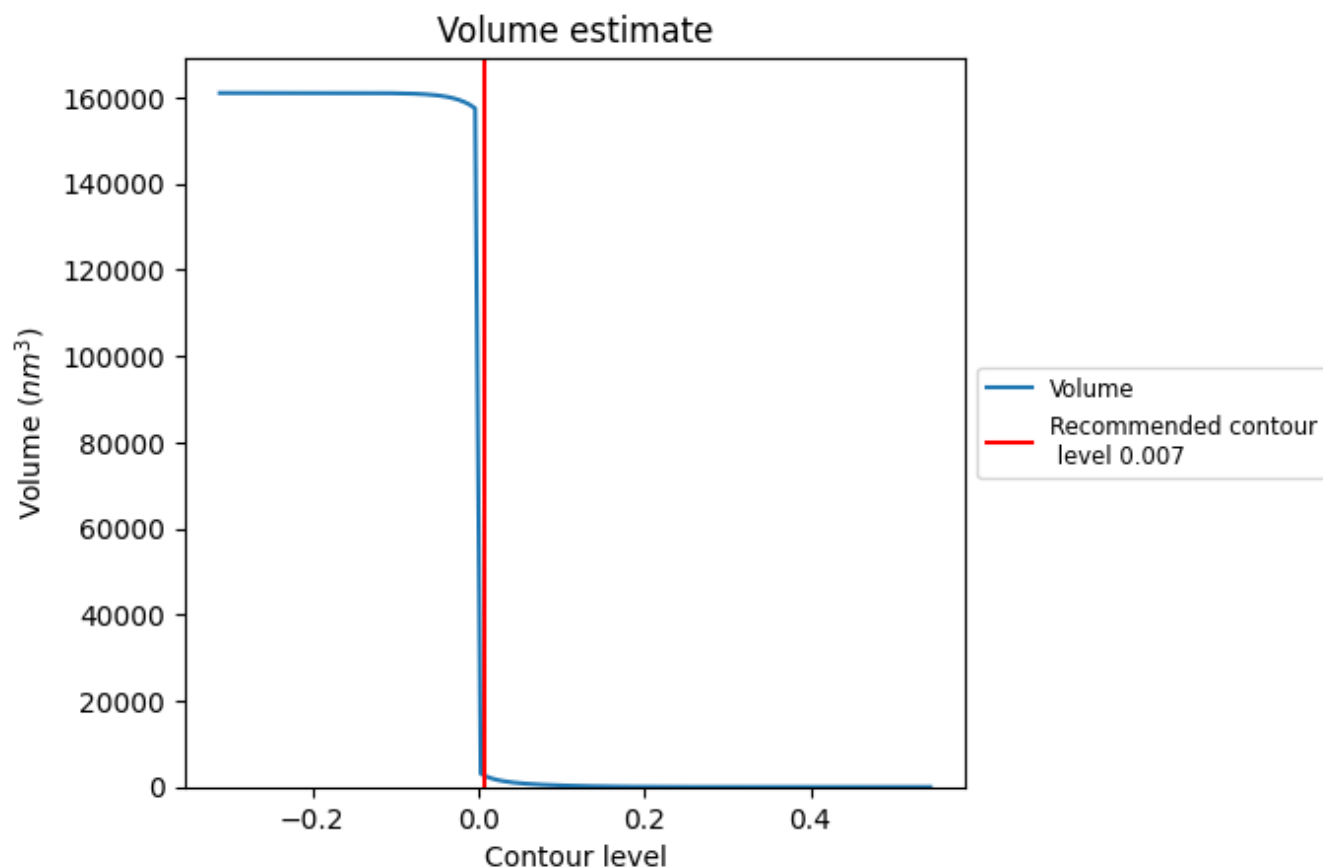
This section contains the results of statistical analysis of the map.

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.

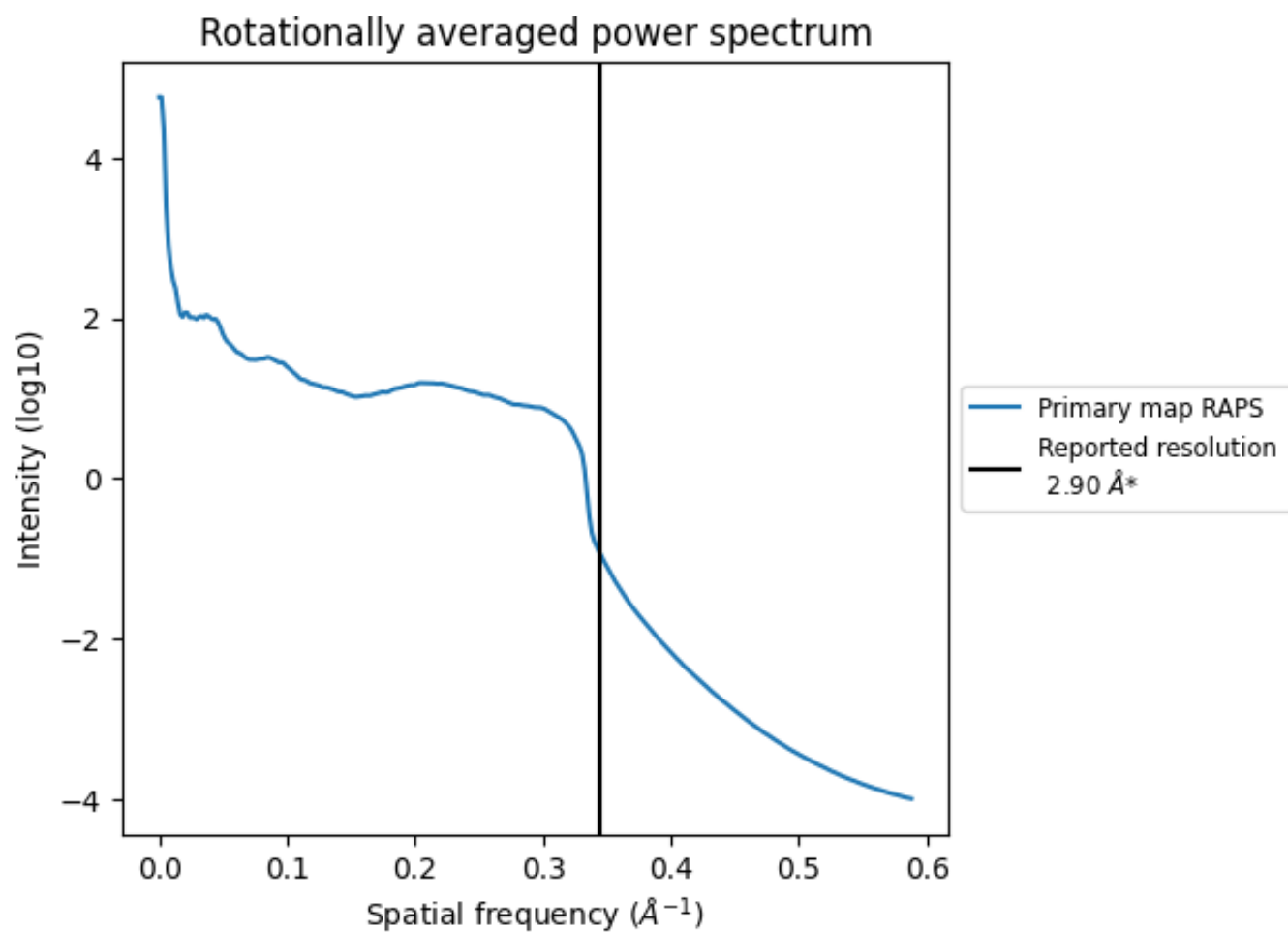
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2699 nm^3 ; this corresponds to an approximate mass of 2438 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 ⓘ

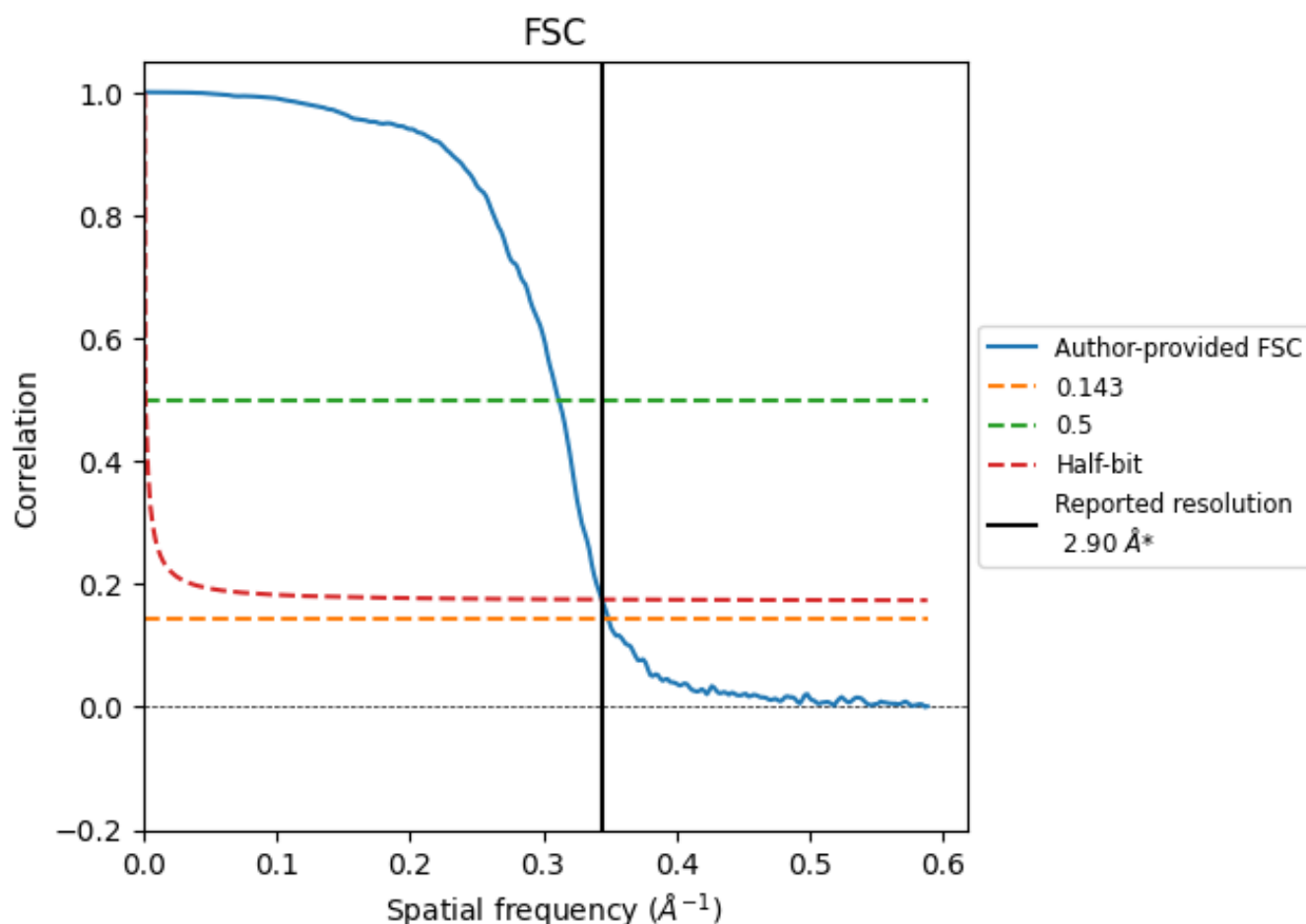


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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](#)

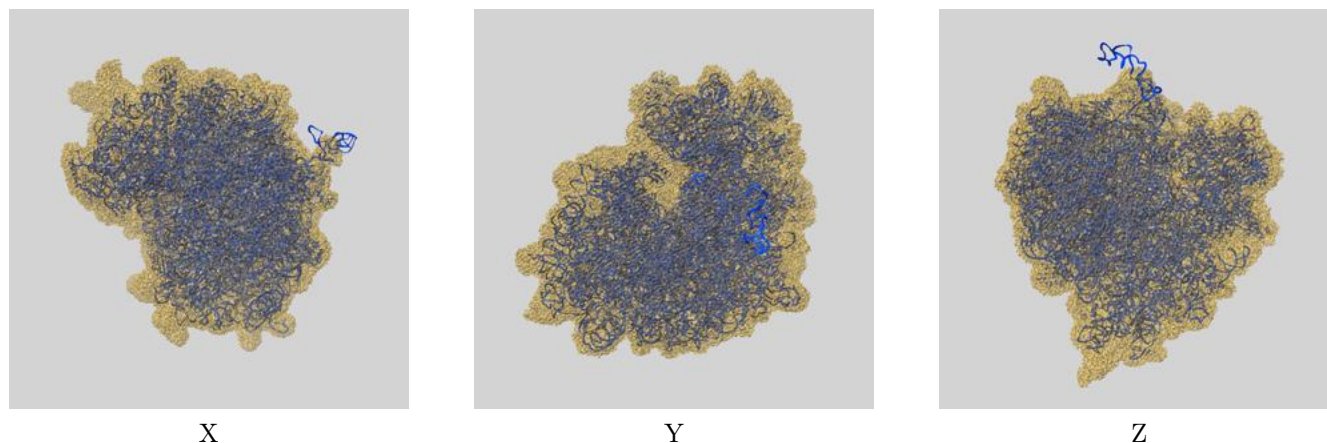
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.21	2.91
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

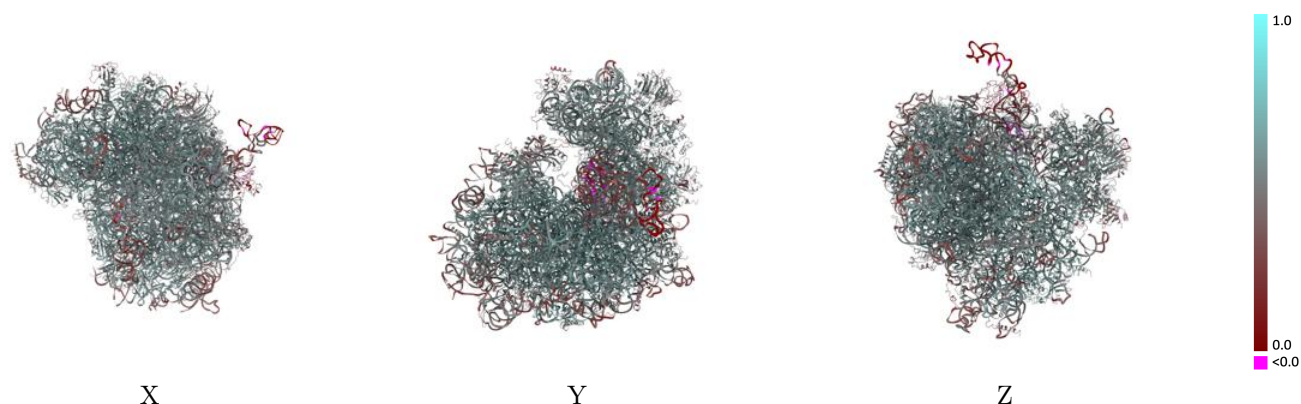
This section contains information regarding the fit between EMDB map EMD-3883 and PDB model 6QZP. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



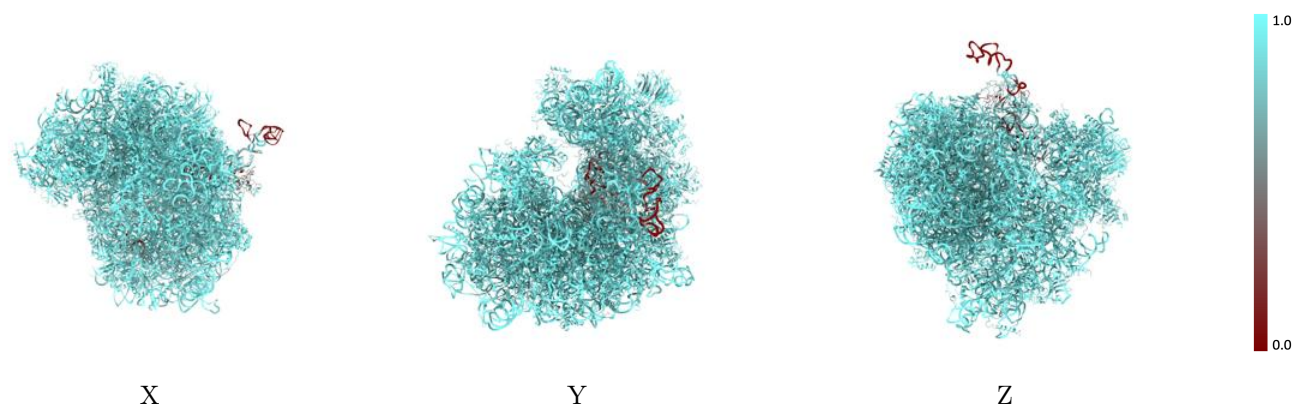
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



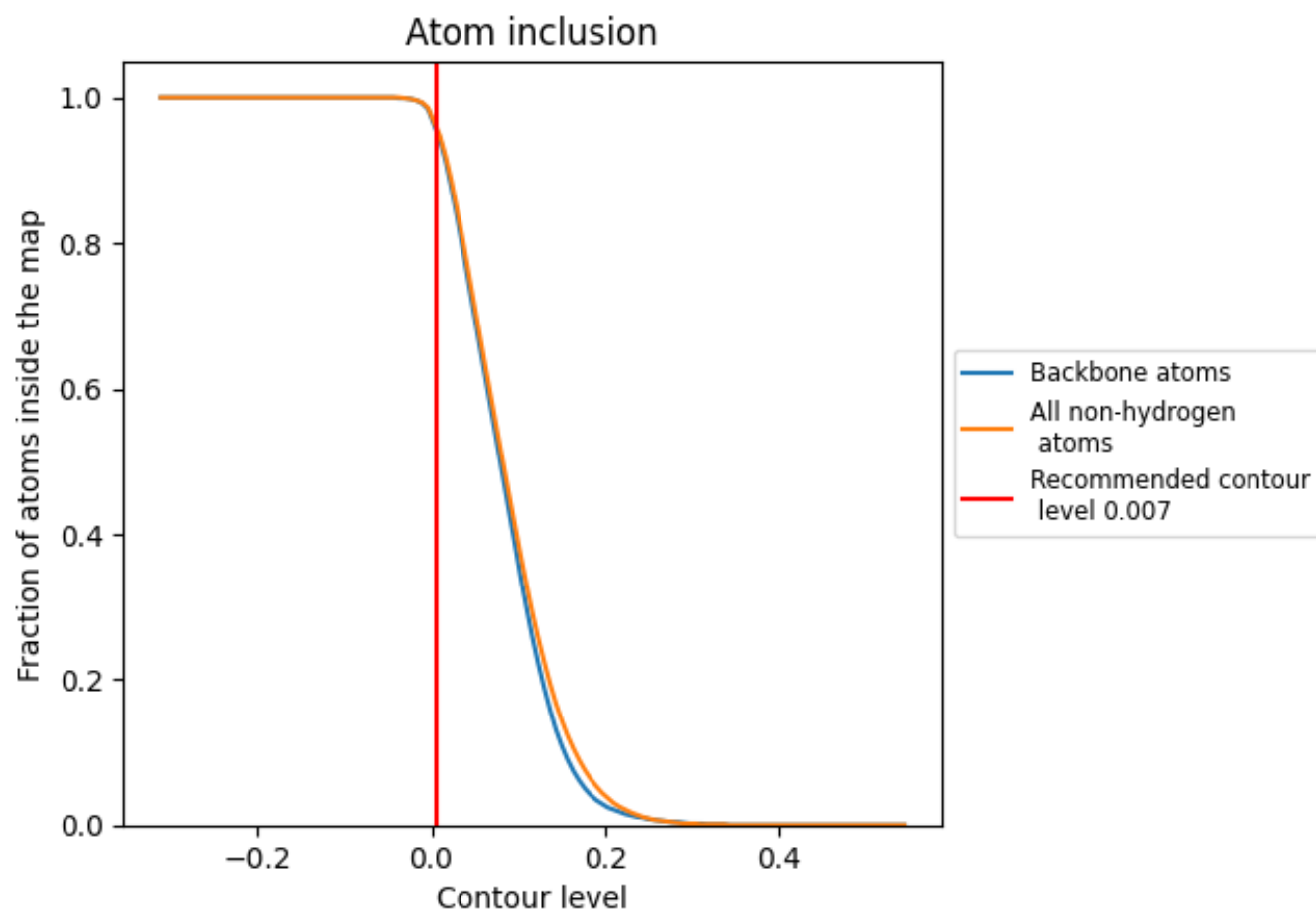
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.5370
L5	 0.9670	 0.5430
L7	 0.9920	 0.5690
L8	 0.9780	 0.5720
LA	 0.9670	 0.5850
LB	 0.9660	 0.5610
LC	 0.9670	 0.5650
LD	 0.9560	 0.5110
LE	 0.9410	 0.5010
LF	 0.9520	 0.5750
LG	 0.9500	 0.5050
LH	 0.9670	 0.5520
LI	 0.9220	 0.5260
LJ	 0.9190	 0.4380
LL	 0.9550	 0.5320
LM	 0.9720	 0.5590
LN	 0.9740	 0.5990
LO	 0.9690	 0.5820
LP	 0.9720	 0.5800
LQ	 0.9610	 0.5770
LR	 0.9540	 0.5310
LS	 0.9810	 0.5840
LT	 0.9660	 0.5590
LU	 0.9420	 0.4470
LV	 0.9690	 0.5640
LW	 0.8980	 0.4490
LX	 0.9530	 0.5540
LY	 0.9580	 0.5470
LZ	 0.9630	 0.5260
La	 0.9750	 0.5890
Lb	 0.9270	 0.5040
Lc	 0.9490	 0.5140
Ld	 0.9560	 0.5430
Le	 0.9620	 0.5860
Lf	 0.9680	 0.5880



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Chain	Atom inclusion	Q-score
Lg	 0.9590	 0.5570
Lh	 0.9600	 0.5420
Li	 0.9650	 0.5340
Lj	 0.9720	 0.5930
Lk	 0.9590	 0.4870
Ll	 0.9600	 0.5650
Lm	 0.9590	 0.5600
Ln	 0.9470	 0.5760
Lo	 0.9640	 0.5550
Lp	 0.9580	 0.5650
Lr	 0.9630	 0.5490
Lz	 0.5030	 0.1930
S2	 0.9820	 0.5540
S6	 0.4870	 0.2120
SA	 0.9690	 0.5320
SB	 0.9600	 0.5330
SC	 0.9620	 0.5510
SD	 0.9410	 0.5010
SE	 0.9670	 0.5650
SF	 0.9180	 0.5040
SG	 0.9540	 0.4980
SH	 0.9390	 0.4620
SI	 0.9540	 0.5330
SJ	 0.9600	 0.5480
SK	 0.9630	 0.5030
SL	 0.9450	 0.5480
SM	 0.8700	 0.3480
SN	 0.9630	 0.5610
SO	 0.9310	 0.5240
SP	 0.9530	 0.5090
SQ	 0.9410	 0.5360
SR	 0.9620	 0.5060
SS	 0.9460	 0.5050
ST	 0.9560	 0.5340
SU	 0.9510	 0.4970
SV	 0.9780	 0.5480
SW	 0.9570	 0.5670
SX	 0.9660	 0.5670
SY	 0.9470	 0.5300
SZ	 0.9360	 0.4770
Sa	 0.9540	 0.5380
Sb	 0.9370	 0.5080

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Chain	Atom inclusion	Q-score
Sc	 0.9200	 0.4630
Sd	 0.9480	 0.5570
Se	 0.9080	 0.4930
Sf	 0.9380	 0.4310
Sg	 0.9440	 0.4810