



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:56 AM UTC

PDB ID : 9I14 / pdb_00009i14
EMDB ID : EMD-52565
Title : CRYO-EM STRUCTURE OF HCT15 POLYSOMES IN HYBRID-PRE STATE
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-01-15
Resolution : 3.34 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 : 2022.3.0, CSD as543be (2022)
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

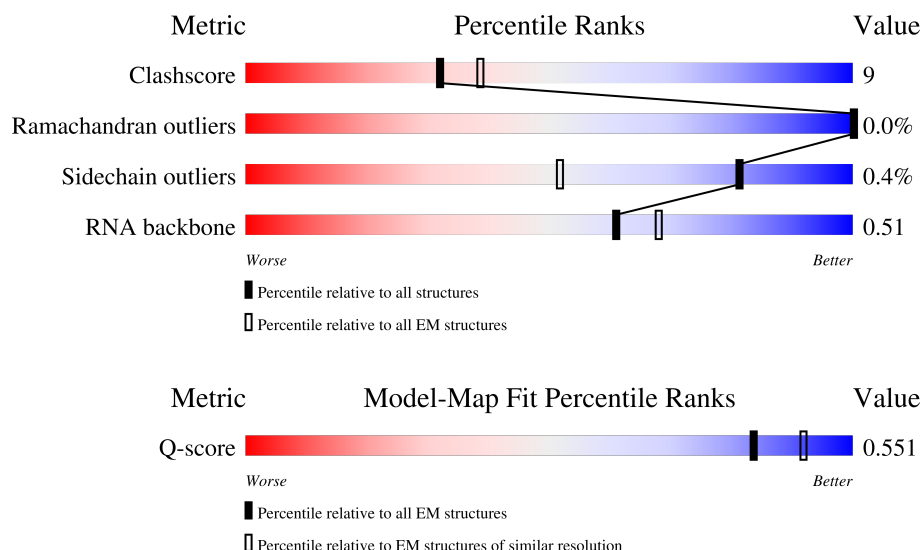
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 3.34 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	14446 (2.84 - 3.84)

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	LA	257	 77% 19% .
2	SA	295	 57% 16% 26%
3	LB	403	 76% 23% .






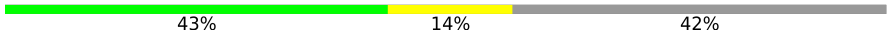



















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Mol	Chain	Length	Quality of chain
4	SB	264	
5	A4	13	
6	B4	75	
7	D4	76	
8	L5	5070	
9	L7	120	
10	L8	156	
11	LC	427	
12	LD	297	
13	LE	288	
14	LF	248	
15	LG	266	
16	LH	192	
17	LJ	178	
18	LL	211	
19	LM	215	
20	LN	204	
21	LO	203	
22	LP	184	
23	LQ	188	
24	LR	196	
25	LS	176	
26	LT	160	
27	LU	128	
28	LV	140	

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Mol	Chain	Length	Quality of chain
29	LW	157	
30	LX	156	
31	LY	145	
32	LZ	136	
33	La	148	
34	Lb	159	
35	Lc	115	
36	Ld	125	
37	Lf	110	
38	Lg	117	
39	Lh	123	
40	Li	105	
41	Lj	97	
42	Lk	70	
43	Ll	51	
44	Lm	128	
45	Ln	25	
46	Lo	106	
47	Lp	92	
48	Lr	137	
49	S2	1869	
50	SC	293	
51	SD	243	
52	SE	263	
53	SF	204	


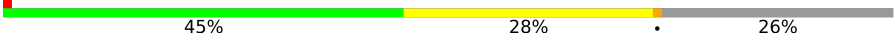


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Mol	Chain	Length	Quality of chain
54	SG	249	
55	SH	194	
56	SI	208	
57	SJ	194	
58	SK	165	
59	SL	158	
60	SN	151	
61	SO	151	
62	SP	145	
63	SQ	146	
64	SR	135	
65	SS	152	
66	ST	145	
67	SU	119	
68	SV	83	
69	SW	130	
70	SX	143	
71	SY	133	
72	SZ	125	
73	Sa	115	
74	Sb	84	
75	Sc	69	
76	Sd	56	
77	Se	59	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	Sg	317	 74% 23%
80	SM	132	 45% 28% 26%
81	Le	135	 73% 21% 6%
82	LI	214	 74% 19% 5%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 206575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	248	Total	C	N	O	S	0	0
			1886	1183	386	311	6		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	217	Total	C	N	O	S	0	0
			1705	1084	300	313	8		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	398	Total	C	N	O	S	0	0
			3147	2008	591	534	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	213	Total	C	N	O	S	0	0
			1727	1096	309	308	14		

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	11	Total	C	N	O	P	0	0
			231	104	37	79	11		

- Molecule 6 is a RNA chain called P/E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B4	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 7 is a RNA chain called A/P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D4	63	Total	C	N	O	P	0	0
			1349	601	243	442	63		

- Molecule 8 is a RNA chain called LSU 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L5	3465	Total	C	N	O	P	0	0
			74335	33126	13606	24139	3464		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 10 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L8	147	Total	C	N	O	P	0	0
			3132	1399	557	1030	146		

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	362	Total	C	N	O	S	0	0
			2874	1808	574	477	15		

- Molecule 12 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	209	Total	C	N	O	S	0	0
			1648	1061	313	270	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	222	Total	C	N	O	S	0	0
			1846	1186	354	297	9		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	224	Total	C	N	O	S	0	0
			1793	1143	343	303	4		

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 17 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	167	Total	C	N	O	S	0	0
			1330	841	249	234	6		

- Molecule 18 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	198	Total	C	N	O	S	0	0
			1588	994	333	257	4		

- Molecule 19 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LM	137	Total	C	N	O	S	0	0
			1121	719	215	180	7		

- Molecule 20 is a protein called 60S ribosomal protein L15.

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

- Molecule 21 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LO	201	Total	C	N	O	S	0	0
			1646	1061	321	259	5		

- Molecule 22 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LP	157	Total	C	N	O	S	0	0
			1267	794	243	221	9		

- Molecule 23 is a protein called 60S ribosomal protein L18.

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

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LR	175	Total	C	N	O	S	0	0
			1458	902	317	230	9		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LS	173	Total	C	N	O	S	0	0
			1431	912	278	232	9		

- Molecule 26 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LT	155	Total	C	N	O	S	0	0
			1247	789	244	208	6		

- Molecule 27 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 28 is a protein called 60S ribosomal protein L23.

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

- Molecule 29 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	89	Total	C	N	O	S	0	0
			663	420	129	112	2		

- Molecule 30 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LX	118	Total	C	N	O	S	0	0
			962	615	180	166	1		

- Molecule 31 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	134	Total	C	N	O	S	0	0
			1103	692	223	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 33 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	La	147	Total	C	N	O	S	0	0
			1159	735	236	185	3		

- Molecule 34 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lb	92	Total	C	N	O	S	0	0
			747	465	163	117	2		

- Molecule 35 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lc	93	Total	C	N	O	S	0	0
			725	462	128	128	7		

- Molecule 36 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ld	106	Total	C	N	O	S	0	0
			871	552	170	147	2		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lf	109	Total	C	N	O	S	0	0
			867	550	173	141	3		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lg	110	Total	C	N	O	S	0	0
			861	539	177	139	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lh	122	Total	C	N	O	S	0	0
			1011	638	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Li	100	Total	C	N	O	S	0	0
			818	512	174	127	5		

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lj	87	Total	C	N	O	S	0	0
			715	440	158	112	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lj	57	THR	ASN	conflict	UNP P61927

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lk	69	Total	C	N	O	S	0	0
			553	356	100	96	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ll	49	Total	C	N	O	S	0	0
			435	275	97	62	1		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lm	51	Total	C	N	O	S	0	0
			411	255	87	63	6		

- Molecule 45 is a protein called 60S ribosomal protein L41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lo	103	Total	C	N	O	S	0	0
			839	525	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lp	91	Total	C	N	O	S	0	0
			707	445	136	119	7		

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lr	125	Total	C	N	O	S	0	0
			992	615	207	166	4		

- Molecule 49 is a RNA chain called SSU 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	1577	Total	C	N	O	P	0	0
			33711	15068	6064	11003	1576		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	220	Total	C	N	O	S	0	0
			1704	1102	293	300	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	223	Total	C	N	O	S	0	0
			1689	1077	304	301	7		

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	258	Total	C	N	O	S	0	0
			2050	1311	381	350	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	187	Total	C	N	O	S	0	0
			1486	929	282	268	7		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	221	Total	C	N	O	S	0	0
			1749	1097	349	296	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	SH	177	Total	C	N	O		
			1360	876	251	233	0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	197	Total	C	N	O	S		
			1582	991	311	275	5	0	0

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	178	Total	C	N	O	S		
			1482	944	296	240	2	0	0

- Molecule 58 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SK	96	Total	C	N	O	S		
			804	527	140	131	6	0	0

- Molecule 59 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	140	Total	C	N	O	S		
			1147	731	216	194	6	0	0

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SN	150	Total	C	N	O	S		
			1205	772	229	203	1	0	0

- Molecule 61 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SO	129	Total	C	N	O	S		
			959	586	190	177	6	0	0

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SP	129	Total	C	N	O	S	0	0
			1060	672	202	179	7		

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SQ	141	Total	C	N	O	S	0	0
			1120	713	212	192	3		

- Molecule 64 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SR	130	Total	C	N	O	S	0	0
			1053	663	197	189	4		

- Molecule 65 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SS	142	Total	C	N	O	S	0	0
			1171	735	239	196	1		

- Molecule 66 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ST	141	Total	C	N	O	S	0	0
			1098	689	210	196	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ST	4	PHE	VAL	conflict	UNP P39019

- Molecule 67 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SU	101	Total	C	N	O	S	0	0
			790	495	152	139	4		

- Molecule 68 is a protein called 40S ribosomal protein S21.

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

- Molecule 69 is a protein called 40S ribosomal protein S15a.

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

- Molecule 70 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SX	141	Total	C	N	O	S	0	0
			1082	685	213	181	3		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SY	123	Total	C	N	O	S	0	0
			988	625	191	167	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	99	Total	C	N	O	S	0	0
			788	490	165	128	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sb	83	Total	C	N	O	S	0	0
			633	398	117	112	6		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sc	63	Total	C	N	O	S	0	0
			489	299	97	91	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sd	52	Total	C	N	O	S	0	0
			436	273	88	70	5		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	50	Total	C	N	O	S	0	0
			400	245	91	63	1		

- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			489	308	91	83	7		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sg	306	Total	C	N	O	S	0	0
			2389	1507	417	453	12		

- Molecule 80 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SM	98	Total	C	N	O	S	0	0
			722	451	134	130	7		

- Molecule 81 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Le	127	Total	C	N	O	S	0	0
			1044	662	214	163	5		

- Molecule 82 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	LI	203	Total	C	N	O	S	0	0
			1641	1042	316	270	13		

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

Mol	Chain	Residues	Atoms		AltConf
83	LA	1	Total	K	0
			1	1	
83	B4	3	Total	K	0
			3	3	
83	L5	17	Total	K	0
			17	17	
83	L8	1	Total	K	0
			1	1	
83	La	1	Total	K	0
			1	1	
83	S2	15	Total	K	0
			15	15	
83	SN	1	Total	K	0
			1	1	
83	Le	1	Total	K	0
			1	1	

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
84	A4	2	Total	Mg	0
			2	2	
84	B4	4	Total	Mg	0
			4	4	
84	D4	1	Total	Mg	0
			1	1	
84	L5	157	Total	Mg	0
			157	157	
84	L7	2	Total	Mg	0
			2	2	
84	L8	3	Total	Mg	0
			3	3	
84	LN	1	Total	Mg	0
			1	1	
84	LP	1	Total	Mg	0
			1	1	

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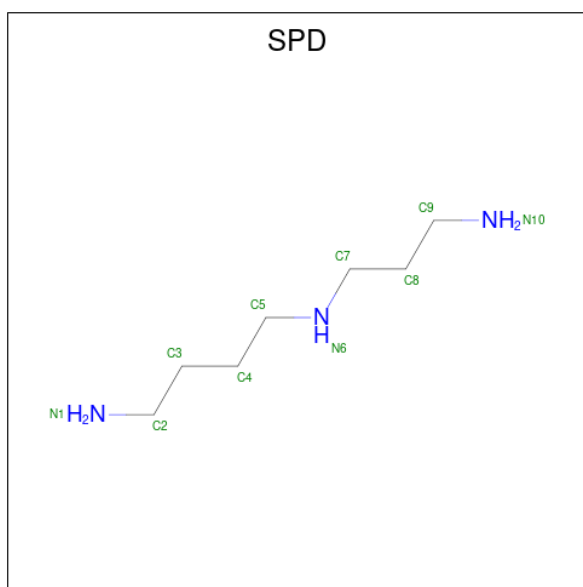
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
84	LT	1	Total 1	Mg 1	0
84	Lp	1	Total 1	Mg 1	0
84	S2	93	Total 93	Mg 93	0
84	LI	1	Total 1	Mg 1	0

- Molecule 85 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

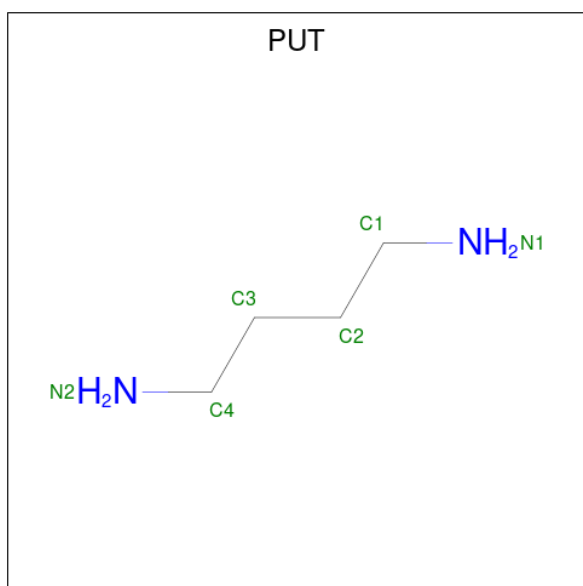
Mol	Chain	Residues	Atoms		AltConf
85	L5	12	Total 12	Na 12	0
85	L7	1	Total 1	Na 1	0
85	L8	1	Total 1	Na 1	0
85	LP	1	Total 1	Na 1	0
85	L1	1	Total 1	Na 1	0
85	S2	7	Total 7	Na 7	0

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
86	L5	1	Total	C	N	0
			10	7	3	

- Molecule 87 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).

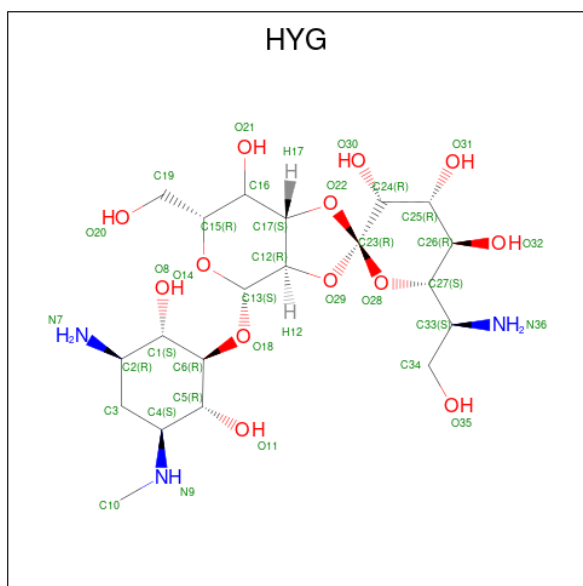


Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			6	4	2	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total	Zn	0
			1	1	
88	Lj	1	Total	Zn	0
			1	1	
88	Lo	1	Total	Zn	0
			1	1	
88	Lp	1	Total	Zn	0
			1	1	
88	Sd	1	Total	Zn	0
			1	1	
88	Sf	1	Total	Zn	0
			1	1	
88	SM	1	Total	Zn	0
			1	1	

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is water.

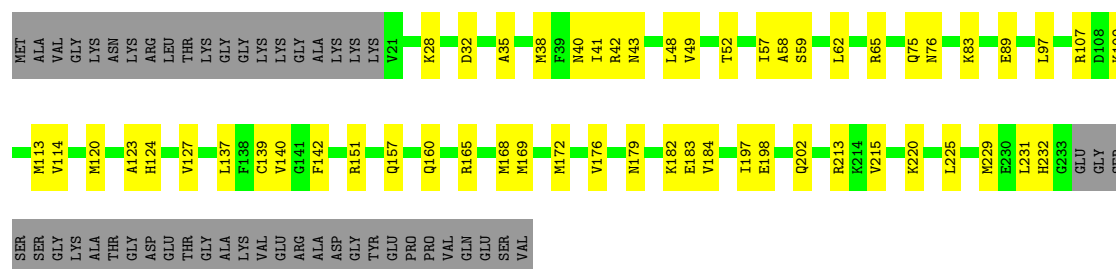
Mol	Chain	Residues	Atoms		AltConf
90	L5	1	Total	O	0
			1	1	

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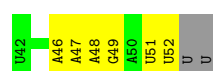
Mol	Chain	Residues	Atoms		AltConf
90	L8	1	Total 1	O 1	0
90	LH	1	Total 1	O 1	0
90	LV	1	Total 1	O 1	0
90	S2	1	Total 1	O 1	0
90	SX	1	Total 1	O 1	0
90	LI	1	Total 1	O 1	0

Chain SB:  60% 21% 19%



• Molecule 5: mRNA

Chain A4:  38% 46% 15%



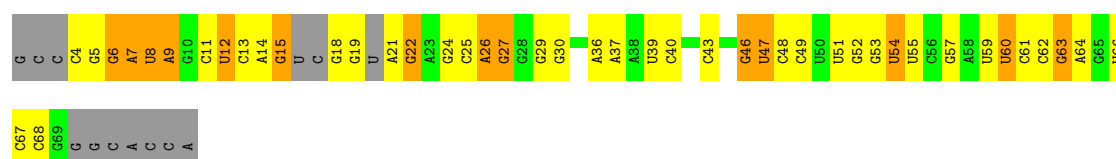
• Molecule 6: P/E tRNA

Chain B4:  47% 40% 13%



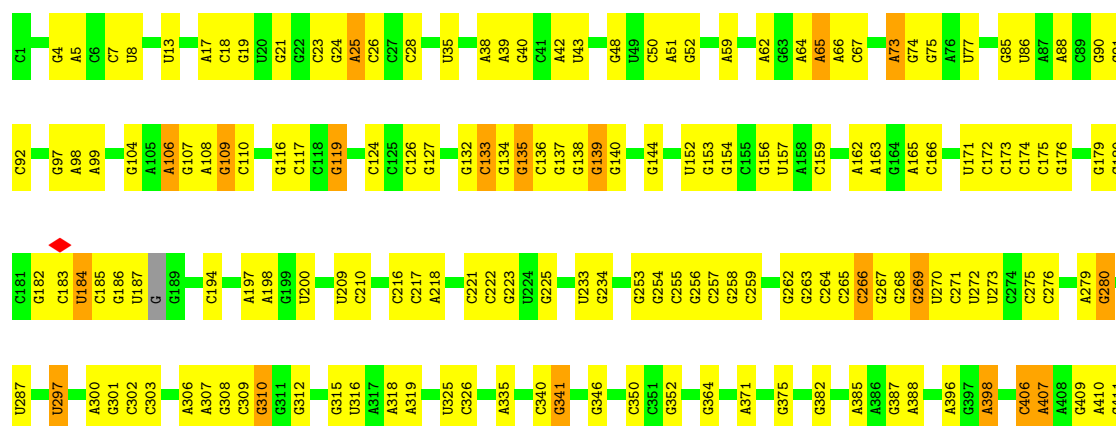
• Molecule 7: A/P tRNA

Chain D4:  24% 41% 18% 17%



• Molecule 8: LSU 28S rRNA

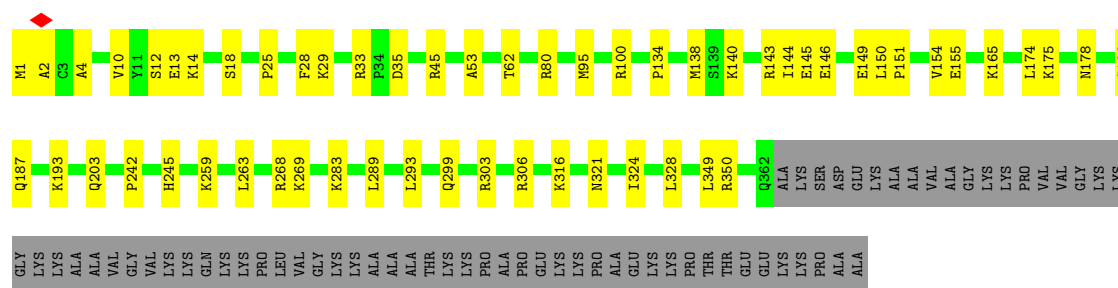
Chain L5:  38% 25% 5% 32%





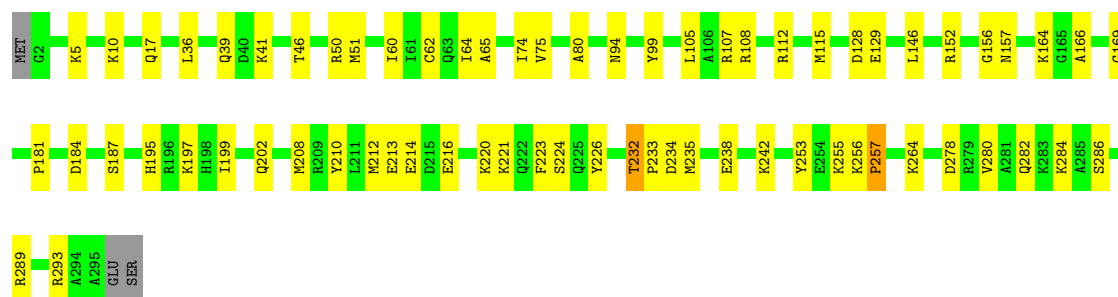






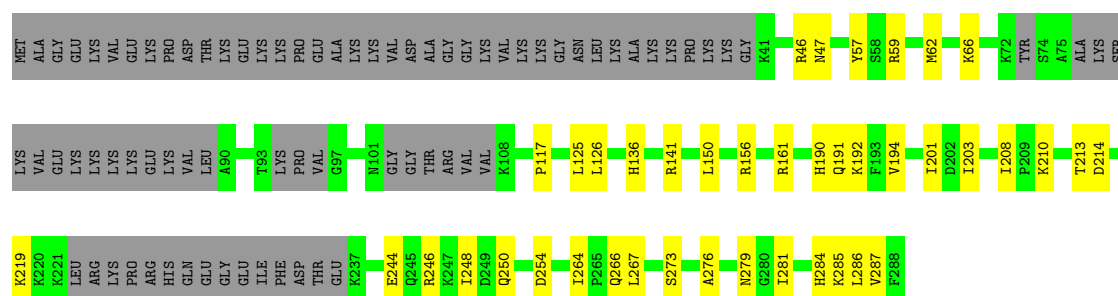
• Molecule 12: 60S ribosomal protein L5

Chain LD: 76% 22% ..



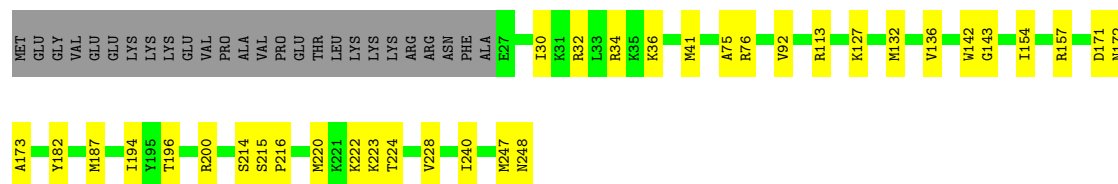
• Molecule 13: Large ribosomal subunit protein eL6

Chain LE: 58% 14% 27%



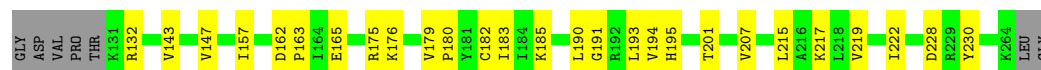
• Molecule 14: Large ribosomal subunit protein uL30

Chain LF: 75% 14% 10%

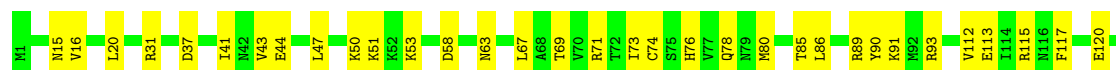


• Molecule 15: 60S ribosomal protein L7a

Chain LG: 70% 14% 16%



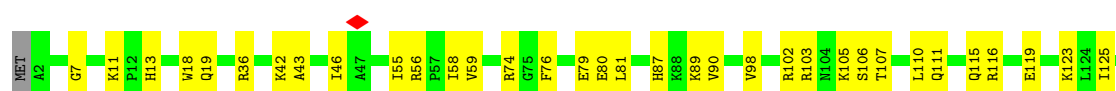
- Molecule 16: 60S ribosomal protein L9



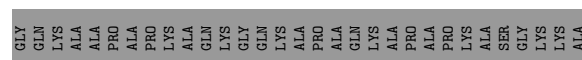
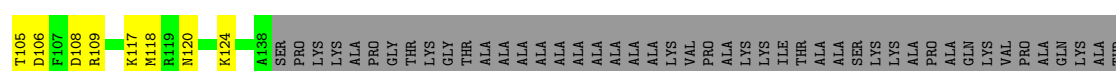
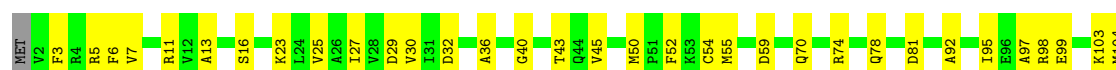
- Molecule 17: 60S ribosomal protein L11



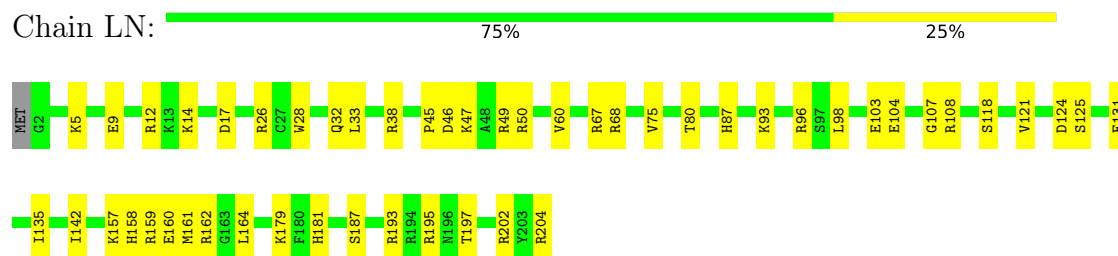
- Molecule 18: 60S ribosomal protein L13



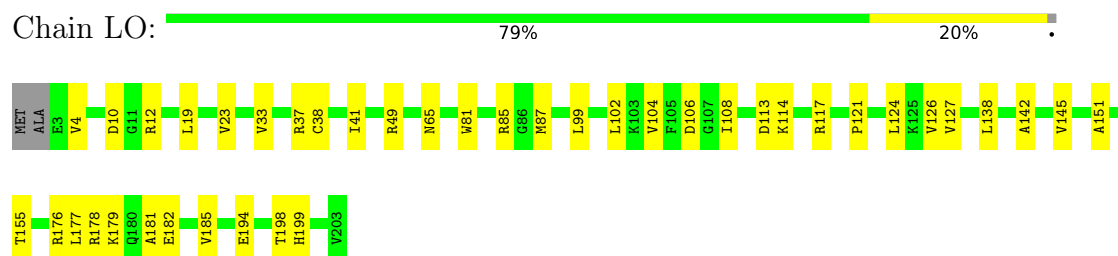
- Molecule 19: 60S ribosomal protein L14



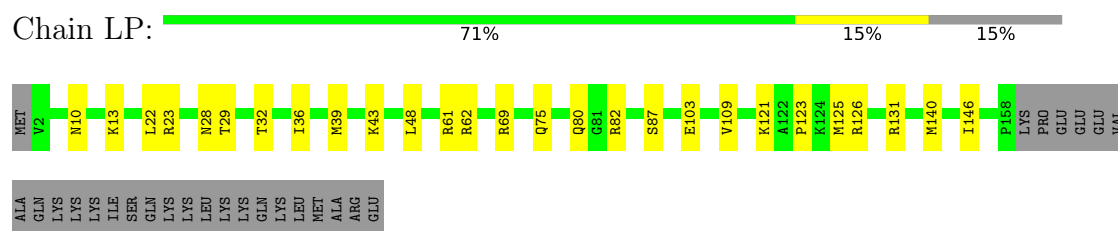
- Molecule 20: 60S ribosomal protein L15



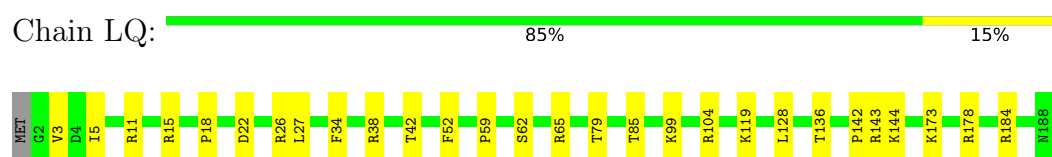
- Molecule 21: 60S ribosomal protein L13a



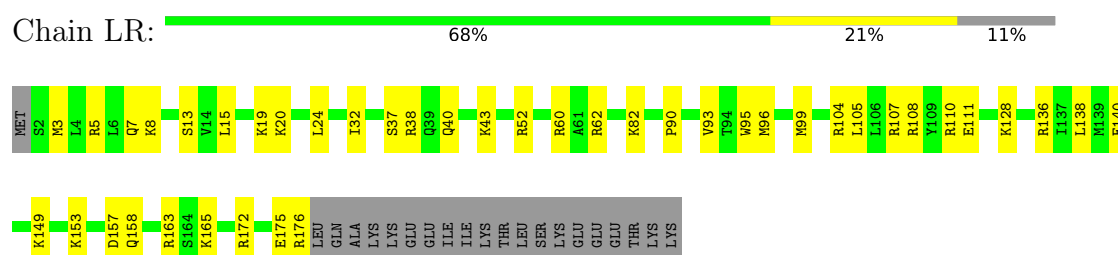
- Molecule 22: 60S ribosomal protein L17



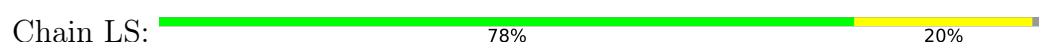
- Molecule 23: 60S ribosomal protein L18

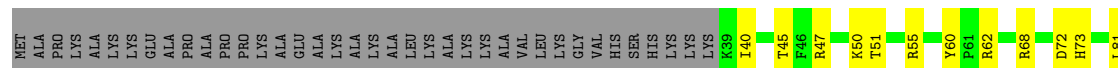


- Molecule 24: 60S ribosomal protein L19

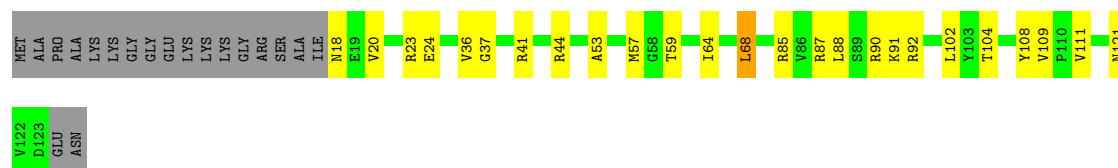


- Molecule 25: 60S ribosomal protein L18a





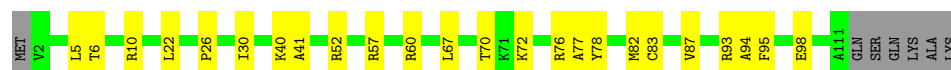

• Molecule 36: 60S ribosomal protein L31

Chain Ld: 

• Molecule 37: 60S ribosomal protein L35a

Chain Lf: 


• Molecule 38: 60S ribosomal protein L34

Chain Lg: 

• Molecule 39: 60S ribosomal protein L35

Chain Lh: 

• Molecule 40: 60S ribosomal protein L36

Chain Li: 

• Molecule 41: Large ribosomal subunit protein eL37

Chain Lj: 

• Molecule 42: 60S ribosomal protein L38

Chain Lk: 



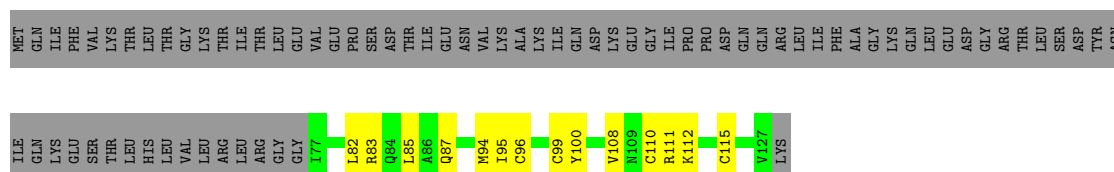
- Molecule 43: 60S ribosomal protein L39

Chain Ll: 71% 25% .



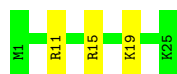
- Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain Lm: 29% 11% 60%



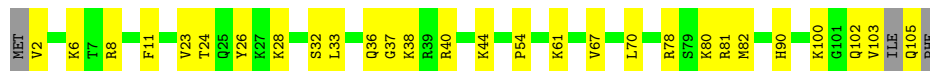
- Molecule 45: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 46: 60S ribosomal protein L36a

Chain Lo: 71% 26% .



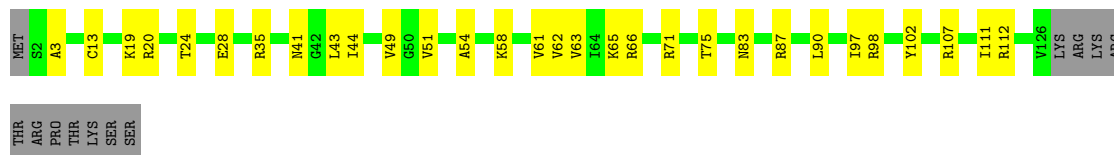
- Molecule 47: 60S ribosomal protein L37a

Chain Lp: 84% 15% .

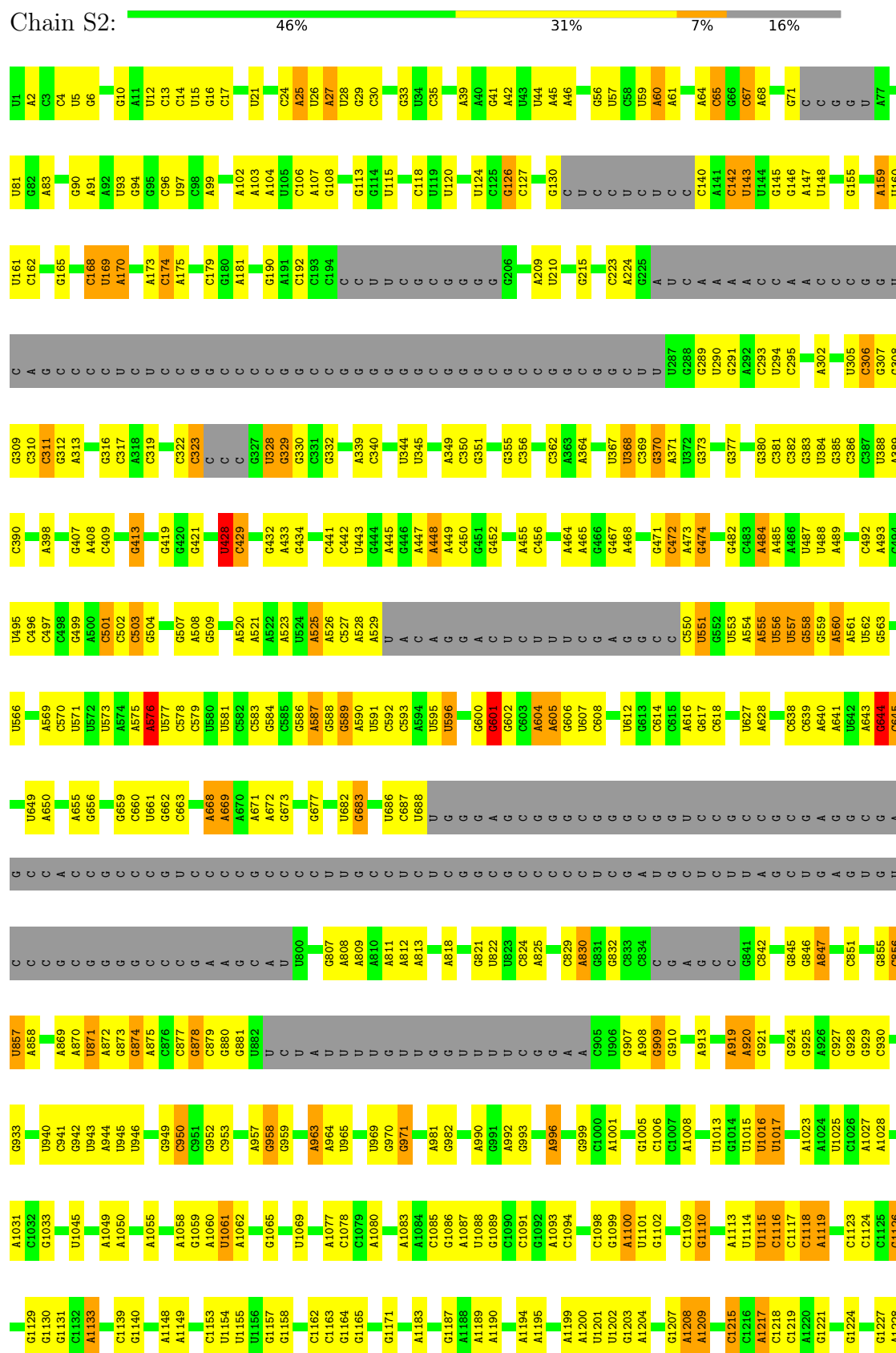


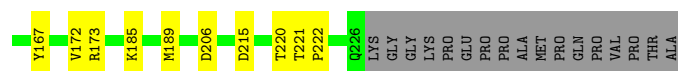
- Molecule 48: 60S ribosomal protein L28

Chain Lr: 69% 22% 9%



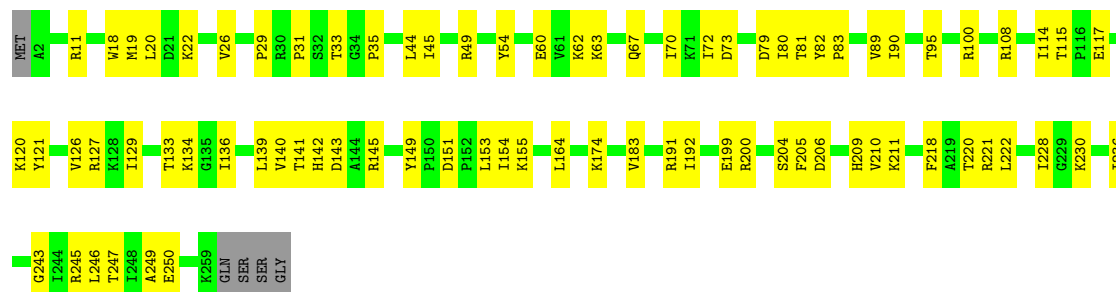
● Molecule 49: SSU 18S rRNA





- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE: 68% 30%



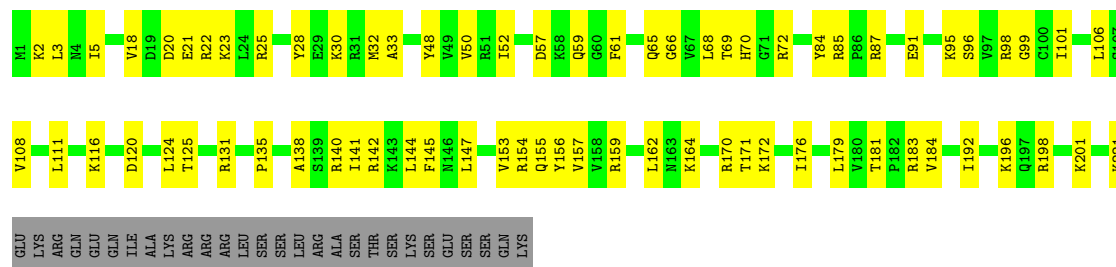
- Molecule 53: 40S ribosomal protein S5

Chain SF: 82% 9% 8%



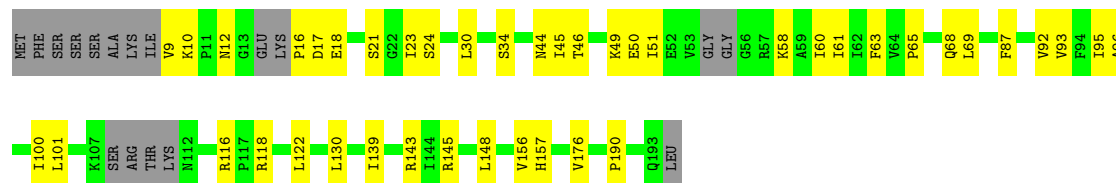
- Molecule 54: 40S ribosomal protein S6

Chain SG: 60% 29% 11%



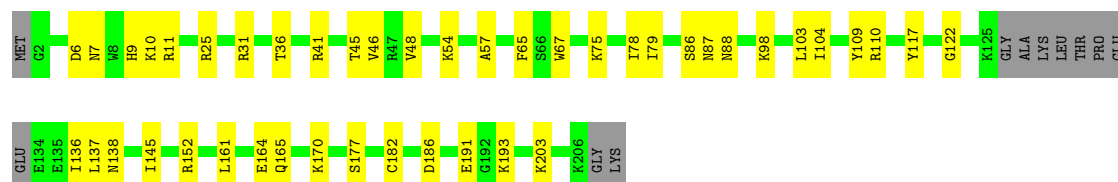
- Molecule 55: 40S ribosomal protein S7

Chain SH: 69% 22% 9%



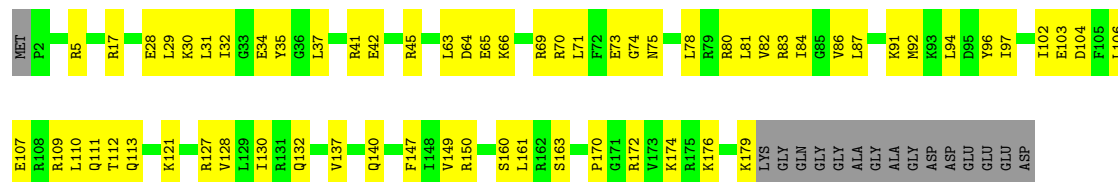
- Molecule 56: 40S ribosomal protein S8

Chain SI: 74% 21% 5%



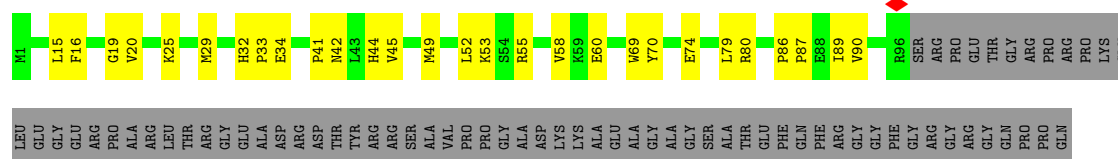
- Molecule 57: 40S ribosomal protein S9

Chain SJ: 59% 33% 8%



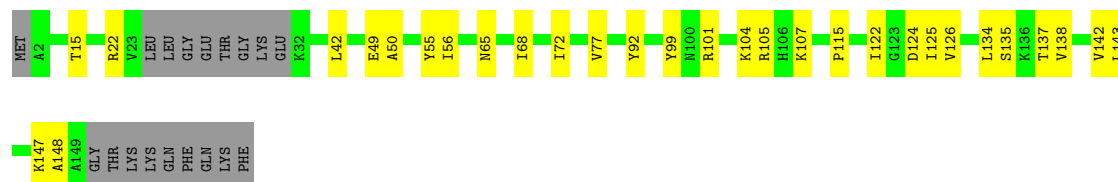
- Molecule 58: 40S ribosomal protein S10

Chain SK: 41% 17% 42%



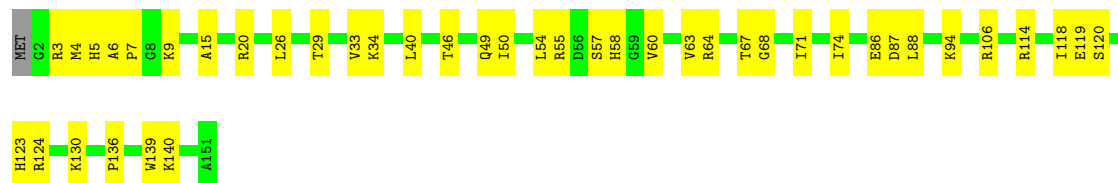
- Molecule 59: 40S ribosomal protein S11

Chain SL: 70% 19% 11%



- Molecule 60: 40S ribosomal protein S13

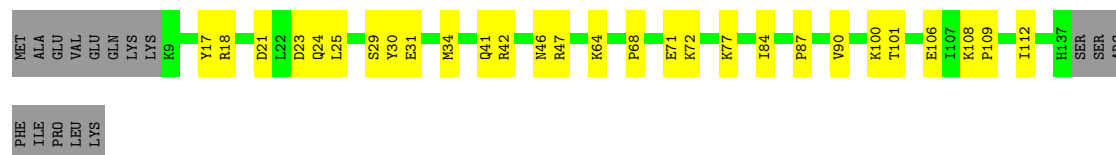
Chain SN: 72% 28%



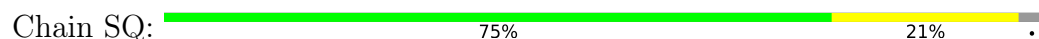
- Molecule 61: 40S ribosomal protein S14

Chain SO: 58% 28% 15%

- Molecule 62: 40S ribosomal protein S15



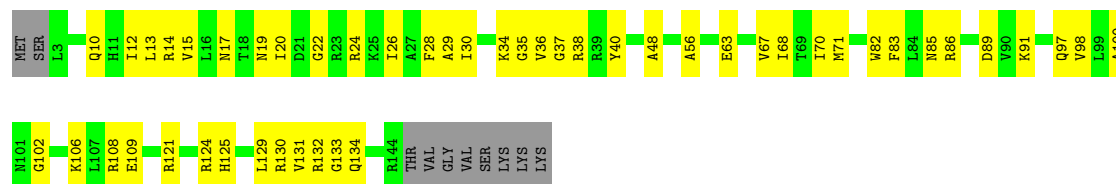
- Molecule 63: 40S ribosomal protein S16



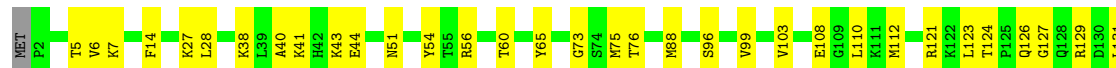
- Molecule 64: 40S ribosomal protein S17



- Molecule 65: 40S ribosomal protein S18



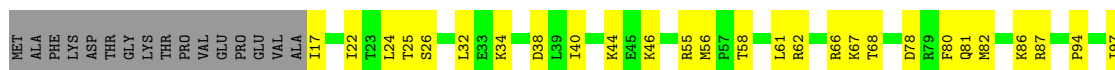
- Molecule 66: Small ribosomal subunit protein eS19





- Molecule 67: 40S ribosomal protein S20

Chain SU: 58% 27% 15%



- Molecule 68: 40S ribosomal protein S21

Chain SV: 83% 17%



- Molecule 69: 40S ribosomal protein S15a

Chain SW: 75% 23% ..



- Molecule 70: 40S ribosomal protein S23

Chain SX: 85% 13% .



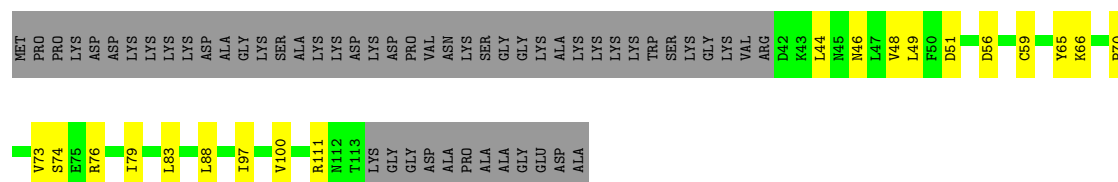
- Molecule 71: 40S ribosomal protein S24

Chain SY: 62% 30% 8%



- Molecule 72: 40S ribosomal protein S25

Chain SZ: 42% 15% 42%



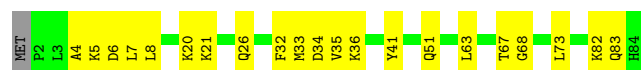
- Molecule 73: 40S ribosomal protein S26

Chain Sa: 70% 17% 14%



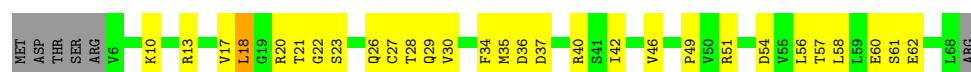
- Molecule 74: 40S ribosomal protein S27

Chain Sb: 74% 25% .



- Molecule 75: 40S ribosomal protein S28

Chain Sc: 49% 41% . 9%



- Molecule 76: 40S ribosomal protein S29

Chain Sd: 62% 29% . 7%



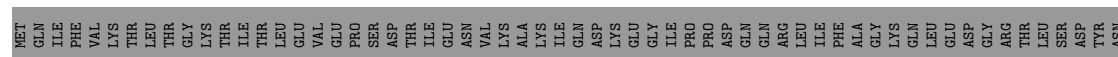
- Molecule 77: 40S ribosomal protein S30

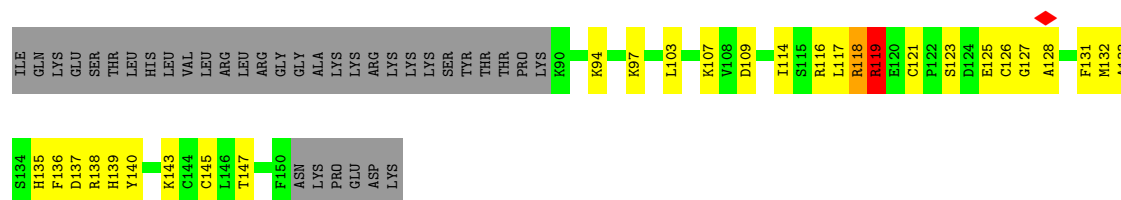
Chain Se: 68% 17% 15%



- Molecule 78: Ubiquitin

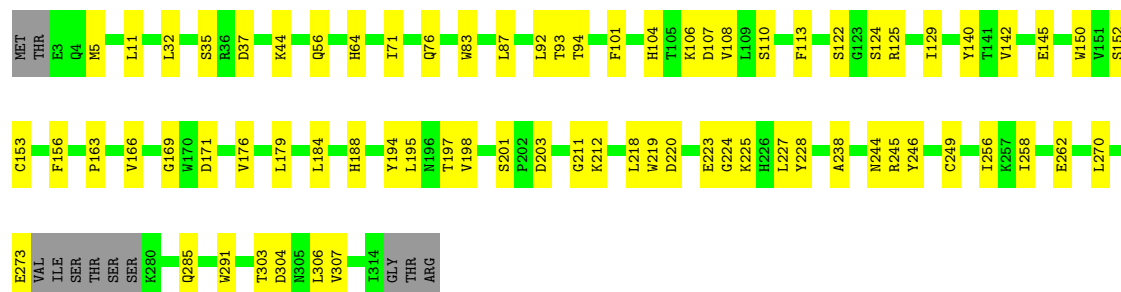
Chain Sf: 21% 17% . 61%





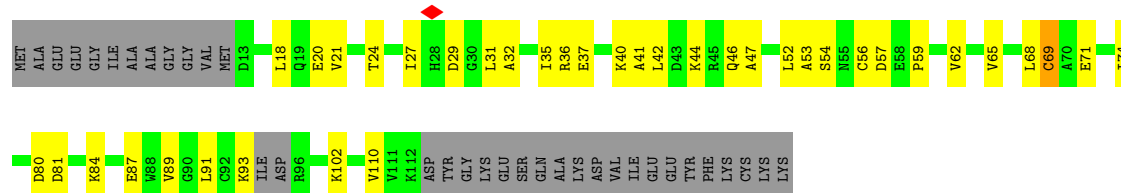
• Molecule 79: Receptor of activated protein C kinase 1

Chain Sg: 74% 23% .



• Molecule 80: 40S ribosomal protein S12

Chain SM: 45% 28% 26% .



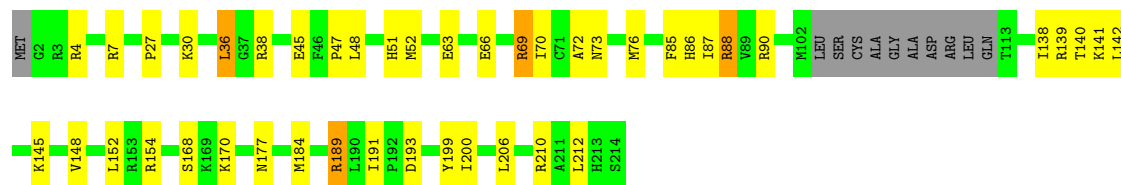
• Molecule 81: 60S ribosomal protein L32

Chain Le: 73% 21% 6% .



• Molecule 82: 60S ribosomal protein L10

Chain LI: 74% 19% 5% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.022	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, SPD, PSU, 4AC, MG, HYG, ZN, UY1, MA6, OMG, 6MZ, OMU, PUT, G7M, B8N, OMC, A2M, NA

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	LA	0.23	0/1924	0.35	0/2581
2	SA	0.22	0/1742	0.46	4/2368 (0.2%)
3	LB	0.20	0/3215	0.31	0/4314
4	SB	0.22	0/1754	0.31	0/2347
5	A4	0.32	0/257	0.36	0/397
6	B4	0.22	0/1795	0.30	0/2798
7	D4	0.20	0/1506	0.35	0/2342
8	L5	0.24	0/81933	0.28	0/127773
9	L7	0.23	0/2836	0.24	0/4421
10	L8	0.23	0/3425	0.28	0/5333
11	LC	0.20	0/2928	0.29	0/3933
12	LD	0.72	7/2437 (0.3%)	0.93	8/3263 (0.2%)
13	LE	0.17	0/1677	0.30	0/2250
14	LF	0.22	0/1880	0.30	0/2505
15	LG	0.18	0/1824	0.29	0/2462
16	LH	0.18	0/1545	0.31	0/2077
17	LJ	0.31	1/1352 (0.1%)	0.36	0/1809
18	LL	0.19	0/1616	0.31	0/2163
19	LM	0.20	0/1143	0.35	0/1530
20	LN	0.23	0/1746	0.30	0/2338
21	LO	0.20	0/1678	0.30	0/2245
22	LP	0.20	0/1294	0.29	0/1739
23	LQ	0.20	0/1537	0.28	0/2052
24	LR	0.19	0/1474	0.28	0/1949
25	LS	0.19	0/1469	0.31	0/1970
26	LT	0.20	0/1272	0.28	0/1698
27	LU	0.14	0/822	0.37	0/1103
28	LV	0.23	0/993	0.35	0/1332
29	LW	0.18	0/676	0.26	0/906
30	LX	0.19	0/979	0.30	0/1319
31	LY	0.18	0/1120	0.28	0/1491

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LZ	0.19	0/1141	0.33	0/1521
33	La	0.21	0/1188	0.28	0/1587
34	Lb	0.20	0/759	0.29	0/1003
35	Lc	0.33	0/736	0.52	0/988
36	Ld	0.19	0/886	0.31	0/1194
37	Lf	0.24	0/886	0.38	0/1189
38	Lg	0.22	0/871	0.29	0/1164
39	Lh	0.17	0/1019	0.31	0/1347
40	Li	0.15	0/829	0.28	0/1097
41	Lj	0.29	0/730	0.40	0/965
42	Lk	0.22	0/559	0.51	1/745 (0.1%)
43	Ll	0.19	0/445	0.25	0/588
44	Lm	0.28	0/417	0.53	0/555
45	Ln	0.26	0/240	0.26	0/305
46	Lo	0.20	0/851	0.31	0/1121
47	Lp	0.22	0/717	0.28	0/953
48	Lr	0.20	0/1007	0.28	0/1351
49	S2	0.27	1/37049 (0.0%)	0.30	0/57713
50	SC	0.21	0/1741	0.36	0/2354
51	SD	0.21	0/1715	0.29	0/2313
52	SE	0.22	0/2092	0.34	0/2816
53	SF	0.21	0/1507	0.29	0/2024
54	SG	0.18	0/1772	0.32	0/2366
55	SH	0.16	0/1380	0.34	0/1856
56	SI	0.21	0/1609	0.33	0/2155
57	SJ	0.17	0/1507	0.32	0/2015
58	SK	0.59	2/828 (0.2%)	1.12	5/1118 (0.4%)
59	SL	0.20	0/1167	0.32	0/1563
60	SN	0.35	1/1229 (0.1%)	0.33	1/1652 (0.1%)
61	SO	0.23	0/971	0.32	0/1302
62	SP	0.25	0/1081	0.36	0/1445
63	SQ	0.20	0/1138	0.29	0/1523
64	SR	0.21	0/1067	0.31	0/1433
65	SS	0.22	0/1189	0.32	0/1592
66	ST	0.20	0/1118	0.27	0/1499
67	SU	0.22	0/800	0.39	0/1075
68	SV	0.17	0/643	0.28	0/860
69	SW	0.21	0/1051	0.30	0/1406
70	SX	0.21	0/1100	0.35	0/1471
71	SY	0.15	0/1005	0.28	0/1340
72	SZ	0.20	0/580	0.36	0/780
73	Sa	0.50	2/801 (0.2%)	0.94	3/1074 (0.3%)
74	Sb	0.19	0/647	0.37	0/870

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sc	0.27	0/491	0.39	0/658
76	Sd	0.21	0/446	0.29	0/591
77	Se	0.16	0/403	0.26	0/527
78	Sf	0.34	0/498	0.61	1/661 (0.2%)
79	Sg	0.17	0/2445	0.33	0/3326
80	SM	0.29	0/727	0.51	0/981
81	Le	0.22	0/1062	0.31	0/1417
82	LI	0.25	0/1679	0.41	1/2243 (0.0%)
All	All	0.25	14/219668 (0.0%)	0.33	24/322500 (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
35	Lc	0	1
41	Lj	0	2
78	Sf	0	3
82	LI	0	3
All	All	0	9

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	LD	257	PRO	CB-CG	21.12	2.55	1.49
12	LD	257	PRO	CG-CD	-17.03	0.92	1.50
12	LD	233	PRO	CG-CD	-15.34	0.98	1.50
58	SK	87	PRO	CB-CG	-11.60	0.91	1.49
60	SN	136	PRO	CA-C	-9.20	1.46	1.51
12	LD	233	PRO	N-CD	7.75	1.58	1.47
73	Sa	97	PRO	CB-CG	-7.62	1.11	1.49
73	Sa	97	PRO	CG-CD	-7.10	1.26	1.50
17	LJ	17	ILE	CG1-CD1	-7.03	1.24	1.51
12	LD	232	THR	C-O	-6.39	1.15	1.23
58	SK	87	PRO	CG-CD	-6.17	1.29	1.50
12	LD	257	PRO	N-CA	-5.83	1.39	1.47
12	LD	257	PRO	N-CD	5.66	1.55	1.47
49	S2	428	OMU	O3'-P	5.52	1.61	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	LD	257	PRO	CB-CG-CD	-32.49	2.13	106.10
12	LD	233	PRO	N-CD-CG	-24.19	66.91	103.20
58	SK	87	PRO	CB-CG-CD	23.08	179.95	106.10
73	Sa	97	PRO	N-CD-CG	-18.80	75.00	103.20
58	SK	87	PRO	CA-CB-CG	-17.06	72.08	104.50
73	Sa	97	PRO	CA-CB-CG	-16.64	72.88	104.50
58	SK	87	PRO	N-CD-CG	-16.29	78.76	103.20
12	LD	233	PRO	CA-CB-CG	-15.56	74.93	104.50
12	LD	257	PRO	CA-N-CD	-13.74	92.77	112.00
12	LD	257	PRO	N-CA-CB	-12.28	92.67	103.35
2	SA	199	PRO	N-CD-CG	-10.30	87.75	103.20
58	SK	87	PRO	CA-N-CD	-10.17	97.77	112.00
12	LD	257	PRO	CA-CB-CG	-9.50	86.46	104.50
73	Sa	97	PRO	CA-N-CD	-8.70	99.82	112.00
58	SK	86	PRO	O-C-N	-8.69	117.31	121.31
2	SA	199	PRO	CA-CB-CG	-8.35	88.64	104.50
12	LD	233	PRO	CA-N-CD	-7.96	100.86	112.00
60	SN	136	PRO	O-C-N	-6.79	118.19	121.31
82	LI	36	LEU	CB-CG-CD1	-6.74	90.49	110.70
42	Lk	62	PRO	CA-N-CD	-6.01	103.58	112.00
2	SA	199	PRO	CA-N-CD	-5.58	104.19	112.00
2	SA	199	PRO	N-CA-CB	-5.40	98.08	103.48
78	Sf	119	ARG	N-CA-C	5.35	118.60	111.75
12	LD	232	THR	O-C-N	-5.07	115.86	121.53

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	LI	189	ARG	Sidechain
82	LI	69	ARG	Sidechain
82	LI	88	ARG	Sidechain
35	Lc	17	ARG	Sidechain
41	Lj	43	ARG	Sidechain
41	Lj	55	ARG	Sidechain
78	Sf	116	ARG	Sidechain
78	Sf	118	ARG	Sidechain
78	Sf	119	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	LA	1886	0	1973	40	0
2	SA	1705	0	1704	35	0
3	LB	3147	0	3237	75	0
4	SB	1727	0	1796	41	0
5	A4	231	0	116	9	0
6	B4	1604	0	816	27	0
7	D4	1349	0	682	34	0
8	L5	74335	0	37632	923	0
9	L7	2538	0	1286	25	0
10	L8	3132	0	1593	48	0
11	LC	2874	0	3043	50	0
12	LD	2391	0	2426	60	0
13	LE	1648	0	1750	31	0
14	LF	1846	0	1976	30	0
15	LG	1793	0	1898	34	0
16	LH	1526	0	1605	37	0
17	LJ	1330	0	1354	38	0
18	LL	1588	0	1682	33	0
19	LM	1121	0	1181	35	0
20	LN	1701	0	1749	40	0
21	LO	1646	0	1790	29	0
22	LP	1267	0	1293	20	0
23	LQ	1513	0	1628	22	0
24	LR	1458	0	1599	38	0
25	LS	1431	0	1461	28	0
26	LT	1247	0	1302	27	0
27	LU	808	0	831	25	0
28	LV	979	0	1039	27	0
29	LW	663	0	612	10	0
30	LX	962	0	1029	25	0
31	LY	1103	0	1177	29	0
32	LZ	1115	0	1195	32	0
33	La	1159	0	1209	26	0
34	Lb	747	0	798	21	0
35	Lc	725	0	763	36	0
36	Ld	871	0	915	16	0
37	Lf	867	0	897	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lg	861	0	937	23	0
39	Lh	1011	0	1137	9	0
40	Li	818	0	899	9	0
41	Lj	715	0	751	15	0
42	Lk	553	0	602	13	0
43	Ll	435	0	472	13	0
44	Lm	411	0	438	14	0
45	Ln	239	0	289	2	0
46	Lo	839	0	902	22	0
47	Lp	707	0	756	12	0
48	Lr	992	0	1045	23	0
49	S2	33711	0	17041	450	0
50	SC	1704	0	1784	37	0
51	SD	1689	0	1734	31	0
52	SE	2050	0	2156	64	0
53	SF	1486	0	1538	13	0
54	SG	1749	0	1875	56	0
55	SH	1360	0	1390	33	0
56	SI	1582	0	1607	32	0
57	SJ	1482	0	1591	49	0
58	SK	804	0	825	21	0
59	SL	1147	0	1207	22	0
60	SN	1205	0	1292	30	0
61	SO	959	0	974	27	0
62	SP	1060	0	1104	20	0
63	SQ	1120	0	1189	24	0
64	SR	1053	0	1109	27	0
65	SS	1171	0	1226	33	0
66	ST	1098	0	1120	31	0
67	SU	790	0	847	30	0
68	SV	636	0	637	9	0
69	SW	1034	0	1080	32	0
70	SX	1082	0	1141	17	0
71	SY	988	0	1034	35	0
72	SZ	574	0	627	13	0
73	Sa	788	0	837	13	0
74	Sb	633	0	631	19	0
75	Sc	489	0	512	17	0
76	Sd	436	0	430	15	0
77	Se	400	0	440	8	0
78	Sf	489	0	486	32	0
79	Sg	2389	0	2343	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	SM	722	0	730	32	0
81	Le	1044	0	1136	21	0
82	LI	1641	0	1683	33	0
83	B4	3	0	0	0	0
83	L5	17	0	0	0	0
83	L8	1	0	0	0	0
83	LA	1	0	0	0	0
83	La	1	0	0	0	0
83	Le	1	0	0	0	0
83	S2	15	0	0	0	0
83	SN	1	0	0	0	0
84	A4	2	0	0	0	0
84	B4	4	0	0	0	0
84	D4	1	0	0	0	0
84	L5	157	0	0	0	0
84	L7	2	0	0	0	0
84	L8	3	0	0	0	0
84	LI	1	0	0	0	0
84	LN	1	0	0	0	0
84	LP	1	0	0	0	0
84	LT	1	0	0	0	0
84	Lp	1	0	0	0	0
84	S2	93	0	0	0	0
85	L5	12	0	0	0	0
85	L7	1	0	0	0	0
85	L8	1	0	0	0	0
85	LP	1	0	0	0	0
85	Ll	1	0	0	0	0
85	S2	7	0	0	0	0
86	L5	10	0	19	2	0
87	L5	6	0	12	1	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	SM	1	0	0	0	0
88	Sd	1	0	0	0	0
88	Sf	1	0	0	0	0
89	S2	36	0	37	0	0
90	L5	1	0	0	0	0
90	L8	1	0	0	0	0
90	LH	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	LI	1	0	0	0	0
90	LV	1	0	0	1	0
90	S2	1	0	0	0	0
90	SX	1	0	0	0	0
All	All	206575	0	152689	3039	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 9.

All (3039) 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)
12:LD:257:PRO:CG	12:LD:257:PRO:N	1.89	1.33
12:LD:257:PRO:CD	12:LD:257:PRO:HG3	1.69	1.17
78:Sf:119:ARG:HG2	78:Sf:132:MET:HE2	1.18	1.09
12:LD:257:PRO:CD	12:LD:257:PRO:HG2	1.69	1.08
12:LD:257:PRO:CG	12:LD:257:PRO:HD3	1.58	1.07
12:LD:257:PRO:CG	12:LD:257:PRO:HD2	1.58	1.06
49:S2:1091:C:HO2'	69:SW:2:VAL:N	1.52	1.05
80:SM:54:SER:OG	80:SM:80:ASP:HA	1.60	1.01
58:SK:53:LYS:NZ	58:SK:60:GLU:OE1	1.96	0.99
12:LD:257:PRO:CG	12:LD:257:PRO:CD	0.92	0.92
78:Sf:119:ARG:HG2	78:Sf:132:MET:CE	1.99	0.92
8:L5:364:G:O6	41:Lj:52:LYS:HE3	1.70	0.91
8:L5:496:G:N2	8:L5:658:C:O2	2.06	0.89
8:L5:184:U:O2	8:L5:254:G:N1	2.06	0.89
82:LI:30:LYS:HG2	82:LI:66:GLU:HG3	1.56	0.88
66:ST:126:GLN:HA	66:ST:126:GLN:HE21	1.39	0.86
8:L5:2520:C:O2	8:L5:2640:G:N2	2.09	0.86
16:LH:128:MET:HE2	16:LH:134:CYS:HB2	1.57	0.85
44:Lm:110:CYS:SG	44:Lm:111:ARG:N	2.47	0.84
10:L8:55:PSU:HN3	10:L8:62:A:H2	1.26	0.82
35:Lc:17:ARG:HD2	35:Lc:108:MET:HE1	1.62	0.82
8:L5:222:C:OP2	11:LC:165:LYS:NZ	2.14	0.81
8:L5:1524:A2M:H61	8:L5:1651:G:H1	1.29	0.81
37:Lf:104:MET:O	37:Lf:105:LEU:HD12	1.80	0.80
49:S2:1849:G:O2'	49:S2:1850:MA6:H8	1.80	0.80
66:ST:126:GLN:HA	66:ST:126:GLN:NE2	1.97	0.80
37:Lf:78:HIS:HB3	37:Lf:83:MET:O	1.81	0.80
62:SP:34:MET:HE1	62:SP:46:ASN:OD1	1.80	0.80
49:S2:190:G:O2'	49:S2:209:A:N6	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D4:8:U:H3	7:D4:13:C:H3'	1.48	0.79
41:Lj:56:ARG:O	41:Lj:57:THR:HG22	1.82	0.79
8:L5:308:G:H2'	40:Li:41:ARG:HH22	1.46	0.78
6:B4:32:C:OP2	63:SQ:146:ARG:NH2	2.16	0.78
49:S2:1488:C:O2'	49:S2:1490:G:OP2	1.99	0.78
7:D4:13:C:O2'	7:D4:22:G:N2	2.14	0.78
1:LA:248:GLY:HA3	49:S2:1069:U:H4'	1.66	0.78
49:S2:952:G:H21	61:SO:52:THR:HG21	1.50	0.77
49:S2:1613:G:OP1	62:SP:42:ARG:NH2	2.16	0.77
8:L5:3722:G:H2'	8:L5:3723:A2M:H8	1.67	0.76
74:Sb:33:MET:HE1	74:Sb:73:LEU:HD11	1.66	0.76
49:S2:1115:U:N3	49:S2:1118:C:N4	2.34	0.76
8:L5:1353:G:N7	23:LQ:104:ARG:NH2	2.34	0.76
49:S2:809:A:O4'	52:SE:221:ARG:NH2	2.18	0.76
49:S2:927:C:O2	74:Sb:51:GLN:NE2	2.17	0.76
8:L5:1468:C:OP1	33:La:132:ARG:NH2	2.19	0.76
66:ST:126:GLN:HE22	66:ST:129:ARG:HD2	1.50	0.76
12:LD:156:GLY:HA2	12:LD:181:PRO:HG3	1.68	0.76
20:LN:124:ASP:OD1	20:LN:125:SER:N	2.19	0.76
46:Lo:23:VAL:HG12	46:Lo:70:LEU:HD22	1.68	0.76
49:S2:1608:U:OP1	65:SS:134:GLN:NE2	2.18	0.76
5:A4:48:A:H61	6:B4:33:C:H42	1.33	0.76
8:L5:496:G:N2	8:L5:658:C:C2	2.54	0.76
46:Lo:11:PHE:O	46:Lo:81:ARG:NH2	2.20	0.75
66:ST:56:ARG:HG2	66:ST:103:VAL:HG21	1.68	0.75
46:Lo:103:VAL:O	46:Lo:105:GLN:N	2.19	0.75
2:SA:40:LYS:NZ	64:SR:101:ASP:OD1	2.19	0.75
54:SG:2:LYS:HB2	54:SG:108:VAL:HG22	1.69	0.75
9:L7:51:G:N2	17:LJ:12:MET:SD	2.60	0.75
48:Lr:58:LYS:O	48:Lr:83:ASN:ND2	2.19	0.75
49:S2:126:G:O2'	49:S2:181:A:N3	2.20	0.74
49:S2:1336:C:O2'	49:S2:1337:4AC:H6	1.87	0.74
20:LN:96:ARG:NH2	20:LN:104:GLU:OE1	2.20	0.74
54:SG:22:ARG:HA	54:SG:25:ARG:HE	1.53	0.74
9:L7:72:U:O2	9:L7:103:A:N6	2.19	0.74
35:Lc:17:ARG:HH11	35:Lc:108:MET:HE1	1.53	0.74
49:S2:1115:U:H3	49:S2:1118:C:N4	1.85	0.74
15:LG:176:LYS:HD2	40:Li:43:MET:HE1	1.68	0.74
57:SJ:140:GLN:NE2	71:SY:64:PHE:O	2.20	0.74
63:SQ:21:ALA:O	63:SQ:87:SER:OG	2.06	0.74
8:L5:1372:A:OP1	20:LN:202:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lc:105:ILE:O	35:Lc:106:ARG:HG2	1.88	0.73
49:S2:1396:A:O2'	49:S2:1398:G:N7	2.21	0.73
49:S2:1285:G:N1	80:SM:57:ASP:OD2	2.21	0.73
67:SU:78:ASP:OD2	76:Sd:54:LYS:NZ	2.18	0.73
6:B4:74:C:O2'	46:Lo:54:PRO:O	2.06	0.73
15:LG:162:ASP:HB2	15:LG:163:PRO:HD3	1.70	0.73
8:L5:435:A:O2'	81:Le:26:ASP:OD2	2.06	0.73
40:Li:2:ALA:N	40:Li:5:TYR:HH	1.86	0.73
15:LG:58:PRO:HD2	15:LG:61:ILE:HD12	1.70	0.73
7:D4:27:G:H22	7:D4:43:C:H5	1.35	0.73
14:LF:182:TYR:HB3	14:LF:200:ARG:HG3	1.69	0.73
19:LM:106:ASP:OD1	19:LM:109:ARG:NH1	2.21	0.73
49:S2:1610:G:OP2	65:SS:132:ARG:NH1	2.21	0.73
35:Lc:17:ARG:HH12	35:Lc:107:SER:CB	2.02	0.73
78:Sf:127:GLY:O	80:SM:44:LYS:NZ	2.21	0.73
31:LY:30:MET:HB3	31:LY:101:PRO:HG2	1.71	0.72
76:Sd:53:ILE:HD11	76:Sd:55:LEU:HD12	1.70	0.72
8:L5:132:G:H2'	8:L5:133:C:H4'	1.70	0.72
8:L5:2400:G:H21	38:Lg:6:THR:HG22	1.54	0.72
57:SJ:63:LEU:HD11	57:SJ:70:ARG:HB2	1.70	0.72
65:SS:12:ILE:HD11	65:SS:19:ASN:HB3	1.72	0.72
62:SP:21:ASP:OD2	62:SP:24:GLN:NE2	2.21	0.72
64:SR:120:THR:HG22	64:SR:121:GLN:H	1.55	0.72
8:L5:2583:C:OP2	38:Lg:76:ARG:NH2	2.22	0.72
8:L5:4122:G:N1	38:Lg:98:GLU:OE1	2.23	0.72
17:LJ:17:ILE:HD12	17:LJ:80:GLU:OE2	1.88	0.72
24:LR:13:SER:OG	24:LR:38:ARG:NH2	2.23	0.71
49:S2:1451:G:N7	64:SR:44:LYS:NZ	2.38	0.71
66:ST:126:GLN:HE22	66:ST:129:ARG:HH11	1.39	0.71
3:LB:246:ARG:NH1	8:L5:4525:C:OP1	2.23	0.71
49:S2:94:G:HO2'	49:S2:508:A:HO2'	1.30	0.71
49:S2:818:A:OP1	57:SJ:80:ARG:NH2	2.24	0.71
60:SN:3:ARG:HB3	60:SN:6:ALA:HB3	1.72	0.71
8:L5:3642:A:HO2'	41:Lj:2:THR:N	1.89	0.71
31:LY:32:SER:OG	31:LY:101:PRO:O	2.08	0.71
13:LE:208:ILE:HG22	13:LE:210:LYS:H	1.55	0.71
42:Lk:50:LYS:O	42:Lk:54:GLU:HG2	1.90	0.71
63:SQ:9:SER:OG	63:SQ:24:HIS:NE2	2.23	0.71
49:S2:687:C:O2'	55:SH:116:ARG:NH2	2.22	0.71
67:SU:78:ASP:OD1	76:Sd:44:ARG:NH1	2.24	0.71
49:S2:556:U:H4'	49:S2:557:U:H5'	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L8:14:OMU:H5''	22:LP:123:PRO:HD3	1.74	0.70
20:LN:193:ARG:O	20:LN:197:THR:HG23	1.91	0.70
49:S2:1729:U:H3	49:S2:1805:G:H1	1.38	0.70
8:L5:438:G:N2	37:Lf:23:GLU:OE1	2.19	0.70
19:LM:36:ALA:HB3	19:LM:55:MET:HE1	1.73	0.70
49:S2:64:A:H2	49:S2:83:A:H62	1.39	0.70
79:Sg:166:VAL:HG12	79:Sg:176:VAL:HG22	1.74	0.70
6:B4:68:U:H2'	6:B4:69:G:H8	1.57	0.70
11:LC:303:ARG:O	23:LQ:38:ARG:NH2	2.19	0.70
13:LE:250:GLN:NE2	13:LE:254:ASP:OD2	2.24	0.70
30:LX:121:VAL:HG13	30:LX:138:VAL:HG13	1.73	0.70
49:S2:24:C:HO2'	49:S2:25:A:H8	1.37	0.70
20:LN:157:LYS:O	20:LN:162:ARG:NH1	2.24	0.70
49:S2:1536:G:H2'	49:S2:1537:A:H8	1.57	0.70
7:D4:27:G:H1	7:D4:43:C:H41	1.38	0.70
3:LB:57:VAL:HG22	3:LB:73:VAL:HG12	1.74	0.70
4:SB:172:MET:O	4:SB:176:VAL:HG12	1.92	0.70
32:LZ:10:VAL:O	32:LZ:83:THR:OG1	2.08	0.70
49:S2:996:A:OP1	60:SN:114:ARG:NH2	2.25	0.70
34:Lb:23:LYS:HG2	34:Lb:24:PRO:HD2	1.73	0.70
65:SS:89:ASP:OD2	65:SS:106:LYS:NZ	2.25	0.70
3:LB:95:THR:HG22	8:L5:4910:G:H4'	1.73	0.69
8:L5:1412:G:H2'	8:L5:1413:C:H6	1.57	0.69
8:L5:4745:G:H1	8:L5:4955:A:H61	1.39	0.69
8:L5:4472:G:O2'	44:Lm:100:TYR:O	2.11	0.69
73:Sa:23:CYS:SG	73:Sa:26:CYS:N	2.65	0.69
8:L5:3641:U:OP2	8:L5:3646:A:N6	2.25	0.69
15:LG:157:ILE:HG22	15:LG:201:THR:OG1	1.93	0.69
49:S2:1745:A:H1'	54:SG:66:GLY:HA2	1.73	0.69
62:SP:34:MET:HE2	62:SP:42:ARG:HG3	1.72	0.69
8:L5:4635:A:H8	8:L5:5048:A:H61	1.40	0.69
49:S2:126:G:OP2	54:SG:198:ARG:NH1	2.25	0.69
3:LB:220:ILE:HG22	3:LB:278:THR:HA	1.73	0.69
8:L5:1178:G:HO2'	12:LD:286:SER:HG	1.36	0.69
81:Le:43:ASN:HB3	81:Le:46:ARG:HG2	1.73	0.69
3:LB:92:TYR:HB2	3:LB:159:VAL:HG13	1.75	0.69
8:L5:2101:C:H2'	8:L5:2102:G:C8	2.27	0.69
51:SD:75:LYS:NZ	58:SK:20:VAL:O	2.24	0.69
61:SO:118:ALA:O	61:SO:122:SER:OG	2.08	0.69
3:LB:258:HIS:NE2	8:L5:3878:C:O2	2.25	0.69
8:L5:2318:G:N2	8:L5:2321:G:OP2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L8:94:G:OP2	41:Lj:72:ARG:NH1	2.26	0.69
49:S2:830:A:OP2	49:S2:846:G:N2	2.25	0.69
60:SN:55:ARG:NH2	74:Sb:51:GLN:OE1	2.26	0.69
22:LP:29:THR:HG21	22:LP:146:ILE:HD11	1.74	0.69
49:S2:1033:G:N1	49:S2:1080:A:O2'	2.25	0.69
78:Sf:128:ALA:HB3	80:SM:44:LYS:NZ	2.07	0.69
4:SB:179:ASN:ND2	4:SB:183:GLU:OE1	2.24	0.69
8:L5:137:G:H2'	8:L5:138:G:H8	1.57	0.69
8:L5:4218:U:OP2	26:LT:9:ARG:NH2	2.26	0.69
60:SN:4:MET:SD	60:SN:124:ARG:NH2	2.65	0.69
12:LD:51:MET:HE3	12:LD:105:LEU:HD23	1.73	0.68
26:LT:43:LYS:O	26:LT:58:HIS:ND1	2.26	0.68
49:S2:921:G:H5'	74:Sb:21:LYS:HE2	1.75	0.68
49:S2:1612:G:OP1	62:SP:18:ARG:NH2	2.27	0.68
49:S2:1623:A:H5''	65:SS:133:GLY:HA3	1.75	0.68
66:ST:126:GLN:NE2	66:ST:129:ARG:HH11	1.91	0.68
8:L5:1187:G:OP2	8:L5:1187:G:N2	2.20	0.68
65:SS:86:ARG:HE	65:SS:106:LYS:HD2	1.58	0.68
82:LI:72:ALA:O	82:LI:76:MET:HG2	1.93	0.68
8:L5:3736:A:O2'	8:L5:3737:A:O5'	2.11	0.68
14:LF:222:LYS:NZ	14:LF:224:THR:OG1	2.27	0.68
8:L5:2262:G:OP2	48:Lr:98:ARG:NH1	2.26	0.68
8:L5:2469:C:H5	8:L5:2471:G:H1	1.42	0.68
79:Sg:256:ILE:HD11	79:Sg:270:LEU:HD12	1.75	0.68
3:LB:56:ILE:HG21	3:LB:365:LEU:HD22	1.76	0.68
8:L5:1405:C:N4	8:L5:1408:G:N3	2.41	0.68
8:L5:4594:U:H2'	8:L5:4595:G:H8	1.58	0.68
7:D4:51:U:H3	7:D4:63:G:H1	0.78	0.68
8:L5:2502:G:O6	30:LX:50:LYS:NZ	2.24	0.68
35:Lc:99:PRO:HB2	35:Lc:102:SER:HB3	1.76	0.68
49:S2:30:C:O2'	49:S2:596:U:OP1	2.10	0.68
8:L5:2338:C:HO2'	48:Lr:13:CYS:HG	1.32	0.68
8:L5:3589:G:N2	8:L5:3590:G:O6	2.27	0.68
16:LH:50:LYS:O	16:LH:51:LYS:HG2	1.94	0.68
44:Lm:83:ARG:O	44:Lm:87:GLN:HG3	1.91	0.68
49:S2:1649:U:H3	49:S2:1675:A:H2	1.42	0.68
79:Sg:220:ASP:HB2	79:Sg:227:LEU:HD11	1.74	0.68
8:L5:654:C:H4'	11:LC:269:LYS:HG3	1.75	0.68
8:L5:2658:G:N2	8:L5:2676:A:OP2	2.27	0.68
20:LN:104:GLU:HA	20:LN:160:GLU:HG3	1.76	0.68
1:LA:3:ARG:HH12	8:L5:1634:A:H62	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SH:65:PRO:HG2	55:SH:68:GLN:HG3	1.76	0.67
3:LB:246:ARG:NH2	8:L5:4558:U:OP2	2.28	0.67
2:SA:173:LEU:O	2:SA:177:MET:HG2	1.95	0.67
3:LB:19:ARG:NH2	8:L5:4623:OMG:OP1	2.27	0.67
8:L5:3765:G:O2'	8:L5:3767:C:N4	2.27	0.67
8:L5:4305:G:N7	26:LT:87:LYS:NZ	2.41	0.67
49:S2:686:U:O2	55:SH:118:ARG:NH2	2.27	0.67
28:LV:50:ASN:ND2	90:LV:201:HOH:O	2.27	0.67
49:S2:1272:C:OP2	78:Sf:94:LYS:NZ	2.27	0.67
49:S2:1546:G:N2	49:S2:1670:C:O2	2.28	0.67
1:LA:207:VAL:HG21	8:L5:1633:G:C6	2.30	0.67
8:L5:4340:U:O2	86:L5:5286:SPD:N10	2.27	0.67
79:Sg:249:CYS:SG	79:Sg:291:TRP:NE1	2.66	0.67
8:L5:308:G:OP2	8:L5:308:G:N2	2.26	0.67
8:L5:1480:C:O2'	8:L5:1482:G:OP2	2.13	0.67
13:LE:117:PRO:O	48:Lr:112:ARG:NH1	2.27	0.67
49:S2:65:C:N4	49:S2:169:U:O2'	2.28	0.67
49:S2:1627:C:H5''	66:ST:41:LYS:HD2	1.76	0.67
13:LE:47:ASN:HB2	13:LE:62:MET:HE2	1.77	0.66
42:Lk:49:ASP:O	42:Lk:50:LYS:HG3	1.95	0.66
8:L5:4076:G:OP1	15:LG:73:ARG:NH1	2.28	0.66
8:L5:4096:C:N4	8:L5:4113:U:O2'	2.28	0.66
28:LV:13:LYS:HB2	28:LV:128:LEU:HD11	1.77	0.66
49:S2:1589:A:N3	49:S2:1653:U:O2'	2.29	0.66
73:Sa:32:LYS:O	73:Sa:37:LYS:NZ	2.28	0.66
8:L5:508:G:O2'	8:L5:510:U:OP2	2.13	0.66
8:L5:4140:C:N3	8:L5:4145:C:O2'	2.24	0.66
35:Lc:17:ARG:NH1	35:Lc:107:SER:CB	2.59	0.66
49:S2:1536:G:H2'	49:S2:1537:A:C8	2.30	0.66
3:LB:268:ARG:NH1	8:L5:3896:C:O2'	2.28	0.66
16:LH:124:ARG:NH1	16:LH:164:ALA:O	2.27	0.66
61:SO:31:CYS:HB2	61:SO:93:LEU:HD22	1.77	0.66
78:Sf:136:PHE:CE2	78:Sf:137:ASP:OD1	2.49	0.66
8:L5:4648:A:OP1	24:LR:62:ARG:NH2	2.28	0.66
19:LM:25:VAL:HG12	19:LM:45:VAL:HG21	1.78	0.66
50:SC:201:GLY:N	50:SC:221:ASP:OD2	2.28	0.66
3:LB:58:ARG:NH2	3:LB:361:GLU:OE2	2.29	0.66
7:D4:25:C:H2'	7:D4:26:A:H8	1.60	0.66
8:L5:664:G:N2	8:L5:666:G:O6	2.24	0.66
8:L5:1443:A:H2	8:L5:2103:G:H1	1.40	0.66
8:L5:1837:A:OP2	26:LT:130:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:3823:G:OP2	8:L5:3823:G:N2	2.23	0.66
52:SE:153:LEU:O	52:SE:174:LYS:NZ	2.28	0.66
2:SA:128:ARG:NH2	2:SA:151:ASP:O	2.29	0.66
8:L5:1173:G:N1	8:L5:1174:A:N3	2.43	0.66
8:L5:4507:A:O2'	28:LV:41:SER:OG	2.14	0.66
24:LR:24:LEU:HD23	24:LR:32:ILE:HG21	1.78	0.66
28:LV:90:ARG:HB2	28:LV:94:VAL:HG23	1.78	0.66
49:S2:857:U:H2'	49:S2:858:A:C8	2.31	0.66
52:SE:63:LYS:O	52:SE:67:GLN:HG3	1.95	0.66
35:Lc:17:ARG:NE	35:Lc:17:ARG:HA	2.10	0.66
35:Lc:105:ILE:O	35:Lc:106:ARG:CG	2.44	0.66
49:S2:65:C:H4'	54:SG:172:LYS:HD3	1.78	0.66
8:L5:1097:C:H2'	8:L5:1098:G:H8	1.61	0.65
16:LH:44:GLU:HG2	16:LH:58:ASP:HB2	1.76	0.65
17:LJ:96:LYS:O	17:LJ:159:LYS:NZ	2.29	0.65
4:SB:229:MET:HA	4:SB:229:MET:HE3	1.79	0.65
8:L5:1412:G:H2'	8:L5:1413:C:C6	2.30	0.65
12:LD:278:ASP:OD2	12:LD:282:GLN:NE2	2.30	0.65
14:LF:32:ARG:HG2	14:LF:36:LYS:HE2	1.78	0.65
49:S2:874:G:H2'	49:S2:875:A:H8	1.61	0.65
78:Sf:119:ARG:CG	78:Sf:132:MET:HE2	2.11	0.65
19:LM:29:ASP:OD1	19:LM:30:VAL:N	2.29	0.65
82:LI:47:PRO:HD2	82:LI:141:LYS:HA	1.77	0.65
8:L5:419:A:N3	8:L5:1332:C:O2'	2.28	0.65
19:LM:120:ASN:O	19:LM:124:LYS:HG3	1.96	0.65
24:LR:15:LEU:HD22	24:LR:52:ARG:HB2	1.79	0.65
57:SJ:30:LYS:O	57:SJ:34:GLU:HG2	1.96	0.65
8:L5:62:A:N3	8:L5:77:U:O2'	2.29	0.65
8:L5:2103:G:H3'	8:L5:2104:G:C8	2.32	0.65
49:S2:1829:G:H1'	49:S2:1850:MA6:H2	1.79	0.65
62:SP:64:LYS:NZ	62:SP:90:VAL:O	2.28	0.65
80:SM:44:LYS:HA	80:SM:44:LYS:HE3	1.78	0.65
54:SG:85:ARG:O	54:SG:87:ARG:NH1	2.28	0.65
66:ST:40:ALA:HB3	66:ST:43:LYS:HG2	1.76	0.65
8:L5:502:C:H5'	8:L5:503:C:H3'	1.79	0.65
8:L5:2562:G:N2	8:L5:2565:A:OP2	2.17	0.65
20:LN:5:LYS:HG2	40:Li:40:VAL:HG11	1.78	0.65
28:LV:10:SER:OG	28:LV:11:GLY:N	2.29	0.65
49:S2:165:G:OP2	49:S2:165:G:N2	2.26	0.65
78:Sf:107:LYS:HE3	78:Sf:109:ASP:OD1	1.96	0.65
8:L5:703:G:H2'	8:L5:704:C:H4'	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:2693:G:OP1	42:Lk:35:LYS:NZ	2.26	0.65
8:L5:4992:G:H2'	8:L5:4993:G:C8	2.31	0.65
8:L5:1268:G:N7	34:Lb:111:ARG:NH2	2.43	0.65
8:L5:1669:A:H4'	8:L5:1685:G:H22	1.61	0.65
8:L5:2338:C:O2'	48:Lr:13:CYS:SG	2.45	0.65
17:LJ:18:ARG:H	17:LJ:134:LEU:HA	1.62	0.65
44:Lm:96:CYS:HB2	44:Lm:99:CYS:H	1.61	0.65
53:SF:102:LEU:HD11	72:SZ:100:VAL:HG21	1.79	0.65
8:L5:1516:G:O2'	18:LL:18:TRP:NE1	2.29	0.65
8:L5:3689:G:O2'	8:L5:3818:U:OP2	2.15	0.65
28:LV:87:SER:OG	29:LW:19:ARG:NH1	2.28	0.65
56:SI:78:ILE:HA	56:SI:104:ILE:HD12	1.79	0.65
28:LV:106:VAL:HA	28:LV:112:MET:HA	1.78	0.64
48:Lr:20:ARG:NH2	81:Le:84:GLU:OE2	2.28	0.64
55:SH:145:ARG:NH1	69:SW:49:GLU:OE1	2.29	0.64
8:L5:4769:G:H5'	21:LO:176:ARG:HD3	1.79	0.64
8:L5:4980:C:N3	22:LP:69:ARG:NH2	2.45	0.64
10:L8:105:C:H4'	10:L8:106:G:H5''	1.79	0.64
49:S2:527:C:O2'	57:SJ:121:LYS:NZ	2.30	0.64
52:SE:18:TRP:HH2	52:SE:31:PRO:HD3	1.62	0.64
79:Sg:87:LEU:HB2	79:Sg:101:PHE:HB2	1.80	0.64
10:L8:52:A:H62	43:Ll:27:ILE:HD13	1.63	0.64
8:L5:2102:G:H1'	8:L5:2103:G:H8	1.62	0.64
49:S2:924:G:H5'	60:SN:4:MET:HE3	1.78	0.64
49:S2:1091:C:O2'	69:SW:2:VAL:N	2.28	0.64
3:LB:300:LYS:HB2	3:LB:311:ASP:HA	1.79	0.64
4:SB:35:ALA:O	4:SB:42:ARG:NH2	2.30	0.64
12:LD:197:LYS:HG3	12:LD:202:GLN:HB2	1.80	0.64
57:SJ:31:LEU:HD21	57:SJ:103:GLU:HG3	1.80	0.64
8:L5:1351:G:OP1	11:LC:33:ARG:NH1	2.31	0.64
10:L8:22:U:OP1	31:LY:11:ARG:NH1	2.30	0.64
49:S2:1528:G:O2'	49:S2:1666:C:OP1	2.14	0.64
57:SJ:74:GLY:O	57:SJ:78:LEU:HD13	1.98	0.64
2:SA:137:ALA:HB1	2:SA:142:LEU:HB3	1.80	0.64
8:L5:1411:C:H41	34:Lb:48:LYS:HE2	1.62	0.64
8:L5:4298:A:O3'	34:Lb:33:LYS:NZ	2.26	0.64
8:L5:4910:G:N2	21:LO:106:ASP:O	2.31	0.64
49:S2:640:A:H2'	49:S2:641:A:C8	2.31	0.64
49:S2:993:G:OP1	49:S2:1131:G:N2	2.25	0.64
78:Sf:103:LEU:O	80:SM:36:ARG:NH2	2.30	0.64
30:LX:114:LYS:NZ	30:LX:120:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:641:A:O2'	49:S2:645:C:OP1	2.16	0.64
61:SO:77:ALA:O	61:SO:81:VAL:HG23	1.98	0.64
68:SV:35:ASN:OD1	68:SV:52:THR:OG1	2.14	0.64
3:LB:224:LYS:NZ	8:L5:4626:A:OP2	2.26	0.64
8:L5:655:C:OP1	11:LC:268:ARG:NH2	2.31	0.64
49:S2:1209:A:OP1	49:S2:1835:A:N6	2.31	0.64
63:SQ:42:ILE:HG22	63:SQ:44:PRO:HD2	1.80	0.64
8:L5:4274:A:H2'	8:L5:4275:G:C8	2.34	0.63
59:SL:42:LEU:HD13	59:SL:72:ILE:HD11	1.79	0.63
26:LT:18:PRO:HG2	26:LT:21:LYS:HB2	1.80	0.63
64:SR:37:GLU:OE2	79:Sg:106:LYS:NZ	2.30	0.63
49:S2:289:G:OP1	52:SE:155:LYS:NZ	2.27	0.63
78:Sf:117:LEU:C	78:Sf:118:ARG:HD2	2.24	0.63
13:LE:161:ARG:NH1	13:LE:273:SER:OG	2.31	0.63
16:LH:93:ARG:HD2	16:LH:143:GLU:HG3	1.80	0.63
43:Ll:24:PRO:HD2	43:Ll:27:ILE:HD12	1.79	0.63
49:S2:468:A:OP1	54:SG:96:SER:OG	2.17	0.63
49:S2:809:A:C4'	52:SE:221:ARG:NH2	2.62	0.63
54:SG:21:GLU:N	54:SG:21:GLU:OE2	2.32	0.63
64:SR:98:VAL:HG13	64:SR:102:THR:HB	1.81	0.63
27:LU:20:LYS:HB2	27:LU:73:THR:HG23	1.80	0.63
49:S2:1115:U:H1'	49:S2:1116:C:H2'	1.81	0.63
8:L5:4206:C:OP1	26:LT:5:LYS:NZ	2.31	0.63
16:LH:113:GLU:OE1	16:LH:115:ARG:NH2	2.31	0.63
19:LM:104:MET:HE3	19:LM:109:ARG:HG2	1.81	0.63
8:L5:5066:U:OP1	22:LP:43:LYS:NZ	2.29	0.63
34:Lb:47:LYS:HA	34:Lb:50:ASN:HD22	1.63	0.63
49:S2:1228:A:H2'	49:S2:1229:G:C8	2.33	0.63
80:SM:84:LYS:HA	80:SM:87:GLU:HG3	1.80	0.63
2:SA:52:LYS:HB2	64:SR:109:LEU:HD11	1.81	0.63
8:L5:3599:A:H2'	8:L5:3600:G:C8	2.34	0.63
24:LR:172:ARG:NH1	49:S2:909:G:OP1	2.32	0.63
57:SJ:84:ILE:HG13	57:SJ:86:VAL:HG13	1.79	0.63
8:L5:86:U:O2'	33:La:65:ARG:NH1	2.32	0.62
11:LC:149:GLU:HG2	11:LC:151:PRO:HD2	1.79	0.62
31:LY:43:ASN:ND2	31:LY:127:GLN:OE1	2.32	0.62
8:L5:109:G:OP2	18:LL:74:ARG:NH2	2.32	0.62
8:L5:462:G:H2'	8:L5:463:A:C8	2.34	0.62
79:Sg:244:ASN:OD1	79:Sg:245:ARG:N	2.32	0.62
7:D4:5:G:H2'	7:D4:6:G:C8	2.34	0.62
8:L5:257:C:H2'	8:L5:258:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:2059:C:O2	25:LS:118:ARG:NH2	2.31	0.62
8:L5:4635:A:H2	8:L5:4663:G:H21	1.46	0.62
16:LH:137:SER:OG	16:LH:143:GLU:HB3	1.99	0.62
36:Ld:24:GLU:HG2	36:Ld:87:ARG:HG3	1.81	0.62
49:S2:832:G:O6	71:SY:11:LYS:NZ	2.33	0.62
56:SI:110:ARG:NH2	56:SI:122:GLY:O	2.32	0.62
67:SU:34:LYS:HZ1	67:SU:107:GLU:HG3	1.65	0.62
42:Lk:12:LEU:HB3	42:Lk:16:ARG:HH21	1.62	0.62
71:SY:62:THR:HG23	71:SY:69:THR:HG22	1.81	0.62
2:SA:74:VAL:HG12	2:SA:121:LEU:HB3	1.80	0.62
4:SB:107:ARG:NH2	61:SO:133:THR:O	2.29	0.62
8:L5:4327:C:OP1	26:LT:70:HIS:NE2	2.33	0.62
35:Lc:36:LYS:O	35:Lc:40:GLN:HG2	1.98	0.62
38:Lg:41:ALA:O	38:Lg:52:ARG:NH1	2.33	0.62
49:S2:921:G:OP2	74:Sb:26:GLN:NE2	2.31	0.62
78:Sf:114:ILE:HG12	80:SM:71:GLU:OE2	2.00	0.62
8:L5:2702:C:OP1	27:LU:101:ARG:NH2	2.33	0.62
13:LE:244:GLU:O	13:LE:248:ILE:HG12	1.99	0.62
46:Lo:78:ARG:O	46:Lo:80:LYS:NZ	2.33	0.62
57:SJ:69:ARG:NH1	57:SJ:73:GLU:OE2	2.28	0.62
8:L5:3710:G:N2	8:L5:3712:A:H62	1.97	0.62
8:L5:3777:G:O2'	8:L5:3815:G:O6	2.15	0.62
24:LR:105:LEU:HD23	24:LR:138:LEU:HD23	1.82	0.62
49:S2:1061:U:O4	49:S2:1849:G:N2	2.32	0.62
7:D4:21:A:N6	7:D4:46:G:O2'	2.33	0.62
8:L5:4940:C:OP1	13:LE:156:ARG:NH2	2.32	0.62
54:SG:57:ASP:HA	54:SG:106:LEU:HA	1.81	0.62
81:Le:85:LEU:HD21	81:Le:115:ALA:HB2	1.82	0.62
82:LI:86:HIS:HB3	82:LI:139:ARG:HG2	1.80	0.62
8:L5:724:C:OP1	11:LC:350:ARG:HD2	2.00	0.62
8:L5:4467:A:O2'	8:L5:4510:A:N3	2.30	0.61
11:LC:146:GLU:OE1	11:LC:146:GLU:N	2.33	0.61
55:SH:51:ILE:HD12	55:SH:176:VAL:HG22	1.80	0.61
6:B4:11:C:H2'	6:B4:12:G:H8	1.65	0.61
8:L5:655:C:H2'	8:L5:656:C:O4'	2.00	0.61
8:L5:257:C:H2'	8:L5:258:G:H8	1.65	0.61
8:L5:3932:U:HO2'	8:L5:3933:G:H8	1.48	0.61
8:L5:4274:A:H2'	8:L5:4275:G:H8	1.64	0.61
8:L5:5006:U:H4'	8:L5:5007:A:H5'	1.82	0.61
21:LO:194:GLU:O	21:LO:198:THR:HG23	2.00	0.61
49:S2:1273:C:O2'	49:S2:1506:A:N6	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:151:ARG:NH2	49:S2:1123:C:OP1	2.33	0.61
8:L5:1564:A:OP1	60:SN:140:LYS:NZ	2.31	0.61
8:L5:1661:C:O2'	81:Le:36:ARG:NH1	2.33	0.61
18:LL:180:ALA:O	18:LL:184:MET:HG3	2.00	0.61
49:S2:1289:U:OP2	78:Sf:97:LYS:NZ	2.32	0.61
49:S2:1585:U:O2'	49:S2:1586:U:O5'	2.19	0.61
8:L5:2100:A:H2'	8:L5:2101:C:C2	2.35	0.61
12:LD:184:ASP:OD2	12:LD:187:SER:OG	2.18	0.61
1:LA:54:ARG:NH2	8:L5:3680:U:OP1	2.34	0.61
7:D4:37:A:OP1	77:Se:74:LYS:N	2.33	0.61
49:S2:1337:4AC:H2'	49:S2:1338:G:C8	2.36	0.61
51:SD:163:PRO:O	51:SD:167:TYR:HB2	2.00	0.61
1:LA:128:ARG:NH1	8:L5:3681:G:OP2	2.33	0.61
7:D4:64:A:H4'	82:LI:27:PRO:HA	1.81	0.61
8:L5:1326:A2M:OP2	8:L5:4445:U:O2'	2.18	0.61
8:L5:1778:C:H5''	12:LD:5:LYS:HG2	1.82	0.61
8:L5:1654:G:N2	8:L5:1678:C:OP1	2.33	0.61
49:S2:1230:C:OP1	65:SS:130:ARG:NH2	2.33	0.61
49:S2:1388:A:H61	51:SD:161:GLY:HA3	1.65	0.61
49:S2:1708:C:H2'	49:S2:1709:G:H5''	1.83	0.61
79:Sg:197:THR:HG21	79:Sg:238:ALA:HA	1.82	0.61
8:L5:1750:G:N2	82:LI:193:ASP:OD2	2.34	0.61
18:LL:11:LYS:NZ	33:La:52:TYR:OH	2.34	0.61
35:Lc:57:LYS:O	35:Lc:61:GLU:HG2	1.99	0.61
50:SC:198:ALA:HB1	50:SC:202:THR:HG21	1.82	0.61
8:L5:1095:A:H2	8:L5:1200:G:H1	1.49	0.61
8:L5:1095:A:N1	8:L5:1200:G:O6	2.34	0.61
43:Ll:2:SER:O	43:Ll:5:LYS:NZ	2.34	0.61
8:L5:677:G:H2'	8:L5:678:C:C6	2.36	0.60
8:L5:4363:A:H5''	46:Lo:36:GLN:HG2	1.83	0.60
11:LC:283:LYS:NZ	23:LQ:22:ASP:OD2	2.23	0.60
18:LL:200:LYS:O	18:LL:202:ALA:N	2.33	0.60
35:Lc:17:ARG:HH12	35:Lc:107:SER:HB2	1.66	0.60
59:SL:101:ARG:HB2	70:SX:10:ALA:HB2	1.83	0.60
8:L5:4124:G:N2	15:LG:43:GLN:O	2.34	0.60
51:SD:95:GLY:HA2	51:SD:101:GLN:HE21	1.64	0.60
67:SU:22:ILE:HG23	67:SU:114:VAL:HG12	1.82	0.60
73:Sa:22:ARG:NH1	73:Sa:29:CYS:SG	2.74	0.60
80:SM:42:LEU:HD23	80:SM:68:LEU:HB3	1.83	0.60
8:L5:279:A:OP1	20:LN:50:ARG:NH1	2.34	0.60
62:SP:100:LYS:HG2	62:SP:101:THR:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SU:34:LYS:NZ	67:SU:107:GLU:HG3	2.16	0.60
7:D4:4:C:H2'	7:D4:5:G:C8	2.35	0.60
8:L5:1503:A:H4'	8:L5:1504:G:H5'	1.84	0.60
8:L5:2601:A:N6	8:L5:2744:A:OP2	2.31	0.60
49:S2:1228:A:H2'	49:S2:1229:G:H8	1.66	0.60
8:L5:4238:G:H2'	8:L5:4239:A:H8	1.67	0.60
31:LY:8:THR:HG21	31:LY:13:LYS:HD3	1.83	0.60
48:Lr:19:LYS:HG2	48:Lr:24:THR:HG22	1.82	0.60
49:S2:1563:G:OP1	66:ST:121:ARG:NH1	2.35	0.60
4:SB:137:LEU:HG	4:SB:215:VAL:HG22	1.84	0.60
8:L5:85:G:O2'	8:L5:97:G:O6	2.17	0.60
8:L5:665:C:O2'	8:L5:666:G:N7	2.35	0.60
57:SJ:94:LEU:HA	57:SJ:97:ILE:HG12	1.82	0.60
18:LL:56:ARG:NH1	18:LL:74:ARG:O	2.34	0.60
49:S2:1133:A:H4'	73:Sa:13:LYS:HG2	1.83	0.60
72:SZ:65:TYR:CZ	72:SZ:76:ARG:HD3	2.36	0.60
36:Ld:20:VAL:HG22	36:Ld:91:LYS:HA	1.83	0.60
64:SR:37:GLU:OE1	79:Sg:150:TRP:NE1	2.34	0.60
8:L5:693:C:H2'	8:L5:694:C:H6	1.67	0.60
8:L5:1398:A:OP1	33:La:136:LYS:NZ	2.32	0.60
65:SS:14:ARG:HE	65:SS:17:ASN:HA	1.65	0.60
8:L5:1097:C:H2'	8:L5:1098:G:C8	2.36	0.60
17:LJ:36:ALA:O	17:LJ:39:VAL:HG12	2.01	0.59
35:Lc:28:VAL:HG22	35:Lc:95:ALA:HB3	1.83	0.59
53:SF:30:ILE:HG21	53:SF:36:GLN:HA	1.83	0.59
8:L5:182:G:N1	8:L5:255:C:O2	2.35	0.59
8:L5:2611:A:H5'	8:L5:2688:G:H4'	1.84	0.59
8:L5:4405:G:OP2	82:LI:7:ARG:NH2	2.35	0.59
11:LC:146:GLU:OE2	11:LC:178:ASN:ND2	2.33	0.59
22:LP:22:LEU:HD12	22:LP:146:ILE:HD12	1.83	0.59
49:S2:928:G:H2'	49:S2:929:G:C8	2.37	0.59
49:S2:1354:G:N2	49:S2:1357:A:OP2	2.29	0.59
54:SG:159:ARG:HH21	54:SG:171:THR:HG23	1.66	0.59
66:ST:110:LEU:HD23	66:ST:112:MET:HE2	1.83	0.59
67:SU:34:LYS:HZ1	67:SU:107:GLU:CG	2.15	0.59
67:SU:98:VAL:O	67:SU:102:THR:HG23	2.03	0.59
73:Sa:74:CYS:N	73:Sa:77:CYS:SG	2.75	0.59
8:L5:693:C:H2'	8:L5:694:C:C6	2.36	0.59
8:L5:3615:G:H1'	29:LW:44:ARG:HD3	1.83	0.59
42:Lk:24:LYS:HG2	42:Lk:67:LYS:NZ	2.16	0.59
63:SQ:116:ASP:HB3	63:SQ:119:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sg:145:GLU:HB2	79:Sg:184:LEU:HD11	1.83	0.59
5:A4:46:A:H2'	5:A4:47:A:C8	2.37	0.59
7:D4:51:U:O4	7:D4:63:G:O6	2.21	0.59
8:L5:2758:G:O2'	8:L5:2765:A:N3	2.33	0.59
8:L5:4478:G:O2'	8:L5:4602:A:N1	2.35	0.59
12:LD:232:THR:HG22	12:LD:234:ASP:H	1.67	0.59
15:LG:207:VAL:HG21	15:LG:215:LEU:HD22	1.83	0.59
76:Sd:21:CYS:HB2	76:Sd:39:CYS:SG	2.42	0.59
8:L5:3717:A:H2'	8:L5:3718:A2M:H8	1.84	0.59
11:LC:293:LEU:O	11:LC:299:GLN:NE2	2.31	0.59
55:SH:10:LYS:NZ	55:SH:12:ASN:OD1	2.29	0.59
79:Sg:110:SER:OG	79:Sg:152:SER:O	2.20	0.59
3:LB:228:TYR:O	8:L5:2835:A:O2'	2.21	0.59
8:L5:490:C:H2'	8:L5:491:G:H8	1.67	0.59
8:L5:4670:C:O2'	8:L5:4672:A:OP2	2.20	0.59
7:D4:53:G:H2'	7:D4:54:U:C6	2.38	0.59
10:L8:75:OMG:OP2	31:LY:74:TYR:OH	2.18	0.59
54:SG:59:GLN:OE1	54:SG:72:ARG:NH2	2.36	0.59
1:LA:244:GLY:HA3	8:L5:3746:A:H5''	1.85	0.59
8:L5:715:G:OP1	11:LC:321:ASN:ND2	2.35	0.59
8:L5:4162:C:O2	15:LG:73:ARG:NH2	2.34	0.59
16:LH:85:THR:HG23	16:LH:86:LEU:HG	1.85	0.59
35:Lc:17:ARG:HH11	35:Lc:108:MET:CE	2.16	0.59
46:Lo:100:LYS:O	46:Lo:102:GLN:NE2	2.35	0.59
49:S2:1387:G:N1	51:SD:206:ASP:OD2	2.30	0.59
52:SE:100:ARG:NH2	52:SE:121:TYR:O	2.34	0.59
79:Sg:184:LEU:H	79:Sg:184:LEU:HD12	1.67	0.59
6:B4:11:C:H2'	6:B4:12:G:C8	2.37	0.59
8:L5:4093:G:H2'	8:L5:4094:G:C8	2.37	0.59
12:LD:107:ARG:NH1	12:LD:169:GLY:O	2.34	0.59
52:SE:151:ASP:HB3	52:SE:154:ILE:HG13	1.83	0.59
57:SJ:64:ASP:OD1	57:SJ:65:GLU:N	2.36	0.59
8:L5:1364:U:OP2	18:LL:36:ARG:NH1	2.27	0.59
8:L5:1443:A:N6	8:L5:1444:G:O6	2.35	0.59
8:L5:4882:U:OP1	19:LM:117:LYS:NZ	2.36	0.59
15:LG:108:GLN:OE1	15:LG:108:GLN:N	2.30	0.59
32:LZ:83:THR:HG22	38:Lg:95:PHE:CZ	2.38	0.59
50:SC:161:SER:O	50:SC:161:SER:OG	2.18	0.59
70:SX:107:ARG:HD3	70:SX:112:VAL:HG12	1.83	0.59
8:L5:666:G:H1'	8:L5:667:A:H3'	1.84	0.58
9:L7:54:A:O2'	17:LJ:13:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LO:121:PRO:HA	21:LO:124:LEU:HD12	1.84	0.58
72:SZ:65:TYR:CE2	72:SZ:76:ARG:HD3	2.37	0.58
8:L5:1577:G:O2'	8:L5:1612:G:H4'	2.03	0.58
8:L5:1870:C:H2'	8:L5:1871:A2M:H8	1.85	0.58
8:L5:3910:C:H2'	8:L5:3911:C:C6	2.38	0.58
11:LC:1:MET:HG3	11:LC:2:ALA:H	1.68	0.58
15:LG:165:GLU:OE1	20:LN:26:ARG:NH1	2.29	0.58
52:SE:115:THR:HG22	52:SE:117:GLU:H	1.67	0.58
64:SR:90:ALA:O	64:SR:93:GLN:NE2	2.36	0.58
16:LH:31:ARG:NH1	16:LH:188:GLN:OE1	2.35	0.58
19:LM:7:VAL:HG23	19:LM:27:ILE:HD13	1.85	0.58
76:Sd:15:GLY:O	76:Sd:19:ARG:NH1	2.36	0.58
2:SA:189:ILE:HG22	2:SA:191:ARG:H	1.67	0.58
52:SE:127:ARG:HH21	52:SE:142:HIS:HB2	1.68	0.58
24:LR:107:ARG:O	24:LR:111:GLU:HG2	2.01	0.58
46:Lo:2:VAL:N	46:Lo:90:HIS:O	2.36	0.58
55:SH:61:ILE:HG13	55:SH:93:VAL:HG23	1.85	0.58
82:LI:48:LEU:HB2	82:LI:142:LEU:HD23	1.84	0.58
8:L5:1942:A:H2'	8:L5:1943:A:C8	2.38	0.58
8:L5:1968:G:H2'	8:L5:1969:G:C8	2.39	0.58
8:L5:5064:G:N2	22:LP:75:GLN:OE1	2.36	0.58
23:LQ:3:VAL:HG22	23:LQ:5:ILE:HG23	1.85	0.58
8:L5:690:C:H2'	8:L5:691:C:C6	2.38	0.58
8:L5:2640:G:H2'	8:L5:2641:A:C8	2.38	0.58
12:LD:65:ALA:HB2	12:LD:74:ILE:HD13	1.85	0.58
32:LZ:66:SER:O	32:LZ:66:SER:OG	2.19	0.58
65:SS:36:VAL:HG12	65:SS:40:TYR:CD1	2.39	0.58
9:L7:28:C:H1'	9:L7:54:A:H61	1.68	0.58
11:LC:143:ARG:NH1	11:LC:145:GLU:OE2	2.37	0.58
25:LS:76:LYS:NZ	25:LS:100:LEU:O	2.36	0.58
8:L5:423:G:OP1	22:LP:62:ARG:NH1	2.37	0.58
8:L5:2019:C:O2'	8:L5:2020:U:OP1	2.19	0.58
49:S2:521:A:OP1	57:SJ:45:ARG:NH1	2.33	0.58
54:SG:50:VAL:HB	54:SG:111:LEU:HD12	1.86	0.58
62:SP:72:LYS:HE2	62:SP:106:GLU:HG3	1.86	0.58
64:SR:71:ILE:HG13	64:SR:74:GLN:HB2	1.86	0.58
72:SZ:70:PRO:O	72:SZ:74:SER:OG	2.21	0.58
1:LA:177:LYS:HB2	47:Lp:29:ILE:HD13	1.86	0.58
8:L5:4272:G:OP2	8:L5:4272:G:N2	2.27	0.58
8:L5:4347:G:H2'	8:L5:4348:A:C8	2.38	0.58
8:L5:4541:G:N2	8:L5:4544:A:OP2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LU:35:ASP:OD2	27:LU:94:ASN:ND2	2.36	0.58
49:S2:919:A:OP1	60:SN:20:ARG:NH1	2.33	0.58
63:SQ:53:GLU:OE1	63:SQ:85:ARG:NH1	2.36	0.58
79:Sg:201:SER:OG	79:Sg:203:ASP:OD1	2.22	0.58
3:LB:222:VAL:O	3:LB:343:ARG:NH1	2.36	0.57
8:L5:3910:C:H2'	8:L5:3911:C:H6	1.69	0.57
49:S2:507:G:O6	71:SY:105:LYS:NZ	2.36	0.57
49:S2:925:G:H1	49:S2:1017:U:H3	1.52	0.57
49:S2:981:A:H2'	49:S2:982:G:C8	2.39	0.57
52:SE:183:VAL:HG11	52:SE:220:THR:HG21	1.86	0.57
6:B4:64:C:H2'	6:B4:65:C:H6	1.69	0.57
8:L5:74:G:H5'	18:LL:59:VAL:HB	1.85	0.57
8:L5:2520:C:H2'	8:L5:2521:G:H8	1.68	0.57
14:LF:132:MET:O	14:LF:136:VAL:HG12	2.05	0.57
30:LX:148:ASP:O	30:LX:152:LYS:NZ	2.34	0.57
55:SH:44:ASN:OD1	55:SH:68:GLN:NE2	2.38	0.57
57:SJ:71:LEU:O	57:SJ:75:ASN:ND2	2.33	0.57
3:LB:217:ILE:HD12	3:LB:347:LEU:HB3	1.86	0.57
8:L5:1332:C:H2'	8:L5:1333:A:H8	1.69	0.57
20:LN:135:ILE:HG23	20:LN:142:ILE:HD13	1.86	0.57
49:S2:1115:U:C2	49:S2:1118:C:N4	2.72	0.57
54:SG:5:ILE:HG21	54:SG:124:LEU:HD21	1.86	0.57
54:SG:162:LEU:HD12	54:SG:170:ARG:HG2	1.85	0.57
1:LA:33:ASP:N	1:LA:33:ASP:OD1	2.36	0.57
1:LA:51:ASP:HB2	1:LA:58:LEU:HD22	1.86	0.57
1:LA:209:HIS:CE1	1:LA:235:VAL:HG11	2.40	0.57
2:SA:85:ARG:HH21	2:SA:201:LEU:HD12	1.69	0.57
4:SB:89:GLU:OE2	4:SB:220:LYS:NZ	2.36	0.57
8:L5:442:G:OP1	37:Lf:68:ARG:NH1	2.37	0.57
8:L5:4699:U:H1'	8:L5:4700:A:H5''	1.87	0.57
38:Lg:94:ALA:O	38:Lg:98:GLU:HG2	2.05	0.57
1:LA:37:ARG:NH2	8:L5:4088:C:OP1	2.37	0.57
8:L5:407:A:O2'	8:L5:410:A:OP1	2.16	0.57
22:LP:10:ASN:ND2	22:LP:13:LYS:HD2	2.20	0.57
35:Lc:19:GLN:CD	35:Lc:20:LEU:H	2.13	0.57
38:Lg:10:ARG:NH2	43:Ll:3:SER:OG	2.37	0.57
49:S2:1497:G:O6	58:SK:25:LYS:NZ	2.38	0.57
49:S2:1745:A:H8	54:SG:65:GLN:HG3	1.69	0.57
51:SD:62:LYS:O	51:SD:67:ARG:NH2	2.35	0.57
56:SI:65:PHE:O	56:SI:109:TYR:OH	2.21	0.57
65:SS:98:VAL:HG11	65:SS:106:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sg:124:SER:OG	79:Sg:125:ARG:N	2.37	0.57
8:L5:4594:U:H2'	8:L5:4595:G:C8	2.39	0.57
19:LM:81:ASP:N	19:LM:81:ASP:OD1	2.36	0.57
30:LX:145:ASP:O	30:LX:149:VAL:HG23	2.05	0.57
48:Lr:28:GLU:OE2	48:Lr:41:ASN:ND2	2.36	0.57
49:S2:367:U:H4'	49:S2:371:A:C8	2.39	0.57
57:SJ:170:PRO:HB3	57:SJ:174:LYS:HD2	1.86	0.57
36:Ld:68:LEU:HB3	36:Ld:108:TYR:HB2	1.86	0.57
37:Lf:37:ASP:OD1	37:Lf:37:ASP:N	2.38	0.57
49:S2:1126:G:OP2	64:SR:129:LYS:NZ	2.34	0.57
49:S2:1543:U:OP1	63:SQ:37:ARG:NH1	2.38	0.57
55:SH:148:LEU:HA	69:SW:42:MET:HE3	1.86	0.57
55:SH:148:LEU:HD22	69:SW:49:GLU:HG3	1.87	0.57
57:SJ:106:LEU:HD23	57:SJ:109:ARG:HD2	1.86	0.57
73:Sa:2:THR:OG1	73:Sa:3:LYS:N	2.28	0.57
2:SA:149:ASN:HB2	2:SA:165:ASN:HB2	1.87	0.57
8:L5:2322:G:OP1	81:Le:36:ARG:NH2	2.38	0.57
50:SC:194:ARG:HD3	50:SC:196:ILE:HD11	1.87	0.57
5:A4:49:G:H1	7:D4:36:A:H2	1.52	0.57
11:LC:12:SER:HA	11:LC:155:GLU:HG2	1.87	0.57
19:LM:11:ARG:HB3	19:LM:27:ILE:HD12	1.86	0.57
49:S2:1025:U:O3'	49:S2:1089:G:N2	2.37	0.57
50:SC:116:THR:OG1	50:SC:119:GLY:O	2.21	0.57
56:SI:177:SER:HB2	56:SI:186:ASP:HB2	1.86	0.57
79:Sg:5:MET:HB2	79:Sg:270:LEU:HD21	1.86	0.57
79:Sg:171:ASP:OD1	79:Sg:171:ASP:N	2.38	0.57
8:L5:1969:G:H3'	8:L5:1970:A:H8	1.69	0.56
20:LN:46:ASP:OD2	20:LN:50:ARG:NH2	2.37	0.56
49:S2:1544:C:H2'	49:S2:1545:A:H5''	1.87	0.56
51:SD:215:ASP:N	51:SD:215:ASP:OD1	2.37	0.56
5:A4:49:G:H22	7:D4:36:A:H2	1.54	0.56
8:L5:3710:G:H4'	8:L5:3711:A:H5'	1.87	0.56
8:L5:4120:U:O2'	38:Lg:93:ARG:NH1	2.36	0.56
8:L5:4260:U:H2'	8:L5:4261:C:C6	2.39	0.56
8:L5:4763:U:O2'	25:LS:174:THR:OG1	2.22	0.56
15:LG:143:VAL:HG21	15:LG:201:THR:HG22	1.87	0.56
16:LH:180:TYR:HB2	44:Lm:85:LEU:HD21	1.85	0.56
49:S2:600:G:H2'	49:S2:601:OMG:H5''	1.85	0.56
1:LA:27:ALA:O	1:LA:128:ARG:NH2	2.38	0.56
8:L5:66:A:O2'	8:L5:326:C:O2	2.20	0.56
8:L5:662:C:H2'	8:L5:663:G:H8	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:691:C:H2'	8:L5:692:A:C8	2.41	0.56
8:L5:2102:G:H1'	8:L5:2103:G:C8	2.39	0.56
8:L5:2566:G:H2'	8:L5:2567:G:H8	1.70	0.56
8:L5:4313:A:H4'	26:LT:71:ALA:HB3	1.87	0.56
14:LF:171:ASP:OD1	14:LF:172:ASN:N	2.38	0.56
19:LM:105:THR:OG1	19:LM:108:ASP:OD2	2.17	0.56
38:Lg:67:LEU:O	38:Lg:72:LYS:NZ	2.39	0.56
49:S2:223:C:H2'	49:S2:224:A:C8	2.39	0.56
50:SC:209:VAL:HG13	50:SC:210:PRO:HD3	1.86	0.56
54:SG:70:HIS:HB3	54:SG:101:ILE:HB	1.87	0.56
64:SR:98:VAL:HG21	64:SR:117:LEU:HD22	1.86	0.56
69:SW:51:GLU:OE1	74:Sb:8:LEU:HD21	2.05	0.56
74:Sb:35:VAL:HG21	74:Sb:63:LEU:HD21	1.88	0.56
8:L5:43:U:O2	46:Lo:44:LYS:NZ	2.37	0.56
8:L5:2744:A:H2'	8:L5:2745:A:C8	2.40	0.56
8:L5:2898:G:OP1	24:LR:104:ARG:NH1	2.37	0.56
19:LM:5:ARG:NE	19:LM:59:ASP:OD1	2.34	0.56
25:LS:2:LYS:HD3	25:LS:43:ARG:HD2	1.87	0.56
61:SO:136:PRO:HB2	61:SO:139:SER:HB3	1.88	0.56
77:Se:75:VAL:O	77:Se:76:HIS:ND1	2.38	0.56
8:L5:2566:G:H2'	8:L5:2567:G:C8	2.41	0.56
17:LJ:136:ARG:NH1	17:LJ:156:ARG:O	2.39	0.56
30:LX:148:ASP:HB3	30:LX:152:LYS:NZ	2.19	0.56
56:SI:46:VAL:HG22	56:SI:54:LYS:HB3	1.87	0.56
34:Lb:36:ASP:HB3	34:Lb:39:PHE:HB3	1.88	0.56
49:S2:604:A:N3	49:S2:639:C:O2'	2.36	0.56
49:S2:1171:G:O2'	49:S2:1187:G:O6	2.23	0.56
67:SU:81:GLN:NE2	76:Sd:56:ASP:OD2	2.38	0.56
78:Sf:117:LEU:O	78:Sf:118:ARG:HD2	2.06	0.56
78:Sf:119:ARG:HB3	78:Sf:132:MET:HG3	1.88	0.56
82:LI:30:LYS:HD3	82:LI:63:GLU:HG3	1.87	0.56
8:L5:2474:G:N2	8:L5:2502:G:O2'	2.39	0.56
9:L7:26:C:O2'	17:LJ:147:ARG:NH1	2.38	0.56
12:LD:257:PRO:N	12:LD:257:PRO:HG2	2.01	0.56
21:LO:178:ARG:O	21:LO:182:GLU:HG3	2.05	0.56
24:LR:136:ARG:O	24:LR:140:GLU:HG2	2.06	0.56
26:LT:28:ALA:O	26:LT:32:ARG:HG2	2.06	0.56
49:S2:96:C:H2'	49:S2:97:U:C6	2.41	0.56
49:S2:959:G:OP2	61:SO:38:ASN:ND2	2.33	0.56
1:LA:54:ARG:HG3	1:LA:56:ALA:H	1.70	0.56
1:LA:108:PRO:O	1:LA:111:THR:OG1	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:297:U:O2'	20:LN:179:LYS:O	2.24	0.56
8:L5:3811:G:O2'	8:L5:3814:U:OP2	2.24	0.56
12:LD:62:CYS:HB3	12:LD:105:LEU:HD22	1.88	0.56
20:LN:103:GLU:OE2	20:LN:118:SER:OG	2.20	0.56
38:Lg:22:LEU:HD12	38:Lg:30:ILE:HG21	1.87	0.56
49:S2:145:G:H2'	49:S2:146:G:C8	2.41	0.56
51:SD:5:ILE:HD12	51:SD:9:ARG:HG2	1.88	0.56
56:SI:136:ILE:HG13	56:SI:137:LEU:H	1.71	0.56
71:SY:41:ARG:NH2	71:SY:52:PRO:O	2.39	0.56
80:SM:52:LEU:HD12	80:SM:53:ALA:H	1.71	0.56
8:L5:3614:G:O2'	8:L5:3615:G:OP1	2.15	0.56
8:L5:4700:A:H2	16:LH:69:THR:HG22	1.69	0.56
17:LJ:100:SER:HG	17:LJ:131:TYR:HH	1.47	0.56
35:Lc:17:ARG:NH2	35:Lc:19:GLN:HE21	2.03	0.56
49:S2:1648:G:N2	49:S2:1675:A:OP2	2.27	0.56
70:SX:68:LYS:HB3	70:SX:91:LEU:HD22	1.88	0.56
79:Sg:93:THR:HG23	79:Sg:94:THR:HG23	1.87	0.56
8:L5:268:G:H2'	8:L5:269:G:H8	1.71	0.56
8:L5:2573:A:H1'	32:LZ:112:ARG:HH22	1.69	0.56
8:L5:4935:C:H2'	8:L5:4936:G:C8	2.41	0.56
17:LJ:65:ASN:ND2	46:Lo:102:GLN:OE1	2.39	0.56
8:L5:1210:C:O2'	8:L5:1211:G:O5'	2.20	0.55
49:S2:1337:4AC:H2'	49:S2:1338:G:H8	1.70	0.55
49:S2:1568:C:O2	49:S2:1627:C:O2'	2.23	0.55
8:L5:280:G:H5''	20:LN:14:LYS:HE2	1.88	0.55
8:L5:2579:G:N2	8:L5:2582:A:OP2	2.30	0.55
17:LJ:136:ARG:NH2	17:LJ:161:GLU:OE1	2.39	0.55
27:LU:47:ILE:HD12	27:LU:63:ILE:HD11	1.88	0.55
49:S2:373:G:OP1	59:SL:137:THR:OG1	2.19	0.55
52:SE:221:ARG:HG3	52:SE:221:ARG:O	2.05	0.55
56:SI:31:ARG:HH12	56:SI:48:VAL:HG12	1.70	0.55
2:SA:85:ARG:HH12	2:SA:205:ARG:HD3	1.72	0.55
2:SA:126:ASP:OD1	2:SA:165:ASN:ND2	2.38	0.55
8:L5:497:G:H4'	8:L5:498:C:H5'	1.87	0.55
8:L5:1324:A:O2'	8:L5:1326:A2M:OP1	2.23	0.55
24:LR:90:PRO:HB2	24:LR:93:VAL:HG22	1.88	0.55
49:S2:419:G:N2	49:S2:661:U:O2	2.40	0.55
49:S2:1661:A:H8	76:Sd:14:PHE:HB2	1.71	0.55
59:SL:99:TYR:O	59:SL:101:ARG:N	2.39	0.55
8:L5:935:A:N1	19:LM:70:GLN:NE2	2.48	0.55
8:L5:1320:U:O2'	8:L5:1891:A:N1	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:1523:A:N3	8:L5:4389:C:O2'	2.34	0.55
8:L5:4250:G:OP1	17:LJ:98:ASN:ND2	2.39	0.55
8:L5:4291:G:H5'	8:L5:4293:U:C6	2.40	0.55
30:LX:155:ILE:HG13	30:LX:156:ILE:HG23	1.88	0.55
49:S2:1446:A:H5''	67:SU:58:THR:HG23	1.88	0.55
49:S2:1599:U:H5''	72:SZ:44:LEU:HD12	1.89	0.55
54:SG:57:ASP:HB3	54:SG:98:ARG:HD2	1.87	0.55
8:L5:194:C:O2	31:LY:121:ARG:NH1	2.39	0.55
35:Lc:48:LEU:HD21	35:Lc:60:ILE:HG21	1.88	0.55
37:Lf:39:THR:HG21	37:Lf:77:ALA:HB2	1.89	0.55
49:S2:659:G:O2'	49:S2:662:G:O2'	2.21	0.55
51:SD:172:VAL:HG13	51:SD:185:LYS:HG2	1.88	0.55
8:L5:307:A:N3	8:L5:310:G:O2'	2.38	0.55
8:L5:2033:A:O3'	25:LS:86:SER:OG	2.24	0.55
8:L5:4238:G:H2'	8:L5:4239:A:C8	2.41	0.55
8:L5:4279:A:H5'	8:L5:4281:A:H1'	1.89	0.55
12:LD:256:LYS:C	12:LD:257:PRO:CG	2.75	0.55
14:LF:220:MET:HE1	14:LF:223:LYS:HE3	1.88	0.55
29:LW:56:ARG:HH21	29:LW:61:LYS:HB3	1.71	0.55
52:SE:129:ILE:HD11	52:SE:139:LEU:HD12	1.88	0.55
57:SJ:78:LEU:HD23	57:SJ:92:MET:HG3	1.87	0.55
63:SQ:116:ASP:OD1	63:SQ:118:THR:OG1	2.21	0.55
3:LB:252:ALA:HB1	8:L5:4524:G:C2	2.41	0.55
8:L5:1563:A:N6	49:S2:1028:A:N1	2.55	0.55
8:L5:4322:G:N2	8:L5:4325:A:OP2	2.33	0.55
20:LN:38:ARG:HH21	20:LN:60:VAL:HG22	1.71	0.55
28:LV:107:ASN:OD1	28:LV:108:ASN:N	2.40	0.55
31:LY:44:VAL:HG21	31:LY:119:LEU:HD13	1.88	0.55
49:S2:1091:C:OP1	60:SN:9:LYS:NZ	2.38	0.55
72:SZ:79:ILE:HB	72:SZ:83:LEU:HD23	1.88	0.55
3:LB:121:ASN:OD1	8:L5:4987:C:N4	2.40	0.55
8:L5:210:C:OP1	31:LY:59:ARG:NH1	2.40	0.55
12:LD:39:GLN:HE21	12:LD:46:THR:HB	1.71	0.55
43:Ll:38:ASN:HB3	43:Ll:41:ARG:HG3	1.89	0.55
49:S2:349:A:H2'	49:S2:350:C:C6	2.41	0.55
49:S2:920:A:OP1	69:SW:57:ARG:NE	2.38	0.55
55:SH:46:THR:HG23	55:SH:65:PRO:HD3	1.88	0.55
69:SW:42:MET:HB2	69:SW:47:ILE:HG13	1.88	0.55
8:L5:662:C:H2'	8:L5:663:G:C8	2.42	0.55
8:L5:690:C:OP1	48:Lr:87:ARG:NH1	2.39	0.55
49:S2:1124:C:O2'	64:SR:126:MET:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:130:SER:HB2	1:LA:171:GLY:HA3	1.88	0.55
27:LU:63:ILE:O	27:LU:63:ILE:HG22	2.06	0.55
49:S2:1218:C:H2'	49:S2:1219:C:H6	1.71	0.55
73:Sa:23:CYS:HB2	73:Sa:74:CYS:H	1.72	0.55
73:Sa:51:ARG:O	73:Sa:55:GLU:HG2	2.06	0.55
4:SB:40:ASN:OD1	4:SB:41:ILE:HD13	2.06	0.54
8:L5:17:A:OP1	39:Lh:84:ARG:NH2	2.28	0.54
8:L5:92:C:OP1	86:L5:5286:SPD:N10	2.40	0.54
8:L5:759:G:H22	8:L5:904:C:H2'	1.72	0.54
8:L5:1942:A:H2'	8:L5:1943:A:H8	1.71	0.54
16:LH:128:MET:HE1	16:LH:146:LEU:HD22	1.89	0.54
49:S2:969:U:O2	49:S2:971:G:N1	2.40	0.54
69:SW:90:GLN:OE1	69:SW:113:HIS:ND1	2.38	0.54
8:L5:253:G:H2'	8:L5:254:G:C8	2.42	0.54
8:L5:977:C:OP2	13:LE:59:ARG:NH1	2.40	0.54
13:LE:287:VAL:O	19:LM:109:ARG:NH2	2.40	0.54
17:LJ:17:ILE:HD12	17:LJ:80:GLU:CD	2.32	0.54
27:LU:18:VAL:N	27:LU:75:GLU:OE1	2.41	0.54
36:Ld:36:VAL:HG21	36:Ld:44:ARG:HG2	1.89	0.54
50:SC:94:ILE:HG21	50:SC:162:ILE:HD12	1.89	0.54
8:L5:490:C:H2'	8:L5:491:G:C8	2.41	0.54
8:L5:1604:G:H2'	8:L5:1605:G:C8	2.43	0.54
8:L5:1669:A:H4'	8:L5:1685:G:N2	2.22	0.54
8:L5:5057:C:H2'	8:L5:5058:A:C8	2.42	0.54
11:LC:154:VAL:HG11	11:LC:174:LEU:HD11	1.89	0.54
22:LP:23:ARG:HG2	22:LP:125:MET:HE1	1.90	0.54
35:Lc:17:ARG:NH1	35:Lc:107:SER:OG	2.39	0.54
49:S2:29:G:H4'	70:SX:129:SER:HB2	1.89	0.54
49:S2:520:A:O2'	49:S2:825:A:N3	2.39	0.54
49:S2:1098:C:H2'	49:S2:1099:G:C8	2.43	0.54
60:SN:40:LEU:HD12	60:SN:50:ILE:HG23	1.88	0.54
8:L5:1359:G:N2	20:LN:204:ARG:OXT	2.39	0.54
8:L5:2297:G:H4'	11:LC:242:PRO:HB2	1.89	0.54
8:L5:2781:G:O2'	43:Ll:3:SER:O	2.25	0.54
8:L5:4930:C:OP1	13:LE:266:GLN:NE2	2.39	0.54
8:L5:5005:G:N2	8:L5:5041:G:O2'	2.41	0.54
21:LO:12:ARG:O	25:LS:171:ARG:NH2	2.40	0.54
23:LQ:99:LYS:HD2	23:LQ:119:LYS:HE2	1.89	0.54
32:LZ:90:PRO:O	32:LZ:117:LYS:NZ	2.40	0.54
49:S2:17:C:O2'	49:S2:1194:A:N1	2.34	0.54
49:S2:509:G:H4'	52:SE:26:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1285:G:H3'	49:S2:1286:G:H5'	1.88	0.54
49:S2:1546:G:H21	49:S2:1670:C:H1'	1.73	0.54
54:SG:84:TYR:OH	54:SG:91:GLU:O	2.19	0.54
75:Sc:13:ARG:NH2	75:Sc:35:MET:SD	2.81	0.54
80:SM:47:ALA:O	80:SM:74:ILE:HD12	2.07	0.54
1:LA:142:GLU:C	1:LA:144:LYS:H	2.15	0.54
8:L5:223:G:OP2	11:LC:165:LYS:HE2	2.08	0.54
8:L5:462:G:H2'	8:L5:463:A:H8	1.72	0.54
8:L5:2573:A:H1'	32:LZ:112:ARG:NH2	2.22	0.54
8:L5:4672:A:OP1	28:LV:15:ARG:NH2	2.40	0.54
30:LX:152:LYS:HD3	30:LX:152:LYS:N	2.22	0.54
49:S2:942:G:H2'	49:S2:943:U:C6	2.43	0.54
8:L5:1092:G:H2'	8:L5:1093:C:C6	2.43	0.54
8:L5:1244:G:H2'	8:L5:1245:C:H6	1.73	0.54
8:L5:4913:G:H4'	8:L5:4914:C:O5'	2.07	0.54
18:LL:125:ILE:HD11	39:Lh:122:LYS:HB2	1.89	0.54
79:Sg:32:LEU:HG	79:Sg:71:ILE:HD11	1.89	0.54
8:L5:2611:A:H2'	8:L5:2612:G:C8	2.42	0.54
36:Ld:23:ARG:HG2	36:Ld:121:ASN:HA	1.90	0.54
49:S2:126:G:C6	54:SG:196:LYS:HG2	2.43	0.54
49:S2:307:G:H1'	56:SI:45:THR:HG22	1.90	0.54
49:S2:526:A:OP1	77:Se:108:ARG:NH1	2.41	0.54
50:SC:271:ASP:OD1	50:SC:271:ASP:N	2.40	0.54
60:SN:57:SER:OG	60:SN:58:HIS:ND1	2.41	0.54
78:Sf:128:ALA:HB3	80:SM:44:LYS:HZ1	1.72	0.54
8:L5:2263:A:OP1	48:Lr:107:ARG:NH1	2.32	0.54
8:L5:2303:C:OP1	81:Le:107:ASN:ND2	2.36	0.54
16:LH:90:TYR:CE1	16:LH:184:LYS:HG2	2.43	0.54
17:LJ:100:SER:OG	17:LJ:131:TYR:OH	2.20	0.54
32:LZ:41:ALA:HB2	32:LZ:77:TYR:HE1	1.73	0.54
37:Lf:59:THR:OG1	37:Lf:65:ASN:OD1	2.24	0.54
49:S2:612:U:O2'	77:Se:84:LYS:NZ	2.40	0.54
52:SE:45:ILE:HB	52:SE:80:ILE:HG23	1.90	0.54
8:L5:4239:A:H2'	8:L5:4240:G:C8	2.43	0.54
28:LV:126:ALA:HB2	28:LV:139:ILE:HD12	1.88	0.54
49:S2:223:C:H2'	49:S2:224:A:H8	1.73	0.54
49:S2:1446:A:H1'	67:SU:55:ARG:HD2	1.90	0.54
52:SE:95:THR:HG23	71:SY:16:ARG:HH12	1.73	0.54
56:SI:79:ILE:HG21	56:SI:170:LYS:HE2	1.90	0.54
4:SB:97:LEU:CD2	4:SB:229:MET:HE1	2.39	0.53
8:L5:500:G:N3	8:L5:504:G:O2'	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:1818:G:OP2	8:L5:1818:G:N2	2.32	0.53
8:L5:1968:G:H2'	8:L5:1969:G:H8	1.72	0.53
8:L5:2705:G:H22	8:L5:2710:C:H5	1.56	0.53
8:L5:4537:C:H2'	8:L5:4538:G:C8	2.43	0.53
14:LF:136:VAL:HG22	14:LF:136:VAL:O	2.07	0.53
17:LJ:144:LYS:O	17:LJ:148:THR:OG1	2.26	0.53
49:S2:67:C:OP2	54:SG:172:LYS:NZ	2.31	0.53
49:S2:807:G:H2'	49:S2:808:A:H8	1.72	0.53
49:S2:964:A:H2'	49:S2:965:U:H6	1.72	0.53
52:SE:199:GLU:OE2	52:SE:209:HIS:NE2	2.41	0.53
52:SE:210:VAL:HG13	52:SE:218:PHE:CE2	2.43	0.53
67:SU:67:LYS:HG3	67:SU:67:LYS:O	2.08	0.53
4:SB:97:LEU:HD21	4:SB:229:MET:HE1	1.89	0.53
7:D4:63:G:H2'	7:D4:64:A:H8	1.73	0.53
8:L5:1269:G:O2'	8:L5:1270:A:O4'	2.24	0.53
8:L5:1426:G:N1	8:L5:1458:C:OP2	2.28	0.53
8:L5:3717:A:H2'	8:L5:3718:A2M:C8	2.39	0.53
8:L5:4373:G:N7	46:Lo:61:LYS:NZ	2.56	0.53
8:L5:4954:G:H2'	8:L5:4955:A:C8	2.43	0.53
15:LG:50:ASP:OD1	30:LX:40:ILE:HD12	2.08	0.53
18:LL:79:GLU:HG2	18:LL:110:LEU:HD11	1.91	0.53
38:Lg:22:LEU:HD12	38:Lg:30:ILE:CG2	2.38	0.53
49:S2:847:A:OP1	52:SE:108:ARG:NH2	2.41	0.53
51:SD:8:LYS:HB3	67:SU:61:LEU:HD21	1.90	0.53
82:LI:51:HIS:CD2	82:LI:168:SER:HB2	2.42	0.53
8:L5:661:C:H2'	8:L5:662:C:C6	2.43	0.53
8:L5:1932:A:OP1	21:LO:49:ARG:NH2	2.41	0.53
11:LC:4:ALA:O	11:LC:29:LYS:NZ	2.41	0.53
12:LD:75:VAL:O	12:LD:112:ARG:NH1	2.42	0.53
49:S2:377:G:H5'	56:SI:98:LYS:HB3	1.91	0.53
49:S2:1114:U:H3	49:S2:1119:A:H61	1.56	0.53
52:SE:31:PRO:HA	52:SE:81:THR:HB	1.90	0.53
8:L5:2411:C:H2'	8:L5:2412:A:H8	1.73	0.53
28:LV:45:ILE:HG21	28:LV:53:PRO:HB3	1.91	0.53
32:LZ:5:MET:O	32:LZ:28:ASN:ND2	2.42	0.53
36:Ld:57:MET:SD	36:Ld:90:ARG:HB2	2.49	0.53
66:ST:28:LEU:HD13	66:ST:110:LEU:HD22	1.90	0.53
71:SY:37:LYS:HA	71:SY:40:ILE:HD12	1.89	0.53
8:L5:287:U:O2	20:LN:93:LYS:NZ	2.35	0.53
8:L5:2588:C:H41	38:Lg:70:THR:HG21	1.72	0.53
8:L5:4730:C:H2'	8:L5:4731:G:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LL:107:THR:HB	40:Li:18:THR:HG23	1.90	0.53
49:S2:142:C:N4	49:S2:330:G:OP2	2.31	0.53
49:S2:306:C:OP2	56:SI:41:ARG:NH1	2.42	0.53
52:SE:54:TYR:O	71:SY:15:ASN:ND2	2.42	0.53
66:ST:108:GLU:OE2	66:ST:121:ARG:NE	2.21	0.53
80:SM:56:CYS:SG	80:SM:62:VAL:HG12	2.48	0.53
3:LB:214:ASP:HB3	3:LB:283:LYS:HZ2	1.74	0.53
7:D4:8:U:H1'	7:D4:15:G:H1	1.74	0.53
8:L5:67:C:OP2	8:L5:312:G:N2	2.37	0.53
8:L5:690:C:H2'	8:L5:691:C:H6	1.73	0.53
8:L5:1406:G:O6	8:L5:1408:G:O2'	2.22	0.53
8:L5:2499:C:H2'	8:L5:2500:U:H6	1.72	0.53
8:L5:2685:C:OP1	38:Lg:57:ARG:NH1	2.40	0.53
8:L5:4344:U:H2'	8:L5:4345:C:C6	2.43	0.53
21:LO:33:VAL:HG13	21:LO:102:LEU:HD12	1.90	0.53
49:S2:659:G:HO2'	49:S2:662:G:HO2'	1.53	0.53
49:S2:1130:G:OP2	49:S2:1130:G:N2	2.37	0.53
55:SH:17:ASP:OD1	55:SH:17:ASP:N	2.40	0.53
61:SO:121:ARG:HH12	75:Sc:62:GLU:HB2	1.74	0.53
67:SU:17:ILE:HG12	67:SU:94:PRO:HB3	1.90	0.53
8:L5:4874:A:O2'	25:LS:170:LYS:NZ	2.42	0.53
9:L7:49:A:H5''	12:LD:224:SER:HB3	1.91	0.53
24:LR:163:ARG:NH1	49:S2:873:G:OP1	2.42	0.53
25:LS:24:THR:O	25:LS:24:THR:OG1	2.22	0.53
49:S2:170:A:OP2	54:SG:140:ARG:NH1	2.41	0.53
62:SP:31:GLU:O	62:SP:34:MET:HB2	2.09	0.53
75:Sc:61:SER:O	75:Sc:62:GLU:HG2	2.07	0.53
11:LC:140:LYS:HE2	11:LC:242:PRO:HD2	1.90	0.53
19:LM:16:SER:OG	19:LM:54:CYS:O	2.27	0.53
27:LU:33:ILE:HD11	27:LU:100:LEU:HD21	1.90	0.53
35:Lc:17:ARG:NH1	35:Lc:107:SER:HB2	2.20	0.53
46:Lo:33:LEU:HA	46:Lo:38:LYS:HG2	1.90	0.53
49:S2:28:U:H2'	49:S2:29:G:H8	1.74	0.53
54:SG:154:ARG:O	54:SG:155:GLN:HG2	2.09	0.53
82:LI:200:ILE:HD12	82:LI:212:LEU:HD21	1.90	0.53
8:L5:478:G:OP1	48:Lr:66:ARG:NH1	2.38	0.53
8:L5:677:G:H2'	8:L5:678:C:H6	1.73	0.53
8:L5:1749:A:H2'	8:L5:1750:G:C8	2.43	0.53
10:L8:154:G:H3'	15:LG:89:ARG:HH22	1.73	0.53
49:S2:952:G:H2'	49:S2:953:C:C6	2.43	0.53
63:SQ:32:ILE:HG21	63:SQ:39:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:ST:124:THR:HG23	66:ST:127:GLY:H	1.74	0.53
75:Sc:21:THR:OG1	75:Sc:22:GLY:N	2.42	0.53
79:Sg:218:LEU:HD21	79:Sg:228:TYR:CD1	2.43	0.53
2:SA:81:ASN:HA	2:SA:84:GLN:NE2	2.23	0.53
8:L5:1533:A:H5'	8:L5:1623:A:H61	1.73	0.53
8:L5:2755:A:OP2	32:LZ:51:ARG:NH2	2.29	0.53
8:L5:4093:G:H2'	8:L5:4094:G:H8	1.72	0.53
10:L8:54:C:H2'	10:L8:55:PSU:C6	2.43	0.53
16:LH:117:PHE:O	16:LH:120:GLU:HG3	2.08	0.53
49:S2:1204:A:H62	49:S2:1694:U:H3	1.57	0.53
50:SC:68:ARG:NH2	50:SC:72:ASP:OD1	2.42	0.53
50:SC:78:LEU:HD11	50:SC:94:ILE:HD13	1.91	0.53
52:SE:79:ASP:HB3	52:SE:82:TYR:HB2	1.91	0.53
60:SN:130:LYS:NZ	60:SN:139:TRP:O	2.41	0.53
80:SM:20:GLU:O	80:SM:24:THR:OG1	2.20	0.53
3:LB:80:GLU:OE1	3:LB:323:TYR:OH	2.24	0.52
8:L5:1933:G:H2'	8:L5:1934:A:C8	2.44	0.52
8:L5:2520:C:H2'	8:L5:2521:G:C8	2.43	0.52
18:LL:103:ARG:HH11	18:LL:105:LYS:HD2	1.73	0.52
40:Li:73:ILE:O	40:Li:77:VAL:HG22	2.09	0.52
49:S2:161:U:O2'	54:SG:87:ARG:NE	2.42	0.52
49:S2:1077:A:OP1	60:SN:106:ARG:NH2	2.42	0.52
55:SH:139:ILE:HG23	55:SH:156:VAL:HG13	1.90	0.52
71:SY:102:THR:HG23	71:SY:107:ARG:HE	1.73	0.52
2:SA:58:LEU:HD21	2:SA:177:MET:HB2	1.90	0.52
3:LB:156:TYR:OH	8:L5:4912:G:N2	2.42	0.52
8:L5:513:U:H3	8:L5:515:C:H3'	1.74	0.52
8:L5:1970:A:H5'	8:L5:2000:G:N1	2.24	0.52
8:L5:2623:A:OP1	27:LU:101:ARG:NH1	2.42	0.52
11:LC:138:MET:HG3	48:Lr:43:LEU:HD13	1.91	0.52
49:S2:1714:U:H2'	49:S2:1715:A:C8	2.45	0.52
50:SC:188:CYS:SG	50:SC:238:LYS:HG3	2.49	0.52
56:SI:177:SER:OG	56:SI:182:CYS:SG	2.67	0.52
62:SP:68:PRO:HG2	62:SP:71:GLU:HB3	1.89	0.52
4:SB:114:VAL:O	49:S2:1869:A:N6	2.42	0.52
8:L5:1633:G:H5'	8:L5:1634:A:OP1	2.09	0.52
61:SO:54:CYS:SG	61:SO:81:VAL:HG13	2.50	0.52
78:Sf:128:ALA:HB3	80:SM:44:LYS:HZ2	1.74	0.52
2:SA:199:PRO:HG2	2:SA:200:ASP:N	2.22	0.52
3:LB:117:ARG:HG2	3:LB:180:LEU:HD12	1.91	0.52
7:D4:63:G:H2'	7:D4:64:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:382:G:N1	8:L5:385:A:OP2	2.37	0.52
8:L5:2303:C:H5''	81:Le:104:SER:HB3	1.90	0.52
8:L5:2539:C:H2'	8:L5:2540:C:C6	2.44	0.52
8:L5:2611:A:H2'	8:L5:2612:G:H8	1.73	0.52
8:L5:3868:G:H22	8:L5:3900:G:H1'	1.74	0.52
16:LH:91:LYS:HB2	16:LH:183:GLU:HB2	1.90	0.52
49:S2:107:A:H2'	49:S2:108:G:C8	2.44	0.52
52:SE:228:ILE:HD11	52:SE:236:ILE:HD11	1.89	0.52
71:SY:45:ALA:HB2	71:SY:52:PRO:HB3	1.92	0.52
72:SZ:51:ASP:OD1	72:SZ:51:ASP:N	2.33	0.52
49:S2:106:C:H2'	49:S2:107:A:H8	1.73	0.52
49:S2:368:U:OP1	49:S2:369:C:O2'	2.28	0.52
49:S2:433:A:H2'	49:S2:434:G:C8	2.45	0.52
49:S2:1013:U:OP1	49:S2:1129:G:O2'	2.27	0.52
49:S2:1617:G:N1	49:S2:1620:A:OP2	2.43	0.52
57:SJ:32:ILE:HG22	57:SJ:37:LEU:HD12	1.92	0.52
66:ST:60:THR:HG23	66:ST:75:MET:HE2	1.92	0.52
74:Sb:34:ASP:HB3	74:Sb:82:LYS:HE2	1.91	0.52
11:LC:33:ARG:NH2	11:LC:35:ASP:OD2	2.38	0.52
28:LV:117:ILE:HB	28:LV:136:ALA:HA	1.92	0.52
31:LY:4:ASN:HB3	31:LY:7:VAL:HG22	1.92	0.52
49:S2:1256:G:H8	67:SU:66:ARG:HB2	1.74	0.52
49:S2:1614:A:H2'	49:S2:1615:U:H6	1.74	0.52
65:SS:24:ARG:HB2	65:SS:29:ALA:HB2	1.91	0.52
65:SS:108:ARG:NH2	65:SS:109:GLU:OE2	2.43	0.52
78:Sf:135:HIS:HB2	78:Sf:138:ARG:HG2	1.91	0.52
5:A4:51:U:O2'	5:A4:52:U:O2	2.24	0.52
7:D4:53:G:H2'	7:D4:54:U:C5	2.44	0.52
19:LM:13:ALA:HB1	19:LM:55:MET:HB2	1.91	0.52
48:Lr:90:LEU:HG	48:Lr:111:ILE:HG23	1.90	0.52
49:S2:1109:C:O2'	49:S2:1110:G:H8	1.93	0.52
49:S2:1360:U:O2'	49:S2:1379:A:OP2	2.28	0.52
55:SH:23:ILE:HD13	55:SH:87:PHE:HE2	1.75	0.52
60:SN:119:GLU:O	60:SN:123:HIS:ND1	2.42	0.52
8:L5:420:A:H62	10:L8:14:OMU:H5	1.74	0.52
8:L5:666:G:O6	8:L5:668:C:N4	2.43	0.52
8:L5:4992:G:H2'	8:L5:4993:G:H8	1.71	0.52
9:L7:12:U:OP2	9:L7:67:C:O2'	2.26	0.52
14:LF:171:ASP:OD1	14:LF:173:ALA:N	2.32	0.52
16:LH:112:VAL:HB	16:LH:126:VAL:HG22	1.91	0.52
20:LN:17:ASP:N	20:LN:17:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LV:87:SER:HA	28:LV:97:TYR:HB3	1.92	0.52
63:SQ:12:VAL:HG11	63:SQ:90:LYS:HB3	1.91	0.52
78:Sf:118:ARG:HB3	78:Sf:131:PHE:HB3	1.91	0.52
1:LA:116:LEU:HD12	1:LA:117:GLU:H	1.75	0.52
7:D4:4:C:H2'	7:D4:5:G:H8	1.74	0.52
12:LD:278:ASP:O	12:LD:282:GLN:HG3	2.09	0.52
15:LG:182:CYS:HB2	15:LG:222:ILE:HD13	1.91	0.52
33:La:84:GLU:O	33:La:88:VAL:HG13	2.10	0.52
49:S2:554:A:H2'	49:S2:555:A:C5	2.45	0.52
60:SN:34:LYS:HG2	60:SN:74:ILE:HD13	1.92	0.52
65:SS:48:ALA:HB2	65:SS:70:ILE:HD12	1.91	0.52
8:L5:737:C:C6	8:L5:739:G:H5''	2.45	0.52
20:LN:38:ARG:NH2	20:LN:60:VAL:HG22	2.25	0.52
22:LP:103:GLU:HG3	22:LP:109:VAL:HG21	1.92	0.52
49:S2:370:G:O2'	56:SI:10:LYS:NZ	2.43	0.52
49:S2:586:G:OP1	57:SJ:176:LYS:NZ	2.37	0.52
49:S2:1531:A:H4'	49:S2:1605:G:H4'	1.92	0.52
57:SJ:78:LEU:HD11	57:SJ:94:LEU:HB3	1.92	0.52
3:LB:107:ALA:HB1	3:LB:202:GLU:HG3	1.92	0.51
4:SB:124:HIS:HA	4:SB:137:LEU:O	2.09	0.51
8:L5:2823:G:N7	24:LR:20:LYS:HD2	2.25	0.51
8:L5:4173:G:H2'	8:L5:4174:U:C6	2.45	0.51
21:LO:181:ALA:O	21:LO:185:VAL:HG22	2.10	0.51
23:LQ:178:ARG:NH2	33:La:46:ASP:OD2	2.42	0.51
27:LU:107:LYS:HE2	27:LU:108:GLU:HG2	1.91	0.51
49:S2:1549:U:OP2	51:SD:8:LYS:NZ	2.43	0.51
52:SE:44:LEU:HD12	52:SE:72:ILE:HD11	1.92	0.51
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.92	0.51
8:L5:325:U:H2'	8:L5:326:C:C6	2.46	0.51
8:L5:4935:C:H2'	8:L5:4936:G:H8	1.76	0.51
11:LC:328:LEU:HD22	14:LF:187:MET:HG3	1.93	0.51
12:LD:152:ARG:O	12:LD:157:ASN:ND2	2.43	0.51
18:LL:146:LEU:O	18:LL:148:THR:OG1	2.23	0.51
20:LN:159:ARG:HB2	20:LN:164:LEU:HB2	1.92	0.51
28:LV:104:VAL:HG11	28:LV:117:ILE:HD11	1.93	0.51
35:Lc:38:ILE:HD11	35:Lc:46:VAL:HG21	1.93	0.51
49:S2:1533:A:H2	49:S2:1536:G:N3	2.07	0.51
49:S2:1658:G:OP2	49:S2:1660:C:N4	2.42	0.51
52:SE:133:THR:HG22	52:SE:134:LYS:HG3	1.91	0.51
54:SG:120:ASP:O	54:SG:125:THR:OG1	2.27	0.51
80:SM:80:ASP:OD1	80:SM:80:ASP:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:109:LYS:O	4:SB:113:MET:HG2	2.10	0.51
8:L5:1283:G:N1	8:L5:2076:G:OP1	2.37	0.51
8:L5:4139:G:H21	8:L5:4140:C:H41	1.58	0.51
15:LG:193:LEU:HD12	15:LG:194:VAL:HG13	1.91	0.51
28:LV:97:TYR:OH	29:LW:37:GLU:OE2	2.15	0.51
56:SI:117:TYR:HD1	56:SI:152:ARG:HB3	1.75	0.51
8:L5:139:G:H2'	8:L5:140:G:H8	1.75	0.51
8:L5:1967:A:H61	8:L5:2020:U:H3	1.59	0.51
25:LS:164:LYS:HB3	25:LS:165:PRO:HD3	1.91	0.51
30:LX:73:HIS:CD2	30:LX:115:LYS:HG2	2.46	0.51
36:Ld:85:ARG:HD3	36:Ld:111:VAL:HG21	1.90	0.51
49:S2:526:A:N6	49:S2:588:G:H22	2.08	0.51
49:S2:855:G:HO2'	49:S2:856:C:P	2.34	0.51
63:SQ:40:GLU:OE1	63:SQ:40:GLU:N	2.43	0.51
72:SZ:65:TYR:OH	72:SZ:76:ARG:HD3	2.10	0.51
3:LB:45:ALA:HB3	3:LB:183:ILE:HG23	1.93	0.51
48:Lr:65:LYS:O	48:Lr:102:TYR:OH	2.26	0.51
49:S2:96:C:H1'	49:S2:474:G:H5'	1.92	0.51
49:S2:855:G:O2'	49:S2:856:C:O5'	2.29	0.51
49:S2:928:G:H1	49:S2:1013:U:H3	1.58	0.51
54:SG:33:ALA:N	54:SG:52:ILE:O	2.41	0.51
57:SJ:160:SER:O	57:SJ:163:SER:OG	2.29	0.51
65:SS:13:LEU:HB2	65:SS:20:ILE:HG12	1.91	0.51
65:SS:15:VAL:HG12	65:SS:68:ILE:HD11	1.92	0.51
71:SY:12:PHE:HD1	71:SY:23:MET:HG2	1.75	0.51
81:Le:38:PRO:HB2	81:Le:46:ARG:HB3	1.91	0.51
1:LA:183:GLY:HA2	8:L5:1613:A:H5''	1.92	0.51
8:L5:138:G:H2'	8:L5:139:G:H8	1.75	0.51
8:L5:267:G:H2'	8:L5:268:G:H8	1.76	0.51
8:L5:978:G:H2'	8:L5:979:C:H6	1.75	0.51
8:L5:2526:C:N4	30:LX:84:GLU:OE2	2.43	0.51
18:LL:42:LYS:O	18:LL:46:ILE:HG12	2.09	0.51
19:LM:92:ALA:HA	19:LM:95:ILE:HG12	1.91	0.51
49:S2:562:U:O4'	57:SJ:132:GLN:NE2	2.44	0.51
56:SI:86:SER:O	56:SI:88:ASN:N	2.42	0.51
8:L5:1217:G:H2'	8:L5:1218:G:O4'	2.10	0.51
8:L5:1873:A:OP2	34:Lb:5:LYS:NZ	2.38	0.51
8:L5:2765:A:H2'	8:L5:2766:A:C8	2.46	0.51
8:L5:2899:C:OP1	24:LR:108:ARG:NH2	2.43	0.51
49:S2:443:U:H3	49:S2:447:A:H62	1.57	0.51
52:SE:246:LEU:HB2	52:SE:250:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:SM:31:LEU:HB2	80:SM:110:VAL:O	2.11	0.51
80:SM:89:VAL:HG13	80:SM:91:LEU:HD13	1.92	0.51
4:SB:127:VAL:HG11	4:SB:176:VAL:HG11	1.93	0.51
8:L5:1198:G:H2'	8:L5:1199:G:C8	2.45	0.51
8:L5:2704:C:H2'	8:L5:2705:G:H8	1.75	0.51
30:LX:81:LEU:HD22	30:LX:97:VAL:HG11	1.92	0.51
38:Lg:78:TYR:HB3	38:Lg:82:MET:HB2	1.92	0.51
49:S2:1713:C:H2'	49:S2:1714:U:C6	2.46	0.51
53:SF:113:VAL:O	53:SF:117:ILE:HG23	2.11	0.51
67:SU:44:LYS:C	67:SU:46:LYS:H	2.19	0.51
80:SM:32:ALA:HB1	80:SM:37:GLU:HB3	1.92	0.51
3:LB:357:ARG:HD2	8:L5:4615:C:H5''	1.91	0.51
8:L5:1241:C:O2	34:Lb:115:GLY:HA2	2.10	0.51
8:L5:1739:G:N3	8:L5:1742:A:N6	2.59	0.51
8:L5:1877:G:O6	34:Lb:10:HIS:NE2	2.36	0.51
8:L5:2570:U:H2'	8:L5:2571:C:C6	2.46	0.51
16:LH:74:CYS:O	16:LH:78:GLN:HG3	2.10	0.51
49:S2:1298:G:H5''	62:SP:77:LYS:HB2	1.92	0.51
56:SI:136:ILE:C	56:SI:138:ASN:H	2.19	0.51
74:Sb:67:THR:HG22	74:Sb:68:GLY:H	1.76	0.51
8:L5:1198:G:H2'	8:L5:1199:G:H8	1.74	0.51
8:L5:1290:G:H5''	13:LE:219:LYS:HD2	1.93	0.51
8:L5:1521:C:H5'	11:LC:95:MET:HE1	1.92	0.51
8:L5:3736:A:O2'	8:L5:3737:A:C8	2.63	0.51
8:L5:4174:U:H2'	8:L5:4175:G:H8	1.75	0.51
25:LS:29:ARG:HB2	26:LT:148:PRO:HB2	1.93	0.51
27:LU:26:THR:O	27:LU:30:GLU:HG2	2.11	0.51
49:S2:919:A:OP2	60:SN:64:ARG:NH1	2.42	0.51
49:S2:924:G:H21	60:SN:87:ASP:CG	2.19	0.51
49:S2:1653:U:H2'	49:S2:1654:G:C8	2.45	0.51
3:LB:385:LYS:NZ	8:L5:5002:U:OP2	2.44	0.50
8:L5:162:A:H2'	8:L5:163:A:C8	2.46	0.50
8:L5:1920:C:H3'	8:L5:1921:C:H5''	1.92	0.50
8:L5:4459:U:H2'	8:L5:4460:U:C6	2.46	0.50
8:L5:4736:C:H2'	8:L5:4737:G:H8	1.77	0.50
23:LQ:79:THR:HB	23:LQ:136:THR:HG22	1.92	0.50
52:SE:191:ARG:HH11	52:SE:245:ARG:HE	1.59	0.50
71:SY:15:ASN:ND2	71:SY:22:GLN:OE1	2.43	0.50
8:L5:1961:G:H21	8:L5:2025:A:H62	1.58	0.50
8:L5:3641:U:H5	8:L5:3646:A:N7	2.09	0.50
8:L5:4344:U:O2'	46:Lo:28:LYS:O	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L8:102:G:OP2	10:L8:104:A:O2'	2.27	0.50
17:LJ:22:LEU:HA	17:LJ:130:PHE:HB3	1.93	0.50
44:Lm:94:MET:C	44:Lm:95:ILE:HD13	2.37	0.50
49:S2:1217:A:H2'	49:S2:1218:C:C6	2.46	0.50
49:S2:1286:G:H8	49:S2:1286:G:OP2	1.95	0.50
49:S2:1628:C:H2'	49:S2:1629:C:C6	2.46	0.50
69:SW:86:LEU:HD21	69:SW:113:HIS:HB2	1.92	0.50
2:SA:56:GLU:HG2	68:SV:79:VAL:HG13	1.93	0.50
6:B4:18:G:N3	6:B4:56:G:N2	2.59	0.50
7:D4:5:G:O2'	7:D4:6:G:H5'	2.12	0.50
7:D4:8:U:O2'	7:D4:15:G:N2	2.44	0.50
8:L5:1328:G:O2'	8:L5:2349:A:OP1	2.28	0.50
31:LY:82:ILE:HG22	31:LY:83:GLU:H	1.76	0.50
49:S2:57:U:OP1	49:S2:504:G:O2'	2.29	0.50
49:S2:60:A:N3	49:S2:316:G:O2'	2.36	0.50
52:SE:136:ILE:HG23	52:SE:149:TYR:CZ	2.46	0.50
8:L5:258:G:H2'	8:L5:259:C:H6	1.76	0.50
8:L5:3600:G:H2'	8:L5:3601:C:C6	2.45	0.50
19:LM:43:THR:O	19:LM:43:THR:HG22	2.11	0.50
47:Lp:27:LYS:O	47:Lp:31:ILE:HG23	2.12	0.50
49:S2:1863:A:OP2	73:Sa:4:LYS:NZ	2.43	0.50
50:SC:125:LYS:HB3	50:SC:143:CYS:HB2	1.93	0.50
52:SE:247:THR:HG23	52:SE:249:ALA:H	1.76	0.50
57:SJ:83:ARG:HG2	57:SJ:150:ARG:HD2	1.94	0.50
7:D4:51:U:O2	7:D4:63:G:N2	2.30	0.50
8:L5:352:G:C8	11:LC:193:LYS:HD3	2.47	0.50
8:L5:433:A:C2	8:L5:3867:A:H4'	2.46	0.50
8:L5:3923:A:H2'	8:L5:3924:C:C6	2.46	0.50
49:S2:571:U:O2'	71:SY:60:PHE:O	2.27	0.50
49:S2:846:G:OP2	52:SE:108:ARG:NH1	2.35	0.50
49:S2:1253:A:OP2	49:S2:1526:G:N2	2.32	0.50
49:S2:1345:G:OP1	49:S2:1688:C:O2'	2.28	0.50
52:SE:11:ARG:NH1	52:SE:20:LEU:HB3	2.27	0.50
55:SH:49:LYS:HG3	55:SH:63:PHE:HE1	1.75	0.50
56:SI:103:LEU:HG	56:SI:170:LYS:HB3	1.92	0.50
64:SR:14:ARG:HG2	64:SR:69:ILE:HG13	1.93	0.50
4:SB:107:ARG:NH1	61:SO:135:ILE:HD12	2.25	0.50
7:D4:8:U:H1'	7:D4:15:G:N1	2.26	0.50
8:L5:2362:U:H2'	8:L5:2363:A2M:H8	1.93	0.50
8:L5:2563:C:H2'	8:L5:2564:G:O4'	2.11	0.50
16:LH:44:GLU:CG	16:LH:58:ASP:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LL:116:ARG:NH2	18:LL:155:MET:O	2.39	0.50
20:LN:107:GLY:HA3	20:LN:160:GLU:OE1	2.12	0.50
49:S2:525:A:OP2	77:Se:99:LYS:NZ	2.30	0.50
2:SA:34:MET:HE2	2:SA:149:ASN:O	2.12	0.50
8:L5:1690:C:OP2	23:LQ:11:ARG:NH2	2.39	0.50
11:LC:14:LYS:N	11:LC:14:LYS:HD3	2.27	0.50
35:Lc:17:ARG:HD2	35:Lc:108:MET:CE	2.39	0.50
49:S2:1232:U:H2'	49:S2:1233:G:H8	1.77	0.50
49:S2:1664:A:O2'	49:S2:1665:G:OP1	2.21	0.50
49:S2:1736:G:H2'	49:S2:1737:G:H8	1.76	0.50
49:S2:1865:C:OP2	73:Sa:5:ARG:NH1	2.45	0.50
52:SE:70:ILE:HD11	52:SE:90:ILE:HG22	1.94	0.50
82:LI:189:ARG:NH1	82:LI:199:TYR:OH	2.45	0.50
3:LB:59:GLU:HG3	3:LB:366:LYS:HD2	1.94	0.50
4:SB:157:GLN:HB2	4:SB:160:GLN:HG3	1.94	0.50
8:L5:172:C:H4'	8:L5:173:C:H5'	1.94	0.50
8:L5:256:G:H2'	8:L5:257:C:C6	2.47	0.50
8:L5:1249:C:H2'	8:L5:1250:C:H6	1.77	0.50
8:L5:1504:G:H2'	8:L5:1505:C:C6	2.46	0.50
8:L5:4862:G:H2'	8:L5:4863:G:C8	2.47	0.50
17:LJ:39:VAL:HG21	17:LJ:112:HIS:CD2	2.46	0.50
30:LX:55:ARG:HH11	30:LX:55:ARG:HG3	1.76	0.50
39:Lh:88:THR:OG1	39:Lh:91:MET:HG2	2.12	0.50
48:Lr:54:ALA:HA	48:Lr:61:VAL:HG23	1.92	0.50
49:S2:1395:C:HO2'	49:S2:1396:A:C5'	2.25	0.50
50:SC:66:LEU:HD11	50:SC:81:ILE:HG12	1.94	0.50
61:SO:34:PHE:HB3	61:SO:41:PHE:HB2	1.93	0.50
64:SR:120:THR:HG22	64:SR:121:GLN:N	2.23	0.50
79:Sg:64:HIS:HD2	79:Sg:83:TRP:HB3	1.77	0.50
79:Sg:304:ASP:O	79:Sg:306:LEU:N	2.44	0.50
1:LA:13:GLY:O	1:LA:17:ARG:NH1	2.45	0.50
1:LA:177:LYS:HD2	47:Lp:29:ILE:HG21	1.93	0.50
8:L5:1731:C:OP1	26:LT:100:LYS:NZ	2.37	0.50
12:LD:99:TYR:CD2	12:LD:199:ILE:HD13	2.47	0.50
35:Lc:17:ARG:CD	35:Lc:108:MET:HE1	2.39	0.50
49:S2:118:C:H1'	49:S2:445:A:C5	2.47	0.50
49:S2:311:C:H5'	49:S2:312:G:H5''	1.94	0.50
51:SD:122:VAL:O	51:SD:126:ILE:HG23	2.11	0.50
59:SL:77:VAL:HG23	59:SL:122:ILE:HA	1.94	0.50
62:SP:17:TYR:HB3	62:SP:25:LEU:HD11	1.93	0.50
82:LI:85:PHE:HD2	82:LI:87:ILE:HG13	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LB:77:THR:HG21	3:LB:337:VAL:HG13	1.94	0.49
8:L5:263:G:N1	8:L5:264:C:O2	2.45	0.49
8:L5:3652:A:H2'	8:L5:3653:A:C8	2.47	0.49
49:S2:12:U:H2'	49:S2:13:C:C6	2.46	0.49
52:SE:126:VAL:HA	52:SE:141:THR:HA	1.94	0.49
75:Sc:17:VAL:HG22	75:Sc:30:VAL:HG12	1.94	0.49
78:Sf:135:HIS:HB3	78:Sf:138:ARG:NH1	2.27	0.49
8:L5:978:G:H2'	8:L5:979:C:C6	2.47	0.49
8:L5:2614:C:O2'	8:L5:2808:G:OP1	2.26	0.49
8:L5:4504:C:H2'	8:L5:4505:C:C6	2.46	0.49
24:LR:7:GLN:OE1	24:LR:7:GLN:N	2.45	0.49
49:S2:1862:G:O2'	49:S2:1864:U:OP2	2.29	0.49
69:SW:11:LEU:HD12	69:SW:74:VAL:HB	1.95	0.49
82:LI:88:ARG:HD2	82:LI:90:ARG:HD2	1.94	0.49
3:LB:92:TYR:HB2	3:LB:159:VAL:CG1	2.43	0.49
8:L5:422:C:H2'	8:L5:423:G:H8	1.77	0.49
8:L5:4537:C:H2'	8:L5:4538:G:H8	1.76	0.49
8:L5:4600:G:O2'	8:L5:4609:G:O6	2.28	0.49
10:L8:142:U:OP1	20:LN:38:ARG:NH2	2.44	0.49
13:LE:150:LEU:HD13	13:LE:194:VAL:HG11	1.93	0.49
49:S2:581:U:H4'	71:SY:66:GLY:HA2	1.94	0.49
49:S2:1413:G:H2'	49:S2:1414:A:H8	1.77	0.49
50:SC:270:THR:O	50:SC:274:VAL:HG23	2.10	0.49
52:SE:247:THR:HG22	52:SE:250:GLU:HG3	1.93	0.49
55:SH:60:ILE:HG13	55:SH:92:VAL:HA	1.94	0.49
57:SJ:78:LEU:O	57:SJ:82:VAL:HG13	2.11	0.49
78:Sf:107:LYS:O	78:Sf:114:ILE:HA	2.13	0.49
4:SB:58:ALA:O	4:SB:62:LEU:HD23	2.12	0.49
5:A4:47:A:N1	6:B4:34:A:N1	2.60	0.49
6:B4:52:G:H2'	6:B4:53:A:H8	1.77	0.49
8:L5:956:A:H1'	8:L5:2076:G:H5''	1.93	0.49
8:L5:2521:G:H4'	38:Lg:26:PRO:HD2	1.94	0.49
8:L5:3610:A:H2'	8:L5:3611:A:H8	1.77	0.49
8:L5:3715:U:H2'	8:L5:3716:C:O4'	2.13	0.49
10:L8:141:C:H2'	10:L8:142:U:C6	2.47	0.49
16:LH:43:VAL:HG21	16:LH:73:ILE:HD12	1.93	0.49
17:LJ:63:ARG:HD3	46:Lo:103:VAL:CG1	2.43	0.49
21:LO:142:ALA:HA	21:LO:145:VAL:HG22	1.94	0.49
31:LY:80:ILE:HG23	31:LY:101:PRO:HG3	1.93	0.49
42:Lk:56:LEU:HA	42:Lk:59:SER:OG	2.11	0.49
49:S2:29:G:H2'	49:S2:30:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:29:G:OP1	70:SX:124:LYS:NZ	2.46	0.49
49:S2:104:A:H62	49:S2:356:C:H5	1.60	0.49
49:S2:878:G:O6	49:S2:908:A:N1	2.46	0.49
49:S2:1546:G:N3	49:S2:1670:C:O2'	2.42	0.49
63:SQ:18:THR:O	63:SQ:18:THR:OG1	2.28	0.49
65:SS:85:ASN:OD1	65:SS:86:ARG:N	2.38	0.49
67:SU:34:LYS:O	67:SU:38:ASP:OD1	2.30	0.49
82:LI:36:LEU:HD13	82:LI:73:ASN:OD1	2.12	0.49
2:SA:52:LYS:HB2	64:SR:109:LEU:CD1	2.41	0.49
8:L5:711:A:H2'	8:L5:712:C:C6	2.47	0.49
8:L5:2086:G:H5''	11:LC:306:ARG:HH21	1.78	0.49
8:L5:2758:G:H2'	8:L5:2759:G:C5	2.48	0.49
8:L5:3615:G:O3'	29:LW:44:ARG:NH1	2.45	0.49
8:L5:3861:A:H2'	8:L5:3862:A:H8	1.75	0.49
21:LO:126:VAL:HG13	21:LO:127:VAL:HG13	1.93	0.49
35:Lc:17:ARG:C	35:Lc:19:GLN:H	2.20	0.49
35:Lc:21:VAL:HG23	35:Lc:22:MET:H	1.77	0.49
49:S2:996:A:H5''	60:SN:7:PRO:HG3	1.95	0.49
49:S2:1232:U:H2'	49:S2:1233:G:C8	2.47	0.49
49:S2:1337:4AC:P	76:Sd:44:ARG:HH22	2.35	0.49
50:SC:275:LYS:HG3	50:SC:276:THR:HG23	1.95	0.49
52:SE:191:ARG:NH1	52:SE:245:ARG:HE	2.10	0.49
55:SH:101:LEU:HB2	55:SH:116:ARG:HD3	1.93	0.49
71:SY:27:VAL:HG21	71:SY:35:VAL:HG21	1.93	0.49
79:Sg:44:LYS:NZ	79:Sg:56:GLN:OE1	2.30	0.49
82:LI:51:HIS:HD2	82:LI:168:SER:HB2	1.76	0.49
8:L5:1719:A:H2'	8:L5:1720:C:C6	2.48	0.49
8:L5:2704:C:H2'	8:L5:2705:G:C8	2.48	0.49
8:L5:4638:U:H2'	8:L5:4639:G:N3	2.27	0.49
8:L5:4967:A:H2'	8:L5:4968:A:C8	2.47	0.49
10:L8:26:C:O2'	11:LC:53:ALA:O	2.28	0.49
16:LH:126:VAL:HG21	16:LH:161:ILE:HG12	1.95	0.49
19:LM:99:GLU:O	19:LM:103:LYS:HG2	2.11	0.49
21:LO:151:ALA:O	21:LO:155:THR:HG23	2.13	0.49
36:Ld:92:ARG:HA	36:Ld:102:LEU:HD13	1.94	0.49
41:Lj:20:ARG:NH2	41:Lj:39:TYR:OH	2.41	0.49
49:S2:644:OMG:H5'	57:SJ:41:ARG:HH22	1.77	0.49
51:SD:95:GLY:HA2	51:SD:101:GLN:NE2	2.27	0.49
82:LI:76:MET:HE2	82:LI:138:ILE:HG21	1.95	0.49
4:SB:52:THR:HB	4:SB:58:ALA:H	1.77	0.49
8:L5:1296:G:H2'	8:L5:1297:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:1339:U:H2'	8:L5:1340:OMC:C6	2.48	0.49
8:L5:3861:A:H2'	8:L5:3862:A:C8	2.48	0.49
8:L5:4584:A:H2'	8:L5:4585:U:O4'	2.13	0.49
10:L8:144:U:H2'	10:L8:145:C:C6	2.48	0.49
12:LD:128:ASP:OD1	12:LD:129:GLU:N	2.42	0.49
21:LO:121:PRO:HD3	25:LS:168:THR:HG22	1.95	0.49
34:Lb:94:ASP:OD1	34:Lb:94:ASP:N	2.44	0.49
49:S2:588:G:H4'	49:S2:589:G:H5'	1.95	0.49
49:S2:829:C:OP1	52:SE:22:LYS:HG2	2.13	0.49
49:S2:1798:C:H2'	49:S2:1799:G:O4'	2.12	0.49
8:L5:742:G:N2	8:L5:743:G:O6	2.46	0.49
8:L5:1349:G:OP1	23:LQ:15:ARG:NH2	2.46	0.49
8:L5:1739:G:H2'	8:L5:1740:C:C6	2.48	0.49
12:LD:235:MET:O	12:LD:238:GLU:HG2	2.12	0.49
24:LR:157:ASP:OD1	24:LR:158:GLN:N	2.45	0.49
36:Ld:18:ASN:O	36:Ld:90:ARG:NH1	2.45	0.49
49:S2:677:G:OP1	60:SN:120:SER:OG	2.31	0.49
50:SC:70:VAL:HG21	50:SC:93:ILE:HG23	1.95	0.49
78:Sf:121:CYS:HB2	78:Sf:132:MET:HG2	1.94	0.49
8:L5:1333:A:H2'	8:L5:1334:A:C8	2.48	0.49
8:L5:4336:A:H5''	8:L5:4337:C:H5'	1.95	0.49
8:L5:4967:A:H2'	8:L5:4968:A:H8	1.77	0.49
24:LR:3:MET:HE1	24:LR:5:ARG:NE	2.28	0.49
38:Lg:5:LEU:HD23	38:Lg:5:LEU:H	1.76	0.49
41:Lj:56:ARG:O	41:Lj:57:THR:CG2	2.59	0.49
49:S2:1849:G:HO2'	49:S2:1850:MA6:H8	1.77	0.49
50:SC:173:LYS:HB3	68:SV:3:ASN:HA	1.95	0.49
55:SH:9:VAL:N	55:SH:24:SER:OG	2.46	0.49
55:SH:30:LEU:O	55:SH:34:SER:OG	2.27	0.49
75:Sc:51:ARG:N	75:Sc:54:ASP:OD2	2.35	0.49
8:L5:308:G:O6	20:LN:12:ARG:NH1	2.46	0.49
8:L5:1969:G:H3'	8:L5:1970:A:C8	2.46	0.49
8:L5:2664:G:OP1	24:LR:110:ARG:NH1	2.46	0.49
8:L5:4251:A:C2	17:LJ:127:GLY:HA3	2.47	0.49
8:L5:4563:U:H2'	8:L5:4564:A:H8	1.78	0.49
12:LD:51:MET:HE1	12:LD:166:ALA:HB2	1.94	0.49
17:LJ:44:THR:OG1	17:LJ:45:GLY:N	2.45	0.49
20:LN:9:GLU:HB2	40:Li:44:ILE:HG13	1.94	0.49
31:LY:37:GLU:HG3	31:LY:38:LEU:N	2.27	0.49
36:Ld:64:ILE:HG23	36:Ld:68:LEU:HD21	1.94	0.49
49:S2:845:G:H2'	49:S2:846:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1189:A:H2'	49:S2:1190:A:H8	1.78	0.49
49:S2:1221:G:O2'	49:S2:1676:U:O2	2.25	0.49
54:SG:181:THR:HG22	54:SG:184:VAL:HG23	1.95	0.49
60:SN:46:THR:HG22	60:SN:86:GLU:OE1	2.12	0.49
65:SS:22:GLY:HA2	65:SS:56:ALA:HB3	1.94	0.49
79:Sg:218:LEU:HD11	79:Sg:228:TYR:CZ	2.47	0.49
18:LL:43:ALA:O	18:LL:149:GLN:NE2	2.35	0.48
49:S2:855:G:O2'	49:S2:856:C:H6	1.94	0.48
79:Sg:163:PRO:HB2	79:Sg:179:LEU:HB2	1.95	0.48
2:SA:148:CYS:SG	2:SA:160:ALA:HB1	2.53	0.48
8:L5:73:A:OP1	18:LL:106:SER:OG	2.31	0.48
8:L5:1802:A:N3	26:LT:130:ARG:NH2	2.59	0.48
8:L5:2848:G:N2	8:L5:3839:G:OP2	2.39	0.48
8:L5:3736:A:HO2'	8:L5:3737:A:H8	1.58	0.48
8:L5:3925:OMU:HM23	8:L5:3925:OMU:H1'	1.52	0.48
10:L8:66:A:H2'	10:L8:67:U:C6	2.48	0.48
13:LE:141:ARG:NH2	13:LE:191:GLN:O	2.47	0.48
28:LV:107:ASN:HB3	28:LV:111:GLU:HG2	1.95	0.48
34:Lb:91:ARG:HB2	34:Lb:94:ASP:OD1	2.12	0.48
49:S2:4:C:H4'	50:SC:207:ALA:HB2	1.94	0.48
49:S2:209:A:H2'	49:S2:210:U:O4'	2.14	0.48
50:SC:234:GLY:O	50:SC:238:LYS:HG2	2.13	0.48
60:SN:46:THR:O	60:SN:50:ILE:HG13	2.13	0.48
1:LA:186:TYR:HB2	1:LA:196:TRP:CZ3	2.48	0.48
3:LB:13:SER:HB2	8:L5:4622:A:H4'	1.94	0.48
8:L5:371:A:N3	8:L5:1531:U:O2'	2.45	0.48
8:L5:425:U:H2'	8:L5:426:A:H8	1.77	0.48
8:L5:444:G:H2'	8:L5:445:U:C6	2.48	0.48
8:L5:2079:G:H2'	8:L5:2080:U:C6	2.47	0.48
8:L5:2458:C:H1'	8:L5:3671:G:H21	1.78	0.48
8:L5:2601:A:OP1	38:Lg:40:LYS:NZ	2.38	0.48
8:L5:3701:OMC:H4'	8:L5:3702:A:O5'	2.13	0.48
16:LH:15:ASN:OD1	16:LH:16:VAL:HG23	2.13	0.48
16:LH:93:ARG:NH1	44:Lm:82:LEU:HD21	2.28	0.48
25:LS:69:GLU:HG3	25:LS:101:THR:HG22	1.95	0.48
27:LU:28:PRO:HB2	27:LU:34:MET:HB2	1.95	0.48
38:Lg:60:ARG:HA	38:Lg:60:ARG:HD2	1.70	0.48
50:SC:132:ASP:C	50:SC:132:ASP:OD1	2.56	0.48
61:SO:84:ARG:HH11	61:SO:88:LEU:HD21	1.77	0.48
82:LI:206:LEU:HD23	82:LI:210:ARG:HH21	1.79	0.48
8:L5:162:A:H2'	8:L5:163:A:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:364:G:C6	41:Lj:52:LYS:HE3	2.47	0.48
8:L5:1478:C:H2'	8:L5:1479:G:H8	1.78	0.48
8:L5:1912:G:N2	21:LO:87:MET:SD	2.86	0.48
8:L5:2323:C:H2'	8:L5:2324:C:H6	1.78	0.48
8:L5:2324:C:O2'	81:Le:98:GLU:OE1	2.32	0.48
8:L5:3845:A:H2'	8:L5:3846:C:C6	2.49	0.48
17:LJ:108:GLY:HA2	17:LJ:129:ASP:HA	1.96	0.48
32:LZ:83:THR:HG22	38:Lg:95:PHE:CE1	2.47	0.48
49:S2:15:U:H2'	49:S2:16:G:O4'	2.13	0.48
49:S2:809:A:H4'	52:SE:221:ARG:NH2	2.28	0.48
49:S2:1405:A:H2'	49:S2:1406:G:O4'	2.13	0.48
52:SE:183:VAL:CG1	52:SE:220:THR:HG21	2.43	0.48
54:SG:141:ILE:HD13	54:SG:157:VAL:HG12	1.95	0.48
56:SI:161:LEU:O	56:SI:165:GLN:HG2	2.12	0.48
59:SL:134:LEU:HB2	59:SL:138:VAL:HG23	1.96	0.48
67:SU:56:MET:HB2	67:SU:86:LYS:HB3	1.95	0.48
69:SW:23:ARG:HG3	74:Sb:4:ALA:HB2	1.94	0.48
3:LB:3:HIS:HB2	8:L5:4516:G:N7	2.28	0.48
3:LB:291:TYR:CE1	3:LB:299:ILE:HG22	2.49	0.48
4:SB:127:VAL:HG21	4:SB:176:VAL:HG13	1.96	0.48
8:L5:186:G:H4'	8:L5:187:U:H5'	1.95	0.48
8:L5:3809:G:OP2	8:L5:3809:G:N2	2.32	0.48
8:L5:4691:A:H5'	16:LH:71:ARG:HE	1.78	0.48
32:LZ:16:GLY:O	32:LZ:19:SER:OG	2.30	0.48
32:LZ:112:ARG:O	32:LZ:112:ARG:HD3	2.13	0.48
49:S2:1005:G:H2'	49:S2:1006:C:H6	1.77	0.48
65:SS:28:PHE:HE1	65:SS:38:ARG:HD3	1.77	0.48
71:SY:21:LYS:HB2	71:SY:75:ILE:HB	1.94	0.48
8:L5:364:G:N7	41:Lj:55:ARG:NH1	2.61	0.48
8:L5:1371:A:N1	10:L8:28:C:O2'	2.46	0.48
8:L5:1617:G:H1'	8:L5:2513:A:N6	2.29	0.48
8:L5:2017:A:H2'	8:L5:2017:A:N3	2.28	0.48
8:L5:2847:G:H1'	28:LV:21:PRO:HD2	1.95	0.48
35:Lc:103:ASP:O	35:Lc:107:SER:HB3	2.14	0.48
49:S2:562:U:O2'	49:S2:563:G:H8	1.97	0.48
49:S2:958:G:H2'	49:S2:959:G:C8	2.48	0.48
49:S2:1628:C:H2'	49:S2:1629:C:H6	1.79	0.48
56:SI:88:ASN:O	56:SI:88:ASN:ND2	2.46	0.48
65:SS:125:HIS:NE2	65:SS:131:VAL:HG21	2.29	0.48
71:SY:79:LEU:C	71:SY:81:TYR:H	2.22	0.48
74:Sb:83:GLN:OE1	74:Sb:83:GLN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:165:ARG:HG2	4:SB:169:MET:HE2	1.96	0.48
7:D4:66:U:H2'	7:D4:67:C:C6	2.49	0.48
8:L5:280:G:OP1	20:LN:47:LYS:HE2	2.14	0.48
8:L5:1079:C:H2'	8:L5:1080:C:H6	1.79	0.48
8:L5:1345:A:H2'	8:L5:1346:C:C6	2.49	0.48
8:L5:4126:C:H5''	8:L5:4127:A:H5''	1.95	0.48
20:LN:80:THR:OG1	20:LN:80:THR:O	2.32	0.48
24:LR:175:GLU:O	24:LR:176:ARG:HG2	2.14	0.48
25:LS:99:ASP:OD1	25:LS:100:LEU:N	2.45	0.48
48:Lr:51:VAL:HG12	48:Lr:62:VAL:HG22	1.95	0.48
49:S2:190:G:H5''	56:SI:145:ILE:HD12	1.96	0.48
49:S2:528:A:H2'	49:S2:529:A:C8	2.48	0.48
80:SM:54:SER:OG	80:SM:80:ASP:CA	2.47	0.48
1:LA:183:GLY:CA	8:L5:1613:A:H5''	2.44	0.48
8:L5:1857:C:H2'	8:L5:1858:A:C8	2.49	0.48
8:L5:2580:U:OP1	32:LZ:36:ARG:NH1	2.35	0.48
8:L5:4771:C:H2'	8:L5:4772:C:C6	2.49	0.48
17:LJ:30:GLY:O	17:LJ:34:THR:HG23	2.14	0.48
19:LM:108:ASP:HB3	21:LO:199:HIS:NE2	2.29	0.48
21:LO:113:ASP:OD1	21:LO:114:LYS:HG3	2.13	0.48
44:Lm:96:CYS:CB	44:Lm:99:CYS:H	2.26	0.48
49:S2:569:A:H2'	49:S2:570:C:O4'	2.14	0.48
49:S2:1158:G:O3'	69:SW:76:SER:OG	2.19	0.48
49:S2:1839:U:H2'	49:S2:1840:U:C6	2.49	0.48
61:SO:45:THR:HA	61:SO:52:THR:HA	1.96	0.48
66:ST:65:TYR:HB2	66:ST:123:LEU:HD22	1.96	0.48
67:SU:40:ILE:HG23	67:SU:44:LYS:HE2	1.96	0.48
69:SW:102:ILE:H	69:SW:113:HIS:HD2	1.61	0.48
70:SX:40:PRO:O	70:SX:77:ASN:ND2	2.46	0.48
1:LA:175:ILE:HD13	8:L5:3683:C:O4'	2.13	0.48
8:L5:1443:A:H61	8:L5:2104:G:N2	2.11	0.48
8:L5:2529:A:O2'	8:L5:2531:C:OP2	2.32	0.48
8:L5:3723:A2M:HM'3	8:L5:3723:A2M:H1'	1.63	0.48
8:L5:4918:C:H2'	8:L5:4919:G:C8	2.49	0.48
9:L7:23:A:H2'	9:L7:24:C:C6	2.48	0.48
10:L8:8:U:H2'	10:L8:9:A:C8	2.49	0.48
11:LC:13:GLU:HG3	11:LC:14:LYS:HD3	1.96	0.48
12:LD:210:TYR:HA	12:LD:213:GLU:HG2	1.95	0.48
24:LR:172:ARG:HH12	49:S2:909:G:P	2.37	0.48
49:S2:957:A:H2'	49:S2:958:G:H21	1.79	0.48
51:SD:7:LYS:HD3	67:SU:25:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SE:62:LYS:HB2	52:SE:80:ILE:HD11	1.95	0.48
53:SF:204:ARG:CZ	75:Sc:60:GLU:HG2	2.44	0.48
79:Sg:246:TYR:HD2	79:Sg:262:GLU:HG2	1.78	0.48
2:SA:85:ARG:NH1	2:SA:205:ARG:HD3	2.28	0.48
2:SA:154:LEU:HD22	2:SA:157:VAL:HG21	1.96	0.48
8:L5:4:G:H2'	8:L5:5:A:H8	1.79	0.48
8:L5:2103:G:H2'	8:L5:2103:G:N3	2.29	0.48
37:Lf:45:LYS:HA	37:Lf:107:PRO:HD2	1.94	0.48
39:Lh:34:ALA:HA	39:Lh:37:THR:HG22	1.96	0.48
49:S2:1109:C:HO2'	49:S2:1110:G:H8	1.61	0.48
62:SP:29:SER:OG	62:SP:30:TYR:N	2.47	0.48
71:SY:109:GLU:HB3	71:SY:113:ARG:NH2	2.29	0.48
2:SA:41:ARG:NH1	49:S2:1126:G:OP1	2.22	0.47
8:L5:126:C:H2'	8:L5:127:G:H8	1.79	0.47
8:L5:175:C:H2'	8:L5:176:G:H8	1.78	0.47
8:L5:175:C:H2'	8:L5:176:G:C8	2.49	0.47
8:L5:418:A:N6	10:L8:16:G:H1'	2.29	0.47
8:L5:2745:A:H2'	8:L5:2746:A:H8	1.79	0.47
8:L5:4137:C:H2'	8:L5:4138:C:C6	2.49	0.47
8:L5:4612:C:C2	16:LH:120:GLU:HB3	2.49	0.47
10:L8:14:OMU:HM23	10:L8:14:OMU:H1'	1.55	0.47
15:LG:175:ARG:HD3	15:LG:230:TYR:CD2	2.49	0.47
49:S2:1745:A:C8	54:SG:65:GLN:HG3	2.49	0.47
61:SO:94:HIS:HA	61:SO:127:GLY:O	2.13	0.47
62:SP:106:GLU:OE1	62:SP:108:LYS:HE3	2.14	0.47
3:LB:29:VAL:HG22	3:LB:220:ILE:HD11	1.96	0.47
3:LB:168:MET:HA	3:LB:171:LEU:HD12	1.95	0.47
8:L5:1521:C:OP1	11:LC:100:ARG:NH2	2.46	0.47
8:L5:1964:A:N6	8:L5:2023:C:O2'	2.42	0.47
8:L5:2545:U:H3'	8:L5:2546:G:H4'	1.95	0.47
49:S2:1005:G:H2'	49:S2:1006:C:C6	2.48	0.47
51:SD:76:ARG:O	51:SD:76:ARG:NH1	2.41	0.47
55:SH:10:LYS:O	55:SH:10:LYS:HG3	2.13	0.47
70:SX:128:VAL:HG23	70:SX:133:LEU:HD11	1.95	0.47
79:Sg:195:LEU:HA	79:Sg:211:GLY:HA3	1.96	0.47
2:SA:42:LYS:HG3	2:SA:48:ILE:HD11	1.96	0.47
8:L5:4694:G:OP1	8:L5:4694:G:N2	2.48	0.47
17:LJ:19:LYS:HE2	17:LJ:133:VAL:HG11	1.97	0.47
21:LO:38:CYS:O	21:LO:138:LEU:HD21	2.14	0.47
24:LR:163:ARG:HD3	49:S2:871:U:H1'	1.95	0.47
49:S2:388:U:H2'	49:S2:389:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1158:G:H5''	69:SW:76:SER:HB2	1.95	0.47
49:S2:1614:A:H2'	49:S2:1615:U:C6	2.50	0.47
8:L5:171:U:H5''	8:L5:172:C:C5	2.49	0.47
8:L5:1448:G:H2'	8:L5:1449:C:H6	1.79	0.47
8:L5:2517:A:N3	8:L5:2539:C:O2'	2.47	0.47
8:L5:2602:G:H2'	8:L5:2603:C:C6	2.50	0.47
8:L5:2667:C:O4'	24:LR:96:MET:HG2	2.15	0.47
8:L5:3586:G:H2'	8:L5:3586:G:N3	2.28	0.47
8:L5:4212:A:N1	26:LT:3:ASN:ND2	2.47	0.47
8:L5:4260:U:H2'	8:L5:4261:C:H6	1.79	0.47
8:L5:4723:A:H2'	8:L5:4724:A:C8	2.50	0.47
10:L8:60:G:O6	10:L8:96:C:O2'	2.26	0.47
12:LD:164:LYS:HG2	12:LD:195:HIS:CE1	2.49	0.47
51:SD:142:LEU:HD12	51:SD:148:LYS:HG3	1.96	0.47
78:Sf:123:SER:HB3	78:Sf:126:CYS:HB2	1.96	0.47
1:LA:223:SER:HB3	8:L5:3748:A:O2'	2.14	0.47
4:SB:65:ARG:HH12	61:SO:51:GLU:HG3	1.80	0.47
8:L5:23:C:H2'	8:L5:24:G:O4'	2.14	0.47
8:L5:138:G:H2'	8:L5:139:G:C8	2.49	0.47
8:L5:491:G:H2'	8:L5:492:U:H6	1.79	0.47
8:L5:1199:G:H2'	8:L5:1200:G:C8	2.48	0.47
8:L5:1244:G:H2'	8:L5:1245:C:C6	2.49	0.47
8:L5:1669:A:P	34:Lb:18:ARG:HH12	2.38	0.47
8:L5:2803:U:H2'	8:L5:2804:OMC:H6	1.78	0.47
8:L5:3917:A:H2'	8:L5:3918:G:H8	1.79	0.47
8:L5:4940:C:O2'	13:LE:246:ARG:NH2	2.47	0.47
21:LO:19:LEU:O	21:LO:23:VAL:HG13	2.15	0.47
31:LY:52:ASP:HB2	31:LY:110:LYS:HG2	1.96	0.47
49:S2:1650:A:H2'	49:S2:1651:A:O4'	2.14	0.47
49:S2:1736:G:H2'	49:S2:1737:G:C8	2.49	0.47
54:SG:98:ARG:NH1	54:SG:101:ILE:O	2.43	0.47
61:SO:113:GLN:OE1	73:Sa:46:GLU:N	2.47	0.47
63:SQ:6:PRO:O	63:SQ:27:ARG:NH2	2.48	0.47
67:SU:68:THR:O	76:Sd:40:ARG:NH1	2.41	0.47
79:Sg:218:LEU:HD21	79:Sg:228:TYR:CE1	2.49	0.47
79:Sg:223:GLU:OE1	79:Sg:225:LYS:HE3	2.14	0.47
4:SB:28:LYS:HD3	4:SB:48:LEU:HD12	1.97	0.47
8:L5:423:G:H2'	8:L5:424:U:C6	2.50	0.47
8:L5:1443:A:C5	8:L5:1444:G:N7	2.83	0.47
8:L5:1890:G:OP2	8:L5:1890:G:N2	2.38	0.47
13:LE:213:THR:HG22	13:LE:214:ASP:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:53:LYS:HD3	16:LH:53:LYS:HA	1.63	0.47
33:La:71:PRO:HG2	33:La:108:TYR:HA	1.96	0.47
49:S2:964:A:H2'	49:S2:965:U:C6	2.48	0.47
49:S2:1259:A:H1'	49:S2:1264:C:H42	1.80	0.47
49:S2:1849:G:O2'	49:S2:1850:MA6:O5'	2.29	0.47
50:SC:168:GLY:N	50:SC:179:THR:O	2.37	0.47
52:SE:80:ILE:HG22	52:SE:81:THR:HG23	1.96	0.47
52:SE:141:THR:OG1	52:SE:143:ASP:OD1	2.33	0.47
54:SG:48:TYR:HE1	54:SG:116:LYS:HG3	1.80	0.47
58:SK:16:PHE:HE2	58:SK:89:ILE:HG22	1.79	0.47
81:Le:35:TRP:CZ2	81:Le:56:PRO:HD2	2.50	0.47
1:LA:58:LEU:HD23	1:LA:75:LEU:HD12	1.96	0.47
3:LB:257:TRP:CD1	3:LB:257:TRP:C	2.93	0.47
6:B4:37:A:O2'	49:S2:1058:A:OP1	2.27	0.47
8:L5:99:A:H4'	20:LN:181:HIS:CD2	2.50	0.47
8:L5:198:A:OP2	31:LY:126:ARG:NH2	2.48	0.47
8:L5:919:C:H2'	8:L5:920:C:H6	1.80	0.47
8:L5:1197:C:H2'	8:L5:1198:G:C8	2.50	0.47
8:L5:1326:A2M:HM'3	8:L5:1326:A2M:H1'	1.67	0.47
8:L5:1443:A:N1	8:L5:2103:G:O6	2.47	0.47
8:L5:1450:C:H2'	8:L5:1451:G:O4'	2.14	0.47
8:L5:1865:G:N2	8:L5:1868:A:OP2	2.42	0.47
8:L5:2306:G:H1'	8:L5:2332:A:N6	2.30	0.47
8:L5:2809:G:O2'	8:L5:4644:G:OP1	2.28	0.47
8:L5:2844:A:O2'	8:L5:4631:G:H4'	2.15	0.47
8:L5:3673:C:OP2	20:LN:67:ARG:NH2	2.43	0.47
8:L5:3934:G:H2'	8:L5:3935:C:C6	2.49	0.47
8:L5:4305:G:C6	26:LT:80:VAL:HG11	2.50	0.47
8:L5:4745:G:H1	8:L5:4955:A:N6	2.10	0.47
8:L5:4891:G:N2	19:LM:118:MET:HE1	2.29	0.47
15:LG:147:VAL:HG12	15:LG:179:VAL:HG11	1.97	0.47
18:LL:119:GLU:O	18:LL:123:LYS:HG2	2.14	0.47
20:LN:158:HIS:HB3	20:LN:161:MET:HG3	1.97	0.47
24:LR:95:TRP:CH2	24:LR:99:MET:HE3	2.50	0.47
30:LX:55:ARG:HG3	30:LX:55:ARG:NH1	2.30	0.47
39:Lh:80:PRO:HD2	39:Lh:83:LEU:HD12	1.97	0.47
49:S2:26:U:H2'	49:S2:27:A2M:H8	1.97	0.47
52:SE:18:TRP:CH2	52:SE:31:PRO:HD3	2.47	0.47
55:SH:18:GLU:O	55:SH:21:SER:OG	2.31	0.47
57:SJ:111:GLN:OE1	57:SJ:127:ARG:HB2	2.14	0.47
59:SL:126:VAL:HG13	59:SL:142:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Sc:40:ARG:HH21	75:Sc:42:ILE:HD11	1.80	0.47
3:LB:252:ALA:HB3	8:L5:4457:U:O2	2.15	0.47
4:SB:75:GLN:HG3	4:SB:76:ASN:H	1.79	0.47
8:L5:179:G:H2'	8:L5:180:C:C6	2.50	0.47
8:L5:1098:G:H2'	8:L5:1099:C:C6	2.49	0.47
8:L5:1443:A:C2	8:L5:2103:G:N1	2.74	0.47
8:L5:1541:C:O2'	8:L5:2448:G:N3	2.48	0.47
8:L5:4323:A:C2	12:LD:146:LEU:HD23	2.50	0.47
8:L5:4535:A:H2'	8:L5:4536:OMC:H6	1.79	0.47
8:L5:4970:C:C2	8:L5:4971:A:C8	3.02	0.47
12:LD:60:ILE:HB	12:LD:80:ALA:HB2	1.97	0.47
12:LD:256:LYS:HA	12:LD:257:PRO:HG2	1.97	0.47
30:LX:94:ASN:ND2	30:LX:94:ASN:O	2.48	0.47
35:Lc:98:ASP:C	35:Lc:98:ASP:OD2	2.58	0.47
49:S2:168:C:O2'	54:SG:131:ARG:O	2.31	0.47
49:S2:455:A:H2'	49:S2:456:C:C6	2.50	0.47
63:SQ:112:LEU:HD22	63:SQ:119:LEU:HD23	1.97	0.47
67:SU:62:ARG:HB3	67:SU:62:ARG:HH11	1.80	0.47
79:Sg:11:LEU:HB2	79:Sg:307:VAL:HB	1.96	0.47
82:LI:36:LEU:HD13	82:LI:73:ASN:CG	2.40	0.47
8:L5:492:U:H2'	8:L5:493:G:C8	2.50	0.47
8:L5:908:G:H2'	8:L5:909:A:H8	1.79	0.47
8:L5:1173:G:C2	8:L5:1174:A:H1'	2.50	0.47
8:L5:1175:A:H2'	8:L5:1176:C:O4'	2.15	0.47
8:L5:1857:C:H2'	8:L5:1858:A:H8	1.80	0.47
22:LP:36:ILE:HG21	22:LP:48:LEU:HD21	1.97	0.47
31:LY:30:MET:SD	31:LY:78:TYR:HA	2.55	0.47
34:Lb:32:LEU:HD13	34:Lb:43:MET:HE1	1.97	0.47
49:S2:24:C:O2'	49:S2:25:A:H8	1.96	0.47
49:S2:455:A:H2'	49:S2:456:C:H6	1.80	0.47
49:S2:573:U:O2	49:S2:576:A2M:H8	2.15	0.47
49:S2:1162:C:H2'	49:S2:1163:C:O4'	2.14	0.47
53:SF:52:SER:O	53:SF:52:SER:OG	2.30	0.47
65:SS:68:ILE:HA	65:SS:71:MET:HE2	1.96	0.47
72:SZ:73:VAL:HG21	72:SZ:88:LEU:HD21	1.96	0.47
3:LB:47:LEU:HD23	3:LB:346:THR:HG22	1.96	0.47
8:L5:1686:C:O2'	34:Lb:18:ARG:NH1	2.48	0.47
8:L5:2875:C:OP1	47:Lp:23:ARG:NH2	2.47	0.47
8:L5:4239:A:H2'	8:L5:4240:G:H8	1.80	0.47
42:Lk:24:LYS:HG2	42:Lk:67:LYS:HZ2	1.78	0.47
49:S2:1500:G:H2'	49:S2:1501:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1539:U:OP1	66:ST:44:GLU:N	2.48	0.47
57:SJ:28:GLU:O	57:SJ:32:ILE:HG23	2.15	0.47
61:SO:136:PRO:CB	61:SO:139:SER:HB3	2.44	0.47
68:SV:17:CYS:HB2	68:SV:56:CYS:HB3	1.97	0.47
8:L5:38:A:H5''	33:La:35:ALA:HB2	1.97	0.46
8:L5:1332:C:H2'	8:L5:1333:A:C8	2.49	0.46
8:L5:1840:G:H5''	14:LF:113:ARG:HD3	1.97	0.46
8:L5:1932:A:H2'	8:L5:1933:G:C8	2.50	0.46
8:L5:2709:C:H5'	24:LR:43:LYS:NZ	2.30	0.46
8:L5:3938:G:H4'	8:L5:3939:G:O5'	2.15	0.46
9:L7:3:C:H2'	9:L7:4:U:C6	2.50	0.46
9:L7:66:G:OP1	12:LD:10:LYS:NZ	2.39	0.46
32:LZ:76:ASN:OD1	32:LZ:77:TYR:N	2.48	0.46
47:Lp:16:THR:O	47:Lp:16:THR:OG1	2.30	0.46
49:S2:811:A:H2'	49:S2:812:A:C8	2.50	0.46
49:S2:1203:G:H2'	49:S2:1204:A:N3	2.30	0.46
49:S2:1215:C:O2'	49:S2:1645:C:OP2	2.34	0.46
58:SK:32:HIS:NE2	58:SK:34:GLU:OE1	2.48	0.46
61:SO:56:VAL:HG13	61:SO:60:MET:HE2	1.96	0.46
72:SZ:56:ASP:HA	72:SZ:59:CYS:SG	2.55	0.46
1:LA:5:ILE:HG12	1:LA:8:GLN:HB2	1.97	0.46
4:SB:225:LEU:HD23	4:SB:225:LEU:HA	1.76	0.46
8:L5:3626:G:H2'	8:L5:3627:OMG:O4'	2.15	0.46
8:L5:4887:C:H42	8:L5:4932:U:H3	1.63	0.46
20:LN:45:PRO:O	20:LN:49:ARG:HG3	2.15	0.46
36:Ld:24:GLU:OE1	36:Ld:109:VAL:HG11	2.15	0.46
48:Lr:75:THR:O	48:Lr:75:THR:HG23	2.15	0.46
8:L5:271:C:H2'	8:L5:272:U:H6	1.80	0.46
8:L5:2897:G:C4	8:L5:3603:G:N2	2.83	0.46
8:L5:4475:G:OP2	16:LH:173:ARG:NH2	2.44	0.46
8:L5:4625:C:O2'	8:L5:4626:A:H5'	2.16	0.46
8:L5:4752:U:H4'	21:LO:4:VAL:HG21	1.97	0.46
13:LE:150:LEU:HB3	13:LE:194:VAL:HG13	1.97	0.46
18:LL:111:GLN:O	18:LL:115:GLN:HG2	2.14	0.46
20:LN:68:ARG:HA	20:LN:98:LEU:HD21	1.96	0.46
25:LS:69:GLU:OE2	25:LS:102:THR:N	2.40	0.46
49:S2:5:U:H2'	49:S2:6:G:H8	1.80	0.46
49:S2:1442:OMU:HM23	49:S2:1442:OMU:H1'	1.50	0.46
49:S2:1500:G:H2'	49:S2:1501:C:H6	1.79	0.46
49:S2:1512:C:H5''	76:Sd:8:TRP:HZ3	1.79	0.46
49:S2:1741:U:H2'	49:S2:1742:C:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D4:48:C:H2'	7:D4:59:U:H1'	1.98	0.46
8:L5:406:C:O2'	8:L5:407:A:OP1	2.29	0.46
8:L5:1308:C:H2'	8:L5:1309:C:C6	2.51	0.46
8:L5:1816:C:C6	34:Lb:42:ASN:OD1	2.68	0.46
8:L5:1866:U:OP1	82:LI:4:ARG:NH1	2.44	0.46
8:L5:2415:U:H2'	8:L5:2416:G:C8	2.51	0.46
8:L5:2591:A:H2'	8:L5:2592:U:H6	1.81	0.46
8:L5:3599:A:H2'	8:L5:3600:G:H8	1.77	0.46
8:L5:3619:G:H22	8:L5:3624:A:H1'	1.80	0.46
8:L5:4243:C:OP2	8:L5:4264:G:N1	2.42	0.46
15:LG:182:CYS:SG	15:LG:183:ILE:N	2.88	0.46
25:LS:107:THR:O	25:LS:111:ARG:HG2	2.14	0.46
29:LW:52:THR:O	29:LW:56:ARG:HG2	2.15	0.46
54:SG:192:ILE:O	54:SG:196:LYS:HG3	2.15	0.46
59:SL:15:THR:HG22	59:SL:15:THR:O	2.16	0.46
59:SL:92:TYR:OH	59:SL:107:LYS:NZ	2.48	0.46
62:SP:109:PRO:O	62:SP:112:ILE:HG12	2.16	0.46
67:SU:34:LYS:HE3	67:SU:107:GLU:OE2	2.15	0.46
69:SW:102:ILE:H	69:SW:113:HIS:CD2	2.33	0.46
74:Sb:6:ASP:O	74:Sb:8:LEU:N	2.48	0.46
80:SM:65:VAL:O	80:SM:69:CYS:HB2	2.14	0.46
2:SA:135:THR:O	2:SA:138:SER:OG	2.32	0.46
7:D4:39:U:H2'	7:D4:40:C:C6	2.51	0.46
8:L5:271:C:H2'	8:L5:272:U:C6	2.49	0.46
8:L5:655:C:P	11:LC:268:ARG:NH2	2.88	0.46
8:L5:1416:G:H2'	8:L5:1417:C:H6	1.81	0.46
8:L5:1447:C:O2'	8:L5:1448:G:H5'	2.16	0.46
8:L5:1958:A:O2'	8:L5:2025:A:N1	2.46	0.46
8:L5:1962:A:OP2	8:L5:2024:G:N2	2.41	0.46
8:L5:3672:G:H3'	8:L5:3673:C:H5''	1.98	0.46
8:L5:3718:A2M:H2	8:L5:3934:G:O4'	2.15	0.46
8:L5:4563:U:H2'	8:L5:4564:A:C8	2.50	0.46
10:L8:155:C:P	15:LG:89:ARG:HH12	2.38	0.46
49:S2:949:G:H2'	49:S2:950:C:C6	2.51	0.46
51:SD:41:VAL:HB	51:SD:46:THR:HG23	1.98	0.46
81:Le:44:ARG:CZ	81:Le:52:GLN:HE22	2.29	0.46
82:LI:170:LYS:HA	82:LI:177:ASN:HA	1.97	0.46
8:L5:106:A:O2'	8:L5:335:A:N3	2.47	0.46
8:L5:375:G:OP1	11:LC:62:THR:HG23	2.16	0.46
8:L5:1249:C:H2'	8:L5:1250:C:C6	2.51	0.46
8:L5:2469:C:H5'	8:L5:2470:C:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L8:47:C:H1'	10:L8:61:A:H2'	1.96	0.46
12:LD:208:MET:O	12:LD:212:MET:HG2	2.15	0.46
19:LM:23:LYS:HB3	19:LM:43:THR:HG21	1.97	0.46
21:LO:85:ARG:HG3	21:LO:99:LEU:HD22	1.97	0.46
32:LZ:52:LYS:O	32:LZ:65:ARG:NH2	2.47	0.46
34:Lb:110:ALA:O	34:Lb:114:LYS:HG2	2.15	0.46
37:Lf:43:LEU:HD23	37:Lf:43:LEU:HA	1.78	0.46
49:S2:496:C:H5'	52:SE:29:PRO:HA	1.98	0.46
56:SI:161:LEU:HA	56:SI:164:GLU:OE2	2.15	0.46
6:B4:68:U:H2'	6:B4:69:G:C8	2.45	0.46
8:L5:52:G:H4'	8:L5:1529:G:H4'	1.97	0.46
8:L5:960:A:N6	13:LE:125:LEU:O	2.47	0.46
8:L5:1397:A:OP1	33:La:132:ARG:HD3	2.15	0.46
8:L5:2264:C:H2'	8:L5:2265:G:O4'	2.15	0.46
8:L5:2630:U:O4	27:LU:89:LYS:NZ	2.48	0.46
8:L5:3656:A:H2'	8:L5:3657:U:H6	1.80	0.46
8:L5:3732:A:H2'	8:L5:3733:A:C8	2.51	0.46
8:L5:3932:U:O2'	8:L5:3933:G:H8	1.97	0.46
8:L5:4147:G:H2'	8:L5:4148:C:C6	2.51	0.46
11:LC:10:VAL:O	11:LC:18:SER:OG	2.26	0.46
11:LC:186:SER:OG	11:LC:187:GLN:N	2.43	0.46
49:S2:945:U:H2'	49:S2:946:U:C6	2.51	0.46
56:SI:103:LEU:HD12	56:SI:103:LEU:HA	1.83	0.46
57:SJ:84:ILE:HA	57:SJ:150:ARG:HG2	1.98	0.46
64:SR:20:TYR:HD2	64:SR:23:ARG:HD3	1.79	0.46
65:SS:26:ILE:O	65:SS:30:ILE:HG12	2.15	0.46
67:SU:24:LEU:HD23	67:SU:112:VAL:HG22	1.97	0.46
79:Sg:256:ILE:HG12	79:Sg:270:LEU:HB2	1.98	0.46
3:LB:55:HIS:NE2	3:LB:369:ASP:OD2	2.49	0.46
8:L5:711:A:N3	13:LE:136:HIS:HE1	2.14	0.46
8:L5:1079:C:H2'	8:L5:1080:C:C6	2.50	0.46
8:L5:1656:U:OP2	33:La:26:ARG:NH2	2.33	0.46
8:L5:2652:G:N2	47:Lp:58:GLY:O	2.48	0.46
8:L5:3823:G:H2'	8:L5:3824:A:C8	2.51	0.46
8:L5:4261:C:O2'	17:LJ:102:THR:HG21	2.15	0.46
8:L5:4458:C:H2'	8:L5:4459:U:C6	2.51	0.46
13:LE:46:ARG:C	13:LE:62:MET:HE1	2.41	0.46
15:LG:157:ILE:HG22	15:LG:201:THR:HG1	1.81	0.46
20:LN:28:TRP:O	20:LN:32:GLN:HG2	2.16	0.46
49:S2:550:C:H2'	49:S2:551:U:C6	2.51	0.46
55:SH:145:ARG:HB2	69:SW:51:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SL:104:LYS:HE3	70:SX:8:ARG:HH21	1.80	0.46
75:Sc:46:VAL:HG12	75:Sc:56:LEU:HD21	1.97	0.46
78:Sf:138:ARG:HD2	78:Sf:147:THR:CG2	2.45	0.46
81:Le:98:GLU:HG3	81:Le:123:THR:OG1	2.16	0.46
82:LI:69:ARG:NH2	82:LI:70:ILE:HG13	2.31	0.46
2:SA:50:ASN:O	2:SA:54:THR:HG23	2.16	0.46
6:B4:20:A:N6	6:B4:45:G:H1'	2.31	0.46
8:L5:1448:G:H2'	8:L5:1449:C:C6	2.50	0.46
8:L5:1786:A:H2'	8:L5:1789:C:C5	2.51	0.46
8:L5:1811:G:H2'	8:L5:1812:C:C6	2.50	0.46
8:L5:4538:G:H2'	8:L5:4539:U:C6	2.51	0.46
15:LG:217:LYS:HB3	15:LG:217:LYS:HE2	1.70	0.46
17:LJ:40:LEU:HD23	17:LJ:40:LEU:HA	1.84	0.46
19:LM:40:GLY:H	19:LM:45:VAL:HG23	1.81	0.46
19:LM:43:THR:O	19:LM:43:THR:CG2	2.64	0.46
32:LZ:16:GLY:O	38:Lg:76:ARG:HG3	2.16	0.46
48:Lr:58:LYS:O	48:Lr:58:LYS:HG3	2.16	0.46
49:S2:1093:A:H2'	49:S2:1094:C:C6	2.50	0.46
49:S2:1630:A:H5''	65:SS:37:GLY:H	1.81	0.46
50:SC:132:ASP:OD1	50:SC:134:ASN:N	2.36	0.46
51:SD:132:LYS:HB2	51:SD:189:MET:HG2	1.98	0.46
2:SA:70:ASN:HB3	2:SA:73:ASP:OD2	2.16	0.46
3:LB:56:ILE:HD12	3:LB:368:ILE:HA	1.98	0.46
3:LB:288:GLY:HA3	3:LB:330:PHE:CE1	2.51	0.46
8:L5:644:G:H2'	8:L5:645:G:O4'	2.16	0.46
8:L5:1202:C:N3	8:L5:1203:G:O2'	2.47	0.46
8:L5:1625:OMG:N1	8:L5:3918:G:OP1	2.42	0.46
8:L5:2080:U:H2'	8:L5:2081:C:C6	2.51	0.46
8:L5:3873:G:H2'	8:L5:3874:G:C8	2.52	0.46
8:L5:4481:U:H2'	8:L5:4482:U:H6	1.81	0.46
10:L8:54:C:H2'	10:L8:55:PSU:H6	1.81	0.46
15:LG:191:GLY:HA2	15:LG:194:VAL:HG22	1.98	0.46
17:LJ:22:LEU:HB3	17:LJ:128:LEU:HD21	1.98	0.46
17:LJ:80:GLU:OE1	17:LJ:80:GLU:HA	2.16	0.46
25:LS:7:LEU:O	25:LS:103:ALA:HB1	2.16	0.46
33:La:37:GLY:H	33:La:41:HIS:HB2	1.80	0.46
49:S2:807:G:H2'	49:S2:808:A:C8	2.50	0.46
49:S2:1541:G:P	66:ST:56:ARG:HH21	2.39	0.46
49:S2:1588:A:HO2'	49:S2:1589:A:H8	1.57	0.46
58:SK:74:GLU:OE2	58:SK:74:GLU:N	2.45	0.46
59:SL:124:ASP:OD1	59:SL:147:LYS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SW:86:LEU:HB3	69:SW:117:ARG:NH2	2.31	0.46
6:B4:8:U:O4	6:B4:14:A:N7	2.49	0.45
8:L5:318:A:H2'	8:L5:319:A:H8	1.81	0.45
8:L5:1396:G:O2'	8:L5:1468:C:O2'	2.31	0.45
8:L5:4273:A:H2'	8:L5:4274:A:C8	2.51	0.45
8:L5:4292:A:O2'	46:Lo:8:ARG:NH2	2.49	0.45
8:L5:4425:G:OP1	44:Lm:100:TYR:OH	2.29	0.45
8:L5:4578:G:H2'	8:L5:4579:U:C6	2.51	0.45
32:LZ:77:TYR:CD2	35:Lc:39:ARG:HD3	2.51	0.45
33:La:38:LEU:O	33:La:42:ARG:NH1	2.49	0.45
35:Lc:18:LEU:O	35:Lc:19:GLN:C	2.59	0.45
49:S2:344:U:H2'	49:S2:345:U:C6	2.51	0.45
49:S2:570:C:O2	71:SY:34:THR:OG1	2.25	0.45
49:S2:1531:A:H2'	49:S2:1532:C:C6	2.51	0.45
50:SC:166:ARG:O	50:SC:181:PRO:HD3	2.16	0.45
58:SK:29:MET:HE3	58:SK:29:MET:HB2	1.85	0.45
58:SK:41:PRO:HD2	58:SK:44:HIS:ND1	2.30	0.45
59:SL:125:ILE:HD13	59:SL:148:ALA:HB2	1.98	0.45
78:Sf:118:ARG:CB	78:Sf:131:PHE:HB3	2.45	0.45
6:B4:57:A:O2'	6:B4:59:A:OP2	2.21	0.45
6:B4:61:C:H2'	6:B4:62:A:H8	1.80	0.45
19:LM:3:PHE:H	25:LS:175:PHE:HZ	1.63	0.45
31:LY:36:LYS:O	31:LY:40:GLN:NE2	2.48	0.45
32:LZ:77:TYR:HD2	35:Lc:39:ARG:HD3	1.81	0.45
48:Lr:3:ALA:O	48:Lr:44:ILE:HD11	2.16	0.45
49:S2:682:U:O2'	69:SW:4:MET:SD	2.69	0.45
52:SE:192:ILE:HG13	52:SE:243:GLY:HA3	1.99	0.45
54:SG:95:LYS:HB3	54:SG:95:LYS:HE3	1.73	0.45
55:SH:50:GLU:OE1	55:SH:60:ILE:HG22	2.16	0.45
79:Sg:108:VAL:HA	79:Sg:124:SER:HA	1.98	0.45
1:LA:200:ARG:HE	1:LA:200:ARG:HB2	1.54	0.45
2:SA:81:ASN:HA	2:SA:84:GLN:HE22	1.81	0.45
7:D4:9:A:OP2	7:D4:13:C:N4	2.48	0.45
8:L5:1248:C:H2'	8:L5:1249:C:C6	2.51	0.45
8:L5:2370:A:N1	8:L5:2390:G:O2'	2.44	0.45
8:L5:2494:U:O2'	8:L5:2495:U:O4'	2.31	0.45
10:L8:140:C:H2'	10:L8:141:C:C6	2.52	0.45
10:L8:154:G:H5''	15:LG:89:ARG:NH1	2.32	0.45
14:LF:157:ARG:NH2	14:LF:248:ASN:O	2.36	0.45
49:S2:311:C:H5'	49:S2:312:G:C5'	2.47	0.45
49:S2:428:OMU:H4'	49:S2:429:C:OP2	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:448:A:H5''	56:SI:25:ARG:HA	1.98	0.45
49:S2:1407:U:H2'	49:S2:1408:U:C6	2.52	0.45
49:S2:1597:C:H4'	49:S2:1603:G:O6	2.16	0.45
51:SD:220:THR:HG23	51:SD:222:PRO:HD3	1.98	0.45
56:SI:67:TRP:CD1	56:SI:191:GLU:OE2	2.70	0.45
65:SS:34:LYS:HE2	65:SS:34:LYS:HB3	1.69	0.45
68:SV:77:GLY:HA2	68:SV:81:LYS:NZ	2.31	0.45
80:SM:40:LYS:O	80:SM:44:LYS:HG2	2.15	0.45
4:SB:168:MET:HG2	4:SB:197:ILE:HD13	1.98	0.45
8:L5:171:U:H5''	8:L5:172:C:H5	1.82	0.45
8:L5:270:U:H2'	8:L5:271:C:C6	2.52	0.45
8:L5:491:G:H2'	8:L5:492:U:C6	2.52	0.45
8:L5:1662:C:H2'	8:L5:1663:C:C6	2.51	0.45
8:L5:3697:U:H5''	8:L5:3698:G:H5'	1.97	0.45
8:L5:4137:C:H2'	8:L5:4138:C:H6	1.81	0.45
9:L7:12:U:O3'	9:L7:109:U:O2'	2.34	0.45
11:LC:146:GLU:HG2	11:LC:175:LYS:HB3	1.97	0.45
28:LV:84:GLN:HG2	28:LV:86:LYS:H	1.80	0.45
49:S2:317:C:OP2	54:SG:183:ARG:NH1	2.47	0.45
49:S2:601:OMG:H1'	49:S2:601:OMG:HM23	1.71	0.45
49:S2:1643:U:H2'	49:S2:1644:C:C6	2.51	0.45
52:SE:35:PRO:HD2	52:SE:83:PRO:HG2	1.98	0.45
1:LA:8:GLN:O	8:L5:3668:C:H5'	2.17	0.45
1:LA:30:ARG:O	1:LA:163:ARG:NH1	2.40	0.45
7:D4:6:G:H1'	7:D4:7:A:C8	2.52	0.45
8:L5:398:A2M:H8	8:L5:398:A2M:OP2	2.15	0.45
8:L5:919:C:H2'	8:L5:920:C:C6	2.51	0.45
8:L5:1730:U:H2'	8:L5:1731:C:C6	2.52	0.45
8:L5:2499:C:H2'	8:L5:2500:U:C6	2.51	0.45
8:L5:2539:C:H2'	8:L5:2540:C:H6	1.80	0.45
8:L5:2702:C:H4'	27:LU:103:VAL:HG11	1.99	0.45
8:L5:3736:A:O2'	8:L5:3737:A:H8	1.99	0.45
8:L5:4688:C:H2'	8:L5:4689:U:C6	2.52	0.45
13:LE:201:ILE:HG13	13:LE:203:ILE:HG23	1.99	0.45
14:LF:154:ILE:HD11	14:LF:194:ILE:HD12	1.98	0.45
49:S2:10:G:H21	50:SC:114:LYS:HA	1.81	0.45
49:S2:1678:A2M:O2'	49:S2:1679:A:H5'	2.16	0.45
51:SD:72:VAL:HG21	58:SK:70:TYR:HE1	1.81	0.45
56:SI:6:ASP:OD1	56:SI:9:HIS:ND1	2.49	0.45
56:SI:137:LEU:O	56:SI:137:LEU:HD12	2.15	0.45
58:SK:60:GLU:HB2	58:SK:69:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SS:35:GLY:O	65:SS:97:GLN:NE2	2.49	0.45
2:SA:12:GLU:O	2:SA:15:VAL:HG12	2.17	0.45
3:LB:240:LEU:HB2	3:LB:248:LEU:HA	1.99	0.45
3:LB:300:LYS:HG3	3:LB:304:SER:OG	2.17	0.45
8:L5:268:G:H2'	8:L5:269:G:C8	2.52	0.45
8:L5:1481:C:H5''	8:L5:1482:G:OP2	2.16	0.45
8:L5:1895:G:O2'	8:L5:1907:A:N3	2.42	0.45
8:L5:2521:G:H5'	8:L5:2640:G:H1'	1.99	0.45
8:L5:4174:U:H2'	8:L5:4175:G:C8	2.51	0.45
8:L5:4342:C:O3'	46:Lo:37:GLY:HA3	2.16	0.45
14:LF:127:LYS:HB2	26:LT:133:ALA:HB3	1.99	0.45
16:LH:151:ILE:HA	16:LH:154:VAL:HG22	1.99	0.45
21:LO:41:ILE:HB	21:LO:138:LEU:HD22	1.98	0.45
32:LZ:68:ILE:O	32:LZ:115:LYS:NZ	2.40	0.45
49:S2:1491:G:H2'	49:S2:1492:U:C6	2.52	0.45
63:SQ:19:ALA:HB2	63:SQ:75:GLY:HA3	1.98	0.45
63:SQ:21:ALA:HB2	63:SQ:72:VAL:HG23	1.98	0.45
3:LB:44:THR:HG21	3:LB:186:ASN:HD22	1.81	0.45
4:SB:176:VAL:HG23	4:SB:184:VAL:HG21	1.98	0.45
8:L5:1390:G:N2	8:L5:1393:G:OP2	2.39	0.45
8:L5:2361:G:O2'	8:L5:3859:G:O6	2.29	0.45
8:L5:2439:G:H5'	8:L5:2778:G:OP2	2.17	0.45
8:L5:2811:G:N2	8:L5:2814:C:OP2	2.39	0.45
8:L5:4088:C:H2'	8:L5:4089:G:H8	1.82	0.45
8:L5:4190:U:O2'	8:L5:4382:G:OP2	2.34	0.45
8:L5:4415:A:OP1	82:LI:154:ARG:NH1	2.50	0.45
8:L5:4621:C:OP1	28:LV:48:ARG:HD2	2.17	0.45
10:L8:60:G:OP1	30:LX:68:ARG:NH2	2.49	0.45
10:L8:141:C:H5''	20:LN:60:VAL:HG21	1.99	0.45
12:LD:223:PHE:HB3	12:LD:226:TYR:HB2	1.98	0.45
49:S2:558:G:H2'	49:S2:559:G:C8	2.51	0.45
49:S2:1438:A:H2'	49:S2:1439:A:C8	2.52	0.45
52:SE:204:SER:OG	52:SE:205:PHE:N	2.41	0.45
79:Sg:104:HIS:NE2	79:Sg:122:SER:OG	2.46	0.45
81:Le:91:CYS:HB2	81:Le:95:TYR:HD2	1.81	0.45
82:LI:191:ILE:HG12	82:LI:200:ILE:HG13	1.98	0.45
8:L5:2634:C:H2'	8:L5:2635:U:H6	1.81	0.45
8:L5:2765:A:H2'	8:L5:2766:A:H8	1.82	0.45
8:L5:2803:U:H2'	8:L5:2804:OMC:C6	2.52	0.45
8:L5:4265:U:N3	12:LD:17:GLN:O	2.50	0.45
8:L5:4377:G:O6	33:La:42:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L8:13:G:O2'	22:LP:121:LYS:O	2.35	0.45
18:LL:162:LYS:H	18:LL:162:LYS:HG2	1.56	0.45
49:S2:107:A:H2'	49:S2:108:G:H8	1.81	0.45
49:S2:322:C:H2'	49:S2:323:C:C6	2.52	0.45
49:S2:508:A:H3'	49:S2:509:G:H8	1.81	0.45
49:S2:1016:U:O2	49:S2:1016:U:H2'	2.16	0.45
49:S2:1521:C:OP1	65:SS:124:ARG:NH1	2.50	0.45
49:S2:1664:A:HO2'	49:S2:1665:G:P	2.39	0.45
49:S2:1845:A:H2'	49:S2:1846:G:C8	2.51	0.45
58:SK:80:ARG:NH1	58:SK:89:ILE:O	2.49	0.45
59:SL:68:ILE:HG21	59:SL:143:LEU:HD11	1.99	0.45
68:SV:65:SER:O	68:SV:69:ILE:HG12	2.16	0.45
75:Sc:18:LEU:O	75:Sc:29:GLN:HB3	2.16	0.45
82:LI:140:THR:OG1	82:LI:141:LYS:N	2.50	0.45
3:LB:55:HIS:C	3:LB:56:ILE:HD13	2.42	0.45
8:L5:1081:C:N4	8:L5:1082:C:H41	2.15	0.45
8:L5:1906:U:H2'	8:L5:1907:A:H8	1.81	0.45
8:L5:2587:A:OP2	38:Lg:70:THR:OG1	2.23	0.45
8:L5:2668:G:OP1	24:LR:128:LYS:NZ	2.50	0.45
8:L5:4211:C:OP1	87:L5:5287:PUT:N1	2.43	0.45
8:L5:4438:U:H2'	8:L5:4439:U:O4'	2.17	0.45
12:LD:256:LYS:C	12:LD:257:PRO:HG2	2.40	0.45
26:LT:147:GLU:HG3	26:LT:148:PRO:HD2	1.98	0.45
49:S2:563:G:N7	57:SJ:172:ARG:NH2	2.65	0.45
49:S2:1189:A:H2'	49:S2:1190:A:C8	2.52	0.45
49:S2:1797:U:H2'	49:S2:1798:C:C6	2.51	0.45
57:SJ:102:ILE:HG22	57:SJ:106:LEU:HD12	1.99	0.45
59:SL:22:ARG:HD3	59:SL:22:ARG:H	1.80	0.45
62:SP:87:PRO:O	62:SP:90:VAL:HG12	2.17	0.45
4:SB:182:LYS:HG3	4:SB:231:LEU:HD22	1.98	0.45
8:L5:119:G:N3	15:LG:132:ARG:NH1	2.64	0.45
8:L5:1669:A:OP1	34:Lb:11:ASN:ND2	2.49	0.45
8:L5:1821:G:H2'	8:L5:1821:G:N3	2.31	0.45
8:L5:2458:C:O2	8:L5:3671:G:N2	2.49	0.45
8:L5:2562:G:N2	8:L5:2564:G:H3'	2.32	0.45
8:L5:2755:A:OP1	32:LZ:65:ARG:NH1	2.48	0.45
8:L5:4481:U:H2'	8:L5:4482:U:C6	2.51	0.45
8:L5:4535:A:H2'	8:L5:4536:OMC:C6	2.51	0.45
14:LF:41:MET:HA	14:LF:41:MET:HE3	1.99	0.45
16:LH:129:ARG:HG2	16:LH:157:SER:HB3	1.99	0.45
36:Ld:53:ALA:HA	36:Ld:88:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lm:94:MET:O	44:Lm:95:ILE:HD13	2.17	0.45
49:S2:846:G:C4	52:SE:19:MET:HE3	2.51	0.45
49:S2:1373:C:O2'	64:SR:10:LYS:HE3	2.17	0.45
50:SC:105:GLU:OE1	50:SC:212:LYS:HD3	2.17	0.45
52:SE:230:LYS:HE3	52:SE:230:LYS:HB2	1.70	0.45
57:SJ:110:LEU:HG	57:SJ:130:ILE:HD11	1.98	0.45
57:SJ:137:VAL:HG21	57:SJ:147:PHE:CE2	2.52	0.45
1:LA:173:GLY:O	47:Lp:69:TRP:NE1	2.48	0.44
8:L5:2459:G:H2'	8:L5:2461:G:OP2	2.17	0.44
9:L7:43:U:H4'	17:LJ:143:ASP:O	2.17	0.44
10:L8:19:C:H2'	10:L8:20:A:C8	2.52	0.44
11:LC:259:LYS:HG2	11:LC:263:LEU:HD13	1.98	0.44
18:LL:58:ILE:HG12	18:LL:116:ARG:HE	1.82	0.44
23:LQ:22:ASP:O	23:LQ:26:ARG:HG3	2.17	0.44
24:LR:165:LYS:HE2	24:LR:165:LYS:HB3	1.90	0.44
27:LU:101:ARG:HB2	27:LU:115:PHE:HE1	1.82	0.44
49:S2:14:C:H2'	49:S2:15:U:C6	2.52	0.44
49:S2:1236:G:H2'	49:S2:1237:C:C6	2.52	0.44
53:SF:68:ILE:HD11	53:SF:151:ILE:HD11	1.99	0.44
54:SG:3:LEU:HD22	54:SG:18:VAL:HG21	1.97	0.44
54:SG:135:PRO:HG2	54:SG:141:ILE:HG12	1.99	0.44
66:ST:129:ARG:O	66:ST:133:ARG:HG3	2.17	0.44
71:SY:57:VAL:HB	71:SY:60:PHE:CE2	2.52	0.44
81:Le:105:SER:O	81:Le:109:LYS:HG3	2.16	0.44
3:LB:252:ALA:HB1	8:L5:4524:G:N3	2.32	0.44
3:LB:348:ARG:HH12	3:LB:351:LEU:HG	1.82	0.44
4:SB:32:ASP:OD1	4:SB:43:ASN:ND2	2.50	0.44
4:SB:49:VAL:HG11	4:SB:62:LEU:HD21	1.99	0.44
7:D4:11:C:H2'	7:D4:12:U:C6	2.52	0.44
8:L5:135:G:P	8:L5:135:G:H8	2.40	0.44
8:L5:1633:G:O6	8:L5:3918:G:O2'	2.30	0.44
8:L5:3610:A:H2'	8:L5:3611:A:C8	2.51	0.44
8:L5:4344:U:H2'	8:L5:4345:C:H6	1.81	0.44
9:L7:35:U:O2	9:L7:45:U:O2'	2.33	0.44
10:L8:7:U:H2'	10:L8:8:U:C6	2.52	0.44
21:LO:10:ASP:CG	21:LO:37:ARG:HH21	2.25	0.44
33:La:75:LEU:HD11	33:La:133:ALA:HA	1.99	0.44
36:Ld:59:THR:OG1	36:Ld:104:THR:OG1	2.30	0.44
40:Li:84:LYS:HE3	40:Li:84:LYS:HB3	1.67	0.44
49:S2:1139:C:H2'	49:S2:1140:G:O4'	2.18	0.44
49:S2:1649:U:N3	49:S2:1675:A:H2	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SE:73:ASP:HA	52:SE:164:LEU:HD13	1.99	0.44
52:SE:206:ASP:OD1	52:SE:206:ASP:N	2.51	0.44
80:SM:41:ALA:HB1	80:SM:46:GLN:HB2	2.00	0.44
2:SA:110:ASN:ND2	49:S2:1351:G:O4'	2.51	0.44
8:L5:97:G:N7	18:LL:13:HIS:NE2	2.61	0.44
8:L5:485:C:H3'	8:L5:486:C:H5''	2.00	0.44
8:L5:1214:C:O4'	34:Lb:91:ARG:NH2	2.50	0.44
8:L5:1316:OMG:H1'	8:L5:1316:OMG:HM23	1.73	0.44
8:L5:2079:G:H2'	8:L5:2080:U:H6	1.82	0.44
8:L5:2323:C:H2'	8:L5:2324:C:C6	2.52	0.44
8:L5:3611:A:H2	8:L5:5016:A:C8	2.36	0.44
8:L5:4474:A:OP2	8:L5:4476:C:N4	2.47	0.44
9:L7:3:C:H2'	9:L7:4:U:H6	1.81	0.44
12:LD:280:VAL:HG12	12:LD:284:LYS:HD2	1.99	0.44
15:LG:143:VAL:O	15:LG:147:VAL:HG13	2.17	0.44
21:LO:81:TRP:HB2	21:LO:104:VAL:HG21	2.00	0.44
22:LP:39:MET:HG2	22:LP:43:LYS:HD3	1.99	0.44
49:S2:561:A:O2'	49:S2:562:U:H5'	2.17	0.44
49:S2:943:U:C2	49:S2:944:A:C8	3.06	0.44
49:S2:1542:C:C2	49:S2:1543:U:H5	2.36	0.44
54:SG:48:TYR:CD1	54:SG:116:LYS:HA	2.52	0.44
58:SK:15:LEU:O	58:SK:19:GLY:HA2	2.17	0.44
64:SR:27:ASP:HB3	64:SR:30:THR:HG22	1.98	0.44
66:ST:96:SER:HB3	66:ST:99:VAL:HG12	1.99	0.44
78:Sf:132:MET:HE3	78:Sf:139:HIS:HB3	1.98	0.44
79:Sg:76:GLN:O	79:Sg:92:LEU:HB2	2.17	0.44
8:L5:25:A:C8	8:L5:341:G:C8	3.05	0.44
8:L5:262:G:H2'	8:L5:263:G:C8	2.53	0.44
8:L5:318:A:H2'	8:L5:319:A:C8	2.52	0.44
8:L5:1333:A:H2'	8:L5:1334:A:H8	1.81	0.44
8:L5:4593:C:H2'	8:L5:4594:U:H6	1.83	0.44
16:LH:89:ARG:HH21	16:LH:187:VAL:HG13	1.82	0.44
20:LN:121:VAL:HG11	20:LN:131:GLU:HG3	1.99	0.44
42:Lk:33:LYS:HG2	42:Lk:46:VAL:HG22	1.99	0.44
49:S2:146:G:O2'	49:S2:147:A:H5'	2.17	0.44
49:S2:963:A:H2'	49:S2:964:A:C8	2.53	0.44
49:S2:1374:C:H2'	49:S2:1375:G:O4'	2.18	0.44
49:S2:1406:G:H2'	49:S2:1407:U:C6	2.53	0.44
49:S2:1620:A:H1'	49:S2:1624:U:OP2	2.17	0.44
49:S2:1752:C:H2'	49:S2:1753:C:O4'	2.17	0.44
49:S2:1801:A:H2'	49:S2:1802:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:164:LYS:O	54:SG:164:LYS:HD3	2.18	0.44
66:ST:51:ASN:HB3	66:ST:54:TYR:HD2	1.83	0.44
69:SW:3:ARG:HD3	69:SW:6:VAL:HG12	1.99	0.44
69:SW:62:VAL:HG21	74:Sb:8:LEU:HD13	1.99	0.44
79:Sg:156:PHE:HE1	79:Sg:179:LEU:HD11	1.82	0.44
1:LA:137:ILE:HD11	1:LA:149:LYS:HB2	1.99	0.44
3:LB:121:ASN:HD22	3:LB:124:LYS:HB2	1.82	0.44
4:SB:42:ARG:HH11	4:SB:42:ARG:HG3	1.82	0.44
8:L5:272:U:H2'	8:L5:273:U:C6	2.53	0.44
8:L5:1189:G:H2'	8:L5:1190:C:C6	2.52	0.44
8:L5:1447:C:C2'	8:L5:1448:G:H5'	2.48	0.44
8:L5:2020:U:H2'	8:L5:2021:G:H8	1.83	0.44
8:L5:2461:G:H5'	20:LN:104:GLU:OE2	2.18	0.44
8:L5:4323:A:H2	12:LD:146:LEU:HD23	1.83	0.44
8:L5:4759:C:H2'	8:L5:4760:G:C8	2.52	0.44
8:L5:5002:U:H2'	8:L5:5003:U:C6	2.52	0.44
13:LE:126:LEU:HD23	13:LE:126:LEU:HA	1.88	0.44
19:LM:23:LYS:HB3	19:LM:43:THR:CG2	2.47	0.44
22:LP:32:THR:HG21	22:LP:87:SER:HB3	2.00	0.44
24:LR:3:MET:HE1	24:LR:5:ARG:HE	1.83	0.44
52:SE:200:ARG:O	52:SE:200:ARG:HG3	2.18	0.44
55:SH:69:LEU:HD22	55:SH:96:ALA:HB2	1.98	0.44
79:Sg:273:GLU:H	79:Sg:273:GLU:CD	2.23	0.44
82:LI:206:LEU:O	82:LI:210:ARG:HG2	2.18	0.44
3:LB:184:GLN:OE1	3:LB:186:ASN:ND2	2.50	0.44
4:SB:225:LEU:O	4:SB:229:MET:HG2	2.17	0.44
8:L5:28:C:OP1	20:LN:187:SER:OG	2.35	0.44
8:L5:65:A:N6	8:L5:75:G:H1'	2.33	0.44
8:L5:139:G:H2'	8:L5:140:G:C8	2.52	0.44
8:L5:1646:A:O2'	41:Lj:49:TRP:O	2.35	0.44
8:L5:2295:C:H2'	8:L5:2296:G:H8	1.81	0.44
8:L5:2619:G:OP1	27:LU:79:SER:OG	2.34	0.44
8:L5:4253:A:H4'	8:L5:4254:G:O5'	2.18	0.44
14:LF:196:THR:O	14:LF:196:THR:OG1	2.35	0.44
23:LQ:18:PRO:HD3	23:LQ:52:PHE:CD1	2.53	0.44
25:LS:29:ARG:HE	26:LT:150:LEU:HD13	1.83	0.44
30:LX:72:ASP:N	30:LX:72:ASP:OD1	2.48	0.44
31:LY:30:MET:HE2	31:LY:75:ARG:HG2	1.99	0.44
49:S2:21:U:O2	57:SJ:17:ARG:NH2	2.50	0.44
49:S2:1201:U:H2'	49:S2:1202:U:C6	2.53	0.44
49:S2:1521:C:H5''	65:SS:129:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:144:LEU:HD23	54:SG:145:PHE:CD1	2.53	0.44
55:SH:10:LYS:NZ	55:SH:46:THR:O	2.45	0.44
58:SK:74:GLU:CD	58:SK:74:GLU:H	2.22	0.44
74:Sb:5:LYS:HG3	74:Sb:7:LEU:CD2	2.48	0.44
79:Sg:153:CYS:HB3	79:Sg:198:VAL:HG12	1.98	0.44
1:LA:20:VAL:HA	1:LA:23:ARG:HG3	1.98	0.44
1:LA:117:GLU:HB2	1:LA:122:ASP:OD1	2.18	0.44
2:SA:38:ILE:HD13	2:SA:47:TYR:HD2	1.83	0.44
4:SB:38:MET:H	4:SB:38:MET:HG3	1.51	0.44
6:B4:26:C:H2'	6:B4:27:U:C6	2.53	0.44
7:D4:46:G:H3'	7:D4:47:U:H5''	1.99	0.44
8:L5:258:G:H2'	8:L5:259:C:C6	2.51	0.44
8:L5:1209:U:O2'	8:L5:1211:G:H5''	2.18	0.44
8:L5:1445:U:H2'	8:L5:1446:C:C5	2.53	0.44
8:L5:4376:A:O2'	33:La:42:ARG:NH1	2.51	0.44
8:L5:4646:U:OP2	24:LR:62:ARG:NH1	2.33	0.44
10:L8:94:G:C6	41:Lj:84:PRO:HG3	2.52	0.44
11:LC:316:LYS:HB2	11:LC:324:ILE:HD12	2.00	0.44
17:LJ:10:ASN:HB3	17:LJ:13:ARG:HG2	2.00	0.44
20:LN:108:ARG:CZ	20:LN:161:MET:HE1	2.48	0.44
25:LS:30:MET:HE1	25:LS:47:PHE:HB3	2.00	0.44
47:Lp:22:LEU:O	47:Lp:26:VAL:HG12	2.18	0.44
49:S2:27:A2M:HM'3	49:S2:27:A2M:H1'	1.78	0.44
49:S2:1336:C:O2'	49:S2:1337:4AC:O5'	2.34	0.44
49:S2:1407:U:H2'	49:S2:1408:U:H6	1.82	0.44
49:S2:1407:U:HO2'	63:SQ:11:GLN:HE22	1.61	0.44
50:SC:179:THR:OG1	50:SC:221:ASP:O	2.27	0.44
80:SM:81:ASP:CB	80:SM:84:LYS:HB2	2.47	0.44
81:Le:22:ARG:HB3	81:Le:25:SER:HB3	1.99	0.44
4:SB:120:MET:HE3	4:SB:142:PHE:CE2	2.53	0.44
8:L5:1188:C:H2'	8:L5:1189:G:H8	1.83	0.44
8:L5:1416:G:H2'	8:L5:1417:C:C6	2.53	0.44
8:L5:1847:C:H2'	8:L5:1848:C:C6	2.53	0.44
8:L5:4589:A:N1	8:L5:4621:C:O2'	2.44	0.44
11:LC:293:LEU:HD22	23:LQ:34:PHE:CD2	2.53	0.44
18:LL:123:LYS:HB2	39:Lh:122:LYS:O	2.18	0.44
22:LP:69:ARG:HA	22:LP:80:GLN:HA	2.00	0.44
32:LZ:30:ASP:OD1	32:LZ:30:ASP:N	2.34	0.44
36:Ld:57:MET:HG3	36:Ld:88:LEU:HD23	1.99	0.44
48:Lr:49:VAL:HG11	48:Lr:97:ILE:HD11	1.99	0.44
49:S2:90:G:H2'	49:S2:91:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1849:G:O2'	49:S2:1850:MA6:P	2.76	0.44
54:SG:72:ARG:HE	54:SG:72:ARG:HB2	1.57	0.44
57:SJ:82:VAL:HG12	57:SJ:87:LEU:HB3	2.00	0.44
66:ST:65:TYR:CD1	66:ST:65:TYR:C	2.95	0.44
76:Sd:53:ILE:CD1	76:Sd:55:LEU:HD12	2.46	0.44
1:LA:132:ASN:O	1:LA:169:VAL:HG12	2.18	0.44
6:B4:8:U:H3	6:B4:14:A:H62	1.66	0.44
8:L5:106:A:H2'	8:L5:107:G:O4'	2.18	0.44
8:L5:756:G:H2'	8:L5:757:G:H8	1.83	0.44
8:L5:2308:A:N3	10:L8:19:C:O2'	2.48	0.44
8:L5:2845:A:H61	8:L5:3843:C:H42	1.65	0.44
8:L5:3760:A2M:H4'	8:L5:3761:C:H5''	1.99	0.44
8:L5:3933:G:H2'	8:L5:3934:G:H8	1.83	0.44
8:L5:4536:OMC:HM22	8:L5:4537:C:O4'	2.18	0.44
8:L5:4607:A:H8	8:L5:4607:A:O5'	2.01	0.44
46:Lo:26:TYR:HB3	46:Lo:67:VAL:HB	2.00	0.44
49:S2:140:C:H42	49:S2:313:A:H61	1.64	0.44
49:S2:472:C:H4'	49:S2:474:G:OP1	2.17	0.44
49:S2:1243:U:H2'	49:S2:1244:U:O4'	2.18	0.44
49:S2:1438:A:H2'	49:S2:1439:A:H8	1.83	0.44
52:SE:206:ASP:HB2	52:SE:222:LEU:HD23	1.99	0.44
53:SF:163:PHE:CD2	53:SF:164:ARG:HG3	2.53	0.44
64:SR:67:ARG:HG2	64:SR:68:GLY:N	2.33	0.44
3:LB:261:ARG:HB3	8:L5:4564:A:O2'	2.18	0.43
8:L5:2622:G:O6	27:LU:81:ARG:NH1	2.51	0.43
23:LQ:178:ARG:HA	23:LQ:184:ARG:O	2.18	0.43
37:Lf:18:LEU:HG	37:Lf:19:ARG:HG3	2.00	0.43
49:S2:605:A:HO2'	49:S2:638:C:HO2'	1.66	0.43
49:S2:1511:U:H2'	49:S2:1512:C:C6	2.54	0.43
50:SC:233:LEU:HD23	50:SC:233:LEU:O	2.18	0.43
75:Sc:10:LYS:HD2	75:Sc:34:PHE:HE2	1.83	0.43
79:Sg:188:HIS:HD2	79:Sg:219:TRP:CD2	2.36	0.43
1:LA:106:THR:HG22	1:LA:106:THR:O	2.18	0.43
7:D4:55:U:O2'	7:D4:57:G:N7	2.46	0.43
8:L5:425:U:H2'	8:L5:426:A:C8	2.53	0.43
8:L5:3614:G:HO2'	8:L5:3615:G:P	2.36	0.43
11:LC:150:LEU:HB3	11:LC:151:PRO:HD3	2.00	0.43
12:LD:256:LYS:HA	12:LD:257:PRO:CG	2.48	0.43
17:LJ:93:GLU:HB2	17:LJ:175:LEU:HD11	2.00	0.43
19:LM:7:VAL:HG21	19:LM:52:PHE:CE1	2.53	0.43
22:LP:126:ARG:HG3	22:LP:140:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LY:48:PRO:O	31:LY:115:ARG:NH2	2.36	0.43
49:S2:120:U:H1'	52:SE:33:THR:O	2.18	0.43
49:S2:1335:G:O2'	49:S2:1336:C:H5'	2.18	0.43
51:SD:64:ARG:O	51:SD:68:GLU:HG3	2.18	0.43
52:SE:19:MET:HB3	52:SE:19:MET:HE2	1.57	0.43
54:SG:5:ILE:CG2	54:SG:124:LEU:HD21	2.48	0.43
61:SO:61:LYS:HD2	61:SO:76:LEU:HB3	2.00	0.43
73:Sa:74:CYS:SG	73:Sa:77:CYS:N	2.78	0.43
76:Sd:16:GLN:O	76:Sd:27:ARG:HD3	2.18	0.43
4:SB:57:ILE:HG22	4:SB:59:SER:H	1.83	0.43
5:A4:46:A:H2'	5:A4:47:A:H8	1.81	0.43
6:B4:52:G:H2'	6:B4:53:A:C8	2.53	0.43
7:D4:18:G:H4'	7:D4:60:U:C5	2.54	0.43
8:L5:346:G:OP1	31:LY:8:THR:HG23	2.18	0.43
8:L5:1879:C:O2'	8:L5:1891:A:N3	2.50	0.43
8:L5:2580:U:O2'	32:LZ:79:HIS:ND1	2.47	0.43
8:L5:4154:G:H2'	8:L5:4155:C:C6	2.54	0.43
11:LC:134:PRO:O	11:LC:138:MET:HG2	2.17	0.43
13:LE:281:ILE:HG23	13:LE:286:LEU:HD11	1.99	0.43
16:LH:37:ASP:C	16:LH:37:ASP:OD1	2.61	0.43
17:LJ:40:LEU:O	17:LJ:44:THR:HG23	2.18	0.43
17:LJ:159:LYS:O	17:LJ:163:MET:HG3	2.18	0.43
24:LR:8:LYS:HE3	24:LR:24:LEU:HD13	2.01	0.43
37:Lf:5:LEU:HD23	37:Lf:5:LEU:HA	1.85	0.43
43:Ll:21:ARG:HG2	43:Ll:22:PRO:HD2	2.00	0.43
49:S2:656:G:N2	49:S2:663:C:H5''	2.33	0.43
49:S2:1059:G:O6	49:S2:1060:A:N6	2.51	0.43
58:SK:52:LEU:HB3	58:SK:58:VAL:HG22	2.00	0.43
61:SO:57:THR:OG1	61:SO:60:MET:HG3	2.19	0.43
61:SO:98:ARG:HE	61:SO:134:PRO:HD3	1.83	0.43
77:Se:98:LYS:HA	77:Se:98:LYS:HD3	1.66	0.43
78:Sf:143:LYS:HB3	78:Sf:143:LYS:HE3	1.78	0.43
82:LI:38:ARG:NH1	82:LI:45:GLU:OE1	2.48	0.43
82:LI:184:MET:HE2	82:LI:189:ARG:CD	2.48	0.43
3:LB:117:ARG:NH2	3:LB:178:ALA:O	2.41	0.43
6:B4:33:C:H2'	6:B4:34:A:C8	2.53	0.43
8:L5:454:U:H2'	8:L5:455:C:C6	2.53	0.43
8:L5:682:G:H2'	8:L5:683:C:C6	2.54	0.43
8:L5:1391:A:N3	8:L5:4364:G:O2'	2.39	0.43
8:L5:2265:G:OP1	48:Lr:35:ARG:NH2	2.32	0.43
8:L5:2399:G:O2'	8:L5:2822:G:O2'	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:5001:U:H2'	8:L5:5002:U:O4'	2.18	0.43
9:L7:63:C:H1'	12:LD:280:VAL:HG11	1.99	0.43
10:L8:69:U:H2'	10:L8:70:G:O4'	2.18	0.43
29:LW:20:ARG:HE	29:LW:20:ARG:HB2	1.68	0.43
49:S2:1109:C:O2'	49:S2:1110:G:O4'	2.33	0.43
52:SE:211:LYS:HB3	52:SE:211:LYS:HE2	1.87	0.43
54:SG:32:MET:HE2	54:SG:65:GLN:HB2	2.01	0.43
60:SN:26:LEU:HD21	60:SN:60:VAL:HG12	1.99	0.43
67:SU:61:LEU:HD22	67:SU:82:MET:HE2	2.00	0.43
3:LB:80:GLU:CD	3:LB:326:VAL:HG23	2.43	0.43
3:LB:214:ASP:HB3	3:LB:283:LYS:NZ	2.33	0.43
3:LB:238:LYS:HE2	3:LB:238:LYS:HB2	1.76	0.43
5:A4:51:U:O2'	5:A4:52:U:O4'	2.36	0.43
8:L5:2413:U:H2'	8:L5:2414:G:H8	1.81	0.43
8:L5:2676:A:OP2	8:L5:2676:A:H8	2.02	0.43
8:L5:4642:U:H2'	8:L5:4643:G:C8	2.53	0.43
8:L5:4875:G:H2'	25:LS:169:THR:HB	2.00	0.43
8:L5:5004:C:H2'	8:L5:5005:G:O4'	2.18	0.43
12:LD:289:ARG:HD3	12:LD:293:ARG:NH2	2.33	0.43
14:LF:75:ALA:HB2	26:LT:140:PHE:CE2	2.53	0.43
16:LH:20:LEU:HD12	16:LH:47:LEU:HB2	2.01	0.43
17:LJ:59:SER:C	17:LJ:61:GLY:H	2.27	0.43
19:LM:52:PHE:CD1	19:LM:55:MET:HE3	2.54	0.43
27:LU:19:LEU:HD13	27:LU:77:PRO:HA	2.00	0.43
27:LU:56:LEU:HB3	27:LU:61:VAL:HB	2.01	0.43
33:La:82:VAL:HG13	33:La:101:ILE:HG23	1.99	0.43
49:S2:59:U:H5''	49:S2:503:C:N4	2.34	0.43
57:SJ:29:LEU:HD23	77:Se:115:PHE:HE2	1.83	0.43
57:SJ:179:LYS:HD2	57:SJ:179:LYS:HA	1.77	0.43
4:SB:48:LEU:HD23	4:SB:48:LEU:H	1.84	0.43
8:L5:424:U:H2'	8:L5:425:U:C6	2.53	0.43
8:L5:683:C:H2'	8:L5:684:G:O4'	2.19	0.43
8:L5:2624:G:H2'	8:L5:2625:U:H6	1.84	0.43
8:L5:2675:G:H4'	8:L5:2676:A:O5'	2.18	0.43
8:L5:3619:G:H5''	8:L5:3620:G:H5''	2.01	0.43
8:L5:4661:G:H2'	8:L5:4662:C:C6	2.54	0.43
10:L8:64:U:C2	10:L8:65:A:C8	3.07	0.43
14:LF:92:VAL:HG13	14:LF:142:TRP:HB3	2.00	0.43
17:LJ:143:ASP:N	17:LJ:143:ASP:OD1	2.52	0.43
25:LS:164:LYS:HD2	25:LS:164:LYS:HA	1.87	0.43
31:LY:82:ILE:HG22	31:LY:83:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lc:99:PRO:CB	35:Lc:102:SER:HB3	2.47	0.43
42:Lk:31:ASN:HB3	42:Lk:48:THR:HG22	2.00	0.43
49:S2:1100:A:OP1	64:SR:129:LYS:HE3	2.18	0.43
49:S2:1164:G:O2'	49:S2:1165:G:H5'	2.18	0.43
49:S2:1199:A:H2'	49:S2:1200:A:C8	2.54	0.43
49:S2:1288:OMU:HN3	49:S2:1311:C:H42	1.67	0.43
57:SJ:78:LEU:HD11	57:SJ:94:LEU:CB	2.48	0.43
70:SX:94:ILE:HD13	70:SX:125:VAL:HG23	2.00	0.43
75:Sc:35:MET:HE3	75:Sc:35:MET:HB3	1.76	0.43
82:LI:200:ILE:HG21	82:LI:212:LEU:CD2	2.48	0.43
7:D4:24:G:H2'	7:D4:25:C:C6	2.53	0.43
8:L5:1341:U:H2'	8:L5:1342:A:C8	2.54	0.43
8:L5:1341:U:H2'	8:L5:1342:A:H8	1.84	0.43
8:L5:1971:C:C2	8:L5:2000:G:H2'	2.54	0.43
8:L5:3700:C:O2'	8:L5:3774:A:N3	2.45	0.43
8:L5:4705:A:H2'	8:L5:4706:G:O4'	2.19	0.43
10:L8:153:C:H5'	15:LG:185:LYS:HD3	2.00	0.43
15:LG:180:PRO:HG2	15:LG:219:VAL:HG13	2.00	0.43
16:LH:41:ILE:HD12	16:LH:73:ILE:HD11	1.99	0.43
19:LM:50:MET:HE3	19:LM:50:MET:HB2	1.77	0.43
49:S2:1099:G:H2'	49:S2:1100:A:O4'	2.19	0.43
49:S2:1378:A:H4'	49:S2:1379:A:O5'	2.18	0.43
51:SD:93:THR:O	51:SD:93:THR:OG1	2.36	0.43
56:SI:203:LYS:HD2	56:SI:203:LYS:HA	1.74	0.43
59:SL:104:LYS:CE	70:SX:8:ARG:HH21	2.32	0.43
60:SN:67:THR:OG1	60:SN:68:GLY:N	2.51	0.43
61:SO:97:LEU:HD21	61:SO:112:ALA:HB1	2.01	0.43
70:SX:105:PHE:CE2	70:SX:112:VAL:HG22	2.53	0.43
80:SM:59:PRO:HA	80:SM:62:VAL:HG22	2.00	0.43
2:SA:205:ARG:NH2	2:SA:210:ILE:HG12	2.34	0.43
8:L5:266:C:H2'	8:L5:267:G:C8	2.54	0.43
8:L5:1733:G:N3	8:L5:4214:A:H2'	2.33	0.43
8:L5:3611:A:H2	8:L5:5016:A:H8	1.67	0.43
8:L5:4085:A:OP1	30:LX:45:THR:HG22	2.18	0.43
8:L5:4136:G:H2'	8:L5:4137:C:C6	2.54	0.43
8:L5:4342:C:H2'	8:L5:4343:U:H6	1.84	0.43
8:L5:4372:U:O2	8:L5:4377:G:O2'	2.23	0.43
8:L5:4749:C:H2'	8:L5:4750:G:O4'	2.18	0.43
10:L8:3:A:O2'	22:LP:61:ARG:HD2	2.18	0.43
13:LE:264:ILE:HD12	13:LE:267:LEU:HD22	2.01	0.43
14:LF:247:MET:HE2	14:LF:247:MET:HB3	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LL:80:GLU:OE2	18:LL:102:ARG:NH2	2.51	0.43
19:LM:6:PHE:O	19:LM:11:ARG:HD3	2.18	0.43
26:LT:46:GLY:O	26:LT:49:GLN:NE2	2.51	0.43
30:LX:145:ASP:C	30:LX:145:ASP:OD2	2.61	0.43
31:LY:108:ARG:HB3	31:LY:108:ARG:CZ	2.48	0.43
32:LZ:126:LYS:HD3	32:LZ:126:LYS:N	2.34	0.43
33:La:100:ILE:HG12	33:La:123:ILE:HB	2.00	0.43
42:Lk:26:LYS:HB2	42:Lk:69:LEU:HD12	2.01	0.43
49:S2:106:C:H2'	49:S2:107:A:C8	2.51	0.43
49:S2:604:A:O2'	49:S2:605:A:OP1	2.34	0.43
49:S2:1387:G:H2'	49:S2:1388:A:O4'	2.19	0.43
52:SE:115:THR:HG22	52:SE:117:GLU:N	2.32	0.43
54:SG:176:ILE:HB	54:SG:179:LEU:HD12	2.01	0.43
79:Sg:107:ASP:OD2	79:Sg:125:ARG:NH1	2.52	0.43
80:SM:29:ASP:C	80:SM:29:ASP:OD1	2.62	0.43
80:SM:93:LYS:HB3	80:SM:102:LYS:H	1.83	0.43
1:LA:28:ARG:HB2	1:LA:123:ARG:HB2	2.01	0.43
3:LB:307:TYR:HD2	3:LB:366:LYS:HA	1.84	0.43
8:L5:418:A:H4'	8:L5:2311:C:H5'	2.01	0.43
8:L5:952:G:H2'	8:L5:953:C:C6	2.54	0.43
8:L5:1251:C:H2'	8:L5:1252:C:C6	2.54	0.43
8:L5:1576:G:OP2	8:L5:1576:G:H8	2.02	0.43
8:L5:4220:A:OP2	26:LT:2:THR:HG23	2.18	0.43
8:L5:4538:G:H2'	8:L5:4539:U:H6	1.84	0.43
8:L5:4586:G:O6	8:L5:4717:A:N6	2.52	0.43
8:L5:4700:A:C2	16:LH:69:THR:HG22	2.52	0.43
8:L5:4891:G:H21	19:LM:118:MET:HE1	1.84	0.43
9:L7:23:A:C2	9:L7:118:C:H1'	2.53	0.43
14:LF:30:ILE:O	14:LF:34:ARG:HG3	2.18	0.43
14:LF:228:VAL:HA	25:LS:39:VAL:HG22	2.00	0.43
31:LY:98:GLY:C	31:LY:99:ILE:HD12	2.44	0.43
37:Lf:106:TYR:HB2	37:Lf:107:PRO:HD3	2.01	0.43
49:S2:1101:U:H2'	49:S2:1102:G:H8	1.83	0.43
51:SD:72:VAL:HG21	58:SK:70:TYR:CE1	2.54	0.43
59:SL:135:SER:HB3	59:SL:138:VAL:HG22	2.00	0.43
60:SN:88:LEU:HD12	60:SN:88:LEU:HA	1.86	0.43
66:ST:14:PHE:HZ	66:ST:131:LEU:HG	1.84	0.43
66:ST:73:GLY:H	66:ST:76:THR:HG23	1.83	0.43
69:SW:3:ARG:HH22	69:SW:28:ARG:HH21	1.66	0.43
3:LB:103:LYS:HB2	3:LB:103:LYS:HE2	1.78	0.43
3:LB:285:TYR:CE1	3:LB:334:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:198:GLU:O	4:SB:202:GLN:NE2	2.49	0.43
8:L5:1431:C:H2'	8:L5:1432:G:O4'	2.19	0.43
8:L5:1969:G:OP2	8:L5:1970:A:N6	2.48	0.43
8:L5:2309:G:O2'	10:L8:18:U:O2	2.36	0.43
8:L5:2465:C:H2'	8:L5:2466:G:O4'	2.19	0.43
8:L5:2782:U:OP2	43:L1:10:LYS:NZ	2.43	0.43
8:L5:4139:G:N2	8:L5:4140:C:H41	2.17	0.43
8:L5:4417:C:H2'	8:L5:4418:G:O4'	2.19	0.43
8:L5:4577:U:H2'	8:L5:4578:G:C8	2.54	0.43
10:L8:93:C:OP1	41:Lj:76:HIS:NE2	2.42	0.43
11:LC:138:MET:HB3	11:LC:144:ILE:HG12	2.00	0.43
18:LL:7:GLY:O	33:La:49:HIS:NE2	2.46	0.43
32:LZ:22:LYS:NZ	32:LZ:132:GLN:O	2.34	0.43
32:LZ:25:ILE:HA	32:LZ:43:VAL:HG12	2.01	0.43
37:Lf:29:LYS:HB2	37:Lf:83:MET:SD	2.59	0.43
47:Lp:45:THR:O	47:Lp:45:THR:OG1	2.32	0.43
49:S2:484:A:H8	49:S2:484:A:OP2	2.02	0.43
49:S2:1713:C:H2'	49:S2:1714:U:H6	1.83	0.43
50:SC:232:THR:HG22	50:SC:234:GLY:H	1.84	0.43
51:SD:220:THR:OG1	51:SD:221:THR:N	2.52	0.43
56:SI:193:LYS:HD3	56:SI:193:LYS:HA	1.83	0.43
63:SQ:42:ILE:HD13	63:SQ:42:ILE:HA	1.85	0.43
66:ST:88:MET:HE2	66:ST:88:MET:HB3	1.88	0.43
69:SW:26:LEU:HB2	74:Sb:7:LEU:HD12	2.00	0.43
4:SB:123:ALA:HB2	4:SB:165:ARG:HG3	2.00	0.42
8:L5:223:G:H4'	8:L5:225:G:C8	2.54	0.42
8:L5:1295:C:H4'	8:L5:1296:G:C8	2.54	0.42
8:L5:3588:C:H3'	8:L5:3589:G:H8	1.84	0.42
8:L5:4685:U:OP1	44:Lm:112:LYS:HD2	2.19	0.42
10:L8:52:A:O2'	43:Ll:19:GLN:O	2.37	0.42
15:LG:106:THR:HG22	15:LG:195:HIS:CE1	2.54	0.42
15:LG:228:ASP:OD1	15:LG:228:ASP:N	2.52	0.42
18:LL:129:ARG:HE	18:LL:129:ARG:HB3	1.60	0.42
19:LM:95:ILE:C	19:LM:97:ALA:H	2.27	0.42
35:Lc:38:ILE:HG21	35:Lc:63:TYR:HB3	2.00	0.42
38:Lg:76:ARG:HG2	38:Lg:77:ALA:N	2.34	0.42
49:S2:1665:G:C8	66:ST:88:MET:HE3	2.53	0.42
49:S2:1700:C:O2	49:S2:1834:A:N6	2.52	0.42
59:SL:55:TYR:CD2	59:SL:115:PRO:HG2	2.54	0.42
61:SO:82:ALA:HB2	61:SO:119:LEU:HD23	2.01	0.42
68:SV:2:GLN:NE2	68:SV:8:PHE:HE1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sg:223:GLU:OE1	79:Sg:225:LYS:HG2	2.19	0.42
80:SM:68:LEU:HD23	80:SM:68:LEU:HA	1.87	0.42
8:L5:270:U:H2'	8:L5:271:C:H6	1.84	0.42
8:L5:1187:G:H2'	8:L5:1188:C:O4'	2.19	0.42
8:L5:1504:G:H2'	8:L5:1505:C:H6	1.84	0.42
8:L5:3744:OMG:HM23	8:L5:3744:OMG:H1'	1.84	0.42
8:L5:4460:U:H2'	8:L5:4461:C:H6	1.84	0.42
8:L5:4642:U:H2'	8:L5:4643:G:H8	1.82	0.42
12:LD:234:ASP:O	12:LD:235:MET:HG2	2.19	0.42
23:LQ:85:THR:HA	23:LQ:104:ARG:O	2.19	0.42
28:LV:74:LYS:HE2	28:LV:74:LYS:HB3	1.71	0.42
28:LV:96:LEU:HD13	29:LW:20:ARG:HG2	2.01	0.42
32:LZ:36:ARG:HG2	32:LZ:38:TYR:CZ	2.54	0.42
36:Ld:37:GLY:O	36:Ld:41:ARG:HG2	2.19	0.42
40:Li:79:THR:OG1	40:Li:82:ARG:HG3	2.19	0.42
48:Lr:97:ILE:HG21	48:Lr:107:ARG:HB2	2.01	0.42
49:S2:553:U:H5	49:S2:554:A:C4	2.38	0.42
49:S2:560:A:H5'	57:SJ:174:LYS:HB2	2.01	0.42
49:S2:1227:G:C2	49:S2:1228:A:C8	3.06	0.42
49:S2:1383:A2M:HM'3	49:S2:1383:A2M:H1'	1.78	0.42
49:S2:1544:C:O2'	63:SQ:75:GLY:O	2.13	0.42
49:S2:1633:A:H2'	49:S2:1634:A:C8	2.54	0.42
50:SC:165:VAL:HG21	50:SC:217:ALA:HB1	2.01	0.42
54:SG:153:VAL:HG23	54:SG:176:ILE:HD13	2.00	0.42
58:SK:15:LEU:HD23	58:SK:79:LEU:HD11	2.00	0.42
61:SO:31:CYS:HA	61:SO:43:HIS:O	2.19	0.42
62:SP:41:GLN:HG3	62:SP:84:ILE:HG21	2.01	0.42
69:SW:30:CYS:SG	69:SW:31:SER:N	2.91	0.42
71:SY:92:ALA:HB2	71:SY:97:TYR:HB3	2.01	0.42
8:L5:40:G:N2	8:L5:4380:A:H62	2.17	0.42
8:L5:1346:C:H2'	8:L5:1347:G:H8	1.84	0.42
12:LD:242:LYS:HB2	12:LD:242:LYS:HE3	1.83	0.42
13:LE:190:HIS:ND1	13:LE:192:LYS:HB2	2.34	0.42
15:LG:63:LEU:HD22	20:LN:33:LEU:HD21	2.02	0.42
23:LQ:65:ARG:HH12	23:LQ:142:PRO:HB3	1.85	0.42
25:LS:147:ASP:N	25:LS:147:ASP:OD1	2.47	0.42
26:LT:71:ALA:HA	26:LT:92:ARG:HA	2.00	0.42
29:LW:4:GLU:OE2	29:LW:20:ARG:NH2	2.52	0.42
32:LZ:115:LYS:NZ	32:LZ:119:GLU:OE2	2.38	0.42
36:Ld:68:LEU:CB	36:Ld:108:TYR:HB2	2.48	0.42
51:SD:162:ASP:N	51:SD:163:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:75:LYS:HB3	56:SI:75:LYS:HE2	1.86	0.42
71:SY:4:THR:HB	71:SY:5:VAL:H	1.70	0.42
8:L5:153:G:H2'	8:L5:154:G:H8	1.84	0.42
8:L5:500:G:H1'	8:L5:504:G:H3'	2.01	0.42
8:L5:654:C:H2'	8:L5:655:C:C6	2.54	0.42
8:L5:1246:G:H2'	8:L5:1247:U:H6	1.85	0.42
8:L5:1248:C:H2'	8:L5:1249:C:H6	1.83	0.42
8:L5:1518:A:N6	18:LL:19:GLN:OE1	2.53	0.42
8:L5:2411:C:H2'	8:L5:2412:A:C8	2.53	0.42
8:L5:2844:A:N6	8:L5:3839:G:O2'	2.53	0.42
8:L5:4112:C:H2'	8:L5:4113:U:H5'	2.00	0.42
13:LE:276:ALA:HB1	37:Lf:3:GLY:HA3	2.00	0.42
24:LR:157:ASP:OD1	24:LR:157:ASP:C	2.61	0.42
35:Lc:19:GLN:OE1	35:Lc:20:LEU:N	2.52	0.42
37:Lf:57:THR:HG21	37:Lf:68:ARG:HG2	2.02	0.42
49:S2:5:U:H2'	49:S2:6:G:C8	2.55	0.42
49:S2:388:U:H2'	49:S2:389:A:C8	2.54	0.42
52:SE:60:GLU:OE1	71:SY:20:ARG:NH2	2.49	0.42
52:SE:89:VAL:HG13	52:SE:114:ILE:HD11	2.02	0.42
53:SF:142:SER:OG	75:Sc:49:PRO:O	2.26	0.42
54:SG:61:PHE:CD2	54:SG:72:ARG:HD3	2.54	0.42
57:SJ:174:LYS:HB2	57:SJ:174:LYS:HE3	1.71	0.42
65:SS:40:TYR:HA	65:SS:83:PHE:HE2	1.85	0.42
67:SU:55:ARG:HG2	67:SU:87:ARG:CD	2.50	0.42
71:SY:16:ARG:CZ	71:SY:16:ARG:HB2	2.49	0.42
71:SY:23:MET:HE1	71:SY:44:LEU:HD11	2.00	0.42
75:Sc:23:SER:O	75:Sc:26:GLN:NE2	2.53	0.42
79:Sg:129:ILE:HB	79:Sg:142:VAL:HG23	2.01	0.42
82:LI:87:ILE:HG12	82:LI:138:ILE:HG12	2.00	0.42
3:LB:108:GLU:OE2	3:LB:138:GLN:NE2	2.52	0.42
3:LB:161:ARG:HG2	3:LB:184:GLN:HA	2.02	0.42
8:L5:754:U:H2'	8:L5:755:C:C6	2.55	0.42
8:L5:958:G:H21	13:LE:125:LEU:H	1.68	0.42
8:L5:2055:G:H4'	8:L5:2056:G:OP2	2.20	0.42
8:L5:3635:A:C8	8:L5:3692:A:C8	3.08	0.42
8:L5:4578:G:H2'	8:L5:4579:U:H6	1.83	0.42
8:L5:4699:U:H4'	8:L5:4700:A:OP1	2.20	0.42
8:L5:4868:G:O2'	8:L5:4872:G:OP1	2.38	0.42
9:L7:58:A:H2'	9:L7:59:G:H8	1.84	0.42
10:L8:66:A:H2'	10:L8:67:U:H6	1.83	0.42
11:LC:25:PRO:HG2	11:LC:28:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:75:ALA:HB2	26:LT:140:PHE:HE2	1.83	0.42
18:LL:55:ILE:HG23	18:LL:76:PHE:HE1	1.84	0.42
21:LO:121:PRO:HD2	25:LS:166:ARG:O	2.19	0.42
24:LR:19:LYS:HB2	24:LR:19:LYS:HE3	1.84	0.42
24:LR:149:LYS:HB3	24:LR:149:LYS:HE2	1.70	0.42
31:LY:54:GLU:HB2	31:LY:108:ARG:HB2	2.01	0.42
49:S2:96:C:H2'	49:S2:97:U:H6	1.84	0.42
49:S2:496:C:P	52:SE:49:ARG:HH12	2.42	0.42
49:S2:677:G:P	60:SN:5:HIS:HE2	2.42	0.42
49:S2:1015:U:OP2	74:Sb:20:LYS:NZ	2.40	0.42
49:S2:1208:A:O2'	49:S2:1209:A:H8	2.01	0.42
49:S2:1542:C:O2'	49:S2:1543:U:O5'	2.35	0.42
71:SY:102:THR:CG2	71:SY:107:ARG:HE	2.31	0.42
79:Sg:32:LEU:HD11	79:Sg:92:LEU:HD11	2.02	0.42
79:Sg:218:LEU:HD23	79:Sg:218:LEU:H	1.85	0.42
81:Le:23:HIS:HA	81:Le:53:ILE:HD12	2.02	0.42
82:LI:145:LYS:HA	82:LI:148:VAL:HG12	2.00	0.42
8:L5:980:U:H2'	8:L5:981:C:C6	2.54	0.42
8:L5:1095:A:N1	8:L5:1200:G:C6	2.87	0.42
8:L5:1221:G:H4'	8:L5:1222:A:H5'	2.01	0.42
8:L5:1655:C:O2	8:L5:4390:A:O2'	2.37	0.42
8:L5:1685:G:H5'	8:L5:1686:C:OP2	2.19	0.42
8:L5:2374:A:H2'	8:L5:2375:A:H8	1.85	0.42
8:L5:2434:G:O2'	8:L5:2527:A:N1	2.48	0.42
8:L5:2542:G:H2'	8:L5:2543:A:C8	2.54	0.42
8:L5:4232:U:H4'	8:L5:4233:A:O4'	2.20	0.42
8:L5:4729:A:H5''	8:L5:4965:U:H1'	2.01	0.42
8:L5:4934:A:H2'	8:L5:4935:C:C6	2.55	0.42
9:L7:38:U:N3	9:L7:41:G:OP2	2.39	0.42
11:LC:80:ARG:HA	11:LC:80:ARG:HD2	1.82	0.42
15:LG:190:LEU:HD23	15:LG:190:LEU:HA	1.86	0.42
16:LH:63:ASN:O	16:LH:67:LEU:HG	2.19	0.42
18:LL:140:SER:C	18:LL:142:GLU:H	2.26	0.42
26:LT:91:VAL:HG23	26:LT:96:ILE:HD11	2.02	0.42
51:SD:99:ILE:HG23	51:SD:173:ARG:HH21	1.84	0.42
54:SG:138:ALA:HB1	54:SG:153:VAL:HG11	2.00	0.42
57:SJ:104:ASP:OD1	57:SJ:104:ASP:C	2.62	0.42
63:SQ:73:LYS:HE2	63:SQ:73:LYS:HB2	1.88	0.42
8:L5:908:G:H2'	8:L5:909:A:C8	2.54	0.42
8:L5:2505:C:H4'	8:L5:2506:G:O4'	2.19	0.42
8:L5:2727:C:H2'	8:L5:2728:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:3684:G:H2'	8:L5:3685:C:C6	2.55	0.42
8:L5:4080:C:H2'	8:L5:4081:G:H8	1.85	0.42
8:L5:4233:A:C5	8:L5:4235:G:C8	3.08	0.42
8:L5:4905:C:H2'	8:L5:4906:C:H6	1.85	0.42
9:L7:82:G:H2'	9:L7:83:A:C8	2.53	0.42
10:L8:45:C:P	43:L1:15:LYS:HD3	2.60	0.42
12:LD:255:LYS:O	12:LD:257:PRO:HG2	2.19	0.42
27:LU:40:GLU:HG2	27:LU:63:ILE:HG22	2.02	0.42
32:LZ:113:GLU:OE2	32:LZ:117:LYS:HG2	2.19	0.42
46:Lo:26:TYR:HB2	46:Lo:82:MET:HE1	2.01	0.42
49:S2:1628:C:OP1	66:ST:38:LYS:NZ	2.45	0.42
49:S2:1839:U:H1'	49:S2:1863:A:H2	1.84	0.42
51:SD:71:ALA:O	51:SD:74:GLN:HG3	2.20	0.42
52:SE:117:GLU:HA	52:SE:120:LYS:HD2	2.01	0.42
55:SH:10:LYS:HE3	55:SH:16:PRO:HA	2.02	0.42
57:SJ:104:ASP:O	57:SJ:107:GLU:HG2	2.19	0.42
71:SY:91:LEU:HD22	71:SY:96:LEU:HD12	2.02	0.42
79:Sg:188:HIS:HD2	79:Sg:219:TRP:CG	2.38	0.42
81:Le:85:LEU:HD22	81:Le:111:ILE:HG23	2.01	0.42
3:LB:56:ILE:HD12	3:LB:368:ILE:HG12	2.02	0.42
6:B4:21:G:N7	6:B4:45:G:O6	2.53	0.42
8:L5:182:G:H22	8:L5:255:C:H2'	1.84	0.42
8:L5:1246:G:H2'	8:L5:1247:U:C6	2.54	0.42
8:L5:1460:C:H5''	23:LQ:144:LYS:HG3	2.01	0.42
8:L5:1502:G:OP2	23:LQ:62:SER:OG	2.32	0.42
8:L5:1590:C:H4'	8:L5:2857:A:H5'	2.01	0.42
8:L5:1907:A:H4'	14:LF:220:MET:HE1	2.01	0.42
8:L5:2730:U:H2'	8:L5:2731:C:C6	2.54	0.42
8:L5:4892:A:H2'	8:L5:4893:A:O4'	2.20	0.42
9:L7:111:C:H2'	9:L7:112:U:O4'	2.20	0.42
12:LD:41:LYS:HB2	26:LT:68:THR:O	2.19	0.42
12:LD:256:LYS:CA	12:LD:257:PRO:HG2	2.49	0.42
16:LH:120:GLU:CD	16:LH:124:ARG:HH21	2.28	0.42
16:LH:168:LYS:HB3	16:LH:168:LYS:HE2	1.80	0.42
19:LM:74:ARG:O	19:LM:78:GLN:HG3	2.20	0.42
20:LN:75:VAL:HG11	20:LN:80:THR:HG22	2.00	0.42
28:LV:90:ARG:NE	28:LV:124:GLU:OE1	2.52	0.42
49:S2:39:A:OP2	57:SJ:5:ARG:NH1	2.52	0.42
49:S2:443:U:O4	49:S2:447:A:N7	2.53	0.42
49:S2:959:G:O2'	49:S2:1065:G:H4'	2.19	0.42
49:S2:1101:U:OP1	64:SR:132:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1520:G:H2'	49:S2:1520:G:N3	2.35	0.42
56:SI:36:THR:HG22	56:SI:57:ALA:O	2.20	0.42
62:SP:34:MET:CE	62:SP:46:ASN:OD1	2.59	0.42
8:L5:731:G:C6	8:L5:932:A:C4	3.07	0.42
8:L5:1099:C:H2'	8:L5:1100:U:O4'	2.20	0.42
8:L5:1715:C:H2'	8:L5:1716:G:C4	2.55	0.42
8:L5:2562:G:C2	8:L5:2566:G:C6	3.08	0.42
8:L5:2676:A:C4	8:L5:2677:G:C8	3.07	0.42
8:L5:3588:C:H2'	8:L5:3589:G:O4'	2.20	0.42
8:L5:3756:A:C2'	8:L5:3757:G:H5'	2.50	0.42
8:L5:4208:U:OP2	26:LT:4:THR:OG1	2.30	0.42
8:L5:5003:U:H2'	8:L5:5004:C:C6	2.54	0.42
12:LD:36:LEU:HG	12:LD:50:ARG:HD2	2.01	0.42
13:LE:47:ASN:HD21	13:LE:57:TYR:H	1.67	0.42
25:LS:74:ARG:NH1	25:LS:74:ARG:HB3	2.35	0.42
27:LU:31:ASP:OD2	27:LU:114:TYR:OH	2.23	0.42
31:LY:109:LEU:HD12	31:LY:109:LEU:HA	1.87	0.42
33:La:76:ASP:OD1	33:La:77:LYS:N	2.52	0.42
44:Lm:99:CYS:HB3	44:Lm:115:CYS:HB3	1.35	0.42
49:S2:669:A:N3	49:S2:1164:G:O2'	2.48	0.42
53:SF:43:GLU:C	53:SF:45:TYR:H	2.27	0.42
54:SG:68:LEU:HD23	54:SG:68:LEU:HA	1.81	0.42
55:SH:50:GLU:HG3	55:SH:58:LYS:HE2	2.01	0.42
63:SQ:26:LYS:O	63:SQ:66:VAL:HA	2.19	0.42
65:SS:100:ALA:C	65:SS:102:GLY:H	2.27	0.42
67:SU:97:ILE:HD12	67:SU:97:ILE:HA	1.87	0.42
73:Sa:60:ASP:OD1	73:Sa:60:ASP:N	2.51	0.42
80:SM:18:LEU:HA	80:SM:21:VAL:HG12	2.01	0.42
82:LI:52:MET:HB2	82:LI:152:LEU:HD22	2.02	0.42
3:LB:213:GLN:NE2	3:LB:285:TYR:O	2.53	0.42
8:L5:174:C:N3	8:L5:263:G:N1	2.68	0.42
8:L5:1428:U:H5''	23:LQ:42:THR:HB	2.01	0.42
8:L5:1513:U:H2'	8:L5:1514:U:O4'	2.20	0.42
8:L5:2104:G:H2'	8:L5:2105:A:C4	2.54	0.42
8:L5:2859:G:H2'	8:L5:2860:C:H6	1.85	0.42
8:L5:3709:U:H2'	8:L5:3710:G:H5'	2.01	0.42
8:L5:3799:A:N3	8:L5:4506:C:O2'	2.38	0.42
8:L5:4966:A:H2'	8:L5:4967:A:O4'	2.19	0.42
11:LC:187:GLN:HG2	11:LC:203:GLN:HG2	2.01	0.42
14:LF:220:MET:CE	14:LF:223:LYS:HB3	2.50	0.42
14:LF:220:MET:CE	14:LF:223:LYS:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LG:97:LYS:HE2	15:LG:97:LYS:HB2	1.74	0.42
20:LN:181:HIS:O	20:LN:195:ARG:NH2	2.50	0.42
27:LU:94:ASN:N	27:LU:94:ASN:OD1	2.53	0.42
29:LW:55:TYR:CD1	29:LW:55:TYR:C	2.97	0.42
44:Lm:95:ILE:HG22	44:Lm:96:CYS:O	2.20	0.42
49:S2:16:G:H2'	49:S2:17:C:C6	2.55	0.42
49:S2:35:C:H5''	49:S2:579:C:H5''	2.02	0.42
49:S2:174:OMC:HM23	49:S2:174:OMC:H1'	1.91	0.42
49:S2:344:U:H2'	49:S2:345:U:H6	1.84	0.42
49:S2:575:A:H2'	49:S2:576:A2M:O4'	2.19	0.42
51:SD:54:ARG:HB2	51:SD:57:ASN:HB2	2.02	0.42
53:SF:201:LYS:HG3	53:SF:204:ARG:NH1	2.34	0.42
70:SX:101:LEU:HD22	70:SX:124:LYS:HD3	2.02	0.42
71:SY:44:LEU:HD23	71:SY:44:LEU:HA	1.82	0.42
78:Sf:118:ARG:HB2	78:Sf:131:PHE:CD2	2.55	0.42
6:B4:47:C:C4	6:B4:58:A:C8	3.08	0.41
8:L5:423:G:H2'	8:L5:424:U:H6	1.85	0.41
8:L5:1882:U:C4	8:L5:2279:A:C2	3.08	0.41
8:L5:1893:C:H1'	8:L5:1937:C:O2	2.19	0.41
8:L5:2804:OMC:HM23	8:L5:2804:OMC:H1'	1.78	0.41
8:L5:2808:G:O3'	24:LR:60:ARG:NH1	2.53	0.41
8:L5:4088:C:H2'	8:L5:4089:G:C8	2.55	0.41
8:L5:4460:U:H2'	8:L5:4461:C:C6	2.55	0.41
8:L5:4880:C:OP1	19:LM:124:LYS:NZ	2.44	0.41
10:L8:67:U:OP1	41:Lj:87:LYS:HG2	2.20	0.41
12:LD:213:GLU:HG3	12:LD:214:GLU:N	2.35	0.41
14:LF:214:SER:OG	14:LF:215:SER:N	2.53	0.41
17:LJ:129:ASP:OD2	17:LJ:129:ASP:C	2.62	0.41
18:LL:89:LYS:HA	18:LL:89:LYS:HD3	1.87	0.41
21:LO:108:ILE:HD13	21:LO:117:ARG:HD3	2.01	0.41
24:LR:37:SER:OG	24:LR:40:GLN:HG3	2.20	0.41
27:LU:36:ALA:C	27:LU:38:ASN:N	2.78	0.41
31:LY:112:ASP:H	31:LY:115:ARG:HB3	1.85	0.41
49:S2:587:A:H2	57:SJ:172:ARG:HH12	1.67	0.41
49:S2:1456:G:H2'	49:S2:1457:U:C6	2.55	0.41
59:SL:65:ASN:O	59:SL:65:ASN:ND2	2.50	0.41
66:ST:43:LYS:HA	66:ST:43:LYS:HD3	1.73	0.41
67:SU:32:LEU:HD21	67:SU:87:ARG:HG2	2.02	0.41
69:SW:55:ASP:N	69:SW:55:ASP:OD1	2.52	0.41
78:Sf:140:TYR:HE1	78:Sf:145:CYS:HB2	1.85	0.41
79:Sg:285:GLN:O	79:Sg:303:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LB:252:ALA:HB3	8:L5:4457:U:H1'	2.01	0.41
8:L5:757:G:H3'	8:L5:758:G:H8	1.85	0.41
8:L5:2722:G:H2'	8:L5:2723:U:O4'	2.19	0.41
8:L5:3724:A2M:HM'3	8:L5:3724:A2M:H1'	1.72	0.41
9:L7:16:A:H2'	9:L7:17:C:C6	2.55	0.41
9:L7:30:C:O2'	12:LD:221:LYS:NZ	2.36	0.41
24:LR:82:LYS:HE2	24:LR:82:LYS:HB3	1.94	0.41
27:LU:80:LYS:O	27:LU:110:TYR:HE2	2.03	0.41
28:LV:126:ALA:HB2	28:LV:139:ILE:CD1	2.51	0.41
30:LX:122:ALA:N	30:LX:139:ARG:O	2.52	0.41
32:LZ:112:ARG:HD3	32:LZ:112:ARG:C	2.45	0.41
49:S2:1265:A:O2'	49:S2:1266:C:H6	2.02	0.41
55:SH:130:LEU:HD22	55:SH:139:ILE:HD11	2.03	0.41
58:SK:45:VAL:O	58:SK:49:MET:HG2	2.21	0.41
59:SL:56:ILE:HD13	59:SL:56:ILE:HA	1.85	0.41
60:SN:63:VAL:HG11	60:SN:71:ILE:HG12	2.02	0.41
78:Sf:135:HIS:CD2	78:Sf:140:TYR:HB3	2.56	0.41
3:LB:122:TRP:CH2	3:LB:127:LYS:HG2	2.55	0.41
8:L5:300:A:H2'	8:L5:301:G:H8	1.86	0.41
8:L5:494:U:H2'	8:L5:495:C:C6	2.55	0.41
8:L5:1173:G:C4	8:L5:1174:A:H1'	2.55	0.41
8:L5:1563:A:H2'	8:L5:1564:A:O4'	2.20	0.41
8:L5:1816:C:C4	8:L5:1817:U:C4	3.08	0.41
8:L5:2362:U:OP1	22:LP:82:ARG:NH2	2.54	0.41
8:L5:2380:G:N2	8:L5:2424:OMG:H5'	2.35	0.41
8:L5:2664:G:H4'	8:L5:2677:G:H4'	2.02	0.41
8:L5:4591:U:H2'	8:L5:4592:C:C6	2.55	0.41
8:L5:4743:G:H2'	8:L5:4744:A:C8	2.55	0.41
9:L7:4:U:H2'	9:L7:5:A:H8	1.84	0.41
10:L8:14:OMU:H6	10:L8:14:OMU:HM22	2.03	0.41
11:LC:349:LEU:HD12	11:LC:349:LEU:HA	1.89	0.41
12:LD:195:HIS:O	12:LD:199:ILE:HG13	2.20	0.41
18:LL:143:GLU:O	18:LL:147:ALA:HB2	2.21	0.41
21:LO:179:LYS:HA	21:LO:179:LYS:HD2	1.55	0.41
28:LV:20:LEU:HB2	28:LV:55:ALA:O	2.21	0.41
37:Lf:45:LYS:HD2	37:Lf:105:LEU:HA	2.01	0.41
49:S2:328:U:O2'	49:S2:329:G:O5'	2.36	0.41
49:S2:413:G:H5'	49:S2:813:A:H61	1.85	0.41
49:S2:562:U:HO2'	49:S2:563:G:H8	1.69	0.41
49:S2:639:C:H2'	49:S2:640:A:C8	2.56	0.41
49:S2:1285:G:C6	80:SM:57:ASP:OD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:32:HIS:ND1	58:SK:33:PRO:HD2	2.36	0.41
62:SP:23:ASP:N	62:SP:23:ASP:OD1	2.52	0.41
64:SR:77:GLU:HG2	64:SR:80:ARG:NH2	2.36	0.41
69:SW:117:ARG:HE	69:SW:117:ARG:HB2	1.72	0.41
71:SY:105:LYS:HA	71:SY:105:LYS:HD3	1.85	0.41
72:SZ:66:LYS:NZ	72:SZ:111:ARG:HH21	2.17	0.41
79:Sg:110:SER:OG	79:Sg:153:CYS:HA	2.20	0.41
6:B4:58:A:H3'	6:B4:59:A:C8	2.55	0.41
8:L5:473:C:H2'	8:L5:474:C:C6	2.56	0.41
8:L5:1350:C:H2'	8:L5:1351:G:C8	2.55	0.41
8:L5:2045:G:O2'	8:L5:2046:G:H5''	2.21	0.41
8:L5:2475:G:H5''	8:L5:2476:G:C8	2.55	0.41
8:L5:2862:G:N3	8:L5:3624:A:H2'	2.36	0.41
10:L8:75:OMG:HM23	10:L8:75:OMG:H1'	1.81	0.41
11:LC:140:LYS:NZ	11:LC:245:HIS:HB2	2.36	0.41
12:LD:64:ILE:HG12	12:LD:105:LEU:HD21	2.02	0.41
25:LS:81:TRP:HE3	25:LS:128:LYS:O	2.04	0.41
26:LT:14:MET:HE2	26:LT:58:HIS:CG	2.55	0.41
28:LV:139:ILE:HD13	28:LV:139:ILE:HA	1.80	0.41
33:La:134:GLU:HG3	33:La:135:GLU:N	2.34	0.41
42:Lk:24:LYS:HG2	42:Lk:67:LYS:HZ3	1.83	0.41
49:S2:140:C:O2	49:S2:143:U:O2'	2.38	0.41
49:S2:495:U:H2'	49:S2:496:C:O4'	2.19	0.41
49:S2:649:U:OP2	70:SX:108:LYS:NZ	2.53	0.41
49:S2:1285:G:C3'	49:S2:1286:G:H5'	2.50	0.41
49:S2:1585:U:H1'	49:S2:1586:U:OP1	2.20	0.41
49:S2:1690:U:H2'	49:S2:1691:U:C6	2.55	0.41
49:S2:1831:A:N6	49:S2:1832:6MZ:H9	2.35	0.41
50:SC:78:LEU:HD23	50:SC:81:ILE:HD12	2.02	0.41
50:SC:121:ARG:NH2	50:SC:123:ARG:HH21	2.17	0.41
50:SC:196:ILE:HB	50:SC:223:TYR:HB2	2.01	0.41
54:SG:142:ARG:HA	54:SG:147:LEU:HD12	2.02	0.41
66:ST:6:VAL:HG12	66:ST:135:ALA:HB2	2.02	0.41
74:Sb:36:LYS:HD3	74:Sb:36:LYS:HA	1.70	0.41
75:Sc:36:ASP:OD1	75:Sc:37:ASP:N	2.52	0.41
2:SA:142:LEU:O	68:SV:60:ARG:NH2	2.53	0.41
8:L5:18:C:H2'	8:L5:19:G:H8	1.85	0.41
8:L5:509:A:C2	33:La:101:ILE:HA	2.56	0.41
8:L5:509:A:C6	33:La:105:ARG:HD3	2.55	0.41
8:L5:1260:G:H2'	8:L5:1261:G:H8	1.85	0.41
8:L5:2100:A:N7	8:L5:2101:C:N4	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:2669:C:OP2	24:LR:128:LYS:NZ	2.41	0.41
8:L5:3651:A:H2'	8:L5:3652:A:C8	2.55	0.41
8:L5:4342:C:H2'	8:L5:4343:U:C6	2.55	0.41
8:L5:4968:A:H2'	8:L5:4969:C:C6	2.55	0.41
12:LD:107:ARG:HA	12:LD:107:ARG:HD2	1.84	0.41
13:LE:284:HIS:CD2	13:LE:285:LYS:HG2	2.56	0.41
15:LG:87:LEU:HD22	15:LG:182:CYS:SG	2.61	0.41
21:LO:177:LEU:HD23	21:LO:177:LEU:HA	1.83	0.41
23:LQ:59:PRO:HG3	23:LQ:143:ARG:HA	2.03	0.41
32:LZ:103:ASP:HB3	32:LZ:106:LEU:HD12	2.02	0.41
35:Lc:17:ARG:NH1	35:Lc:108:MET:SD	2.93	0.41
35:Lc:17:ARG:NH1	35:Lc:108:MET:HE1	2.29	0.41
41:Lj:67:LEU:HD23	41:Lj:67:LEU:HA	1.82	0.41
47:Lp:90:LYS:HB2	47:Lp:90:LYS:HE3	1.84	0.41
49:S2:656:G:H5'	49:S2:662:G:N2	2.35	0.41
49:S2:1533:A:C8	49:S2:1604:G:H1'	2.55	0.41
49:S2:1549:U:OP1	76:Sd:34:TYR:OH	2.24	0.41
49:S2:1567:G:C6	65:SS:82:TRP:CG	3.08	0.41
49:S2:1579:A:O2'	49:S2:1581:C:OP2	2.24	0.41
49:S2:1667:U:H2'	49:S2:1668:U:C6	2.55	0.41
49:S2:1705:C:H2'	49:S2:1706:G:C8	2.56	0.41
55:SH:145:ARG:HD2	69:SW:49:GLU:OE1	2.20	0.41
57:SJ:128:VAL:O	57:SJ:132:GLN:HG3	2.20	0.41
58:SK:42:ASN:HA	58:SK:45:VAL:HG12	2.02	0.41
70:SX:105:PHE:HB2	70:SX:119:ARG:C	2.44	0.41
71:SY:9:THR:HG23	71:SY:23:MET:HB3	2.03	0.41
71:SY:26:ASP:OD1	71:SY:26:ASP:N	2.53	0.41
79:Sg:44:LYS:HB2	79:Sg:56:GLN:HB2	2.03	0.41
3:LB:196:TRP:O	3:LB:199:GLU:HG2	2.19	0.41
3:LB:322:HIS:O	3:LB:342:LYS:HE3	2.21	0.41
8:L5:4:G:H2'	8:L5:5:A:C8	2.56	0.41
8:L5:7:C:H2'	8:L5:8:U:C6	2.56	0.41
8:L5:2049:G:O2'	8:L5:3884:U:O2'	2.24	0.41
8:L5:2756:G:H2'	8:L5:2757:A:C8	2.55	0.41
8:L5:4099:G:O2'	8:L5:4100:C:O4'	2.22	0.41
8:L5:4691:A:H2'	8:L5:4692:A:O4'	2.21	0.41
13:LE:62:MET:O	13:LE:66:LYS:HG2	2.21	0.41
22:LP:28:ASN:O	22:LP:32:THR:HG22	2.21	0.41
41:Lj:20:ARG:HH21	41:Lj:39:TYR:HH	1.62	0.41
42:Lk:54:GLU:HA	42:Lk:57:LYS:HD2	2.01	0.41
49:S2:339:A:H2'	49:S2:340:C:H5	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:389:A:H2'	49:S2:390:C:C6	2.56	0.41
49:S2:921:G:C5	69:SW:28:ARG:HD3	2.56	0.41
49:S2:1446:A:O2'	49:S2:1447:G:H5''	2.21	0.41
49:S2:1447:G:C2'	49:S2:1448:A:H5'	2.50	0.41
49:S2:1842:4AC:O5'	49:S2:1842:4AC:H6	2.21	0.41
53:SF:51:HIS:O	63:SQ:50:LYS:HE2	2.20	0.41
54:SG:157:VAL:HG11	54:SG:176:ILE:HD11	2.02	0.41
57:SJ:91:LYS:HE3	57:SJ:96:TYR:CD2	2.55	0.41
65:SS:63:GLU:O	65:SS:67:VAL:HG13	2.20	0.41
69:SW:111:MET:SD	69:SW:115:GLU:HG2	2.61	0.41
77:Se:101:LYS:HD2	77:Se:105:ALA:HB1	2.03	0.41
78:Sf:125:GLU:OE1	78:Sf:125:GLU:N	2.43	0.41
79:Sg:249:CYS:HB3	79:Sg:258:ILE:HG12	2.03	0.41
1:LA:70:LYS:NZ	8:L5:4084:G:O6	2.51	0.41
2:SA:184:ARG:HB3	2:SA:191:ARG:NH1	2.36	0.41
3:LB:57:VAL:HB	3:LB:367:PHE:HB3	2.03	0.41
3:LB:224:LYS:HG3	8:L5:4625:C:OP1	2.21	0.41
6:B4:62:A:C6	6:B4:63:U:C4	3.09	0.41
8:L5:88:A:N7	23:LQ:173:LYS:NZ	2.68	0.41
8:L5:156:G:N2	8:L5:157:U:O4	2.53	0.41
8:L5:730:G:OP2	14:LF:76:ARG:NE	2.49	0.41
8:L5:1721:G:H2'	8:L5:1722:C:C6	2.56	0.41
8:L5:2464:C:HO2'	8:L5:2465:C:H6	1.67	0.41
8:L5:2861:OMC:HM23	8:L5:2861:OMC:H1'	1.76	0.41
8:L5:3799:A:C5	28:LV:40:ILE:HD12	2.56	0.41
8:L5:4529:G:H2'	8:L5:4530:U:O4'	2.20	0.41
8:L5:4593:C:H2'	8:L5:4594:U:C6	2.55	0.41
8:L5:4680:G:H2'	8:L5:4681:A:C8	2.55	0.41
12:LD:108:ARG:CZ	12:LD:253:TYR:HB2	2.51	0.41
12:LD:216:GLU:HB3	12:LD:220:LYS:NZ	2.36	0.41
12:LD:264:LYS:HA	12:LD:264:LYS:HD2	1.85	0.41
14:LF:143:GLY:HA3	14:LF:240:ILE:HB	2.03	0.41
24:LR:104:ARG:HD3	24:LR:108:ARG:NH2	2.36	0.41
25:LS:80:ILE:HG23	25:LS:129:VAL:HG22	2.01	0.41
31:LY:54:GLU:O	31:LY:107:THR:OG1	2.37	0.41
45:Ln:15:ARG:O	45:Ln:19:LYS:HG3	2.21	0.41
46:Lo:6:LYS:O	46:Lo:23:VAL:HG22	2.21	0.41
49:S2:124:U:OP1	54:SG:201:LYS:NZ	2.45	0.41
49:S2:639:C:H2'	49:S2:640:A:H8	1.85	0.41
49:S2:644:OMG:H1'	49:S2:644:OMG:HM23	1.78	0.41
49:S2:809:A:C1'	52:SE:221:ARG:HH21	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1388:A:N6	51:SD:161:GLY:HA3	2.32	0.41
49:S2:1585:U:O2'	49:S2:1587:G:OP2	2.32	0.41
59:SL:49:GLU:OE1	59:SL:49:GLU:N	2.40	0.41
60:SN:29:THR:O	60:SN:33:VAL:HG22	2.21	0.41
66:ST:126:GLN:HE21	66:ST:126:GLN:CA	2.14	0.41
74:Sb:41:TYR:O	74:Sb:41:TYR:CG	2.73	0.41
79:Sg:179:LEU:HD23	79:Sg:179:LEU:HA	1.84	0.41
82:LI:76:MET:HG3	82:LI:87:ILE:HD11	2.02	0.41
3:LB:253:CYS:SG	8:L5:4521:U:H1'	2.60	0.41
8:L5:186:G:H8	8:L5:186:G:OP2	2.03	0.41
8:L5:1383:G:H2'	8:L5:1384:C:C6	2.56	0.41
8:L5:2408:U:OP2	43:Ll:42:ARG:NH2	2.41	0.41
8:L5:2675:G:O6	35:Lc:30:GLY:HA3	2.21	0.41
8:L5:3848:U:H2'	8:L5:3849:A:H8	1.85	0.41
8:L5:4755:G:N7	13:LE:279:ASN:ND2	2.68	0.41
9:L7:28:C:O2'	9:L7:54:A:N1	2.54	0.41
11:LC:149:GLU:OE2	48:Lr:71:ARG:NE	2.51	0.41
14:LF:36:LYS:N	14:LF:36:LYS:HD3	2.35	0.41
14:LF:216:PRO:HB3	14:LF:247:MET:HG2	2.02	0.41
18:LL:87:HIS:HB3	18:LL:90:VAL:HG23	2.02	0.41
34:Lb:11:ASN:OD1	34:Lb:14:ARG:HD3	2.21	0.41
39:Lh:35:LYS:HA	39:Lh:44:LEU:HD21	2.03	0.41
41:Lj:44:LYS:HE2	41:Lj:44:LYS:HB3	1.98	0.41
49:S2:102:A:H4'	49:S2:104:A:C8	2.56	0.41
49:S2:809:A:C4'	52:SE:221:ARG:HH21	2.21	0.41
49:S2:1370:A:N3	49:S2:1372:U:H5'	2.36	0.41
50:SC:145:LYS:HG2	50:SC:146:GLU:HG3	2.03	0.41
51:SD:16:ILE:HD11	76:Sd:36:LEU:HD23	2.03	0.41
53:SF:126:THR:HG21	75:Sc:27:CYS:SG	2.61	0.41
65:SS:10:GLN:H	65:SS:10:GLN:HG3	1.59	0.41
67:SU:80:PHE:HB3	76:Sd:52:PHE:HB3	2.03	0.41
71:SY:55:ILE:HG12	71:SY:75:ILE:HG12	2.03	0.41
79:Sg:152:SER:H	79:Sg:169:GLY:HA2	1.86	0.41
80:SM:27:ILE:HD13	80:SM:27:ILE:HA	1.89	0.41
2:SA:12:GLU:HG2	64:SR:114:LEU:HD21	2.02	0.41
2:SA:94:THR:HG23	2:SA:186:ARG:HH12	1.84	0.41
3:LB:121:ASN:ND2	3:LB:124:LYS:HB2	2.35	0.41
3:LB:285:TYR:N	3:LB:332:MET:O	2.53	0.41
6:B4:49:A:H2'	6:B4:50:U:C6	2.56	0.41
8:L5:468:U:C4	8:L5:686:A:N3	2.89	0.41
8:L5:1305:C:OP1	10:L8:7:U:O2'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:1443:A:C6	8:L5:1444:G:N7	2.89	0.41
8:L5:1662:C:H2'	8:L5:1663:C:H6	1.86	0.41
8:L5:2052:G:O2'	8:L5:2057:A:N1	2.51	0.41
8:L5:2376:A:H2'	8:L5:2377:C:C6	2.56	0.41
8:L5:2381:A:H1'	8:L5:2383:C:OP2	2.21	0.41
8:L5:2407:G:O6	43:L1:2:SER:N	2.53	0.41
8:L5:2693:G:H2'	8:L5:2694:G:N2	2.35	0.41
8:L5:2870:A:H2'	8:L5:2871:A:C8	2.56	0.41
8:L5:2876:OMG:OP1	47:Lp:8:VAL:HG22	2.21	0.41
8:L5:2876:OMG:HM22	8:L5:2877:G:H5'	2.03	0.41
8:L5:3654:G:O2'	8:L5:3693:U:OP1	2.38	0.41
8:L5:4154:G:H2'	8:L5:4155:C:H6	1.86	0.41
8:L5:4192:A:H2'	8:L5:4193:C:H6	1.85	0.41
8:L5:4228:OMG:H5''	8:L5:4229:U:O4'	2.20	0.41
8:L5:4385:A:H61	8:L5:4531:U:H5'	1.86	0.41
8:L5:4565:C:OP1	21:LO:65:ASN:ND2	2.54	0.41
9:L7:58:A:H2'	9:L7:59:G:C8	2.56	0.41
12:LD:99:TYR:CE2	12:LD:199:ILE:HD13	2.56	0.41
14:LF:220:MET:HE2	14:LF:223:LYS:HB3	2.02	0.41
15:LG:73:ARG:HD3	15:LG:73:ARG:HA	1.69	0.41
18:LL:81:LEU:HD11	18:LL:98:VAL:HG22	2.02	0.41
25:LS:173:ASN:OD1	25:LS:174:THR:N	2.54	0.41
30:LX:147:LEU:HD23	30:LX:147:LEU:HA	1.82	0.41
49:S2:355:G:OP1	59:SL:105:ARG:NH1	2.48	0.41
49:S2:367:U:OP1	56:SI:11:ARG:NH1	2.54	0.41
49:S2:432:G:H2'	49:S2:433:A:C8	2.56	0.41
49:S2:576:A2M:HM'2	49:S2:577:U:H5'	2.03	0.41
49:S2:1217:A:H2'	49:S2:1218:C:H6	1.85	0.41
49:S2:1309:C:OP1	78:Sf:133:ALA:HA	2.21	0.41
49:S2:1445:U:O2'	49:S2:1446:A:H5'	2.21	0.41
49:S2:1493:C:O2'	49:S2:1499:U:O4	2.39	0.41
49:S2:1562:C:H2'	49:S2:1563:G:H8	1.86	0.41
49:S2:1599:U:OP2	72:SZ:46:ASN:ND2	2.53	0.41
49:S2:1616:U:O2	49:S2:1661:A:H2	2.04	0.41
49:S2:1678:A2M:OP2	53:SF:63:LYS:NZ	2.41	0.41
50:SC:120:GLN:H	50:SC:120:GLN:HG2	1.66	0.41
50:SC:160:LEU:HD23	50:SC:160:LEU:HA	1.94	0.41
51:SD:103:GLU:OE2	51:SD:173:ARG:NE	2.39	0.41
54:SG:154:ARG:C	54:SG:156:TYR:H	2.29	0.41
55:SH:61:ILE:HD11	55:SH:95:ILE:HG13	2.03	0.41
57:SJ:37:LEU:HB3	57:SJ:42:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SJ:113:GLN:HG3	57:SJ:149:VAL:HG21	2.03	0.41
58:SK:60:GLU:HB2	58:SK:69:TRP:NE1	2.36	0.41
59:SL:50:ALA:HA	59:SL:55:TYR:HE1	1.86	0.41
63:SQ:50:LYS:NZ	63:SQ:53:GLU:OE2	2.54	0.41
64:SR:20:TYR:CD1	64:SR:38:ILE:HD12	2.55	0.41
65:SS:91:LYS:HB3	65:SS:91:LYS:HE3	1.76	0.41
67:SU:26:SER:OG	67:SU:32:LEU:HB2	2.21	0.41
68:SV:81:LYS:HA	68:SV:81:LYS:HD3	1.87	0.41
69:SW:66:THR:OG1	69:SW:68:ARG:HG3	2.21	0.41
70:SX:96:GLU:OE1	70:SX:96:GLU:HA	2.21	0.41
71:SY:35:VAL:HG23	71:SY:40:ILE:HD11	2.03	0.41
72:SZ:48:VAL:HG13	72:SZ:49:LEU:HG	2.03	0.41
74:Sb:32:PHE:O	74:Sb:82:LYS:HB3	2.20	0.41
80:SM:35:ILE:HD13	80:SM:35:ILE:HA	1.85	0.41
2:SA:16:LEU:HD21	64:SR:114:LEU:HD22	2.03	0.41
4:SB:83:LYS:HB2	4:SB:83:LYS:HE3	1.79	0.41
4:SB:140:VAL:HG12	4:SB:213:ARG:HB2	2.03	0.41
8:L5:198:A:O2'	8:L5:221:C:O2	2.36	0.41
8:L5:757:G:C4	8:L5:758:G:C8	3.09	0.41
8:L5:758:G:N3	8:L5:758:G:H2'	2.35	0.41
8:L5:1340:OMC:HM23	8:L5:1340:OMC:H1'	1.85	0.41
8:L5:1693:U:H2'	8:L5:1694:C:O4'	2.21	0.41
8:L5:1947:U:C5	44:Lm:108:VAL:HG11	2.56	0.41
8:L5:2347:A:C4	81:Le:31:ILE:HD11	2.57	0.41
8:L5:2366:A:N3	8:L5:3850:C:O2'	2.51	0.41
8:L5:2480:G:H2'	8:L5:2481:G:H8	1.85	0.41
8:L5:2538:U:H2'	8:L5:2539:C:C6	2.56	0.41
8:L5:3816:A:OP1	8:L5:3818:U:H5	2.03	0.41
8:L5:4968:A:H2'	8:L5:4969:C:H6	1.86	0.41
10:L8:67:U:H2'	10:L8:68:G:H8	1.84	0.41
11:LC:289:LEU:HD13	23:LQ:27:LEU:HD22	2.03	0.41
16:LH:76:HIS:O	16:LH:80:MET:HG3	2.20	0.41
17:LJ:19:LYS:HG3	17:LJ:133:VAL:CG1	2.51	0.41
27:LU:105:ASN:OD1	27:LU:109:SER:OG	2.21	0.41
28:LV:45:ILE:HD13	28:LV:45:ILE:HA	1.99	0.41
34:Lb:5:LYS:HE3	34:Lb:8:THR:HB	2.03	0.41
37:Lf:4:ARG:HG2	37:Lf:6:TRP:O	2.21	0.41
39:Lh:105:LYS:HE2	39:Lh:105:LYS:HB2	1.89	0.41
46:Lo:100:LYS:HB3	46:Lo:102:GLN:NE2	2.36	0.41
49:S2:67:C:O2'	54:SG:164:LYS:HD2	2.21	0.41
49:S2:1148:A:H4'	49:S2:1149:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1619:A:OP2	62:SP:47:ARG:NH1	2.53	0.41
58:SK:52:LEU:HD12	58:SK:55:ARG:HH21	1.85	0.41
64:SR:58:MET:HE3	64:SR:58:MET:HB3	1.83	0.41
71:SY:29:HIS:O	71:SY:29:HIS:ND1	2.54	0.41
8:L5:1563:A:H8	8:L5:1563:A:O5'	2.03	0.40
8:L5:1601:A:N7	8:L5:3643:A:C4	2.89	0.40
8:L5:1715:C:H3'	8:L5:1716:G:C8	2.56	0.40
8:L5:2296:G:O4'	11:LC:45:ARG:NH1	2.54	0.40
8:L5:2815:A2M:H2'	8:L5:2816:G:C8	2.56	0.40
10:L8:87:G:H8	10:L8:87:G:OP2	2.04	0.40
31:LY:89:LYS:HE3	31:LY:89:LYS:HB3	1.86	0.40
33:La:26:ARG:HD3	33:La:26:ARG:HA	1.78	0.40
35:Lc:17:ARG:NE	35:Lc:17:ARG:CA	2.81	0.40
39:Lh:116:LEU:H	39:Lh:116:LEU:HD12	1.86	0.40
49:S2:441:C:H2'	49:S2:442:C:C6	2.56	0.40
49:S2:909:G:H2'	49:S2:910:G:C8	2.57	0.40
49:S2:940:U:H2'	49:S2:941:C:C6	2.56	0.40
50:SC:221:ASP:N	50:SC:221:ASP:OD1	2.54	0.40
57:SJ:65:GLU:OE1	57:SJ:66:LYS:N	2.36	0.40
60:SN:46:THR:OG1	60:SN:49:GLN:HB2	2.21	0.40
60:SN:94:LYS:HG2	60:SN:118:ILE:HD13	2.03	0.40
75:Sc:20:ARG:HD2	75:Sc:28:THR:HG23	2.02	0.40
79:Sg:224:GLY:O	79:Sg:225:LYS:HD3	2.21	0.40
1:LA:171:GLY:O	47:Lp:68:ALA:HB2	2.21	0.40
3:LB:11:HIS:NE2	8:L5:4458:C:OP1	2.55	0.40
3:LB:324:GLY:HA2	8:L5:5051:C:H4'	2.03	0.40
5:A4:47:A:H4'	49:S2:1830:U:C4	2.56	0.40
6:B4:50:U:C4	6:B4:51:G:N7	2.89	0.40
6:B4:63:U:H2'	6:B4:64:C:C6	2.57	0.40
8:L5:267:G:H2'	8:L5:268:G:C8	2.55	0.40
8:L5:652:G:H2'	8:L5:653:U:C6	2.57	0.40
8:L5:1720:C:H2'	8:L5:1721:G:O4'	2.20	0.40
8:L5:1888:A:C8	8:L5:2049:G:O4'	2.74	0.40
8:L5:1961:G:N2	8:L5:2025:A:H62	2.19	0.40
8:L5:2385:U:OP1	24:LR:5:ARG:NH1	2.55	0.40
8:L5:2408:U:P	43:Ll:42:ARG:HH22	2.42	0.40
8:L5:2689:C:H2'	8:L5:2690:C:C6	2.57	0.40
8:L5:2690:C:H2'	8:L5:2691:U:O4'	2.21	0.40
8:L5:2758:G:H2'	8:L5:2759:G:N7	2.36	0.40
8:L5:3841:OMC:HM23	8:L5:3841:OMC:H1'	1.70	0.40
8:L5:3848:U:H2'	8:L5:3849:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:3925:OMU:H2'	8:L5:3926:C:O4'	2.21	0.40
8:L5:4872:G:O6	19:LM:98:ARG:NH1	2.54	0.40
8:L5:4897:G:H2'	8:L5:4898:G:H8	1.87	0.40
8:L5:4905:C:H2'	8:L5:4906:C:C6	2.56	0.40
17:LJ:112:HIS:CE1	17:LJ:125:ILE:HA	2.56	0.40
30:LX:148:ASP:HB3	30:LX:152:LYS:HZ3	1.85	0.40
31:LY:14:ASN:HD22	31:LY:14:ASN:HA	1.65	0.40
32:LZ:92:ASP:OD1	32:LZ:94:THR:N	2.54	0.40
37:Lf:47:CYS:SG	37:Lf:74:VAL:HG23	2.62	0.40
46:Lo:32:SER:O	46:Lo:33:LEU:HB3	2.22	0.40
49:S2:126:G:H5'	49:S2:127:C:OP2	2.21	0.40
49:S2:382:C:H2'	49:S2:383:G:H8	1.86	0.40
49:S2:496:C:H2'	49:S2:497:C:C6	2.55	0.40
49:S2:499:G:H2'	49:S2:501:C:O2	2.21	0.40
49:S2:566:U:H3	49:S2:584:G:H1	1.68	0.40
49:S2:943:U:H2'	49:S2:944:A:H8	1.85	0.40
49:S2:1829:G:H1'	49:S2:1850:MA6:C2	2.49	0.40
54:SG:221:LYS:HD2	54:SG:221:LYS:HA	1.83	0.40
55:SH:143:ARG:HB3	69:SW:51:GLU:OE2	2.21	0.40
60:SN:54:LEU:HB3	60:SN:60:VAL:CG2	2.51	0.40
61:SO:45:THR:OG1	61:SO:49:GLY:HA2	2.21	0.40
66:ST:27:LYS:HB2	66:ST:110:LEU:CD1	2.51	0.40
79:Sg:194:TYR:CZ	79:Sg:212:LYS:HB2	2.56	0.40
81:Le:9:LYS:HE3	81:Le:9:LYS:HB2	1.81	0.40
8:L5:50:C:C2	8:L5:51:A:C8	3.09	0.40
8:L5:410:A:O2'	8:L5:414:C:O2'	2.29	0.40
8:L5:1241:C:H2'	8:L5:1242:G:O4'	2.21	0.40
8:L5:1669:A:OP1	34:Lb:18:ARG:NH1	2.53	0.40
8:L5:1819:G:O2'	12:LD:115:MET:HE1	2.20	0.40
8:L5:3587:C:H2'	8:L5:3588:C:C6	2.57	0.40
8:L5:3877:A:O2'	8:L5:4400:G:N2	2.45	0.40
8:L5:4188:U:H2'	8:L5:4189:U:C6	2.55	0.40
8:L5:4371:G:O2'	8:L5:4372:U:OP2	2.34	0.40
8:L5:4424:A:C4	8:L5:4425:G:C8	3.10	0.40
12:LD:94:ASN:OD1	12:LD:94:ASN:N	2.55	0.40
13:LE:125:LEU:HD12	13:LE:125:LEU:HA	1.89	0.40
21:LO:113:ASP:OD1	21:LO:113:ASP:C	2.64	0.40
30:LX:47:ARG:HE	30:LX:47:ARG:HB3	1.58	0.40
33:La:134:GLU:O	33:La:138:LYS:HG3	2.21	0.40
35:Lc:17:ARG:O	35:Lc:19:GLN:N	2.52	0.40
49:S2:28:U:H2'	49:S2:29:G:C8	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:616:A:OP1	70:SX:68:LYS:NZ	2.53	0.40
49:S2:650:A:OP2	70:SX:108:LYS:HG2	2.21	0.40
49:S2:1252:C:N4	63:SQ:146:ARG:OXT	2.45	0.40
50:SC:180:VAL:HG13	50:SC:219:ILE:HD13	2.03	0.40
54:SG:28:TYR:O	54:SG:30:LYS:HG2	2.21	0.40
57:SJ:81:LEU:HD13	57:SJ:97:ILE:HD12	2.02	0.40
79:Sg:35:SER:OG	79:Sg:37:ASP:OD1	2.39	0.40
1:LA:199:VAL:HG21	8:L5:1631:A:N7	2.37	0.40
3:LB:254:ILE:HG12	8:L5:3897:G:H4'	2.03	0.40
3:LB:305:THR:C	3:LB:307:TYR:H	2.29	0.40
4:SB:97:LEU:HG	4:SB:232:HIS:CE1	2.57	0.40
8:L5:35:U:H4'	8:L5:1525:A:C2	2.57	0.40
8:L5:1084:C:H2'	8:L5:1085:C:H6	1.85	0.40
8:L5:1257:A:H3'	8:L5:1258:G:H8	1.86	0.40
8:L5:2296:G:O2'	11:LC:242:PRO:O	2.34	0.40
8:L5:3702:A:C6	8:L5:3703:G:C8	3.09	0.40
8:L5:3860:A:N3	22:LP:131:ARG:NH1	2.68	0.40
17:LJ:99:PHE:CD2	17:LJ:105:PHE:HB3	2.56	0.40
23:LQ:128:LEU:HD23	23:LQ:128:LEU:HA	1.88	0.40
27:LU:62:THR:O	27:LU:72:VAL:HA	2.22	0.40
32:LZ:92:ASP:OD1	32:LZ:92:ASP:C	2.64	0.40
33:La:75:LEU:HD22	33:La:117:LEU:HD11	2.03	0.40
38:Lg:83:CYS:O	38:Lg:87:VAL:HG13	2.21	0.40
45:Ln:11:ARG:O	45:Ln:15:ARG:HG3	2.22	0.40
49:S2:389:A:H1'	56:SI:87:ASN:H	1.86	0.40
49:S2:1365:G:H2'	49:S2:1366:G:H8	1.85	0.40
52:SE:95:THR:HG23	71:SY:16:ARG:NH1	2.35	0.40
52:SE:140:VAL:HA	52:SE:145:ARG:O	2.21	0.40
54:SG:20:ASP:OD2	54:SG:23:LYS:N	2.48	0.40
65:SS:121:ARG:HG3	65:SS:131:VAL:HG13	2.03	0.40
66:ST:5:THR:HG22	66:ST:7:LYS:H	1.87	0.40
69:SW:5:ASN:HB3	69:SW:8:ALA:HB3	2.04	0.40
79:Sg:140:TYR:HE1	79:Sg:142:VAL:HG13	1.86	0.40
81:Le:46:ARG:HG3	81:Le:47:ARG:N	2.36	0.40
1:LA:141:PRO:O	1:LA:144:LYS:HD3	2.22	0.40
3:LB:201:LEU:HD12	3:LB:201:LEU:HA	1.98	0.40
3:LB:357:ARG:CD	8:L5:4615:C:H5''	2.52	0.40
8:L5:90:G:OP2	46:Lo:40:ARG:NH1	2.54	0.40
8:L5:302:C:H2'	8:L5:303:C:H6	1.87	0.40
8:L5:1446:C:N3	8:L5:2100:A:H2	2.19	0.40
8:L5:2475:G:N1	30:LX:51:THR:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L5:2608:G:H2'	8:L5:2609:G:H8	1.86	0.40
8:L5:2745:A:H2'	8:L5:2746:A:C8	2.57	0.40
8:L5:4753:U:OP1	37:Lf:100:ARG:NH2	2.48	0.40
24:LR:153:LYS:HE3	24:LR:153:LYS:HB3	1.80	0.40
26:LT:103:ASP:OD1	26:LT:103:ASP:C	2.64	0.40
30:LX:60:TYR:O	30:LX:62:ARG:NH1	2.54	0.40
33:La:119:LYS:H	33:La:119:LYS:HG2	1.68	0.40
42:Lk:51:GLU:C	42:Lk:55:LYS:HE3	2.47	0.40
49:S2:1016:U:H5''	60:SN:15:ALA:O	2.22	0.40
49:S2:1446:A:N3	67:SU:55:ARG:NE	2.69	0.40
54:SG:69:THR:O	54:SG:99:GLY:HA3	2.22	0.40
55:SH:100:ILE:HD11	55:SH:122:LEU:HD12	2.04	0.40
57:SJ:35:TYR:HD1	57:SJ:112:THR:HG21	1.87	0.40
61:SO:40:THR:HG21	61:SO:74:ALA:HB2	2.03	0.40
61:SO:96:LYS:HB3	61:SO:132:VAL:HG21	2.02	0.40
64:SR:37:GLU:CD	79:Sg:150:TRP:HE1	2.30	0.40
78:Sf:138:ARG:HD2	78:Sf:147:THR:HG21	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	
1	LA	246/257 (96%)	225 (92%)	21 (8%)	0	100	100
2	SA	215/295 (73%)	206 (96%)	9 (4%)	0	100	100
3	LB	396/403 (98%)	367 (93%)	29 (7%)	0	100	100
4	SB	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
11	LC	360/427 (84%)	342 (95%)	18 (5%)	0	100	100
12	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
13	LE	197/288 (68%)	181 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	LF	220/248 (89%)	214 (97%)	6 (3%)	0	100	100
15	LG	220/266 (83%)	211 (96%)	9 (4%)	0	100	100
16	LH	189/192 (98%)	181 (96%)	8 (4%)	0	100	100
17	LJ	163/178 (92%)	153 (94%)	10 (6%)	0	100	100
18	LL	192/211 (91%)	171 (89%)	21 (11%)	0	100	100
19	LM	135/215 (63%)	126 (93%)	8 (6%)	1 (1%)	18	49
20	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
21	LO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
22	LP	155/184 (84%)	150 (97%)	5 (3%)	0	100	100
23	LQ	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
24	LR	173/196 (88%)	171 (99%)	2 (1%)	0	100	100
25	LS	169/176 (96%)	158 (94%)	11 (6%)	0	100	100
26	LT	151/160 (94%)	146 (97%)	5 (3%)	0	100	100
27	LU	97/128 (76%)	89 (92%)	8 (8%)	0	100	100
28	LV	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
29	LW	83/157 (53%)	81 (98%)	2 (2%)	0	100	100
30	LX	116/156 (74%)	110 (95%)	6 (5%)	0	100	100
31	LY	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
32	LZ	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
33	La	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
34	Lb	88/159 (55%)	86 (98%)	2 (2%)	0	100	100
35	Lc	91/115 (79%)	83 (91%)	7 (8%)	1 (1%)	11	40
36	Ld	104/125 (83%)	100 (96%)	4 (4%)	0	100	100
37	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
38	Lg	108/117 (92%)	104 (96%)	4 (4%)	0	100	100
39	Lh	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
40	Li	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
41	Lj	85/97 (88%)	82 (96%)	3 (4%)	0	100	100
42	Lk	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
43	Ll	47/51 (92%)	43 (92%)	4 (8%)	0	100	100
44	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Ln	23/25 (92%)	23 (100%)	0	0	100	100
46	Lo	100/106 (94%)	92 (92%)	8 (8%)	0	100	100
47	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
48	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
50	SC	218/293 (74%)	208 (95%)	10 (5%)	0	100	100
51	SD	219/243 (90%)	211 (96%)	8 (4%)	0	100	100
52	SE	256/263 (97%)	242 (94%)	14 (6%)	0	100	100
53	SF	183/204 (90%)	173 (94%)	10 (6%)	0	100	100
54	SG	219/249 (88%)	204 (93%)	15 (7%)	0	100	100
55	SH	169/194 (87%)	160 (95%)	9 (5%)	0	100	100
56	SI	193/208 (93%)	182 (94%)	11 (6%)	0	100	100
57	SJ	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
58	SK	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
59	SL	136/158 (86%)	127 (93%)	9 (7%)	0	100	100
60	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
61	SO	127/151 (84%)	117 (92%)	10 (8%)	0	100	100
62	SP	127/145 (88%)	123 (97%)	4 (3%)	0	100	100
63	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
64	SR	128/135 (95%)	122 (95%)	6 (5%)	0	100	100
65	SS	140/152 (92%)	130 (93%)	10 (7%)	0	100	100
66	ST	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
67	SU	99/119 (83%)	90 (91%)	9 (9%)	0	100	100
68	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
69	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
70	SX	139/143 (97%)	128 (92%)	11 (8%)	0	100	100
71	SY	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
72	SZ	70/125 (56%)	63 (90%)	7 (10%)	0	100	100
73	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
74	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
75	Sc	61/69 (88%)	53 (87%)	8 (13%)	0	100	100
76	Sd	50/56 (89%)	48 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Se	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
78	Sf	59/156 (38%)	46 (78%)	13 (22%)	0	100	100
79	Sg	302/317 (95%)	279 (92%)	23 (8%)	0	100	100
80	SM	94/132 (71%)	86 (92%)	8 (8%)	0	100	100
81	Le	125/135 (93%)	121 (97%)	4 (3%)	0	100	100
82	LI	199/214 (93%)	194 (98%)	5 (2%)	0	100	100
All	All	10966/12688 (86%)	10396 (95%)	568 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	LM	32	ASP
35	Lc	99	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LA	187/199 (94%)	187 (100%)	0	100	100
2	SA	178/243 (73%)	177 (99%)	1 (1%)	78	81
3	LB	330/349 (95%)	328 (99%)	2 (1%)	78	81
4	SB	193/231 (84%)	192 (100%)	1 (0%)	81	82
11	LC	299/348 (86%)	299 (100%)	0	100	100
12	LD	247/250 (99%)	247 (100%)	0	100	100
13	LE	175/252 (69%)	175 (100%)	0	100	100
14	LF	192/215 (89%)	192 (100%)	0	100	100
15	LG	189/223 (85%)	189 (100%)	0	100	100
16	LH	170/171 (99%)	170 (100%)	0	100	100
17	LJ	138/149 (93%)	137 (99%)	1 (1%)	76	79
18	LL	161/177 (91%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LM	115/161 (71%)	115 (100%)	0	100	100
20	LN	171/172 (99%)	170 (99%)	1 (1%)	78	81
21	LO	172/174 (99%)	172 (100%)	0	100	100
22	LP	137/163 (84%)	137 (100%)	0	100	100
23	LQ	164/165 (99%)	164 (100%)	0	100	100
24	LR	153/175 (87%)	153 (100%)	0	100	100
25	LS	152/157 (97%)	152 (100%)	0	100	100
26	LT	132/140 (94%)	132 (100%)	0	100	100
27	LU	89/115 (77%)	89 (100%)	0	100	100
28	LV	101/107 (94%)	99 (98%)	2 (2%)	48	67
29	LW	57/126 (45%)	57 (100%)	0	100	100
30	LX	105/133 (79%)	105 (100%)	0	100	100
31	LY	121/135 (90%)	121 (100%)	0	100	100
32	LZ	118/118 (100%)	118 (100%)	0	100	100
33	La	119/121 (98%)	119 (100%)	0	100	100
34	Lb	75/126 (60%)	75 (100%)	0	100	100
35	Lc	78/97 (80%)	78 (100%)	0	100	100
36	Ld	94/110 (86%)	93 (99%)	1 (1%)	65	75
37	Lf	86/89 (97%)	86 (100%)	0	100	100
38	Lg	91/100 (91%)	91 (100%)	0	100	100
39	Lh	108/110 (98%)	108 (100%)	0	100	100
40	Li	85/89 (96%)	84 (99%)	1 (1%)	63	74
41	Lj	74/80 (92%)	74 (100%)	0	100	100
42	Lk	60/65 (92%)	60 (100%)	0	100	100
43	Ll	46/48 (96%)	46 (100%)	0	100	100
44	Lm	45/116 (39%)	45 (100%)	0	100	100
45	Ln	24/24 (100%)	24 (100%)	0	100	100
46	Lo	90/94 (96%)	89 (99%)	1 (1%)	65	75
47	Lp	74/75 (99%)	73 (99%)	1 (1%)	59	72
48	Lr	105/121 (87%)	104 (99%)	1 (1%)	68	75
50	SC	185/225 (82%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	SD	174/202 (86%)	174 (100%)	0	100	100
52	SE	221/225 (98%)	221 (100%)	0	100	100
53	SF	159/170 (94%)	158 (99%)	1 (1%)	78	81
54	SG	183/218 (84%)	183 (100%)	0	100	100
55	SH	139/174 (80%)	138 (99%)	1 (1%)	76	79
56	SI	162/180 (90%)	161 (99%)	1 (1%)	78	81
57	SJ	158/168 (94%)	157 (99%)	1 (1%)	78	81
58	SK	86/136 (63%)	85 (99%)	1 (1%)	63	74
59	SL	126/142 (89%)	126 (100%)	0	100	100
60	SN	129/131 (98%)	129 (100%)	0	100	100
61	SO	98/119 (82%)	96 (98%)	2 (2%)	48	67
62	SP	114/130 (88%)	114 (100%)	0	100	100
63	SQ	116/121 (96%)	115 (99%)	1 (1%)	70	77
64	SR	117/122 (96%)	117 (100%)	0	100	100
65	SS	121/132 (92%)	121 (100%)	0	100	100
66	ST	111/115 (96%)	111 (100%)	0	100	100
67	SU	89/107 (83%)	89 (100%)	0	100	100
68	SV	67/67 (100%)	66 (98%)	1 (2%)	57	71
69	SW	112/113 (99%)	110 (98%)	2 (2%)	51	69
70	SX	110/115 (96%)	110 (100%)	0	100	100
71	SY	103/115 (90%)	102 (99%)	1 (1%)	68	75
72	SZ	64/103 (62%)	63 (98%)	1 (2%)	55	71
73	Sa	85/98 (87%)	84 (99%)	1 (1%)	63	74
74	Sb	69/76 (91%)	69 (100%)	0	100	100
75	Sc	54/62 (87%)	51 (94%)	3 (6%)	19	47
76	Sd	46/49 (94%)	45 (98%)	1 (2%)	45	65
77	Se	40/48 (83%)	40 (100%)	0	100	100
78	Sf	52/140 (37%)	52 (100%)	0	100	100
79	Sg	265/275 (96%)	264 (100%)	1 (0%)	84	83
80	SM	74/108 (68%)	73 (99%)	1 (1%)	59	72
81	Le	113/121 (93%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	LI	172/181 (95%)	172 (100%)	0	100	100
All	All	9414/10801 (87%)	9381 (100%)	33 (0%)	81	83

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	145	ILE
3	LB	214	ASP
3	LB	345	LEU
4	SB	139	CYS
17	LJ	125	ILE
20	LN	87	HIS
28	LV	22	VAL
28	LV	117	ILE
36	Ld	68	LEU
40	Li	41	ARG
46	Lo	24	THR
47	Lp	78	THR
48	Lr	63	VAL
53	SF	55	ARG
55	SH	45	ILE
56	SI	7	ASN
57	SJ	161	LEU
58	SK	90	VAL
61	SO	66	ARG
61	SO	75	MET
63	SQ	67	ASP
68	SV	39	VAL
69	SW	26	LEU
69	SW	80	ASP
71	SY	26	ASP
72	SZ	97	ILE
73	Sa	94	ASP
75	Sc	18	LEU
75	Sc	57	THR
75	Sc	58	LEU
76	Sd	16	GLN
79	Sg	113	PHE
80	SM	69	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	LA	83	HIS
1	LA	205	ASN
2	SA	113	GLN
2	SA	132	GLN
3	LB	184	GLN
3	LB	186	ASN
3	LB	289	GLN
3	LB	322	HIS
11	LC	21	ASN
11	LC	187	GLN
11	LC	198	ASN
11	LC	203	GLN
11	LC	329	ASN
12	LD	122	GLN
12	LD	267	ASN
12	LD	275	GLN
13	LE	47	ASN
13	LE	256	GLN
13	LE	268	GLN
14	LF	80	ASN
14	LF	116	GLN
14	LF	119	ASN
14	LF	126	ASN
14	LF	241	ASN
15	LG	38	ASN
15	LG	46	GLN
15	LG	141	ASN
15	LG	153	GLN
15	LG	236	HIS
16	LH	98	HIS
16	LH	102	ASN
17	LJ	10	ASN
17	LJ	65	ASN
17	LJ	98	ASN
17	LJ	112	HIS
19	LM	56	GLN
20	LN	87	HIS
20	LN	158	HIS
21	LO	26	GLN
22	LP	10	ASN
22	LP	21	ASN
22	LP	72	GLN
22	LP	80	GLN

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Mol	Chain	Res	Type
22	LP	137	ASN
23	LQ	44	ASN
23	LQ	125	GLN
24	LR	34	ASN
26	LT	49	GLN
26	LT	66	ASN
28	LV	50	ASN
29	LW	63	GLN
30	LX	73	HIS
31	LY	43	ASN
31	LY	61	HIS
31	LY	127	GLN
33	La	39	HIS
33	La	62	HIS
34	Lb	6	ASN
35	Lc	72	HIS
36	Ld	79	ASN
36	Ld	121	ASN
37	Lf	21	GLN
38	Lg	28	ASN
39	Lh	98	HIS
40	Li	15	HIS
40	Li	20	ASN
41	Lj	30	GLN
43	Ll	17	GLN
44	Lm	87	GLN
44	Lm	120	ASN
46	Lo	3	ASN
48	Lr	21	ASN
48	Lr	30	ASN
51	SD	101	GLN
53	SF	83	ASN
53	SF	118	ASN
54	SG	155	GLN
54	SG	177	GLN
55	SH	68	GLN
56	SI	64	ASN
57	SJ	132	GLN
59	SL	11	GLN
59	SL	13	GLN
61	SO	103	ASN
64	SR	93	GLN

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Mol	Chain	Res	Type
66	ST	126	GLN
68	SV	2	GLN
69	SW	5	ASN
69	SW	91	ASN
75	Sc	26	GLN
76	Sd	26	ASN
77	Se	95	GLN
78	Sf	139	HIS
79	Sg	64	HIS
79	Sg	188	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	L8	144/156 (92%)	27 (18%)	0
49	S2	1561/1869 (83%)	347 (22%)	6 (0%)
5	A4	10/13 (76%)	0	0
6	B4	74/75 (98%)	18 (24%)	0
7	D4	60/76 (78%)	23 (38%)	0
8	L5	3436/5070 (67%)	666 (19%)	16 (0%)
9	L7	118/120 (98%)	11 (9%)	0
All	All	5403/7379 (73%)	1092 (20%)	22 (0%)

All (1092) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B4	8	U
6	B4	10	G
6	B4	11	C
6	B4	12	G
6	B4	17	G
6	B4	18	G
6	B4	19	A
6	B4	20	A
6	B4	21	G
6	B4	46	U
6	B4	48	G
6	B4	51	G
6	B4	52	G
6	B4	55	C
6	B4	56	G

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Mol	Chain	Res	Type
6	B4	60	C
6	B4	74	C
6	B4	75	A
7	D4	6	G
7	D4	7	A
7	D4	8	U
7	D4	9	A
7	D4	12	U
7	D4	14	A
7	D4	15	G
7	D4	19	G
7	D4	22	G
7	D4	26	A
7	D4	27	G
7	D4	29	G
7	D4	30	G
7	D4	46	G
7	D4	47	U
7	D4	49	C
7	D4	52	G
7	D4	54	U
7	D4	60	U
7	D4	61	C
7	D4	62	C
7	D4	63	G
7	D4	68	C
8	L5	13	U
8	L5	21	G
8	L5	25	A
8	L5	26	C
8	L5	39	A
8	L5	42	A
8	L5	48	G
8	L5	59	A
8	L5	64	A
8	L5	65	A
8	L5	73	A
8	L5	91	G
8	L5	98	A
8	L5	104	G
8	L5	106	A
8	L5	108	A

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Mol	Chain	Res	Type
8	L5	109	G
8	L5	110	C
8	L5	116	G
8	L5	117	C
8	L5	119	G
8	L5	124	C
8	L5	133	C
8	L5	134	G
8	L5	135	G
8	L5	136	C
8	L5	139	G
8	L5	144	G
8	L5	152	U
8	L5	159	C
8	L5	165	A
8	L5	166	C
8	L5	183	C
8	L5	184	U
8	L5	185	C
8	L5	197	A
8	L5	200	U
8	L5	209	U
8	L5	216	C
8	L5	217	C
8	L5	218	A
8	L5	233	U
8	L5	234	G
8	L5	265	C
8	L5	266	C
8	L5	269	G
8	L5	275	C
8	L5	276	C
8	L5	280	G
8	L5	297	U
8	L5	306	A
8	L5	309	C
8	L5	310	G
8	L5	315	G
8	L5	316	U
8	L5	340	C
8	L5	341	G
8	L5	350	C

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Mol	Chain	Res	Type
8	L5	387	G
8	L5	388	A
8	L5	396	A
8	L5	407	A
8	L5	409	G
8	L5	411	G
8	L5	412	G
8	L5	414	C
8	L5	415	G
8	L5	449	C
8	L5	450	G
8	L5	452	A
8	L5	454	U
8	L5	456	C
8	L5	457	G
8	L5	465	G
8	L5	468	U
8	L5	473	C
8	L5	483	G
8	L5	484	U
8	L5	485	C
8	L5	486	C
8	L5	489	C
8	L5	497	G
8	L5	498	C
8	L5	500	G
8	L5	502	C
8	L5	503	C
8	L5	504	G
8	L5	505	G
8	L5	506	C
8	L5	509	A
8	L5	510	U
8	L5	512	U
8	L5	513	U
8	L5	514	U
8	L5	515	C
8	L5	516	C
8	L5	517	C
8	L5	519	C
8	L5	643	C
8	L5	644	G

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Mol	Chain	Res	Type
8	L5	646	G
8	L5	654	C
8	L5	655	C
8	L5	656	C
8	L5	657	C
8	L5	659	G
8	L5	665	C
8	L5	666	G
8	L5	667	A
8	L5	668	C
8	L5	674	G
8	L5	686	A
8	L5	687	U
8	L5	696	C
8	L5	703	G
8	L5	704	C
8	L5	706	C
8	L5	731	G
8	L5	739	G
8	L5	740	G
8	L5	741	C
8	L5	742	G
8	L5	743	G
8	L5	744	G
8	L5	745	G
8	L5	758	G
8	L5	759	G
8	L5	904	C
8	L5	905	C
8	L5	914	U
8	L5	915	A
8	L5	917	A
8	L5	932	A
8	L5	933	G
8	L5	934	C
8	L5	935	A
8	L5	944	A
8	L5	945	U
8	L5	956	A
8	L5	959	G
8	L5	960	A
8	L5	961	G

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Mol	Chain	Res	Type
8	L5	982	U
8	L5	1075	G
8	L5	1082	C
8	L5	1083	U
8	L5	1169	G
8	L5	1171	G
8	L5	1172	C
8	L5	1173	G
8	L5	1174	A
8	L5	1176	C
8	L5	1182	C
8	L5	1183	C
8	L5	1200	G
8	L5	1202	C
8	L5	1203	G
8	L5	1210	C
8	L5	1211	G
8	L5	1214	C
8	L5	1215	C
8	L5	1218	G
8	L5	1220	G
8	L5	1221	G
8	L5	1235	G
8	L5	1241	C
8	L5	1243	C
8	L5	1244	G
8	L5	1258	G
8	L5	1259	G
8	L5	1266	G
8	L5	1271	G
8	L5	1272	C
8	L5	1273	G
8	L5	1280	C
8	L5	1284	G
8	L5	1287	G
8	L5	1293	G
8	L5	1294	A
8	L5	1301	C
8	L5	1326	A2M
8	L5	1339	U
8	L5	1354	A
8	L5	1358	G

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Mol	Chain	Res	Type
8	L5	1359	G
8	L5	1365	C
8	L5	1366	G
8	L5	1377	G
8	L5	1381	U
8	L5	1387	A
8	L5	1393	G
8	L5	1394	G
8	L5	1397	A
8	L5	1398	A
8	L5	1399	G
8	L5	1402	C
8	L5	1403	G
8	L5	1404	G
8	L5	1405	C
8	L5	1407	C
8	L5	1408	G
8	L5	1409	C
8	L5	1410	U
8	L5	1414	C
8	L5	1420	A
8	L5	1421	G
8	L5	1439	C
8	L5	1447	C
8	L5	1448	G
8	L5	1482	G
8	L5	1483	C
8	L5	1497	A
8	L5	1498	G
8	L5	1502	G
8	L5	1518	A
8	L5	1525	A
8	L5	1534	A
8	L5	1547	A
8	L5	1566	C
8	L5	1576	G
8	L5	1578	U
8	L5	1591	U
8	L5	1596	U
8	L5	1612	G
8	L5	1624	G
8	L5	1625	OMG

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Mol	Chain	Res	Type
8	L5	1631	A
8	L5	1633	G
8	L5	1634	A
8	L5	1638	A
8	L5	1640	C
8	L5	1641	G
8	L5	1642	A
8	L5	1654	G
8	L5	1661	C
8	L5	1663	C
8	L5	1676	C
8	L5	1677	U
8	L5	1681	G
8	L5	1684	A
8	L5	1685	G
8	L5	1691	G
8	L5	1694	C
8	L5	1717	C
8	L5	1718	C
8	L5	1719	A
8	L5	1731	C
8	L5	1734	G
8	L5	1740	C
8	L5	1742	A
8	L5	1750	G
8	L5	1783	C
8	L5	1787	A
8	L5	1803	G
8	L5	1804	A
8	L5	1810	G
8	L5	1815	G
8	L5	1820	C
8	L5	1821	G
8	L5	1822	U
8	L5	1836	G
8	L5	1837	A
8	L5	1842	G
8	L5	1855	G
8	L5	1869	G
8	L5	1897	A
8	L5	1918	U
8	L5	1919	G

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Mol	Chain	Res	Type
8	L5	1920	C
8	L5	1921	C
8	L5	1922	G
8	L5	1931	C
8	L5	1932	A
8	L5	1936	C
8	L5	1940	G
8	L5	1948	G
8	L5	1955	G
8	L5	1959	U
8	L5	1960	A
8	L5	1961	G
8	L5	1962	A
8	L5	1966	C
8	L5	1968	G
8	L5	1970	A
8	L5	1971	C
8	L5	1998	A
8	L5	1999	A
8	L5	2000	G
8	L5	2018	C
8	L5	2020	U
8	L5	2022	C
8	L5	2024	G
8	L5	2025	A
8	L5	2026	A
8	L5	2033	A
8	L5	2046	G
8	L5	2048	U
8	L5	2055	G
8	L5	2056	G
8	L5	2069	A
8	L5	2070	U
8	L5	2084	C
8	L5	2085	G
8	L5	2101	C
8	L5	2102	G
8	L5	2104	G
8	L5	2106	G
8	L5	2107	C
8	L5	2289	C
8	L5	2300	A

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Mol	Chain	Res	Type
8	L5	2301	G
8	L5	2313	A
8	L5	2333	G
8	L5	2348	G
8	L5	2351	OMC
8	L5	2366	A
8	L5	2370	A
8	L5	2389	A
8	L5	2395	A
8	L5	2396	A
8	L5	2397	G
8	L5	2401	A2M
8	L5	2410	C
8	L5	2417	A
8	L5	2421	G
8	L5	2422	OMC
8	L5	2424	OMG
8	L5	2425	U
8	L5	2441	C
8	L5	2450	G
8	L5	2464	C
8	L5	2465	C
8	L5	2471	G
8	L5	2474	G
8	L5	2475	G
8	L5	2483	G
8	L5	2484	A
8	L5	2492	C
8	L5	2493	G
8	L5	2494	U
8	L5	2496	G
8	L5	2504	C
8	L5	2506	G
8	L5	2513	A
8	L5	2514	G
8	L5	2519	U
8	L5	2520	C
8	L5	2529	A
8	L5	2537	A
8	L5	2544	G
8	L5	2546	G
8	L5	2547	G

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Mol	Chain	Res	Type
8	L5	2554	U
8	L5	2555	G
8	L5	2556	G
8	L5	2560	C
8	L5	2567	G
8	L5	2568	C
8	L5	2573	A
8	L5	2583	C
8	L5	2586	G
8	L5	2587	A
8	L5	2589	C
8	L5	2618	G
8	L5	2627	C
8	L5	2653	C
8	L5	2662	G
8	L5	2669	C
8	L5	2675	G
8	L5	2676	A
8	L5	2687	U
8	L5	2694	G
8	L5	2695	A
8	L5	2696	A
8	L5	2703	G
8	L5	2711	G
8	L5	2712	G
8	L5	2714	G
8	L5	2717	G
8	L5	2724	G
8	L5	2726	G
8	L5	2728	U
8	L5	2732	G
8	L5	2739	C
8	L5	2742	G
8	L5	2743	A
8	L5	2754	G
8	L5	2759	G
8	L5	2761	U
8	L5	2763	U
8	L5	2764	A
8	L5	2769	U
8	L5	2770	C
8	L5	2788	U

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Mol	Chain	Res	Type
8	L5	2790	U
8	L5	2804	OMC
8	L5	2814	C
8	L5	2826	U
8	L5	2827	G
8	L5	2829	U
8	L5	2842	G
8	L5	2855	G
8	L5	2856	C
8	L5	2876	OMG
8	L5	2877	G
8	L5	2892	C
8	L5	2897	G
8	L5	2900	U
8	L5	2902	G
8	L5	2903	G
8	L5	2904	U
8	L5	2905	C
8	L5	3585	G
8	L5	3587	C
8	L5	3588	C
8	L5	3590	G
8	L5	3591	C
8	L5	3592	G
8	L5	3594	C
8	L5	3595	U
8	L5	3596	A
8	L5	3597	G
8	L5	3599	A
8	L5	3604	A
8	L5	3605	C
8	L5	3606	U
8	L5	3615	G
8	L5	3618	C
8	L5	3619	G
8	L5	3620	G
8	L5	3626	G
8	L5	3630	A
8	L5	3635	A
8	L5	3644	U
8	L5	3646	A
8	L5	3662	A

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Mol	Chain	Res	Type
8	L5	3663	A
8	L5	3673	C
8	L5	3674	G
8	L5	3701	OMC
8	L5	3702	A
8	L5	3710	G
8	L5	3711	A
8	L5	3717	A
8	L5	3735	G
8	L5	3736	A
8	L5	3737	A
8	L5	3748	A
8	L5	3750	G
8	L5	3757	G
8	L5	3761	C
8	L5	3769	C
8	L5	3771	C
8	L5	3773	U
8	L5	3774	A
8	L5	3776	G
8	L5	3777	G
8	L5	3784	A
8	L5	3785	A
8	L5	3786	U
8	L5	3801	U
8	L5	3802	U
8	L5	3811	G
8	L5	3813	A
8	L5	3814	U
8	L5	3817	A
8	L5	3818	U
8	L5	3819	G
8	L5	3838	U
8	L5	3839	G
8	L5	3840	U
8	L5	3851	U
8	L5	3867	A
8	L5	3877	A
8	L5	3878	C
8	L5	3879	G
8	L5	3892	U
8	L5	3897	G

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Mol	Chain	Res	Type
8	L5	3901	A
8	L5	3906	A
8	L5	3907	G
8	L5	3908	A
8	L5	3915	U
8	L5	3926	C
8	L5	3927	U
8	L5	3933	G
8	L5	3938	G
8	L5	3939	G
8	L5	3942	C
8	L5	4076	G
8	L5	4084	G
8	L5	4085	A
8	L5	4086	G
8	L5	4091	G
8	L5	4097	G
8	L5	4099	G
8	L5	4100	C
8	L5	4113	U
8	L5	4114	C
8	L5	4115	G
8	L5	4116	C
8	L5	4117	U
8	L5	4119	C
8	L5	4121	G
8	L5	4122	G
8	L5	4127	A
8	L5	4141	G
8	L5	4142	C
8	L5	4143	G
8	L5	4144	C
8	L5	4146	G
8	L5	4149	C
8	L5	4150	G
8	L5	4160	C
8	L5	4162	C
8	L5	4163	U
8	L5	4170	A
8	L5	4183	G
8	L5	4184	G
8	L5	4191	G

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Mol	Chain	Res	Type
8	L5	4201	G
8	L5	4203	A
8	L5	4205	A
8	L5	4212	A
8	L5	4222	G
8	L5	4229	U
8	L5	4233	A
8	L5	4234	A
8	L5	4251	A
8	L5	4254	G
8	L5	4256	A
8	L5	4257	A
8	L5	4265	U
8	L5	4273	A
8	L5	4284	C
8	L5	4291	G
8	L5	4297	G
8	L5	4304	A
8	L5	4305	G
8	L5	4306	U
8	L5	4314	C
8	L5	4330	G
8	L5	4332	C
8	L5	4339	A
8	L5	4349	C
8	L5	4354	U
8	L5	4373	G
8	L5	4377	G
8	L5	4378	A
8	L5	4379	A
8	L5	4381	A
8	L5	4387	C
8	L5	4394	A
8	L5	4421	C
8	L5	4422	A
8	L5	4444	C
8	L5	4448	G
8	L5	4449	A
8	L5	4453	C
8	L5	4464	A
8	L5	4466	C
8	L5	4475	G

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Mol	Chain	Res	Type
8	L5	4500	U
8	L5	4512	U
8	L5	4513	A
8	L5	4515	G
8	L5	4519	C
8	L5	4524	G
8	L5	4525	C
8	L5	4532	U
8	L5	4545	G
8	L5	4548	A
8	L5	4549	G
8	L5	4554	G
8	L5	4560	C
8	L5	4567	G
8	L5	4573	G
8	L5	4575	G
8	L5	4584	A
8	L5	4589	A
8	L5	4590	A2M
8	L5	4619	U
8	L5	4620	OMU
8	L5	4623	OMG
8	L5	4624	A
8	L5	4635	A
8	L5	4636	U
8	L5	4637	OMG
8	L5	4648	A
8	L5	4652	G
8	L5	4656	A
8	L5	4658	G
8	L5	4670	C
8	L5	4672	A
8	L5	4687	A
8	L5	4700	A
8	L5	4708	A
8	L5	4709	U
8	L5	4719	G
8	L5	4730	C
8	L5	4731	G
8	L5	4733	C
8	L5	4734	A
8	L5	4740	G

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Mol	Chain	Res	Type
8	L5	4741	C
8	L5	4742	G
8	L5	4745	G
8	L5	4747	C
8	L5	4751	G
8	L5	4754	G
8	L5	4757	C
8	L5	4759	C
8	L5	4761	G
8	L5	4765	G
8	L5	4772	C
8	L5	4773	C
8	L5	4775	C
8	L5	4776	G
8	L5	4859	C
8	L5	4861	G
8	L5	4864	U
8	L5	4870	G
8	L5	4871	C
8	L5	4875	G
8	L5	4877	G
8	L5	4881	U
8	L5	4882	U
8	L5	4883	C
8	L5	4886	C
8	L5	4889	G
8	L5	4895	C
8	L5	4896	G
8	L5	4897	G
8	L5	4898	G
8	L5	4900	C
8	L5	4901	G
8	L5	4910	G
8	L5	4912	G
8	L5	4914	C
8	L5	4916	G
8	L5	4917	C
8	L5	4923	C
8	L5	4934	A
8	L5	4937	C
8	L5	4938	A
8	L5	4940	C

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Mol	Chain	Res	Type
8	L5	4943	A
8	L5	4949	G
8	L5	4951	G
8	L5	4955	A
8	L5	4960	G
8	L5	4963	G
8	L5	4966	A
8	L5	4967	A
8	L5	4976	U
8	L5	4985	U
8	L5	5009	G
8	L5	5013	C
8	L5	5014	A
8	L5	5017	G
8	L5	5034	A
8	L5	5041	G
8	L5	5047	C
8	L5	5050	C
8	L5	5058	A
8	L5	5069	U
9	L7	7	G
9	L7	24	C
9	L7	27	G
9	L7	41	G
9	L7	53	U
9	L7	54	A
9	L7	63	C
9	L7	64	G
9	L7	97	G
9	L7	100	A
9	L7	111	C
10	L8	22	U
10	L8	23	C
10	L8	34	U
10	L8	35	C
10	L8	39	G
10	L8	48	A
10	L8	51	U
10	L8	52	A
10	L8	55	PSU
10	L8	59	A
10	L8	62	A

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Mol	Chain	Res	Type
10	L8	63	U
10	L8	85	U
10	L8	86	U
10	L8	87	G
10	L8	88	A
10	L8	94	G
10	L8	103	A
10	L8	105	C
10	L8	106	G
10	L8	107	C
10	L8	110	U
10	L8	111	U
10	L8	114	G
10	L8	147	G
10	L8	153	C
10	L8	156	U
49	S2	2	A
49	S2	25	A
49	S2	33	G
49	S2	41	G
49	S2	42	A
49	S2	44	U
49	S2	45	A
49	S2	46	A
49	S2	56	G
49	S2	60	A
49	S2	61	A
49	S2	65	C
49	S2	67	C
49	S2	68	A
49	S2	71	G
49	S2	81	U
49	S2	93	U
49	S2	99	A
49	S2	103	A
49	S2	113	G
49	S2	115	U
49	S2	126	G
49	S2	130	G
49	S2	142	C
49	S2	143	U
49	S2	148	U

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Mol	Chain	Res	Type
49	S2	155	G
49	S2	159	A2M
49	S2	160	U
49	S2	162	C
49	S2	168	C
49	S2	169	U
49	S2	170	A
49	S2	173	A
49	S2	175	A
49	S2	179	C
49	S2	192	C
49	S2	215	G
49	S2	290	U
49	S2	291	G
49	S2	293	C
49	S2	294	U
49	S2	295	C
49	S2	302	A
49	S2	305	U
49	S2	306	C
49	S2	308	G
49	S2	309	G
49	S2	310	C
49	S2	311	C
49	S2	319	C
49	S2	323	C
49	S2	328	U
49	S2	329	G
49	S2	332	G
49	S2	351	G
49	S2	362	C
49	S2	364	A
49	S2	368	U
49	S2	370	G
49	S2	380	G
49	S2	381	C
49	S2	384	U
49	S2	385	G
49	S2	386	C
49	S2	398	A
49	S2	407	G
49	S2	408	A

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Mol	Chain	Res	Type
49	S2	409	C
49	S2	413	G
49	S2	421	G
49	S2	428	OMU
49	S2	429	C
49	S2	448	A
49	S2	449	A
49	S2	450	C
49	S2	452	G
49	S2	464	A
49	S2	465	A
49	S2	467	G
49	S2	471	G
49	S2	472	C
49	S2	473	A
49	S2	474	G
49	S2	482	G
49	S2	484	A
49	S2	485	A
49	S2	487	U
49	S2	488	U
49	S2	489	A
49	S2	492	C
49	S2	493	A
49	S2	501	C
49	S2	502	C
49	S2	503	C
49	S2	523	A
49	S2	525	A
49	S2	551	U
49	S2	555	A
49	S2	556	U
49	S2	557	U
49	S2	558	G
49	S2	560	A
49	S2	576	A2M
49	S2	578	C
49	S2	583	C
49	S2	587	A
49	S2	589	G
49	S2	590	A
49	S2	591	U

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Mol	Chain	Res	Type
49	S2	592	C
49	S2	593	C
49	S2	595	U
49	S2	596	U
49	S2	601	OMG
49	S2	602	G
49	S2	604	A
49	S2	605	A
49	S2	606	G
49	S2	607	U
49	S2	608	C
49	S2	614	C
49	S2	617	G
49	S2	618	C
49	S2	627	U
49	S2	628	A
49	S2	643	A
49	S2	644	OMG
49	S2	645	C
49	S2	655	A
49	S2	660	C
49	S2	668	A2M
49	S2	669	A
49	S2	671	A
49	S2	672	A
49	S2	673	G
49	S2	683	OMG
49	S2	688	U
49	S2	821	G
49	S2	822	U
49	S2	824	C
49	S2	830	A
49	S2	842	C
49	S2	847	A
49	S2	851	C
49	S2	856	C
49	S2	857	U
49	S2	869	A
49	S2	870	A
49	S2	871	U
49	S2	872	A
49	S2	874	G

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Mol	Chain	Res	Type
49	S2	877	C
49	S2	878	G
49	S2	879	C
49	S2	880	G
49	S2	881	G
49	S2	907	G
49	S2	909	G
49	S2	913	A
49	S2	919	A
49	S2	920	A
49	S2	930	C
49	S2	933	G
49	S2	950	C
49	S2	958	G
49	S2	963	A
49	S2	970	G
49	S2	971	G
49	S2	990	A
49	S2	992	A
49	S2	996	A
49	S2	999	G
49	S2	1001	A
49	S2	1008	A
49	S2	1016	U
49	S2	1017	U
49	S2	1023	A
49	S2	1027	A
49	S2	1045	U
49	S2	1049	A
49	S2	1050	A
49	S2	1055	A
49	S2	1061	U
49	S2	1062	A
49	S2	1078	C
49	S2	1083	A
49	S2	1085	C
49	S2	1086	G
49	S2	1087	A
49	S2	1088	U
49	S2	1100	A
49	S2	1110	G
49	S2	1113	A

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Mol	Chain	Res	Type
49	S2	1115	U
49	S2	1116	C
49	S2	1117	C
49	S2	1118	C
49	S2	1119	A
49	S2	1126	G
49	S2	1133	A
49	S2	1153	C
49	S2	1154	U
49	S2	1155	U
49	S2	1157	G
49	S2	1183	A
49	S2	1195	A
49	S2	1207	G
49	S2	1208	A
49	S2	1209	A
49	S2	1215	C
49	S2	1217	A
49	S2	1224	G
49	S2	1238	U
49	S2	1242	U
49	S2	1243	U
49	S2	1247	C
49	S2	1248	B8N
49	S2	1251	A
49	S2	1253	A
49	S2	1256	G
49	S2	1257	G
49	S2	1259	A
49	S2	1265	A
49	S2	1269	G
49	S2	1271	C
49	S2	1274	G
49	S2	1275	G
49	S2	1277	C
49	S2	1282	A
49	S2	1286	G
49	S2	1288	OMU
49	S2	1298	G
49	S2	1299	A
49	S2	1301	A
49	S2	1302	G

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Mol	Chain	Res	Type
49	S2	1303	C
49	S2	1304	U
49	S2	1308	U
49	S2	1309	C
49	S2	1327	G
49	S2	1330	G
49	S2	1331	C
49	S2	1337	4AC
49	S2	1342	U
49	S2	1348	G
49	S2	1371	U
49	S2	1372	U
49	S2	1373	C
49	S2	1378	A
49	S2	1382	A
49	S2	1396	A
49	S2	1402	A
49	S2	1403	C
49	S2	1406	G
49	S2	1409	A
49	S2	1415	C
49	S2	1440	C
49	S2	1448	A
49	S2	1449	G
49	S2	1450	G
49	S2	1452	A
49	S2	1454	A
49	S2	1474	A
49	S2	1477	U
49	S2	1487	A
49	S2	1489	A
49	S2	1490	G
49	S2	1495	G
49	S2	1498	A
49	S2	1505	U
49	S2	1506	A
49	S2	1508	A
49	S2	1519	U
49	S2	1520	G
49	S2	1521	C
49	S2	1522	A
49	S2	1528	G

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Mol	Chain	Res	Type
49	S2	1533	A
49	S2	1543	U
49	S2	1544	C
49	S2	1546	G
49	S2	1552	G
49	S2	1553	C
49	S2	1569	A
49	S2	1570	G
49	S2	1574	C
49	S2	1578	U
49	S2	1580	A
49	S2	1585	U
49	S2	1586	U
49	S2	1588	A
49	S2	1589	A
49	S2	1599	U
49	S2	1601	A
49	S2	1604	G
49	S2	1606	G
49	S2	1607	A
49	S2	1621	U
49	S2	1623	A
49	S2	1624	U
49	S2	1633	A
49	S2	1634	A
49	S2	1646	C
49	S2	1648	G
49	S2	1652	G
49	S2	1654	G
49	S2	1661	A
49	S2	1662	U
49	S2	1663	A
49	S2	1664	A
49	S2	1665	G
49	S2	1671	G
49	S2	1680	G
49	S2	1683	C
49	S2	1695	A
49	S2	1698	C
49	S2	1709	G
49	S2	1715	A
49	S2	1719	A

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Mol	Chain	Res	Type
49	S2	1722	G
49	S2	1726	G
49	S2	1729	U
49	S2	1742	C
49	S2	1743	G
49	S2	1744	G
49	S2	1813	A
49	S2	1822	A
49	S2	1823	A
49	S2	1824	A
49	S2	1829	G
49	S2	1831	A
49	S2	1832	6MZ
49	S2	1834	A
49	S2	1835	A
49	S2	1837	G
49	S2	1838	U
49	S2	1849	G
49	S2	1850	MA6
49	S2	1851	MA6
49	S2	1852	C
49	S2	1861	G
49	S2	1862	G
49	S2	1863	A
49	S2	1865	C
49	S2	1868	U
49	S2	1869	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	L5	233	U
8	L5	406	C
8	L5	667	A
8	L5	1082	C
8	L5	1210	C
8	L5	1271	G
8	L5	2019	C
8	L5	2416	G
8	L5	2675	G
8	L5	2760	G
8	L5	3614	G

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Mol	Chain	Res	Type
8	L5	3673	C
8	L5	3701	OMC
8	L5	4699	U
8	L5	4740	G
8	L5	4913	G
49	S2	601	OMG
49	S2	604	A
49	S2	1395	C
49	S2	1519	U
49	S2	1585	U
49	S2	1664	A

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

76 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	$\# Z > 2$
49	MA6	S2	1851	49	23,26,27	1.47	4 (17%)	33,38,41	3.34	11 (33%)
8	OMG	L5	4499	8	23,26,27	2.40	9 (39%)	32,38,41	2.59	10 (31%)
49	OMG	S2	601	49	23,26,27	2.43	9 (39%)	32,38,41	2.78	9 (28%)
8	A2M	L5	2363	8,84	22,25,26	3.55	9 (40%)	30,36,39	2.36	11 (36%)
8	OMG	L5	3627	8	23,26,27	2.40	9 (39%)	32,38,41	2.51	12 (37%)
8	PSU	L5	1683	8	18,21,22	4.54	7 (38%)	21,30,33	1.93	5 (23%)
8	OMG	L5	4618	8	23,26,27	2.39	9 (39%)	32,38,41	2.54	11 (34%)
49	OMC	S2	1703	49	19,22,23	2.95	8 (42%)	25,31,34	0.67	0
49	A2M	S2	159	49	22,25,26	3.56	9 (40%)	30,36,39	2.42	12 (40%)
49	A2M	S2	1678	49	22,25,26	3.60	9 (40%)	30,36,39	2.46	13 (43%)
49	OMG	S2	644	49	23,26,27	2.42	9 (39%)	32,38,41	2.64	10 (31%)
49	A2M	S2	668	84,49	22,25,26	3.52	9 (40%)	30,36,39	2.42	12 (40%)
49	4AC	S2	1842	49	21,24,25	3.34	9 (42%)	28,34,37	1.06	4 (14%)
8	OMG	L5	4494	8	23,26,27	2.44	9 (39%)	32,38,41	2.64	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	B8N	S2	1248	49	25,29,30	3.31	9 (36%)	28,42,45	2.22	10 (35%)
8	OMG	L5	1316	8	23,26,27	2.42	9 (39%)	32,38,41	2.66	10 (31%)
8	OMG	L5	2364	8	23,26,27	2.39	9 (39%)	32,38,41	2.58	11 (34%)
8	A2M	L5	3718	8	22,25,26	3.54	9 (40%)	30,36,39	2.38	12 (40%)
8	A2M	L5	1871	8	22,25,26	3.58	9 (40%)	30,36,39	2.39	12 (40%)
8	OMC	L5	2351	8	19,22,23	2.96	8 (42%)	25,31,34	0.86	0
8	A2M	L5	2815	8	22,25,26	3.50	9 (40%)	30,36,39	2.41	11 (36%)
8	PSU	L5	3729	8	18,21,22	4.55	7 (38%)	21,30,33	1.91	5 (23%)
8	OMC	L5	2861	8	19,22,23	2.92	8 (42%)	25,31,34	0.71	0
49	OMC	S2	1391	49	19,22,23	2.96	8 (42%)	25,31,34	0.76	0
8	PSU	L5	3758	8	18,21,22	4.53	7 (38%)	21,30,33	1.95	5 (23%)
49	A2M	S2	1383	49	22,25,26	3.51	9 (40%)	30,36,39	2.38	10 (33%)
8	OMC	L5	1881	8,84	19,22,23	2.92	8 (42%)	25,31,34	0.79	0
8	OMG	L5	3744	8	23,26,27	2.40	9 (39%)	32,38,41	2.56	11 (34%)
10	PSU	L8	55	10	18,21,22	4.55	7 (38%)	21,30,33	1.77	4 (19%)
49	OMU	S2	428	49	19,22,23	3.06	8 (42%)	25,31,34	1.79	5 (20%)
49	OMC	S2	174	49	19,22,23	2.99	8 (42%)	25,31,34	0.76	0
8	OMC	L5	2422	8,84	19,22,23	2.96	8 (42%)	25,31,34	0.75	0
8	OMG	L5	3792	8	23,26,27	2.40	9 (39%)	32,38,41	2.66	10 (31%)
8	OMG	L5	2876	8	23,26,27	2.38	9 (39%)	32,38,41	2.72	10 (31%)
49	6MZ	S2	1832	49	22,25,26	2.44	4 (18%)	29,36,39	2.26	10 (34%)
8	OMG	L5	1625	8	23,26,27	2.42	9 (39%)	32,38,41	2.63	10 (31%)
8	A2M	L5	4590	8,84	22,25,26	3.54	9 (40%)	30,36,39	2.45	12 (40%)
8	A2M	L5	3825	8	22,25,26	3.56	9 (40%)	30,36,39	2.34	11 (36%)
8	A2M	L5	398	8	22,25,26	3.54	9 (40%)	30,36,39	2.37	11 (36%)
8	A2M	L5	1524	8	22,25,26	3.55	10 (45%)	30,36,39	2.28	10 (33%)
8	OMG	L5	2424	8	23,26,27	2.46	9 (39%)	32,38,41	2.62	10 (31%)
8	OMU	L5	3925	8	19,22,23	2.89	8 (42%)	25,31,34	1.77	5 (20%)
8	OMU	L5	4620	8	19,22,23	2.96	8 (42%)	25,31,34	1.90	5 (20%)
49	G7M	S2	1639	49,6	23,26,27	2.64	9 (39%)	34,39,42	2.55	11 (32%)
8	OMG	L5	4228	8	23,26,27	2.37	9 (39%)	32,38,41	2.50	12 (37%)
49	OMG	S2	1328	49	23,26,27	2.40	9 (39%)	32,38,41	2.57	10 (31%)
49	MA6	S2	1850	49	23,26,27	1.51	4 (17%)	33,38,41	3.03	11 (33%)
8	OMC	L5	4536	8	19,22,23	2.90	8 (42%)	25,31,34	0.77	0
8	A2M	L5	1326	8	22,25,26	3.54	9 (40%)	30,36,39	2.37	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	L5	3734	8	18,21,22	4.70	7 (38%)	21,30,33	1.92	5 (23%)
8	OMC	L5	1340	8	19,22,23	2.92	8 (42%)	25,31,34	0.74	0
8	OMC	L5	2365	8	19,22,23	2.95	8 (42%)	25,31,34	0.76	0
8	OMC	L5	3701	8,84	19,22,23	2.94	8 (42%)	25,31,34	0.74	0
8	A2M	L5	3724	8	22,25,26	3.54	9 (40%)	30,36,39	2.38	12 (40%)
8	OMC	L5	3841	8	19,22,23	2.88	8 (42%)	25,31,34	0.65	0
8	PSU	L5	4353	8	18,21,22	4.57	7 (38%)	21,30,33	1.97	5 (23%)
8	OMG	L5	4637	8	23,26,27	2.44	9 (39%)	32,38,41	2.74	10 (31%)
8	PSU	L5	1782	8	18,21,22	4.60	7 (38%)	21,30,33	1.86	4 (19%)
49	A2M	S2	27	84,49	22,25,26	3.56	9 (40%)	30,36,39	2.39	10 (33%)
49	UY1	S2	1326	84,49	19,22,23	4.18	7 (36%)	21,31,34	1.97	5 (23%)
49	A2M	S2	576	49	22,25,26	3.53	9 (40%)	30,36,39	2.37	12 (40%)
8	A2M	L5	3760	8	22,25,26	3.56	10 (45%)	30,36,39	2.31	9 (30%)
8	OMG	L5	4623	8	23,26,27	2.38	9 (39%)	32,38,41	2.54	11 (34%)
49	A2M	S2	1031	49,83	22,25,26	3.55	9 (40%)	30,36,39	2.39	10 (33%)
8	A2M	L5	2787	8,84	22,25,26	3.51	9 (40%)	30,36,39	2.34	11 (36%)
8	OMG	L5	4370	8	23,26,27	2.40	9 (39%)	32,38,41	2.58	10 (31%)
8	A2M	L5	2401	8	22,25,26	3.52	9 (40%)	30,36,39	2.33	11 (36%)
49	OMG	S2	683	49	23,26,27	2.41	9 (39%)	32,38,41	2.54	13 (40%)
10	OMG	L8	75	10	23,26,27	2.41	9 (39%)	32,38,41	2.59	10 (31%)
49	4AC	S2	1337	49	21,24,25	3.33	9 (42%)	28,34,37	1.22	4 (14%)
49	OMU	S2	1442	84,49	19,22,23	2.99	8 (42%)	25,31,34	1.83	5 (20%)
8	OMC	L5	2804	8	19,22,23	2.88	8 (42%)	25,31,34	0.71	0
8	OMG	L5	1522	8	23,26,27	2.37	9 (39%)	32,38,41	2.57	10 (31%)
8	A2M	L5	3723	8	22,25,26	3.55	9 (40%)	30,36,39	2.30	11 (36%)
49	OMU	S2	1288	49	19,22,23	3.02	8 (42%)	25,31,34	1.80	5 (20%)
10	OMU	L8	14	10	19,22,23	3.10	8 (42%)	25,31,34	1.93	7 (28%)

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
49	MA6	S2	1851	49	-	3/11/29/30	0/3/3/3
8	OMG	L5	4499	8	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	OMG	S2	601	49	-	5/9/27/28	0/3/3/3
8	A2M	L5	2363	8,84	-	0/9/27/28	0/3/3/3
8	OMG	L5	3627	8	-	2/9/27/28	0/3/3/3
8	PSU	L5	1683	8	-	0/7/25/26	0/2/2/2
8	OMG	L5	4618	8	-	0/9/27/28	0/3/3/3
49	OMC	S2	1703	49	-	2/9/27/28	0/2/2/2
49	A2M	S2	159	49	-	2/9/27/28	0/3/3/3
49	A2M	S2	1678	49	-	1/9/27/28	0/3/3/3
49	OMG	S2	644	49	-	4/9/27/28	0/3/3/3
49	A2M	S2	668	84,49	-	3/9/27/28	0/3/3/3
49	4AC	S2	1842	49	-	0/11/29/30	0/2/2/2
8	OMG	L5	4494	8	-	0/9/27/28	0/3/3/3
49	B8N	S2	1248	49	-	8/16/34/35	0/2/2/2
8	OMG	L5	1316	8	-	1/9/27/28	0/3/3/3
8	OMG	L5	2364	8	-	2/9/27/28	0/3/3/3
8	A2M	L5	3718	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	1871	8	-	0/9/27/28	0/3/3/3
8	OMC	L5	2351	8	-	5/9/27/28	0/2/2/2
8	A2M	L5	2815	8	-	0/9/27/28	0/3/3/3
8	PSU	L5	3729	8	-	2/7/25/26	0/2/2/2
8	OMC	L5	2861	8	-	1/9/27/28	0/2/2/2
49	OMC	S2	1391	49	-	0/9/27/28	0/2/2/2
8	PSU	L5	3758	8	-	0/7/25/26	0/2/2/2
49	A2M	S2	1383	49	-	1/9/27/28	0/3/3/3
8	OMC	L5	1881	8,84	-	0/9/27/28	0/2/2/2
8	OMG	L5	3744	8	-	0/9/27/28	0/3/3/3
10	PSU	L8	55	10	-	2/7/25/26	0/2/2/2
49	OMU	S2	428	49	-	6/9/27/28	0/2/2/2
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2
8	OMC	L5	2422	8,84	-	2/9/27/28	0/2/2/2
8	OMG	L5	3792	8	-	0/9/27/28	0/3/3/3
8	OMG	L5	2876	8	-	2/9/27/28	0/3/3/3
49	6MZ	S2	1832	49	-	4/9/27/28	0/3/3/3
8	OMG	L5	1625	8	-	2/9/27/28	0/3/3/3
8	A2M	L5	4590	8,84	-	2/9/27/28	0/3/3/3
8	A2M	L5	3825	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	398	8	-	2/9/27/28	0/3/3/3
8	A2M	L5	1524	8	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMG	L5	2424	8	-	2/9/27/28	0/3/3/3
8	OMU	L5	3925	8	-	1/9/27/28	0/2/2/2
8	OMU	L5	4620	8	-	2/9/27/28	0/2/2/2
49	G7M	S2	1639	49,6	-	1/7/25/26	0/3/3/3
8	OMG	L5	4228	8	-	0/9/27/28	0/3/3/3
49	OMG	S2	1328	49	-	0/9/27/28	0/3/3/3
49	MA6	S2	1850	49	-	1/11/29/30	0/3/3/3
8	OMC	L5	4536	8	-	0/9/27/28	0/2/2/2
8	A2M	L5	1326	8	-	1/9/27/28	0/3/3/3
8	PSU	L5	3734	8	-	2/7/25/26	0/2/2/2
8	OMC	L5	1340	8	-	0/9/27/28	0/2/2/2
8	OMC	L5	2365	8	-	0/9/27/28	0/2/2/2
8	OMC	L5	3701	8,84	-	5/9/27/28	0/2/2/2
8	A2M	L5	3724	8	-	1/9/27/28	0/3/3/3
8	OMC	L5	3841	8	-	1/9/27/28	0/2/2/2
8	PSU	L5	4353	8	-	0/7/25/26	0/2/2/2
8	OMG	L5	4637	8	-	0/9/27/28	0/3/3/3
8	PSU	L5	1782	8	-	0/7/25/26	0/2/2/2
49	A2M	S2	27	84,49	-	1/9/27/28	0/3/3/3
49	UY1	S2	1326	84,49	-	0/9/27/28	0/2/2/2
49	A2M	S2	576	49	-	3/9/27/28	0/3/3/3
8	A2M	L5	3760	8	-	0/9/27/28	0/3/3/3
8	OMG	L5	4623	8	-	2/9/27/28	0/3/3/3
49	A2M	S2	1031	49,83	-	0/9/27/28	0/3/3/3
8	A2M	L5	2787	8,84	-	3/9/27/28	0/3/3/3
8	OMG	L5	4370	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	2401	8	-	2/9/27/28	0/3/3/3
49	OMG	S2	683	49	-	2/9/27/28	0/3/3/3
10	OMG	L8	75	10	-	0/9/27/28	0/3/3/3
49	4AC	S2	1337	49	-	0/11/29/30	0/2/2/2
49	OMU	S2	1442	84,49	-	1/9/27/28	0/2/2/2
8	OMC	L5	2804	8	-	1/9/27/28	0/2/2/2
8	OMG	L5	1522	8	-	0/9/27/28	0/3/3/3
8	A2M	L5	3723	8	-	1/9/27/28	0/3/3/3
49	OMU	S2	1288	49	-	2/9/27/28	0/2/2/2
10	OMU	L8	14	10	-	5/9/27/28	0/2/2/2

All (636) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	3734	PSU	C6-C5	12.44	1.49	1.35
8	L5	1782	PSU	C6-C5	12.06	1.48	1.35
10	L8	55	PSU	C6-C5	12.01	1.48	1.35
8	L5	1683	PSU	C6-C5	11.93	1.48	1.35
8	L5	4353	PSU	C6-C5	11.91	1.48	1.35
8	L5	3729	PSU	C6-C5	11.83	1.48	1.35
8	L5	3758	PSU	C6-C5	11.73	1.48	1.35
49	S2	1326	UY1	C6-C5	11.30	1.47	1.35
8	L5	3734	PSU	C2-N1	10.09	1.49	1.36
8	L5	4353	PSU	C2-N1	9.95	1.49	1.36
8	L5	1782	PSU	C2-N1	9.87	1.49	1.36
49	S2	1832	6MZ	C6-N6	9.85	1.45	1.34
8	L5	3758	PSU	C2-N1	9.79	1.49	1.36
49	S2	1326	UY1	C2-N1	9.78	1.49	1.36
8	L5	1683	PSU	C2-N1	9.69	1.49	1.36
8	L5	3729	PSU	C2-N1	9.69	1.49	1.36
49	S2	1248	B8N	C4-N3	-9.67	1.23	1.40
10	L8	55	PSU	C2-N1	9.56	1.49	1.36
49	S2	27	A2M	C2'-C1'	-9.41	1.29	1.53
8	L5	2363	A2M	C2'-C1'	-9.39	1.30	1.53
49	S2	1678	A2M	C2'-C1'	-9.38	1.30	1.53
8	L5	3760	A2M	C2'-C1'	-9.38	1.30	1.53
8	L5	3825	A2M	C2'-C1'	-9.36	1.30	1.53
8	L5	1871	A2M	C2'-C1'	-9.29	1.30	1.53
49	S2	1031	A2M	C2'-C1'	-9.24	1.30	1.53
8	L5	2401	A2M	C2'-C1'	-9.23	1.30	1.53
8	L5	2787	A2M	C2'-C1'	-9.22	1.30	1.53
49	S2	576	A2M	C2'-C1'	-9.22	1.30	1.53
8	L5	1326	A2M	C2'-C1'	-9.21	1.30	1.53
8	L5	398	A2M	C2'-C1'	-9.18	1.30	1.53
8	L5	1524	A2M	C2'-C1'	-9.17	1.30	1.53
8	L5	2815	A2M	C2'-C1'	-9.15	1.30	1.53
8	L5	3723	A2M	C2'-C1'	-9.15	1.30	1.53
49	S2	159	A2M	C2'-C1'	-9.15	1.30	1.53
8	L5	3718	A2M	C2'-C1'	-9.11	1.30	1.53
8	L5	3724	A2M	C2'-C1'	-9.07	1.30	1.53
8	L5	4590	A2M	C2'-C1'	-9.06	1.30	1.53
49	S2	1383	A2M	C2'-C1'	-9.06	1.30	1.53
49	S2	668	A2M	C2'-C1'	-9.04	1.30	1.53
8	L5	398	A2M	O4'-C1'	8.89	1.62	1.42
8	L5	3718	A2M	O4'-C1'	8.87	1.62	1.42
8	L5	4590	A2M	O4'-C1'	8.83	1.62	1.42
8	L5	3723	A2M	O4'-C1'	8.83	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	1871	A2M	O4'-C1'	8.83	1.62	1.42
49	S2	1383	A2M	O4'-C1'	8.82	1.62	1.42
8	L5	3724	A2M	O4'-C1'	8.82	1.62	1.42
49	S2	1678	A2M	O4'-C1'	8.81	1.62	1.42
49	S2	576	A2M	O4'-C1'	8.77	1.62	1.42
49	S2	159	A2M	O4'-C1'	8.77	1.62	1.42
8	L5	3825	A2M	O4'-C1'	8.68	1.62	1.42
8	L5	2787	A2M	O4'-C1'	8.68	1.62	1.42
8	L5	2815	A2M	O4'-C1'	8.67	1.62	1.42
8	L5	1524	A2M	O4'-C1'	8.63	1.61	1.42
8	L5	2401	A2M	O4'-C1'	8.61	1.61	1.42
49	S2	27	A2M	O4'-C1'	8.57	1.61	1.42
49	S2	1031	A2M	O4'-C1'	8.57	1.61	1.42
8	L5	2363	A2M	O4'-C1'	8.55	1.61	1.42
8	L5	1326	A2M	O4'-C1'	8.52	1.61	1.42
8	L5	3760	A2M	O4'-C1'	8.43	1.61	1.42
49	S2	668	A2M	O4'-C1'	8.40	1.61	1.42
8	L5	3734	PSU	C2-N3	7.84	1.50	1.37
8	L5	3729	PSU	C2-N3	7.77	1.50	1.37
8	L5	1782	PSU	C2-N3	7.73	1.50	1.37
10	L8	55	PSU	C2-N3	7.72	1.50	1.37
8	L5	1683	PSU	C2-N3	7.64	1.50	1.37
8	L5	3758	PSU	C2-N3	7.62	1.50	1.37
8	L5	4353	PSU	C2-N3	7.61	1.50	1.37
10	L8	14	OMU	C2-N1	7.45	1.50	1.38
49	S2	1326	UY1	C2-N3	7.34	1.49	1.37
49	S2	428	OMU	C2-N1	7.13	1.49	1.38
49	S2	1337	4AC	C4-N3	7.05	1.44	1.32
49	S2	1842	4AC	C4-N3	6.97	1.44	1.32
49	S2	1288	OMU	C2-N3	6.92	1.50	1.38
49	S2	1248	B8N	C6-N1	6.92	1.53	1.36
49	S2	1288	OMU	C2-N1	6.92	1.49	1.38
49	S2	668	A2M	O4'-C4'	-6.88	1.29	1.45
49	S2	428	OMU	C2-N3	6.86	1.49	1.38
49	S2	1442	OMU	C2-N1	6.86	1.49	1.38
10	L8	14	OMU	C2-N3	6.82	1.49	1.38
49	S2	1031	A2M	O4'-C4'	-6.82	1.29	1.45
49	S2	1442	OMU	C2-N3	6.81	1.49	1.38
8	L5	4620	OMU	C2-N1	6.73	1.49	1.38
8	L5	4620	OMU	C2-N3	6.68	1.49	1.38
49	S2	1678	A2M	O4'-C4'	-6.65	1.30	1.45
8	L5	2363	A2M	O4'-C4'	-6.64	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	4494	OMG	C4-N3	6.63	1.49	1.34
8	L5	3925	OMU	C2-N1	6.61	1.48	1.38
8	L5	1524	A2M	O4'-C4'	-6.60	1.30	1.45
8	L5	4637	OMG	C4-N3	6.60	1.49	1.34
8	L5	2424	OMG	C4-N3	6.59	1.49	1.34
8	L5	3825	A2M	O4'-C4'	-6.55	1.30	1.45
8	L5	3925	OMU	C2-N3	6.54	1.49	1.38
49	S2	644	OMG	C4-N3	6.53	1.49	1.34
8	L5	3723	A2M	O4'-C4'	-6.53	1.30	1.45
8	L5	1326	A2M	O4'-C4'	-6.52	1.30	1.45
8	L5	3792	OMG	C4-N3	6.52	1.49	1.34
8	L5	4590	A2M	O4'-C4'	-6.51	1.30	1.45
8	L5	4370	OMG	C4-N3	6.51	1.49	1.34
8	L5	1625	OMG	C4-N3	6.48	1.49	1.34
8	L5	1871	A2M	O4'-C4'	-6.45	1.30	1.45
49	S2	159	A2M	O4'-C4'	-6.45	1.30	1.45
49	S2	1328	OMG	C4-N3	6.45	1.49	1.34
8	L5	3760	A2M	O4'-C4'	-6.45	1.30	1.45
49	S2	1842	4AC	C6-C5	6.44	1.50	1.35
8	L5	4499	OMG	C4-N3	6.44	1.49	1.34
8	L5	3744	OMG	C4-N3	6.43	1.49	1.34
8	L5	3724	A2M	O4'-C4'	-6.43	1.30	1.45
10	L8	75	OMG	C4-N3	6.43	1.49	1.34
49	S2	27	A2M	O4'-C4'	-6.42	1.30	1.45
8	L5	2876	OMG	C4-N3	6.42	1.48	1.34
8	L5	1316	OMG	C4-N3	6.41	1.48	1.34
49	S2	1383	A2M	O4'-C4'	-6.41	1.30	1.45
49	S2	174	OMC	C2-N3	6.41	1.49	1.36
49	S2	683	OMG	C4-N3	6.40	1.48	1.34
49	S2	1639	G7M	C4-N3	6.40	1.48	1.34
8	L5	3718	A2M	O4'-C4'	-6.37	1.30	1.45
8	L5	2351	OMC	C2-N3	6.37	1.49	1.36
8	L5	3627	OMG	C4-N3	6.36	1.48	1.34
8	L5	2815	A2M	O4'-C4'	-6.36	1.30	1.45
8	L5	4618	OMG	C4-N3	6.36	1.48	1.34
8	L5	398	A2M	O4'-C4'	-6.35	1.30	1.45
8	L5	1340	OMC	C2-N3	6.35	1.48	1.36
8	L5	1522	OMG	C4-N3	6.35	1.48	1.34
8	L5	2364	OMG	C4-N3	6.33	1.48	1.34
8	L5	2401	A2M	O4'-C4'	-6.32	1.30	1.45
49	S2	1248	B8N	C4-C5	6.32	1.61	1.47
8	L5	2787	A2M	O4'-C4'	-6.32	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	576	A2M	O4'-C4'	-6.31	1.31	1.45
8	L5	3701	OMC	C2-N3	6.30	1.48	1.36
8	L5	2422	OMC	C2-N3	6.30	1.48	1.36
8	L5	4623	OMG	C4-N3	6.27	1.48	1.34
49	S2	601	OMG	C4-N3	6.27	1.48	1.34
8	L5	2365	OMC	C2-N3	6.27	1.48	1.36
49	S2	1391	OMC	C2-N3	6.26	1.48	1.36
8	L5	4536	OMC	C2-N3	6.24	1.48	1.36
8	L5	2861	OMC	C2-N3	6.23	1.48	1.36
8	L5	4228	OMG	C4-N3	6.22	1.48	1.34
8	L5	1881	OMC	C2-N3	6.21	1.48	1.36
49	S2	1337	4AC	C6-C5	6.19	1.49	1.35
8	L5	2804	OMC	C2-N3	6.18	1.48	1.36
8	L5	3841	OMC	C2-N3	6.17	1.48	1.36
49	S2	1703	OMC	C2-N3	6.16	1.48	1.36
49	S2	1337	4AC	C2-N3	6.08	1.48	1.36
49	S2	174	OMC	C6-C5	5.97	1.48	1.35
49	S2	1703	OMC	C6-C5	5.94	1.48	1.35
8	L5	1340	OMC	C6-C5	5.91	1.48	1.35
8	L5	2365	OMC	C6-C5	5.90	1.48	1.35
8	L5	2422	OMC	C6-C5	5.90	1.48	1.35
8	L5	2861	OMC	C6-C5	5.89	1.48	1.35
8	L5	3701	OMC	C6-C5	5.88	1.48	1.35
8	L5	4536	OMC	C6-C5	5.88	1.48	1.35
49	S2	1391	OMC	C6-C5	5.88	1.48	1.35
8	L5	2351	OMC	C6-C5	5.84	1.48	1.35
8	L5	3841	OMC	C6-C5	5.84	1.48	1.35
49	S2	1842	4AC	C2-N3	5.80	1.47	1.36
8	L5	1881	OMC	C6-C5	5.80	1.48	1.35
49	S2	428	OMU	C6-C5	5.69	1.48	1.35
8	L5	2804	OMC	C6-C5	5.67	1.48	1.35
49	S2	1288	OMU	C6-C5	5.63	1.48	1.35
8	L5	4620	OMU	C6-C5	5.60	1.48	1.35
10	L8	14	OMU	C6-C5	5.58	1.48	1.35
49	S2	1442	OMU	C6-C5	5.57	1.48	1.35
49	S2	1248	B8N	C2-N1	5.53	1.55	1.39
49	S2	1337	4AC	C7-N4	5.48	1.48	1.37
8	L5	3734	PSU	C6-N1	5.43	1.45	1.36
49	S2	1248	B8N	C6-C5	5.42	1.42	1.35
8	L5	3925	OMU	C6-C5	5.42	1.47	1.35
8	L5	4637	OMG	C2-N3	5.37	1.46	1.33
49	S2	601	OMG	C2-N3	5.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	2424	OMG	C2-N3	5.34	1.46	1.33
8	L5	3758	PSU	C6-N1	5.32	1.45	1.36
49	S2	1842	4AC	C7-N4	5.30	1.48	1.37
8	L5	1782	PSU	C6-N1	5.30	1.45	1.36
10	L8	55	PSU	C6-N1	5.28	1.44	1.36
8	L5	4494	OMG	C2-N3	5.28	1.46	1.33
8	L5	4353	PSU	C6-N1	5.27	1.44	1.36
49	S2	644	OMG	C2-N3	5.25	1.45	1.33
8	L5	1625	OMG	C2-N3	5.22	1.45	1.33
49	S2	1639	G7M	C2-N3	5.21	1.45	1.33
8	L5	3729	PSU	C6-N1	5.20	1.44	1.36
49	S2	1639	G7M	C5-N7	-5.20	1.33	1.39
10	L8	75	OMG	C2-N3	5.19	1.45	1.33
8	L5	4370	OMG	C2-N3	5.18	1.45	1.33
8	L5	4499	OMG	C2-N3	5.17	1.45	1.33
8	L5	3701	OMC	C4-N3	5.14	1.44	1.34
8	L5	1316	OMG	C2-N3	5.13	1.45	1.33
8	L5	3792	OMG	C2-N3	5.11	1.45	1.33
49	S2	1391	OMC	C4-N3	5.11	1.44	1.34
49	S2	174	OMC	C4-N3	5.11	1.44	1.34
8	L5	1683	PSU	C6-N1	5.10	1.44	1.36
8	L5	2365	OMC	C4-N3	5.10	1.44	1.34
49	S2	1328	OMG	C2-N3	5.09	1.45	1.33
49	S2	683	OMG	C2-N3	5.09	1.45	1.33
8	L5	2422	OMC	C4-N3	5.08	1.44	1.34
8	L5	4618	OMG	C2-N3	5.07	1.45	1.33
49	S2	1703	OMC	C4-N3	5.05	1.44	1.34
8	L5	2876	OMG	C2-N3	5.04	1.45	1.33
49	S2	1326	UY1	C6-N1	5.03	1.44	1.36
8	L5	2364	OMG	C2-N3	5.03	1.45	1.33
8	L5	3744	OMG	C2-N3	5.00	1.45	1.33
8	L5	2351	OMC	C4-N3	5.00	1.44	1.34
8	L5	2804	OMC	C4-N3	5.00	1.44	1.34
8	L5	1340	OMC	C4-N3	4.99	1.44	1.34
8	L5	4623	OMG	C2-N3	4.96	1.45	1.33
8	L5	2861	OMC	C4-N3	4.94	1.44	1.34
49	S2	1703	OMC	C4-N4	4.94	1.45	1.33
8	L5	1522	OMG	C2-N3	4.92	1.45	1.33
8	L5	1881	OMC	C4-N3	4.92	1.44	1.34
8	L5	3841	OMC	C4-N3	4.91	1.44	1.34
8	L5	4536	OMC	C4-N3	4.90	1.44	1.34
49	S2	601	OMG	C2-N2	4.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	174	OMC	C4-N4	4.90	1.45	1.33
8	L5	2365	OMC	C4-N4	4.86	1.45	1.33
8	L5	2804	OMC	C4-N4	4.85	1.45	1.33
8	L5	3627	OMG	C2-N3	4.85	1.44	1.33
8	L5	4228	OMG	C2-N3	4.85	1.44	1.33
49	S2	1391	OMC	C4-N4	4.84	1.45	1.33
8	L5	2422	OMC	C4-N4	4.83	1.45	1.33
8	L5	2861	OMC	C4-N4	4.78	1.45	1.33
8	L5	2424	OMG	C2-N2	4.78	1.45	1.34
8	L5	1340	OMC	C4-N4	4.76	1.45	1.33
8	L5	4536	OMC	C4-N4	4.76	1.45	1.33
8	L5	1625	OMG	C2-N2	4.73	1.45	1.34
8	L5	1316	OMG	C2-N2	4.72	1.45	1.34
8	L5	2351	OMC	C4-N4	4.72	1.45	1.33
8	L5	1881	OMC	C4-N4	4.72	1.45	1.33
10	L8	75	OMG	C2-N2	4.72	1.45	1.34
8	L5	3792	OMG	C2-N2	4.71	1.45	1.34
49	S2	1639	G7M	C2-N2	4.71	1.45	1.34
8	L5	3701	OMC	C4-N4	4.70	1.45	1.33
49	S2	683	OMG	C2-N2	4.70	1.45	1.34
8	L5	4499	OMG	C2-N2	4.69	1.45	1.34
8	L5	3841	OMC	C4-N4	4.69	1.45	1.33
49	S2	644	OMG	C2-N2	4.64	1.45	1.34
8	L5	2876	OMG	C2-N2	4.61	1.45	1.34
8	L5	4623	OMG	C2-N2	4.61	1.45	1.34
8	L5	2364	OMG	C2-N2	4.61	1.45	1.34
8	L5	4494	OMG	C2-N2	4.60	1.44	1.34
8	L5	4618	OMG	C2-N2	4.60	1.44	1.34
8	L5	3758	PSU	C1'-C5	-4.60	1.39	1.50
8	L5	4637	OMG	C2-N2	4.60	1.44	1.34
49	S2	1328	OMG	C2-N2	4.59	1.44	1.34
8	L5	3744	OMG	C2-N2	4.56	1.44	1.34
8	L5	4370	OMG	C2-N2	4.56	1.44	1.34
8	L5	4353	PSU	C1'-C5	-4.55	1.40	1.50
8	L5	3627	OMG	C2-N2	4.55	1.44	1.34
8	L5	3729	PSU	C1'-C5	-4.53	1.40	1.50
8	L5	1683	PSU	C1'-C5	-4.53	1.40	1.50
10	L8	55	PSU	C1'-C5	-4.52	1.40	1.50
8	L5	1522	OMG	C2-N2	4.52	1.44	1.34
8	L5	2351	OMC	C2-N1	4.51	1.49	1.40
49	S2	1391	OMC	C2-N1	4.51	1.49	1.40
8	L5	4228	OMG	C2-N2	4.46	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	27	A2M	C6-N6	4.45	1.45	1.34
49	S2	576	A2M	C6-N6	4.41	1.45	1.34
8	L5	3701	OMC	C2-N1	4.40	1.49	1.40
8	L5	3723	A2M	C6-N6	4.39	1.45	1.34
49	S2	174	OMC	C2-N1	4.39	1.49	1.40
8	L5	1326	A2M	C6-N6	4.39	1.45	1.34
8	L5	3724	A2M	C6-N6	4.37	1.45	1.34
8	L5	398	A2M	C6-N6	4.36	1.45	1.34
8	L5	2422	OMC	C2-N1	4.36	1.49	1.40
8	L5	1524	A2M	C6-N6	4.35	1.45	1.34
8	L5	4590	A2M	C6-N6	4.35	1.45	1.34
8	L5	2787	A2M	C6-N6	4.34	1.45	1.34
8	L5	3718	A2M	C6-N6	4.34	1.45	1.34
8	L5	3734	PSU	C1'-C5	-4.34	1.40	1.50
8	L5	1871	A2M	C6-N6	4.34	1.45	1.34
49	S2	668	A2M	C6-N6	4.34	1.45	1.34
8	L5	2815	A2M	C6-N6	4.33	1.45	1.34
8	L5	1881	OMC	C2-N1	4.33	1.49	1.40
49	S2	1842	4AC	O2-C2	-4.33	1.15	1.23
49	S2	1337	4AC	O2-C2	-4.33	1.15	1.23
8	L5	2401	A2M	C6-N6	4.33	1.45	1.34
8	L5	3825	A2M	C6-N6	4.31	1.45	1.34
49	S2	1031	A2M	C6-N6	4.30	1.45	1.34
49	S2	1678	A2M	C6-N6	4.28	1.45	1.34
8	L5	1782	PSU	C1'-C5	-4.28	1.40	1.50
8	L5	2861	OMC	C2-N1	4.27	1.49	1.40
49	S2	159	A2M	C6-N6	4.26	1.45	1.34
8	L5	3760	A2M	C6-N6	4.23	1.45	1.34
49	S2	1288	OMU	C4-N3	4.23	1.45	1.38
8	L5	2365	OMC	C2-N1	4.22	1.48	1.40
49	S2	428	OMU	C4-N3	4.21	1.45	1.38
49	S2	1383	A2M	C6-N6	4.20	1.44	1.34
8	L5	2363	A2M	C6-N6	4.20	1.44	1.34
49	S2	1703	OMC	C2-N1	4.19	1.48	1.40
8	L5	4536	OMC	C2-N1	4.16	1.48	1.40
10	L8	14	OMU	C4-N3	4.15	1.45	1.38
8	L5	3841	OMC	C2-N1	4.14	1.48	1.40
8	L5	1340	OMC	C2-N1	4.12	1.48	1.40
8	L5	2804	OMC	C2-N1	4.12	1.48	1.40
49	S2	1842	4AC	C5-C4	4.07	1.50	1.41
49	S2	1842	4AC	C2-N1	4.06	1.48	1.40
49	S2	1442	OMU	C4-N3	4.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	4620	OMU	C4-N3	3.92	1.45	1.38
8	L5	3925	OMU	C4-N3	3.90	1.45	1.38
49	S2	1337	4AC	C5-C4	3.90	1.49	1.41
49	S2	1850	MA6	C6-N6	3.89	1.47	1.36
8	L5	3734	PSU	C4-N3	3.88	1.46	1.38
49	S2	1337	4AC	C2-N1	3.87	1.48	1.40
49	S2	1851	MA6	C6-N6	3.85	1.47	1.36
49	S2	1639	G7M	C5-C6	3.82	1.53	1.43
8	L5	3729	PSU	C4-N3	3.80	1.46	1.38
49	S2	1337	4AC	C4-N4	3.79	1.45	1.39
8	L5	1782	PSU	C4-N3	3.79	1.46	1.38
8	L5	4353	PSU	C4-N3	3.60	1.45	1.38
49	S2	1842	4AC	C4-N4	3.60	1.45	1.39
8	L5	3758	PSU	C4-N3	3.59	1.45	1.38
10	L8	55	PSU	C4-N3	3.58	1.45	1.38
8	L5	1683	PSU	C4-N3	3.53	1.45	1.38
49	S2	1326	UY1	C4-N3	3.41	1.45	1.38
49	S2	159	A2M	C5-C4	-3.39	1.33	1.39
8	L5	1326	A2M	C5-C4	-3.39	1.33	1.39
8	L5	3760	A2M	C5-C4	-3.36	1.33	1.39
49	S2	1851	MA6	C5-C4	-3.31	1.33	1.39
49	S2	1031	A2M	C5-C4	-3.30	1.33	1.39
8	L5	1871	A2M	C5-C4	-3.28	1.33	1.39
49	S2	1842	4AC	C6-N1	3.26	1.45	1.38
8	L5	3825	A2M	C5-C4	-3.26	1.33	1.39
49	S2	668	A2M	C5-C4	-3.26	1.33	1.39
8	L5	2401	A2M	C5-C4	-3.21	1.33	1.39
8	L5	4590	A2M	C5-C4	-3.20	1.33	1.39
8	L5	2363	A2M	C5-C4	-3.20	1.33	1.39
49	S2	1678	A2M	C5-C4	-3.20	1.33	1.39
8	L5	3718	A2M	C5-C4	-3.19	1.33	1.39
8	L5	3724	A2M	C5-C4	-3.16	1.33	1.39
8	L5	398	A2M	C5-C4	-3.15	1.33	1.39
8	L5	2351	OMC	C6-N1	3.15	1.45	1.38
8	L5	3760	A2M	C5-N7	-3.15	1.33	1.39
49	S2	27	A2M	C5-C4	-3.15	1.33	1.39
49	S2	159	A2M	O3'-C3'	-3.15	1.35	1.43
8	L5	2787	A2M	C5-C4	-3.13	1.33	1.39
8	L5	1881	OMC	C6-N1	3.12	1.45	1.38
8	L5	1524	A2M	C5-C4	-3.11	1.33	1.39
49	S2	174	OMC	C6-N1	3.09	1.45	1.38
49	S2	1383	A2M	C5-C4	-3.09	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1703	OMC	C6-N1	3.09	1.45	1.38
8	L5	4620	OMU	O4-C4	-3.08	1.18	1.24
8	L5	2815	A2M	C5-C4	-3.07	1.33	1.39
8	L5	2365	OMC	C6-N1	3.06	1.45	1.38
8	L5	1871	A2M	C5-N7	-3.05	1.33	1.39
49	S2	1678	A2M	O3'-C3'	-3.05	1.35	1.43
8	L5	3723	A2M	C5-C4	-3.04	1.33	1.39
49	S2	576	A2M	C5-C4	-3.02	1.33	1.39
8	L5	2422	OMC	C6-N1	3.01	1.45	1.38
8	L5	2401	A2M	C5-N7	-3.01	1.33	1.39
8	L5	1316	OMG	C5-N7	-3.01	1.33	1.39
8	L5	3925	OMU	O4-C4	-3.01	1.18	1.24
49	S2	1442	OMU	O4-C4	-3.00	1.18	1.24
49	S2	1850	MA6	C5-N7	-3.00	1.33	1.39
8	L5	1524	A2M	O3'-C3'	-3.00	1.35	1.43
8	L5	1871	A2M	O3'-C3'	-3.00	1.35	1.43
49	S2	159	A2M	C5-N7	-3.00	1.33	1.39
8	L5	3701	OMC	C6-N1	2.99	1.45	1.38
8	L5	4499	OMG	C5-N7	-2.99	1.33	1.39
8	L5	3841	OMC	C6-N1	2.99	1.45	1.38
8	L5	3718	A2M	C5-N7	-2.98	1.33	1.39
8	L5	4494	OMG	C5-N7	-2.98	1.33	1.39
8	L5	3627	OMG	C5-N7	-2.98	1.33	1.39
49	S2	1391	OMC	C6-N1	2.98	1.45	1.38
8	L5	2363	A2M	O3'-C3'	-2.98	1.35	1.43
49	S2	1703	OMC	O2-C2	-2.97	1.18	1.23
8	L5	3760	A2M	O3'-C3'	-2.97	1.35	1.43
8	L5	3724	A2M	O2'-C2'	2.97	1.49	1.42
8	L5	398	A2M	O3'-C3'	-2.97	1.35	1.43
8	L5	3723	A2M	O3'-C3'	-2.97	1.35	1.43
8	L5	1326	A2M	O3'-C3'	-2.96	1.35	1.43
8	L5	4637	OMG	C5-N7	-2.96	1.33	1.39
49	S2	428	OMU	O4-C4	-2.95	1.18	1.24
8	L5	3792	OMG	C5-N7	-2.95	1.33	1.39
8	L5	1522	OMG	C5-N7	-2.95	1.33	1.39
8	L5	1524	A2M	C5-N7	-2.95	1.33	1.39
8	L5	2861	OMC	C6-N1	2.95	1.45	1.38
8	L5	3825	A2M	O3'-C3'	-2.94	1.35	1.43
8	L5	2424	OMG	C5-N7	-2.94	1.33	1.39
49	S2	1850	MA6	C8-N9	-2.94	1.32	1.37
8	L5	3724	A2M	O3'-C3'	-2.94	1.35	1.43
49	S2	644	OMG	C5-N7	-2.93	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	1340	OMC	C6-N1	2.93	1.45	1.38
49	S2	576	A2M	O3'-C3'	-2.93	1.35	1.43
8	L5	3758	PSU	O4-C4	-2.93	1.18	1.23
8	L5	4590	A2M	O3'-C3'	-2.91	1.35	1.43
49	S2	1383	A2M	O2'-C2'	2.91	1.49	1.42
49	S2	1678	A2M	O2'-C2'	2.91	1.49	1.42
8	L5	1326	A2M	C5-N7	-2.91	1.33	1.39
8	L5	2876	OMG	C5-N7	-2.90	1.33	1.39
49	S2	1288	OMU	O4-C4	-2.90	1.18	1.24
49	S2	159	A2M	O2'-C2'	2.90	1.49	1.42
8	L5	2787	A2M	C5-N7	-2.90	1.33	1.39
10	L8	14	OMU	O4-C4	-2.89	1.18	1.24
49	S2	27	A2M	O3'-C3'	-2.89	1.35	1.43
49	S2	1031	A2M	O2'-C2'	2.89	1.49	1.42
8	L5	1625	OMG	C5-N7	-2.89	1.33	1.39
49	S2	668	A2M	O2'-C2'	2.89	1.49	1.42
8	L5	4590	A2M	O2'-C2'	2.89	1.49	1.42
8	L5	2363	A2M	O2'-C2'	2.89	1.49	1.42
8	L5	3723	A2M	O2'-C2'	2.89	1.49	1.42
49	S2	1383	A2M	O3'-C3'	-2.88	1.35	1.43
8	L5	2363	A2M	C5-N7	-2.88	1.33	1.39
49	S2	27	A2M	C5-N7	-2.88	1.33	1.39
8	L5	2815	A2M	C5-N7	-2.88	1.33	1.39
10	L8	75	OMG	C5-N7	-2.88	1.33	1.39
8	L5	4228	OMG	C2-N1	2.87	1.44	1.37
10	L8	14	OMU	C6-N1	2.87	1.44	1.38
49	S2	576	A2M	C5-N7	-2.87	1.33	1.39
10	L8	14	OMU	O2-C2	-2.87	1.18	1.23
49	S2	1328	OMG	C5-N7	-2.86	1.33	1.39
49	S2	576	A2M	O2'-C2'	2.86	1.49	1.42
8	L5	4590	A2M	C5-N7	-2.86	1.33	1.39
49	S2	1832	6MZ	C5-C4	-2.86	1.34	1.39
49	S2	1678	A2M	C5-N7	-2.86	1.33	1.39
8	L5	3825	A2M	O2'-C2'	2.86	1.49	1.42
49	S2	428	OMU	C6-N1	2.86	1.44	1.38
49	S2	1031	A2M	O3'-C3'	-2.86	1.35	1.43
8	L5	2364	OMG	C2-N1	2.86	1.44	1.37
8	L5	3723	A2M	C5-N7	-2.85	1.33	1.39
8	L5	3744	OMG	C5-N7	-2.85	1.33	1.39
49	S2	1850	MA6	C5-C4	-2.84	1.34	1.39
49	S2	601	OMG	C5-N7	-2.84	1.33	1.39
8	L5	2861	OMC	O2-C2	-2.84	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	2364	OMG	C5-N7	-2.84	1.33	1.39
8	L5	4623	OMG	C5-N7	-2.84	1.33	1.39
8	L5	4618	OMG	C5-N7	-2.84	1.33	1.39
8	L5	2815	A2M	O3'-C3'	-2.84	1.35	1.43
49	S2	601	OMG	C2-N1	2.84	1.44	1.37
8	L5	2804	OMC	C6-N1	2.83	1.44	1.38
8	L5	3718	A2M	O3'-C3'	-2.83	1.35	1.43
49	S2	683	OMG	C2-N1	2.83	1.44	1.37
8	L5	3627	OMG	C2-N1	2.83	1.44	1.37
8	L5	1871	A2M	O2'-C2'	2.83	1.49	1.42
8	L5	4536	OMC	C6-N1	2.82	1.44	1.38
8	L5	2401	A2M	O2'-C2'	2.82	1.49	1.42
8	L5	2365	OMC	O2-C2	-2.82	1.18	1.23
8	L5	2787	A2M	O3'-C3'	-2.82	1.36	1.43
8	L5	398	A2M	C5-N7	-2.82	1.33	1.39
8	L5	1326	A2M	O2'-C2'	2.82	1.49	1.42
8	L5	4228	OMG	C5-N7	-2.82	1.33	1.39
8	L5	3825	A2M	C5-N7	-2.81	1.33	1.39
8	L5	4370	OMG	C5-N7	-2.81	1.33	1.39
8	L5	2401	A2M	O3'-C3'	-2.81	1.36	1.43
8	L5	3744	OMG	C2-N1	2.80	1.44	1.37
8	L5	2351	OMC	O2-C2	-2.80	1.18	1.23
49	S2	27	A2M	O2'-C2'	2.80	1.49	1.42
8	L5	2422	OMC	O2-C2	-2.80	1.18	1.23
8	L5	3724	A2M	C5-N7	-2.80	1.34	1.39
8	L5	398	A2M	O2'-C2'	2.80	1.49	1.42
8	L5	2804	OMC	O2-C2	-2.80	1.18	1.23
10	L8	75	OMG	C2-N1	2.80	1.44	1.37
8	L5	2815	A2M	O2'-C2'	2.80	1.49	1.42
8	L5	4536	OMC	O2-C2	-2.79	1.18	1.23
8	L5	1625	OMG	C2-N1	2.78	1.44	1.37
49	S2	668	A2M	C5-N7	-2.78	1.34	1.39
8	L5	3841	OMC	O2-C2	-2.78	1.18	1.23
49	S2	683	OMG	C5-N7	-2.78	1.33	1.39
8	L5	4353	PSU	O4-C4	-2.78	1.18	1.23
49	S2	1337	4AC	C6-N1	2.78	1.44	1.38
49	S2	668	A2M	O3'-C3'	-2.77	1.36	1.43
8	L5	1524	A2M	O2'-C2'	2.77	1.49	1.42
8	L5	2787	A2M	O2'-C2'	2.77	1.49	1.42
8	L5	1340	OMC	O2-C2	-2.77	1.18	1.23
49	S2	1391	OMC	O2-C2	-2.77	1.18	1.23
49	S2	1031	A2M	C5-N7	-2.76	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	1881	OMC	O2-C2	-2.75	1.18	1.23
8	L5	4618	OMG	C2-N1	2.75	1.44	1.37
49	S2	1639	G7M	C2-N1	2.75	1.44	1.37
49	S2	1288	OMU	C6-N1	2.74	1.44	1.38
8	L5	3718	A2M	O2'-C2'	2.74	1.49	1.42
8	L5	1683	PSU	O4-C4	-2.74	1.18	1.23
8	L5	2424	OMG	C2-N1	2.73	1.44	1.37
49	S2	1326	UY1	O4-C4	-2.73	1.18	1.23
49	S2	1678	A2M	C8-N9	-2.71	1.32	1.37
8	L5	3760	A2M	O2'-C2'	2.71	1.49	1.42
8	L5	3627	OMG	O6-C6	-2.70	1.18	1.23
8	L5	4623	OMG	C2-N1	2.70	1.44	1.37
8	L5	4494	OMG	C2-N1	2.70	1.44	1.37
8	L5	1522	OMG	C2-N1	2.69	1.44	1.37
49	S2	601	OMG	O6-C6	-2.69	1.18	1.23
49	S2	174	OMC	O2-C2	-2.69	1.18	1.23
49	S2	1383	A2M	C5-N7	-2.69	1.34	1.39
49	S2	1442	OMU	C6-N1	2.69	1.44	1.38
8	L5	1782	PSU	O4-C4	-2.69	1.18	1.23
49	S2	1328	OMG	C2-N1	2.68	1.44	1.37
49	S2	644	OMG	C2-N1	2.68	1.44	1.37
8	L5	1316	OMG	C2-N1	2.68	1.44	1.37
49	S2	1832	6MZ	C8-N9	-2.67	1.33	1.37
8	L5	1625	OMG	O6-C6	-2.67	1.18	1.23
8	L5	4637	OMG	O6-C6	-2.66	1.18	1.23
8	L5	4620	OMU	O2-C2	-2.65	1.18	1.23
8	L5	1522	OMG	O6-C6	-2.65	1.18	1.23
49	S2	644	OMG	O6-C6	-2.64	1.18	1.23
8	L5	3925	OMU	O2-C2	-2.64	1.18	1.23
49	S2	1328	OMG	O6-C6	-2.64	1.18	1.23
8	L5	4494	OMG	O6-C6	-2.64	1.18	1.23
49	S2	1832	6MZ	C5-N7	-2.64	1.34	1.39
8	L5	4370	OMG	C2-N1	2.64	1.44	1.37
8	L5	2876	OMG	O6-C6	-2.63	1.18	1.23
8	L5	4637	OMG	C2-N1	2.63	1.44	1.37
8	L5	4623	OMG	O6-C6	-2.63	1.18	1.23
8	L5	4499	OMG	C2-N1	2.61	1.44	1.37
10	L8	55	PSU	O4-C4	-2.60	1.18	1.23
8	L5	2424	OMG	O6-C6	-2.60	1.18	1.23
8	L5	3792	OMG	C2-N1	2.60	1.43	1.37
49	S2	1639	G7M	O6-C6	-2.60	1.18	1.23
8	L5	4228	OMG	C4-N9	-2.59	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	2876	OMG	C2-N1	2.59	1.43	1.37
8	L5	3718	A2M	C8-N9	-2.58	1.33	1.37
8	L5	4228	OMG	O6-C6	-2.57	1.18	1.23
8	L5	3825	A2M	C8-N9	-2.57	1.33	1.37
8	L5	2364	OMG	O6-C6	-2.57	1.18	1.23
8	L5	3627	OMG	C4-N9	-2.56	1.31	1.38
8	L5	3734	PSU	O4-C4	-2.56	1.18	1.23
49	S2	1442	OMU	O2-C2	-2.56	1.18	1.23
8	L5	4228	OMG	C6-N1	2.56	1.43	1.38
8	L5	3744	OMG	O6-C6	-2.55	1.18	1.23
49	S2	683	OMG	O6-C6	-2.55	1.18	1.23
8	L5	4590	A2M	C8-N9	-2.54	1.33	1.37
8	L5	1326	A2M	C8-N9	-2.54	1.33	1.37
8	L5	4618	OMG	O6-C6	-2.54	1.18	1.23
49	S2	1851	MA6	C5-N7	-2.54	1.34	1.39
10	L8	75	OMG	O6-C6	-2.54	1.18	1.23
8	L5	3760	A2M	C8-N9	-2.54	1.33	1.37
8	L5	3729	PSU	O4-C4	-2.53	1.18	1.23
49	S2	1031	A2M	C8-N9	-2.53	1.33	1.37
8	L5	3701	OMC	O2-C2	-2.53	1.19	1.23
49	S2	428	OMU	O2-C2	-2.53	1.18	1.23
8	L5	2363	A2M	C8-N9	-2.53	1.33	1.37
8	L5	4370	OMG	O6-C6	-2.52	1.18	1.23
8	L5	1871	A2M	C8-N9	-2.52	1.33	1.37
8	L5	4620	OMU	C6-N1	2.52	1.44	1.38
49	S2	159	A2M	C8-N9	-2.52	1.33	1.37
8	L5	4499	OMG	O6-C6	-2.51	1.18	1.23
8	L5	3744	OMG	C6-N1	2.51	1.43	1.38
8	L5	3925	OMU	C6-N1	2.50	1.44	1.38
8	L5	3792	OMG	O6-C6	-2.50	1.18	1.23
49	S2	27	A2M	C8-N9	-2.49	1.33	1.37
8	L5	2401	A2M	C8-N9	-2.47	1.33	1.37
49	S2	601	OMG	C5-C6	2.47	1.53	1.44
49	S2	576	A2M	C8-N9	-2.47	1.33	1.37
8	L5	4370	OMG	C5-C6	2.47	1.53	1.44
8	L5	1316	OMG	O6-C6	-2.46	1.18	1.23
8	L5	3724	A2M	C8-N9	-2.45	1.33	1.37
8	L5	4228	OMG	C5-C6	2.45	1.53	1.44
8	L5	4618	OMG	C5-C6	2.44	1.53	1.44
49	S2	668	A2M	C8-N9	-2.44	1.33	1.37
8	L5	4618	OMG	C6-N1	2.43	1.43	1.38
10	L8	75	OMG	C6-N1	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	3744	OMG	C5-C6	2.43	1.53	1.44
49	S2	1383	A2M	C8-N9	-2.42	1.33	1.37
49	S2	1288	OMU	O2-C2	-2.42	1.18	1.23
49	S2	683	OMG	C4-N9	-2.42	1.31	1.38
49	S2	683	OMG	C5-C6	2.41	1.53	1.44
8	L5	2364	OMG	C5-C6	2.41	1.53	1.44
49	S2	683	OMG	C6-N1	2.40	1.43	1.38
8	L5	4494	OMG	C6-N1	2.40	1.43	1.38
8	L5	1625	OMG	C5-C6	2.40	1.53	1.44
49	S2	1328	OMG	C5-C6	2.40	1.53	1.44
8	L5	3723	A2M	C8-N9	-2.40	1.33	1.37
8	L5	1316	OMG	C5-C6	2.39	1.53	1.44
10	L8	75	OMG	C5-C6	2.39	1.53	1.44
8	L5	4623	OMG	C4-N9	-2.39	1.32	1.38
8	L5	2424	OMG	C5-C6	2.39	1.53	1.44
8	L5	2364	OMG	C4-N9	-2.39	1.32	1.38
8	L5	4637	OMG	C5-C6	2.39	1.53	1.44
8	L5	2424	OMG	C6-N1	2.38	1.43	1.38
8	L5	3627	OMG	C6-N1	2.38	1.43	1.38
49	S2	644	OMG	C5-C6	2.38	1.53	1.44
8	L5	2364	OMG	C6-N1	2.37	1.43	1.38
8	L5	3792	OMG	C5-C6	2.37	1.53	1.44
8	L5	4618	OMG	C4-N9	-2.37	1.32	1.38
8	L5	4494	OMG	C5-C6	2.37	1.53	1.44
49	S2	1248	B8N	O2-C2	-2.37	1.18	1.22
8	L5	1522	OMG	C4-N9	-2.37	1.32	1.38
8	L5	4623	OMG	C5-C6	2.36	1.53	1.44
49	S2	1703	OMC	C5-C4	2.35	1.48	1.42
8	L5	1522	OMG	C5-C6	2.35	1.53	1.44
8	L5	2365	OMC	C5-C4	2.35	1.48	1.42
49	S2	1248	B8N	O4-C4	-2.34	1.18	1.23
8	L5	398	A2M	C8-N9	-2.33	1.33	1.37
8	L5	3744	OMG	C4-N9	-2.33	1.32	1.38
8	L5	4499	OMG	C5-C6	2.33	1.53	1.44
8	L5	3627	OMG	C5-C6	2.32	1.53	1.44
8	L5	2422	OMC	C5-C4	2.32	1.48	1.42
49	S2	174	OMC	C5-C4	2.32	1.48	1.42
8	L5	1524	A2M	C4-N9	-2.32	1.32	1.37
8	L5	4623	OMG	C6-N1	2.31	1.43	1.38
49	S2	1288	OMU	C5-C4	2.31	1.48	1.43
49	S2	1328	OMG	C6-N1	2.31	1.43	1.38
8	L5	1316	OMG	C6-N1	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L5	2815	A2M	C8-N9	-2.30	1.33	1.37
8	L5	2876	OMG	C5-C6	2.30	1.53	1.44
8	L5	4499	OMG	C4-N9	-2.30	1.32	1.38
49	S2	1639	G7M	C6-N1	2.30	1.43	1.38
8	L5	2876	OMG	C4-N9	-2.30	1.32	1.38
8	L5	4370	OMG	C6-N1	2.29	1.43	1.38
8	L5	1881	OMC	C5-C4	2.28	1.48	1.42
49	S2	1328	OMG	C4-N9	-2.28	1.32	1.38
49	S2	1248	B8N	C2-N3	2.28	1.42	1.38
8	L5	2787	A2M	C8-N9	-2.27	1.33	1.37
49	S2	428	OMU	C5-C4	2.27	1.48	1.43
49	S2	1851	MA6	C8-N9	-2.25	1.33	1.37
49	S2	601	OMG	C4-N9	-2.25	1.32	1.38
8	L5	1316	OMG	C4-N9	-2.25	1.32	1.38
8	L5	2876	OMG	C6-N1	2.25	1.43	1.38
8	L5	1625	OMG	C4-N9	-2.25	1.32	1.38
8	L5	4370	OMG	C4-N9	-2.25	1.32	1.38
8	L5	1522	OMG	C6-N1	2.24	1.43	1.38
8	L5	1625	OMG	C6-N1	2.23	1.43	1.38
8	L5	2861	OMC	C5-C4	2.22	1.48	1.42
49	S2	1391	OMC	C5-C4	2.22	1.48	1.42
49	S2	644	OMG	C6-N1	2.22	1.43	1.38
10	L8	75	OMG	C4-N9	-2.22	1.32	1.38
8	L5	1340	OMC	C5-C4	2.21	1.48	1.42
8	L5	3792	OMG	C4-N9	-2.21	1.32	1.38
8	L5	4637	OMG	C6-N1	2.20	1.43	1.38
49	S2	644	OMG	C4-N9	-2.20	1.32	1.38
8	L5	2424	OMG	C4-N9	-2.20	1.32	1.38
8	L5	4494	OMG	C4-N9	-2.20	1.32	1.38
8	L5	4499	OMG	C6-N1	2.16	1.42	1.38
49	S2	1639	G7M	C4-N9	-2.16	1.32	1.38
8	L5	4536	OMC	C5-C4	2.15	1.47	1.42
10	L8	14	OMU	C5-C4	2.15	1.48	1.43
49	S2	1442	OMU	C5-C4	2.14	1.48	1.43
49	S2	1326	UY1	O2-C2	-2.13	1.18	1.23
8	L5	4637	OMG	C4-N9	-2.12	1.32	1.38
8	L5	3841	OMC	C5-C4	2.11	1.47	1.42
49	S2	601	OMG	C6-N1	2.10	1.42	1.38
8	L5	3792	OMG	C6-N1	2.10	1.42	1.38
8	L5	4620	OMU	C5-C4	2.08	1.48	1.43
8	L5	1524	A2M	C8-N9	-2.08	1.34	1.37
8	L5	3701	OMC	C5-C4	2.07	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1248	B8N	C1'-C5	2.06	1.54	1.50
8	L5	3760	A2M	C4-N9	-2.06	1.33	1.37
8	L5	2351	OMC	C5-C4	2.06	1.47	1.42
8	L5	3925	OMU	C5-C4	2.05	1.48	1.43
8	L5	2804	OMC	C5-C4	2.03	1.47	1.42

All (586) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1851	MA6	N1-C6-N6	-12.24	101.94	116.86
49	S2	1850	MA6	N1-C6-N6	-10.19	104.44	116.86
49	S2	601	OMG	C1'-N9-C8	-8.87	101.52	126.73
8	L5	2876	OMG	C1'-N9-C8	-8.58	102.35	126.73
8	L5	4637	OMG	C1'-N9-C8	-8.48	102.64	126.73
8	L5	3792	OMG	C1'-N9-C8	-8.29	103.17	126.73
49	S2	1851	MA6	C5-C6-N6	8.11	138.17	125.33
8	L5	1625	OMG	C1'-N9-C8	-8.10	103.72	126.73
8	L5	1316	OMG	C1'-N9-C8	-7.99	104.02	126.73
8	L5	2424	OMG	C1'-N9-C8	-7.93	104.21	126.73
8	L5	4494	OMG	C1'-N9-C8	-7.92	104.22	126.73
8	L5	4499	OMG	C1'-N9-C8	-7.91	104.27	126.73
49	S2	644	OMG	C1'-N9-C8	-7.89	104.33	126.73
8	L5	2364	OMG	C1'-N9-C8	-7.86	104.41	126.73
49	S2	601	OMG	C1'-N9-C4	7.82	149.59	126.49
10	L8	75	OMG	C1'-N9-C8	-7.81	104.55	126.73
8	L5	4370	OMG	C1'-N9-C8	-7.80	104.56	126.73
49	S2	1328	OMG	C1'-N9-C8	-7.78	104.63	126.73
8	L5	1522	OMG	C1'-N9-C8	-7.71	104.84	126.73
49	S2	1639	G7M	C1'-N9-C4	7.63	149.02	126.49
8	L5	4623	OMG	C1'-N9-C8	-7.62	105.08	126.73
8	L5	4618	OMG	C1'-N9-C8	-7.58	105.20	126.73
8	L5	3744	OMG	C1'-N9-C8	-7.54	105.32	126.73
49	S2	1639	G7M	C1'-N9-C8	-7.43	101.65	126.74
49	S2	683	OMG	C1'-N9-C8	-7.42	105.66	126.73
8	L5	4637	OMG	C1'-N9-C4	7.33	148.13	126.49
8	L5	2876	OMG	C1'-N9-C4	7.31	148.09	126.49
8	L5	3627	OMG	C1'-N9-C8	-7.31	105.95	126.73
8	L5	4228	OMG	C1'-N9-C8	-7.21	106.25	126.73
8	L5	3792	OMG	C1'-N9-C4	7.17	147.67	126.49
49	S2	1850	MA6	C5-C6-N6	7.01	136.43	125.33
8	L5	1625	OMG	C1'-N9-C4	6.98	147.09	126.49
8	L5	2424	OMG	C1'-N9-C4	6.94	146.98	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	4494	OMG	C1'-N9-C4	6.88	146.80	126.49
8	L5	4499	OMG	C1'-N9-C4	6.82	146.62	126.49
8	L5	1316	OMG	C1'-N9-C4	6.80	146.56	126.49
10	L8	75	OMG	C1'-N9-C4	6.77	146.49	126.49
49	S2	644	OMG	C1'-N9-C4	6.73	146.37	126.49
8	L5	4370	OMG	C1'-N9-C4	6.71	146.30	126.49
8	L5	2364	OMG	C1'-N9-C4	6.67	146.18	126.49
49	S2	1328	OMG	C1'-N9-C4	6.67	146.18	126.49
8	L5	1522	OMG	C1'-N9-C4	6.62	146.04	126.49
8	L5	4618	OMG	C1'-N9-C4	6.57	145.90	126.49
8	L5	4623	OMG	C1'-N9-C4	6.49	145.65	126.49
8	L5	3744	OMG	C1'-N9-C4	6.44	145.50	126.49
8	L5	3760	A2M	N3-C2-N1	-6.15	119.27	128.58
8	L5	3627	OMG	C1'-N9-C4	6.14	144.63	126.49
49	S2	683	OMG	C1'-N9-C4	6.11	144.53	126.49
49	S2	27	A2M	N3-C2-N1	-6.02	119.46	128.58
8	L5	4228	OMG	C1'-N9-C4	6.00	144.20	126.49
49	S2	1832	6MZ	N1-C2-N3	-5.98	119.52	128.58
8	L5	1871	A2M	N3-C2-N1	-5.96	119.57	128.58
8	L5	1326	A2M	N3-C2-N1	-5.91	119.64	128.58
49	S2	1248	B8N	C31-N3-C2	5.90	126.34	117.64
8	L5	4590	A2M	N3-C2-N1	-5.87	119.69	128.58
8	L5	2815	A2M	N3-C2-N1	-5.80	119.80	128.58
49	S2	1851	MA6	N1-C2-N3	-5.76	119.86	128.58
49	S2	668	A2M	N3-C2-N1	-5.75	119.88	128.58
8	L5	3724	A2M	N3-C2-N1	-5.75	119.88	128.58
49	S2	1031	A2M	N3-C2-N1	-5.74	119.89	128.58
8	L5	3723	A2M	N3-C2-N1	-5.74	119.90	128.58
8	L5	2363	A2M	N3-C2-N1	-5.73	119.90	128.58
8	L5	398	A2M	N3-C2-N1	-5.72	119.92	128.58
8	L5	2401	A2M	N3-C2-N1	-5.72	119.92	128.58
8	L5	4620	OMU	C4-N3-C2	-5.72	119.52	126.61
49	S2	1383	A2M	N3-C2-N1	-5.69	119.97	128.58
8	L5	2787	A2M	N3-C2-N1	-5.65	120.02	128.58
49	S2	1442	OMU	C4-N3-C2	-5.65	119.60	126.61
49	S2	576	A2M	N3-C2-N1	-5.57	120.14	128.58
49	S2	428	OMU	C4-N3-C2	-5.56	119.70	126.61
49	S2	1288	OMU	C4-N3-C2	-5.55	119.72	126.61
49	S2	159	A2M	N3-C2-N1	-5.55	120.19	128.58
49	S2	1678	A2M	N3-C2-N1	-5.54	120.20	128.58
8	L5	3825	A2M	N3-C2-N1	-5.48	120.28	128.58
8	L5	3925	OMU	C4-N3-C2	-5.47	119.82	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	3718	A2M	N3-C2-N1	-5.44	120.34	128.58
8	L5	1524	A2M	N3-C2-N1	-5.43	120.36	128.58
49	S2	1678	A2M	C5-C4-N3	-5.42	119.25	126.72
49	S2	1031	A2M	C5-C4-N3	-5.42	119.26	126.72
8	L5	2815	A2M	C5-C4-N3	-5.40	119.28	126.72
49	S2	1850	MA6	C4-C5-C6	5.35	121.44	115.91
49	S2	1850	MA6	C5-C4-N3	-5.30	119.42	126.72
10	L8	14	OMU	C4-N3-C2	-5.29	120.04	126.61
49	S2	576	A2M	C5-C4-N3	-5.28	119.44	126.72
8	L5	3825	A2M	C5-C4-N3	-5.26	119.47	126.72
49	S2	1850	MA6	N1-C2-N3	-5.22	120.68	128.58
49	S2	159	A2M	C5-C4-N3	-5.21	119.54	126.72
8	L5	2363	A2M	C5-C4-N3	-5.20	119.56	126.72
8	L5	4590	A2M	C5-C4-N3	-5.18	119.59	126.72
8	L5	2787	A2M	C5-C4-N3	-5.14	119.64	126.72
8	L5	3718	A2M	C5-C4-N3	-5.14	119.64	126.72
49	S2	1326	UY1	C4-N3-C2	-5.12	119.31	126.37
49	S2	1383	A2M	N6-C6-N1	-5.11	107.00	118.38
8	L5	398	A2M	C5-C4-N3	-5.10	119.69	126.72
8	L5	4637	OMG	C5-C4-N3	-5.09	120.29	128.39
8	L5	1326	A2M	C5-C4-N3	-5.07	119.74	126.72
8	L5	2401	A2M	C5-C4-N3	-5.07	119.74	126.72
49	S2	601	OMG	C5-C4-N3	-5.06	120.33	128.39
8	L5	3724	A2M	C5-C4-N3	-5.05	119.76	126.72
8	L5	2363	A2M	N6-C6-N1	-5.02	107.20	118.38
49	S2	159	A2M	N6-C6-N1	-5.01	107.21	118.38
49	S2	1248	B8N	C4-N3-C2	-5.01	119.46	125.62
49	S2	1383	A2M	C5-C4-N3	-5.00	119.83	126.72
49	S2	27	A2M	N6-C6-N1	-5.00	107.23	118.38
8	L5	2815	A2M	N6-C6-N1	-4.96	107.32	118.38
8	L5	4590	A2M	N6-C6-N1	-4.94	107.38	118.38
49	S2	668	A2M	N6-C6-N1	-4.93	107.39	118.38
49	S2	1678	A2M	N6-C6-N1	-4.91	107.45	118.38
8	L5	1871	A2M	C5-C4-N3	-4.90	119.97	126.72
49	S2	1248	B8N	C5-C4-N3	4.89	125.03	116.15
8	L5	4494	OMG	C5-C4-N3	-4.89	120.61	128.39
8	L5	3718	A2M	N6-C6-N1	-4.89	107.49	118.38
8	L5	3723	A2M	C5-C4-N3	-4.86	120.02	126.72
8	L5	1524	A2M	N6-C6-N1	-4.85	107.58	118.38
49	S2	1851	MA6	C5-C4-N3	-4.84	120.05	126.72
8	L5	3825	A2M	N6-C6-N1	-4.83	107.62	118.38
8	L5	398	A2M	N6-C6-N1	-4.83	107.62	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	4353	PSU	C4-N3-C2	-4.83	119.72	126.37
8	L5	2787	A2M	N6-C6-N1	-4.83	107.63	118.38
49	S2	27	A2M	C5-C4-N3	-4.83	120.07	126.72
49	S2	644	OMG	C5-C4-N3	-4.82	120.72	128.39
8	L5	3724	A2M	N6-C6-N1	-4.81	107.66	118.38
8	L5	3758	PSU	C4-N3-C2	-4.80	119.76	126.37
8	L5	1316	OMG	C5-C4-N3	-4.78	120.79	128.39
8	L5	2424	OMG	C5-C4-N3	-4.78	120.79	128.39
49	S2	1832	6MZ	C5-C4-N3	-4.77	120.14	126.72
8	L5	3723	A2M	N6-C6-N1	-4.77	107.76	118.38
8	L5	3792	OMG	C5-C4-N3	-4.74	120.85	128.39
49	S2	1031	A2M	N6-C6-N1	-4.72	107.86	118.38
8	L5	3760	A2M	N6-C6-N1	-4.71	107.88	118.38
8	L5	2401	A2M	N6-C6-N1	-4.71	107.89	118.38
49	S2	668	A2M	C5-C4-N3	-4.71	120.24	126.72
8	L5	1625	OMG	C5-C4-N3	-4.70	120.91	128.39
8	L5	4499	OMG	C5-C4-N3	-4.69	120.92	128.39
10	L8	75	OMG	C5-C4-N3	-4.68	120.94	128.39
8	L5	1326	A2M	N6-C6-N1	-4.68	107.96	118.38
8	L5	4370	OMG	C5-C4-N3	-4.66	120.97	128.39
8	L5	2876	OMG	C5-C4-N3	-4.66	120.97	128.39
8	L5	1871	A2M	N6-C6-N1	-4.65	108.01	118.38
49	S2	576	A2M	N6-C6-N1	-4.64	108.05	118.38
8	L5	1683	PSU	C4-N3-C2	-4.62	120.00	126.37
49	S2	1328	OMG	C5-C4-N3	-4.58	121.11	128.39
8	L5	4494	OMG	C2-N3-C4	4.57	120.17	112.30
8	L5	1782	PSU	C4-N3-C2	-4.57	120.08	126.37
49	S2	601	OMG	C2-N3-C4	4.56	120.16	112.30
49	S2	1639	G7M	C2-N3-C4	4.54	120.12	112.30
8	L5	4618	OMG	C5-C4-N3	-4.52	121.20	128.39
8	L5	3744	OMG	C5-C4-N3	-4.51	121.21	128.39
8	L5	2424	OMG	C2-N3-C4	4.51	120.06	112.30
8	L5	1522	OMG	C5-C4-N3	-4.51	121.22	128.39
8	L5	3729	PSU	C4-N3-C2	-4.50	120.17	126.37
8	L5	3734	PSU	N1-C2-N3	4.49	119.90	115.17
8	L5	1316	OMG	C2-N3-C4	4.49	120.03	112.30
49	S2	644	OMG	C2-N3-C4	4.49	120.03	112.30
8	L5	3744	OMG	C2-N3-C4	4.45	119.96	112.30
8	L5	3760	A2M	C5-C4-N3	-4.42	120.63	126.72
8	L5	1683	PSU	N1-C2-N3	4.42	119.83	115.17
49	S2	1851	MA6	N9-C8-N7	-4.41	107.68	113.94
8	L5	2364	OMG	C5-C4-N3	-4.41	121.38	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	3734	PSU	C4-N3-C2	-4.40	120.31	126.37
10	L8	75	OMG	C2-N3-C4	4.40	119.87	112.30
8	L5	4353	PSU	N1-C2-N3	4.39	119.79	115.17
49	S2	1326	UY1	N1-C2-N3	4.38	119.79	115.17
49	S2	1328	OMG	C2-N3-C4	4.38	119.84	112.30
8	L5	4370	OMG	C2-N3-C4	4.38	119.84	112.30
8	L5	1522	OMG	C2-N3-C4	4.38	119.84	112.30
8	L5	4637	OMG	C2-N3-C4	4.37	119.82	112.30
49	S2	668	A2M	N9-C8-N7	-4.36	107.75	113.94
8	L5	2876	OMG	C2-N3-C4	4.36	119.80	112.30
8	L5	4623	OMG	C5-C4-N3	-4.36	121.46	128.39
8	L5	3792	OMG	C2-N3-C4	4.35	119.80	112.30
8	L5	4618	OMG	C2-N3-C4	4.32	119.75	112.30
8	L5	4499	OMG	C2-N3-C4	4.32	119.74	112.30
49	S2	683	OMG	C5-C4-N3	-4.31	121.53	128.39
8	L5	4623	OMG	C2-N3-C4	4.30	119.71	112.30
8	L5	1625	OMG	C2-N3-C4	4.30	119.70	112.30
8	L5	1782	PSU	N1-C2-N3	4.28	119.69	115.17
8	L5	3729	PSU	N1-C2-N3	4.27	119.67	115.17
8	L5	2364	OMG	C2-N3-C4	4.27	119.65	112.30
8	L5	3627	OMG	C2-N3-C4	4.27	119.65	112.30
49	S2	683	OMG	C2-N3-C4	4.25	119.62	112.30
8	L5	3627	OMG	C5-C4-N3	-4.21	121.69	128.39
8	L5	4228	OMG	C2-N3-C4	4.21	119.55	112.30
8	L5	3758	PSU	N1-C2-N3	4.19	119.59	115.17
8	L5	1326	A2M	N9-C8-N7	-4.18	108.01	113.94
49	S2	1832	6MZ	N9-C8-N7	-4.18	108.01	113.94
10	L8	14	OMU	N3-C2-N1	4.17	120.33	114.89
8	L5	3724	A2M	N9-C8-N7	-4.16	108.03	113.94
8	L5	4620	OMU	N3-C2-N1	4.16	120.31	114.89
8	L5	4590	A2M	N9-C8-N7	-4.15	108.05	113.94
49	S2	159	A2M	N9-C8-N7	-4.14	108.06	113.94
10	L8	55	PSU	C6-N1-C2	-4.11	118.88	122.69
49	S2	1639	G7M	C5-C4-N3	-4.09	120.42	128.15
8	L5	4228	OMG	C5-C4-N3	-4.07	121.91	128.39
49	S2	1678	A2M	N9-C8-N7	-4.07	108.17	113.94
49	S2	1851	MA6	C4-C5-C6	4.06	120.10	115.91
8	L5	1524	A2M	C5-C4-N3	-4.05	121.13	126.72
8	L5	398	A2M	N9-C8-N7	-4.00	108.26	113.94
10	L8	55	PSU	N1-C2-N3	4.00	119.39	115.17
8	L5	3760	A2M	N9-C8-N7	-3.99	108.28	113.94
8	L5	1524	A2M	C5-C6-N6	3.98	133.13	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1031	A2M	N9-C8-N7	-3.97	108.31	113.94
8	L5	3723	A2M	N9-C8-N7	-3.96	108.31	113.94
49	S2	1442	OMU	N3-C2-N1	3.96	120.04	114.89
49	S2	1383	A2M	N9-C8-N7	-3.96	108.32	113.94
8	L5	3825	A2M	N9-C8-N7	-3.95	108.33	113.94
49	S2	27	A2M	N9-C8-N7	-3.95	108.33	113.94
8	L5	1871	A2M	N9-C8-N7	-3.95	108.34	113.94
8	L5	2815	A2M	N9-C8-N7	-3.93	108.36	113.94
49	S2	576	A2M	N9-C8-N7	-3.92	108.37	113.94
8	L5	2401	A2M	N9-C8-N7	-3.92	108.38	113.94
49	S2	27	A2M	C5-C6-N6	3.91	132.97	123.29
8	L5	3718	A2M	N9-C8-N7	-3.89	108.42	113.94
8	L5	2787	A2M	N9-C8-N7	-3.89	108.42	113.94
49	S2	668	A2M	C5-C6-N6	3.88	132.89	123.29
49	S2	683	OMG	N9-C8-N7	-3.86	106.24	113.40
49	S2	1639	G7M	C5-C6-N1	3.86	119.82	111.84
8	L5	2363	A2M	N9-C8-N7	-3.86	108.46	113.94
49	S2	1383	A2M	C5-C6-N6	3.84	132.79	123.29
8	L5	3925	OMU	N3-C2-N1	3.83	119.88	114.89
49	S2	1288	OMU	N3-C2-N1	3.82	119.87	114.89
8	L5	1524	A2M	N9-C8-N7	-3.80	108.54	113.94
8	L5	3718	A2M	C5-C6-N6	3.79	132.67	123.29
49	S2	428	OMU	N3-C2-N1	3.79	119.82	114.89
8	L5	4228	OMG	N9-C8-N7	-3.78	106.39	113.40
49	S2	159	A2M	C5-C6-N6	3.75	132.58	123.29
8	L5	3734	PSU	C6-N1-C2	-3.74	119.22	122.69
10	L8	55	PSU	C4-N3-C2	-3.73	121.23	126.37
49	S2	1832	6MZ	C4-C5-C6	3.72	119.87	116.78
8	L5	2815	A2M	C5-C6-N6	3.71	132.48	123.29
8	L5	4590	A2M	C5-C6-N6	3.71	132.48	123.29
8	L5	2363	A2M	C5-C6-N6	3.71	132.47	123.29
8	L5	3760	A2M	C5-C6-N6	3.71	132.46	123.29
8	L5	3723	A2M	C5-C6-N6	3.67	132.38	123.29
49	S2	1678	A2M	C5-C6-N6	3.67	132.37	123.29
8	L5	1316	OMG	N9-C8-N7	-3.65	106.63	113.40
8	L5	2787	A2M	C5-C6-N6	3.65	132.32	123.29
8	L5	2815	A2M	C2-N3-C4	3.64	120.72	111.83
49	S2	428	OMU	C5-C4-N3	3.63	119.89	114.80
8	L5	3724	A2M	C5-C6-N6	3.63	132.28	123.29
8	L5	398	A2M	C5-C6-N6	3.63	132.27	123.29
49	S2	1850	MA6	N3-C4-N9	3.63	133.34	127.17
49	S2	644	OMG	N9-C8-N7	-3.63	106.68	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1442	OMU	C5-C4-N3	3.62	119.88	114.80
49	S2	1031	A2M	C2-N3-C4	3.62	120.68	111.83
8	L5	2401	A2M	C5-C6-N6	3.62	132.24	123.29
8	L5	3627	OMG	N9-C8-N7	-3.62	106.69	113.40
8	L5	2876	OMG	N9-C8-N7	-3.61	106.70	113.40
8	L5	3825	A2M	C5-C6-N6	3.59	132.17	123.29
8	L5	2364	OMG	N9-C8-N7	-3.59	106.75	113.40
8	L5	4623	OMG	N9-C8-N7	-3.57	106.77	113.40
8	L5	3744	OMG	N9-C8-N7	-3.56	106.80	113.40
8	L5	1683	PSU	C6-N1-C2	-3.56	119.39	122.69
8	L5	4590	A2M	C2-N3-C4	3.54	120.48	111.83
8	L5	1326	A2M	C5-C6-N6	3.54	132.04	123.29
8	L5	1326	A2M	C2-N3-C4	3.54	120.47	111.83
8	L5	1871	A2M	C5-C6-N6	3.53	132.03	123.29
8	L5	2363	A2M	C2-N3-C4	3.53	120.45	111.83
49	S2	1678	A2M	C2-N3-C4	3.52	120.44	111.83
49	S2	576	A2M	C5-C6-N6	3.52	132.00	123.29
49	S2	1288	OMU	C5-C4-N3	3.51	119.72	114.80
8	L5	3925	OMU	C5-C4-N3	3.51	119.71	114.80
49	S2	1328	OMG	N9-C8-N7	-3.50	106.92	113.40
10	L8	14	OMU	C1'-N1-C2	3.48	123.85	117.59
8	L5	398	A2M	C2-N3-C4	3.47	120.30	111.83
8	L5	3825	A2M	C2-N3-C4	3.47	120.30	111.83
8	L5	4620	OMU	C5-C4-N3	3.47	119.65	114.80
8	L5	1871	A2M	C2-N3-C4	3.46	120.28	111.83
8	L5	1522	OMG	N9-C8-N7	-3.46	106.99	113.40
8	L5	2787	A2M	C2-N3-C4	3.46	120.27	111.83
49	S2	27	A2M	C2-N3-C4	3.46	120.27	111.83
8	L5	3724	A2M	C2-N3-C4	3.45	120.26	111.83
49	S2	576	A2M	C2-N3-C4	3.44	120.23	111.83
49	S2	159	A2M	C2-N3-C4	3.43	120.21	111.83
49	S2	1851	MA6	C2-N3-C4	3.43	120.20	111.83
8	L5	4370	OMG	N9-C8-N7	-3.42	107.05	113.40
49	S2	1383	A2M	C2-N3-C4	3.42	120.19	111.83
49	S2	1248	B8N	N3-C2-N1	3.42	120.90	116.72
8	L5	3792	OMG	N9-C8-N7	-3.41	107.08	113.40
8	L5	1625	OMG	N9-C8-N7	-3.41	107.08	113.40
8	L5	3729	PSU	C6-N1-C2	-3.40	119.54	122.69
8	L5	3758	PSU	C6-N1-C2	-3.40	119.54	122.69
49	S2	1832	6MZ	C2-N3-C4	3.39	120.11	111.83
8	L5	1782	PSU	C6-N1-C2	-3.39	119.55	122.69
8	L5	2401	A2M	C2-N3-C4	3.38	120.09	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L8	14	OMU	C5-C4-N3	3.37	119.52	114.80
8	L5	4637	OMG	N9-C8-N7	-3.37	107.15	113.40
49	S2	1031	A2M	C5-C6-N6	3.37	131.63	123.29
10	L8	75	OMG	N9-C8-N7	-3.37	107.16	113.40
8	L5	3718	A2M	C2-N3-C4	3.36	120.04	111.83
8	L5	3723	A2M	C2-N3-C4	3.36	120.03	111.83
8	L5	1524	A2M	C2'-C1'-N9	-3.35	108.24	113.75
49	S2	668	A2M	C2-N3-C4	3.33	119.97	111.83
8	L5	4494	OMG	N9-C8-N7	-3.32	107.24	113.40
49	S2	576	A2M	N3-C4-N9	3.32	132.82	127.17
8	L5	4499	OMG	N9-C8-N7	-3.32	107.24	113.40
49	S2	1851	MA6	C2-N1-C6	3.31	119.91	111.83
8	L5	4618	OMG	N9-C8-N7	-3.30	107.28	113.40
49	S2	1031	A2M	N3-C4-N9	3.29	132.77	127.17
49	S2	1850	MA6	C2-N1-C6	3.29	119.87	111.83
8	L5	4637	OMG	N9-C4-N3	3.27	132.49	125.95
8	L5	3760	A2M	C2-N3-C4	3.27	119.81	111.83
49	S2	1678	A2M	N3-C4-N9	3.23	132.67	127.17
8	L5	2815	A2M	N3-C4-N9	3.21	132.63	127.17
8	L5	4353	PSU	C6-N1-C2	-3.20	119.72	122.69
8	L5	4637	OMG	C2-N1-C6	-3.17	119.36	125.11
8	L5	2424	OMG	N9-C8-N7	-3.17	107.52	113.40
49	S2	1832	6MZ	C5-N7-C8	3.17	108.43	103.45
49	S2	1337	4AC	N4-C4-N3	3.13	118.95	113.87
49	S2	1850	MA6	C2-N3-C4	3.13	119.47	111.83
49	S2	1639	G7M	O6-C6-C5	-3.11	121.07	128.01
49	S2	1639	G7M	N9-C4-N3	3.10	132.16	125.95
49	S2	601	OMG	N9-C4-N3	3.09	132.14	125.95
8	L5	3825	A2M	N3-C4-N9	3.07	132.40	127.17
49	S2	601	OMG	N9-C8-N7	-3.07	107.71	113.40
8	L5	1326	A2M	N3-C4-N9	3.06	132.38	127.17
8	L5	2363	A2M	N3-C4-N9	3.06	132.37	127.17
49	S2	159	A2M	N3-C4-N9	3.05	132.36	127.17
8	L5	4590	A2M	N3-C4-N9	3.04	132.34	127.17
49	S2	601	OMG	C2-N1-C6	-3.04	119.60	125.11
8	L5	398	A2M	N3-C4-N9	3.02	132.30	127.17
8	L5	4590	A2M	C5-N7-C8	3.02	108.19	103.45
8	L5	4228	OMG	C2-N1-C6	-3.01	119.64	125.11
8	L5	2424	OMG	C2-N1-C6	-2.99	119.68	125.11
49	S2	1639	G7M	C2-N1-C6	-2.99	119.68	125.11
49	S2	1851	MA6	N3-C4-N9	2.99	132.26	127.17
49	S2	668	A2M	C5-N7-C8	2.99	108.14	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1678	A2M	C5-N7-C8	2.98	108.14	103.45
8	L5	1625	OMG	C2-N1-C6	-2.98	119.71	125.11
8	L5	2401	A2M	N3-C4-N9	2.98	132.23	127.17
49	S2	1850	MA6	N9-C8-N7	-2.97	109.72	113.94
8	L5	1871	A2M	C2'-C1'-N9	-2.97	108.87	113.75
8	L5	3724	A2M	C5-N7-C8	2.97	108.11	103.45
8	L5	2787	A2M	N3-C4-N9	2.97	132.21	127.17
49	S2	159	A2M	C5-N7-C8	2.96	108.11	103.45
8	L5	4620	OMU	O4-C4-C5	-2.96	120.05	125.16
49	S2	1442	OMU	O4-C4-C5	-2.96	120.05	125.16
49	S2	428	OMU	O4-C4-C5	-2.95	120.08	125.16
8	L5	4494	OMG	N9-C4-N3	2.94	131.84	125.95
49	S2	644	OMG	C2-N1-C6	-2.94	119.78	125.11
8	L5	1871	A2M	N3-C4-N9	2.94	132.16	127.17
8	L5	3718	A2M	N3-C4-N9	2.93	132.15	127.17
8	L5	1316	OMG	C2-N1-C6	-2.93	119.80	125.11
8	L5	4618	OMG	C2-N1-C6	-2.93	119.80	125.11
8	L5	1524	A2M	C2-N3-C4	2.92	118.97	111.83
8	L5	1326	A2M	C5-N7-C8	2.92	108.04	103.45
8	L5	3724	A2M	N3-C4-N9	2.92	132.13	127.17
49	S2	1288	OMU	O4-C4-C5	-2.92	120.13	125.16
8	L5	2815	A2M	C5-N7-C8	2.92	108.04	103.45
10	L8	75	OMG	C2-N1-C6	-2.92	119.82	125.11
8	L5	2876	OMG	C2-N1-C6	-2.91	119.83	125.11
8	L5	1522	OMG	C2-N1-C6	-2.91	119.83	125.11
49	S2	1832	6MZ	C4-C5-N7	-2.90	107.27	110.58
8	L5	4494	OMG	C2-N1-C6	-2.89	119.88	125.11
49	S2	683	OMG	C2-N1-C6	-2.88	119.89	125.11
8	L5	4499	OMG	C2-N1-C6	-2.88	119.89	125.11
8	L5	2424	OMG	N9-C4-N3	2.87	131.70	125.95
8	L5	2876	OMG	N9-C4-N3	2.87	131.70	125.95
8	L5	3744	OMG	C2-N1-C6	-2.87	119.91	125.11
49	S2	644	OMG	N9-C4-N3	2.87	131.69	125.95
8	L5	3792	OMG	N9-C4-N3	2.86	131.67	125.95
8	L5	3718	A2M	C5-N7-C8	2.86	107.94	103.45
8	L5	1316	OMG	N9-C4-N3	2.85	131.65	125.95
8	L5	4370	OMG	C2-N1-C6	-2.85	119.95	125.11
8	L5	4499	OMG	N9-C4-N3	2.85	131.65	125.95
8	L5	3792	OMG	C2-N1-C6	-2.84	119.96	125.11
8	L5	2364	OMG	C2-N1-C6	-2.84	119.97	125.11
8	L5	3723	A2M	N3-C4-N9	2.83	131.98	127.17
8	L5	4623	OMG	C2-N1-C6	-2.83	119.98	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	2787	A2M	C5-N7-C8	2.82	107.89	103.45
8	L5	1625	OMG	N9-C4-N3	2.82	131.59	125.95
8	L5	2363	A2M	C5-N7-C8	2.82	107.88	103.45
8	L5	3925	OMU	O4-C4-C5	-2.82	120.30	125.16
8	L5	3825	A2M	C5-N7-C8	2.81	107.87	103.45
8	L5	3729	PSU	C6-C5-C4	2.80	120.06	118.17
8	L5	2401	A2M	C5-N7-C8	2.80	107.85	103.45
8	L5	2424	OMG	C5-C6-N1	2.79	120.36	113.25
49	S2	1031	A2M	C5-N7-C8	2.79	107.84	103.45
49	S2	1383	A2M	N3-C4-N9	2.79	131.91	127.17
8	L5	398	A2M	C5-N7-C8	2.79	107.83	103.45
8	L5	3723	A2M	C5-N7-C8	2.78	107.82	103.45
49	S2	576	A2M	C5-N7-C8	2.78	107.81	103.45
10	L8	14	OMU	O4-C4-C5	-2.77	120.38	125.16
49	S2	1383	A2M	C5-N7-C8	2.77	107.80	103.45
8	L5	4353	PSU	C6-C5-C4	2.77	120.04	118.17
49	S2	1248	B8N	O4-C4-C5	-2.76	117.81	122.58
49	S2	1328	OMG	C2-N1-C6	-2.75	120.12	125.11
49	S2	1326	UY1	C6-C5-C4	2.74	120.03	118.17
8	L5	4637	OMG	C5-C6-N1	2.74	120.24	113.25
49	S2	1326	UY1	C6-N1-C2	-2.74	120.15	122.69
8	L5	4370	OMG	N9-C4-N3	2.74	131.43	125.95
49	S2	1851	MA6	C5-N7-C8	2.74	107.75	103.45
49	S2	27	A2M	C5-N7-C8	2.73	107.74	103.45
49	S2	1337	4AC	C5-C4-N3	-2.73	118.33	122.60
49	S2	27	A2M	N3-C4-N9	2.73	131.80	127.17
8	L5	3627	OMG	C2-N1-C6	-2.72	120.18	125.11
49	S2	644	OMG	C5-C6-N1	2.71	120.16	113.25
10	L8	75	OMG	N9-C4-N3	2.71	131.37	125.95
49	S2	668	A2M	N3-C4-N9	2.71	131.77	127.17
8	L5	3718	A2M	C2'-C1'-N9	-2.71	109.30	113.75
49	S2	1832	6MZ	N3-C4-N9	2.70	131.76	127.17
8	L5	4494	OMG	C5-C6-N1	2.69	120.10	113.25
49	S2	1851	MA6	C4-N9-C8	2.69	108.56	105.74
8	L5	1871	A2M	C5-N7-C8	2.67	107.65	103.45
8	L5	1625	OMG	C5-C6-N1	2.67	120.04	113.25
8	L5	3729	PSU	O2-C2-N1	-2.66	120.04	122.79
8	L5	2876	OMG	C5-C6-N1	2.66	120.02	113.25
49	S2	601	OMG	C5-C6-N1	2.65	120.00	113.25
49	S2	1639	G7M	CN7-N7-C5	2.65	130.10	126.80
8	L5	1522	OMG	C5-C6-N1	2.64	119.98	113.25
8	L5	4499	OMG	C5-C6-N1	2.64	119.96	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	3792	OMG	C5-C6-N1	2.64	119.96	113.25
8	L5	4370	OMG	C5-C6-N1	2.63	119.95	113.25
49	S2	683	OMG	C5-C6-N1	2.61	119.90	113.25
49	S2	1328	OMG	N9-C4-N3	2.61	131.17	125.95
8	L5	4228	OMG	C5-C6-N1	2.61	119.90	113.25
8	L5	1316	OMG	C5-C6-N1	2.60	119.88	113.25
8	L5	4618	OMG	C5-C6-N1	2.60	119.87	113.25
10	L8	75	OMG	C5-C6-N1	2.60	119.87	113.25
8	L5	3744	OMG	C5-C6-N1	2.59	119.86	113.25
8	L5	4623	OMG	C5-C6-N1	2.59	119.84	113.25
8	L5	1683	PSU	O2-C2-N1	-2.59	120.12	122.79
49	S2	1328	OMG	C5-C6-N1	2.57	119.79	113.25
8	L5	3760	A2M	C5-N7-C8	2.57	107.49	103.45
8	L5	4637	OMG	O6-C6-C5	-2.56	119.77	126.53
8	L5	1782	PSU	O2-C2-N1	-2.56	120.15	122.79
8	L5	3758	PSU	O2-C2-N1	-2.56	120.15	122.79
8	L5	2424	OMG	O6-C6-C5	-2.55	119.81	126.53
8	L5	1522	OMG	N9-C4-N3	2.54	131.02	125.95
8	L5	3627	OMG	C5-C6-N1	2.54	119.71	113.25
49	S2	683	OMG	C8-N7-C5	2.53	108.78	104.26
8	L5	2364	OMG	N9-C4-N3	2.53	131.02	125.95
8	L5	3760	A2M	N3-C4-N9	2.53	131.46	127.17
8	L5	2364	OMG	C5-C6-N1	2.53	119.68	113.25
8	L5	1316	OMG	C8-N7-C5	2.52	108.76	104.26
49	S2	1842	4AC	N4-C4-N3	2.52	117.96	113.87
8	L5	4494	OMG	O6-C6-C5	-2.52	119.89	126.53
49	S2	1678	A2M	C4-C5-N7	-2.50	107.72	110.58
10	L8	75	OMG	O6-C6-C5	-2.49	119.96	126.53
8	L5	4228	OMG	N2-C2-N1	2.49	122.01	116.76
10	L8	55	PSU	O2-C2-N1	-2.49	120.22	122.79
49	S2	1248	B8N	C32-C31-N3	2.48	116.49	112.16
49	S2	644	OMG	C8-N7-C5	2.48	108.68	104.26
8	L5	2876	OMG	O6-C6-C5	-2.48	119.99	126.53
8	L5	4618	OMG	N9-C4-N3	2.47	130.89	125.95
8	L5	1625	OMG	O6-C6-C5	-2.47	120.02	126.53
8	L5	3744	OMG	N9-C4-N3	2.46	130.88	125.95
8	L5	4618	OMG	O6-C6-C5	-2.46	120.04	126.53
8	L5	4228	OMG	O6-C6-C5	-2.46	120.04	126.53
8	L5	4353	PSU	O2-C2-N1	-2.45	120.26	122.79
8	L5	2364	OMG	O6-C6-C5	-2.45	120.07	126.53
8	L5	4590	A2M	C4-C5-N7	-2.44	107.79	110.58
49	S2	576	A2M	C2'-C1'-N9	-2.44	109.73	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	4499	OMG	O6-C6-C5	-2.44	120.09	126.53
8	L5	4228	OMG	C8-N7-C5	2.43	108.59	104.26
8	L5	3734	PSU	O2-C2-N1	-2.43	120.28	122.79
8	L5	3744	OMG	O6-C6-C5	-2.43	120.11	126.53
49	S2	683	OMG	O6-C6-C5	-2.43	120.12	126.53
8	L5	3724	A2M	C4-C5-N7	-2.42	107.81	110.58
49	S2	1248	B8N	O2-C2-N1	-2.42	116.21	121.21
49	S2	683	OMG	N9-C4-N3	2.41	130.78	125.95
49	S2	1326	UY1	O2-C2-N1	-2.41	120.30	122.79
8	L5	1522	OMG	O6-C6-C5	-2.40	120.19	126.53
8	L5	3718	A2M	C4-C5-N7	-2.39	107.84	110.58
8	L5	3744	OMG	C8-N7-C5	2.39	108.52	104.26
49	S2	1850	MA6	C6-C5-N7	-2.39	129.62	133.43
8	L5	3627	OMG	O6-C6-C5	-2.39	120.23	126.53
49	S2	1383	A2M	C4-C5-N7	-2.39	107.85	110.58
8	L5	1316	OMG	O6-C6-C5	-2.38	120.25	126.53
8	L5	3734	PSU	C6-C5-C4	2.38	119.78	118.17
49	S2	644	OMG	O6-C6-C5	-2.38	120.26	126.53
49	S2	668	A2M	C4-N9-C8	2.38	108.23	105.74
8	L5	3792	OMG	O6-C6-C5	-2.37	120.27	126.53
8	L5	4623	OMG	N9-C4-N3	2.37	130.70	125.95
49	S2	668	A2M	C4-C5-N7	-2.36	107.88	110.58
8	L5	2364	OMG	C8-N7-C5	2.36	108.47	104.26
8	L5	2876	OMG	C8-N7-C5	2.35	108.44	104.26
49	S2	1832	6MZ	C4-N9-C8	2.34	108.20	105.74
8	L5	4623	OMG	C8-N7-C5	2.34	108.42	104.26
49	S2	1328	OMG	C8-N7-C5	2.34	108.42	104.26
8	L5	4620	OMU	O2-C2-N1	-2.33	119.76	122.80
49	S2	576	A2M	C6-C5-C4	2.33	120.36	117.18
8	L5	4370	OMG	O6-C6-C5	-2.33	120.38	126.53
8	L5	3627	OMG	C8-N7-C5	2.33	108.41	104.26
8	L5	3792	OMG	C8-N7-C5	2.33	108.41	104.26
49	S2	159	A2M	C4-C5-N7	-2.32	107.92	110.58
8	L5	3825	A2M	C4-C5-N7	-2.32	107.93	110.58
8	L5	1524	A2M	C5-N7-C8	2.32	107.09	103.45
8	L5	3718	A2M	C6-C5-C4	2.31	120.33	117.18
49	S2	1328	OMG	O6-C6-C5	-2.30	120.46	126.53
8	L5	1522	OMG	C8-N7-C5	2.30	108.36	104.26
8	L5	3627	OMG	N2-C2-N1	2.30	121.61	116.76
8	L5	4370	OMG	C8-N7-C5	2.29	108.34	104.26
8	L5	4623	OMG	O6-C6-C5	-2.29	120.49	126.53
8	L5	2815	A2M	C4-C5-N7	-2.29	107.96	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	2363	A2M	C4-C5-N7	-2.29	107.97	110.58
8	L5	1683	PSU	C6-C5-C4	2.29	119.72	118.17
8	L5	4637	OMG	C8-N7-C5	2.29	108.33	104.26
8	L5	4494	OMG	C8-N7-C5	2.28	108.32	104.26
49	S2	1678	A2M	C6-C5-C4	2.28	120.29	117.18
8	L5	3627	OMG	N9-C4-N3	2.27	130.49	125.95
49	S2	1678	A2M	C2'-C1'-N9	2.27	117.48	113.75
49	S2	1337	4AC	CM7-C7-N4	2.26	118.91	115.27
49	S2	601	OMG	O6-C6-C5	-2.26	120.58	126.53
49	S2	1842	4AC	C5-C4-N3	-2.26	119.07	122.60
49	S2	1639	G7M	N9-C8-N7	-2.25	107.01	112.48
8	L5	3744	OMG	N2-C2-N1	2.25	121.51	116.76
49	S2	27	A2M	C4-C5-N7	-2.25	108.01	110.58
49	S2	1383	A2M	C5-C4-N9	2.25	108.26	105.81
8	L5	1625	OMG	C8-N7-C5	2.24	108.26	104.26
8	L5	2787	A2M	C4-C5-N7	-2.24	108.02	110.58
49	S2	159	A2M	C6-C5-C4	2.24	120.23	117.18
10	L8	75	OMG	C8-N7-C5	2.23	108.23	104.26
10	L8	14	OMU	C6-N1-C2	-2.23	118.29	121.00
8	L5	2401	A2M	C6-C5-C4	2.22	120.21	117.18
49	S2	1031	A2M	C4-C5-N7	-2.22	108.04	110.58
8	L5	3723	A2M	C4-C5-N7	-2.22	108.04	110.58
49	S2	1842	4AC	C6-C5-C4	2.22	119.67	117.00
8	L5	1326	A2M	C4-C5-N7	-2.20	108.06	110.58
8	L5	3718	A2M	C5-C4-N9	2.20	108.21	105.81
49	S2	1842	4AC	CM7-C7-N4	2.20	118.81	115.27
8	L5	2401	A2M	C4-C5-N7	-2.17	108.10	110.58
8	L5	1524	A2M	C5-C4-N9	2.17	108.17	105.81
49	S2	1639	G7M	CN7-N7-C8	-2.16	121.52	124.79
49	S2	1288	OMU	O2-C2-N1	-2.16	119.99	122.80
8	L5	398	A2M	C4-C5-N7	-2.15	108.12	110.58
8	L5	1326	A2M	C4-N9-C8	2.15	108.00	105.74
49	S2	1442	OMU	O2-C2-N1	-2.15	120.00	122.80
8	L5	2787	A2M	C5-C4-N9	2.14	108.15	105.81
8	L5	2364	OMG	N2-C2-N1	2.14	121.28	116.76
8	L5	4499	OMG	C8-N7-C5	2.14	108.08	104.26
8	L5	4618	OMG	C8-N7-C5	2.14	108.07	104.26
49	S2	1337	4AC	C6-C5-C4	2.14	119.58	117.00
49	S2	668	A2M	C3'-C2'-C1'	2.13	106.89	102.81
49	S2	1248	B8N	C31-N3-C4	-2.13	114.17	117.18
8	L5	3825	A2M	C5-C4-N9	2.13	108.13	105.81
8	L5	2815	A2M	C6-C5-C4	2.13	120.08	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	3825	A2M	C6-C5-C4	2.12	120.08	117.18
49	S2	27	A2M	C5-C4-N9	2.12	108.12	105.81
10	L8	14	OMU	O2-C2-N3	-2.11	117.59	121.49
49	S2	1248	B8N	O36-C34-O35	-2.11	119.30	124.08
49	S2	576	A2M	C4-C5-N7	-2.10	108.18	110.58
8	L5	3724	A2M	C5-C4-N9	2.10	108.10	105.81
49	S2	159	A2M	C5-C4-N9	2.10	108.10	105.81
49	S2	428	OMU	O2-C2-N1	-2.10	120.07	122.80
8	L5	2815	A2M	C5-C4-N9	2.10	108.10	105.81
49	S2	1832	6MZ	C5-C4-N9	2.10	108.10	105.81
8	L5	3724	A2M	C4-N9-C8	2.10	107.94	105.74
8	L5	2787	A2M	C6-C5-C4	2.09	120.04	117.18
49	S2	683	OMG	C2'-C1'-N9	-2.08	110.29	114.24
49	S2	1678	A2M	C5-C4-N9	2.08	108.07	105.81
8	L5	2363	A2M	C5-C4-N9	2.07	108.07	105.81
8	L5	3723	A2M	C6-C5-C4	2.07	120.01	117.18
8	L5	1524	A2M	N3-C4-N9	2.07	130.69	127.17
8	L5	4590	A2M	C5-C4-N9	2.07	108.07	105.81
8	L5	2424	OMG	C8-N7-C5	2.07	107.94	104.26
49	S2	1031	A2M	C6-C5-C4	2.07	120.00	117.18
8	L5	398	A2M	C6-C5-C4	2.06	120.00	117.18
8	L5	4228	OMG	N9-C4-N3	2.06	130.08	125.95
8	L5	3724	A2M	C6-C5-C4	2.06	119.99	117.18
49	S2	1248	B8N	C1'-C5-C4	2.06	120.73	117.61
8	L5	4618	OMG	N2-C2-N1	2.06	121.10	116.76
8	L5	4590	A2M	C4-N9-C8	2.06	107.90	105.74
8	L5	3758	PSU	C6-C5-C4	2.06	119.56	118.17
49	S2	576	A2M	C4-N9-C8	2.06	107.90	105.74
8	L5	3760	A2M	C4-N9-C8	2.05	107.89	105.74
49	S2	1850	MA6	C5-N7-C8	2.05	106.68	103.45
8	L5	3925	OMU	O2-C2-N1	-2.05	120.12	122.80
8	L5	4590	A2M	C6-C5-C4	2.05	119.97	117.18
49	S2	1678	A2M	C4-N9-C8	2.05	107.89	105.74
8	L5	4623	OMG	N2-C2-N1	2.03	121.05	116.76
8	L5	2401	A2M	C5-C4-N9	2.03	108.03	105.81
8	L5	1871	A2M	C4-N9-C8	2.03	107.87	105.74
8	L5	4228	OMG	C4-C5-N7	-2.03	107.45	110.67
49	S2	159	A2M	C2'-C1'-N9	-2.02	110.42	113.75
8	L5	4494	OMG	N1-C2-N3	-2.02	119.63	123.32
8	L5	3627	OMG	C2'-C1'-N9	-2.01	110.42	114.24
8	L5	1326	A2M	C6-C5-C4	2.01	119.93	117.18
8	L5	1871	A2M	C4-C5-N7	-2.01	108.28	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	398	A2M	C5-C4-N9	2.01	108.00	105.81
8	L5	3723	A2M	C5-C4-N9	2.01	108.00	105.81
49	S2	683	OMG	C8-N9-C4	2.01	109.78	106.03
8	L5	1871	A2M	C6-C5-C4	2.00	119.92	117.18
8	L5	2363	A2M	C6-C5-C4	2.00	119.91	117.18
49	S2	683	OMG	C4-C5-N7	-2.00	107.50	110.67
49	S2	668	A2M	C5-C4-N9	2.00	107.99	105.81

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L8	14	OMU	O4'-C1'-N1-C2
10	L8	14	OMU	O4'-C1'-N1-C6
10	L8	14	OMU	C1'-C2'-O2'-CM2
10	L8	55	PSU	O4'-C4'-C5'-O5'
8	L5	1316	OMG	C1'-C2'-O2'-CM2
8	L5	1326	A2M	C1'-C2'-O2'-CM'
8	L5	1625	OMG	O4'-C4'-C5'-O5'
8	L5	2351	OMC	C1'-C2'-O2'-CM2
8	L5	2401	A2M	C3'-C4'-C5'-O5'
8	L5	2424	OMG	O4'-C4'-C5'-O5'
8	L5	2861	OMC	C1'-C2'-O2'-CM2
8	L5	2876	OMG	O4'-C4'-C5'-O5'
8	L5	3701	OMC	C2'-C1'-N1-C2
8	L5	3701	OMC	C2'-C1'-N1-C6
8	L5	3723	A2M	C1'-C2'-O2'-CM'
8	L5	3724	A2M	C1'-C2'-O2'-CM'
8	L5	3841	OMC	C1'-C2'-O2'-CM2
8	L5	3925	OMU	C1'-C2'-O2'-CM2
8	L5	4590	A2M	C4'-C5'-O5'-P
8	L5	4620	OMU	O4'-C4'-C5'-O5'
49	S2	27	A2M	C1'-C2'-O2'-CM'
49	S2	601	OMG	C1'-C2'-O2'-CM2
49	S2	601	OMG	O4'-C1'-N9-C4
49	S2	644	OMG	O4'-C4'-C5'-O5'
49	S2	644	OMG	C3'-C4'-C5'-O5'
49	S2	644	OMG	C1'-C2'-O2'-CM2
49	S2	683	OMG	O4'-C4'-C5'-O5'
49	S2	1248	B8N	C2'-C1'-C5-C4
49	S2	1248	B8N	C32-C31-N3-C2
49	S2	1248	B8N	C32-C31-N3-C4

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Mol	Chain	Res	Type	Atoms
49	S2	1288	OMU	O4'-C4'-C5'-O5'
49	S2	1383	A2M	C1'-C2'-O2'-CM'
49	S2	1442	OMU	C1'-C2'-O2'-CM2
49	S2	1678	A2M	C1'-C2'-O2'-CM'
49	S2	1832	6MZ	N1-C6-N6-C9
49	S2	1832	6MZ	O4'-C4'-C5'-O5'
49	S2	1851	MA6	O4'-C4'-C5'-O5'
10	L8	55	PSU	C3'-C4'-C5'-O5'
8	L5	2424	OMG	C3'-C4'-C5'-O5'
8	L5	3627	OMG	O4'-C4'-C5'-O5'
8	L5	4623	OMG	O4'-C4'-C5'-O5'
8	L5	4623	OMG	C3'-C4'-C5'-O5'
49	S2	159	A2M	O4'-C4'-C5'-O5'
49	S2	159	A2M	C3'-C4'-C5'-O5'
49	S2	601	OMG	O4'-C1'-N9-C8
10	L8	14	OMU	C3'-C4'-C5'-O5'
10	L8	14	OMU	O4'-C4'-C5'-O5'
8	L5	398	A2M	C3'-C4'-C5'-O5'
8	L5	1625	OMG	C3'-C4'-C5'-O5'
8	L5	2364	OMG	O4'-C4'-C5'-O5'
8	L5	2401	A2M	O4'-C4'-C5'-O5'
8	L5	2422	OMC	C3'-C4'-C5'-O5'
8	L5	3729	PSU	O4'-C4'-C5'-O5'
49	S2	428	OMU	C3'-C4'-C5'-O5'
49	S2	428	OMU	O4'-C4'-C5'-O5'
49	S2	601	OMG	O4'-C4'-C5'-O5'
49	S2	1832	6MZ	C3'-C4'-C5'-O5'
8	L5	2876	OMG	C3'-C4'-C5'-O5'
49	S2	668	A2M	C3'-C4'-C5'-O5'
49	S2	683	OMG	C3'-C4'-C5'-O5'
49	S2	1288	OMU	C3'-C4'-C5'-O5'
49	S2	1851	MA6	C3'-C4'-C5'-O5'
8	L5	2351	OMC	O4'-C4'-C5'-O5'
8	L5	3627	OMG	C3'-C4'-C5'-O5'
8	L5	4620	OMU	C3'-C4'-C5'-O5'
49	S2	601	OMG	C3'-C4'-C5'-O5'
49	S2	668	A2M	O4'-C4'-C5'-O5'
8	L5	398	A2M	O4'-C4'-C5'-O5'
8	L5	2422	OMC	O4'-C4'-C5'-O5'
8	L5	3734	PSU	O4'-C4'-C5'-O5'
49	S2	1850	MA6	C5-C6-N6-C10
49	S2	1851	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
49	S2	1703	OMC	O4'-C4'-C5'-O5'
8	L5	2787	A2M	C2'-C1'-N9-C8
49	S2	428	OMU	C2'-C1'-N1-C6
8	L5	2804	OMC	C1'-C2'-O2'-CM2
8	L5	2351	OMC	C3'-C4'-C5'-O5'
49	S2	576	A2M	C3'-C4'-C5'-O5'
49	S2	644	OMG	C4'-C5'-O5'-P
49	S2	428	OMU	O4'-C1'-N1-C6
49	S2	1832	6MZ	C5-C6-N6-C9
8	L5	3729	PSU	C3'-C4'-C5'-O5'
49	S2	576	A2M	C4'-C5'-O5'-P
8	L5	1524	A2M	C3'-C2'-O2'-CM'
49	S2	1248	B8N	O4'-C1'-C5-C4
8	L5	2787	A2M	C2'-C1'-N9-C4
8	L5	2364	OMG	C3'-C4'-C5'-O5'
49	S2	1248	B8N	O4'-C4'-C5'-O5'
8	L5	3701	OMC	O4'-C1'-N1-C6
49	S2	428	OMU	O4'-C1'-N1-C2
8	L5	3734	PSU	C3'-C4'-C5'-O5'
8	L5	4590	A2M	C3'-C4'-C5'-O5'
49	S2	428	OMU	C2'-C1'-N1-C2
49	S2	1639	G7M	C3'-C4'-C5'-O5'
49	S2	668	A2M	C2'-C1'-N9-C8
8	L5	3701	OMC	O4'-C1'-N1-C2
8	L5	2351	OMC	C2'-C1'-N1-C2
8	L5	2787	A2M	O4'-C1'-N9-C8
8	L5	3701	OMC	C4'-C5'-O5'-P
49	S2	576	A2M	O4'-C4'-C5'-O5'
49	S2	1703	OMC	C3'-C4'-C5'-O5'
49	S2	1248	B8N	N3-C31-C32-C33
8	L5	2351	OMC	C4'-C5'-O5'-P
49	S2	1248	B8N	N34-C33-C34-O35
49	S2	1248	B8N	N34-C33-C34-O36

There are no ring outliers.

42 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	601	OMG	2	0
8	L5	2363	A2M	1	0
8	L5	3627	OMG	1	0
49	S2	1678	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	644	OMG	2	0
49	S2	1842	4AC	1	0
8	L5	1316	OMG	1	0
8	L5	3718	A2M	3	0
8	L5	1871	A2M	1	0
8	L5	2815	A2M	1	0
8	L5	2861	OMC	1	0
49	S2	1383	A2M	1	0
8	L5	3744	OMG	1	0
10	L8	55	PSU	3	0
49	S2	428	OMU	1	0
49	S2	174	OMC	1	0
8	L5	2876	OMG	2	0
49	S2	1832	6MZ	1	0
8	L5	1625	OMG	1	0
8	L5	398	A2M	1	0
8	L5	1524	A2M	1	0
8	L5	2424	OMG	1	0
8	L5	3925	OMU	2	0
8	L5	4228	OMG	1	0
49	S2	1850	MA6	6	0
8	L5	4536	OMC	3	0
8	L5	1326	A2M	3	0
8	L5	1340	OMC	2	0
8	L5	3701	OMC	1	0
8	L5	3724	A2M	1	0
8	L5	3841	OMC	1	0
49	S2	27	A2M	2	0
49	S2	576	A2M	3	0
8	L5	3760	A2M	1	0
8	L5	4623	OMG	1	0
10	L8	75	OMG	2	0
49	S2	1337	4AC	5	0
49	S2	1442	OMU	1	0
8	L5	2804	OMC	3	0
8	L5	3723	A2M	2	0
49	S2	1288	OMU	1	0
10	L8	14	OMU	4	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 340 ligands modelled in this entry, 337 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	SPD	L5	5286	-	9,9,9	0.43	0	8,8,8	0.39	0
89	HYG	S2	1901	84	36,39,39	2.51	10 (27%)	44,60,60	1.22	5 (11%)
87	PUT	L5	5287	-	5,5,5	0.25	0	4,4,4	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPD	L5	5286	-	-	0/7/7/7	-
89	HYG	S2	1901	84	-	4/12/87/87	0/4/4/4
87	PUT	L5	5287	-	-	0/3/3/3	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	S2	1901	HYG	O29-C12	8.26	1.57	1.43
89	S2	1901	HYG	O22-C17	6.25	1.53	1.43
89	S2	1901	HYG	O14-C13	5.86	1.56	1.41
89	S2	1901	HYG	C17-C12	-3.78	1.45	1.53
89	S2	1901	HYG	C16-C15	3.37	1.60	1.53
89	S2	1901	HYG	C25-C24	-3.05	1.48	1.53
89	S2	1901	HYG	O28-C23	2.86	1.43	1.40
89	S2	1901	HYG	C16-C17	-2.64	1.45	1.52
89	S2	1901	HYG	O18-C13	-2.34	1.35	1.41
89	S2	1901	HYG	C13-C12	-2.12	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	S2	1901	HYG	O14-C13-C12	-3.57	102.55	109.49
89	S2	1901	HYG	O22-C17-C16	3.36	119.25	111.22
89	S2	1901	HYG	O29-C23-O22	2.48	108.71	105.90
89	S2	1901	HYG	O11-C5-C4	-2.33	104.56	109.40
89	S2	1901	HYG	C23-O28-C27	-2.05	108.08	112.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

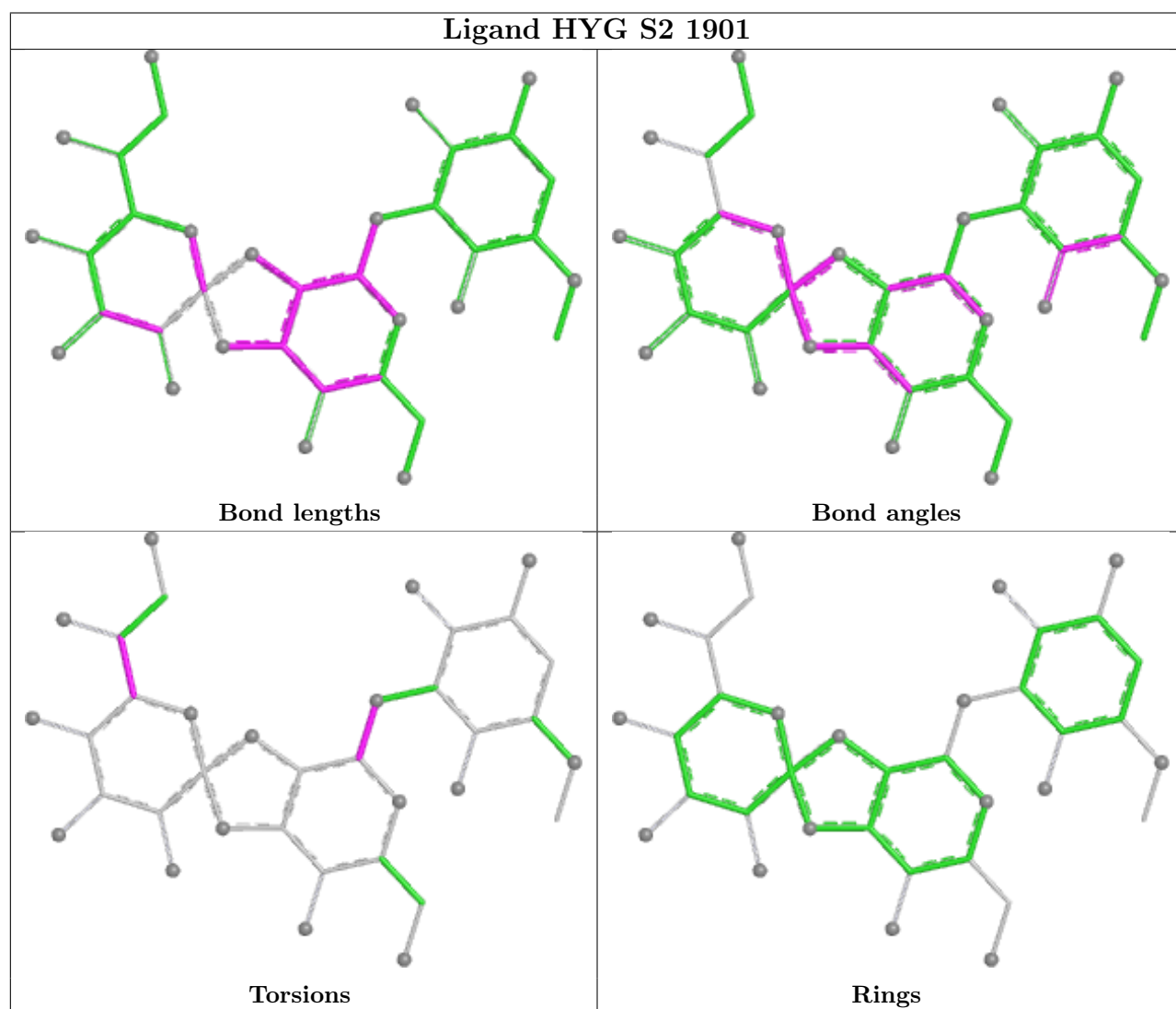
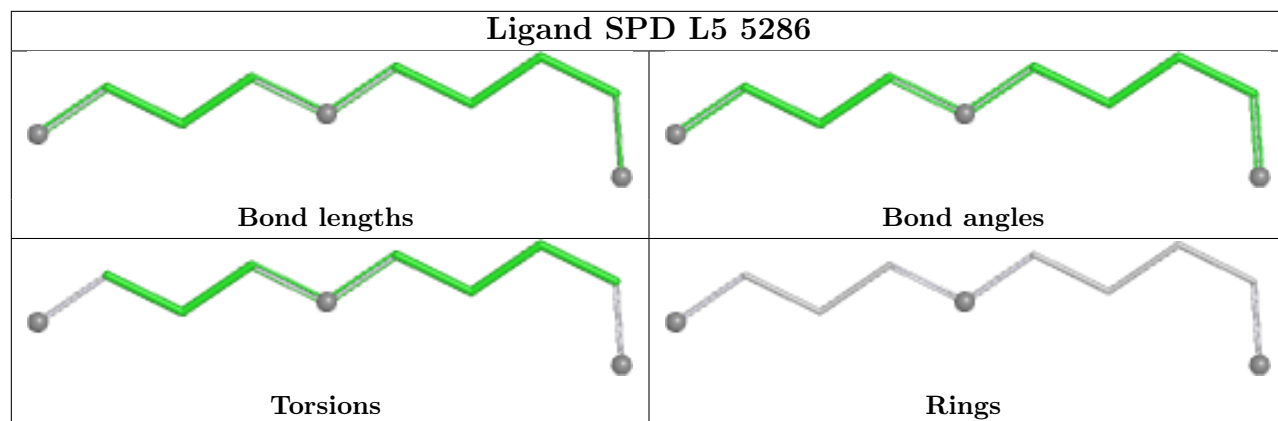
Mol	Chain	Res	Type	Atoms
89	S2	1901	HYG	C26-C27-C33-C34
89	S2	1901	HYG	O28-C27-C33-C34
89	S2	1901	HYG	O14-C13-O18-C6
89	S2	1901	HYG	C12-C13-O18-C6

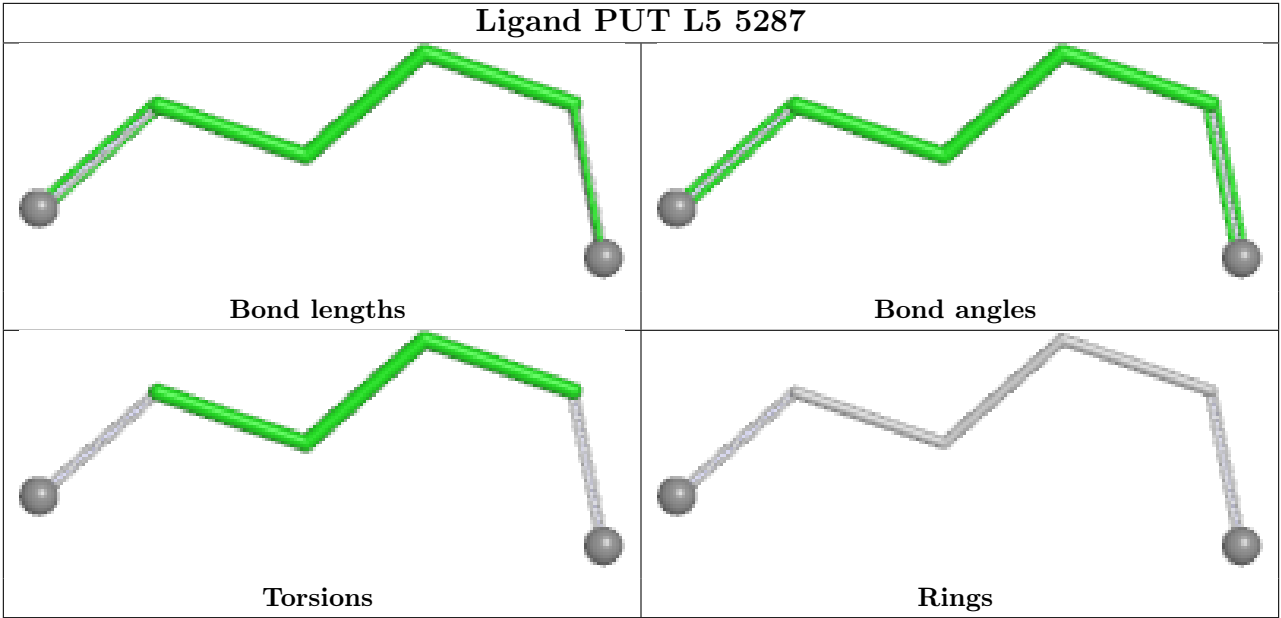
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5286	SPD	2	0
87	L5	5287	PUT	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	S2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1832:6MZ	O3'	1833:C	P	4.54
1	S2	1248:B8N	O3'	1249:C	P	3.93

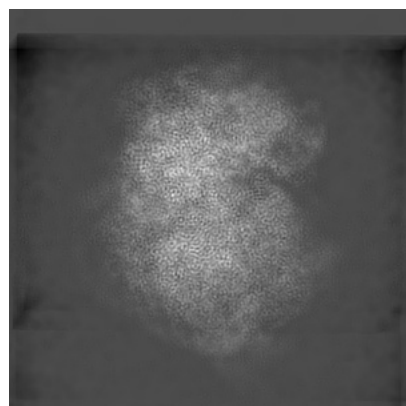
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52565. These allow visual inspection of the internal detail of the map and identification of artifacts.

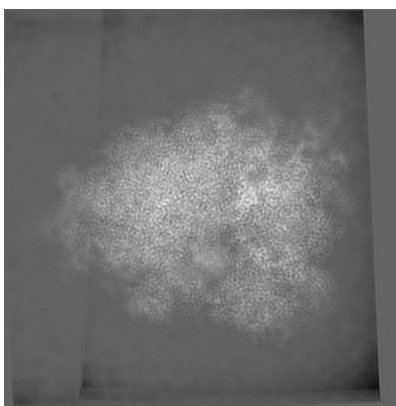
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

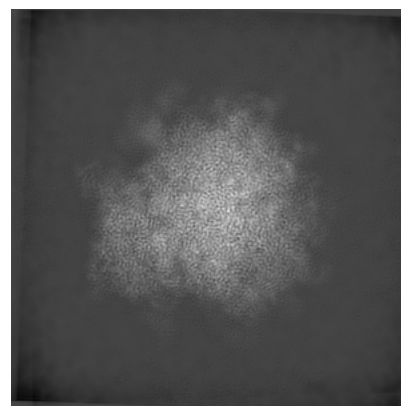
6.1.1 Primary map



X

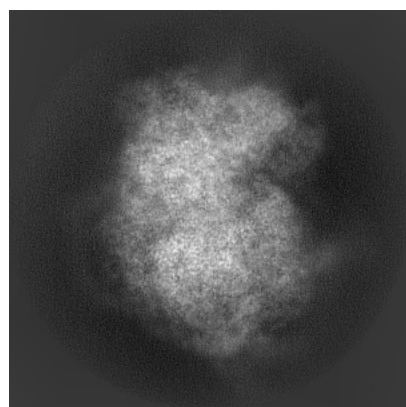


Y

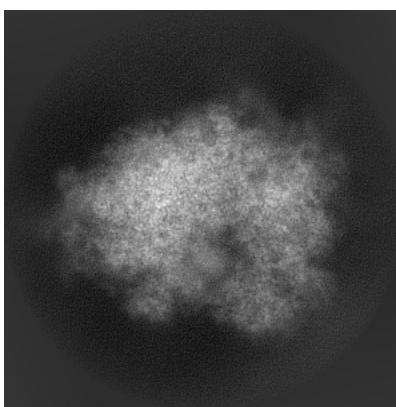


Z

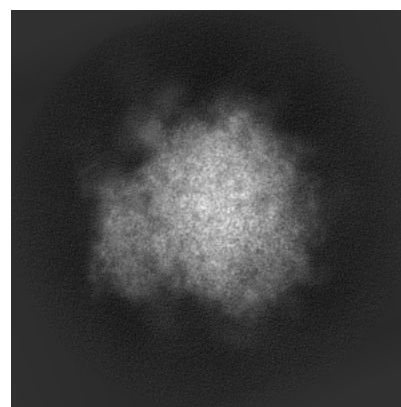
6.1.2 Raw map



X



Y

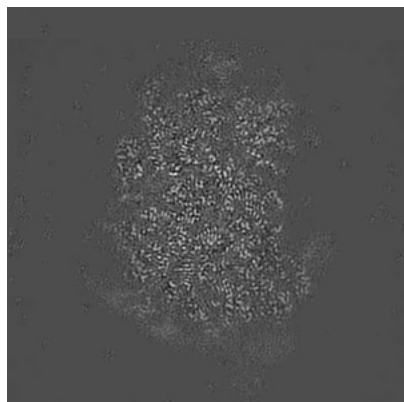


Z

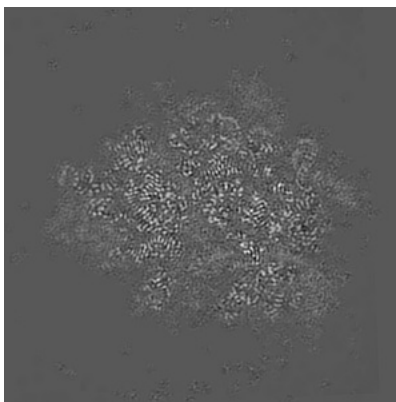
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

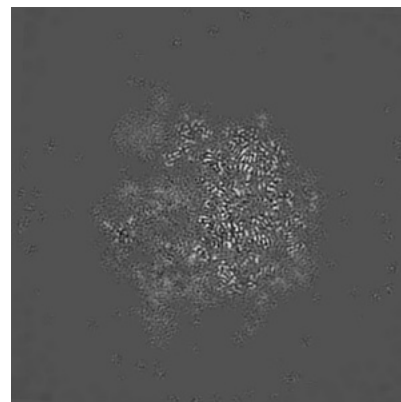
6.2.1 Primary map



X Index: 240

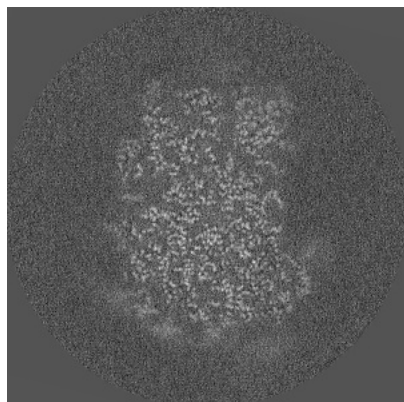


Y Index: 240

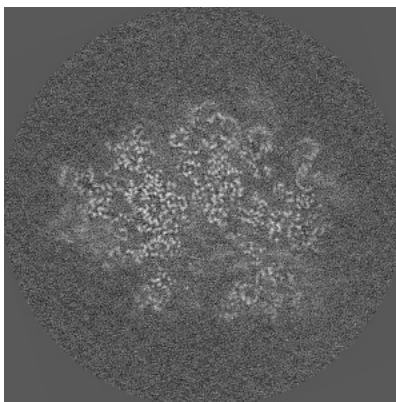


Z Index: 240

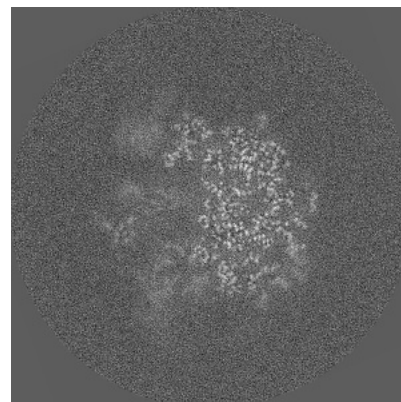
6.2.2 Raw map



X Index: 240



Y Index: 240

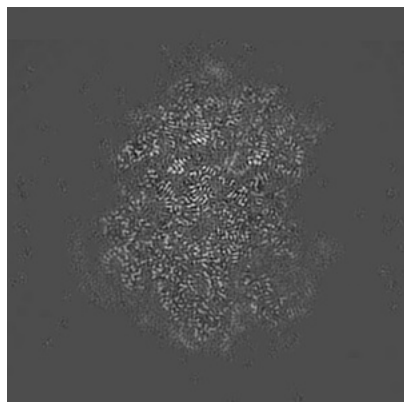


Z Index: 240

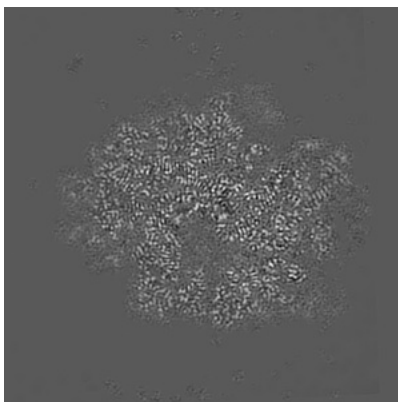
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

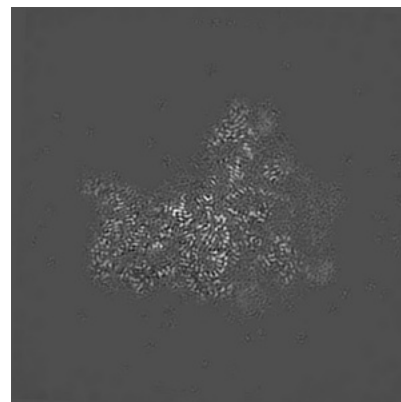
6.3.1 Primary map



X Index: 261

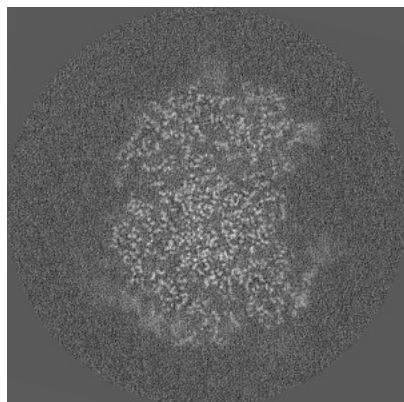


Y Index: 220

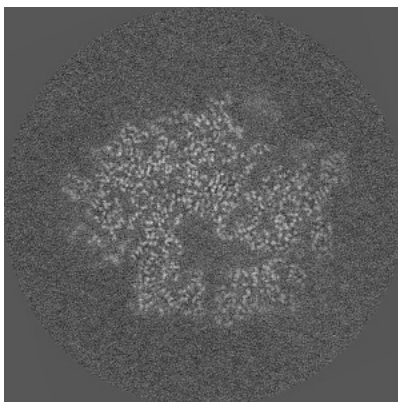


Z Index: 288

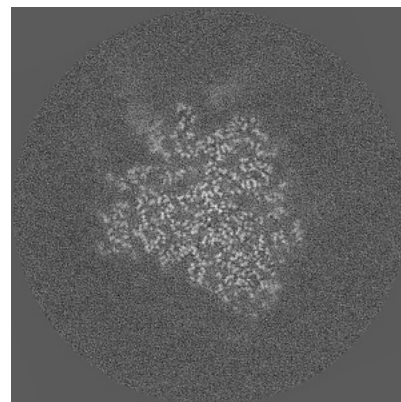
6.3.2 Raw map



X Index: 254



Y Index: 221

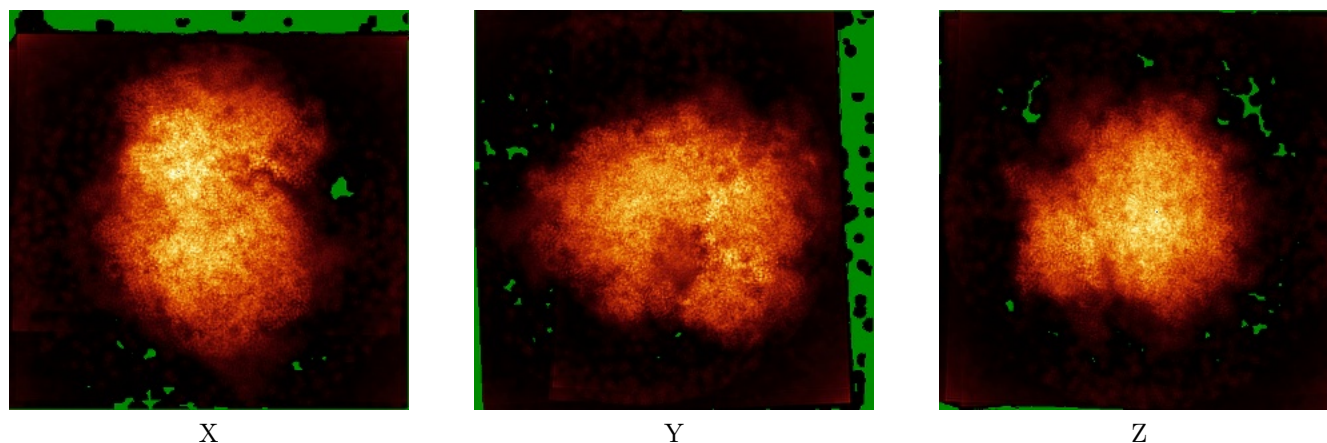


Z Index: 197

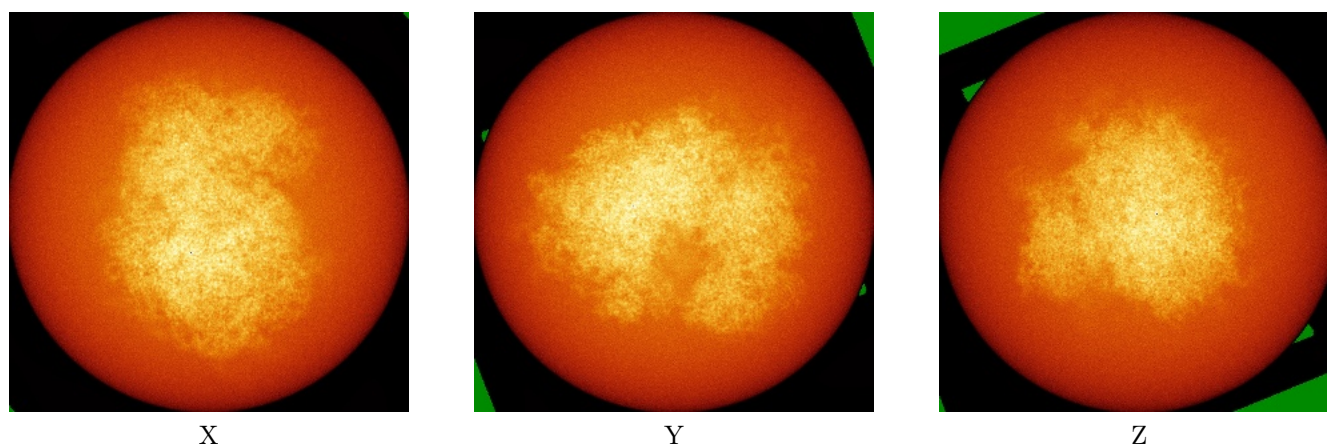
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

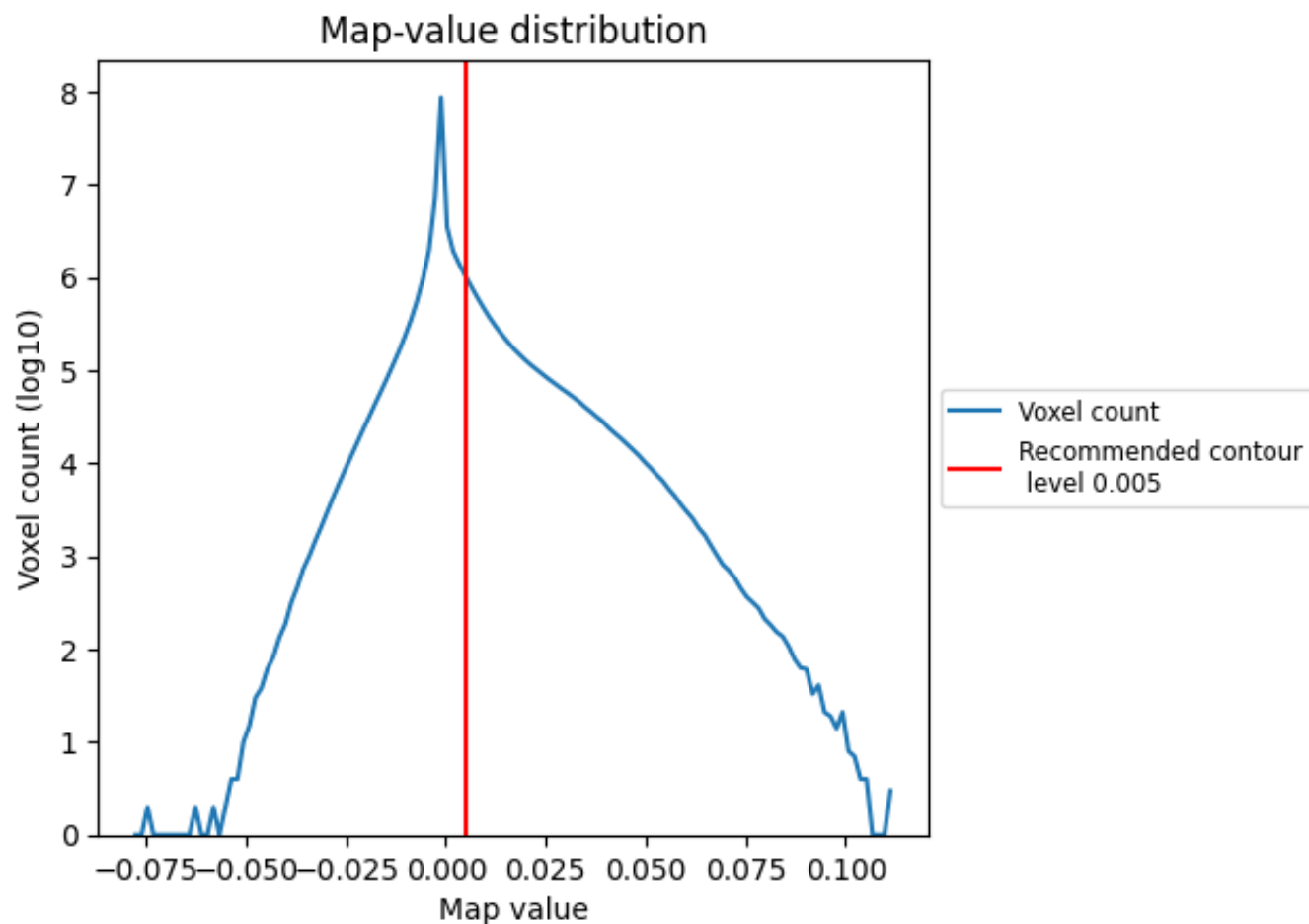
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

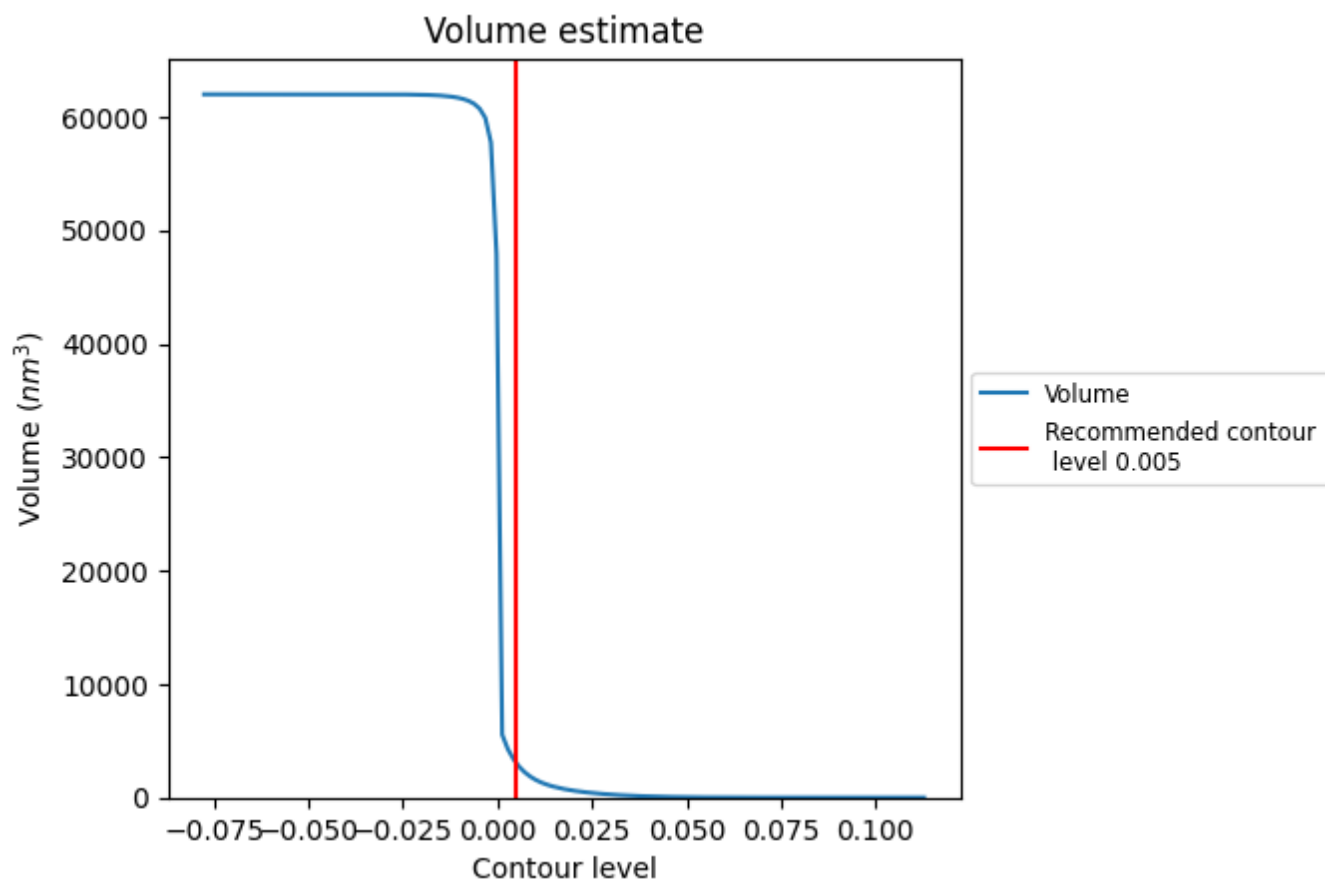
This section contains the results of statistical analysis of the map.

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.

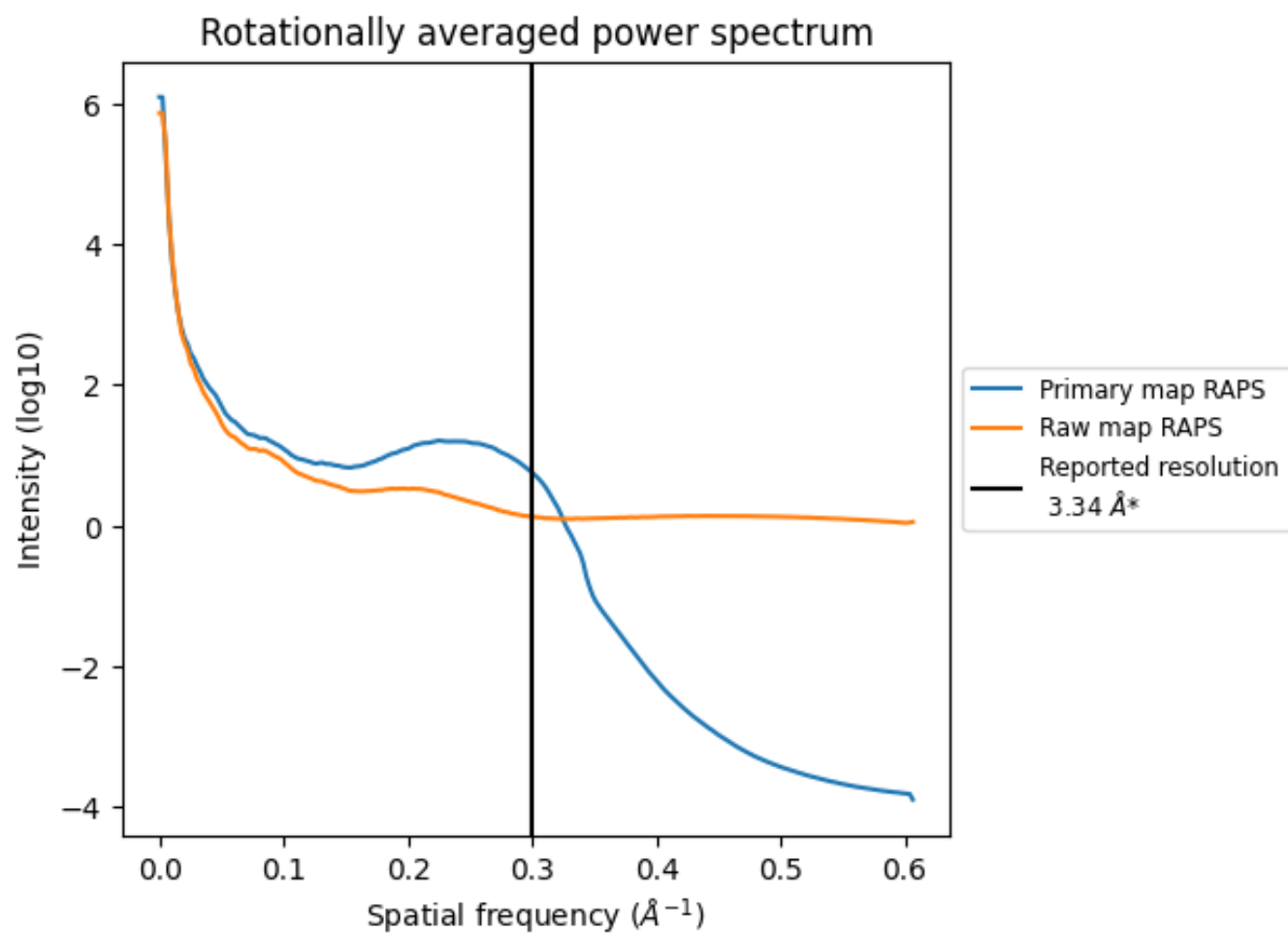
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3036 nm^3 ; this corresponds to an approximate mass of 2742 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 ⓘ

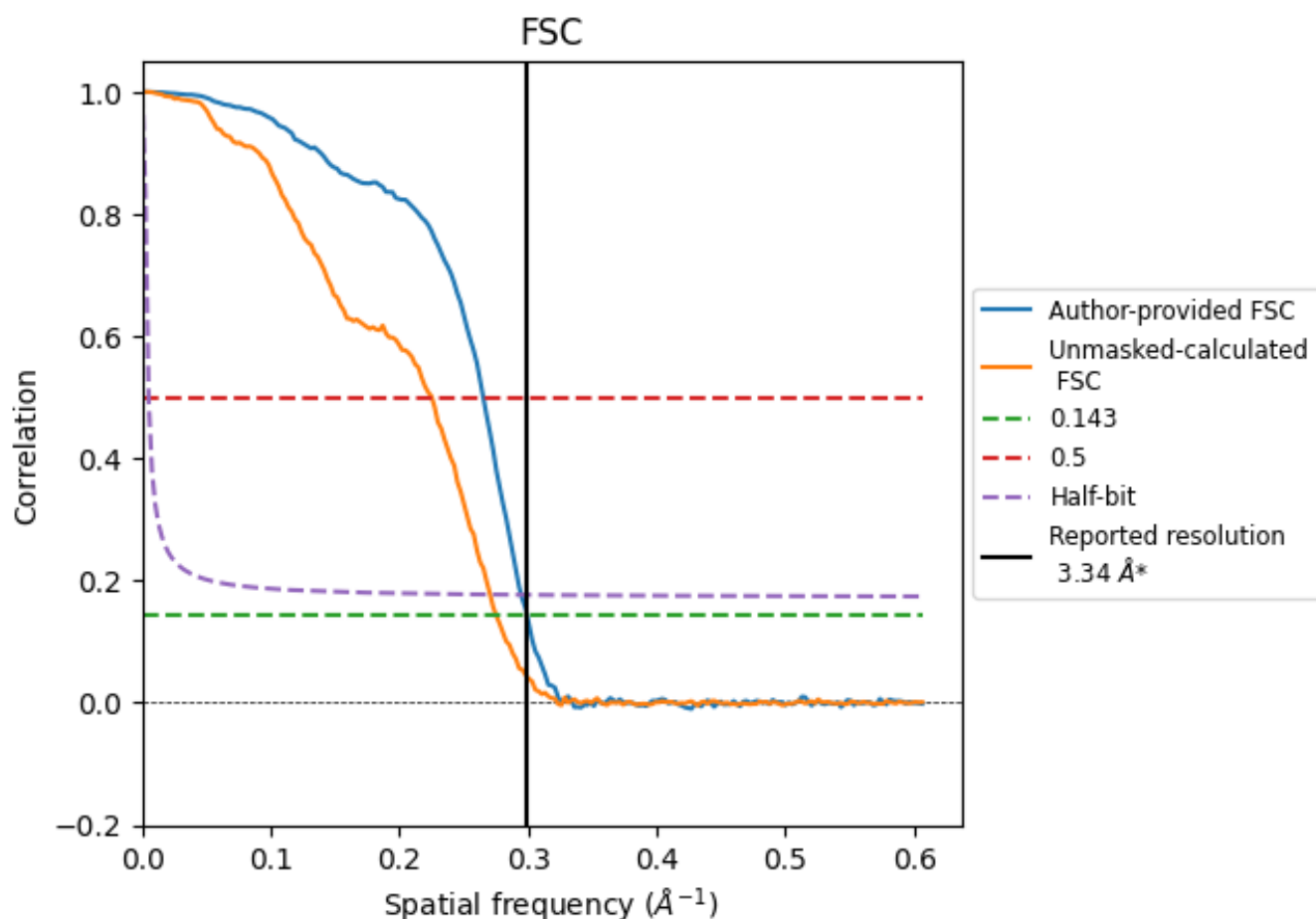


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 \AA^{-1}

8.2 Resolution estimates [i](#)

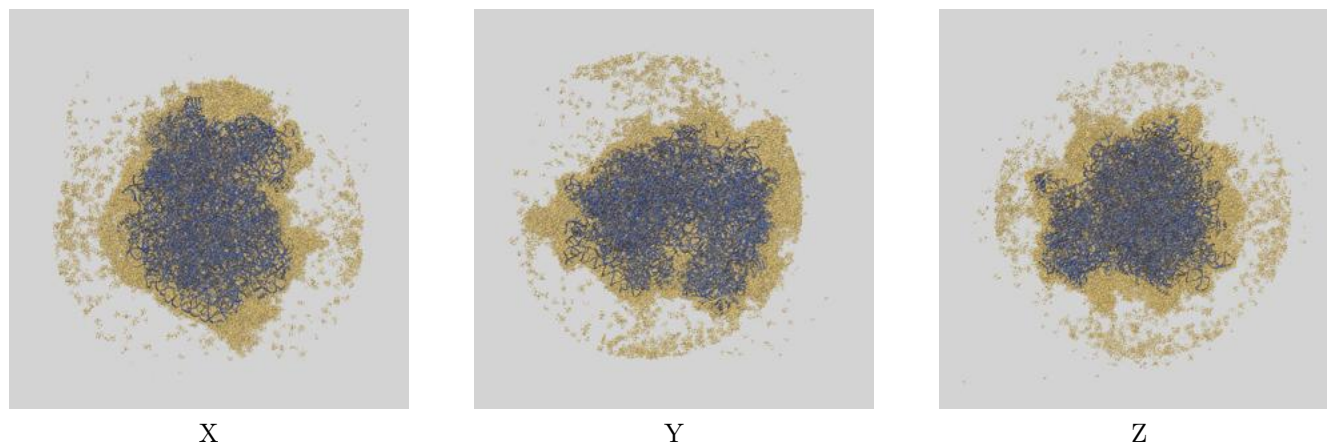
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.77	3.39
Unmasked-calculated*	3.63	4.44	3.70

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

9 Map-model fit [i](#)

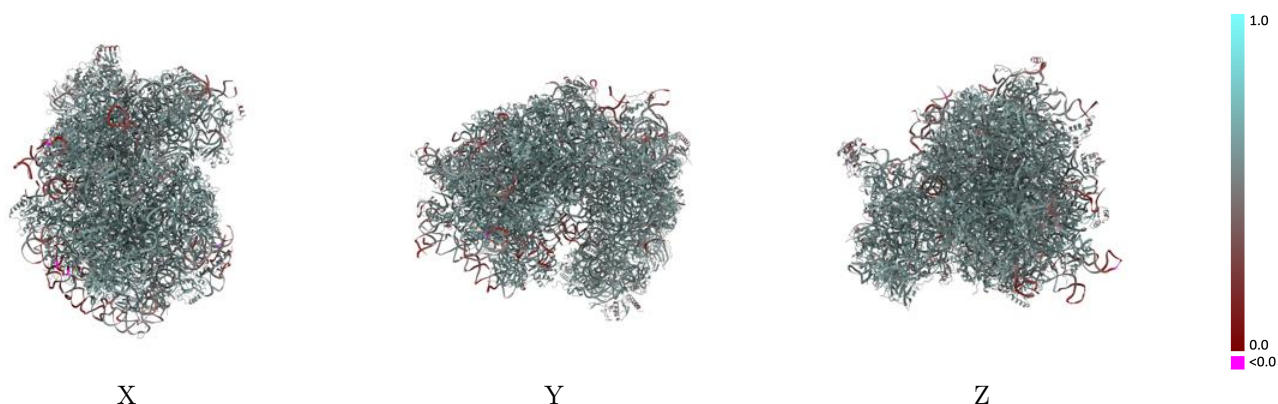
This section contains information regarding the fit between EMDB map EMD-52565 and PDB model 9I14. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.005 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](#)

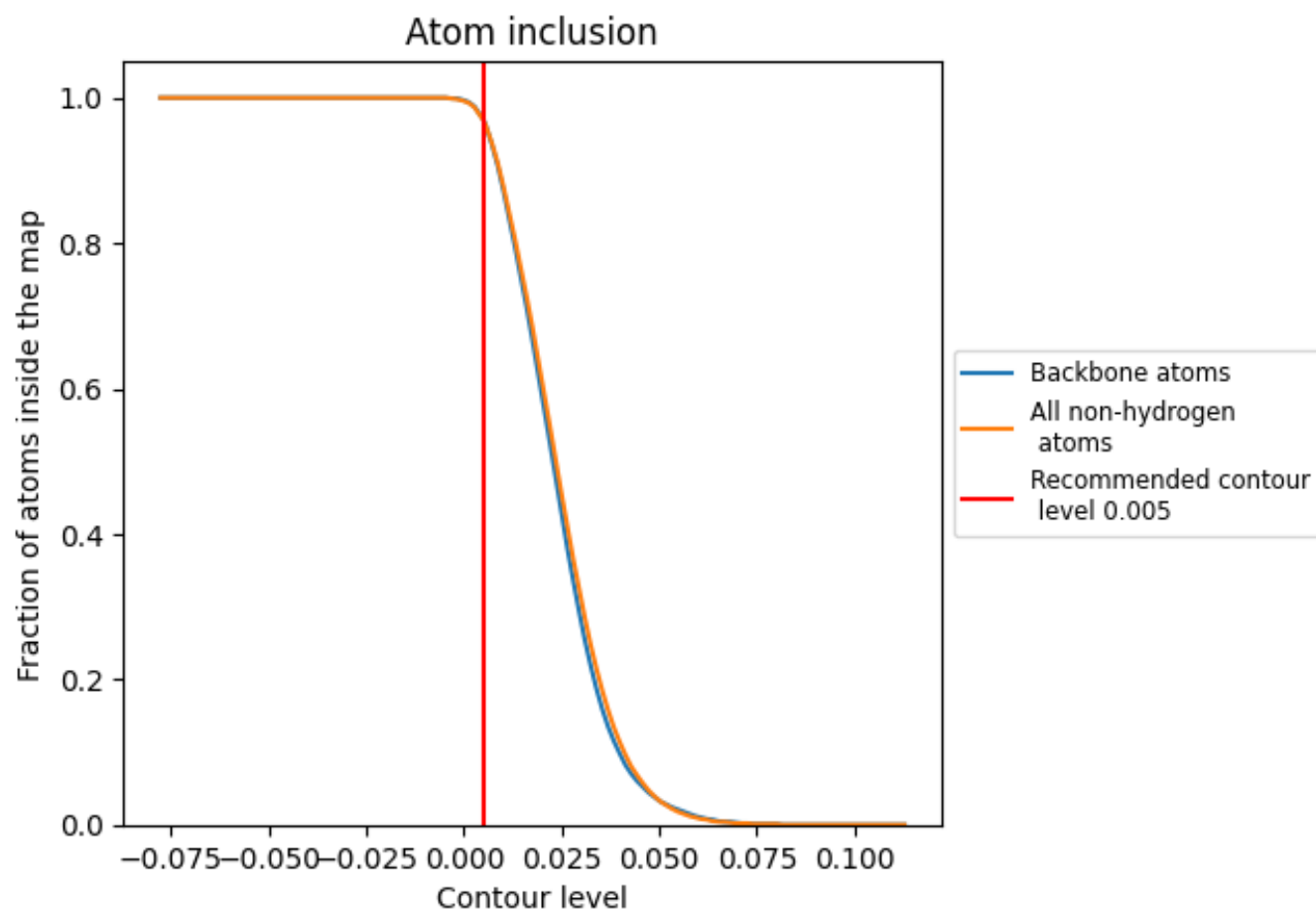


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5510
A4	 0.9790	 0.5320
B4	 0.9500	 0.4080
D4	 0.9110	 0.3570
L5	 0.9660	 0.5340
L7	 0.9930	 0.5760
L8	 0.9860	 0.5630
LA	 0.9840	 0.5980
LB	 0.9760	 0.5860
LC	 0.9720	 0.5850
LD	 0.9590	 0.5690
LE	 0.9680	 0.5660
LF	 0.9690	 0.5850
LG	 0.9560	 0.5580
LH	 0.9590	 0.5740
LI	 0.9660	 0.5810
LJ	 0.9660	 0.5630
LL	 0.9640	 0.5700
LM	 0.9650	 0.5730
LN	 0.9830	 0.6020
LO	 0.9710	 0.5850
LP	 0.9690	 0.5900
LQ	 0.9810	 0.5980
LR	 0.9760	 0.5660
LS	 0.9800	 0.5970
LT	 0.9750	 0.5820
LU	 0.9290	 0.5080
LV	 0.9840	 0.5830
LW	 0.9800	 0.5490
LX	 0.9710	 0.5760
LY	 0.9630	 0.5860
LZ	 0.9710	 0.5710
La	 0.9770	 0.5980
Lb	 0.9670	 0.5600
Lc	 0.9630	 0.5530















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Chain	Atom inclusion	Q-score
Ld	 0.9770	 0.5780
Le	 0.9870	 0.5970
Lf	 0.9860	 0.6000
Lg	 0.9770	 0.5790
Lh	 0.9560	 0.5650
Li	 0.9550	 0.5630
Lj	 0.9870	 0.5950
Lk	 0.9460	 0.5290
Ll	 0.9780	 0.5860
Lm	 0.9750	 0.5720
Ln	 0.9950	 0.5820
Lo	 0.9820	 0.5770
Lp	 0.9910	 0.5870
Lr	 0.9740	 0.5860
S2	 0.9830	 0.5550
SA	 0.9500	 0.5560
SB	 0.9680	 0.5670
SC	 0.9750	 0.5670
SD	 0.9560	 0.5470
SE	 0.9650	 0.5630
SF	 0.9680	 0.5670
SG	 0.9720	 0.5400
SH	 0.9390	 0.5080
SI	 0.9810	 0.5510
SJ	 0.9580	 0.5460
SK	 0.9430	 0.5620
SL	 0.9780	 0.5670
SM	 0.8330	 0.4440
SN	 0.9790	 0.5650
SO	 0.9680	 0.5710
SP	 0.9730	 0.5650
SQ	 0.9610	 0.5770
SR	 0.9340	 0.5310
SS	 0.9650	 0.5680
ST	 0.9640	 0.5780
SU	 0.9280	 0.5270
SV	 0.9410	 0.5610
SW	 0.9770	 0.5750
SX	 0.9630	 0.5640
SY	 0.9660	 0.5580
SZ	 0.9550	 0.5570
Sa	 0.9750	 0.5740

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Chain	Atom inclusion	Q-score
Sb	 0.9440	 0.5090
Sc	 0.9830	 0.5520
Sd	 0.9810	 0.5830
Se	 0.9820	 0.5640
Sf	 0.8910	 0.4750
Sg	 0.9330	 0.5460