



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 04:42 PM EDT

PDB ID : 8G5Z / pdb_00008g5z
EMDB ID : EMD-29758
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (GA state)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-14
Resolution : 2.64 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.dev133
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) : 2.50

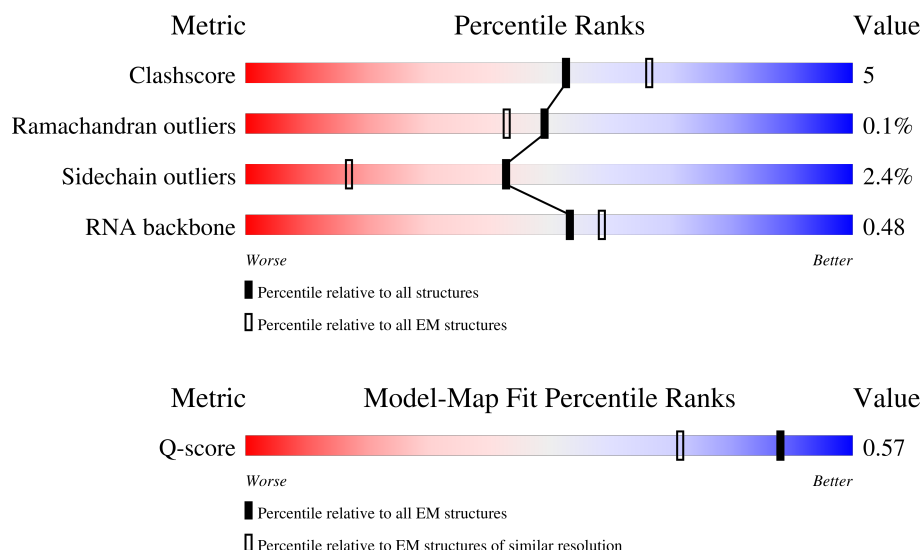
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 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	8968 (2.14 - 3.14)

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	S2	1701	
2	L8	156	
3	L5	3687	

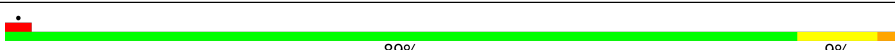
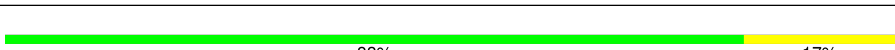
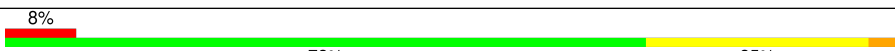
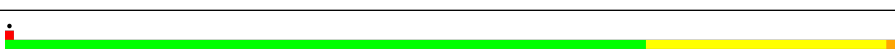
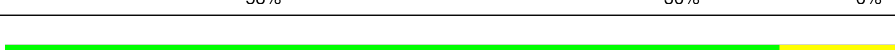
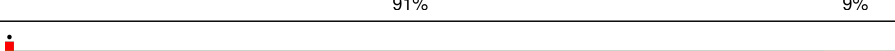
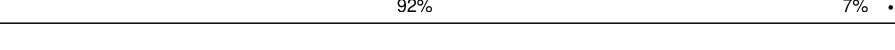
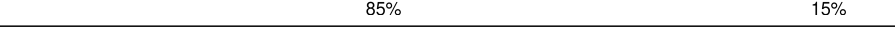
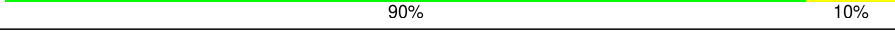
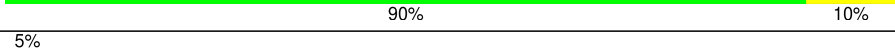
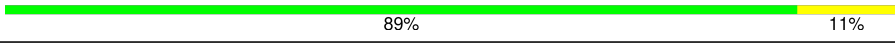
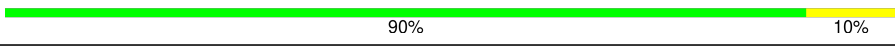
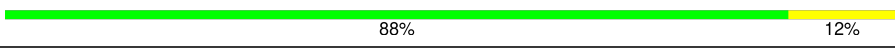
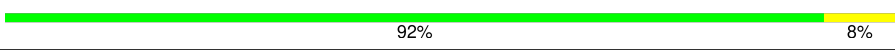
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Mol	Chain	Length	Quality of chain
4	L7	120	 78%19%
5	SB	223	 86%14%
6	SA	222	 78%21%
7	SD	226	 77%22%
8	SJ	185	 78%22%
9	SE	262	 77%22%
10	SC	222	 86%14%
11	SG	237	 88%12%
12	SF	189	 87%12%
13	SH	189	 78%20%
14	SW	129	 87%12%
15	SI	206	 83%16%
16	SQ	141	 81%18%
17	SU	101	 74%24%
18	SK	96	 72%26%
19	SO	135	 89%9%
20	SX	142	 84%14%
21	SM	122	 11%68%29%
22	SS	148	 82%18%
23	Sd	55	 89%11%
24	SN	150	 84%15%
25	SL	143	 82%16%
26	SR	134	 76%21%
27	SP	133	 84%15%
28	ST	143	 88%11%

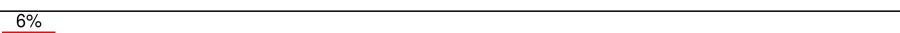
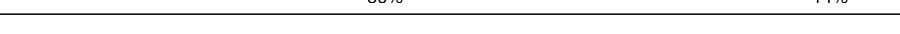
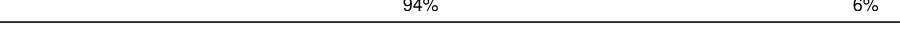
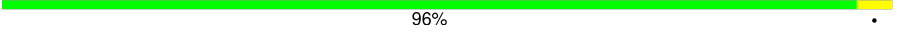
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	131	
31	SZ	84	
32	Sa	99	
33	Sb	83	
34	Sc	64	
35	Se	59	
36	Sf	75	
37	Sg	313	
38	Lz	211	
39	LA	251	
40	LB	402	
41	LC	368	
42	LJ	169	
43	LH	190	
44	LE	223	
45	LG	239	
46	Lq	196	
47	LK	147	
48	LO	201	
49	LL	206	
50	LV	140	
51	LM	136	
52	La	147	
53	LN	203	

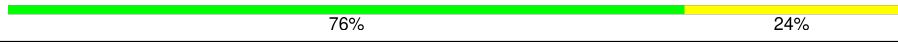
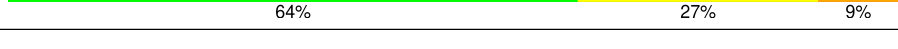
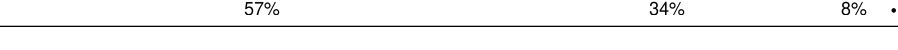
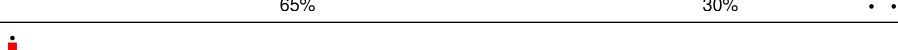
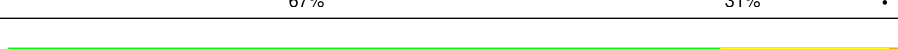
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Mol	Chain	Length	Quality of chain
54	LI	205	
55	LD	294	
56	LQ	187	
57	LR	187	
58	LS	176	
59	LT	159	
60	LP	153	
61	LU	99	
62	LX	118	
63	LY	134	
64	LW	118	
65	LZ	135	
66	Lr	125	
67	Lh	122	
68	Lb	109	
69	LF	225	
70	Lc	98	
71	Ld	107	
72	Le	128	
73	Lf	109	
74	Lg	114	
75	Li	102	
76	Lj	86	
77	Lk	69	
78	Ll	50	

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Mol	Chain	Length	Quality of chain
79	Lm	52	
80	Ln	25	
81	Lo	105	
82	Lp	91	
83	mR	11	
84	At	76	
85	Pt	77	
86	5A	143	
87	EF	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
66	SAC	Lr	2	-	X	-	-

2 Entry composition [i](#)

There are 99 unique types of molecules in this entry. The entry contains 227372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1701	Total	C	N	O	P	0	0
			36364	16257	6517	11889	1701		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3687	Total	C	N	O	P	2	0
			79168	35292	14483	25704	3689		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2562	1141	456	845	120		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SB	?	-	LYS	deletion	UNP P61247
SB	?	-	GLY	deletion	UNP P61247
SB	?	-	GLY	deletion	UNP P61247

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Chain	Residue	Modelled	Actual	Comment	Reference
SB	?	-	LYS	deletion	UNP P61247
SB	?	-	LYS	deletion	UNP P61247
SB	?	-	GLY	deletion	UNP P61247
SB	?	-	ALA	deletion	UNP P61247
SB	?	-	LYS	deletion	UNP P61247
SB	?	-	LYS	deletion	UNP P61247
SB	?	-	LYS	deletion	UNP P61247

- Molecule 6 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	222	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 8 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 9 is a protein called eS4.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 17 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 18 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 19 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 20 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SX	142	Total	C	N	O	S	0	0
			1105	696	220	186	3		

- Molecule 21 is a protein called eS12.

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

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	143	Total	C	N	O	S	0	0
			1171	746	221	198	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 27 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	133	Total	C	N	O	S	0	0
			1093	695	206	185	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

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

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 31 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 33 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 34 is a protein called 40S ribosomal protein S28.

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

- Molecule 35 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 36 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	75	Total	C	N	O	S	0	0
			615	388	118	102	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	211	Total	C	N	O	S	0	0
			1701	1089	307	297	8		

- Molecule 39 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LA	251	Total	C	N	O	S	0	0
			1922	1204	393	319	6		

- Molecule 40 is a protein called 60S ribosomal protein L3.

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

- Molecule 41 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1359	859	253	241	6		

- Molecule 43 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LH	190	Total	C	N	O	S	0	0
			1519	956	284	273	6		

- Molecule 44 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	223	Total	C	N	O	S	1	0
			1793	1155	340	294	4		

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1910	1217	368	321	4		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lq	196	Total	C	N	O	S	0	0
			1507	958	263	277	9		

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LK	147	Total	C	N	O	S	0	0
			1122	700	211	208	3		

- Molecule 48 is a protein called 60S ribosomal protein L13a.

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

- Molecule 49 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LL	206	Total	C	N	O	S	0	0
			1665	1041	345	275	4		

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LV	140	Total	C	N	O	S	0	0
			1042	653	200	183	6		

- Molecule 51 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LM	136	Total	C	N	O	S	0	0
			1121	719	215	180	7		

- Molecule 52 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 53 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 54 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	?	-	CYS	deletion	UNP P27635
LI	?	-	ALA	deletion	UNP P27635
LI	?	-	GLY	deletion	UNP P27635
LI	?	-	ALA	deletion	UNP P27635
LI	?	-	ASP	deletion	UNP P27635
LI	?	-	ARG	deletion	UNP P27635
LI	?	-	LEU	deletion	UNP P27635
LI	?	-	GLN	deletion	UNP P27635

- Molecule 55 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LD	294	Total	C	N	O	S	0	0
			2392	1513	436	429	14		

- Molecule 56 is a protein called 60S ribosomal protein L18.

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

- Molecule 57 is a protein called 60S ribosomal protein L19.

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

- Molecule 58 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 59 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LU	99	Total	C	N	O	S	0	0
			809	518	141	148	2		

- Molecule 62 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 63 is a protein called 60S ribosomal protein L26.

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

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 65 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lr	125	Total	C	N	O	S	0	0
			1006	624	207	170	5		

- Molecule 67 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 68 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 69 is a protein called 60S ribosomal protein L7.

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

- Molecule 70 is a protein called 60S ribosomal protein L30.

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

- Molecule 71 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ld	107	Total	C	N	O	S	0	0
			889	560	171	156	2		

- Molecule 72 is a protein called 60S ribosomal protein L32.

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

- Molecule 73 is a protein called 60S ribosomal protein L35a.

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

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Li	102	Total	C	N	O	S	0	0
			833	521	177	130	5		

- Molecule 76 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 77 is a protein called 60S ribosomal protein L38.

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

- Molecule 78 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 79 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 80 is a protein called 60S ribosomal protein L41.

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

- Molecule 81 is a protein called Ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 82 is a protein called 60S ribosomal protein L37a.

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mR	11	Total	C	N	O	P	1	0
			252	113	41	86	12		

- Molecule 84 is a RNA chain called A-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace	
84	At	76	Total	C	N	O	P	S	0	0
			1630	730	290	532	76	2		

- Molecule 85 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

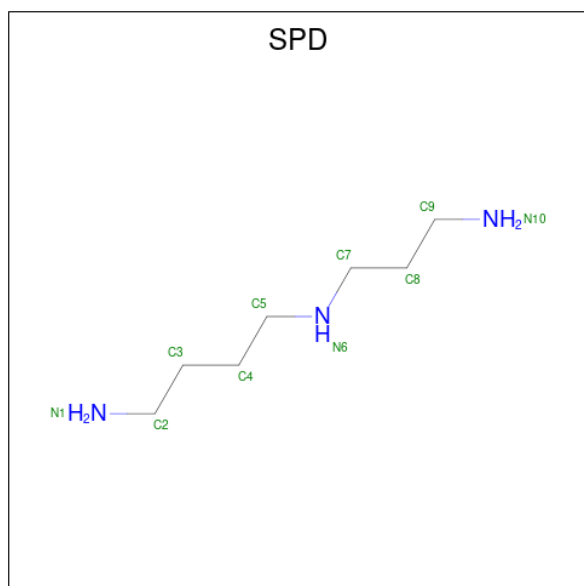
- Molecule 86 is a protein called eIF5A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	5A	143	Total	C	N	O	S	0	0
			1089	682	187	211	9		

- Molecule 87 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	EF	444	Total	C	N	O	S	0	0
			3405	2167	585	636	17		

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
88	S2	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 89 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
89	S2	9	Total	K	0
			9	9	
89	L8	1	Total	K	0
			1	1	
89	L5	30	Total	K	0
			30	30	
89	L7	1	Total	K	0
			1	1	
89	LA	1	Total	K	0
			1	1	
89	LB	1	Total	K	0
			1	1	
89	Lf	1	Total	K	0
			1	1	
89	mR	1	Total	K	0
			1	1	

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	S2	108	Total	Mg	0
			108	108	
90	L8	6	Total	Mg	0
			6	6	
90	L5	284	Total	Mg	0
			284	284	
90	L7	5	Total	Mg	0
			5	5	
90	SE	1	Total	Mg	0
			1	1	
90	SG	1	Total	Mg	0
			1	1	
90	SO	1	Total	Mg	0
			1	1	

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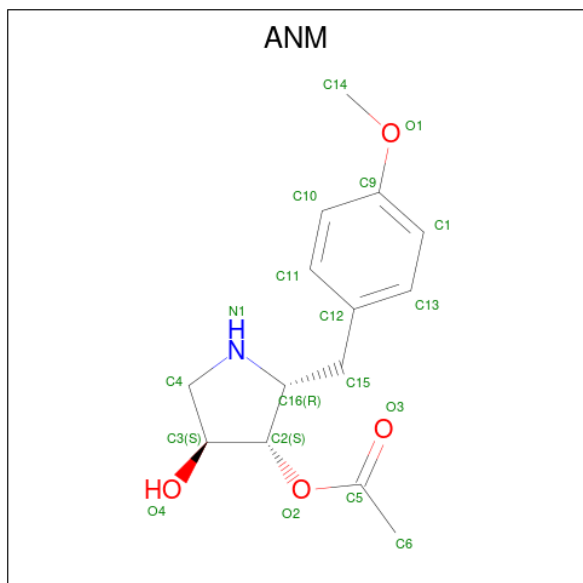
Mol	Chain	Residues	Atoms		AltConf
90	SX	2	Total 2	Mg 2	0
90	Sd	1	Total 1	Mg 1	0
90	ST	1	Total 1	Mg 1	0
90	Sa	1	Total 1	Mg 1	0
90	LA	1	Total 1	Mg 1	0
90	LB	1	Total 1	Mg 1	0
90	LC	1	Total 1	Mg 1	0
90	LJ	1	Total 1	Mg 1	0
90	LH	1	Total 1	Mg 1	0
90	LV	1	Total 1	Mg 1	0
90	LN	1	Total 1	Mg 1	0
90	LI	1	Total 1	Mg 1	0
90	LS	1	Total 1	Mg 1	0
90	LP	1	Total 1	Mg 1	0
90	LW	1	Total 1	Mg 1	0
90	Lr	1	Total 1	Mg 1	0
90	Le	1	Total 1	Mg 1	0
90	Lg	2	Total 2	Mg 2	0
90	Lj	1	Total 1	Mg 1	0
90	mR	1	Total 1	Mg 1	0
90	At	1	Total 1	Mg 1	0

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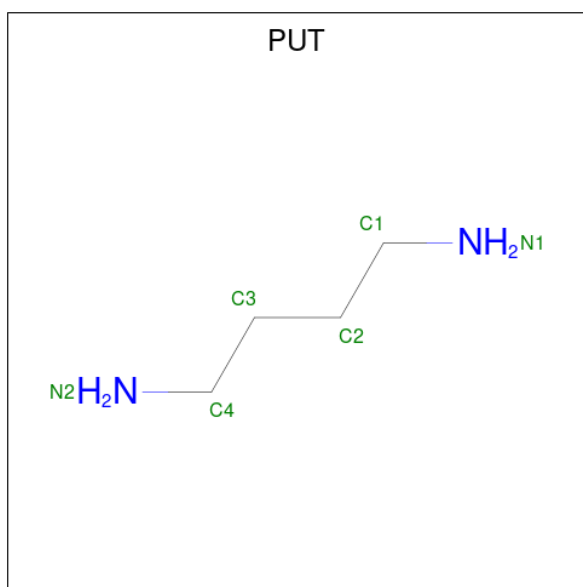
Mol	Chain	Residues	Atoms		AltConf
90	Pt	2	Total	Mg	0
			2	2	
90	EF	2	Total	Mg	0
			2	2	

- Molecule 91 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$) (labeled as "Ligand of Interest" by depositor).



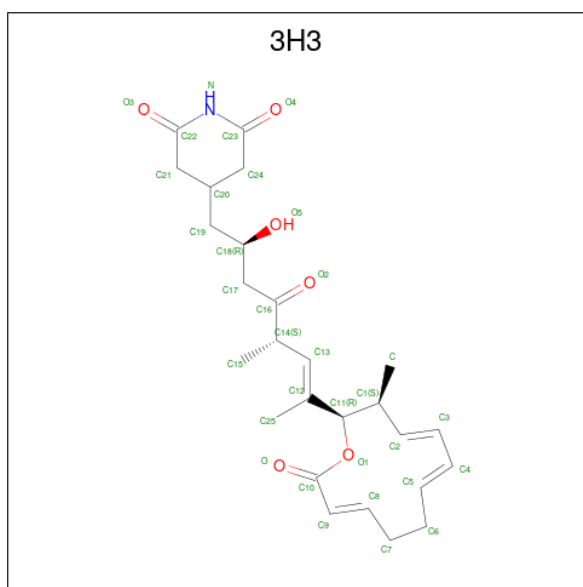
Mol	Chain	Residues	Atoms				AltConf
91	L5	1	Total	C	N	O	0
			19	14	1	4	

- Molecule 92 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

- Molecule 93 is 4-[(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo-oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl]piperidine-2,6-dione (CCD ID: 3H3) (formula: C₂₆H₃₅NO₆) (labeled as "Ligand of Interest" by depositor).

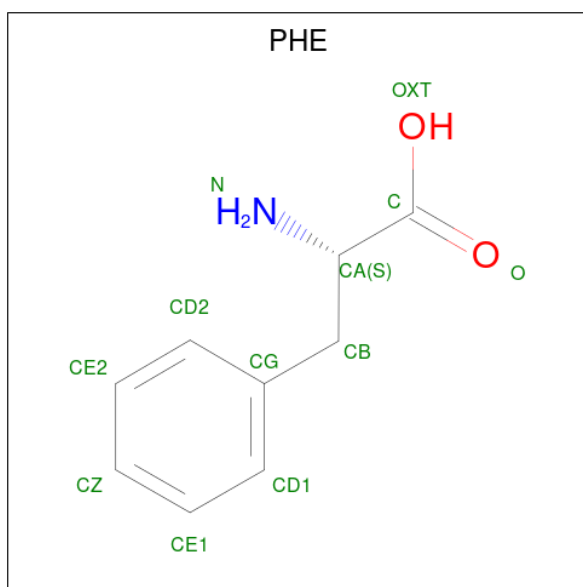


Mol	Chain	Residues	Atoms				AltConf
93	L5	1	Total	C	N	O	0
			33	26	1	6	

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

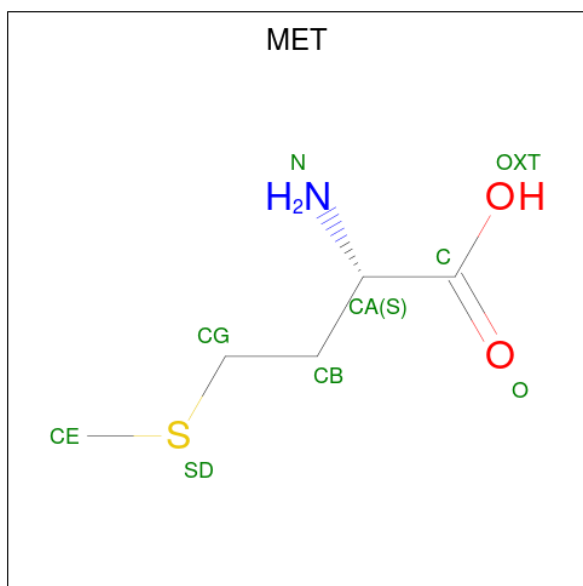
Mol	Chain	Residues	Atoms		AltConf
94	Sd	1	Total	Zn	0
			1	1	
94	Sa	1	Total	Zn	0
			1	1	
94	Sf	1	Total	Zn	0
			1	1	
94	Lg	1	Total	Zn	0
			1	1	
94	Lj	1	Total	Zn	0
			1	1	
94	Lm	1	Total	Zn	0
			1	1	
94	Lo	1	Total	Zn	0
			1	1	
94	Lp	1	Total	Zn	0
			1	1	

- Molecule 95 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



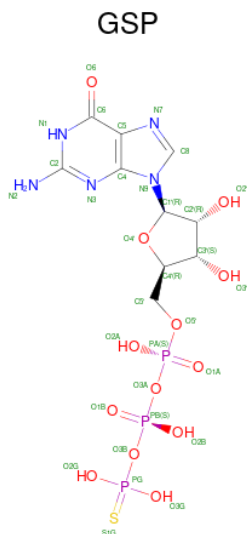
Mol	Chain	Residues	Atoms				AltConf
95	At	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 96 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



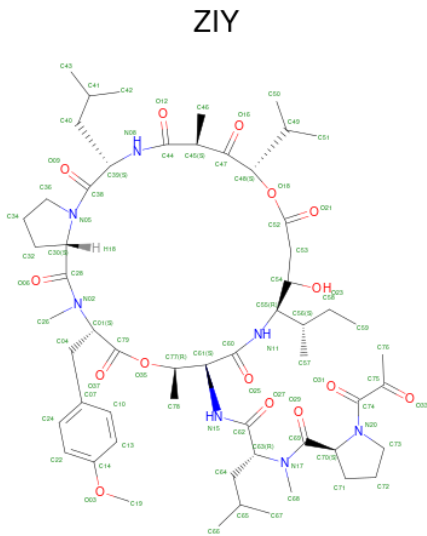
Mol	Chain	Residues	Atoms					AltConf
96	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 97 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						AltConf
97	EF	1	Total 32	C 10	N 5	O 13	P 3	S 1	0

- Molecule 98 is plitidepsin (CCD ID: ZIY) (formula: $C_{57}H_{87}N_7O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
98	EF	1	Total	C	N	O	0
			79	57	7	15	

- Molecule 99 is water.

Mol	Chain	Residues	Atoms	AltConf
99	S2	21	Total O 21 21	0
99	L8	4	Total O 4 4	0
99	L5	304	Total O 304 304	0
99	L7	3	Total O 3 3	0
99	SE	1	Total O 1 1	0
99	SS	1	Total O 1 1	0
99	SN	1	Total O 1 1	0
99	Sa	1	Total O 1 1	0
99	LA	1	Total O 1 1	0
99	LB	3	Total O 3 3	0
99	LC	2	Total O 2 2	0
99	LO	1	Total O 1 1	0
99	LV	1	Total O 1 1	0
99	LM	1	Total O 1 1	0
99	La	4	Total O 4 4	0
99	LI	1	Total O 1 1	0
99	LQ	1	Total O 1 1	0
99	LP	3	Total O 3 3	0
99	Lr	1	Total O 1 1	0
99	Lb	1	Total O 1 1	0
99	LF	1	Total O 1 1	0
99	Li	1	Total O 1 1	0

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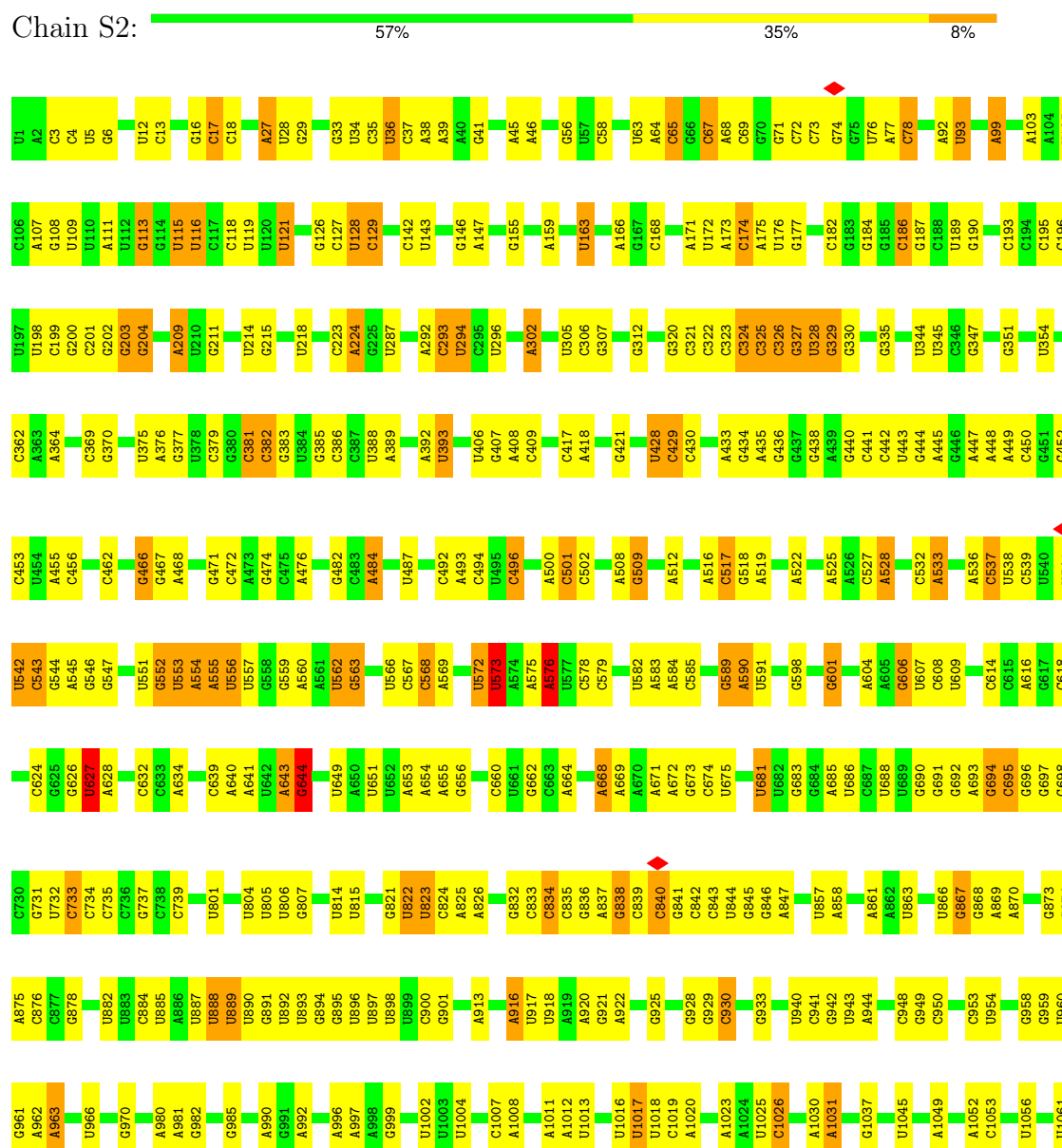
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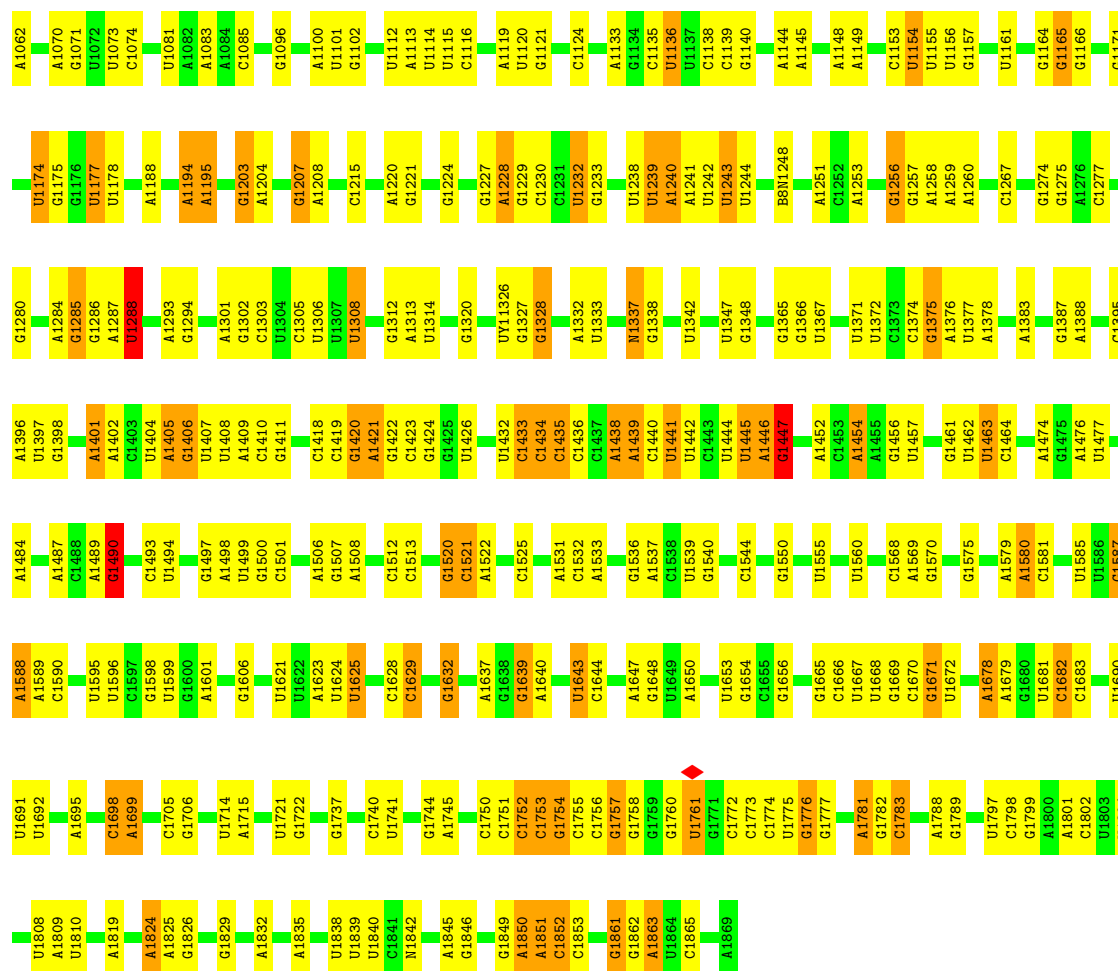
Mol	Chain	Residues	Atoms		AltConf
99	Lj	2	Total 2	O 2	0
99	Lo	2	Total 2	O 2	0
99	EF	3	Total 3	O 3	0

3 Residue-property plots

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

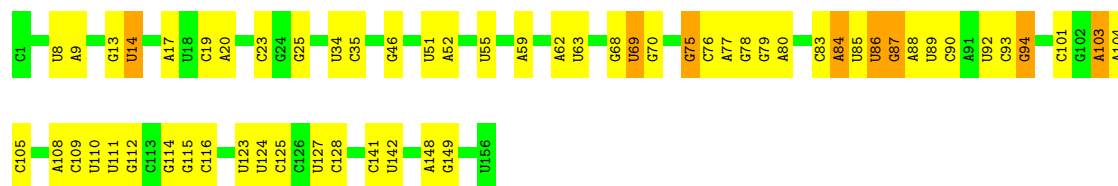
• Molecule 1: 18S rRNA





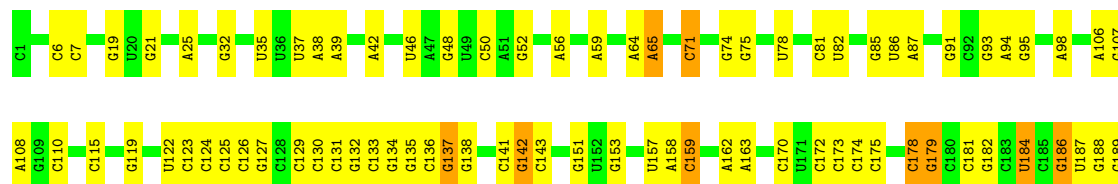
• Molecule 2: 5.8S rRNA

Chain L8: 62% 33% 5%



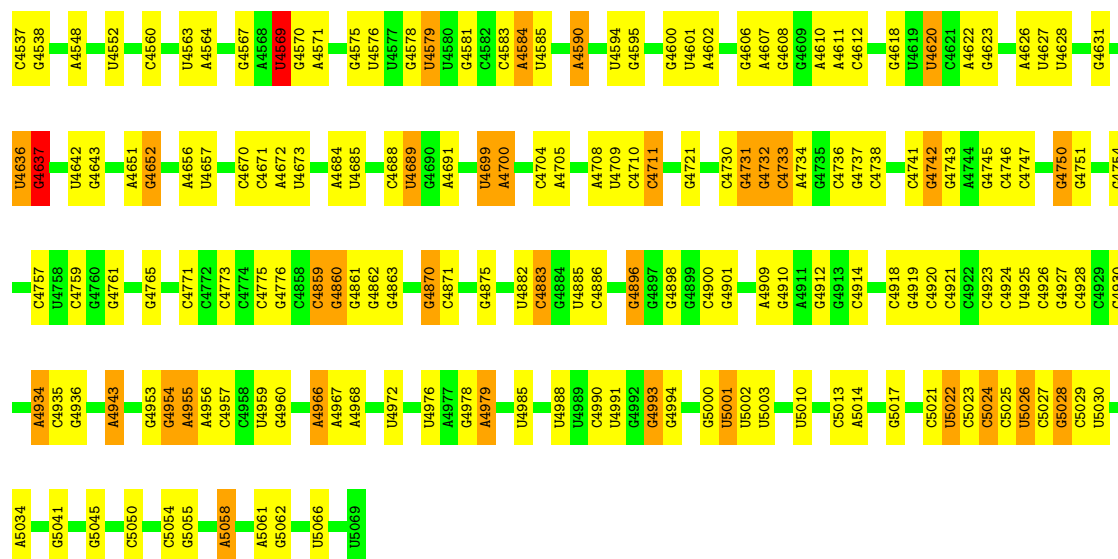
• Molecule 3: 28S rRNA

Chain L5: 62% 32% 6%



C1993	C1994	A1896	C1789	A1701	G1604	G1451	G1358	G1071	G912	C673	G462	C340	U200
C1995	C1996	A1897	U1792	C1702	G1605	G1457	G1359	C1072	U913	G677	A463	A344	C201
C1997	C1998	C1703	A1793	C1704	G1458	C1458	C1365	G1073	U914	C678	G464	C350	C202
U1997	U1918	C1705	A1794	A1706	G1612	A1459	C1366	G1074	A916	C679	A465	C361	U206
A1999	G1919	A1707	A1802	G1721	G1613	C1460	C1369	C1075	A917	G680	A466	U207	G207
G2000	C1920	A1803	A1803	U1725	G1614	C1464	G1370	C1076	C921	C683	A469	A208	A208
C2001	C1921	A1804	A1805	U1726	G1617	C1472	G1377	C1082	C922	G684	A470	U209	U209
A2002	G1922	A1806	G1624	U1727	G1625	U1473	G1380	U1083	C925	G685	G483	G373	A218
G2003	G1925	G1810	G1625	U1728	G1631	C1480	G1387	C1085	G926	U688	G484	G374	G219
U2004	U1930	G1811	A1632	A1729	A1631	C1481	A1387	G1092	C928	G689	G485	G375	G223
U2008	C1931	G1812	A1633	U1730	A1632	C1482	A1392	C1093	A929	G696	G486	G376	U224
C2011	A1932	G1815	A1634	C1731	A1634	C1483	G1393	G1094	C930	C696	G487	G377	G225
C2014	C1933	G1820	A1634	C1732	A1634	C1483	G1394	A1095	C931	C699	G488	G378	U231
U2015	A1934	G1820	G1640	C1733	A1641	A1491	G1395	G1096	A932	G700	G489	A377	G232
C2016	C1937	G1834	G1641	G1734	A1642	G1498	G1396	C1097	C933	G701	G490	A378	U233
C2019	G1940	G1835	A1642	G1739	C1645	G1502	A1397	G1098	A934	G702	G491	A377	G234
U2020	A1941	G1836	A1646	A1743	C1646	G1503	A1398	G1170	A935	G703	G492	A377	A235
A2025	A1942	A1837	U1647	U1744	U1647	G1504	G1402	G1177	U937	G704	G493	A377	G254
A2026	A1943	G1842	G1648	A1749	G1648	G1504	G1403	G1178	C938	G707	G494	A377	C255
A2029	G1948	A1843	U1649	G1750	U1649	U1514	G1404	G1179	C939	G708	G495	A377	G256
A2030	G1951	G1846	G1654	G1753	G1654	A1515	G1405	U1179	C940	A711	G496	A377	C257
A2042	G1952	C1847	G1654	U1754	G1654	A1515	G1406	C1181	C941	C712	G497	A377	G258
A2043	G1955	C1848	G1661	C1755	G1661	A1524	G1407	C1182	A943	C713	G498	A377	C259
A2044	A1956	U1852	G1662	U1756	G1662	A1525	G1408	C1183	A944	U717	G499	A377	C260
G2045	U1957	G1853	G1663	U1757	G1663	A1525	G1409	U1184	U945	C718	G500	A377	G261
G2046	G1960	G1854	A1669	U1758	A1669	G1529	U1411	C1185	G955	U728	G501	A377	G262
A2047	G1961	G1855	G1670	G1759	G1670	A1534	G1412	C1186	A956	U729	G502	A377	G263
U2048	G1962	G1856	U1671	G1760	U1671	C1535	G1413	C1187	U957	G730	G503	A377	C266
G2055	G1963	C1857	U1672	G1761	U1672	U1536	G1414	C1192	G959	G731	G504	A377	U273
G2056	G1964	G1858	U1673	C1762	U1673	U1536	G1415	G1198	A960	C738	G505	A377	C274
A2069	A1970	G1859	C1674	G1763	U1674	A1547	G1416	G1199	G961	G739	G506	A377	G278
C2084	C1971	U1860	C1675	G1764	C1675	G1548	G1417	G1200	C962	G740	G507	A377	G279
G2085	G1972	U1861	C1676	A1765	C1676	G1549	G1418	U1201	A963	G741	G508	A377	G280
C2091	U1973	U1862	U1677	A1766	U1677	A1564	G1419	G1211	G965	G742	G509	A377	G284
G2092	U1974	U1863	C1678	A1767	C1678	A1565	G1420	G1212	A966	U746	G510	A377	U297
A2093	A1979	U1864	U1683	C1768	U1683	C1566	G1432	C1214	C967	A747	G511	A377	A306
G2094	U1980	G1865	U1687	A1770	U1687	U1577	G1436	C1215	C968	G751	G512	A377	G315
A2095	G1981	U1866	G1688	U1771	U1688	G1578	U1437	C1216	C969	G752	G513	A377	U316
G2096	G1982	A1867	G1689	C1772	G1689	U1578	U1438	G1241	U971	G753	G514	A377	A317
U2097	U1983	U1868	C1690	U1773	C1690	U1578	U1439	G1242	C979	G754	G515	A377	A318
G2098	U1984	U1869	G1691	C1774	G1691	U1582	U1440	G1243	U980	G755	G516	A377	A319
G2099	U1985	U1870	G1692	A1775	G1692	U1582	U1441	G1244	U981	G756	G517	A377	A320
A2100	C1987	U1871	C1693	A1776	C1693	U1582	U1442	G1245	U982	G757	G518	A377	U325
C2101	U1988	U1872	C1694	U1777	C1694	U1582	U1443	G1246	C983	G758	G519	A377	C326
G2102	U1989	U1873	G1695	U1778	G1695	U1582	U1444	G1247	C984	G759	G520	A377	A336
G2103	U1990	U1874	G1696	U1779	G1696	U1582	U1445	G1248	U985	G760	G521	A377	G457
G2104	U1991	U1875	G1697	U1780	G1697	U1582	U1446	G1249	C986	G761	G522	A377	G458
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		U1877	G1699	U1782	G1699	U1582	U1448	G1251	C988	G763	G524	A377	G460
		U1878	G1700	U1783	G1700	U1582	U1449	G1252	C989	G764	G525	A377	G461
				U1784		U1582	U1450	G1253	C990	G765	G526	A377	G462
				U1785		U1582	U1451	G1254	C991	G766	G527	A377	G463
				U1786		U1582	U1452	G1255	C992	G767	G528	A377	G464
				U1787		U1582	U1453	G1256	C993	G768	G529	A377	G465
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						U1582	U1456	G1259	C996	G771	G532	A377	G468
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						U1582	U1458	G1261	C998	G773	G534	A377	G470
						U1582	U1459	G1262	C999	G774	G535	A377	G471
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						U1582	U1461	G1264	C1001	G776	G537	A377	G473
						U1582	U1462	G1265	C1002	G777	G538	A377	G474
						U1582	U1463	G1266	C1003	G778	G539	A377	G475
						U1582	U1464	G1267	C1004	G779	G540	A377	G476
						U1582	U1465	G1268	C1005	G780	G541	A377	G477
						U1582	U1466	G1269	C1006	G781	G542	A377	G478
						U1582	U1467	G1270	C1007	G782	G543	A377	G479
						U1582	U1468	G1271	C1008	G783	G544	A377	G480
						U1582	U1469	G1272	C1009	G784	G545	A377	G481
						U1582	U1470	G1273	C1010	G785	G546	A377	G482
						U1582	U1471	G1274	C1011	G786	G547	A377	G483
						U1582	U1472	G1275	C1012	G787	G548	A377	G484
						U1582	U1473	G1276	C1013	G788	G549	A377	G485
						U1582	U1474	G1277	C1014	G789	G550	A377	G486
						U1582	U1475	G1278	C1015	G790	G551	A377	G487
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						U1582	U1481	G1284	C1021	G796	G557	A377	G493
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						U1582	U1483	G1286	C1023	G798	G559	A377	G495
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						U1582	U1488	G1291	C1028	G803	G564	A377	G500
						U1582	U1489	G1292	C1029	G804	G565	A377	G501
						U1582	U1490	G1293	C1030	G805	G566	A377	G502
						U1582	U1491	G1294	C1031	G806	G567	A377	G503
						U1582	U1492	G1295	C1032	G807	G568	A377	G504
						U1582	U1493	G1296	C1033	G808	G569	A377	G505
						U1582	U1494	G1297	C1034	G809	G570	A377	G506
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						U1582	U1497	G1300	C1037	G812	G573	A377	G509
						U1582	U1498	G1301	C1038	G813	G574	A377	G510
						U1582	U1499	G1302	C1039	G814	G575	A377	G511
						U1582	U1500	G1303	C1040	G815	G576	A377	G512
						U1582	U1501	G1304	C1041	G816	G577	A377	G513
						U1582	U1502	G1305	C1042	G817	G578	A377	G514
						U1582	U1503	G1306	C1043	G818	G579	A377	G515
						U1582	U1504	G1307	C1044	G819	G580	A377	G516
						U1582	U1505	G1308	C1045	G820	G581	A377	G517
						U1582	U1506	G1309	C1046	G821	G582	A377	G518
						U1582	U1507	G1310	C1047	G822	G583	A377	G519
						U1582	U1508	G1311	C1048	G823	G584	A377	G520
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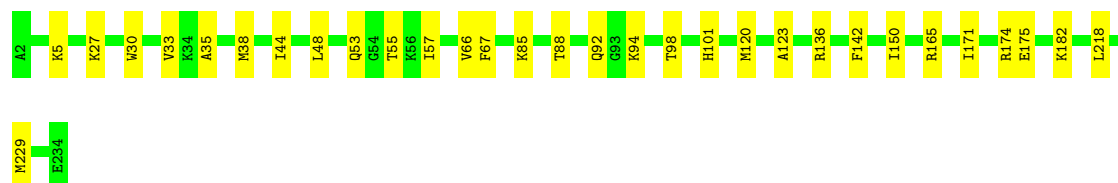
• Molecule 4: 5S rRNA

Chain L7: 78% 19% .



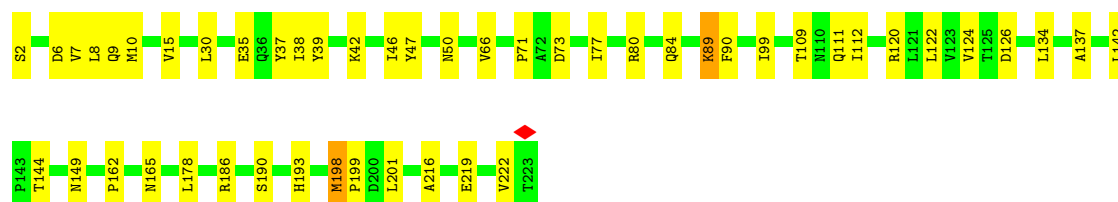
• Molecule 5: 40S ribosomal protein S3a

Chain SB: 86% 14% .



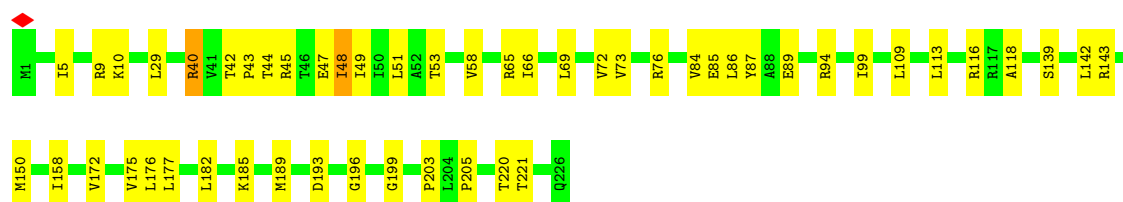
• Molecule 6: 40S ribosomal protein SA

Chain SA: 78% 21% .

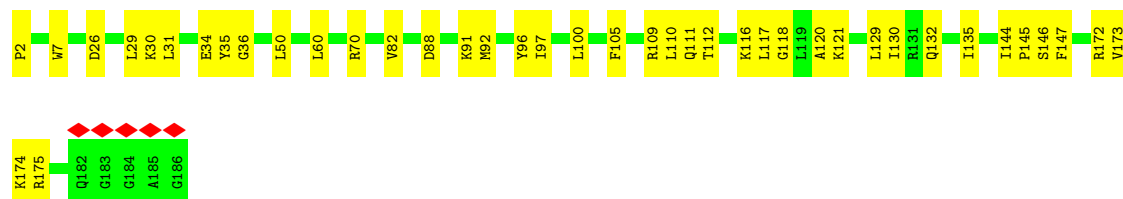
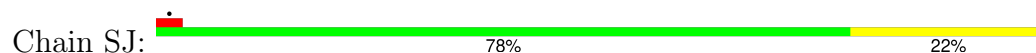


• Molecule 7: 40S ribosomal protein S3

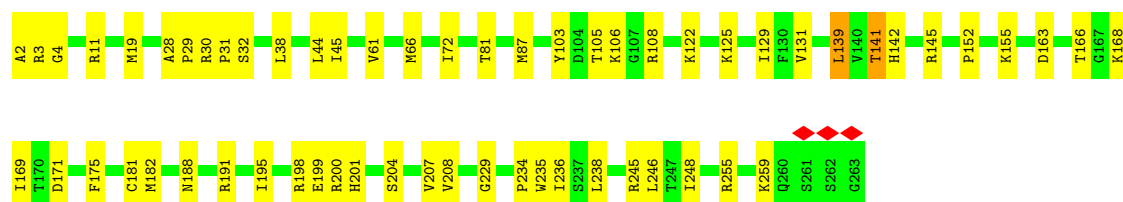
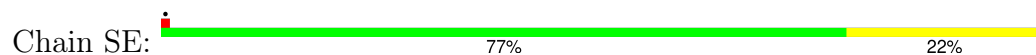
Chain SD: 77% 22% .



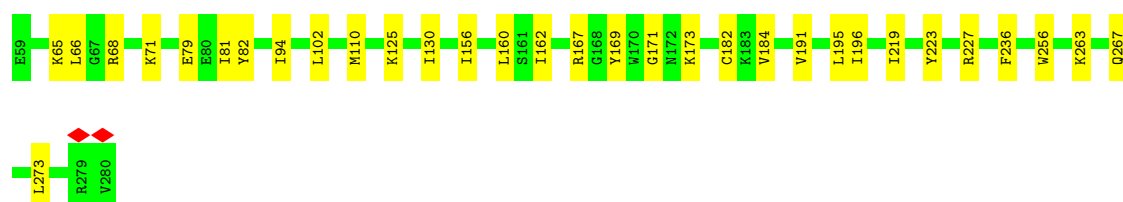
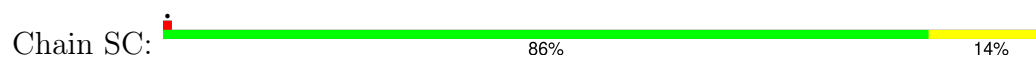
• Molecule 8: 40S ribosomal protein S9



• Molecule 9: eS4



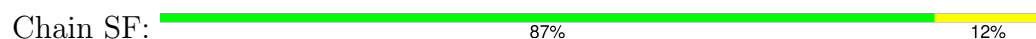
• Molecule 10: 40S ribosomal protein S2



• Molecule 11: 40S ribosomal protein S6



• Molecule 12: 40S ribosomal protein S5





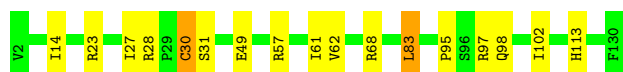
- Molecule 13: 40S ribosomal protein S7

Chain SH: 78% 20%



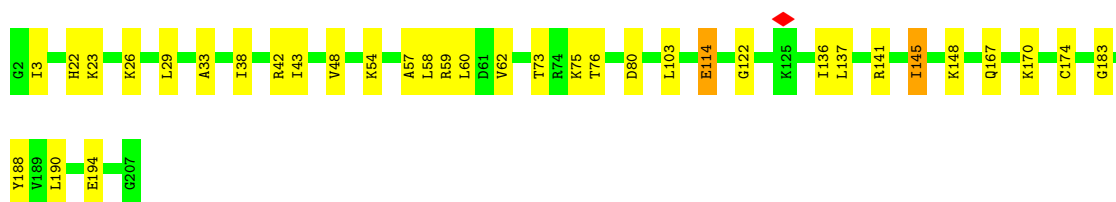
- Molecule 14: 40S ribosomal protein S15a

Chain SW: 87% 12%



- Molecule 15: 40S ribosomal protein S8

Chain SI: 83% 16%



- Molecule 16: uS9

Chain SQ: 81% 18%



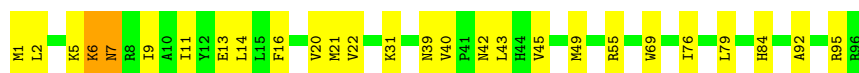
- Molecule 17: uS10

Chain SU: 74% 24%

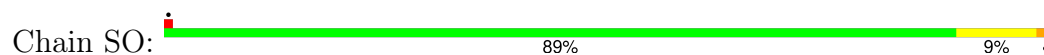


- Molecule 18: eS10

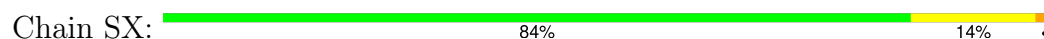
Chain SK: 72% 26%



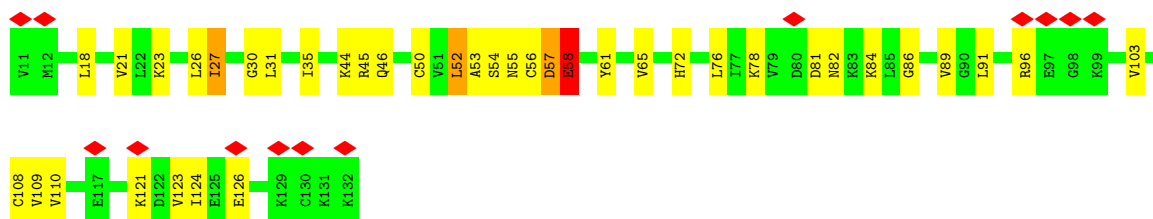
• Molecule 19: uS11



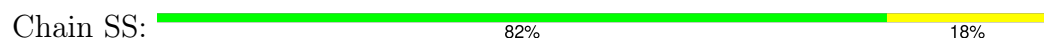
• Molecule 20: uS12



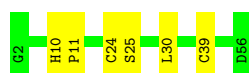
• Molecule 21: eS12



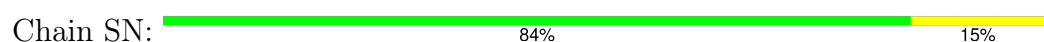
• Molecule 22: uS13



• Molecule 23: 40S ribosomal protein S29



• Molecule 24: 40S ribosomal protein S13



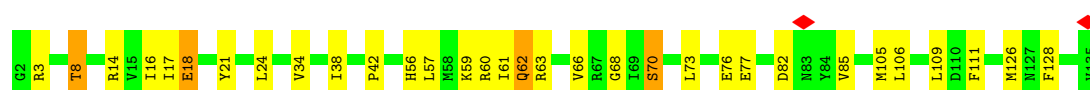
• Molecule 25: uS17

Chain SL:  82% 16%



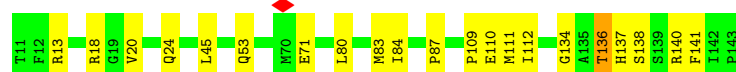
- Molecule 26: 40S ribosomal protein S17

Chain SR:  76% 21%



- Molecule 27: uS19

Chain SP:  84% 15%



- Molecule 28: 40S ribosomal protein S19

Chain ST:  88% 11%



- Molecule 29: 40S ribosomal protein S21

Chain SV:  86% 13%



- Molecule 30: 40S ribosomal protein S24

Chain SY:  6% 77% 22%



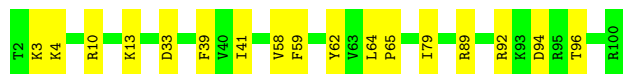
- Molecule 31: eS25

Chain SZ:  68% 31%



- Molecule 32: 40S ribosomal protein S26

Chain Sa:  83% 17%



- Molecule 33: eS27

Chain Sb:  89% 11%



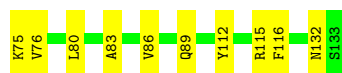
- Molecule 34: 40S ribosomal protein S28

Chain Sc:  89% 9%



- Molecule 35: 40S ribosomal protein S30

Chain Se:  83% 17%



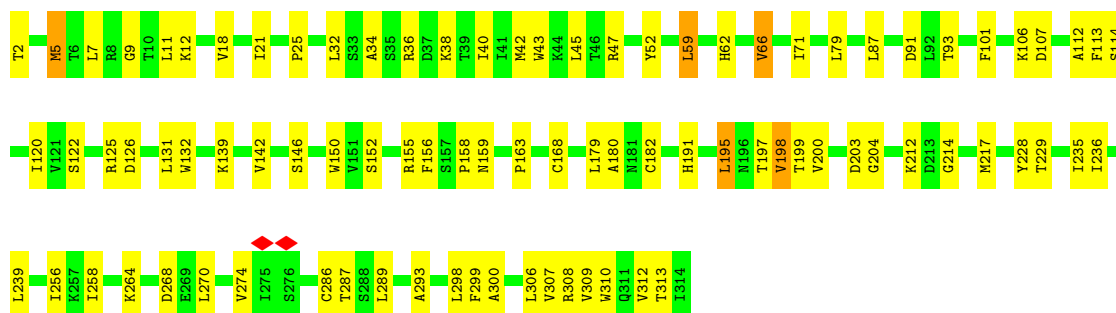
- Molecule 36: eS31

Chain Sf:  8% 72% 25%

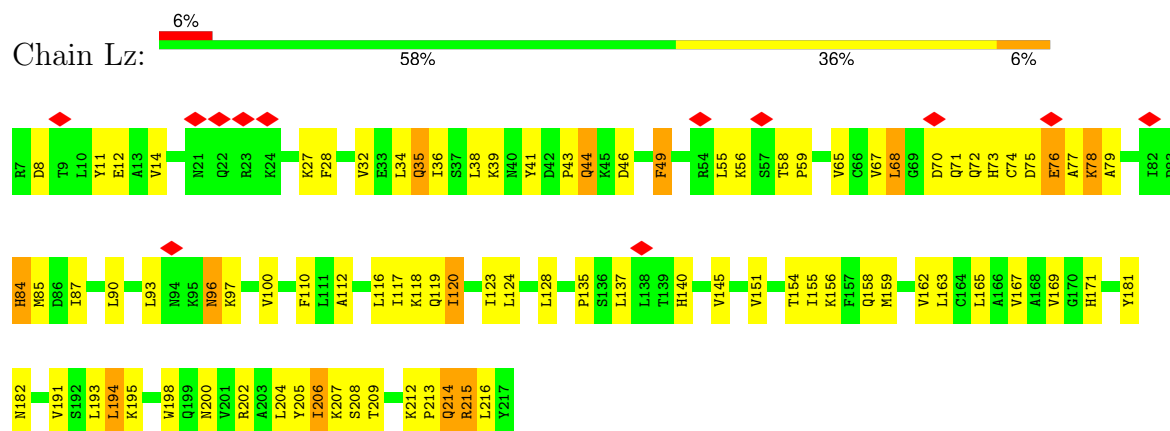


- Molecule 37: Receptor of activated protein C kinase 1

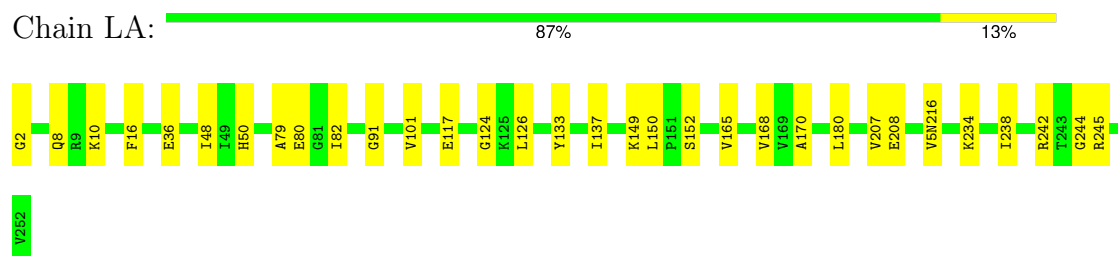
Chain Sg:  72% 27%



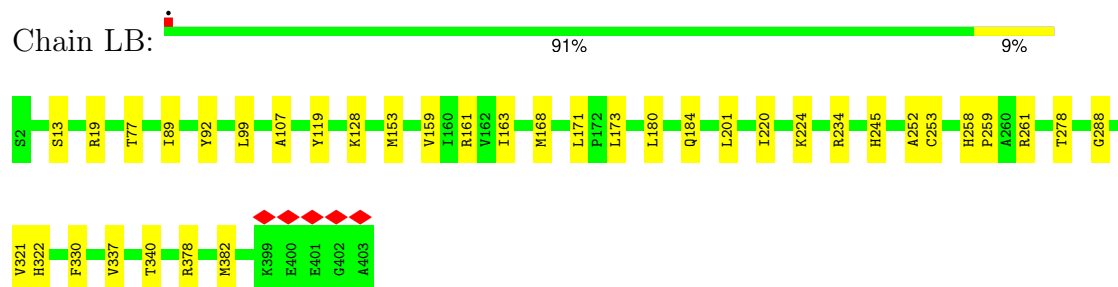
- Molecule 38: uL1



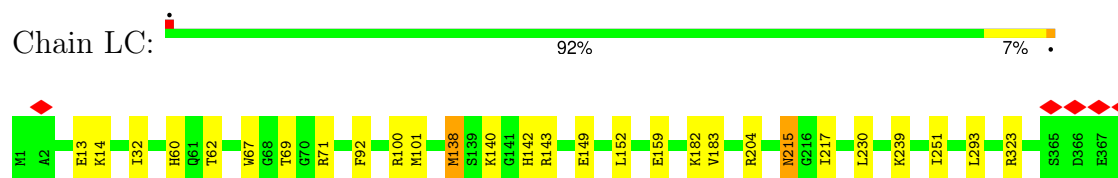
- Molecule 39: uL2



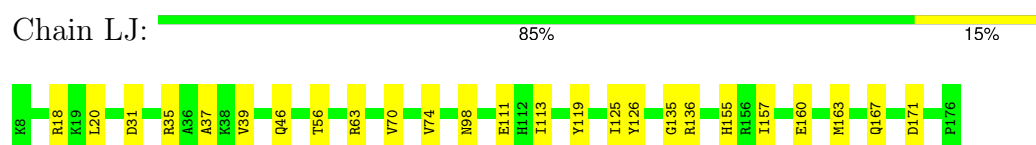
- Molecule 40: 60S ribosomal protein L3



- Molecule 41: 60S ribosomal protein L4



- Molecule 42: 60S ribosomal protein L11



- Molecule 43: 60S ribosomal protein L9

Chain LH:  90% 10%



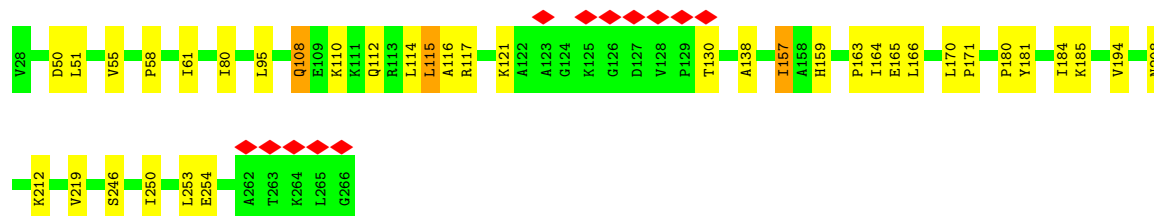
- Molecule 44: eL6

Chain LE:  90% 10%



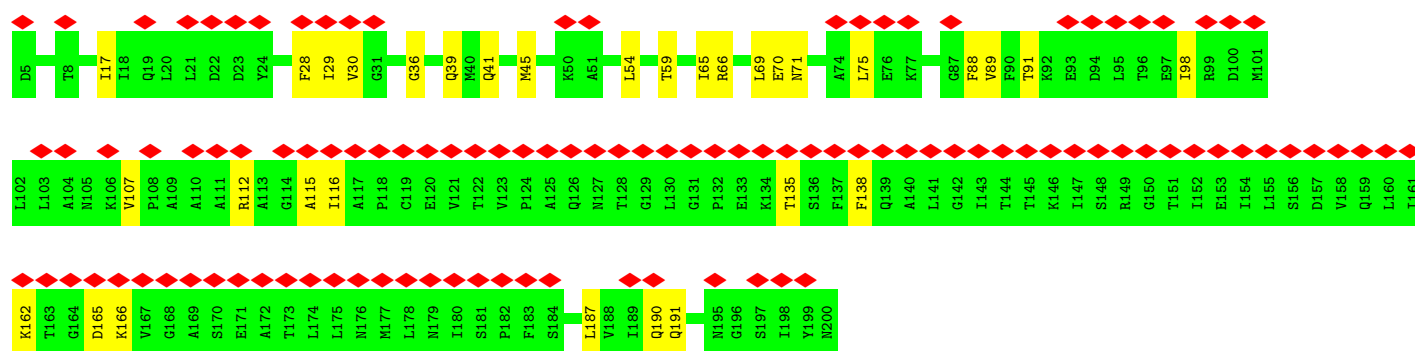
- Molecule 45: 60S ribosomal protein L7a

Chain LG:  5% 85% 14%



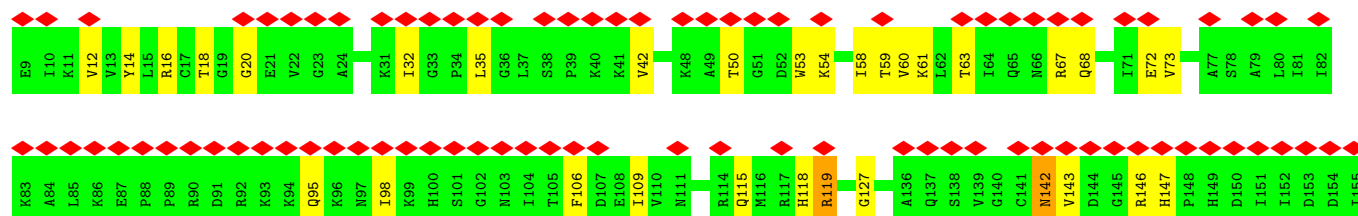
- Molecule 46: 60S acidic ribosomal protein P0

Chain Lq:  56% 84% 16%



- Molecule 47: 60S ribosomal protein L12

Chain LK:  59% 78% 20%



- Molecule 48: 60S ribosomal protein L13a

Chain LO:  89% 11%



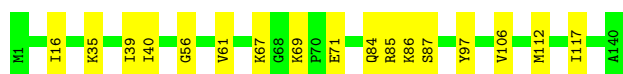
- Molecule 49: 60S ribosomal protein L13

Chain LL:  90% 10%



- Molecule 50: 60S ribosomal protein L23

Chain LV:  88% 12%



- Molecule 51: 60S ribosomal protein L14

Chain LM:  92% 8%



- Molecule 52: 60S ribosomal protein L27a

Chain La:  86% 14%



- Molecule 53: 60S ribosomal protein L15

Chain LN:  89% 11%



- Molecule 54: 60S ribosomal protein L10

Chain LI:  86% 14%



- Molecule 55: 60S ribosomal protein L5

Chain LD:  90% 10%



- Molecule 56: 60S ribosomal protein L18

Chain LQ:  89% 11%



- Molecule 57: 60S ribosomal protein L19

Chain LR:  90% 10%



- Molecule 58: 60S ribosomal protein L18a

Chain LS:  90% 10%



- Molecule 59: 60S ribosomal protein L21

Chain LT:  84% 14% ..



- Molecule 60: 60S ribosomal protein L17

Chain LP:  90% 10%



- Molecule 61: 60S ribosomal protein L22

Chain LU:  82% 16% .



- Molecule 62: uL23

Chain LX:  86% 14%



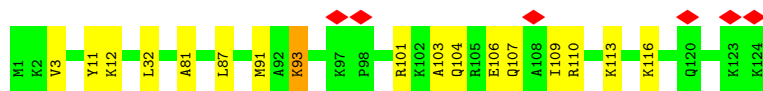
- Molecule 63: 60S ribosomal protein L26

Chain LY:  89% 10%



- Molecule 64: eL24

Chain LW:  5% 86% 14%



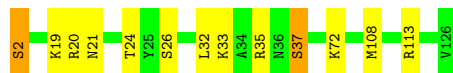
- Molecule 65: 60S ribosomal protein L27

Chain LZ:  87% 13%



- Molecule 66: 60S ribosomal protein L28

Chain Lr:  90% 9%



- Molecule 67: 60S ribosomal protein L35

Chain Lh:  93% 7%



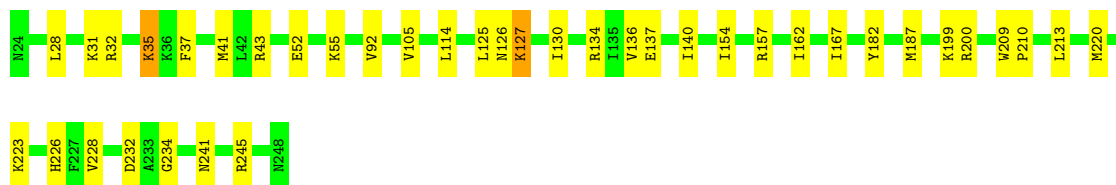
- Molecule 68: eL29

Chain Lb:  6% 86% 14%



- Molecule 69: 60S ribosomal protein L7

Chain LF:  83% 16%

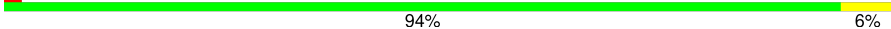


- Molecule 70: 60S ribosomal protein L30

Chain Lc:  84% 16%



- Molecule 71: 60S ribosomal protein L31

Chain Ld:  94% 6%



- Molecule 72: 60S ribosomal protein L32

Chain Le:  91% 8%



- Molecule 73: 60S ribosomal protein L35a

Chain Lf:  90% 10%



- Molecule 74: 60S ribosomal protein L34

Chain Lg:  91% 8%



- Molecule 75: 60S ribosomal protein L36

Chain Li:  94% 5%



- Molecule 76: 60S ribosomal protein L37

Chain Lj: 90% 9%



- Molecule 77: 60S ribosomal protein L38

Chain Lk: 96%



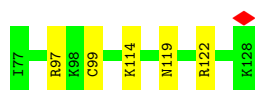
- Molecule 78: 60S ribosomal protein L39

Chain Ll: 86% 14%



- Molecule 79: eL40

Chain Lm: 90% 10%



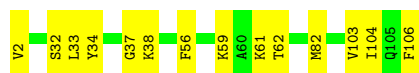
- Molecule 80: 60S ribosomal protein L41

Chain Ln: 76% 24%



- Molecule 81: Ribosomal protein L36a

Chain Lo: 87% 13%



- Molecule 82: 60S ribosomal protein L37a

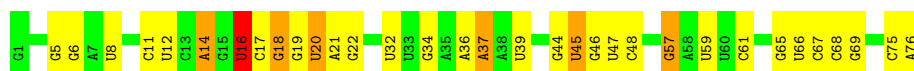
Chain Lp: 89% 11%



- Molecule 83: mRNA



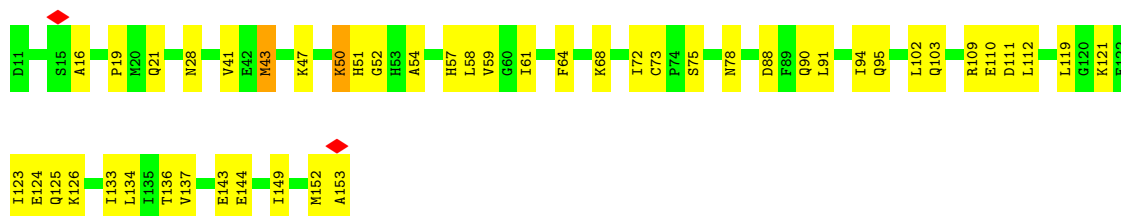
- Molecule 84: A-site tRNA Phe



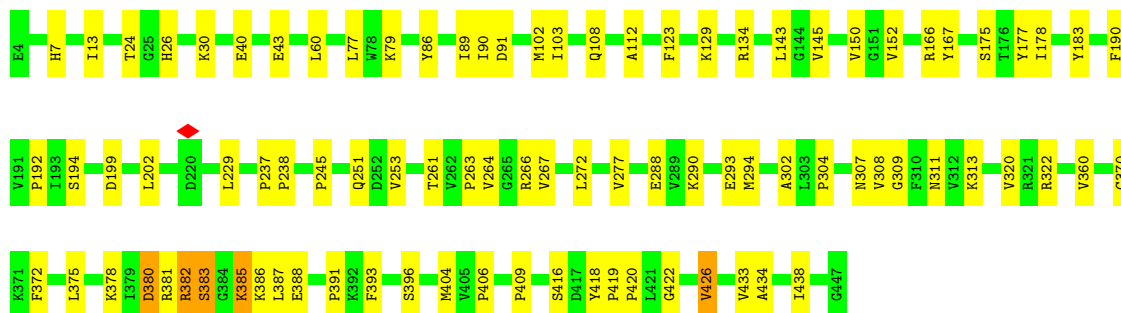
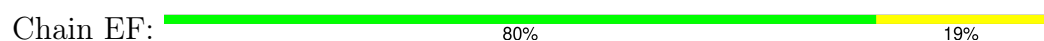
- Molecule 85: P-site tRNA fMet



- Molecule 86: eIF5A1



- Molecule 87: Elongation factor 1-alpha 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20290	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	528.64, 528.64, 528.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82600003, 0.82600003, 0.82600003	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, HIC, A2M, UR3, MLZ, UY1, 4AC, K, G7M, H2U, 6MZ, OMU, 5MC, MG, 3H3, M3L, ANM, MIA, 1MA, B8N, MA6, OMC, 4SU, MLY, V5N, SPD, OMG, 5CT, HY3, AME, ZIY, GSP, PUT, ZN, PSU

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	S2	0.38	5/38635 (0.0%)	0.55	0/60214
2	L8	0.36	0/3613	0.51	0/5627
3	L5	0.36	8/85497 (0.0%)	0.51	1/133383 (0.0%)
4	L7	0.33	0/2862	0.46	0/4459
5	SB	0.34	0/1832	0.51	0/2449
6	SA	0.39	0/1778	0.54	0/2416
7	SD	0.54	0/1784	0.72	0/2403
8	SJ	0.55	0/1550	0.90	0/2069
9	SE	0.51	0/2118	0.80	0/2849
10	SC	0.47	0/1762	0.69	0/2381
11	SG	0.47	0/1946	0.74	0/2590
12	SF	0.46	0/1515	0.69	0/2037
13	SH	0.61	0/1540	0.89	0/2064
14	SW	0.50	0/1051	0.72	0/1406
15	SI	0.40	0/1715	0.64	0/2287
16	SQ	0.63	0/1141	0.86	0/1528
17	SU	0.71	0/813	1.01	0/1092
18	SK	0.52	0/834	0.83	0/1125
19	SO	0.57	0/1022	0.92	3/1372 (0.2%)
20	SX	0.54	0/1113	0.79	0/1483
21	SM	0.68	0/950	0.93	0/1275
22	SS	0.54	0/1232	0.84	0/1651
23	Sd	0.50	0/469	0.75	0/623
24	SN	0.52	0/1242	0.76	0/1671
25	SL	0.47	0/1191	0.69	1/1593 (0.1%)
26	SR	0.61	0/1098	0.97	0/1474
27	SP	0.48	0/1116	0.69	0/1493
28	ST	0.55	0/1131	0.83	0/1515
29	SV	0.48	0/635	0.73	0/850
30	SY	0.30	0/1083	0.54	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SZ	0.60	0/682	0.95	0/911
32	Sa	0.27	0/805	0.46	0/1079
33	Sb	0.34	0/664	0.53	0/891
34	Sc	0.60	0/508	0.94	0/680
35	Se	0.49	0/473	0.76	0/623
36	Sf	0.77	0/627	1.07	0/829
37	Sg	0.57	0/2493	0.84	0/3394
38	Lz	0.86	0/1729	1.17	0/2320
39	LA	0.48	0/1947	0.69	1/2609 (0.0%)
40	LB	0.38	0/3294	0.55	0/4406
41	LC	0.38	0/2981	0.56	0/4002
42	LJ	0.40	0/1382	0.63	0/1847
43	LH	0.40	0/1538	0.60	0/2066
44	LE	0.40	0/1830	0.57	0/2453
45	LG	0.57	0/1943	0.78	0/2616
46	Lq	0.24	0/1530	0.42	0/2063
47	LK	0.45	0/1136	0.64	0/1529
48	LO	0.49	0/1682	0.71	1/2250 (0.0%)
49	LL	0.57	0/1696	0.79	0/2270
50	LV	0.48	0/1056	0.69	1/1412 (0.1%)
51	LM	0.36	0/1143	0.52	0/1527
52	La	0.42	0/1179	0.61	0/1573
53	LN	0.43	0/1745	0.65	0/2338
54	LI	0.58	0/1698	0.86	1/2266 (0.0%)
55	LD	0.42	0/2438	0.61	0/3263
56	LQ	0.39	0/1536	0.60	0/2052
57	LR	0.35	0/1582	0.55	0/2091
58	LS	0.44	0/1500	0.63	0/2013
59	LT	0.35	0/1325	0.54	0/1770
60	LP	0.42	0/1268	0.66	0/1701
61	LU	0.53	0/823	0.76	0/1103
62	LX	0.29	0/984	0.43	0/1323
63	LY	0.47	0/1132	0.68	0/1504
64	LW	0.54	0/964	0.77	0/1278
65	LZ	0.53	0/1129	0.81	0/1507
66	Lr	0.46	0/1012	0.69	0/1356
67	Lh	0.42	0/1022	0.61	0/1351
68	Lb	0.47	0/887	0.72	0/1171
69	LF	0.36	0/1905	0.54	0/2539
70	Lc	0.25	0/774	0.39	0/1038
71	Ld	0.50	0/904	0.76	0/1216
72	Le	0.52	0/1071	0.66	0/1429
73	Lf	0.34	0/895	0.45	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Lg	0.43	0/916	0.63	0/1220
75	Li	0.62	0/844	0.91	0/1115
76	Lj	0.41	0/731	0.63	0/967
77	Lk	0.40	0/575	0.65	0/761
78	Ll	0.65	0/453	0.85	0/599
79	Lm	0.39	0/426	0.76	0/564
80	Ln	0.46	0/240	0.84	0/305
81	Lo	0.39	0/877	0.60	0/1156
82	Lp	0.38	0/718	0.58	0/953
83	mR	0.21	0/280	0.33	0/433
84	At	0.37	1/1650 (0.1%)	0.48	0/2566
85	Pt	0.43	1/1721 (0.1%)	0.55	0/2679
86	5A	0.58	0/1088	0.83	1/1463 (0.1%)
87	EF	0.39	0/3428	0.59	0/4644
All	All	0.42	15/237127 (0.0%)	0.60	10/347099 (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
87	EF	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	Pt	47	G7M	O3'-P	9.64	1.65	1.56
1	S2	166	A2M	O3'-P	7.68	1.64	1.56
3	L5	3785	A2M	O3'-P	6.77	1.63	1.56
1	S2	1288	OMU	O3'-P	6.53	1.62	1.56
3	L5	3825	A2M	O3'-P	6.02	1.62	1.56
84	At	8	4SU	O3'-P	5.97	1.62	1.56
3	L5	3718	A2M	O3'-P	5.90	1.62	1.56
1	S2	668	A2M	O3'-P	5.74	1.61	1.56
3	L5	3867	A2M	O3'-P	5.71	1.61	1.56
3	L5	398	A2M	O3'-P	5.64	1.61	1.56
3	L5	4571	A2M	O3'-P	5.55	1.61	1.56
3	L5	1326	A2M	O3'-P	5.46	1.61	1.56
1	S2	484	A2M	O3'-P	5.24	1.61	1.56
3	L5	3760	A2M	O3'-P	5.21	1.61	1.56
1	S2	27	A2M	O3'-P	5.14	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	LI	81	GLY	CA-C-O	-6.63	117.53	122.37
50	LV	40	ILE	N-CA-C	-6.47	107.56	113.71
19	SO	138	ASP	CB-CA-C	6.21	122.78	110.42
86	5A	16	ALA	N-CA-C	-5.70	105.07	111.28
19	SO	137	SER	N-CA-C	-5.67	103.65	111.81
39	LA	244	GLY	CA-C-O	-5.56	118.13	122.52
3	L5	2098	G	C4'-C3'-O3'	-5.22	101.58	109.40
48	LO	109	PRO	CB-CA-C	-5.20	104.58	110.92
25	SL	50	ALA	N-CA-C	-5.18	107.09	113.41
19	SO	146	ARG	N-CA-C	-5.01	106.68	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
87	EF	381	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36364	0	18406	348	0
2	L8	3320	0	1686	26	0
3	L5	79168	0	40078	605	0
4	L7	2562	0	1295	13	0
5	SB	1806	0	1888	17	0
6	SA	1750	0	1755	28	0
7	SD	1756	0	1852	34	0
8	SJ	1525	0	1640	29	0
9	SE	2076	0	2177	39	0
10	SC	1725	0	1813	21	0
11	SG	1923	0	2089	25	0
12	SF	1494	0	1549	20	0
13	SH	1517	0	1605	30	0
14	SW	1034	0	1080	17	0
15	SI	1686	0	1772	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	SQ	1123	0	1193	17	0
17	SU	803	0	873	16	0
18	SK	810	0	836	22	0
19	SO	1009	0	1034	9	0
20	SX	1105	0	1167	20	0
21	SM	940	0	965	33	0
22	SS	1214	0	1275	23	0
23	Sd	458	0	448	3	0
24	SN	1214	0	1301	16	0
25	SL	1171	0	1241	14	0
26	SR	1083	0	1137	23	0
27	SP	1093	0	1139	13	0
28	ST	1112	0	1146	11	0
29	SV	639	0	638	5	0
30	SY	1065	0	1142	20	0
31	SZ	674	0	748	18	0
32	Sa	792	0	841	12	0
33	Sb	650	0	672	8	0
34	Sc	506	0	536	7	0
35	Se	467	0	516	9	0
36	Sf	615	0	639	12	0
37	Sg	2436	0	2393	51	0
38	Lz	1701	0	1810	68	0
39	LA	1922	0	2015	17	0
40	LB	3239	0	3377	27	0
41	LC	2927	0	3104	20	0
42	LJ	1359	0	1396	13	0
43	LH	1519	0	1601	10	0
44	LE	1793	0	1958	18	0
45	LG	1910	0	2052	22	0
46	Lq	1507	0	1562	20	0
47	LK	1122	0	1184	19	0
48	LO	1650	0	1794	14	0
49	LL	1665	0	1773	13	0
50	LV	1042	0	1109	10	0
51	LM	1121	0	1187	7	0
52	La	1163	0	1206	14	0
53	LN	1700	0	1749	16	0
54	LI	1660	0	1710	15	0
55	LD	2392	0	2426	21	0
56	LQ	1512	0	1628	11	0
57	LR	1566	0	1729	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	LS	1460	0	1502	14	0
59	LT	1297	0	1366	20	0
60	LP	1242	0	1269	10	0
61	LU	809	0	831	10	0
62	LX	967	0	1040	11	0
63	LY	1115	0	1205	8	0
64	LW	950	0	999	16	0
65	LZ	1106	0	1182	9	0
66	Lr	1006	0	1072	8	0
67	Lh	1014	0	1148	5	0
68	Lb	885	0	967	10	0
69	LF	1870	0	1996	27	0
70	Lc	764	0	804	10	0
71	Ld	889	0	930	4	0
72	Le	1053	0	1147	6	0
73	Lf	876	0	910	9	0
74	Lg	906	0	998	8	0
75	Li	833	0	917	5	0
76	Lj	712	0	744	9	0
77	Lk	569	0	637	1	0
78	Ll	443	0	483	5	0
79	Lm	432	0	470	2	0
80	Ln	239	0	289	4	0
81	Lo	870	0	936	20	0
82	Lp	708	0	756	6	0
83	mR	252	0	127	8	0
84	At	1630	0	839	12	0
85	Pt	1645	0	843	8	0
86	5A	1089	0	1096	33	0
87	EF	3405	0	3465	57	0
88	L5	90	0	171	3	0
88	S2	10	0	19	0	0
89	L5	30	0	0	0	0
89	L7	1	0	0	0	0
89	L8	1	0	0	0	0
89	LA	1	0	0	0	0
89	LB	1	0	0	0	0
89	Lf	1	0	0	0	0
89	S2	9	0	0	0	0
89	mR	1	0	0	0	0
90	At	1	0	0	0	0
90	EF	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	L5	284	0	0	0	0
90	L7	5	0	0	0	0
90	L8	6	0	0	0	0
90	LA	1	0	0	0	0
90	LB	1	0	0	0	0
90	LC	1	0	0	0	0
90	LH	1	0	0	0	0
90	LI	1	0	0	0	0
90	LJ	1	0	0	0	0
90	LN	1	0	0	0	0
90	LP	1	0	0	0	0
90	LS	1	0	0	0	0
90	LV	1	0	0	0	0
90	LW	1	0	0	0	0
90	Le	1	0	0	0	0
90	Lg	2	0	0	0	0
90	Lj	1	0	0	0	0
90	Lr	1	0	0	0	0
90	Pt	2	0	0	0	0
90	S2	108	0	0	0	0
90	SE	1	0	0	0	0
90	SG	1	0	0	0	0
90	SO	1	0	0	0	0
90	ST	1	0	0	0	0
90	SX	2	0	0	0	0
90	Sa	1	0	0	0	0
90	Sd	1	0	0	0	0
90	mR	1	0	0	0	0
91	L5	19	0	18	0	0
92	L5	48	0	96	0	0
93	L5	33	0	35	13	0
94	Lg	1	0	0	0	0
94	Lj	1	0	0	0	0
94	Lm	1	0	0	0	0
94	Lo	1	0	0	0	0
94	Lp	1	0	0	0	0
94	Sa	1	0	0	0	0
94	Sd	1	0	0	0	0
94	Sf	1	0	0	0	0
95	At	11	0	8	0	0
96	Pt	8	0	8	0	0
97	EF	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
98	EF	79	0	0	0	0
99	EF	3	0	0	0	0
99	L5	304	0	0	4	0
99	L7	3	0	0	0	0
99	L8	4	0	0	0	0
99	LA	1	0	0	0	0
99	LB	3	0	0	0	0
99	LC	2	0	0	0	0
99	LF	1	0	0	0	0
99	LI	1	0	0	0	0
99	LM	1	0	0	0	0
99	LO	1	0	0	0	0
99	LP	3	0	0	0	0
99	LQ	1	0	0	0	0
99	LV	1	0	0	0	0
99	La	4	0	0	0	0
99	Lb	1	0	0	0	0
99	Li	1	0	0	0	0
99	Lj	2	0	0	0	0
99	Lo	2	0	0	0	0
99	Lr	1	0	0	0	0
99	S2	21	0	0	0	0
99	SE	1	0	0	0	0
99	SN	1	0	0	0	0
99	SS	1	0	0	0	0
99	Sa	1	0	0	0	0
All	All	227372	0	170270	2085	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2085) 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)
93:L5:5119:3H3:H3	81:Lo:59:LYS:NZ	1.63	1.14
1:S2:327:G:H2'	1:S2:329:G:H5''	1.40	1.03
93:L5:5119:3H3:H3	81:Lo:59:LYS:CE	1.90	1.01
9:SE:198:ARG:HG3	9:SE:208:VAL:HG22	1.48	0.94
21:SM:81:ASP:HB2	21:SM:84:LYS:HB2	1.50	0.93
99:L5:5664:HOH:O	52:La:32:ARG:HD2	1.70	0.92
3:L5:2097:U:H2'	3:L5:2098:G:H3'	1.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SH:160:LYS:HD2	13:SH:191:GLU:HA	1.53	0.88
17:SU:24:LEU:HB2	17:SU:87:ARG:HB2	1.60	0.84
85:Pt:17:C:H1'	86:5A:28:ASN:HD21	1.45	0.82
46:Lq:190:GLN:HG3	46:Lq:191:GLN:HG2	1.62	0.81
21:SM:76:LEU:HD21	21:SM:78:LYS:HG3	1.60	0.81
1:S2:560:A:H5'	8:SJ:174:LYS:HB2	1.63	0.81
81:Lo:62:THR:HG22	86:5A:19:PRO:HD2	1.63	0.81
38:Lz:207:LYS:HG3	38:Lz:213:PRO:HD2	1.64	0.80
21:SM:81:ASP:CB	21:SM:84:LYS:HB2	2.11	0.80
3:L5:1242:G:H4'	68:Lb:122:LYS:HA	1.63	0.80
38:Lz:90:LEU:HD21	38:Lz:124:LEU:HD12	1.62	0.80
38:Lz:68:LEU:HD11	38:Lz:77:ALA:HB2	1.65	0.79
37:Sg:87:LEU:HB2	37:Sg:101:PHE:HB2	1.64	0.79
21:SM:35:ILE:HD12	36:Sf:102:VAL:HG21	1.64	0.78
3:L5:4530:UR3:H2'	3:L5:4531:PSU:H2'	1.64	0.78
36:Sf:126:CYS:HB2	36:Sf:130:VAL:HG21	1.66	0.78
93:L5:5119:3H3:H3	81:Lo:59:LYS:HZ1	1.45	0.78
13:SH:137:SER:HA	13:SH:162:GLN:HG3	1.66	0.77
3:L5:3946:G:H1	3:L5:4067:U:H3	1.32	0.77
1:S2:1285:G:O6	21:SM:56:CYS:HA	1.83	0.77
1:S2:16:G:H2'	1:S2:17:C:C6	2.21	0.75
38:Lz:77:ALA:HB3	38:Lz:84:HIS:HB3	1.69	0.74
18:SK:21:MET:HG3	18:SK:49:MET:HE3	1.68	0.74
1:S2:1639:G7M:H2'	1:S2:1640:A:C8	2.23	0.73
87:EF:245:PRO:HG2	87:EF:418:TYR:OH	1.89	0.73
10:SC:171:GLY:HA2	14:SW:98:GLN:HE22	1.54	0.73
22:SS:98:VAL:HG11	22:SS:106:LYS:HG3	1.70	0.73
6:SA:134:LEU:HD22	6:SA:144:THR:HG21	1.71	0.72
1:S2:925:G:H1	1:S2:1017:U:H3	1.37	0.72
93:L5:5119:3H3:C8	81:Lo:59:LYS:CE	2.67	0.72
46:Lq:29:ILE:HB	46:Lq:191:GLN:HG3	1.72	0.71
26:SR:17:ILE:HG21	26:SR:61:ILE:HD12	1.72	0.70
46:Lq:91:THR:HG21	46:Lq:98:ILE:HG12	1.73	0.70
19:SO:53:ILE:HG23	19:SO:88:LEU:HD23	1.74	0.69
65:LZ:46:ILE:HG23	65:LZ:68:ILE:HG23	1.74	0.69
43:LH:115:ARG:HG2	43:LH:123:ILE:HG12	1.75	0.69
3:L5:1703:C:H2'	3:L5:1704:C:O4'	1.92	0.69
3:L5:3697:U:H2'	39:LA:245:ARG:HH22	1.57	0.68
1:S2:944:A:H5''	19:SO:134:PRO:HB2	1.75	0.68
87:EF:294:MET:HB2	87:EF:308:VAL:HG12	1.76	0.68
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:928:G:H1	1:S2:1013:U:H3	1.41	0.68
18:SK:84:HIS:ND1	21:SM:27:ILE:HG13	2.08	0.68
84:At:14:A:H61	84:At:21:A:H1'	1.59	0.68
38:Lz:14:VAL:HB	38:Lz:214:GLN:HE21	1.58	0.67
38:Lz:119:GLN:HG3	38:Lz:123:ILE:HB	1.76	0.67
87:EF:419:PRO:HB2	87:EF:420:PRO:HD3	1.76	0.67
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.30	0.67
37:Sg:79:LEU:HB2	37:Sg:113:PHE:CZ	2.28	0.67
1:S2:327:G:H2'	1:S2:329:G:C5'	2.21	0.67
47:LK:50:THR:HB	47:LK:53:TRP:HD1	1.59	0.67
86:5A:91:LEU:HD21	86:5A:94:ILE:HD11	1.76	0.67
49:LL:58:ILE:HD12	49:LL:116:ARG:HD2	1.77	0.67
55:LD:211:LEU:HB3	55:LD:219:TYR:HB2	1.77	0.67
3:L5:37:U:H5''	52:La:32:ARG:HD3	1.76	0.66
46:Lq:17:ILE:HG22	46:Lq:54:LEU:HD21	1.77	0.66
1:S2:328:U:H5'	64:LW:109:ILE:HD11	1.76	0.66
37:Sg:32:LEU:HD21	37:Sg:42:MET:HG2	1.78	0.66
3:L5:1590:C:H4'	3:L5:2857:A:H5'	1.78	0.65
1:S2:190:G:H1'	1:S2:209:A:H61	1.62	0.65
18:SK:1:MET:HE1	18:SK:43:LEU:HG	1.78	0.65
1:S2:888:U:H1'	1:S2:889:U:H2'	1.79	0.65
3:L5:4896:G:N2	3:L5:4926:C:H41	1.94	0.65
93:L5:5119:3H3:C8	81:Lo:59:LYS:NZ	2.53	0.65
3:L5:5025:C:H2'	3:L5:5026:U:H4'	1.79	0.65
40:LB:107:ALA:HB2	40:LB:201:LEU:HD22	1.77	0.65
3:L5:1447:C:H1'	3:L5:2098:G:H22	1.61	0.65
3:L5:32:G:H21	3:L5:50:C:H5	1.45	0.65
3:L5:4896:G:H21	3:L5:4926:C:H41	1.44	0.65
37:Sg:5:MET:HE2	37:Sg:312:VAL:HG12	1.78	0.65
13:SH:163:GLN:HG2	13:SH:167:GLU:HG3	1.78	0.65
53:LN:138:PHE:HA	53:LN:143:ARG:HD2	1.78	0.65
1:S2:582:U:H2'	1:S2:583:A:H8	1.62	0.65
1:S2:1520:G:N3	1:S2:1520:G:H2'	2.13	0.64
27:SP:137:HIS:HA	27:SP:140:ARG:HG2	1.80	0.64
93:L5:5119:3H3:C8	81:Lo:59:LYS:HE3	2.27	0.64
64:LW:101:ARG:HA	64:LW:104:GLN:OE1	1.98	0.64
11:SG:70:HIS:HB3	11:SG:103:ASP:OD2	1.98	0.64
59:LT:121:GLU:O	59:LT:122:LYS:HB2	1.97	0.64
66:Lr:35:ARG:HG3	66:Lr:37:SER:HB3	1.80	0.64
9:SE:105:THR:CG2	9:SE:245:ARG:HA	2.28	0.63
37:Sg:168:CYS:HB3	37:Sg:198:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:LL:58:ILE:CD1	49:LL:116:ARG:HD2	2.28	0.63
86:5A:47:LYS:HA	86:5A:54:ALA:HA	1.80	0.63
1:S2:1536:G:H2'	1:S2:1537:A:C8	2.32	0.63
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.33	0.63
3:L5:2786:C:H5''	3:L5:2787:A2M:H5'	1.81	0.63
10:SC:196:ILE:HB	10:SC:223:TYR:HB2	1.81	0.63
3:L5:451:C:H2'	3:L5:1294:A:C8	2.33	0.63
18:SK:7:ASN:ND2	18:SK:40:VAL:HG22	2.13	0.63
38:Lz:49:PHE:HB2	38:Lz:193:LEU:HD13	1.79	0.63
69:LF:182:TYR:HB3	69:LF:200:ARG:HG3	1.80	0.63
3:L5:4733:C:H4'	3:L5:4734:A:H5'	1.80	0.62
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.35	0.62
12:SF:128:ILE:HD11	34:Sc:22:GLY:HA2	1.81	0.62
38:Lz:68:LEU:HD11	38:Lz:77:ALA:CB	2.29	0.62
87:EF:382:ARG:HB3	87:EF:382:ARG:HH21	1.63	0.62
1:S2:92:A:O2'	9:SE:4:GLY:HA3	1.98	0.62
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.80	0.62
3:L5:3975:C:H2'	3:L5:4036:G:H1	1.63	0.62
9:SE:201:HIS:HB2	9:SE:204:SER:HB3	1.80	0.62
38:Lz:77:ALA:CB	38:Lz:84:HIS:HB3	2.28	0.62
1:S2:1824:A:OP1	20:SX:60:LYS:HA	1.99	0.62
7:SD:47:GLU:HG2	7:SD:87:TYR:HE2	1.64	0.62
9:SE:45:ILE:HG13	9:SE:61:VAL:HG21	1.82	0.62
22:SS:23:ARG:HG2	31:SZ:48:VAL:CG1	2.30	0.62
1:S2:1650:A:H5''	16:SQ:139:ALA:HB2	1.80	0.62
11:SG:70:HIS:HA	11:SG:98:ARG:HH12	1.64	0.62
20:SX:140:ARG:O	20:SX:142:ARG:HG3	2.00	0.61
38:Lz:75:ASP:HA	38:Lz:78:LYS:HD2	1.81	0.61
40:LB:220:ILE:HG12	40:LB:278:THR:HG23	1.82	0.61
1:S2:582:U:H2'	1:S2:583:A:C8	2.35	0.61
17:SU:21:ARG:HA	17:SU:89:ILE:O	2.00	0.61
58:LS:15:ARG:HB3	58:LS:27:LEU:HD23	1.80	0.61
21:SM:58:GLU:HG2	21:SM:58:GLU:O	1.99	0.61
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.82	0.61
83:mR:36[A]:U:H2'	83:mR:37:A:C8	2.35	0.61
37:Sg:87:LEU:HD21	37:Sg:122:SER:HB3	1.82	0.61
1:S2:190:G:H1'	1:S2:209:A:N6	2.15	0.61
9:SE:175:PHE:HE2	9:SE:198:ARG:HD2	1.65	0.61
20:SX:68:LYS:HE2	35:Se:83:ALA:HB2	1.81	0.61
1:S2:1444:U:H2'	1:S2:1445:PSU:C6	2.35	0.61
30:SY:15:ASN:HD21	30:SY:18:LEU:HD23	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1706:G:H5'	80:Ln:1:MET:HB2	1.83	0.61
13:SH:73:GLN:HE21	13:SH:135:PHE:HD1	1.46	0.61
38:Lz:32:VAL:HG22	38:Lz:208:SER:HB3	1.82	0.61
5:SB:33:VAL:HG12	5:SB:44:ILE:HD13	1.82	0.61
32:Sa:64:LEU:HD12	32:Sa:65:PRO:HD2	1.83	0.61
3:L5:1739:G:H5''	4:L7:102:U:H1'	1.83	0.60
7:SD:40:ARG:HA	7:SD:40:ARG:HH11	1.64	0.60
20:SX:68:LYS:HE3	35:Se:80:LEU:HA	1.82	0.60
69:LF:105:VAL:HG13	69:LF:136:VAL:HG12	1.83	0.60
3:L5:184:U:H2'	3:L5:186:G:H1'	1.83	0.60
13:SH:84:GLU:HG3	13:SH:92:VAL:HG22	1.82	0.60
39:LA:234:LYS:HG2	39:LA:238:ILE:HG12	1.83	0.60
81:Lo:56:PHE:HE2	81:Lo:59:LYS:HD3	1.67	0.60
2:L8:86:U:H3'	2:L8:87:G:H5'	1.83	0.60
1:S2:1444:U:H2'	1:S2:1445:PSU:H6	1.66	0.60
3:L5:2458:C:H5''	53:LN:67:ARG:HD2	1.84	0.60
70:Lc:20:LEU:HB3	70:Lc:102:SER:HB3	1.84	0.60
1:S2:1740:C:H5''	15:SI:58:LEU:HD21	1.83	0.60
3:L5:4731:G:H1'	3:L5:4732:G:C2	2.37	0.60
37:Sg:113:PHE:O	37:Sg:156:PHE:HD2	1.84	0.60
39:LA:36:GLU:HG3	39:LA:91:GLY:HA2	1.83	0.60
12:SF:76:MET:HB2	12:SF:89:THR:HG21	1.82	0.60
60:LP:128:ARG:HH21	60:LP:136:ILE:HD13	1.67	0.60
1:S2:1587:G:H5''	28:ST:77:LYS:HD2	1.84	0.59
54:LI:51:HIS:CD2	54:LI:168:SER:HB2	2.37	0.59
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.37	0.59
18:SK:84:HIS:HB3	21:SM:27:ILE:HG23	1.83	0.59
1:S2:543:C:H3'	1:S2:544:G:H8	1.68	0.59
38:Lz:215:ARG:C	38:Lz:215:ARG:HD2	2.28	0.59
48:LO:37:ARG:HD2	48:LO:108:ILE:HD11	1.84	0.59
87:EF:77:LEU:HG	87:EF:90:ILE:HG13	1.82	0.59
5:SB:171:ILE:HD13	5:SB:174:ARG:HH12	1.66	0.59
38:Lz:120:ILE:HD12	38:Lz:124:LEU:HD13	1.83	0.59
3:L5:2008:U:H1'	3:L5:2011:C:H5	1.68	0.59
3:L5:4060:U:H2'	3:L5:4061:G:C8	2.38	0.59
3:L5:4521:PSU:H1'	40:LB:253:CYS:SG	2.43	0.59
8:SJ:82:VAL:HG21	8:SJ:92:MET:HE1	1.83	0.59
3:L5:4385:A:C4	86:5A:50:5CT:H13	2.37	0.59
15:SI:57:ALA:HB2	15:SI:183:GLY:HA2	1.85	0.59
16:SQ:53:GLU:HB2	16:SQ:54:PRO:HD3	1.83	0.59
87:EF:386:LYS:O	87:EF:387:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SD:220:THR:HG23	7:SD:221:THR:HG23	1.85	0.59
20:SX:140:ARG:O	20:SX:142:ARG:N	2.35	0.59
21:SM:121:LYS:HA	21:SM:124:ILE:HG12	1.84	0.59
12:SF:76:MET:HB2	12:SF:89:THR:CG2	2.32	0.58
1:S2:1401:A:H2'	1:S2:1402:A:C8	2.38	0.58
37:Sg:25:PRO:HA	37:Sg:293:ALA:HB2	1.84	0.58
75:Li:80:HIS:HE2	75:Li:84:LYS:HE2	1.66	0.58
87:EF:108:GLN:HB2	87:EF:266:ARG:HD3	1.86	0.58
28:ST:115:LYS:HA	28:ST:121:ARG:HG3	1.85	0.58
13:SH:130:LEU:HD21	13:SH:156:VAL:HG21	1.85	0.58
46:Lq:66:ARG:HA	46:Lq:69:LEU:HD23	1.86	0.58
47:LK:143:VAL:HG23	47:LK:147:HIS:CE1	2.38	0.58
57:LR:109:TYR:HB3	57:LR:115:ILE:HG12	1.85	0.58
87:EF:266:ARG:HA	87:EF:307:ASN:HA	1.85	0.58
87:EF:272:LEU:HB3	87:EF:302:ALA:HB3	1.85	0.58
1:S2:545:A:H2'	1:S2:546:G:C8	2.38	0.58
3:L5:260:C:H2'	3:L5:261:G:H5'	1.86	0.58
3:L5:667:A:H2'	3:L5:668:C:C6	2.38	0.58
37:Sg:236:ILE:HG21	37:Sg:239:LEU:HD23	1.86	0.58
47:LK:12:VAL:HG22	47:LK:63:THR:HG22	1.84	0.58
3:L5:162:A:H2'	3:L5:163:A:C8	2.39	0.58
3:L5:4918:C:H2'	3:L5:4919:G:H8	1.69	0.58
6:SA:137:ALA:HB1	6:SA:142:LEU:HB3	1.84	0.58
32:Sa:59:PHE:HB2	32:Sa:62:TYR:HB2	1.86	0.58
1:S2:433:A:H5''	15:SI:22:HIS:HB3	1.85	0.58
21:SM:52:LEU:HD23	21:SM:78:LYS:HG2	1.85	0.58
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.19	0.58
3:L5:1995:G:H5''	3:L5:1996:C:H5	1.68	0.58
3:L5:3603:G:H2'	3:L5:3604:A:C8	2.38	0.58
3:L5:3950:U:H2'	3:L5:3951:G:C8	2.39	0.58
38:Lz:207:LYS:HG3	38:Lz:213:PRO:CD	2.34	0.58
1:S2:1017:U:H5'	24:SN:55:ARG:HD3	1.85	0.58
3:L5:930:G:H2'	3:L5:931:C:C6	2.39	0.58
1:S2:1438:A:H2'	1:S2:1439:A:C8	2.39	0.57
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.39	0.57
3:L5:3712:A:H2'	3:L5:3713:U:C6	2.38	0.57
30:SY:125:VAL:HG12	30:SY:129:LYS:HE2	1.85	0.57
37:Sg:299:PHE:HD1	37:Sg:309:VAL:HG12	1.69	0.57
40:LB:163:ILE:HG22	40:LB:180:LEU:HD11	1.86	0.57
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.39	0.57
9:SE:31:PRO:HG2	9:SE:38:LEU:HG	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:181:CYS:HB3	9:SE:195:ILE:HD11	1.86	0.57
1:S2:1052:A:H2'	1:S2:1053:C:O4'	2.05	0.57
3:L5:454:U:H3	3:L5:702:U:H3	1.52	0.57
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.39	0.57
93:L5:5119:3H3:H3	81:Lo:59:LYS:HZ2	1.63	0.57
86:5A:88:ASP:HB3	86:5A:136:THR:HG22	1.86	0.57
11:SG:145:PHE:HD2	64:LW:93:LYS:HB2	1.70	0.57
37:Sg:163:PRO:HB2	37:Sg:179:LEU:HB2	1.86	0.57
63:LY:10:ASP:HB3	63:LY:13:LYS:HB2	1.87	0.57
1:S2:546:G:H2'	1:S2:547:G:C8	2.40	0.57
3:L5:2478:C:H2'	3:L5:2479:G:C8	2.39	0.57
22:SS:117:ILE:HD13	27:SP:110:GLU:HB2	1.86	0.57
27:SP:20:VAL:HG13	27:SP:24:GLN:HG3	1.86	0.57
44:LE:149:ILE:HD12	44:LE:271:LEU:HD21	1.87	0.57
1:S2:321:C:H2'	1:S2:322:C:C6	2.39	0.57
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.87	0.57
11:SG:67:VAL:HB	11:SG:99:GLY:HA2	1.87	0.57
44:LE:192[A]:LYS:HE3	73:Lf:107:PRO:HB3	1.85	0.57
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.40	0.57
3:L5:1960:A:H4'	46:Lq:59:THR:HB	1.87	0.57
16:SQ:112:LEU:HD22	16:SQ:119:LEU:HD13	1.86	0.57
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.40	0.56
6:SA:7:VAL:HG13	6:SA:8:LEU:HG	1.86	0.56
13:SH:53:VAL:HG11	13:SH:172:THR:HA	1.86	0.56
18:SK:31:LYS:HG2	18:SK:39:ASN:HA	1.87	0.56
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.34	0.56
6:SA:77:ILE:HG12	6:SA:99:ILE:HB	1.86	0.56
3:L5:4859:C:H3'	3:L5:4860:G:H8	1.70	0.56
10:SC:167:ARG:HG2	10:SC:219:ILE:HD13	1.87	0.56
16:SQ:45:ARG:HG2	16:SQ:48:GLN:HE21	1.71	0.56
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.41	0.56
2:L8:70:G:H5''	63:LY:27:ARG:CZ	2.36	0.56
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.40	0.56
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.39	0.56
6:SA:30:LEU:HB2	6:SA:47:TYR:CE2	2.40	0.56
26:SR:106:LEU:HA	26:SR:109:LEU:HB2	1.86	0.56
39:LA:137:ILE:HD11	39:LA:149:LYS:HB2	1.87	0.56
45:LG:110:LYS:O	45:LG:114:LEU:HG	2.05	0.56
1:S2:328:U:H5'	64:LW:109:ILE:CD1	2.36	0.56
22:SS:59:LEU:HG	22:SS:63:GLU:HG3	1.87	0.56
55:LD:208:MET:HB2	55:LD:233:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.70	0.56
37:Sg:11:LEU:HB2	37:Sg:307:VAL:HB	1.87	0.56
43:LH:174:LYS:HG2	43:LH:175:PHE:H	1.71	0.56
54:LI:152:LEU:HB3	54:LI:165:ILE:HD12	1.87	0.56
87:EF:426:VAL:HG22	87:EF:433:VAL:HB	1.88	0.56
1:S2:1824:A:H5''	20:SX:58:GLU:OE1	2.06	0.56
3:L5:495:C:H2'	3:L5:496:G:C8	2.41	0.56
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.40	0.56
27:SP:136:THR:HG21	85:Pt:30:G:OP1	2.05	0.56
49:LL:164:GLU:HG2	49:LL:164:GLU:O	2.06	0.56
55:LD:208:MET:HE2	55:LD:236:MET:HE1	1.86	0.56
75:Li:80:HIS:NE2	75:Li:84:LYS:HE2	2.20	0.56
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.41	0.56
48:LO:34:VAL:HG22	48:LO:103:LYS:HB2	1.88	0.56
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.40	0.56
38:Lz:120:ILE:HA	38:Lz:124:LEU:HB3	1.86	0.56
38:Lz:205:TYR:CE2	38:Lz:215:ARG:HD3	2.41	0.56
3:L5:982:U:H2'	3:L5:983:C:C6	2.41	0.56
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.41	0.56
11:SG:98:ARG:NH2	11:SG:103:ASP:HB2	2.21	0.56
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.41	0.55
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.05	0.55
38:Lz:120:ILE:CG2	38:Lz:128:LEU:HD12	2.36	0.55
1:S2:1588:A:H2'	1:S2:1589:A:C8	2.41	0.55
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.41	0.55
3:L5:4520:G:N2	40:LB:253:CYS:SG	2.79	0.55
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.41	0.55
25:SL:48:LYS:O	25:SL:52:GLU:HG2	2.05	0.55
26:SR:66:VAL:HG23	26:SR:68:GLY:H	1.72	0.55
3:L5:490:C:H2'	3:L5:491:G:C8	2.41	0.55
3:L5:1407:C:H2'	3:L5:1408:G:C8	2.42	0.55
3:L5:1697:G:H2'	3:L5:1698:C:C2	2.42	0.55
3:L5:2583:C:OP1	74:Lg:54:ARG:HB2	2.06	0.55
6:SA:6:ASP:HA	6:SA:9:GLN:HG2	1.89	0.55
37:Sg:11:LEU:HD12	37:Sg:43:TRP:CE3	2.41	0.55
43:LH:114:ILE:HB	43:LH:124:ARG:HB2	1.87	0.55
57:LR:105:LEU:HD22	57:LR:135:LYS:HG2	1.87	0.55
69:LF:125:LEU:HD22	69:LF:130:ILE:HD11	1.86	0.55
1:S2:944:A:H5''	19:SO:134:PRO:CB	2.34	0.55
6:SA:10:MET:HE2	6:SA:15:VAL:HG22	1.88	0.55
17:SU:36:CYS:SG	17:SU:87:ARG:HG3	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:92:TYR:HB3	40:LB:99:LEU:HD22	1.88	0.55
55:LD:62:CYS:HB3	55:LD:105:LEU:HD22	1.88	0.55
79:Lm:99:CYS:HB2	79:Lm:114:LYS:HD2	1.88	0.55
3:L5:256:G:H2'	3:L5:257:C:C6	2.41	0.55
3:L5:492:U:H2'	3:L5:493:G:C8	2.42	0.55
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.41	0.55
3:L5:2363:A2M:H2'	3:L5:2364:OMG:O4'	2.06	0.55
3:L5:2667:C:O4'	57:LR:96:MET:HG2	2.07	0.55
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.72	0.55
17:SU:96:GLU:HA	17:SU:99:LYS:HE2	1.88	0.55
1:S2:92:A:H4'	1:S2:93:PSU:OP2	2.07	0.55
5:SB:92:GLN:HE22	5:SB:229:MET:HE1	1.72	0.55
22:SS:23:ARG:HG2	31:SZ:48:VAL:HG12	1.89	0.55
28:ST:42:HIS:HB3	28:ST:93:SER:HB3	1.88	0.55
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.05	0.55
3:L5:4341:C:C2	93:L5:5119:3H3:H14	2.42	0.55
15:SI:141:ARG:HB2	15:SI:145:ILE:HD11	1.89	0.55
37:Sg:32:LEU:HD12	37:Sg:71:ILE:HG12	1.87	0.55
57:LR:105:LEU:HD23	57:LR:138:LEU:HD23	1.87	0.55
3:L5:711:A:H2'	3:L5:712:C:C6	2.42	0.55
3:L5:1979:A:H2	3:L5:1987:C:H42	1.53	0.55
6:SA:80:ARG:HH21	6:SA:126:ASP:HB2	1.71	0.55
26:SR:56:HIS:HA	26:SR:59:LYS:HE3	1.88	0.55
1:S2:324:C:H2'	1:S2:325:C:C6	2.42	0.55
1:S2:681:PSU:H4'	20:SX:9:THR:HG22	1.89	0.55
3:L5:981:C:H4'	44:LE:39:LYS:HD2	1.87	0.55
8:SJ:34:GLU:HG3	8:SJ:35:TYR:CD2	2.41	0.55
11:SG:63:MET:HG2	11:SG:99:GLY:O	2.07	0.55
3:L5:1408:G:H21	3:L5:1409:C:H42	1.54	0.55
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.42	0.55
3:L5:3961:G:H4'	3:L5:4049:U:H3	1.72	0.55
9:SE:201:HIS:HE1	9:SE:207:VAL:HG23	1.71	0.55
16:SQ:50:LYS:HE2	16:SQ:50:LYS:HA	1.88	0.55
19:SO:75:MET:HG3	19:SO:118:ALA:HB2	1.88	0.55
1:S2:1797:U:H2'	1:S2:1798:C:C6	2.42	0.54
29:SV:37:ALA:HB1	29:SV:46:PHE:CD1	2.42	0.54
59:LT:133:ALA:HB3	69:LF:127:LYS:HB2	1.88	0.54
87:EF:375:LEU:HB3	87:EF:391:PRO:HD2	1.88	0.54
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.41	0.54
23:Sd:24:CYS:O	23:Sd:25:SER:OG	2.24	0.54
43:LH:4:ILE:HG12	43:LH:61:TRP:CH2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LG:108:GLN:O	45:LG:112:GLN:HG3	2.06	0.54
59:LT:51:GLY:HA3	59:LT:92:ARG:HG3	1.89	0.54
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.42	0.54
1:S2:502:C:O4'	9:SE:66:MET:HG3	2.07	0.54
38:Lz:41:TYR:CE2	38:Lz:159:MET:HE2	2.42	0.54
41:LC:140:LYS:HB3	41:LC:142:HIS:HD2	1.73	0.54
69:LF:92:VAL:HG23	69:LF:114:LEU:HD11	1.90	0.54
70:Lc:55:LEU:HD11	74:Lg:92:LYS:HG3	1.89	0.54
1:S2:447:A:H4'	9:SE:3:ARG:HG2	1.90	0.54
1:S2:948:C:H2'	1:S2:949:G:H8	1.71	0.54
1:S2:1536:G:H2'	1:S2:1537:A:H8	1.72	0.54
6:SA:71:PRO:HB3	6:SA:186:ARG:HH22	1.70	0.54
21:SM:81:ASP:CG	21:SM:84:LYS:HD2	2.32	0.54
30:SY:15:ASN:ND2	30:SY:18:LEU:HD23	2.22	0.54
50:LV:112:MET:HE1	50:LV:117:ILE:HG12	1.90	0.54
70:Lc:47:ILE:HD12	70:Lc:94:LEU:HD11	1.89	0.54
78:Ll:42:ARG:HG3	78:Ll:47:THR:HG23	1.89	0.54
1:S2:1454:A:H5''	26:SR:3:ARG:HD2	1.89	0.54
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.73	0.54
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.43	0.54
16:SQ:53:GLU:HG3	16:SQ:85:ARG:HH11	1.72	0.54
38:Lz:155:ILE:HG13	38:Lz:167:VAL:CG1	2.37	0.54
57:LR:136:ARG:O	57:LR:140:GLU:HG2	2.07	0.54
75:Li:2:ALA:N	75:Li:5:TYR:HH	2.04	0.54
87:EF:267:VAL:HG13	87:EF:304:PRO:HA	1.90	0.54
3:L5:131:C:H2'	3:L5:132:G:C8	2.42	0.54
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.43	0.54
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.42	0.54
7:SD:196:GLY:HA2	7:SD:199:GLY:O	2.08	0.54
1:S2:5:U:H2'	1:S2:6:G:H8	1.73	0.54
1:S2:28:U:H2'	1:S2:29:G:H8	1.72	0.54
1:S2:324:C:O2'	1:S2:325:C:H5'	2.08	0.54
1:S2:694:G:H3'	1:S2:695:C:H3'	1.89	0.54
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.42	0.54
4:L7:117:G:H5''	55:LD:256:LYS:HD2	1.90	0.54
1:S2:39:A:H5'	8:SJ:7:TRP:NE1	2.23	0.54
3:L5:1768:C:H3'	3:L5:1769:G:H8	1.73	0.54
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.42	0.54
3:L5:4966:A:H2'	3:L5:4967:A:O4'	2.08	0.54
9:SE:32:SER:HB3	9:SE:81:THR:OG1	2.08	0.54
13:SH:140:VAL:HG12	24:SN:19:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Sg:91:ASP:C	37:Sg:93:THR:H	2.16	0.54
41:LC:159:GLU:HA	41:LC:217:ILE:HB	1.90	0.54
12:SF:127:ARG:HB2	12:SF:134:VAL:HG11	1.90	0.53
36:Sf:121:CYS:HB3	36:Sf:141:CYS:SG	2.47	0.53
1:S2:5:U:H2'	1:S2:6:G:C8	2.43	0.53
3:L5:2673:G:N3	3:L5:2673:G:H5'	2.23	0.53
3:L5:3823:G:N3	3:L5:3823:G:H5''	2.23	0.53
7:SD:48:ILE:HD12	7:SD:73:VAL:HG11	1.89	0.53
8:SJ:120:ALA:HB2	8:SJ:129:LEU:HD12	1.89	0.53
48:LO:121:PRO:HA	48:LO:124:LEU:HD12	1.88	0.53
52:La:2:PRO:HB2	52:La:5:LEU:HD12	1.90	0.53
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.43	0.53
1:S2:640:A:H2'	1:S2:641:A:C8	2.44	0.53
3:L5:1998:A:H2'	3:L5:1999:A:C8	2.42	0.53
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.74	0.53
3:L5:4955:A:H2'	3:L5:4956:A:C8	2.44	0.53
13:SH:60:ILE:HB	13:SH:92:VAL:HG12	1.90	0.53
3:L5:280:G:H5''	53:LN:14:LYS:HE2	1.90	0.53
3:L5:3642:A:HO2'	76:Lj:2:THR:N	2.06	0.53
45:LG:58:PRO:HD2	45:LG:61:ILE:HD12	1.89	0.53
55:LD:106:ALA:HB2	55:LD:166:ALA:HA	1.90	0.53
62:LX:89:LYS:HB3	62:LX:95:THR:HG23	1.91	0.53
68:Lb:35:VAL:HB	68:Lb:40:LEU:HD11	1.90	0.53
87:EF:129:LYS:HA	87:EF:134:ARG:HH12	1.73	0.53
87:EF:264:VAL:HG12	87:EF:309:GLY:HA3	1.90	0.53
3:L5:126:C:H2'	3:L5:127:G:H8	1.74	0.53
3:L5:1983:A:H4'	3:L5:1983:A:OP1	2.07	0.53
3:L5:3668:C:H5'	39:LA:8:GLN:O	2.08	0.53
50:LV:35:LYS:HB2	50:LV:67:LYS:HG3	1.90	0.53
86:5A:64:PHE:HE2	86:5A:143:GLU:HG3	1.74	0.53
3:L5:1730:U:H4'	59:LT:100:LYS:HB2	1.91	0.53
3:L5:4959:U:H2'	3:L5:4960:G:C8	2.44	0.53
30:SY:110:ARG:HH12	30:SY:127:ALA:HA	1.73	0.53
87:EF:152:VAL:HG21	87:EF:167:TYR:HD1	1.72	0.53
1:S2:35:C:H5''	1:S2:579:C:H5''	1.91	0.53
1:S2:1337:4AC:H2'	1:S2:1338:G:C8	2.44	0.53
1:S2:1374:C:H2'	1:S2:1375:G:O4'	2.08	0.53
3:L5:3952:A:H2'	3:L5:3953:G:C8	2.43	0.53
16:SQ:58:LEU:HB3	16:SQ:62:ARG:HD2	1.91	0.53
61:LU:56:LEU:O	61:LU:56:LEU:HD23	2.09	0.53
78:Ll:9:ILE:HD12	78:Ll:51:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L8:101:C:O2'	76:Lj:20:ARG:HG3	2.09	0.53
3:L5:1881:OMC:C2	3:L5:1881:OMC:HM23	2.44	0.53
3:L5:3946:G:H2'	3:L5:3947:A:C8	2.44	0.53
17:SU:28:ASN:HB3	17:SU:31:SER:HB3	1.90	0.53
42:LJ:39:VAL:HG21	42:LJ:126:TYR:HD2	1.74	0.53
1:S2:168:C:O2'	11:SG:133:LEU:HB2	2.09	0.52
1:S2:958:G:H2'	1:S2:959:G:C8	2.44	0.52
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.45	0.52
3:L5:2476:G:H2'	3:L5:2477:A:C8	2.44	0.52
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.44	0.52
10:SC:184:VAL:CG2	10:SC:195:LEU:HB2	2.39	0.52
27:SP:134:GLY:HA2	27:SP:140:ARG:HB3	1.91	0.52
54:LI:47:PRO:HB3	54:LI:171:TRP:CZ2	2.44	0.52
15:SI:26:LYS:HD2	15:SI:29:LEU:HD23	1.91	0.52
50:LV:106:VAL:HG12	50:LV:112:MET:HA	1.91	0.52
54:LI:145:LYS:O	54:LI:149:ILE:HG13	2.08	0.52
1:S2:323:C:H2'	1:S2:326:C:C6	2.45	0.52
1:S2:640:A:P	35:Se:115:ARG:HH22	2.32	0.52
1:S2:1499:U:H4'	7:SD:176:LEU:HD13	1.91	0.52
3:L5:260:C:C2'	3:L5:261:G:H5'	2.40	0.52
46:Lq:39:GLN:HE22	46:Lq:107:VAL:HG11	1.74	0.52
54:LI:166:HIS:HB2	59:LT:158:PHE:HE2	1.74	0.52
86:5A:90:GLN:HA	86:5A:134:LEU:HA	1.91	0.52
1:S2:388:U:H2'	1:S2:389:A:C8	2.44	0.52
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.75	0.52
3:L5:1995:G:N3	3:L5:1995:G:H2'	2.24	0.52
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.08	0.52
18:SK:6:LYS:H	18:SK:6:LYS:CD	2.22	0.52
22:SS:33:ILE:HD13	22:SS:71:MET:HE1	1.92	0.52
34:Sc:32:VAL:HG11	34:Sc:56:LEU:HD12	1.90	0.52
1:S2:186:C:H2'	1:S2:187:G:C8	2.45	0.52
1:S2:1030:A:H2'	1:S2:1031:A2M:H8	1.91	0.52
3:L5:318:A:H2'	3:L5:319:A:C8	2.44	0.52
3:L5:717:U:H2'	3:L5:718:C:C6	2.45	0.52
21:SM:31:LEU:HD13	21:SM:109:VAL:HG13	1.90	0.52
31:SZ:86:ALA:O	31:SZ:89:GLN:HG2	2.09	0.52
46:Lq:41:GLN:HG2	46:Lq:45:MET:HE1	1.90	0.52
71:Ld:37:GLY:O	71:Ld:41:ARG:HG3	2.08	0.52
3:L5:4370:OMG:HM21	93:L5:5119:3H3:O	2.10	0.52
3:L5:4923:C:H2'	3:L5:4924:C:C6	2.45	0.52
10:SC:191:VAL:HG11	10:SC:236:PHE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SF:19:LEU:HD21	12:SF:69:VAL:HG21	1.90	0.52
22:SS:45:LEU:HB3	22:SS:52:LEU:HD21	1.91	0.52
1:S2:189:U:H2'	1:S2:190:G:O4'	2.09	0.52
1:S2:455:A:H5'	11:SG:94:ARG:HH21	1.75	0.52
3:L5:921:C:H2'	3:L5:922:C:C6	2.44	0.52
17:SU:56:MET:HB2	17:SU:86:LYS:HB3	1.91	0.52
64:LW:81:ALA:HB2	64:LW:87:LEU:HB2	1.91	0.52
86:5A:119:LEU:O	86:5A:123:ILE:HG12	2.10	0.52
87:EF:103:ILE:HG23	87:EF:143:LEU:HD11	1.91	0.52
1:S2:553:U:H2'	1:S2:555:A:H8	1.75	0.52
1:S2:562:U:H2'	1:S2:563:G:C8	2.45	0.52
1:S2:1461:G:H2'	1:S2:1464:C:H41	1.74	0.52
41:LC:13:GLU:HG3	41:LC:14:LYS:HD2	1.91	0.52
62:LX:119:ILE:HD12	62:LX:140:LEU:HD22	1.92	0.52
64:LW:104:GLN:HA	64:LW:107:GLN:NE2	2.24	0.52
1:S2:857:U:H2'	1:S2:858:A:C8	2.44	0.52
1:S2:981:A:H2'	1:S2:982:G:C8	2.45	0.52
3:L5:907:C:H2'	3:L5:908:G:C8	2.45	0.52
3:L5:3661:G:N7	39:LA:152:SER:OG	2.38	0.52
3:L5:4345:C:O2'	81:Lo:82:MET:HE3	2.10	0.52
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.44	0.52
93:L5:5119:3H3:C7	81:Lo:59:LYS:HE3	2.39	0.52
11:SG:70:HIS:CE1	11:SG:101:ILE:HG21	2.44	0.52
22:SS:45:LEU:HD22	22:SS:50:ILE:HD11	1.93	0.52
38:Lz:206:ILE:HG12	38:Lz:214:GLN:CG	2.40	0.52
46:Lq:135:THR:HA	46:Lq:138:PHE:HD2	1.75	0.52
52:La:98:ALA:HB2	52:La:121:PRO:HB2	1.90	0.52
65:LZ:87:VAL:HG22	65:LZ:89:ILE:HG13	1.92	0.52
1:S2:1119:A:H2'	1:S2:1120:U:O4'	2.10	0.51
1:S2:1672:U:OP1	16:SQ:18:THR:HG22	2.09	0.51
12:SF:103:LEU:HD21	31:SZ:67:LEU:HD22	1.91	0.51
16:SQ:51:LEU:HD11	16:SQ:81:ILE:HD12	1.92	0.51
25:SL:35:ARG:HD2	25:SL:53:GLY:O	2.10	0.51
40:LB:92:TYR:HB2	40:LB:159:VAL:HB	1.92	0.51
3:L5:699:C:H2'	3:L5:700:G:H8	1.75	0.51
3:L5:2098:G:H1'	3:L5:2099:G:C8	2.45	0.51
3:L5:4200:G:H1	3:L5:4221:C:H42	1.58	0.51
12:SF:49:LEU:HD12	16:SQ:50:LYS:HG2	1.92	0.51
17:SU:19:ARG:H	17:SU:19:ARG:HD3	1.75	0.51
1:S2:627:OMU:H6	1:S2:627:OMU:H5''	1.91	0.51
3:L5:4053:A:H4'	38:Lz:212:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:30:LYS:O	8:SJ:34:GLU:HG2	2.11	0.51
10:SC:171:GLY:HA2	14:SW:98:GLN:NE2	2.22	0.51
38:Lz:34:LEU:HD12	38:Lz:206:ILE:HG22	1.92	0.51
38:Lz:155:ILE:HG13	38:Lz:167:VAL:HG11	1.92	0.51
40:LB:261:ARG:HB2	48:LO:64:THR:HG21	1.91	0.51
48:LO:81:TRP:HB2	48:LO:104:VAL:HG21	1.93	0.51
1:S2:553:U:H2'	1:S2:555:A:C8	2.46	0.51
1:S2:573:PSU:O4	1:S2:576:A2M:H8	2.11	0.51
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.46	0.51
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.45	0.51
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.75	0.51
6:SA:89:LYS:HD3	6:SA:201:LEU:O	2.09	0.51
8:SJ:129:LEU:HB3	8:SJ:135:ILE:HD11	1.92	0.51
15:SI:141:ARG:HB2	15:SI:145:ILE:CD1	2.41	0.51
1:S2:1144:A:H2'	1:S2:1145:A:C8	2.46	0.51
3:L5:728:U:H2'	3:L5:730:G:H5'	1.90	0.51
3:L5:4385:A:OP1	86:5A:50:5CT:H12	2.10	0.51
5:SB:35:ALA:HB2	5:SB:44:ILE:HD11	1.93	0.51
12:SF:35:LEU:HD22	12:SF:147:VAL:HG23	1.93	0.51
37:Sg:131:LEU:HD12	37:Sg:139:LYS:HB2	1.92	0.51
52:La:36:GLY:HA3	52:La:40:HIS:CE1	2.45	0.51
1:S2:201:C:H2'	1:S2:202:G:N3	2.26	0.51
3:L5:4711:C:H5''	48:LO:58:LEU:HD23	1.91	0.51
20:SX:98:ASP:OD2	20:SX:140:ARG:NH1	2.44	0.51
25:SL:111:VAL:HG12	25:SL:140:PHE:HB2	1.91	0.51
1:S2:65:C:OP1	11:SG:136:LYS:HE2	2.11	0.51
1:S2:536:A:H2'	1:S2:537:C:C6	2.46	0.51
1:S2:1698:C:H4'	1:S2:1699:A:OP2	2.10	0.51
3:L5:1971:C:C5	3:L5:2000:G:H2'	2.45	0.51
26:SR:126:MET:HB2	26:SR:128:PHE:HE1	1.74	0.51
86:5A:57:HIS:ND1	86:5A:72:ILE:HG12	2.26	0.51
1:S2:17:C:O2'	1:S2:1194:A:N1	2.40	0.51
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.46	0.51
8:SJ:109:ARG:HG2	8:SJ:146:SER:HA	1.93	0.51
63:LY:24:HIS:CE1	63:LY:25:ILE:HG12	2.46	0.51
81:Lo:33:LEU:HA	81:Lo:38:LYS:HG2	1.91	0.51
1:S2:556:U:H2'	1:S2:557:U:O4'	2.11	0.51
3:L5:1593:A:H5''	3:L5:2839:PSU:H5'	1.92	0.51
3:L5:1699:A:H8	3:L5:1706:A:H5''	1.75	0.51
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.93	0.51
37:Sg:18:VAL:HG11	37:Sg:307:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:56:LYS:HE3	38:Lz:181:TYR:HB3	1.93	0.51
50:LV:87:SER:HA	50:LV:97:TYR:HB3	1.91	0.51
56:LQ:12:LYS:HB2	56:LQ:14:ARG:HH11	1.76	0.51
64:LW:104:GLN:HA	64:LW:107:GLN:HE22	1.76	0.51
1:S2:572:PSU:H4'	30:SY:61:ARG:HE	1.76	0.51
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.93	0.51
3:L5:2000:G:H5''	3:L5:2001:G:H5'	1.92	0.51
31:SZ:79:ILE:HB	31:SZ:83:LEU:HD23	1.93	0.51
37:Sg:125:ARG:HA	37:Sg:150:TRP:HB3	1.93	0.51
38:Lz:85:MET:HG2	38:Lz:90:LEU:HD13	1.92	0.51
47:LK:20:GLY:HA3	47:LK:54:LYS:HA	1.92	0.51
47:LK:115:GLN:HA	47:LK:118:HIS:ND1	2.26	0.51
85:Pt:72:C:H2'	85:Pt:73:A:C8	2.46	0.51
1:S2:1750:C:H2'	1:S2:1751:C:O4'	2.11	0.50
28:ST:65:TYR:HD2	28:ST:66:LEU:HD23	1.76	0.50
44:LE:190:HIS:HB3	44:LE:193:PHE:HD2	1.74	0.50
46:Lq:30:VAL:HG21	46:Lq:187:LEU:CD1	2.40	0.50
1:S2:1337:4AC:H2'	1:S2:1338:G:H8	1.75	0.50
1:S2:1643:PSU:H2'	1:S2:1644:C:C6	2.46	0.50
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.47	0.50
26:SR:16:ILE:HG22	26:SR:24:LEU:HD11	1.94	0.50
32:Sa:4:LYS:HE3	32:Sa:92:ARG:CZ	2.41	0.50
38:Lz:76:GLU:O	38:Lz:79:ALA:HB3	2.11	0.50
38:Lz:159:MET:HA	38:Lz:165:LEU:HD21	1.94	0.50
1:S2:551:U:H2'	1:S2:552:G:C8	2.46	0.50
1:S2:1207:G:N2	83:mR:36[B]:U:H3'	2.25	0.50
1:S2:1531:A:H2'	1:S2:1532:C:C6	2.47	0.50
3:L5:1074:G:H2'	3:L5:1075:G:H8	1.76	0.50
3:L5:4038:C:H5''	3:L5:4039:G:C8	2.47	0.50
13:SH:73:GLN:HB3	13:SH:135:PHE:CE1	2.46	0.50
13:SH:137:SER:HA	13:SH:162:GLN:CG	2.40	0.50
33:Sb:33:MET:HE3	33:Sb:48:SER:HA	1.92	0.50
37:Sg:158:PRO:HD2	37:Sg:204:GLY:HA2	1.92	0.50
38:Lz:194:LEU:HD21	38:Lz:200:ASN:HB2	1.94	0.50
84:At:68:C:H2'	84:At:69:G:H8	1.75	0.50
1:S2:329:G:H2'	1:S2:330:G:O4'	2.11	0.50
7:SD:53:THR:HG21	7:SD:94:ARG:HG3	1.93	0.50
9:SE:129:ILE:HD11	9:SE:139:LEU:HD12	1.94	0.50
36:Sf:94:LYS:HA	36:Sf:94:LYS:HZ2	1.76	0.50
44:LE:186:LEU:HD21	44:LE:253:VAL:HG21	1.92	0.50
3:L5:1766:A:H1'	22:SS:116:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4153:C:H2'	3:L5:4154:G:C8	2.46	0.50
21:SM:52:LEU:O	21:SM:78:LYS:HA	2.10	0.50
38:Lz:36:ILE:HG12	38:Lz:165:LEU:H	1.76	0.50
38:Lz:206:ILE:O	38:Lz:213:PRO:HG2	2.12	0.50
45:LG:50:ASP:HB2	62:LX:40:ILE:HD12	1.93	0.50
2:L8:108:A:H2'	2:L8:109:C:O4'	2.12	0.50
3:L5:141:C:O2'	3:L5:142:G:H5'	2.12	0.50
3:L5:3922:G:C6	86:5A:72:ILE:HG13	2.46	0.50
40:LB:378:ARG:HE	64:LW:32:LEU:HD21	1.76	0.50
60:LP:29:THR:HG21	60:LP:146:ILE:HD11	1.93	0.50
72:Le:10:PRO:HG2	72:Le:69:MET:HE1	1.94	0.50
72:Le:35:TRP:CZ2	72:Le:56:PRO:HD2	2.46	0.50
1:S2:323:C:H4'	1:S2:324:C:C5	2.46	0.50
1:S2:1073:U:H2'	1:S2:1074:C:C6	2.47	0.50
1:S2:1445:PSU:O2'	1:S2:1446:A:H5'	2.11	0.50
3:L5:490:C:H2'	3:L5:491:G:H8	1.75	0.50
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.76	0.50
14:SW:14:ILE:HG13	14:SW:27:ILE:HD11	1.93	0.50
40:LB:288:GLY:HA3	40:LB:330:PHE:CZ	2.47	0.50
47:LK:32:ILE:O	47:LK:35:LEU:HG	2.11	0.50
70:Lc:30:GLY:O	70:Lc:34:THR:OG1	2.28	0.50
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.47	0.50
30:SY:76:TYR:OH	30:SY:86:GLU:OE1	2.23	0.50
35:Se:75:LYS:HD3	84:At:37:MIA:H5''	1.93	0.50
37:Sg:256:ILE:HB	37:Sg:270:LEU:HB2	1.94	0.50
87:EF:253:VAL:HG11	87:EF:320:VAL:HG23	1.94	0.50
1:S2:1419:C:H4'	1:S2:1420:G:H2'	1.94	0.50
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.47	0.50
3:L5:3973:G:H2'	3:L5:3975:C:N4	2.27	0.50
14:SW:57:ARG:HH22	24:SN:16:LEU:HB3	1.76	0.50
15:SI:103:LEU:HD22	15:SI:170:LYS:HB3	1.94	0.50
31:SZ:66:LYS:HG3	31:SZ:111:ARG:HH12	1.77	0.50
39:LA:80:GLU:HB2	39:LA:170:ALA:HA	1.94	0.50
59:LT:75:VAL:HG22	59:LT:88:ARG:HG2	1.92	0.50
3:L5:5027:C:H4'	3:L5:5028:G:H5'	1.94	0.49
3:L5:5045:G:H5''	71:Ld:82:TYR:HD2	1.78	0.49
42:LJ:113:ILE:HG21	42:LJ:119:TYR:HB2	1.94	0.49
47:LK:32:ILE:HG21	47:LK:42:VAL:HG21	1.94	0.49
57:LR:89:MET:HE3	57:LR:90:PRO:HD2	1.93	0.49
87:EF:79:M3L:HD3	87:EF:86:TYR:HE1	1.77	0.49
87:EF:388:GLU:OE2	87:EF:391:PRO:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2400:G:H21	74:Lg:6:THR:HG22	1.77	0.49
17:SU:24:LEU:HB3	17:SU:32:LEU:HD11	1.95	0.49
77:Lk:33:LYS:HG2	77:Lk:46:VAL:HG22	1.93	0.49
1:S2:1406:G:H2'	1:S2:1407:U:C6	2.47	0.49
1:S2:1757:G:H1'	1:S2:1776:G:N1	2.27	0.49
3:L5:1097:C:H2'	3:L5:1098:G:H8	1.77	0.49
3:L5:1241:C:H2'	3:L5:1242:G:C8	2.48	0.49
3:L5:1448:G:H2'	3:L5:1449:C:C6	2.48	0.49
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.48	0.49
3:L5:2903:G:H5''	3:L5:2904:U:H5'	1.94	0.49
8:SJ:111:GLN:HA	8:SJ:130:ILE:CD1	2.43	0.49
15:SI:48:VAL:HG11	15:SI:54:LYS:HE3	1.94	0.49
17:SU:20:ILE:HD12	17:SU:98:VAL:HG21	1.94	0.49
47:LK:142:ASN:HB3	47:LK:146:ARG:HH21	1.76	0.49
70:Lc:34:THR:HG23	70:Lc:95:ALA:HB2	1.94	0.49
1:S2:1754:G:H2'	1:S2:1755:C:C6	2.47	0.49
3:L5:71:C:H5'	49:LL:64:VAL:HG12	1.95	0.49
3:L5:137:G:H2'	3:L5:138:G:H8	1.78	0.49
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.48	0.49
3:L5:4859:C:H3'	3:L5:4860:G:C8	2.47	0.49
7:SD:45:ARG:NH1	7:SD:85:GLU:HG3	2.28	0.49
38:Lz:191:VAL:HG21	38:Lz:198:TRP:CE2	2.47	0.49
38:Lz:206:ILE:O	38:Lz:214:GLN:HB2	2.12	0.49
60:LP:54:GLN:HA	60:LP:83:TRP:CD1	2.48	0.49
1:S2:501:C:O2	1:S2:501:C:H2'	2.12	0.49
1:S2:804:U:H2'	1:S2:805:U:C6	2.47	0.49
3:L5:1281:G:H5'	41:LC:323:ARG:HB2	1.95	0.49
3:L5:5024:C:H2'	3:L5:5025:C:C6	2.48	0.49
10:SC:102:LEU:HD22	10:SC:130:ILE:HG13	1.94	0.49
13:SH:147:LYS:HA	14:SW:49:GLU:HG2	1.93	0.49
24:SN:13:GLN:HG3	33:Sb:21:LYS:HE3	1.92	0.49
82:Lp:51:ALA:HB3	82:Lp:54:ILE:HD12	1.94	0.49
84:At:66:U:H2'	84:At:67:C:C6	2.47	0.49
3:L5:3974:G:H3'	3:L5:3975:C:H6	1.78	0.49
9:SE:141:THR:HG22	9:SE:145:ARG:H	1.76	0.49
22:SS:59:LEU:HD23	22:SS:64:VAL:HG22	1.93	0.49
37:Sg:258:ILE:HD12	37:Sg:268:ASP:HB3	1.94	0.49
58:LS:84:TYR:HE1	58:LS:93:MET:HE3	1.77	0.49
1:S2:940:U:H3	1:S2:1002:U:H3	1.61	0.49
3:L5:78:U:H5''	53:LN:185:GLY:HA2	1.95	0.49
3:L5:86:U:H2'	3:L5:87:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:188:ASN:HB3	9:SE:191:ARG:HD3	1.95	0.49
9:SE:201:HIS:CE1	9:SE:207:VAL:HG23	2.47	0.49
22:SS:23:ARG:HG2	31:SZ:48:VAL:HG11	1.93	0.49
38:Lz:41:TYR:HE2	38:Lz:159:MET:HE2	1.77	0.49
51:LM:24:LEU:HD11	51:LM:86:TRP:CG	2.48	0.49
56:LQ:43:PHE:CD2	56:LQ:133:GLY:HA3	2.47	0.49
75:Li:80:HIS:CD2	75:Li:84:LYS:HE2	2.47	0.49
1:S2:527:C:H2'	1:S2:528:A:C8	2.48	0.49
1:S2:832:G:N2	1:S2:843:C:H1'	2.27	0.49
2:L8:84:A:C6	2:L8:88:A:H4'	2.48	0.49
2:L8:141:C:H2'	2:L8:142:U:C6	2.47	0.49
4:L7:110:G:H2'	4:L7:111:C:C6	2.48	0.49
5:SB:120:MET:HG3	5:SB:142:PHE:CE2	2.48	0.49
14:SW:57:ARG:NH2	24:SN:16:LEU:HB3	2.27	0.49
22:SS:55:ARG:HG3	31:SZ:48:VAL:HG21	1.94	0.49
27:SP:83:MET:HA	27:SP:83:MET:HE3	1.95	0.49
38:Lz:112:ALA:HB3	38:Lz:116:LEU:HB3	1.94	0.49
3:L5:257:C:H2'	3:L5:258:G:C8	2.47	0.49
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.48	0.49
3:L5:4860:G:H5'	48:LO:169:ARG:NE	2.28	0.49
40:LB:161:ARG:HG2	40:LB:184:GLN:HA	1.95	0.49
54:LI:43:VAL:HG21	54:LI:197:VAL:HG13	1.95	0.49
70:Lc:48:LEU:HD13	70:Lc:57:LYS:HG3	1.93	0.49
1:S2:1599:U:C4	12:SF:166:ILE:HA	2.48	0.49
3:L5:2656:U:H2'	3:L5:2657:G:O4'	2.13	0.49
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.47	0.49
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.78	0.49
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.47	0.49
31:SZ:102:LYS:HG3	31:SZ:107:VAL:HG12	1.95	0.49
49:LL:136:LYS:HG2	49:LL:136:LYS:O	2.13	0.49
50:LV:39:ILE:HD12	50:LV:61:VAL:HG21	1.95	0.49
56:LQ:122:THR:OG1	56:LQ:124:ASP:OD1	2.25	0.49
87:EF:277:VAL:HA	87:EF:288:GLU:HA	1.94	0.49
1:S2:527:C:H4'	8:SJ:121:LYS:HD3	1.95	0.48
3:L5:1074:G:H2'	3:L5:1075:G:C8	2.47	0.48
39:LA:101:VAL:HG22	39:LA:165:VAL:HG22	1.95	0.48
1:S2:17:C:H2'	1:S2:18:C:C6	2.48	0.48
1:S2:1308:U:O2'	36:Sf:133:ALA:HB1	2.13	0.48
3:L5:493:G:H2'	3:L5:494:U:C6	2.48	0.48
3:L5:4606:G:H2'	3:L5:4607:A:C8	2.48	0.48
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SA:111:GLN:HG2	6:SA:112:ILE:HG23	1.95	0.48
18:SK:49:MET:HG3	18:SK:69:TRP:CE3	2.49	0.48
20:SX:90:CYS:HA	20:SX:93:PHE:HD2	1.78	0.48
21:SM:52:LEU:HD23	21:SM:78:LYS:CG	2.43	0.48
55:LD:37:VAL:HB	55:LD:67:ALA:HB2	1.95	0.48
1:S2:67:C:C5	11:SG:162:LEU:HB3	2.48	0.48
1:S2:434:G:H5''	15:SI:23:LYS:HE3	1.95	0.48
1:S2:1124:C:H5''	5:SB:150:ILE:HG12	1.95	0.48
1:S2:1293:A:H2'	1:S2:1294:G:C8	2.48	0.48
1:S2:1798:C:H2'	1:S2:1799:G:O4'	2.13	0.48
3:L5:1417:C:H2'	3:L5:1418:C:O4'	2.14	0.48
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.13	0.48
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.28	0.48
3:L5:4518:A:OP2	3:L5:4518:A:H8	1.97	0.48
3:L5:4601:U:H2'	3:L5:4602:A:C8	2.47	0.48
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.78	0.48
4:L7:112:U:H2'	4:L7:113:G:H8	1.77	0.48
6:SA:77:ILE:HD12	6:SA:122:LEU:HD11	1.93	0.48
7:SD:29:LEU:HD21	7:SD:69:LEU:HD11	1.95	0.48
7:SD:42:THR:HB	7:SD:43:PRO:HD2	1.95	0.48
15:SI:38:ILE:HD13	15:SI:80:ASP:HA	1.94	0.48
38:Lz:35:GLN:HB2	38:Lz:205:TYR:HB2	1.95	0.48
38:Lz:78:LYS:HA	38:Lz:84:HIS:CD2	2.48	0.48
1:S2:496:C:OP1	9:SE:29:PRO:HD3	2.13	0.48
1:S2:953:C:H2'	1:S2:954:U:O4'	2.13	0.48
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.14	0.48
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.49	0.48
3:L5:3942:A:H2'	3:L5:3943:A:C8	2.48	0.48
3:L5:4385:A:C5	86:5A:50:5CT:H13	2.48	0.48
16:SQ:82:TYR:O	16:SQ:85:ARG:HG2	2.13	0.48
46:Lq:30:VAL:HG11	46:Lq:187:LEU:HD21	1.95	0.48
67:Lh:35:LYS:HA	67:Lh:44:LEU:HD21	1.94	0.48
1:S2:1256:G:H8	17:SU:66:ARG:HB2	1.79	0.48
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.49	0.48
3:L5:3972:A:H2	3:L5:4040:C:H2'	1.77	0.48
4:L7:39:C:O2'	42:LJ:46:GLN:HB3	2.13	0.48
8:SJ:29:LEU:HD21	35:Se:112:TYR:HA	1.95	0.48
8:SJ:91:LYS:HD2	8:SJ:96:TYR:HD2	1.77	0.48
9:SE:11:ARG:HA	9:SE:28:ALA:HB2	1.96	0.48
13:SH:117:PRO:HG2	13:SH:120:ARG:HD3	1.95	0.48
13:SH:162:GLN:H	13:SH:162:GLN:HG2	1.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lz:120:ILE:HG21	38:Lz:128:LEU:HD12	1.95	0.48
78:Ll:49:LEU:C	78:Ll:51:LEU:H	2.22	0.48
86:5A:90:GLN:HE21	86:5A:102:LEU:HD23	1.79	0.48
86:5A:133:ILE:HG13	86:5A:149:ILE:HD11	1.96	0.48
1:S2:884:C:H2'	1:S2:885:U:C6	2.49	0.48
1:S2:1007:C:H2'	1:S2:1008:A:C8	2.49	0.48
2:L8:80:A:H5''	2:L8:83:C:H5	1.79	0.48
3:L5:1082:C:H2'	3:L5:1083:U:O4'	2.13	0.48
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.48	0.48
3:L5:4301:U:H4'	59:LT:54:HIS:CD2	2.49	0.48
3:L5:4684:A:H2'	3:L5:4685:U:O4'	2.13	0.48
18:SK:6:LYS:H	18:SK:6:LYS:HD2	1.78	0.48
31:SZ:68:ILE:HB	31:SZ:109:TYR:HB2	1.94	0.48
37:Sg:79:LEU:HD22	37:Sg:120:ILE:HD12	1.96	0.48
38:Lz:27:LYS:O	38:Lz:28:PHE:HB3	2.12	0.48
65:LZ:39:SER:HB2	65:LZ:77:TYR:CD2	2.48	0.48
1:S2:115:U:H2'	1:S2:116:OMU:H6	1.96	0.48
1:S2:302:A:H1'	15:SI:73:THR:OG1	2.13	0.48
1:S2:1745:A:H1'	11:SG:66:GLY:HA2	1.95	0.48
3:L5:106:A:H2'	3:L5:107:G:O4'	2.14	0.48
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.48	0.48
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.49	0.48
3:L5:4039:G:H1'	3:L5:4040:C:H5	1.79	0.48
39:LA:48:ILE:HG22	82:Lp:54:ILE:HG12	1.95	0.48
87:EF:383:SER:C	87:EF:385:LYS:H	2.22	0.48
1:S2:928:G:H2'	1:S2:929:G:C8	2.48	0.48
1:S2:929:G:H2'	1:S2:930:C:O4'	2.13	0.48
1:S2:1432:U:H2'	1:S2:1438:A:C8	2.49	0.48
1:S2:1589:A:H2'	1:S2:1590:C:C6	2.49	0.48
3:L5:411:G:H4'	3:L5:412:G:H5'	1.94	0.48
3:L5:1325:C:C4	3:L5:3879:G:H5''	2.48	0.48
3:L5:2389:A:H4'	71:Ld:70:LYS:HG3	1.96	0.48
40:LB:224:LYS:HG2	40:LB:340:THR:HG22	1.96	0.48
53:LN:121:VAL:HG11	53:LN:131:GLU:HG3	1.96	0.48
87:EF:422:GLY:HA2	87:EF:438:ILE:HD12	1.96	0.48
1:S2:693:A:H1'	1:S2:694:G:H2'	1.96	0.48
2:L8:78:G:H2'	2:L8:79:G:C8	2.49	0.48
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.13	0.48
3:L5:1756:U:C2'	3:L5:1757:U:H5'	2.44	0.48
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.14	0.48
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SC:110:MET:HE2	10:SC:125:LYS:HD2	1.94	0.48
11:SG:228:ILE:HA	11:SG:231:ARG:HG2	1.95	0.48
18:SK:1:MET:HE1	18:SK:43:LEU:CG	2.44	0.48
25:SL:68:ILE:HG21	25:SL:143:LEU:HD11	1.95	0.48
83:mR:36[A]:U:H2'	83:mR:37:A:H8	1.76	0.48
1:S2:186:C:H2'	1:S2:187:G:H8	1.78	0.48
1:S2:379:C:H5'	15:SI:33:ALA:HA	1.96	0.48
1:S2:1434:C:H2'	1:S2:1435:C:C6	2.48	0.48
3:L5:462:G:H2'	3:L5:463:A:C8	2.49	0.48
3:L5:934:C:H4'	3:L5:935:A:O5'	2.14	0.48
3:L5:1411:C:H2'	3:L5:1412:G:H8	1.78	0.48
3:L5:4862:G:H2'	3:L5:4863:G:H8	1.79	0.48
6:SA:124:VAL:HG21	6:SA:134:LEU:HD21	1.95	0.48
6:SA:198:MET:HG3	6:SA:199:PRO:HD2	1.96	0.48
22:SS:84:LEU:O	22:SS:87:GLN:HG3	2.14	0.48
30:SY:12:PHE:HZ	30:SY:21:LYS:HD3	1.79	0.48
45:LG:114:LEU:O	45:LG:115:LEU:C	2.57	0.48
87:EF:426:VAL:CG2	87:EF:433:VAL:HB	2.43	0.48
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.49	0.47
18:SK:92:ALA:HA	18:SK:95:ARG:NH2	2.29	0.47
21:SM:55:ASN:HB2	21:SM:82:ASN:H	1.78	0.47
45:LG:157:ILE:HG12	45:LG:170:LEU:HD23	1.96	0.47
69:LF:125:LEU:HD22	69:LF:130:ILE:CD1	2.44	0.47
3:L5:231:U:H4'	63:LY:100:HIS:CD2	2.48	0.47
3:L5:2525:U:P	57:LR:42:ARG:HH22	2.38	0.47
13:SH:76:GLN:NE2	13:SH:94:PHE:HB2	2.29	0.47
22:SS:13:LEU:HB2	22:SS:20:ILE:HB	1.96	0.47
41:LC:67:TRP:HB3	41:LC:71:ARG:HD2	1.96	0.47
50:LV:16:ILE:HD11	50:LV:56:GLY:HA3	1.95	0.47
86:5A:41:VAL:HG11	86:5A:61:ILE:HG23	1.96	0.47
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.49	0.47
3:L5:2096:G:H3'	3:L5:2096:G:N3	2.28	0.47
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.49	0.47
7:SD:51:LEU:HD23	7:SD:89:GLU:HB2	1.96	0.47
9:SE:163:ASP:HB3	9:SE:166:THR:HG22	1.96	0.47
10:SC:184:VAL:HG23	10:SC:195:LEU:HB2	1.96	0.47
14:SW:30:CYS:HB2	14:SW:61:ILE:HG13	1.95	0.47
60:LP:94:MET:SD	60:LP:148:MET:HE3	2.54	0.47
87:EF:382:ARG:HB3	87:EF:382:ARG:NH2	2.28	0.47
3:L5:448:G:H3'	3:L5:449:C:H5'	1.97	0.47
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3596:A:H1'	3:L5:3598:C:C4	2.49	0.47
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.30	0.47
21:SM:23:LYS:O	21:SM:27:ILE:HD13	2.14	0.47
21:SM:55:ASN:ND2	21:SM:81:ASP:HA	2.29	0.47
22:SS:117:ILE:HD11	27:SP:111:MET:HG3	1.96	0.47
31:SZ:69:THR:H	31:SZ:72:VAL:HG12	1.79	0.47
36:Sf:109:ASP:C	36:Sf:110:GLU:HG3	2.40	0.47
1:S2:39:A:H5'	8:SJ:7:TRP:HE1	1.78	0.47
1:S2:382:C:H2'	1:S2:383:G:H8	1.79	0.47
1:S2:1681:U:H2'	1:S2:1682:C:C6	2.49	0.47
1:S2:1808:U:H2'	1:S2:1809:A:C8	2.50	0.47
1:S2:1809:A:H2'	1:S2:1810:U:C6	2.49	0.47
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.78	0.47
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.50	0.47
10:SC:79:GLU:HA	10:SC:82:TYR:HB2	1.97	0.47
13:SH:163:GLN:HG2	13:SH:167:GLU:CG	2.45	0.47
15:SI:136:ILE:HG13	15:SI:137:LEU:HD12	1.96	0.47
21:SM:44:LYS:O	21:SM:44:LYS:HG2	2.14	0.47
30:SY:41:ARG:HA	30:SY:55:ILE:HG21	1.97	0.47
42:LJ:136:ARG:HG3	42:LJ:157:ILE:HD11	1.96	0.47
69:LF:52:GLU:OE2	69:LF:55:LYS:HE2	2.14	0.47
1:S2:12:U:H2'	1:S2:13:C:C6	2.49	0.47
1:S2:685:A:H5''	14:SW:31:SER:OG	2.15	0.47
3:L5:4169:G:H4'	3:L5:4171:C:C2	2.49	0.47
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.49	0.47
13:SH:191:GLU:HG2	13:SH:192:PHE:CD1	2.50	0.47
25:SL:13:GLN:HE22	25:SL:35:ARG:HG3	1.80	0.47
45:LG:180:PRO:HG3	45:LG:219:VAL:HG13	1.97	0.47
87:EF:134:ARG:HB3	87:EF:177:TYR:CZ	2.49	0.47
1:S2:107:A:H2'	1:S2:108:G:C8	2.50	0.47
1:S2:1462:U:H2'	1:S2:1463:U:C6	2.50	0.47
1:S2:1670:C:H2'	1:S2:1671:G:C8	2.49	0.47
1:S2:1752:C:H2'	1:S2:1753:C:O4'	2.15	0.47
1:S2:1760:G:H21	1:S2:1761:U:H4'	1.79	0.47
3:L5:653:U:H2'	3:L5:654:C:C6	2.49	0.47
3:L5:683:C:H2'	3:L5:684:G:O4'	2.15	0.47
3:L5:1396:G:H5''	52:La:132:ARG:HH12	1.80	0.47
3:L5:2094:G:H2'	3:L5:2095:A:H2'	1.96	0.47
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.15	0.47
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.50	0.47
3:L5:4518:A:O5'	3:L5:4520:G:H4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SB:67:PHE:CE1	19:SO:48:SER:HB3	2.50	0.47
9:SE:125:LYS:HB3	9:SE:142:HIS:HB3	1.97	0.47
9:SE:229:GLY:HA3	9:SE:234:PRO:HA	1.96	0.47
12:SF:129:GLY:HA3	12:SF:134:VAL:HA	1.97	0.47
22:SS:98:VAL:CG1	22:SS:106:LYS:HG3	2.44	0.47
25:SL:113:LEU:HD11	25:SL:120:VAL:HG21	1.97	0.47
41:LC:230:LEU:HD11	41:LC:239:LYS:HB2	1.97	0.47
52:La:88:VAL:O	52:La:92:LYS:HG2	2.15	0.47
61:LU:101:ARG:HD2	61:LU:115:PHE:CE1	2.50	0.47
87:EF:60:LEU:HD13	87:EF:91:ASP:HB2	1.97	0.47
87:EF:251:GLN:HA	87:EF:322:ARG:HG3	1.97	0.47
1:S2:375:U:H2'	1:S2:376:A:C8	2.50	0.47
1:S2:1395:C:O2'	1:S2:1396:A:H5'	2.15	0.47
3:L5:396:A:H2'	3:L5:397:G:C8	2.49	0.47
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.63	0.47
3:L5:963:G:H3'	3:L5:963:G:N3	2.30	0.47
3:L5:1759:G:H1	3:L5:1773:U:H3	1.63	0.47
3:L5:1809:C:H2'	3:L5:1810:G:H8	1.79	0.47
3:L5:3607:U:H2'	3:L5:3608:A:H8	1.80	0.47
4:L7:3:C:H2'	4:L7:4:U:C6	2.50	0.47
10:SC:256:TRP:CE2	14:SW:68:ARG:HD3	2.50	0.47
38:Lz:76:GLU:HG2	38:Lz:145:VAL:HG23	1.97	0.47
38:Lz:116:LEU:HD21	38:Lz:137:LEU:HD13	1.96	0.47
41:LC:60:HIS:HA	41:LC:92:PHE:HE1	1.80	0.47
44:LE:258:LEU:O	44:LE:262:LYS:HG2	2.15	0.47
46:Lq:190:GLN:HG3	46:Lq:191:GLN:CG	2.41	0.47
60:LP:59:PRO:HG3	60:LP:76:TRP:CG	2.49	0.47
86:5A:61:ILE:HA	86:5A:68:LYS:HA	1.96	0.47
1:S2:494:C:H42	1:S2:509:OMG:HN22	1.63	0.47
1:S2:562:U:H4'	8:SJ:132:GLN:HB3	1.95	0.47
1:S2:943:U:H2'	1:S2:944:A:C8	2.50	0.47
1:S2:1599:U:O4	12:SF:166:ILE:HA	2.15	0.47
1:S2:1829:G:H1'	1:S2:1850:MA6:H2	1.97	0.47
35:Se:86:VAL:HA	35:Se:89:GLN:HG2	1.97	0.47
36:Sf:94:LYS:HA	36:Sf:94:LYS:HD3	1.59	0.47
46:Lq:29:ILE:HG12	46:Lq:88:PHE:CE1	2.50	0.47
1:S2:567:C:H2'	1:S2:568:C:H5''	1.97	0.47
1:S2:825:A:H2'	1:S2:826:A:C8	2.49	0.47
1:S2:1387:G:N2	26:SR:8:THR:HG21	2.30	0.47
3:L5:294:G:O6	3:L5:315:G:H1'	2.15	0.47
3:L5:488:G:H2'	3:L5:489:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1604:G:N7	88:L5:5108:SPD:H22	2.30	0.47
3:L5:1633:G:H1'	99:L5:5555:HOH:O	2.14	0.47
3:L5:1697:G:N2	3:L5:2085:G:H5''	2.29	0.47
8:SJ:91:LYS:HD2	8:SJ:96:TYR:CD2	2.50	0.47
37:Sg:152:SER:HB3	37:Sg:168:CYS:SG	2.55	0.47
55:LD:208:MET:HG2	55:LD:223:PHE:CE2	2.49	0.47
66:Lr:32:LEU:O	66:Lr:33:LYS:HB2	2.15	0.47
73:Lf:71:TRP:HB2	73:Lf:89:ARG:NH1	2.30	0.47
3:L5:178:C:H2'	3:L5:258:G:H21	1.80	0.46
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.50	0.46
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.51	0.46
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.50	0.46
3:L5:3856:A:H5''	60:LP:83:TRP:O	2.15	0.46
3:L5:4133:C:H2'	3:L5:4134:C:H6	1.80	0.46
3:L5:4885:U:H2'	3:L5:4886:C:H6	1.80	0.46
6:SA:66:VAL:HG11	29:SV:46:PHE:HB2	1.97	0.46
17:SU:61:LEU:HB2	17:SU:82:MET:HB3	1.97	0.46
37:Sg:7:LEU:HD11	37:Sg:308:ARG:HG2	1.97	0.46
55:LD:41:LYS:HD2	59:LT:93:ILE:HD13	1.96	0.46
65:LZ:50:PRO:HD3	65:LZ:68:ILE:HG13	1.97	0.46
1:S2:522:A:H5''	8:SJ:145:PRO:HD2	1.97	0.46
1:S2:532:C:H2'	1:S2:533:A:C8	2.50	0.46
1:S2:1539:U:H2'	1:S2:1540:G:O4'	2.15	0.46
3:L5:153:G:OP2	53:LN:54:LYS:NZ	2.41	0.46
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.50	0.46
3:L5:3640:U:H2'	3:L5:3646:A:N6	2.30	0.46
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.50	0.46
7:SD:40:ARG:HB2	7:SD:47:GLU:HB2	1.96	0.46
20:SX:93:PHE:O	20:SX:140:ARG:NH1	2.48	0.46
37:Sg:9:GLY:O	37:Sg:309:VAL:HG22	2.15	0.46
38:Lz:204:LEU:HB3	38:Lz:216:LEU:HB3	1.97	0.46
42:LJ:160:GLU:HA	42:LJ:163:MET:HE2	1.96	0.46
55:LD:56:THR:HG22	55:LD:57:ASN:H	1.80	0.46
62:LX:73:HIS:ND1	62:LX:112:ALA:HA	2.30	0.46
63:LY:54:GLU:HB2	63:LY:108:ARG:HB3	1.97	0.46
1:S2:321:C:H2'	1:S2:322:C:H6	1.78	0.46
1:S2:1447:OMG:H5''	17:SU:29:VAL:HG13	1.97	0.46
3:L5:65:A:N6	3:L5:75:G:H1'	2.31	0.46
3:L5:3723:A2M:HM'3	3:L5:3723:A2M:H1'	1.54	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.50	0.46
11:SG:215:LYS:O	11:SG:219:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SH:148:LEU:HD22	14:SW:49:GLU:HG3	1.96	0.46
30:SY:10:ARG:HH21	30:SY:24:VAL:HG11	1.79	0.46
54:LI:51:HIS:HD2	54:LI:168:SER:HB2	1.77	0.46
1:S2:443:U:H2'	1:S2:444:G:O4'	2.14	0.46
1:S2:1624:U:H2'	1:S2:1625:PSU:O4'	2.15	0.46
3:L5:126:C:H2'	3:L5:127:G:C8	2.50	0.46
3:L5:707:C:O2'	3:L5:4943:A:N1	2.41	0.46
3:L5:1732:C:H5''	59:LT:43:LYS:HD2	1.97	0.46
3:L5:2858:A:H2'	3:L5:2859:G:O4'	2.16	0.46
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.69	0.46
27:SP:53:GLN:HG3	27:SP:80:LEU:HD23	1.98	0.46
55:LD:56:THR:HG22	55:LD:57:ASN:N	2.29	0.46
56:LQ:49:LYS:HG2	56:LQ:53:MET:HE3	1.97	0.46
64:LW:107:GLN:HA	64:LW:110:ARG:HB2	1.95	0.46
1:S2:67:C:H41	11:SG:164:LYS:H	1.62	0.46
1:S2:960:U:H1'	1:S2:963:A:N7	2.31	0.46
3:L5:677:G:H2'	3:L5:678:C:C6	2.50	0.46
3:L5:1811:G:H2'	3:L5:1812:C:H6	1.80	0.46
3:L5:1969:G:H4'	46:Lq:36:GLY:CA	2.45	0.46
3:L5:2602:G:H2'	3:L5:2603:C:H6	1.80	0.46
38:Lz:119:GLN:O	38:Lz:124:LEU:N	2.49	0.46
39:LA:126:LEU:HD12	39:LA:150:LEU:HD22	1.97	0.46
47:LK:95:GLN:HB3	47:LK:98:ILE:HG22	1.97	0.46
48:LO:118:MET:HG2	58:LS:169:THR:HG22	1.98	0.46
54:LI:48:LEU:HD22	54:LI:142:LEU:HA	1.98	0.46
61:LU:63:ILE:HA	61:LU:71:THR:O	2.16	0.46
73:Lf:8:LYS:HB3	73:Lf:100:ARG:NH1	2.31	0.46
1:S2:1426:U:P	16:SQ:69:ARG:HH21	2.39	0.46
3:L5:93:G:H2'	3:L5:94:A:C8	2.50	0.46
3:L5:700:G:H2'	3:L5:701:G:H8	1.81	0.46
3:L5:2815:A2M:H1'	3:L5:2815:A2M:HM'3	1.65	0.46
3:L5:3887:OMC:H5''	48:LO:71:TYR:CE2	2.51	0.46
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.81	0.46
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.16	0.46
15:SI:3:ILE:H	15:SI:3:ILE:HD12	1.80	0.46
18:SK:16:PHE:HB2	18:SK:79:LEU:HD23	1.96	0.46
18:SK:42:ASN:O	18:SK:43:LEU:C	2.57	0.46
65:LZ:95:VAL:HG12	65:LZ:110:ALA:HA	1.98	0.46
76:Lj:39:TYR:CD1	76:Lj:40:PRO:HA	2.50	0.46
87:EF:123:PHE:HB3	87:EF:166:ARG:NH2	2.30	0.46
1:S2:293:C:O2'	1:S2:294:U:H3'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1306:C:H2'	3:L5:1307:A:C8	2.50	0.46
93:L5:5119:3H3:H2	81:Lo:59:LYS:HE3	1.96	0.46
4:L7:24:C:H2'	4:L7:25:G:O4'	2.16	0.46
10:SC:263:LYS:HA	10:SC:267:GLN:HE21	1.81	0.46
26:SR:57:LEU:O	26:SR:61:ILE:HG13	2.16	0.46
31:SZ:58:LEU:HD12	31:SZ:62:VAL:HG21	1.97	0.46
37:Sg:168:CYS:HB2	37:Sg:195:LEU:HB3	1.97	0.46
37:Sg:286:CYS:SG	37:Sg:300:ALA:HB1	2.56	0.46
38:Lz:44:GLN:HE21	38:Lz:44:GLN:HB3	1.50	0.46
50:LV:69:LYS:HE2	50:LV:71:GLU:OE1	2.15	0.46
76:Lj:60:GLY:HA2	76:Lj:64:MET:HE3	1.98	0.46
84:At:18:G:N2	84:At:57:G:H2'	2.30	0.46
86:5A:95:GLN:HB2	86:5A:110:GLU:OE2	2.15	0.46
1:S2:1112:U:H2'	1:S2:1113:A:C8	2.51	0.46
1:S2:1401:A:H4'	17:SU:52:GLY:HA3	1.98	0.46
3:L5:179:G:C5	3:L5:258:G:N2	2.84	0.46
3:L5:967:C:H5'	3:L5:969:C:H5	1.80	0.46
3:L5:1177:U:H2'	3:L5:1178:G:C8	2.50	0.46
3:L5:1756:U:H2'	3:L5:1757:U:H5'	1.97	0.46
3:L5:2326:G:H5''	72:Le:127:ALA:HB2	1.97	0.46
6:SA:73:ASP:HB3	6:SA:120:ARG:HB2	1.98	0.46
15:SI:43:ILE:HD11	15:SI:60:LEU:HD21	1.97	0.46
21:SM:18:LEU:HA	21:SM:21:VAL:HG12	1.98	0.46
27:SP:45:LEU:HD21	27:SP:84:ILE:HD11	1.97	0.46
30:SY:30:PRO:HA	30:SY:67:GLY:HA2	1.98	0.46
42:LJ:31:ASP:HB3	42:LJ:35:ARG:NH1	2.31	0.46
56:LQ:34:PHE:CE1	56:LQ:38:ARG:HG3	2.51	0.46
1:S2:163:U:O3'	11:SG:83:CYS:HA	2.16	0.46
3:L5:125:C:OP1	53:LN:140:LYS:HG3	2.16	0.46
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.31	0.46
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.51	0.46
3:L5:3763:A:H2'	3:L5:3764:PSU:O4'	2.16	0.46
4:L7:23:A:H2'	4:L7:24:C:C6	2.51	0.46
9:SE:103:TYR:HB2	9:SE:182:MET:HE2	1.98	0.46
16:SQ:28:GLY:H	16:SQ:66:VAL:HA	1.80	0.46
48:LO:177:LEU:HD11	51:LM:130:LEU:HB3	1.98	0.46
49:LL:172:GLU:H	49:LL:172:GLU:CD	2.24	0.46
76:Lj:59:THR:CG2	76:Lj:64:MET:HE1	2.46	0.46
87:EF:79:M3L:HD3	87:EF:86:TYR:CE1	2.51	0.46
1:S2:656:G:H5'	1:S2:662:G:N2	2.31	0.46
3:L5:315:G:C6	53:LN:178:HIS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1730:U:H2'	3:L5:1731:C:C6	2.51	0.46
3:L5:3747:A:C8	39:LA:245:ARG:HG2	2.51	0.46
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.80	0.46
3:L5:4611:A:H2'	3:L5:4612:C:C6	2.51	0.46
8:SJ:110:LEU:HB2	8:SJ:147:PHE:HB3	1.97	0.46
21:SM:61:TYR:OH	21:SM:108:CYS:HB2	2.16	0.46
53:LN:148:THR:O	53:LN:151:ILE:HG22	2.15	0.46
62:LX:129:ARG:HG2	62:LX:133:GLU:O	2.15	0.46
69:LF:157:ARG:HD2	69:LF:213:LEU:HD23	1.98	0.46
69:LF:226:HIS:ND1	69:LF:228:VAL:HG22	2.31	0.46
81:Lo:104:ILE:HG23	81:Lo:106:PHE:H	1.80	0.46
82:Lp:13:LYS:HE3	82:Lp:14:TYR:CZ	2.51	0.46
83:mR:36[A]:U:H4'	83:mR:36[A]:U:OP1	2.15	0.46
1:S2:324:C:C2'	1:S2:325:C:H5'	2.46	0.45
1:S2:575:A:H2'	1:S2:576:A2M:O4'	2.16	0.45
1:S2:948:C:H2'	1:S2:949:G:C8	2.51	0.45
2:L8:93:C:O2'	2:L8:94:G:H8	1.99	0.45
3:L5:174:C:H2'	3:L5:175:C:C6	2.50	0.45
3:L5:3974:G:H3'	3:L5:3975:C:C6	2.52	0.45
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.97	0.45
3:L5:4746:C:H2'	3:L5:4747:C:C6	2.51	0.45
18:SK:31:LYS:CG	18:SK:39:ASN:HA	2.46	0.45
32:Sa:39:PHE:CD2	32:Sa:41:ILE:HD11	2.51	0.45
42:LJ:20:LEU:HB3	42:LJ:74:VAL:HG23	1.97	0.45
58:LS:30:MET:HE1	58:LS:47:PHE:HB3	1.98	0.45
69:LF:187:MET:HE3	69:LF:187:MET:HB3	1.84	0.45
84:At:5:G:H2'	84:At:6:G:H8	1.80	0.45
1:S2:388:U:H2'	1:S2:389:A:H8	1.80	0.45
1:S2:428:OMU:O3'	8:SJ:2:PRO:HD2	2.16	0.45
1:S2:1113:A:H2'	1:S2:1114:U:O4'	2.17	0.45
1:S2:1328:OMG:HM23	1:S2:1328:OMG:H1'	1.57	0.45
1:S2:1781:A:H2'	1:S2:1783:C:C4	2.51	0.45
3:L5:911:U:H2'	3:L5:912:G:O4'	2.16	0.45
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.17	0.45
3:L5:2689:C:H2'	3:L5:2690:C:C6	2.51	0.45
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.80	0.45
3:L5:4370:OMG:CM2	93:L5:5119:3H3:O	2.65	0.45
16:SQ:45:ARG:O	16:SQ:48:GLN:HB2	2.16	0.45
38:Lz:11:TYR:CE1	38:Lz:12:GLU:HG2	2.51	0.45
45:LG:95:LEU:HD23	45:LG:184:ILE:HD12	1.97	0.45
60:LP:94:MET:HE1	60:LP:146:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:LZ:84:ARG:HA	70:Lc:66:LEU:HD21	1.98	0.45
1:S2:93:PSU:OP1	9:SE:2:ALA:HB1	2.17	0.45
1:S2:327:G:C6	1:S2:329:G:C5	3.04	0.45
1:S2:554:A:H62	1:S2:589:G:N2	2.14	0.45
1:S2:1863:A:H1'	32:Sa:79:ILE:HD13	1.97	0.45
3:L5:980:U:H2'	3:L5:981:C:C6	2.51	0.45
3:L5:2323:C:H2'	3:L5:2324:C:H6	1.81	0.45
3:L5:2477:A:H2'	3:L5:2478:C:C6	2.51	0.45
3:L5:4861:G:H2'	3:L5:4862:G:H8	1.81	0.45
12:SF:128:ILE:HG13	34:Sc:68:LEU:CD1	2.46	0.45
37:Sg:180:ALA:C	37:Sg:182:CYS:H	2.24	0.45
57:LR:126:LYS:O	57:LR:131:VAL:HG22	2.15	0.45
87:EF:290:LYS:HB3	87:EF:311:ASN:HB3	1.97	0.45
87:EF:391:PRO:O	87:EF:393:PHE:N	2.49	0.45
1:S2:71:G:H2'	1:S2:72:C:O4'	2.16	0.45
1:S2:1512:C:H2'	1:S2:1513:C:C6	2.51	0.45
2:L8:76:C:H2'	2:L8:77:A:O4'	2.16	0.45
3:L5:516:C:H2'	3:L5:517:C:C6	2.51	0.45
3:L5:1432:G:H2'	3:L5:1451:G:N2	2.31	0.45
3:L5:1766:A:H2'	3:L5:1767:A:C8	2.51	0.45
3:L5:1982:G:H3'	3:L5:1983:A:H5''	1.98	0.45
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.82	0.45
3:L5:4155:C:H2'	3:L5:4156:G:O4'	2.17	0.45
3:L5:4517:A:N6	3:L5:4520:G:C5	2.84	0.45
7:SD:76:ARG:HB2	18:SK:22:VAL:HG11	1.99	0.45
7:SD:116:ARG:NE	7:SD:150:MET:HE2	2.30	0.45
13:SH:80:VAL:HG22	13:SH:92:VAL:HG23	1.98	0.45
25:SL:126:VAL:HG12	25:SL:145:VAL:HG22	1.98	0.45
39:LA:10:LYS:HA	39:LA:16:PHE:CD2	2.52	0.45
51:LM:96:GLU:HA	51:LM:99:GLU:HG3	1.99	0.45
65:LZ:16:GLY:O	74:Lg:76:ARG:HG3	2.16	0.45
73:Lf:71:TRP:HB2	73:Lf:89:ARG:HH12	1.82	0.45
1:S2:466:G:H1'	11:SG:59:GLN:HE21	1.82	0.45
1:S2:961:G:C4	83:mR:34:C:H1'	2.51	0.45
1:S2:1540:G:OP1	28:ST:39:LEU:HD12	2.16	0.45
1:S2:1852:C:H2'	1:S2:1853:C:C6	2.51	0.45
2:L8:92:U:H2'	2:L8:93:C:O4'	2.16	0.45
3:L5:2415:OMU:H1'	3:L5:2415:OMU:HM23	1.75	0.45
3:L5:3595:U:H4'	3:L5:3596:A:H5'	1.99	0.45
3:L5:4861:G:H2'	3:L5:4862:G:C8	2.51	0.45
20:SX:142:ARG:O	87:EF:409:PRO:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SS:5:ILE:HD12	22:SS:6:PRO:HD2	1.97	0.45
23:Sd:30:LEU:HA	23:Sd:39:CYS:HA	1.97	0.45
27:SP:109:PRO:O	27:SP:112:ILE:HG13	2.16	0.45
38:Lz:41:TYR:CD1	38:Lz:195:LYS:HD3	2.51	0.45
64:LW:101:ARG:C	64:LW:103:ALA:N	2.74	0.45
1:S2:1520:G:H5''	1:S2:1521:C:OP2	2.17	0.45
3:L5:1397:A:OP1	52:La:132:ARG:HD2	2.15	0.45
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.51	0.45
3:L5:2521:G:H4'	74:Lg:26:PRO:HD2	1.97	0.45
3:L5:3724:A2M:HM'3	3:L5:3724:A2M:H1'	1.74	0.45
3:L5:4265:U:OP1	55:LD:12:TYR:OH	2.28	0.45
6:SA:219:GLU:HA	6:SA:222:VAL:HG12	1.99	0.45
86:5A:43:MET:HE3	86:5A:43:MET:HB3	1.54	0.45
1:S2:287:U:O2	9:SE:131:VAL:HG21	2.16	0.45
1:S2:874:G:H2'	1:S2:875:A:H8	1.81	0.45
1:S2:1606:G:N2	1:S2:1632:G:H1'	2.31	0.45
1:S2:1628:C:H2'	1:S2:1629:C:C6	2.52	0.45
3:L5:700:G:H2'	3:L5:701:G:C8	2.52	0.45
3:L5:967:C:H42	3:L5:2261:G:H21	1.64	0.45
3:L5:2498:C:H2'	3:L5:2499:C:C6	2.52	0.45
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.31	0.45
14:SW:23:ARG:HG3	33:Sb:4:ALA:HB2	1.99	0.45
18:SK:16:PHE:CE2	18:SK:76:ILE:HG23	2.52	0.45
19:SO:28:PHE:HZ	32:Sa:58:VAL:HG21	1.82	0.45
38:Lz:35:GLN:HE21	38:Lz:35:GLN:HB3	1.55	0.45
40:LB:321:VAL:HG12	40:LB:322:HIS:ND1	2.32	0.45
45:LG:166:LEU:HD21	53:LN:45:PRO:HG2	1.99	0.45
69:LF:199:LYS:HA	69:LF:199:LYS:HD3	1.74	0.45
70:Lc:36:LYS:O	70:Lc:40:GLN:HG3	2.16	0.45
80:Ln:20:MET:HE2	80:Ln:20:MET:HA	1.98	0.45
85:Pt:24:C:H2'	85:Pt:25:U:C6	2.51	0.45
1:S2:113:G:N2	1:S2:292:A:H2'	2.31	0.45
1:S2:1229:G:H2'	1:S2:1230:C:O4'	2.16	0.45
1:S2:1232:PSU:H2'	1:S2:1233:G:C8	2.52	0.45
1:S2:1653:U:H2'	1:S2:1654:G:C8	2.52	0.45
3:L5:979:C:OP2	44:LE:66:LYS:HD3	2.17	0.45
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.52	0.45
5:SB:171:ILE:O	5:SB:175:GLU:HG2	2.16	0.45
34:Sc:44:ARG:HD3	34:Sc:44:ARG:HA	1.66	0.45
41:LC:32:ILE:O	56:LQ:23:ILE:HD11	2.15	0.45
42:LJ:56:THR:HG23	42:LJ:63:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:La:72:THR:HG22	52:La:110:LYS:HB3	1.97	0.45
56:LQ:61:LEU:HD21	56:LQ:66:MET:HB2	1.99	0.45
61:LU:25:CYS:C	61:LU:28:PRO:HD2	2.41	0.45
86:5A:50:5CT:H11	86:5A:50:5CT:H3	1.98	0.45
1:S2:195:C:H2'	1:S2:196:C:C6	2.52	0.45
1:S2:326:C:H1'	1:S2:327:G:C6	2.52	0.45
1:S2:538:U:H2'	1:S2:539:C:C6	2.52	0.45
1:S2:1520:G:N3	1:S2:1520:G:C2'	2.78	0.45
2:L8:127:U:H2'	2:L8:128:C:O4'	2.17	0.45
3:L5:207:G:H2'	3:L5:208:A:C8	2.52	0.45
3:L5:325:U:H2'	3:L5:326:C:C6	2.52	0.45
3:L5:1250:C:H2'	3:L5:1251:C:C6	2.52	0.45
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.52	0.45
3:L5:4637:OMG:H1'	3:L5:4637:OMG:HM23	1.58	0.45
5:SB:85:LYS:HB2	5:SB:101:HIS:HB3	1.99	0.45
9:SE:19:MET:SD	9:SE:108:ARG:HD2	2.57	0.45
18:SK:6:LYS:HG2	18:SK:7:ASN:H	1.81	0.45
21:SM:52:LEU:HD23	21:SM:78:LYS:HD3	1.99	0.45
32:Sa:39:PHE:CE2	32:Sa:41:ILE:HD11	2.52	0.45
41:LC:215:ASN:HD22	41:LC:215:ASN:HA	1.49	0.45
45:LG:246:SER:O	45:LG:250:ILE:HG12	2.17	0.45
53:LN:116:LEU:HD22	53:LN:135:ILE:HD11	1.98	0.45
55:LD:156:GLY:HA2	55:LD:181:PRO:HG3	1.98	0.45
69:LF:137:GLU:OE1	69:LF:234:GLY:HA2	2.16	0.45
80:Ln:2:ARG:HD3	80:Ln:5:TRP:NE1	2.31	0.45
86:5A:134:LEU:HD22	86:5A:152:MET:SD	2.57	0.45
1:S2:838:G:N3	1:S2:841:G:H1'	2.32	0.45
1:S2:1305:C:H2'	1:S2:1306:U:H6	1.82	0.45
3:L5:699:C:H2'	3:L5:700:G:C8	2.52	0.45
3:L5:928:C:H2'	3:L5:929:A:C8	2.52	0.45
3:L5:2310:C:H2'	3:L5:2311:C:H6	1.82	0.45
3:L5:2518:G:H1'	3:L5:2539:C:H1'	1.98	0.45
3:L5:4341:C:N3	93:L5:5119:3H3:H14	2.32	0.45
3:L5:4993:G:H22	3:L5:5058:A:H2	1.64	0.45
7:SD:72:VAL:HB	18:SK:20:VAL:HG21	2.00	0.45
16:SQ:93:VAL:HA	16:SQ:108:ILE:HD11	1.98	0.45
40:LB:258:HIS:HA	40:LB:259:PRO:C	2.41	0.45
46:Lq:116:ILE:HG22	46:Lq:166:LYS:HA	1.99	0.45
46:Lq:162:LYS:HG3	46:Lq:165:ASP:HB2	1.98	0.45
68:Lb:65:MET:HA	68:Lb:68:ARG:HG2	1.98	0.45
80:Ln:2:ARG:HB3	80:Ln:5:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:EF:370:CYS:HA	87:EF:406:PRO:HA	1.97	0.45
87:EF:385:LYS:HE3	87:EF:385:LYS:HB3	1.51	0.45
87:EF:426:VAL:HG13	87:EF:434:ALA:O	2.17	0.45
1:S2:115:U:H2'	1:S2:116:OMU:C6	2.46	0.44
1:S2:806:U:H2'	1:S2:807:G:C8	2.51	0.44
3:L5:375:G:OP1	41:LC:62:THR:OG1	2.33	0.44
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.52	0.44
3:L5:1409:C:C4	3:L5:1410:U:H1'	2.52	0.44
3:L5:2560:C:H2'	3:L5:2561:C:C6	2.51	0.44
12:SF:128:ILE:HG13	34:Sc:68:LEU:HD12	1.99	0.44
13:SH:161:ALA:C	13:SH:163:GLN:H	2.25	0.44
24:SN:140:LYS:HE3	24:SN:140:LYS:HB3	1.56	0.44
25:SL:37:TYR:CE1	25:SL:51:ILE:HG23	2.52	0.44
27:SP:137:HIS:HD1	27:SP:141:PHE:HE2	1.64	0.44
28:ST:134:ILE:O	28:ST:137:GLN:HG2	2.17	0.44
51:LM:3:PHE:CZ	58:LS:155:PRO:HB3	2.52	0.44
54:LI:156:LYS:HG3	54:LI:163:GLN:HB2	1.99	0.44
87:EF:418:TYR:O	87:EF:419:PRO:C	2.59	0.44
3:L5:1762:C:H2'	3:L5:1763:C:C6	2.52	0.44
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.32	0.44
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.52	0.44
37:Sg:289:LEU:HD22	37:Sg:298:LEU:HD11	1.98	0.44
41:LC:183:VAL:HA	41:LC:204:ARG:HG2	1.99	0.44
54:LI:63:GLU:H	54:LI:63:GLU:CD	2.25	0.44
58:LS:1:MET:HG3	58:LS:39:VAL:HG11	1.99	0.44
67:Lh:94:ARG:HE	67:Lh:94:ARG:HB3	1.53	0.44
1:S2:344:U:H2'	1:S2:345:U:C6	2.52	0.44
1:S2:996:A:H2'	1:S2:997:A:C8	2.52	0.44
1:S2:1207:G:H22	83:mR:36[B]:U:H3'	1.82	0.44
1:S2:1654:G:OP1	28:ST:90:SER:HB2	2.18	0.44
2:L8:115:G:H2'	2:L8:116:C:H6	1.82	0.44
3:L5:46:U:OP1	49:LL:16:LYS:HE2	2.17	0.44
3:L5:2258:C:O2	44:LE:91:THR:HG22	2.16	0.44
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.52	0.44
12:SF:73:THR:O	12:SF:89:THR:HG21	2.17	0.44
24:SN:23:PRO:HB3	33:Sb:84:HIS:HB2	2.00	0.44
24:SN:88:LEU:HD22	24:SN:135:LEU:HD11	1.98	0.44
38:Lz:151:VAL:O	38:Lz:154:THR:HG23	2.17	0.44
55:LD:152:ARG:HG3	55:LD:154:THR:HG23	1.99	0.44
59:LT:112:ASN:HD22	59:LT:128:LEU:HD22	1.81	0.44
69:LF:28:LEU:HA	69:LF:31:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Lp:46:LYS:HD3	82:Lp:59:SER:OG	2.16	0.44
1:S2:1240:A:H1'	1:S2:1267:C:HO2'	1.82	0.44
1:S2:1801:A:H2'	1:S2:1802:C:C6	2.53	0.44
2:L8:46:G:OP2	78:L1:15:LYS:HD2	2.18	0.44
2:L8:148:A:H2'	2:L8:149:G:C8	2.52	0.44
3:L5:159:C:OP2	75:Li:25:ARG:HG2	2.17	0.44
3:L5:1250:C:H2'	3:L5:1251:C:H6	1.82	0.44
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.53	0.44
3:L5:1440:U:H2'	3:L5:1441:C:H6	1.82	0.44
3:L5:2091:C:H1'	3:L5:2094:G:H1'	1.99	0.44
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.80	0.44
4:L7:18:C:H2'	4:L7:19:C:C6	2.53	0.44
37:Sg:142:VAL:HG12	37:Sg:146:SER:HB2	1.99	0.44
58:LS:84:TYR:CE1	58:LS:93:MET:HE3	2.53	0.44
1:S2:1277:C:H4'	18:SK:55:ARG:HG3	1.99	0.44
1:S2:1754:G:H2'	1:S2:1755:C:H6	1.81	0.44
1:S2:1808:U:H2'	1:S2:1809:A:H8	1.82	0.44
3:L5:469:C:H2'	3:L5:470:A:C8	2.52	0.44
3:L5:4107:G:C6	3:L5:4108:G:H1'	2.53	0.44
3:L5:4967:A:H5''	40:LB:119:TYR:HE1	1.83	0.44
19:SO:44:VAL:HG11	19:SO:85:CYS:SG	2.57	0.44
45:LG:171:PRO:HB3	45:LG:181:TYR:CE2	2.53	0.44
59:LT:48:VAL:HG21	59:LT:94:GLU:HG2	1.99	0.44
63:LY:38:LEU:HD22	63:LY:42:TYR:HE2	1.81	0.44
63:LY:56:GLN:HG3	63:LY:67:ILE:HD13	2.00	0.44
68:Lb:113:ALA:HB1	69:LF:37:PHE:HZ	1.83	0.44
1:S2:128:U:H3'	1:S2:129:C:C6	2.52	0.44
1:S2:639:C:H2'	1:S2:640:A:C8	2.53	0.44
3:L5:106:A:H1'	3:L5:336:A:N3	2.32	0.44
3:L5:273:U:H2'	3:L5:274:C:H6	1.82	0.44
3:L5:907:C:H2'	3:L5:908:G:H8	1.83	0.44
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.52	0.44
3:L5:1437:C:H1'	3:L5:2098:G:O2'	2.17	0.44
3:L5:1673:U:H2'	3:L5:1674:C:C6	2.53	0.44
3:L5:3627:OMG:HM23	3:L5:3627:OMG:H1'	1.75	0.44
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.53	0.44
24:SN:35:GLU:OE2	24:SN:39:LYS:HE3	2.18	0.44
25:SL:4:ILE:HG12	25:SL:54:THR:O	2.18	0.44
37:Sg:299:PHE:CD1	37:Sg:309:VAL:HG12	2.50	0.44
41:LC:138:MET:HE3	41:LC:138:MET:HB3	1.69	0.44
53:LN:159:ARG:HB3	53:LN:164:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Lj:59:THR:HG23	76:Lj:64:MET:HE1	2.00	0.44
1:S2:874:G:H2'	1:S2:875:A:C8	2.52	0.44
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.53	0.44
3:L5:1920:C:H3'	3:L5:1921:C:H5''	2.00	0.44
8:SJ:26:ASP:HB2	35:Se:116:PHE:HZ	1.82	0.44
12:SF:167:LYS:HA	31:SZ:71:ALA:HB1	1.99	0.44
14:SW:102:ILE:HB	14:SW:113:HIS:HB3	1.99	0.44
16:SQ:113:ILE:HD11	16:SQ:120:LEU:HB2	1.99	0.44
29:SV:38:GLU:CG	29:SV:49:GLN:HB2	2.48	0.44
42:LJ:111:GLU:HB3	42:LJ:125:ILE:HD11	1.99	0.44
44:LE:164:PHE:CE1	44:LE:173:LEU:HB3	2.52	0.44
62:LX:89:LYS:HD3	62:LX:93:ASN:HD22	1.83	0.44
69:LF:41:MET:HA	69:LF:41:MET:HE2	1.99	0.44
69:LF:209:TRP:CD1	69:LF:210:PRO:HD2	2.52	0.44
82:Lp:30:GLU:OE2	82:Lp:34:HIS:HE1	2.00	0.44
1:S2:203:G:H2'	1:S2:204:G:H8	1.83	0.44
1:S2:624:C:H41	20:SX:63:ASN:ND2	2.16	0.44
1:S2:1240:A:H1'	1:S2:1267:C:O2'	2.17	0.44
1:S2:1714:U:H2'	1:S2:1715:A:C8	2.53	0.44
2:L8:19:C:H2'	2:L8:20:A:C8	2.52	0.44
3:L5:1772:C:H2'	3:L5:1773:U:C6	2.53	0.44
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.83	0.44
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.53	0.44
8:SJ:116:LYS:C	8:SJ:118:GLY:N	2.75	0.44
10:SC:182:CYS:HB2	14:SW:95:PRO:HB2	1.98	0.44
39:LA:79:ALA:O	39:LA:82:ILE:HG12	2.18	0.44
51:LM:43:THR:O	51:LM:43:THR:HG22	2.18	0.44
59:LT:43:LYS:HG3	59:LT:58:HIS:NE2	2.32	0.44
1:S2:941:C:H2'	1:S2:942:G:C8	2.53	0.44
1:S2:1654:G:OP1	28:ST:82:ARG:HD2	2.18	0.44
1:S2:1690:U:H2'	1:S2:1691:U:C6	2.53	0.44
1:S2:1845:A:H2'	1:S2:1846:G:C8	2.52	0.44
3:L5:1970:A:H4'	3:L5:2000:G:C8	2.53	0.44
3:L5:2298:U:H5''	41:LC:204:ARG:HH21	1.83	0.44
3:L5:2424:OMG:H1'	3:L5:2424:OMG:HM23	1.58	0.44
3:L5:4208:U:H2'	3:L5:4209:G:C8	2.51	0.44
6:SA:80:ARG:O	6:SA:84:GLN:HG3	2.18	0.44
7:SD:29:LEU:HD23	7:SD:65:ARG:HH21	1.83	0.44
13:SH:134:VAL:O	13:SH:135:PHE:C	2.61	0.44
21:SM:53:ALA:C	21:SM:55:ASN:N	2.76	0.44
32:Sa:94:ASP:OD1	32:Sa:96:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LE:253:VAL:O	44:LE:257:ILE:HG12	2.18	0.44
61:LU:26:THR:HA	61:LU:29:VAL:HG22	1.99	0.44
61:LU:84:LYS:HB2	61:LU:110:TYR:CE2	2.52	0.44
67:Lh:27:GLU:OE2	67:Lh:46:LYS:HE3	2.17	0.44
1:S2:1139:C:H2'	1:S2:1140:G:O4'	2.18	0.43
1:S2:1164:G:O2'	1:S2:1165:G:H5'	2.18	0.43
1:S2:1839:U:H2'	1:S2:1840:U:C6	2.52	0.43
3:L5:741:C:OP2	3:L5:742:G:H5''	2.18	0.43
3:L5:758:G:H5''	43:LH:52:LYS:HE3	2.00	0.43
3:L5:968:C:H5'	44:LE:110:ARG:NH1	2.33	0.43
3:L5:1397:A:OP1	52:La:132:ARG:HB2	2.18	0.43
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.32	0.43
3:L5:4342:C:O3'	81:Lo:37:GLY:HA3	2.18	0.43
8:SJ:50:LEU:HD13	8:SJ:105:PHE:CE2	2.52	0.43
8:SJ:91:LYS:O	8:SJ:92:MET:HE2	2.18	0.43
21:SM:26:LEU:HA	21:SM:30:GLY:HA2	1.99	0.43
22:SS:20:ILE:HD11	22:SS:33:ILE:HG13	1.99	0.43
24:SN:33:VAL:HG21	24:SN:66:VAL:HG11	2.00	0.43
26:SR:62:GLN:O	26:SR:62:GLN:HG2	2.18	0.43
45:LG:80:ILE:HG23	45:LG:164:ILE:HD13	1.99	0.43
47:LK:61:LYS:O	47:LK:72:GLU:HG3	2.18	0.43
64:LW:109:ILE:O	64:LW:113:LYS:HG2	2.18	0.43
68:Lb:108:ALA:O	68:Lb:112:ILE:HG12	2.18	0.43
69:LF:162:ILE:HD12	69:LF:167:ILE:HB	1.99	0.43
76:Lj:25:LYS:HD2	76:Lj:25:LYS:O	2.18	0.43
1:S2:653:A:H2'	1:S2:654:A:O4'	2.18	0.43
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.18	0.43
1:S2:1037:G:H4'	1:S2:1845:A:H4'	1.99	0.43
3:L5:131:C:H2'	3:L5:132:G:H8	1.82	0.43
3:L5:1445:U:H2'	3:L5:1446:C:C6	2.53	0.43
3:L5:1464:C:H5''	68:Lb:32:LEU:HD12	1.99	0.43
3:L5:4232:U:OP2	81:Lo:2:VAL:HA	2.18	0.43
3:L5:4289:U:H2'	3:L5:4290:U:C6	2.53	0.43
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.19	0.43
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.52	0.43
7:SD:47:GLU:O	7:SD:49:ILE:HG13	2.18	0.43
7:SD:109:LEU:HD23	7:SD:182:LEU:HD23	1.99	0.43
8:SJ:88:ASP:HB3	8:SJ:91:LYS:HG2	2.00	0.43
13:SH:134:VAL:O	13:SH:134:VAL:HG23	2.17	0.43
21:SM:44:LYS:O	21:SM:46:GLN:HG2	2.18	0.43
28:ST:39:LEU:HD21	28:ST:52:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SY:12:PHE:CZ	30:SY:21:LYS:HD3	2.52	0.43
30:SY:40:ILE:HD13	30:SY:60:PHE:CE2	2.53	0.43
45:LG:163:PRO:HG3	53:LN:43:THR:O	2.18	0.43
50:LV:85:ARG:HG2	50:LV:85:ARG:HH11	1.82	0.43
51:LM:24:LEU:H	51:LM:43:THR:HG21	1.83	0.43
69:LF:241:ASN:O	69:LF:245:ARG:HG2	2.18	0.43
87:EF:202:LEU:HG	87:EF:229:LEU:HD22	1.99	0.43
1:S2:542:U:H6	1:S2:542:U:H2'	1.64	0.43
1:S2:916:A:C5	24:SN:73:ARG:HD3	2.54	0.43
1:S2:1328:OMG:H4'	36:Sf:78:LYS:HE3	2.00	0.43
1:S2:1440:C:O2'	1:S2:1441:U:H5'	2.18	0.43
1:S2:1740:C:H2'	1:S2:1741:U:C6	2.53	0.43
3:L5:137:G:H2'	3:L5:138:G:C8	2.54	0.43
3:L5:1369:C:OP2	3:L5:1370:G:O2'	2.31	0.43
3:L5:1377:G:H21	3:L5:1380:G:H5'	1.82	0.43
3:L5:1457:G:H5'	56:LQ:72:LEU:HD13	2.00	0.43
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.18	0.43
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.53	0.43
3:L5:4978:G:H2'	3:L5:4979:A:H5''	2.00	0.43
7:SD:10:LYS:HB2	7:SD:10:LYS:HE2	1.83	0.43
30:SY:55:ILE:CD1	30:SY:75:ILE:HD12	2.48	0.43
41:LC:149:GLU:HG3	66:Lr:72:LYS:HG2	2.00	0.43
41:LC:152:LEU:HD23	41:LC:251:ILE:HG12	1.99	0.43
44:LE:276:ALA:HB1	73:Lf:3:GLY:HA3	2.01	0.43
83:mR:34:C:H2'	83:mR:35:G:O4'	2.18	0.43
85:Pt:72:C:H2'	85:Pt:73:A:H8	1.83	0.43
1:S2:1580:A:H8	17:SU:56:MET:HE1	1.83	0.43
1:S2:1666:C:H2'	1:S2:1667:U:O4'	2.18	0.43
3:L5:81:C:H2'	3:L5:82:U:O4'	2.18	0.43
3:L5:679:C:H2'	3:L5:680:G:C8	2.53	0.43
3:L5:1700:G:N2	3:L5:2097:U:H5'	2.33	0.43
3:L5:1918:U:O3'	3:L5:1919:G:H3'	2.18	0.43
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.53	0.43
4:L7:2:U:H2'	4:L7:3:C:C6	2.53	0.43
32:Sa:89:ARG:HD2	32:Sa:89:ARG:HA	1.81	0.43
37:Sg:45:LEU:HB3	37:Sg:47:ARG:HD2	1.99	0.43
40:LB:168:MET:HA	40:LB:171:LEU:HD12	2.00	0.43
42:LJ:167:GLN:O	42:LJ:171:ASP:HA	2.18	0.43
43:LH:41:ILE:HG22	43:LH:43:VAL:HG13	1.99	0.43
69:LF:154:ILE:HG22	69:LF:187:MET:HE1	2.00	0.43
72:Le:82:VAL:HG13	72:Le:114:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:EF:372:PHE:CE1	87:EF:404:MET:HE2	2.53	0.43
87:EF:380:ASP:HB2	87:EF:385:LYS:HZ2	1.83	0.43
1:S2:37:C:H2'	1:S2:38:A:O4'	2.18	0.43
1:S2:381:C:H2'	1:S2:382:C:C6	2.54	0.43
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.53	0.43
3:L5:377:A:H2'	3:L5:378:A:O4'	2.19	0.43
3:L5:450:G:H3'	3:L5:451:C:H6	1.83	0.43
3:L5:966:A:H2'	3:L5:2092:G:N1	2.33	0.43
3:L5:1249:C:H2'	3:L5:1250:C:H6	1.83	0.43
3:L5:1971:C:H41	3:L5:2001:G:P	2.42	0.43
3:L5:3939:G:HO2'	3:L5:4076:G:H1	1.65	0.43
7:SD:49:ILE:HG12	7:SD:87:TYR:HB2	2.00	0.43
7:SD:113:LEU:HD22	7:SD:118:ALA:HB2	2.00	0.43
19:SO:34:PHE:HB3	19:SO:41:PHE:HB2	2.00	0.43
24:SN:120:SER:O	24:SN:124:ARG:HG3	2.18	0.43
37:Sg:12:LYS:HG2	37:Sg:306:LEU:HD22	2.00	0.43
38:Lz:41:TYR:CE1	38:Lz:46:ASP:HB3	2.53	0.43
39:LA:117:GLU:HG2	39:LA:124:GLY:H	1.84	0.43
41:LC:140:LYS:HB3	41:LC:142:HIS:CD2	2.52	0.43
41:LC:293:LEU:HD22	56:LQ:34:PHE:CD2	2.53	0.43
66:Lr:20:ARG:HG2	66:Lr:21:ASN:OD1	2.17	0.43
87:EF:175:SER:HA	87:EF:178:ILE:HG12	2.00	0.43
1:S2:77:A:H2'	1:S2:78:C:C6	2.54	0.43
1:S2:440:G:H5''	1:S2:1798:C:O2'	2.19	0.43
1:S2:823:U:O2'	1:S2:824:C:H5'	2.18	0.43
3:L5:6:C:H2'	3:L5:7:C:C6	2.53	0.43
3:L5:1459:A:H2'	3:L5:1460:C:O4'	2.19	0.43
3:L5:2029:A:H2'	3:L5:2030:A:H8	1.81	0.43
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.99	0.43
8:SJ:60:LEU:HD22	8:SJ:70:ARG:HA	2.01	0.43
12:SF:68:ILE:HD11	12:SF:151:ILE:HD11	2.01	0.43
13:SH:73:GLN:O	13:SH:76:GLN:HB2	2.18	0.43
18:SK:11:ILE:HG12	18:SK:45:VAL:HG22	1.99	0.43
24:SN:89:TYR:CE1	24:SN:150:VAL:HG12	2.54	0.43
32:Sa:13:LYS:HD3	32:Sa:13:LYS:HA	1.82	0.43
37:Sg:214:GLY:HA2	37:Sg:236:ILE:HG12	2.00	0.43
38:Lz:34:LEU:HD11	38:Lz:204:LEU:HD21	2.00	0.43
38:Lz:117:ILE:HG23	38:Lz:118:LYS:HG3	2.01	0.43
70:Lc:65:MET:HE3	70:Lc:65:MET:HB3	1.88	0.43
74:Lg:83:CYS:SG	74:Lg:86:CYS:HB2	2.57	0.43
3:L5:38:A:H5''	52:La:35:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4622:A:H4'	40:LB:13:SER:HB2	2.00	0.43
4:L7:3:C:H2'	4:L7:4:U:H6	1.83	0.43
5:SB:136:ARG:HB2	5:SB:218:LEU:HD11	1.99	0.43
7:SD:58:VAL:HA	7:SD:65:ARG:HD3	2.01	0.43
12:SF:175:ASP:HA	12:SF:178:ILE:HB	2.00	0.43
21:SM:53:ALA:C	21:SM:55:ASN:H	2.27	0.43
31:SZ:73:VAL:HG21	31:SZ:88:LEU:HD21	2.01	0.43
38:Lz:70:ASP:HB3	38:Lz:73:HIS:HB2	2.01	0.43
38:Lz:205:TYR:CZ	38:Lz:215:ARG:HD3	2.53	0.43
54:LI:40:LYS:O	54:LI:41:ALA:C	2.62	0.43
79:Lm:97:ARG:HG3	79:Lm:122:ARG:HG2	1.99	0.43
85:Pt:21:H2U:H1'	86:5A:153:ALA:HB3	1.99	0.43
1:S2:1788:A:H2'	1:S2:1789:G:O4'	2.19	0.43
3:L5:444:G:H2'	3:L5:445:U:C6	2.53	0.43
3:L5:1727:U:H2'	3:L5:1728:U:C6	2.54	0.43
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.53	0.43
3:L5:2900:U:H2'	3:L5:2901:G:C8	2.54	0.43
3:L5:4085:A:H3'	62:LX:44:PRO:HB2	2.00	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.54	0.43
6:SA:90:PHE:HE2	6:SA:178:LEU:HG	1.84	0.43
30:SY:55:ILE:HD13	30:SY:75:ILE:HD12	2.01	0.43
40:LB:288:GLY:HA3	40:LB:330:PHE:CE2	2.54	0.43
42:LJ:18:ARG:HG3	42:LJ:135:GLY:HA3	2.01	0.43
85:Pt:4:G:H2'	85:Pt:5:G:H8	1.82	0.43
87:EF:24:THR:HG23	87:EF:89:ILE:HD13	2.00	0.43
87:EF:264:VAL:HG12	87:EF:309:GLY:CA	2.48	0.43
1:S2:326:C:O2	64:LW:116:LYS:HE2	2.18	0.43
1:S2:888:U:H3	1:S2:900:C:H1'	1.82	0.43
1:S2:960:U:H2'	1:S2:962:A:OP2	2.18	0.43
1:S2:1148:A:H4'	1:S2:1149:A:O4'	2.18	0.43
1:S2:1446:A:O2'	1:S2:1447:OMG:H8	2.02	0.43
2:L8:88:A:H2'	2:L8:89:U:O4'	2.19	0.43
3:L5:129:C:H2'	3:L5:130:C:C6	2.54	0.43
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.54	0.43
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.54	0.43
3:L5:1973:G:H2'	3:L5:1974:U:C5	2.53	0.43
3:L5:4337:C:N3	81:Lo:61:LYS:HE3	2.34	0.43
7:SD:40:ARG:HA	7:SD:40:ARG:HD2	1.38	0.43
12:SF:43:GLU:C	12:SF:45:TYR:H	2.26	0.43
13:SH:163:GLN:HG3	13:SH:189:PHE:CD2	2.54	0.43
36:Sf:78:LYS:HG3	36:Sf:79:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LB:77:THR:HG21	40:LB:337:VAL:HG22	2.00	0.43
40:LB:378:ARG:HD3	64:LW:11:TYR:CD2	2.54	0.43
46:Lq:28:PHE:HB2	46:Lq:89:VAL:HG23	2.00	0.43
86:5A:109:ARG:HH12	86:5A:112:LEU:HD11	1.84	0.43
87:EF:152:VAL:HG23	87:EF:192:PRO:HA	2.01	0.43
1:S2:833:C:H2'	1:S2:834:C:C6	2.54	0.43
1:S2:867:OMG:HM23	1:S2:867:OMG:H1'	1.53	0.43
1:S2:921:G:H5'	33:Sb:21:LYS:HD2	2.01	0.43
1:S2:949:G:H2'	1:S2:950:C:C6	2.54	0.43
2:L8:86:U:C3'	2:L8:87:G:H5'	2.48	0.43
3:L5:1214:C:N3	68:Lb:91:ARG:HA	2.34	0.43
3:L5:1418:C:H2'	3:L5:1419:G:O4'	2.19	0.43
3:L5:2109:G:H22	3:L5:2252:G:N2	2.17	0.43
7:SD:142:LEU:HD12	7:SD:143:ARG:N	2.33	0.43
44:LE:183:ARG:HA	44:LE:183:ARG:HD2	1.89	0.43
58:LS:76:LYS:HE2	58:LS:78:PHE:CZ	2.53	0.43
63:LY:126:ARG:HG3	63:LY:130:LYS:NZ	2.34	0.43
87:EF:40:GLU:HA	87:EF:43:GLU:HB3	2.00	0.43
87:EF:112:ALA:HB2	87:EF:145:VAL:HG11	2.01	0.43
1:S2:392:A:C2'	1:S2:393:U:H5'	2.49	0.42
1:S2:1194:A:H4'	1:S2:1195:A:OP1	2.18	0.42
1:S2:1285:G:C6	21:SM:56:CYS:HA	2.54	0.42
3:L5:1249:C:H2'	3:L5:1250:C:C6	2.53	0.42
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.54	0.42
3:L5:4736:C:H2'	3:L5:4737:G:C8	2.54	0.42
9:SE:44:LEU:HD21	9:SE:72:ILE:HD11	2.00	0.42
12:SF:119:SER:OG	12:SF:189:ALA:HB1	2.19	0.42
15:SI:42:ARG:HH21	15:SI:59:ARG:NH1	2.17	0.42
15:SI:188:TYR:OH	15:SI:194:GLU:OE2	2.33	0.42
16:SQ:47:LEU:O	16:SQ:50:LYS:HB2	2.18	0.42
20:SX:40:PRO:HA	20:SX:79:LYS:HD2	2.01	0.42
22:SS:28:PHE:HA	22:SS:31:THR:HG23	2.00	0.42
36:Sf:119:ARG:O	36:Sf:132:MET:HB2	2.20	0.42
37:Sg:34:ALA:HB1	37:Sg:66:VAL:HG22	2.01	0.42
38:Lz:8:ASP:O	38:Lz:12:GLU:HB2	2.17	0.42
43:LH:43:VAL:HG21	43:LH:73:ILE:HD13	2.01	0.42
52:La:28:HIS:CD2	52:La:32:ARG:HG2	2.54	0.42
54:LI:47:PRO:HB3	54:LI:171:TRP:CE2	2.54	0.42
58:LS:98:ARG:HG3	58:LS:142:VAL:HG13	2.01	0.42
61:LU:63:ILE:HG23	61:LU:70:ILE:HG23	2.01	0.42
82:Lp:38:THR:HA	82:Lp:45:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:63:U:H2'	1:S2:64:A:H5''	2.01	0.42
1:S2:455:A:H2'	1:S2:456:C:C6	2.53	0.42
1:S2:1203:G:H2'	1:S2:1204:A:C8	2.54	0.42
1:S2:1256:G:C8	17:SU:66:ARG:HB2	2.55	0.42
1:S2:1568:C:H2'	1:S2:1569:A:C8	2.54	0.42
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.54	0.42
3:L5:2876:OMG:HM22	3:L5:2877:G:O5'	2.18	0.42
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.85	0.42
3:L5:4208:U:H4'	3:L5:4274:A:H2	1.84	0.42
3:L5:4439:U:H2'	3:L5:4440:G:O4'	2.19	0.42
9:SE:30:ARG:HD2	9:SE:31:PRO:HD2	2.01	0.42
26:SR:17:ILE:O	26:SR:21:TYR:HB2	2.19	0.42
39:LA:2:GLY:HA2	39:LA:207:VAL:HG23	2.01	0.42
60:LP:14:SER:OG	60:LP:151:THR:HG22	2.19	0.42
84:At:68:C:H2'	84:At:69:G:C8	2.54	0.42
1:S2:121:OMU:HM23	1:S2:121:OMU:H1'	1.80	0.42
1:S2:176:U:H2'	1:S2:177:G:C8	2.53	0.42
1:S2:554:A:H62	1:S2:589:G:H21	1.66	0.42
3:L5:666:G:H2'	3:L5:666:G:N3	2.34	0.42
3:L5:968:C:H5'	44:LE:110:ARG:HH11	1.84	0.42
3:L5:1669:A:N3	3:L5:1852:U:O2'	2.46	0.42
3:L5:1730:U:H2'	3:L5:1731:C:H6	1.85	0.42
3:L5:2310:C:H2'	3:L5:2311:C:C6	2.54	0.42
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.54	0.42
9:SE:155:LYS:HA	9:SE:155:LYS:HD3	1.81	0.42
19:SO:88:LEU:HA	19:SO:88:LEU:HD12	1.70	0.42
38:Lz:39:LYS:HB2	38:Lz:202:ARG:HB2	2.01	0.42
55:LD:223:PHE:HB3	55:LD:226:TYR:HB2	2.02	0.42
58:LS:39:VAL:HG22	69:LF:228:VAL:HA	2.00	0.42
87:EF:264:VAL:HA	87:EF:309:GLY:HA2	2.01	0.42
1:S2:484:A2M:HM'3	1:S2:484:A2M:H1'	1.70	0.42
1:S2:1305:C:H2'	1:S2:1306:U:C6	2.54	0.42
1:S2:1861:G:H5''	32:Sa:3:LYS:HA	2.01	0.42
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.53	0.42
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.55	0.42
3:L5:3717:A:N1	3:L5:3933:G:H1'	2.34	0.42
3:L5:4451:G:H2'	3:L5:4522:G:O6	2.19	0.42
3:L5:4524:G:C2	40:LB:252:ALA:HB1	2.54	0.42
7:SD:99:ILE:H	7:SD:99:ILE:HD12	1.84	0.42
13:SH:158:LEU:HD11	13:SH:187:PHE:HD2	1.84	0.42
14:SW:62:VAL:HG11	33:Sb:8:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SK:1:MET:HE1	18:SK:43:LEU:CD2	2.49	0.42
26:SR:57:LEU:HD23	26:SR:57:LEU:HA	1.90	0.42
34:Sc:67:ARG:HD3	34:Sc:67:ARG:HA	1.85	0.42
37:Sg:212:LYS:HA	37:Sg:235:ILE:HG13	2.00	0.42
68:Lb:110:ALA:O	68:Lb:114:LYS:HG2	2.19	0.42
76:Lj:39:TYR:CG	76:Lj:40:PRO:HA	2.54	0.42
86:5A:121:LYS:O	86:5A:124:GLU:HG3	2.19	0.42
1:S2:543:C:H3'	1:S2:544:G:C8	2.51	0.42
1:S2:643:A:H4'	1:S2:644:OMG:H5'	2.02	0.42
1:S2:674:C:H2'	1:S2:675:U:C6	2.55	0.42
1:S2:1177:PSU:H2'	1:S2:1178:U:C6	2.54	0.42
1:S2:1454:A:H2	1:S2:1476:A:H1'	1.83	0.42
1:S2:1525:C:H4'	27:SP:137:HIS:NE2	2.34	0.42
3:L5:94:A:C5	3:L5:95:G:H1'	2.53	0.42
3:L5:123:C:H2'	3:L5:124:C:H6	1.84	0.42
3:L5:208:A:H2	3:L5:233:U:H5''	1.85	0.42
3:L5:1480:C:H1'	3:L5:1482:G:N2	2.35	0.42
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.54	0.42
3:L5:1956:A:H2'	3:L5:1957:U:H6	1.85	0.42
3:L5:2014:C:H2'	3:L5:2015:U:O4'	2.19	0.42
3:L5:2590:G:H2'	3:L5:2754:G:N2	2.34	0.42
3:L5:2859:G:H21	3:L5:3837:C:H1'	1.85	0.42
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.54	0.42
3:L5:4523:A2M:H1'	3:L5:4523:A2M:HM'3	1.71	0.42
20:SX:130:LEU:HD12	20:SX:130:LEU:HA	1.81	0.42
21:SM:45:ARG:HD3	21:SM:72:HIS:HD2	1.85	0.42
31:SZ:50:PHE:HD1	31:SZ:54:THR:OG1	2.01	0.42
33:Sb:42:LYS:NZ	33:Sb:57:VAL:O	2.39	0.42
37:Sg:156:PHE:CE1	37:Sg:179:LEU:HD21	2.54	0.42
38:Lz:55:LEU:HD13	38:Lz:182:ASN:HD22	1.85	0.42
47:LK:50:THR:HG21	47:LK:58:ILE:HD13	2.01	0.42
54:LI:99:ILE:HG12	54:LI:101:LYS:HD2	2.00	0.42
1:S2:99:A2M:H1'	1:S2:99:A2M:HM'3	1.82	0.42
1:S2:509:OMG:H1'	1:S2:509:OMG:HM23	1.68	0.42
1:S2:1395:C:H1'	1:S2:1474:A:C5	2.55	0.42
3:L5:172:C:H2'	3:L5:173:C:C6	2.54	0.42
3:L5:1649:U:O2'	88:L5:5110:SPD:H92	2.19	0.42
3:L5:2390:G:H22	3:L5:2825:A:H2	1.68	0.42
3:L5:4120:U:C4	74:Lg:97:ILE:HG12	2.55	0.42
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.53	0.42
3:L5:4488:A:H4'	3:L5:4489:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4569:PSU:H1'	60:LP:69:ARG:NH1	2.34	0.42
3:L5:5021:C:H2'	3:L5:5022:U:H4'	2.00	0.42
5:SB:88:THR:HA	5:SB:98:THR:HA	2.02	0.42
5:SB:123:ALA:HB2	5:SB:165:ARG:HG3	2.01	0.42
6:SA:39:TYR:CE2	26:SR:105:MET:HB2	2.54	0.42
8:SJ:97:ILE:HG23	8:SJ:100:LEU:HD12	2.01	0.42
8:SJ:116:LYS:C	8:SJ:118:GLY:H	2.27	0.42
9:SE:103:TYR:HA	9:SE:108:ARG:O	2.19	0.42
10:SC:68:ARG:NH2	10:SC:71:LYS:HD3	2.35	0.42
25:SL:61:PRO:HA	25:SL:66:VAL:HG13	2.01	0.42
38:Lz:38:LEU:HB2	38:Lz:163:LEU:HD22	2.00	0.42
48:LO:74:ARG:O	48:LO:142:ALA:HB1	2.19	0.42
55:LD:233:PRO:HA	55:LD:236:MET:HE2	2.01	0.42
66:Lr:32:LEU:HD23	66:Lr:113:ARG:HD3	2.01	0.42
86:5A:21:GLN:HA	86:5A:78:ASN:HA	2.01	0.42
86:5A:125:GLN:NE2	86:5A:126:LYS:HG3	2.35	0.42
87:EF:194:SER:HB3	87:EF:199:ASP:HB2	2.01	0.42
1:S2:583:A:H2'	1:S2:584:A:C8	2.55	0.42
1:S2:1154:U:O4	10:SC:227:ARG:HD2	2.19	0.42
1:S2:1579:A:H4'	1:S2:1581:C:C5	2.55	0.42
3:L5:223:G:H4'	3:L5:225:G:N7	2.35	0.42
3:L5:457:G:H2'	3:L5:458:C:C6	2.55	0.42
3:L5:965:G:O6	3:L5:2093:A:H5''	2.20	0.42
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.55	0.42
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	2.00	0.42
3:L5:5000:G:O3'	40:LB:382:MET:HE1	2.20	0.42
7:SD:139:SER:O	7:SD:182:LEU:HD12	2.19	0.42
9:SE:129:ILE:HD13	9:SE:139:LEU:HA	2.02	0.42
37:Sg:274:VAL:O	37:Sg:274:VAL:HG13	2.20	0.42
44:LE:258:LEU:HD12	44:LE:262:LYS:HE3	2.02	0.42
47:LK:53:TRP:HB2	47:LK:58:ILE:HD11	2.02	0.42
59:LT:58:HIS:HD2	59:LT:59:GLY:N	2.18	0.42
62:LX:77:ILE:HD13	62:LX:100:VAL:HG12	2.00	0.42
73:Lf:6:TRP:CE2	73:Lf:102:ARG:HD3	2.55	0.42
1:S2:128:U:H3'	1:S2:129:C:H6	1.84	0.42
1:S2:440:G:O2'	1:S2:1737:G:H1'	2.20	0.42
1:S2:1500:G:H2'	1:S2:1501:C:O4'	2.20	0.42
3:L5:965:G:N2	3:L5:2092:G:H1'	2.35	0.42
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.83	0.42
3:L5:1700:G:C2	3:L5:2097:U:H5'	2.54	0.42
3:L5:1952:G:H4'	58:LS:93:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4065:G:H2'	3:L5:4066:U:C6	2.55	0.42
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.44	0.42
5:SB:27:LYS:HD2	5:SB:53:GLN:HE22	1.85	0.42
11:SG:14:LYS:HB3	11:SG:124:LEU:HD21	2.01	0.42
30:SY:20:ARG:HB3	30:SY:76:TYR:CD1	2.55	0.42
33:Sb:33:MET:HG2	33:Sb:46:VAL:O	2.19	0.42
40:LB:89:ILE:HG22	40:LB:153:MET:HE1	2.02	0.42
49:LL:150:LEU:HD23	49:LL:154:VAL:HG22	2.01	0.42
49:LL:176:PHE:CE2	49:LL:178:ALA:HA	2.54	0.42
57:LR:180:LYS:HA	57:LR:183:GLU:HG3	2.01	0.42
58:LS:29:ARG:HB2	59:LT:148:PRO:HB2	2.01	0.42
61:LU:25:CYS:O	61:LU:28:PRO:HD2	2.20	0.42
64:LW:106:GLU:O	64:LW:110:ARG:HG3	2.20	0.42
70:Lc:31:TYR:O	70:Lc:35:LEU:HD23	2.19	0.42
81:Lo:56:PHE:CE2	81:Lo:59:LYS:HD3	2.52	0.42
84:At:65:G:H5'	87:EF:360:VAL:HG21	2.01	0.42
87:EF:24:THR:HB	87:EF:60:LEU:HD11	2.02	0.42
1:S2:1388:A:C2	7:SD:205:PRO:HG2	2.54	0.42
1:S2:1410:C:H2'	1:S2:1411:G:C8	2.54	0.42
1:S2:1456:G:H2'	1:S2:1457:U:C6	2.55	0.42
1:S2:1678:A2M:HM'3	1:S2:1678:A2M:H1'	1.60	0.42
1:S2:1705:C:H2'	1:S2:1706:G:C8	2.55	0.42
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.01	0.42
3:L5:678:C:H2'	3:L5:679:C:C6	2.55	0.42
3:L5:1480:C:H1'	3:L5:1482:G:H21	1.84	0.42
3:L5:2741:U:H2'	39:LA:50:HIS:CD2	2.55	0.42
3:L5:2815:A2M:H2'	3:L5:2816:G:C8	2.55	0.42
3:L5:2902:G:H22	3:L5:3596:A:P	2.43	0.42
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.20	0.42
3:L5:4438:U:H2'	3:L5:4439:U:O4'	2.20	0.42
11:SG:7:PHE:HB2	11:SG:113:ILE:HD12	2.02	0.42
28:ST:116:ASP:HB3	28:ST:119:GLY:O	2.19	0.42
30:SY:83:LYS:HD3	30:SY:96:LEU:HD21	2.02	0.42
37:Sg:228:TYR:CD2	37:Sg:264:LYS:HD3	2.55	0.42
44:LE:276:ALA:CB	73:Lf:3:GLY:HA3	2.50	0.42
61:LU:100:LEU:HD13	61:LU:112:LEU:HD23	2.01	0.42
1:S2:223:C:H2'	1:S2:224:A:C8	2.55	0.42
1:S2:1464:C:H5''	26:SR:60:ARG:NE	2.35	0.42
3:L5:254:G:H2'	3:L5:255:C:O4'	2.20	0.42
3:L5:273:U:H2'	3:L5:274:C:C6	2.55	0.42
3:L5:445:U:H2'	3:L5:446:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:962:C:O4'	3:L5:963:G:C2	2.73	0.42
3:L5:1881:OMC:H5''	3:L5:2281:U:H1'	2.02	0.42
3:L5:1882:U:C4	3:L5:2279:A:C2	3.08	0.42
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.55	0.42
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.55	0.42
9:SE:152:PRO:HG2	11:SG:216:ARG:HG3	2.00	0.42
14:SW:83:LEU:HD22	14:SW:83:LEU:HA	1.80	0.42
34:Sc:18:LEU:HD13	34:Sc:18:LEU:HA	1.89	0.42
38:Lz:43:PRO:O	38:Lz:159:MET:HE1	2.20	0.42
40:LB:168:MET:HE1	40:LB:173:LEU:HD12	2.01	0.42
46:Lq:70:GLU:HG2	46:Lq:71:ASN:N	2.34	0.42
52:La:75:LEU:HD11	52:La:133:ALA:HA	2.02	0.42
69:LF:35:LYS:HB3	69:LF:35:LYS:HE2	1.86	0.42
1:S2:1135:C:H2'	1:S2:1136:PSU:C6	2.54	0.41
1:S2:1232:PSU:H2'	1:S2:1233:G:H8	1.85	0.41
1:S2:1490:OMG:H1'	1:S2:1490:OMG:HM23	1.60	0.41
1:S2:1569:A:H5'	28:ST:41:LYS:HD3	2.01	0.41
3:L5:71:C:H5'	49:LL:64:VAL:CG1	2.50	0.41
3:L5:962:C:O2	69:LF:32:ARG:NH2	2.53	0.41
3:L5:1805:A:N6	68:Lb:27:GLN:HA	2.35	0.41
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.85	0.41
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.54	0.41
5:SB:30:TRP:O	5:SB:94:LYS:HD2	2.20	0.41
6:SA:42:LYS:HD3	6:SA:46:ILE:HB	2.02	0.41
11:SG:145:PHE:CD2	64:LW:93:LYS:HB2	2.51	0.41
20:SX:140:ARG:O	20:SX:141:PRO:C	2.64	0.41
26:SR:126:MET:HB2	26:SR:128:PHE:CE1	2.52	0.41
32:Sa:10:ARG:HB2	32:Sa:33:ASP:OD2	2.19	0.41
36:Sf:118:ARG:HB2	36:Sf:131:PHE:HB3	2.01	0.41
40:LB:19:ARG:HB2	40:LB:234:ARG:NH2	2.35	0.41
44:LE:162:VAL:HG12	44:LE:177:GLY:HA2	2.02	0.41
45:LG:208:ASN:O	45:LG:212:LYS:HG3	2.20	0.41
86:5A:102:LEU:HD12	86:5A:103:GLN:H	1.84	0.41
86:5A:112:LEU:HD22	86:5A:144:GLU:OE1	2.20	0.41
1:S2:329:G:H5'	1:S2:329:G:H8	1.85	0.41
2:L8:89:U:H2'	2:L8:90:C:C6	2.56	0.41
3:L5:19:G:P	67:Lh:93:ARG:HE	2.43	0.41
3:L5:206:U:H1'	3:L5:209:U:C4	2.54	0.41
3:L5:434:A:H2'	3:L5:435:A:O4'	2.20	0.41
3:L5:2323:C:H2'	3:L5:2324:C:C6	2.55	0.41
3:L5:2861:OMC:H2'	3:L5:2862:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3816:A:OP1	3:L5:3818:UY1:N1	2.53	0.41
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.20	0.41
3:L5:4524:G:OP2	3:L5:4524:G:H4'	2.20	0.41
6:SA:50:ASN:HA	26:SR:105:MET:HE3	2.02	0.41
9:SE:199:GLU:HG3	9:SE:201:HIS:CE1	2.55	0.41
10:SC:94:ILE:HG21	10:SC:162:ILE:HD12	2.01	0.41
21:SM:123:VAL:O	21:SM:126:GLU:HG2	2.19	0.41
45:LG:138:ALA:HB2	45:LG:194:VAL:HG11	2.01	0.41
69:LF:134:ARG:HA	69:LF:137:GLU:HG2	2.02	0.41
1:S2:731:G:H21	1:S2:733:C:H5''	1.84	0.41
3:L5:123:C:H2'	3:L5:124:C:C6	2.55	0.41
3:L5:446:C:H2'	3:L5:447:C:C6	2.55	0.41
3:L5:465:G:H2'	3:L5:466:A:C8	2.55	0.41
3:L5:1359:G:H4'	53:LN:203:TYR:HB2	2.02	0.41
3:L5:1458:C:H2'	3:L5:1459:A:O4'	2.20	0.41
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.20	0.41
3:L5:1880:G:C8	3:L5:1881:OMC:HM22	2.55	0.41
3:L5:4953:G:O2'	3:L5:4954:G:H5'	2.20	0.41
4:L7:7:G:OP1	55:LD:33:ARG:HD2	2.20	0.41
6:SA:216:ALA:O	6:SA:219:GLU:HG3	2.20	0.41
9:SE:171:ASP:OD2	9:SE:235:TRP:HH2	2.03	0.41
13:SH:133:LEU:O	13:SH:173:PHE:CE1	2.74	0.41
13:SH:134:VAL:HG12	13:SH:173:PHE:CD2	2.55	0.41
22:SS:55:ARG:NE	31:SZ:48:VAL:HG23	2.35	0.41
24:SN:11:LEU:O	24:SN:13:GLN:HG2	2.20	0.41
30:SY:56:PHE:HE2	30:SY:86:GLU:HG2	1.85	0.41
37:Sg:191:HIS:CE1	37:Sg:217:MET:HG3	2.56	0.41
43:LH:117:PHE:O	43:LH:118:LEU:HB2	2.21	0.41
46:Lq:112:ARG:HG3	46:Lq:115:ALA:HB3	2.01	0.41
57:LR:180:LYS:O	57:LR:183:GLU:HG3	2.19	0.41
1:S2:111:A:H5'	25:SL:70:GLY:HA2	2.03	0.41
1:S2:382:C:H2'	1:S2:383:G:C8	2.55	0.41
1:S2:555:A:H2'	1:S2:555:A:N3	2.35	0.41
1:S2:601:OMG:HM23	1:S2:601:OMG:H1'	1.81	0.41
1:S2:606:G:H1'	35:Se:132:ASN:ND2	2.35	0.41
1:S2:824:C:C2	8:SJ:144:ILE:HG12	2.56	0.41
1:S2:1376:A:H2'	1:S2:1377:U:O4'	2.21	0.41
1:S2:1433:C:H2'	1:S2:1434:C:C2	2.54	0.41
3:L5:382:G:N1	3:L5:385:A:OP2	2.49	0.41
3:L5:654:C:H2'	3:L5:655:C:C6	2.56	0.41
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1763:C:H2'	3:L5:1764:G:O4'	2.20	0.41
3:L5:1995:G:O2'	47:LK:127:GLY:HA3	2.21	0.41
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.86	0.41
3:L5:3594:C:H2'	3:L5:3595:U:H2'	2.01	0.41
3:L5:4860:G:H2'	3:L5:4861:G:H8	1.85	0.41
6:SA:35:GLU:O	6:SA:38:ILE:HG12	2.19	0.41
7:SD:175:VAL:HG12	7:SD:177:LEU:HG	2.00	0.41
10:SC:66:LEU:HD11	10:SC:81:ILE:HG12	2.02	0.41
15:SI:174:CYS:HB2	15:SI:190:LEU:HD11	2.02	0.41
26:SR:70:SER:OG	26:SR:73:LEU:HD12	2.20	0.41
38:Lz:156:LYS:NZ	38:Lz:158:GLN:HB2	2.35	0.41
38:Lz:207:LYS:CG	38:Lz:213:PRO:HD2	2.44	0.41
39:LA:133:TYR:HB3	39:LA:168:VAL:HG12	2.02	0.41
45:LG:115:LEU:HD12	45:LG:116:ALA:N	2.35	0.41
46:Lq:65:ILE:HG23	46:Lq:75:LEU:HB3	2.02	0.41
49:LL:183:ARG:HA	49:LL:183:ARG:HD2	1.90	0.41
59:LT:117:LYS:HD3	59:LT:117:LYS:HA	1.88	0.41
65:LZ:51:ARG:HB3	65:LZ:65:ARG:NH2	2.35	0.41
69:LF:136:VAL:O	69:LF:140:ILE:HG12	2.21	0.41
69:LF:220:MET:HB3	69:LF:232:ASP:OD2	2.19	0.41
87:EF:7:HIS:HA	87:EF:86:TYR:O	2.20	0.41
1:S2:429:C:H2'	1:S2:430:C:H6	1.85	0.41
1:S2:518:G:O5'	1:S2:518:G:H8	2.03	0.41
1:S2:584:A:H2'	1:S2:585:C:O4'	2.21	0.41
1:S2:1070:A:H2'	1:S2:1071:G:O4'	2.20	0.41
1:S2:1174:PSU:H2'	1:S2:1175:G:C8	2.56	0.41
1:S2:1365:G:H2'	1:S2:1366:G:H8	1.86	0.41
1:S2:1595:U:H2'	1:S2:1596:U:C6	2.55	0.41
3:L5:218:A:H2'	3:L5:218:A:N3	2.36	0.41
3:L5:939:G:H2'	3:L5:940:C:C6	2.56	0.41
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.56	0.41
3:L5:4277:G:H5''	59:LT:17:ARG:HG2	2.02	0.41
6:SA:15:VAL:HG21	26:SR:111:PHE:CD2	2.56	0.41
10:SC:169:TYR:CG	10:SC:173:LYS:HA	2.55	0.41
20:SX:90:CYS:HA	20:SX:93:PHE:CD2	2.56	0.41
36:Sf:121:CYS:HB2	36:Sf:146:LEU:HD23	2.03	0.41
37:Sg:52:TYR:CD2	37:Sg:309:VAL:HG11	2.55	0.41
45:LG:163:PRO:HB2	45:LG:165:GLU:OE2	2.20	0.41
47:LK:67:ARG:HG2	47:LK:68:GLN:N	2.35	0.41
48:LO:16:LEU:HD12	48:LO:80:PHE:HD1	1.84	0.41
55:LD:125:VAL:HG11	55:LD:199:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:LX:87:MET:HE1	62:LX:155:ILE:HG22	2.02	0.41
66:Lr:2:SAC:H2A1	66:Lr:2:SAC:HA	1.75	0.41
73:Lf:48:ALA:HB2	73:Lf:71:TRP:CZ3	2.55	0.41
73:Lf:50:VAL:HG22	73:Lf:69:VAL:HG22	2.02	0.41
1:S2:841:G:H2'	1:S2:842:C:C6	2.56	0.41
1:S2:1239:PSU:O4	1:S2:1241:A:H8	2.04	0.41
2:L8:8:U:H2'	2:L8:9:A:C8	2.56	0.41
2:L8:103:A:N3	3:L5:21:G:H1'	2.36	0.41
3:L5:449:C:H4'	3:L5:450:G:C5'	2.51	0.41
3:L5:661:C:H2'	3:L5:662:C:C6	2.56	0.41
3:L5:669:C:H2'	3:L5:670:G:C8	2.55	0.41
3:L5:987:C:H2'	3:L5:988:C:H6	1.85	0.41
3:L5:1647:U:OP1	88:L5:5110:SPD:H52	2.20	0.41
3:L5:1703:C:O2'	69:LF:43:ARG:NH1	2.53	0.41
7:SD:66:ILE:HD11	7:SD:86:LEU:HB3	2.03	0.41
9:SE:103:TYR:HB2	9:SE:182:MET:CE	2.50	0.41
17:SU:45:GLU:OE2	17:SU:46:LYS:HG3	2.20	0.41
21:SM:50:CYS:HB2	21:SM:110:VAL:HG22	2.01	0.41
31:SZ:54:THR:O	31:SZ:55:TYR:C	2.63	0.41
37:Sg:106:LYS:HB2	37:Sg:126:ASP:HB3	2.03	0.41
84:At:11:C:H2'	84:At:12:U:C6	2.55	0.41
86:5A:50:5CT:H6	86:5A:50:5CT:H20	1.78	0.41
1:S2:383:G:H4'	25:SL:132:ARG:HD2	2.02	0.41
1:S2:839:C:H3'	1:S2:840:C:C5'	2.51	0.41
1:S2:873:G:C5	25:SL:152:LYS:HG3	2.55	0.41
1:S2:1026:C:H4'	1:S2:1161:U:H4'	2.02	0.41
1:S2:1418:C:N3	1:S2:1421:A:H2	2.19	0.41
1:S2:1667:U:H2'	1:S2:1668:U:C6	2.56	0.41
3:L5:260:C:N4	3:L5:261:G:O6	2.54	0.41
3:L5:1535:C:H2'	3:L5:1536:PSU:O4'	2.21	0.41
3:L5:1743:A:O4'	55:LD:15:ARG:HD2	2.21	0.41
3:L5:3956:G:H21	3:L5:3960:A:H61	1.68	0.41
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.20	0.41
20:SX:87:ASN:HB3	20:SX:134:TYR:CE1	2.55	0.41
21:SM:52:LEU:HD13	21:SM:65:VAL:HG21	2.02	0.41
21:SM:86:GLY:HA2	21:SM:89:VAL:HG22	2.01	0.41
27:SP:87:PRO:HG3	27:SP:112:ILE:HD13	2.03	0.41
37:Sg:40:ILE:HB	37:Sg:59:LEU:HB2	2.03	0.41
38:Lz:96:ASN:O	38:Lz:97:LYS:C	2.64	0.41
47:LK:106:PHE:CD1	47:LK:109:ILE:HD11	2.56	0.41
47:LK:119:ARG:HE	47:LK:119:ARG:HB3	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:LL:184:MET:HE2	49:LL:184:MET:HB3	1.97	0.41
66:Lr:19:LYS:HG2	66:Lr:24:THR:HG23	2.03	0.41
84:At:44:G:H1'	84:At:45:U:H2'	2.01	0.41
87:EF:13:ILE:CG2	87:EF:102:MET:HE3	2.51	0.41
1:S2:846:G:OP1	9:SE:106:LYS:HE2	2.20	0.41
3:L5:122:U:H2'	3:L5:123:C:H6	1.85	0.41
3:L5:1410:U:H4'	3:L5:1411:C:O4'	2.20	0.41
3:L5:1802:A:H4'	59:LT:105:PHE:CE1	2.56	0.41
3:L5:2406:G:N7	78:Ll:2:SER:N	2.69	0.41
3:L5:4250:G:H5''	42:LJ:98:ASN:OD1	2.21	0.41
3:L5:4336:A:H5''	3:L5:4337:C:H5'	2.03	0.41
4:L7:111:C:H2'	4:L7:112:U:O4'	2.20	0.41
7:SD:203:PRO:HG2	26:SR:42:PRO:HB3	2.02	0.41
9:SE:255:ARG:HG2	9:SE:259:LYS:NZ	2.36	0.41
12:SF:44:LYS:HE2	12:SF:44:LYS:HB3	1.89	0.41
15:SI:122:GLY:HA2	15:SI:167:GLN:HA	2.02	0.41
38:Lz:14:VAL:HB	38:Lz:214:GLN:NE2	2.30	0.41
38:Lz:120:ILE:HG23	38:Lz:124:LEU:HD22	2.03	0.41
38:Lz:206:ILE:HG12	38:Lz:214:GLN:CD	2.46	0.41
47:LK:16:ARG:HG2	47:LK:59:THR:OG1	2.21	0.41
48:LO:31:ARG:O	48:LO:33:VAL:HG23	2.21	0.41
48:LO:46:ASN:ND2	48:LO:49:ARG:HG3	2.36	0.41
59:LT:122:LYS:O	59:LT:122:LYS:HD2	2.20	0.41
84:At:5:G:H2'	84:At:6:G:C8	2.55	0.41
84:At:16:H2U:H61	84:At:16:H2U:H2'	1.81	0.41
87:EF:26:HIS:NE2	87:EF:30:LYS:HE2	2.36	0.41
87:EF:178:ILE:HB	87:EF:183:TYR:HB2	2.03	0.41
87:EF:290:LYS:HE3	87:EF:313:LYS:HG2	2.02	0.41
1:S2:27:A2M:HM'3	1:S2:27:A2M:H1'	1.67	0.41
1:S2:69:C:OP2	11:SG:164:LYS:NZ	2.48	0.41
1:S2:116:OMU:H6	1:S2:116:OMU:O5'	2.20	0.41
1:S2:940:U:H2'	1:S2:941:C:C6	2.55	0.41
1:S2:1018:U:H2'	1:S2:1019:C:C6	2.56	0.41
1:S2:1161:U:OP2	20:SX:4:CYS:HB3	2.21	0.41
2:L8:68:G:H2'	2:L8:69:PSU:O4'	2.21	0.41
3:L5:35:U:H4'	3:L5:1525:A:C2	2.55	0.41
3:L5:143:C:H5'	45:LG:108:GLN:HG3	2.03	0.41
3:L5:469:C:H2'	3:L5:470:A:H8	1.86	0.41
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.84	0.41
3:L5:1397:A:C2	3:L5:1498:G:N3	2.89	0.41
3:L5:1437:C:C2	3:L5:2098:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1690:C:H2'	3:L5:1691:G:O4'	2.20	0.41
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.35	0.41
3:L5:1772:C:H2'	3:L5:1773:U:H6	1.85	0.41
3:L5:1809:C:H2'	3:L5:1810:G:C8	2.56	0.41
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.56	0.41
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.21	0.41
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.20	0.41
3:L5:2370:A:C8	71:Ld:39:LYS:HD2	2.56	0.41
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.86	0.41
3:L5:3718:A2M:H1'	3:L5:3718:A2M:HM'3	1.89	0.41
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.56	0.41
3:L5:3899:OMG:HM23	3:L5:3899:OMG:H1'	1.88	0.41
3:L5:4208:U:H4'	3:L5:4274:A:C2	2.56	0.41
3:L5:4704:C:H2'	3:L5:4705:A:C8	2.56	0.41
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.56	0.41
3:L5:4870:G:H5''	51:LM:91:TRP:CD2	2.56	0.41
5:SB:66:VAL:HG11	5:SB:85:LYS:HE2	2.02	0.41
7:SD:158:ILE:HG12	7:SD:189:MET:SD	2.61	0.41
8:SJ:34:GLU:HG2	8:SJ:34:GLU:H	1.59	0.41
9:SE:168:LYS:HD2	9:SE:169:ILE:H	1.86	0.41
10:SC:156:ILE:O	10:SC:160:LEU:HD23	2.21	0.41
11:SG:70:HIS:C	11:SG:98:ARG:NH1	2.79	0.41
13:SH:142:LYS:HB3	13:SH:142:LYS:HE2	1.49	0.41
20:SX:14:ARG:NH1	25:SL:103:GLU:OE1	2.52	0.41
22:SS:12:ILE:C	22:SS:13:LEU:HD12	2.45	0.41
26:SR:14:ARG:O	26:SR:18:GLU:HG2	2.20	0.41
26:SR:61:ILE:HG12	26:SR:66:VAL:HG21	2.03	0.41
30:SY:78:SER:OG	30:SY:80:ASP:OD1	2.33	0.41
37:Sg:5:MET:HB3	37:Sg:270:LEU:HD21	2.03	0.41
37:Sg:112:ALA:HB2	37:Sg:155:ARG:HH11	1.85	0.41
38:Lz:74:CYS:C	38:Lz:78:LYS:HZ2	2.28	0.41
42:LJ:37:ALA:HA	42:LJ:70:VAL:HG11	2.02	0.41
43:LH:129:ARG:HB3	43:LH:153:LEU:HD22	2.02	0.41
45:LG:159:HIS:CE1	45:LG:185:LYS:HD3	2.55	0.41
47:LK:60:VAL:HG12	47:LK:73:VAL:HG22	2.02	0.41
53:LN:19:MET:HE3	53:LN:19:MET:HB3	1.93	0.41
54:LI:61:SER:HA	54:LI:126:VAL:HG12	2.02	0.41
56:LQ:178:ARG:HA	56:LQ:184:ARG:O	2.21	0.41
58:LS:45:TRP:NE1	58:LS:56:LYS:HG3	2.35	0.41
60:LP:4:TYR:CE1	60:LP:16:LYS:HD3	2.55	0.41
83:mR:36[A]:U:O2	85:Pt:38:A:H2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:5A:111:ASP:CG	86:5A:112:LEU:H	2.29	0.41
1:S2:28:U:H2'	1:S2:29:G:C8	2.53	0.41
2:L8:14:OMU:HM23	2:L8:14:OMU:H1'	1.62	0.41
2:L8:109:C:N3	76:Lj:20:ARG:NH1	2.69	0.41
3:L5:316:U:H2'	99:L5:5516:HOH:O	2.21	0.41
3:L5:729:G:H5'	3:L5:729:G:N3	2.35	0.41
3:L5:741:C:H3'	3:L5:742:G:C5'	2.51	0.41
3:L5:2249:C:H2'	3:L5:2250:C:C5	2.56	0.41
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.56	0.41
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.86	0.41
3:L5:4620:OMU:H1'	3:L5:4620:OMU:HM23	1.85	0.41
9:SE:105:THR:HG23	9:SE:245:ARG:HA	2.00	0.41
31:SZ:64:ASN:O	31:SZ:111:ARG:NE	2.52	0.41
37:Sg:36:ARG:C	37:Sg:38:LYS:H	2.29	0.41
37:Sg:217:MET:HA	37:Sg:229:THR:HA	2.03	0.41
43:LH:8:GLN:OE1	43:LH:71:ARG:HG3	2.21	0.41
45:LG:117:ARG:HE	45:LG:117:ARG:HB3	1.58	0.41
45:LG:170:LEU:HD12	45:LG:170:LEU:HA	1.92	0.41
47:LK:14:TYR:CZ	47:LK:59:THR:HG21	2.56	0.41
62:LX:73:HIS:CE1	62:LX:115:LYS:HE3	2.56	0.41
68:Lb:93:LEU:HD23	68:Lb:93:LEU:HA	1.86	0.41
1:S2:35:C:H2'	1:S2:36:PSU:H6	1.85	0.40
1:S2:844:U:H2'	1:S2:845:G:H8	1.85	0.40
1:S2:1220:A:H2'	1:S2:1221:G:O4'	2.21	0.40
1:S2:1227:G:N3	1:S2:1227:G:H2'	2.37	0.40
3:L5:751:G:H2'	3:L5:752:G:O4'	2.21	0.40
3:L5:1762:C:H2'	3:L5:1763:C:H6	1.86	0.40
3:L5:1765:A:H5'	3:L5:1767:A:H62	1.86	0.40
3:L5:3759:A:H5'	3:L5:3765:G:H22	1.86	0.40
3:L5:3783:A:O5'	3:L5:3784:A:H5'	2.21	0.40
3:L5:4966:A:H5''	40:LB:128:LYS:HG3	2.03	0.40
3:L5:5029:C:H2'	3:L5:5030:U:C6	2.56	0.40
5:SB:48:LEU:HD23	5:SB:48:LEU:H	1.86	0.40
6:SA:37:TYR:CD1	6:SA:162:PRO:HG3	2.56	0.40
6:SA:149:ASN:HB2	6:SA:165:ASN:OD1	2.21	0.40
9:SE:87:MET:O	9:SE:122:LYS:HE3	2.21	0.40
11:SG:1:MET:HE3	11:SG:1:MET:HB2	1.95	0.40
20:SX:56:GLY:HA3	35:Se:80:LEU:HD21	2.03	0.40
22:SS:16:LEU:HD11	22:SS:72:GLN:NE2	2.36	0.40
37:Sg:7:LEU:HD12	37:Sg:309:VAL:O	2.21	0.40
50:LV:112:MET:HE1	50:LV:117:ILE:CG1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LI:75:TYR:CZ	54:LI:150:GLU:HG3	2.56	0.40
58:LS:43:ARG:HA	58:LS:43:ARG:HD2	1.93	0.40
64:LW:3:VAL:HG11	64:LW:12:LYS:HE2	2.03	0.40
69:LF:126:ASN:O	69:LF:127:LYS:C	2.63	0.40
74:Lg:56:VAL:HG13	74:Lg:72:LYS:HA	2.03	0.40
86:5A:110:GLU:HG2	86:5A:110:GLU:O	2.21	0.40
1:S2:434:G:H2'	1:S2:435:A:C8	2.56	0.40
1:S2:893:U:H3'	1:S2:894:G:H8	1.86	0.40
1:S2:1011:A:H2'	1:S2:1012:A:O4'	2.21	0.40
1:S2:1288:OMU:HM23	1:S2:1288:OMU:H1'	1.82	0.40
1:S2:1579:A:H4'	1:S2:1581:C:H5	1.86	0.40
3:L5:489:C:H2'	3:L5:490:C:C6	2.57	0.40
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.87	0.40
3:L5:2015:U:H2'	3:L5:2016:C:H6	1.86	0.40
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.56	0.40
3:L5:4103:C:H42	3:L5:4108:G:H1	1.69	0.40
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.86	0.40
7:SD:172:VAL:HG22	7:SD:185:LYS:HG2	2.04	0.40
10:SC:171:GLY:HA3	14:SW:97:ARG:HH21	1.86	0.40
11:SG:70:HIS:CA	11:SG:98:ARG:HH12	2.31	0.40
13:SH:87:PHE:HB3	13:SH:90:LYS:HE2	2.04	0.40
15:SI:42:ARG:HH21	15:SI:59:ARG:HH12	1.69	0.40
22:SS:27:ALA:HB1	22:SS:42:HIS:CE1	2.55	0.40
26:SR:34:VAL:HG12	26:SR:38:ILE:HD13	2.04	0.40
29:SV:16:LYS:HD2	29:SV:21:ASN:OD1	2.22	0.40
30:SY:74:MET:O	30:SY:75:ILE:HD13	2.21	0.40
38:Lz:58:THR:HA	38:Lz:59:PRO:HD3	1.92	0.40
41:LC:100:ARG:HG2	41:LC:101:MET:O	2.21	0.40
53:LN:165:THR:O	53:LN:169:ARG:HG2	2.21	0.40
57:LR:4:LEU:HD22	57:LR:32:ILE:HG22	2.03	0.40
57:LR:78:ILE:HD13	57:LR:78:ILE:HA	1.91	0.40
81:Lo:33:LEU:HD23	81:Lo:33:LEU:O	2.21	0.40
86:5A:47:LYS:HD3	86:5A:52:GLY:H	1.86	0.40
87:EF:261:THR:HG22	87:EF:263:PRO:HD3	2.03	0.40
1:S2:118:C:H1'	1:S2:445:A:C5	2.56	0.40
1:S2:174:OMC:H1'	1:S2:174:OMC:HM23	1.79	0.40
1:S2:441:C:H2'	1:S2:442:C:C6	2.56	0.40
1:S2:921:G:C6	14:SW:28:ARG:HD2	2.57	0.40
1:S2:980:A:H2'	1:S2:981:A:C8	2.57	0.40
2:L8:17:A:H1'	3:L5:418:A:C2	2.56	0.40
2:L8:75:OMG:HM23	2:L8:75:OMG:H1'	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:86:U:H2'	3:L5:87:A:H8	1.85	0.40
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.85	0.40
3:L5:1402:C:H2'	3:L5:1403:G:O4'	2.20	0.40
3:L5:1419:G:C6	52:La:116:LYS:HD2	2.56	0.40
3:L5:1432:G:H2'	3:L5:1451:G:H22	1.86	0.40
3:L5:4152:G:H2'	3:L5:4153:C:O4'	2.22	0.40
3:L5:4524:G:N3	40:LB:252:ALA:HB1	2.36	0.40
6:SA:190:SER:HB3	6:SA:193:HIS:HB3	2.02	0.40
7:SD:47:GLU:HG2	7:SD:87:TYR:CE2	2.48	0.40
10:SC:65:LYS:HG2	10:SC:273:LEU:HD22	2.03	0.40
24:SN:93:LYS:HA	24:SN:150:VAL:HG21	2.04	0.40
37:Sg:5:MET:HG2	37:Sg:310:TRP:HB3	2.03	0.40
38:Lz:72:GLN:H	38:Lz:72:GLN:CD	2.29	0.40
38:Lz:110:PHE:HB2	38:Lz:135:PRO:HA	2.01	0.40
49:LL:194:ILE:HD12	49:LL:194:ILE:HA	1.94	0.40
59:LT:106:LEU:HD23	59:LT:106:LEU:HA	1.92	0.40
61:LU:61:VAL:HG22	61:LU:74:SER:HB2	2.03	0.40
65:LZ:25:ILE:HA	65:LZ:43:VAL:HG12	2.03	0.40
72:Le:126:ASN:HA	72:Le:129:LEU:HD12	2.02	0.40
1:S2:1405:A:H2'	1:S2:1406:G:O4'	2.21	0.40
3:L5:450:G:H3'	3:L5:451:C:C6	2.57	0.40
3:L5:672:C:H2'	3:L5:673:C:C6	2.56	0.40
3:L5:1094:G:H2'	3:L5:1095:A:C8	2.56	0.40
3:L5:1670:G:O2'	3:L5:1853:G:H4'	2.22	0.40
3:L5:2474:G:N2	3:L5:2503:G:H5''	2.37	0.40
3:L5:3906:A:H5''	41:LC:69:THR:OG1	2.21	0.40
3:L5:4343:U:H2'	3:L5:4344:U:C6	2.56	0.40
3:L5:4883:C:OP2	44:LE:274:VAL:HG22	2.21	0.40
7:SD:5:ILE:HG22	7:SD:9:ARG:HB2	2.03	0.40
15:SI:114:GLU:H	15:SI:114:GLU:HG2	1.62	0.40
24:SN:34:LYS:HE2	24:SN:67:THR:HB	2.03	0.40
29:SV:2:GLN:HB3	29:SV:6:GLY:HA2	2.02	0.40
37:Sg:42:MET:HE2	37:Sg:42:MET:HB3	1.87	0.40
38:Lz:120:ILE:HG23	38:Lz:128:LEU:HD12	2.03	0.40
41:LC:143:ARG:HG2	41:LC:182:LYS:HD2	2.02	0.40
45:LG:51:LEU:O	45:LG:55:VAL:HG23	2.21	0.40
50:LV:84:GLN:HE21	50:LV:86:LYS:HB3	1.87	0.40
59:LT:123:GLY:O	59:LT:124:THR:O	2.38	0.40
81:Lo:32:SER:C	81:Lo:34:TYR:H	2.28	0.40
86:5A:109:ARG:HH22	86:5A:137:VAL:HG11	1.86	0.40
1:S2:327:G:H3'	1:S2:327:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:566:U:H2'	1:S2:567:C:O4'	2.22	0.40
1:S2:616:A:N1	1:S2:632:C:H1'	2.37	0.40
1:S2:1019:C:H2'	1:S2:1020:A:O4'	2.21	0.40
1:S2:1285:G:H1	21:SM:57:ASP:CG	2.30	0.40
1:S2:1396:A:O2'	1:S2:1398:G:N7	2.53	0.40
3:L5:175:C:H42	3:L5:260:C:H42	1.68	0.40
3:L5:437:G:H5'	72:Le:53:ILE:HD13	2.03	0.40
3:L5:1749:A:H2'	3:L5:1750:G:C8	2.56	0.40
3:L5:1764:G:H1'	3:L5:1769:G:N2	2.36	0.40
3:L5:2263:A:H5''	66:Lr:108:MET:HG3	2.03	0.40
3:L5:2857:A:H2'	3:L5:2858:A:O4'	2.21	0.40
3:L5:2889:G:H2'	3:L5:2890:C:C6	2.57	0.40
3:L5:4240:G:H5'	55:LD:152:ARG:HD3	2.04	0.40
3:L5:4583:C:H1'	99:L5:5689:HOH:O	2.21	0.40
5:SB:38:MET:SD	5:SB:182:LYS:HG3	2.61	0.40
8:SJ:31:LEU:HD23	8:SJ:31:LEU:HA	1.89	0.40
13:SH:158:LEU:HD11	13:SH:187:PHE:CD2	2.56	0.40
18:SK:14:LEU:HD12	18:SK:14:LEU:HA	1.88	0.40
21:SM:57:ASP:O	21:SM:58:GLU:O	2.40	0.40
23:Sd:10:HIS:HA	23:Sd:11:PRO:HD2	1.91	0.40
26:SR:61:ILE:O	26:SR:61:ILE:HG22	2.22	0.40
30:SY:35:VAL:HG13	30:SY:39:GLU:HB3	2.03	0.40
37:Sg:191:HIS:CD2	37:Sg:195:LEU:HD21	2.57	0.40
55:LD:235:MET:HE2	55:LD:235:MET:HB2	1.75	0.40
56:LQ:59:PRO:HG3	56:LQ:143:ARG:HA	2.04	0.40
62:LX:64:SER:HB2	67:Lh:69:LEU:HD13	2.03	0.40
87:EF:150:VAL:O	87:EF:190:PHE:HA	2.21	0.40
87:EF:237:PRO:HA	87:EF:238:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	219/223 (98%)	213 (97%)	6 (3%)	0	100	100
6	SA	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
7	SD	224/226 (99%)	217 (97%)	6 (3%)	1 (0%)	30	42
8	SJ	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	11	16
9	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
10	SC	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
11	SG	235/237 (99%)	230 (98%)	5 (2%)	0	100	100
12	SF	187/189 (99%)	180 (96%)	7 (4%)	0	100	100
13	SH	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
14	SW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	SI	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
16	SQ	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
17	SU	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	SK	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
19	SO	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
20	SX	139/142 (98%)	136 (98%)	2 (1%)	1 (1%)	18	27
21	SM	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	24
22	SS	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
23	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
24	SN	149/150 (99%)	145 (97%)	4 (3%)	0	100	100
25	SL	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
26	SR	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
27	SP	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
28	ST	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
30	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
31	SZ	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
32	Sa	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
33	Sb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
34	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
35	Se	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
36	Sf	73/75 (97%)	59 (81%)	14 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Sg	311/313 (99%)	286 (92%)	25 (8%)	0	100	100
38	Lz	209/211 (99%)	181 (87%)	26 (12%)	2 (1%)	12	18
39	LA	248/251 (99%)	241 (97%)	7 (3%)	0	100	100
40	LB	399/402 (99%)	391 (98%)	8 (2%)	0	100	100
41	LC	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
42	LJ	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
43	LH	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
44	LE	218/223 (98%)	207 (95%)	11 (5%)	0	100	100
45	LG	237/239 (99%)	231 (98%)	6 (2%)	0	100	100
46	Lq	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
47	LK	145/147 (99%)	132 (91%)	13 (9%)	0	100	100
48	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
49	LL	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
50	LV	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
51	LM	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
52	La	144/147 (98%)	138 (96%)	5 (4%)	1 (1%)	18	27
53	LN	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
54	LI	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
55	LD	292/294 (99%)	287 (98%)	5 (2%)	0	100	100
56	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
57	LR	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
58	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
59	LT	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	9	14
60	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
61	LU	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
62	LX	116/118 (98%)	116 (100%)	0	0	100	100
63	LY	132/134 (98%)	132 (100%)	0	0	100	100
64	LW	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
65	LZ	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
66	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
67	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Lb	104/109 (95%)	98 (94%)	6 (6%)	0	100	100
69	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
70	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
71	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
72	Le	126/128 (98%)	126 (100%)	0	0	100	100
73	Lf	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
74	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
75	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
76	Lj	85/86 (99%)	84 (99%)	1 (1%)	0	100	100
77	Lk	67/69 (97%)	67 (100%)	0	0	100	100
78	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
79	Lm	49/52 (94%)	49 (100%)	0	0	100	100
80	Ln	23/25 (92%)	23 (100%)	0	0	100	100
81	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
82	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
86	5A	140/143 (98%)	125 (89%)	15 (11%)	0	100	100
87	EF	438/444 (99%)	422 (96%)	16 (4%)	0	100	100
All	All	12440/12622 (99%)	11983 (96%)	447 (4%)	10 (0%)	49	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SM	58	GLU
59	LT	122	LYS
59	LT	124	THR
8	SJ	117	LEU
20	SX	141	PRO
52	La	15	VAL
7	SD	48	ILE
8	SJ	36	GLY
38	Lz	65	VAL
38	Lz	87	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SB	202/202 (100%)	199 (98%)	3 (2%)	57	74
6	SA	183/183 (100%)	180 (98%)	3 (2%)	55	73
7	SD	189/189 (100%)	185 (98%)	4 (2%)	47	67
8	SJ	161/161 (100%)	157 (98%)	4 (2%)	42	63
9	SE	224/224 (100%)	217 (97%)	7 (3%)	35	55
10	SC	188/188 (100%)	188 (100%)	0	100	100
11	SG	207/207 (100%)	203 (98%)	4 (2%)	50	70
12	SF	159/159 (100%)	156 (98%)	3 (2%)	50	70
13	SH	168/169 (99%)	157 (94%)	11 (6%)	15	26
14	SW	112/112 (100%)	110 (98%)	2 (2%)	51	71
15	SI	178/178 (100%)	172 (97%)	6 (3%)	32	52
16	SQ	117/117 (100%)	112 (96%)	5 (4%)	26	42
17	SU	93/93 (100%)	87 (94%)	6 (6%)	15	26
18	SK	87/87 (100%)	81 (93%)	6 (7%)	14	23
19	SO	105/105 (100%)	101 (96%)	4 (4%)	29	48
20	SX	113/113 (100%)	108 (96%)	5 (4%)	25	41
21	SM	102/104 (98%)	94 (92%)	8 (8%)	11	18
22	SS	128/128 (100%)	127 (99%)	1 (1%)	73	84
23	Sd	48/48 (100%)	48 (100%)	0	100	100
24	SN	131/130 (101%)	127 (97%)	4 (3%)	35	55
25	SL	129/129 (100%)	124 (96%)	5 (4%)	28	47
26	SR	121/121 (100%)	112 (93%)	9 (7%)	13	20
27	SP	119/119 (100%)	114 (96%)	5 (4%)	26	44
28	ST	113/113 (100%)	111 (98%)	2 (2%)	51	71
29	SV	66/66 (100%)	62 (94%)	4 (6%)	17	29
30	SY	113/113 (100%)	111 (98%)	2 (2%)	51	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SZ	74/74 (100%)	69 (93%)	5 (7%)	14	23
32	Sa	86/86 (100%)	86 (100%)	0	100	100
33	Sb	75/75 (100%)	75 (100%)	0	100	100
34	Sc	57/57 (100%)	56 (98%)	1 (2%)	51	71
35	Se	48/48 (100%)	47 (98%)	1 (2%)	47	67
36	Sf	67/67 (100%)	60 (90%)	7 (10%)	7	9
37	Sg	272/272 (100%)	254 (93%)	18 (7%)	15	25
38	Lz	190/190 (100%)	168 (88%)	22 (12%)	5	7
39	LA	192/192 (100%)	189 (98%)	3 (2%)	55	73
40	LB	347/347 (100%)	347 (100%)	0	100	100
41	LC	306/306 (100%)	304 (99%)	2 (1%)	76	86
42	LJ	143/143 (100%)	142 (99%)	1 (1%)	76	86
43	LH	169/169 (100%)	168 (99%)	1 (1%)	78	87
44	LE	197/196 (100%)	195 (99%)	2 (1%)	68	80
45	LG	201/203 (99%)	194 (96%)	7 (4%)	32	51
46	Lq	164/164 (100%)	164 (100%)	0	100	100
47	LK	122/122 (100%)	119 (98%)	3 (2%)	42	63
48	LO	173/173 (100%)	172 (99%)	1 (1%)	78	87
49	LL	172/172 (100%)	166 (96%)	6 (4%)	32	51
50	LV	107/107 (100%)	107 (100%)	0	100	100
51	LM	116/116 (100%)	113 (97%)	3 (3%)	40	61
52	La	119/119 (100%)	118 (99%)	1 (1%)	73	84
53	LN	171/171 (100%)	170 (99%)	1 (1%)	78	87
54	LI	175/175 (100%)	171 (98%)	4 (2%)	44	65
55	LD	247/247 (100%)	243 (98%)	4 (2%)	55	73
56	LQ	164/164 (100%)	162 (99%)	2 (1%)	63	78
57	LR	166/166 (100%)	166 (100%)	0	100	100
58	LS	157/157 (100%)	157 (100%)	0	100	100
59	LT	139/139 (100%)	138 (99%)	1 (1%)	76	86
60	LP	134/134 (100%)	134 (100%)	0	100	100
61	LU	89/89 (100%)	85 (96%)	4 (4%)	24	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LX	106/106 (100%)	106 (100%)	0	100	100
63	LY	124/124 (100%)	122 (98%)	2 (2%)	55	73
64	LW	95/97 (98%)	93 (98%)	2 (2%)	47	67
65	LZ	117/117 (100%)	114 (97%)	3 (3%)	40	61
66	Lr	108/108 (100%)	106 (98%)	2 (2%)	50	70
67	Lh	109/109 (100%)	108 (99%)	1 (1%)	70	82
68	Lb	89/89 (100%)	88 (99%)	1 (1%)	65	79
69	LF	194/194 (100%)	191 (98%)	3 (2%)	57	74
70	Lc	83/83 (100%)	83 (100%)	0	100	100
71	Ld	98/98 (100%)	97 (99%)	1 (1%)	68	80
72	Le	114/114 (100%)	112 (98%)	2 (2%)	51	71
73	Lf	88/88 (100%)	88 (100%)	0	100	100
74	Lg	98/98 (100%)	97 (99%)	1 (1%)	68	80
75	Li	86/86 (100%)	84 (98%)	2 (2%)	44	65
76	Lj	74/73 (101%)	72 (97%)	2 (3%)	39	60
77	Lk	64/64 (100%)	63 (98%)	1 (2%)	55	73
78	Ll	47/47 (100%)	47 (100%)	0	100	100
79	Lm	47/47 (100%)	46 (98%)	1 (2%)	47	67
80	Ln	24/24 (100%)	22 (92%)	2 (8%)	10	16
81	Lo	93/92 (101%)	92 (99%)	1 (1%)	65	79
82	Lp	74/74 (100%)	74 (100%)	0	100	100
86	5A	116/118 (98%)	110 (95%)	6 (5%)	21	34
87	EF	363/363 (100%)	354 (98%)	9 (2%)	42	63
All	All	10806/10811 (100%)	10551 (98%)	255 (2%)	43	64

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SB	5	LYS
5	SB	55	THR
5	SB	57	ILE
6	SA	89	LYS
6	SA	109	THR
6	SA	198	MET

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Mol	Chain	Res	Type
7	SD	40	ARG
7	SD	44	THR
7	SD	84	VAL
7	SD	193	ASP
8	SJ	112	THR
8	SJ	172	ARG
8	SJ	173	VAL
8	SJ	175	ARG
9	SE	139	LEU
9	SE	141	THR
9	SE	200	ARG
9	SE	236	ILE
9	SE	238	LEU
9	SE	246	LEU
9	SE	248	ILE
11	SG	52	ILE
11	SG	53	SER
11	SG	94	ARG
11	SG	181	THR
12	SF	126	THR
12	SF	127	ARG
12	SF	134	VAL
13	SH	8	ILE
13	SH	74	LYS
13	SH	76	GLN
13	SH	82	GLU
13	SH	83	LEU
13	SH	110	THR
13	SH	132	ASP
13	SH	142	LYS
13	SH	160	LYS
13	SH	162	GLN
13	SH	165	ASN
14	SW	30	CYS
14	SW	83	LEU
15	SI	62	VAL
15	SI	75	LYS
15	SI	76	THR
15	SI	114	GLU
15	SI	145	ILE
15	SI	148	LYS
16	SQ	9	SER

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Mol	Chain	Res	Type
16	SQ	20	THR
16	SQ	46	THR
16	SQ	48	GLN
16	SQ	88	ILE
17	SU	20	ILE
17	SU	50	VAL
17	SU	89	ILE
17	SU	90	ASP
17	SU	91	LEU
17	SU	114	VAL
18	SK	2	LEU
18	SK	5	LYS
18	SK	6	LYS
18	SK	7	ASN
18	SK	9	ILE
18	SK	13	GLU
19	SO	53	ILE
19	SO	88	LEU
19	SO	104	ARG
19	SO	138	ASP
20	SX	105	PHE
20	SX	115	ILE
20	SX	129	SER
20	SX	140	ARG
20	SX	142	ARG
21	SM	27	ILE
21	SM	52	LEU
21	SM	54	SER
21	SM	57	ASP
21	SM	58	GLU
21	SM	91	LEU
21	SM	96	ARG
21	SM	103	VAL
22	SS	12	ILE
24	SN	31	ASP
24	SN	103	GLU
24	SN	133	ARG
24	SN	140	LYS
25	SL	19	ASN
25	SL	48	LYS
25	SL	51	ILE
25	SL	133	PRO

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Mol	Chain	Res	Type
25	SL	152	LYS
26	SR	8	THR
26	SR	18	GLU
26	SR	62	GLN
26	SR	63	ARG
26	SR	70	SER
26	SR	76	GLU
26	SR	77	GLU
26	SR	82	ASP
26	SR	85	VAL
27	SP	13	ARG
27	SP	18	ARG
27	SP	71	GLU
27	SP	136	THR
27	SP	138	SER
28	ST	104	LEU
28	ST	121	ARG
29	SV	4	ASP
29	SV	38	GLU
29	SV	42	VAL
29	SV	45	ARG
30	SY	34	THR
30	SY	39	GLU
31	SZ	36	SER
31	SZ	44	LEU
31	SZ	45	ASN
31	SZ	48	VAL
31	SZ	56	ASP
34	Sc	18	LEU
35	Se	76	VAL
36	Sf	87	THR
36	Sf	92	LYS
36	Sf	94	LYS
36	Sf	97	LYS
36	Sf	98	VAL
36	Sf	108	VAL
36	Sf	132	MET
37	Sg	2	THR
37	Sg	5	MET
37	Sg	21	ILE
37	Sg	59	LEU
37	Sg	62	HIS

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Mol	Chain	Res	Type
37	Sg	66	VAL
37	Sg	107	ASP
37	Sg	114	SER
37	Sg	132	TRP
37	Sg	159	ASN
37	Sg	195	LEU
37	Sg	197	THR
37	Sg	198	VAL
37	Sg	199	THR
37	Sg	200	VAL
37	Sg	203	ASP
37	Sg	287	THR
37	Sg	313	THR
38	Lz	35	GLN
38	Lz	44	GLN
38	Lz	49	PHE
38	Lz	67	VAL
38	Lz	68	LEU
38	Lz	71	GLN
38	Lz	76	GLU
38	Lz	78	LYS
38	Lz	84	HIS
38	Lz	93	LEU
38	Lz	96	ASN
38	Lz	100	VAL
38	Lz	120	ILE
38	Lz	140	HIS
38	Lz	162	VAL
38	Lz	169	VAL
38	Lz	171	HIS
38	Lz	194	LEU
38	Lz	206	ILE
38	Lz	209	THR
38	Lz	214	GLN
38	Lz	215	ARG
39	LA	180	LEU
39	LA	208	GLU
39	LA	242	ARG
41	LC	138	MET
41	LC	215	ASN
42	LJ	155	HIS
43	LH	67	LEU

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Mol	Chain	Res	Type
44	LE	104	THR
44	LE	106	VAL
45	LG	108	GLN
45	LG	115	LEU
45	LG	121	LYS
45	LG	130	THR
45	LG	157	ILE
45	LG	253	LEU
45	LG	254	GLU
47	LK	18	THR
47	LK	119	ARG
47	LK	142	ASN
48	LO	58	LEU
49	LL	44	ARG
49	LL	138	ASP
49	LL	148	THR
49	LL	151	THR
49	LL	158	ARG
49	LL	160	VAL
51	LM	46	ARG
51	LM	112	VAL
51	LM	113	MET
52	La	16	SER
53	LN	10	LEU
54	LI	36	LEU
54	LI	79	SER
54	LI	82	LYS
54	LI	141	LYS
55	LD	41	LYS
55	LD	111	ASN
55	LD	231	VAL
55	LD	232	THR
56	LQ	92	VAL
56	LQ	93	GLN
59	LT	122	LYS
61	LU	26	THR
61	LU	70	ILE
61	LU	105	ASN
61	LU	108	GLU
63	LY	46	SER
63	LY	130	LYS
64	LW	91	MET

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Mol	Chain	Res	Type
64	LW	93	LYS
65	LZ	29	ILE
65	LZ	30	ASP
65	LZ	97	ASN
66	Lr	26	SER
66	Lr	37	SER
67	Lh	87	LYS
68	Lb	118	LEU
69	LF	35	LYS
69	LF	127	LYS
69	LF	223	LYS
71	Ld	107	THR
72	Le	69	MET
72	Le	108	ARG
74	Lg	26	PRO
75	Li	25	ARG
75	Li	63	VAL
76	Lj	20	ARG
76	Lj	50	SER
77	Lk	10	ASP
79	Lm	119	ASN
80	Ln	15	ARG
80	Ln	16	LYS
81	Lo	103	VAL
86	5A	43	MET
86	5A	51	HIS
86	5A	58	LEU
86	5A	59	VAL
86	5A	73	CYS
86	5A	75	SER
87	EF	293	GLU
87	EF	378	LYS
87	EF	380	ASP
87	EF	382	ARG
87	EF	383	SER
87	EF	385	LYS
87	EF	396	SER
87	EF	416	SER
87	EF	426	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
5	SB	186	ASN
6	SA	9	GLN
7	SD	159	HIS
8	SJ	156	HIS
9	SE	67	GLN
9	SE	157	ASN
9	SE	201	HIS
10	SC	267	GLN
12	SF	74	ASN
12	SF	137	GLN
12	SF	203	ASN
13	SH	44	ASN
13	SH	97	GLN
13	SH	114	GLN
13	SH	168	HIS
14	SW	70	ASN
14	SW	98	GLN
15	SI	146	GLN
16	SQ	80	GLN
16	SQ	86	GLN
17	SU	28	ASN
18	SK	7	ASN
20	SX	16	HIS
20	SX	31	HIS
20	SX	73	GLN
21	SM	19	GLN
22	SS	135	HIS
23	Sd	3	HIS
24	SN	105	ASN
25	SL	13	GLN
25	SL	19	ASN
26	SR	26	ASN
27	SP	24	GLN
30	SY	15	ASN
31	SZ	64	ASN
31	SZ	112	ASN
32	Sa	8	ASN
33	Sb	51	GLN
33	Sb	83	GLN
35	Se	89	GLN
36	Sf	111	ASN
37	Sg	4	GLN
37	Sg	15	ASN

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Mol	Chain	Res	Type
37	Sg	117	ASN
37	Sg	285	GLN
38	Lz	44	GLN
38	Lz	71	GLN
38	Lz	84	HIS
38	Lz	141	ASN
38	Lz	199	GLN
39	LA	38	HIS
39	LA	215	ASN
40	LB	145	GLN
40	LB	184	GLN
40	LB	186	ASN
40	LB	203	GLN
41	LC	38	ASN
41	LC	43	ASN
41	LC	142	HIS
41	LC	187	GLN
41	LC	203	GLN
41	LC	215	ASN
41	LC	310	HIS
41	LC	329	ASN
41	LC	346	ASN
41	LC	347	HIS
42	LJ	65	ASN
43	LH	98	HIS
43	LH	106	GLN
44	LE	245	GLN
45	LG	43	GLN
45	LG	66	GLN
45	LG	94	GLN
45	LG	206	GLN
45	LG	208	ASN
46	Lq	85	ASN
46	Lq	179	ASN
47	LK	142	ASN
48	LO	42	ASN
48	LO	50	ASN
49	LL	115	GLN
49	LL	175	ASN
51	LM	34	ASN
51	LM	48	GLN
51	LM	125	ASN

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Mol	Chain	Res	Type
52	La	19	HIS
52	La	34	ASN
52	La	60	HIS
52	La	120	GLN
53	LN	117	ASN
53	LN	145	ASN
54	LI	133	GLN
55	LD	81	HIS
55	LD	122	GLN
55	LD	225	GLN
57	LR	118	HIS
59	LT	54	HIS
59	LT	58	HIS
59	LT	112	ASN
59	LT	114	GLN
60	LP	21	ASN
60	LP	34	GLN
60	LP	97	ASN
60	LP	133	HIS
61	LU	27	HIS
61	LU	38	ASN
61	LU	105	ASN
63	LY	18	HIS
64	LW	95	ASN
64	LW	120	GLN
66	Lr	95	HIS
67	Lh	98	HIS
69	LF	39	GLN
69	LF	239	GLN
70	Lc	72	HIS
72	Le	52	GLN
72	Le	80	HIS
72	Le	107	ASN
76	Lj	57	ASN
78	Ll	17	GLN
78	Ll	25	GLN
78	Ll	33	ASN
81	Lo	25	GLN
86	5A	28	ASN
86	5A	103	GLN
87	EF	307	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1695/1701 (99%)	363 (21%)	29 (1%)
2	L8	155/156 (99%)	25 (16%)	3 (1%)
3	L5	3672/3687 (99%)	690 (18%)	53 (1%)
4	L7	119/120 (99%)	13 (10%)	0
83	mR	9/11 (81%)	1 (11%)	0
84	At	75/76 (98%)	17 (22%)	0
85	Pt	76/77 (98%)	17 (22%)	0
All	All	5801/5828 (99%)	1126 (19%)	85 (1%)

All (1126) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	58	C
1	S2	65	C
1	S2	67	C
1	S2	68	A
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	78	C
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	127	C
1	S2	128	U
1	S2	129	C
1	S2	142	C
1	S2	143	U
1	S2	146	G
1	S2	147	A
1	S2	155	G
1	S2	163	U

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Mol	Chain	Res	Type
1	S2	171	A
1	S2	173	A
1	S2	175	A
1	S2	182	C
1	S2	184	G
1	S2	186	C
1	S2	193	C
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	209	A
1	S2	211	G
1	S2	214	U
1	S2	215	G
1	S2	224	A
1	S2	294	U
1	S2	302	A
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	312	G
1	S2	320	G
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	335	G
1	S2	347	G
1	S2	351	G
1	S2	362	C
1	S2	364	A
1	S2	369	C
1	S2	370	G
1	S2	377	G
1	S2	381	C
1	S2	382	C
1	S2	385	G
1	S2	386	C

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Mol	Chain	Res	Type
1	S2	393	U
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	417	C
1	S2	418	A
1	S2	421	G
1	S2	429	C
1	S2	438	G
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	453	C
1	S2	466	G
1	S2	467	G
1	S2	471	G
1	S2	472	C
1	S2	474	G
1	S2	476	A
1	S2	482	G
1	S2	487	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	501	C
1	S2	508	A
1	S2	516	A
1	S2	517	OMC
1	S2	519	A
1	S2	525	A
1	S2	528	A
1	S2	533	A
1	S2	537	C
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	552	G
1	S2	554	A
1	S2	555	A
1	S2	556	U

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Mol	Chain	Res	Type
1	S2	559	G
1	S2	562	U
1	S2	563	G
1	S2	568	C
1	S2	569	A
1	S2	573	PSU
1	S2	576	A2M
1	S2	578	C
1	S2	589	G
1	S2	590	A2M
1	S2	591	U
1	S2	598	G
1	S2	604	A
1	S2	606	G
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	618	C
1	S2	626	G
1	S2	627	OMU
1	S2	628	A
1	S2	634	A
1	S2	643	A
1	S2	644	OMG
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	688	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	694	G
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	732	U

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Mol	Chain	Res	Type
1	S2	733	C
1	S2	734	C
1	S2	735	C
1	S2	737	G
1	S2	739	C
1	S2	821	G
1	S2	822	PSU
1	S2	823	U
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	840	C
1	S2	847	A
1	S2	861	A
1	S2	869	A
1	S2	870	A
1	S2	876	C
1	S2	878	G
1	S2	882	U
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	901	G
1	S2	913	A
1	S2	916	A
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	930	C
1	S2	933	G
1	S2	963	A
1	S2	970	G
1	S2	985	G

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Mol	Chain	Res	Type
1	S2	990	A
1	S2	992	A
1	S2	999	G
1	S2	1016	U
1	S2	1017	U
1	S2	1023	A
1	S2	1026	C
1	S2	1045	U
1	S2	1049	A
1	S2	1061	U
1	S2	1062	A
1	S2	1083	A
1	S2	1085	C
1	S2	1096	G
1	S2	1100	A
1	S2	1115	U
1	S2	1116	C
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1153	C
1	S2	1154	U
1	S2	1155	U
1	S2	1156	U
1	S2	1157	G
1	S2	1165	G
1	S2	1166	G
1	S2	1171	G
1	S2	1188	A
1	S2	1195	A
1	S2	1203	G
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1224	G
1	S2	1228	A
1	S2	1240	A
1	S2	1242	U
1	S2	1243	PSU
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G

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Mol	Chain	Res	Type
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1260	A
1	S2	1274	G
1	S2	1275	G
1	S2	1280	G
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1288	OMU
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1308	U
1	S2	1312	G
1	S2	1313	A
1	S2	1314	U
1	S2	1320	G
1	S2	1327	G
1	S2	1332	A
1	S2	1333	U
1	S2	1342	U
1	S2	1348	G
1	S2	1371	U
1	S2	1372	U
1	S2	1375	G
1	S2	1378	A
1	S2	1397	U
1	S2	1401	A
1	S2	1404	U
1	S2	1405	A
1	S2	1406	G
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C

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Mol	Chain	Res	Type
1	S2	1436	C
1	S2	1438	A
1	S2	1439	A
1	S2	1441	U
1	S2	1447	OMG
1	S2	1452	A
1	S2	1454	A
1	S2	1463	U
1	S2	1477	U
1	S2	1484	A
1	S2	1487	A
1	S2	1489	A
1	S2	1490	OMG
1	S2	1493	C
1	S2	1494	U
1	S2	1497	G
1	S2	1498	A
1	S2	1506	A
1	S2	1507	G
1	S2	1508	A
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1533	A
1	S2	1544	C
1	S2	1555	U
1	S2	1560	U
1	S2	1570	G
1	S2	1575	G
1	S2	1580	A
1	S2	1585	U
1	S2	1587	G
1	S2	1588	A
1	S2	1598	G
1	S2	1601	A
1	S2	1621	U
1	S2	1623	A
1	S2	1629	C
1	S2	1632	G
1	S2	1637	A
1	S2	1647	A
1	S2	1648	G

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Mol	Chain	Res	Type
1	S2	1656	G
1	S2	1665	G
1	S2	1669	G
1	S2	1671	G
1	S2	1682	C
1	S2	1683	C
1	S2	1695	A
1	S2	1699	A
1	S2	1721	U
1	S2	1722	G
1	S2	1744	G
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1775	U
1	S2	1776	G
1	S2	1777	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1819	A
1	S2	1824	A
1	S2	1825	A
1	S2	1826	G
1	S2	1835	A
1	S2	1838	U
1	S2	1849	G
1	S2	1851	MA6
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
2	L8	13	G
2	L8	23	C

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Mol	Chain	Res	Type
2	L8	25	G
2	L8	34	U
2	L8	35	C
2	L8	51	U
2	L8	52	A
2	L8	59	A
2	L8	62	A
2	L8	63	U
2	L8	84	A
2	L8	85	U
2	L8	86	U
2	L8	87	G
2	L8	94	G
2	L8	103	A
2	L8	104	A
2	L8	105	C
2	L8	110	U
2	L8	111	U
2	L8	112	G
2	L8	114	G
2	L8	123	U
2	L8	124	U
2	L8	125	C
3	L5	25	A
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	71	C
3	L5	74	G
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	108	A
3	L5	110	C
3	L5	115	C
3	L5	119	G
3	L5	133	C
3	L5	134	G

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Mol	Chain	Res	Type
3	L5	135	G
3	L5	136	C
3	L5	137	G
3	L5	142	G
3	L5	151	G
3	L5	158	A
3	L5	159	C
3	L5	170	C
3	L5	178	C
3	L5	179	G
3	L5	181	C
3	L5	182	G
3	L5	184	U
3	L5	186	G
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	202	C
3	L5	209	U
3	L5	219	G
3	L5	234	G
3	L5	235	A
3	L5	257	C
3	L5	258	G
3	L5	259	C
3	L5	260	C
3	L5	261	G
3	L5	262	G
3	L5	263	G
3	L5	266	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	326	C
3	L5	340	C
3	L5	344	A
3	L5	350	C
3	L5	361	C
3	L5	373	G

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Mol	Chain	Res	Type
3	L5	386	A
3	L5	387	G
3	L5	399	G
3	L5	408	A
3	L5	409	G
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U
3	L5	449	C
3	L5	450	G
3	L5	451	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	483	G
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	487	G
3	L5	498	C
3	L5	499	G
3	L5	504	G
3	L5	510	U
3	L5	513	U
3	L5	514	U
3	L5	644	G
3	L5	646	G
3	L5	659	G
3	L5	663	G
3	L5	665	C
3	L5	666	G
3	L5	667	A
3	L5	670	G
3	L5	685	C
3	L5	688	U
3	L5	695	G
3	L5	696	C
3	L5	704	C
3	L5	708	G

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Mol	Chain	Res	Type
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	741	C
3	L5	742	G
3	L5	746	A
3	L5	747	A
3	L5	759	G
3	L5	760	G
3	L5	904	C
3	L5	905	C
3	L5	911	U
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	916	C
3	L5	917	A
3	L5	925	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	937	U
3	L5	941	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	955	G
3	L5	956	A
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C
3	L5	970	G
3	L5	971	U
3	L5	982	U

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Mol	Chain	Res	Type
3	L5	1070	G
3	L5	1072	C
3	L5	1092	G
3	L5	1093	C
3	L5	1094	G
3	L5	1170	G
3	L5	1180	C
3	L5	1182	C
3	L5	1183	C
3	L5	1185	G
3	L5	1186	U
3	L5	1192	C
3	L5	1198	G
3	L5	1199	G
3	L5	1200	G
3	L5	1201	U
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1246	G
3	L5	1254	A
3	L5	1258	G
3	L5	1260	G
3	L5	1261	G
3	L5	1266	G
3	L5	1270	A
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1279	A
3	L5	1280	C
3	L5	1284	G
3	L5	1287	G
3	L5	1295	C
3	L5	1296	G
3	L5	1302	U
3	L5	1303	A
3	L5	1304	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A

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Mol	Chain	Res	Type
3	L5	1358	G
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1403	G
3	L5	1404	G
3	L5	1410	U
3	L5	1411	C
3	L5	1413	C
3	L5	1417	C
3	L5	1418	C
3	L5	1419	G
3	L5	1420	A
3	L5	1436	C
3	L5	1438	U
3	L5	1439	C
3	L5	1443	A
3	L5	1448	G
3	L5	1457	G
3	L5	1480	C
3	L5	1481	C
3	L5	1483	C
3	L5	1491	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1515	A
3	L5	1523	A
3	L5	1534	A2M
3	L5	1535	C
3	L5	1547	A
3	L5	1549	G
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1613	A
3	L5	1614	C

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Mol	Chain	Res	Type
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1640	C
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1670	G
3	L5	1676	C
3	L5	1677	PSU
3	L5	1678	C
3	L5	1691	G
3	L5	1694	C
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1705	G
3	L5	1721	G
3	L5	1734	G
3	L5	1753	G
3	L5	1754	U
3	L5	1755	C
3	L5	1756	U
3	L5	1757	U
3	L5	1760	G
3	L5	1766	A
3	L5	1768	C
3	L5	1775	A
3	L5	1787	A
3	L5	1794	A
3	L5	1804	A
3	L5	1815	G
3	L5	1820	C
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1855	G

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Mol	Chain	Res	Type
3	L5	1869	G
3	L5	1891	A
3	L5	1897	A
3	L5	1898	C
3	L5	1917	A
3	L5	1919	G
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1930	U
3	L5	1931	C
3	L5	1932	A
3	L5	1940	G
3	L5	1948	G
3	L5	1951	G
3	L5	1955	G
3	L5	1961	G
3	L5	1968	G
3	L5	1983	A
3	L5	1984	A
3	L5	1985	G
3	L5	1987	C
3	L5	1990	A
3	L5	1992	U
3	L5	1993	C
3	L5	1996	C
3	L5	1997	U
3	L5	1998	A
3	L5	2002	A
3	L5	2004	U
3	L5	2011	C
3	L5	2025	A
3	L5	2026	A
3	L5	2042	A
3	L5	2043	A
3	L5	2044	U
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C

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Mol	Chain	Res	Type
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2103	G
3	L5	2104	G
3	L5	2109	G
3	L5	2110	C
3	L5	2111	G
3	L5	2112	G
3	L5	2250	C
3	L5	2253	A
3	L5	2255	C
3	L5	2256	C
3	L5	2259	G
3	L5	2260	C
3	L5	2268	A
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2314	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2357	G
3	L5	2360	A
3	L5	2395	A
3	L5	2396	A
3	L5	2397	G
3	L5	2417	A
3	L5	2421	G
3	L5	2425	U
3	L5	2447	U
3	L5	2453	A
3	L5	2474	G
3	L5	2486	G
3	L5	2487	G

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Mol	Chain	Res	Type
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2492	C
3	L5	2503	G
3	L5	2504	C
3	L5	2506	G
3	L5	2513	A
3	L5	2514	G
3	L5	2519	U
3	L5	2554	U
3	L5	2559	G
3	L5	2570	U
3	L5	2573	A
3	L5	2577	C
3	L5	2578	G
3	L5	2583	C
3	L5	2587	A
3	L5	2588	C
3	L5	2601	A
3	L5	2602	G
3	L5	2618	G
3	L5	2627	C
3	L5	2629	C
3	L5	2638	G
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2687	U
3	L5	2688	G
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2697	A
3	L5	2705	G
3	L5	2708	U
3	L5	2711	G
3	L5	2726	G
3	L5	2732	G
3	L5	2733	C
3	L5	2735	G

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Mol	Chain	Res	Type
3	L5	2742	G
3	L5	2743	A
3	L5	2754	G
3	L5	2759	G
3	L5	2760	G
3	L5	2763	U
3	L5	2768	C
3	L5	2769	U
3	L5	2770	C
3	L5	2787	A2M
3	L5	2788	U
3	L5	2790	U
3	L5	2798	A
3	L5	2814	C
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2830	G
3	L5	2855	G
3	L5	2903	G
3	L5	2904	U
3	L5	2906	G
3	L5	2907	G
3	L5	2909	C
3	L5	2910	G
3	L5	3585	G
3	L5	3586	G
3	L5	3589	G
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3596	A
3	L5	3597	G
3	L5	3598	C
3	L5	3606	U
3	L5	3615	G
3	L5	3618	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A

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Mol	Chain	Res	Type
3	L5	3662	A
3	L5	3672	G
3	L5	3673	C
3	L5	3712	A
3	L5	3732	A
3	L5	3736	A
3	L5	3747	A
3	L5	3748	A
3	L5	3750	G
3	L5	3753	G
3	L5	3759	A
3	L5	3760	A2M
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3786	U
3	L5	3787	G
3	L5	3807	A
3	L5	3809	G
3	L5	3810	C
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3816	A
3	L5	3817	A
3	L5	3819	G
3	L5	3822	U
3	L5	3823	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3844	PSU
3	L5	3876	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A

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Mol	Chain	Res	Type
3	L5	3907	G
3	L5	3915	U
3	L5	3949	A
3	L5	3952	A
3	L5	3953	G
3	L5	3954	A
3	L5	3956	G
3	L5	3957	U
3	L5	3958	G
3	L5	3960	A
3	L5	3962	A
3	L5	3964	U
3	L5	3965	A
3	L5	3966	A
3	L5	3967	G
3	L5	3968	U
3	L5	3969	G
3	L5	3971	G
3	L5	3972	A
3	L5	3973	G
3	L5	3974	G
3	L5	3977	C
3	L5	4035	G
3	L5	4037	C
3	L5	4039	G
3	L5	4040	C
3	L5	4041	C
3	L5	4042	G
3	L5	4044	U
3	L5	4048	A
3	L5	4049	U
3	L5	4050	A
3	L5	4051	C
3	L5	4053	A
3	L5	4056	A
3	L5	4064	C
3	L5	4065	G
3	L5	4067	U
3	L5	4069	U
3	L5	4070	U
3	L5	4076	G
3	L5	4084	G

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Mol	Chain	Res	Type
3	L5	4095	G
3	L5	4096	C
3	L5	4103	C
3	L5	4107	G
3	L5	4108	G
3	L5	4115	G
3	L5	4116	C
3	L5	4118	U
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4133	C
3	L5	4136	G
3	L5	4139	G
3	L5	4141	G
3	L5	4142	C
3	L5	4144	C
3	L5	4145	C
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4228	OMG
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4265	U
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4280	A
3	L5	4281	A
3	L5	4289	U
3	L5	4291	G
3	L5	4304	A
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C

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Mol	Chain	Res	Type
3	L5	4326	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4350	C
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4419	U
3	L5	4420	PSU
3	L5	4421	C
3	L5	4422	A
3	L5	4440	G
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4528	G
3	L5	4532	PSU
3	L5	4548	A
3	L5	4560	C
3	L5	4567	G
3	L5	4569	PSU
3	L5	4570	G
3	L5	4575	G
3	L5	4581	G
3	L5	4584	A
3	L5	4590	A2M
3	L5	4600	G

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Mol	Chain	Res	Type
3	L5	4608	G
3	L5	4610	A
3	L5	4626	A
3	L5	4627	U
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C
3	L5	4671	C
3	L5	4672	A
3	L5	4691	A
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4711	C
3	L5	4721	G
3	L5	4730	C
3	L5	4731	G
3	L5	4732	G
3	L5	4733	C
3	L5	4738	C
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4773	C
3	L5	4775	C
3	L5	4776	G
3	L5	4859	C
3	L5	4860	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4882	U

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Mol	Chain	Res	Type
3	L5	4883	C
3	L5	4896	G
3	L5	4898	G
3	L5	4900	C
3	L5	4901	G
3	L5	4909	A
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4928	C
3	L5	4930	C
3	L5	4934	A
3	L5	4943	A
3	L5	4954	G
3	L5	4955	A
3	L5	4957	C
3	L5	4966	A
3	L5	4976	U
3	L5	4979	A
3	L5	4985	U
3	L5	4988	U
3	L5	4990	C
3	L5	4991	U
3	L5	4993	G
3	L5	4994	G
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5026	U
3	L5	5028	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5055	G
3	L5	5058	A
3	L5	5061	A
3	L5	5062	G
3	L5	5066	U
4	L7	2	U

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Mol	Chain	Res	Type
4	L7	3	C
4	L7	33	U
4	L7	42	A
4	L7	53	U
4	L7	63	C
4	L7	64	G
4	L7	76	U
4	L7	97	G
4	L7	100	A
4	L7	106	G
4	L7	110	G
4	L7	120	U
83	mR	37	A
84	At	14	A
84	At	16	H2U
84	At	17	C
84	At	18	G
84	At	19	G
84	At	20	H2U
84	At	22	G
84	At	34	G
84	At	36	A
84	At	45	U
84	At	47	U
84	At	48	C
84	At	57	G
84	At	59	U
84	At	61	C
84	At	75	C
84	At	76	A
85	Pt	2	G
85	Pt	8	4SU
85	Pt	9	G
85	Pt	13	C
85	Pt	16	C
85	Pt	18	C
85	Pt	19	G
85	Pt	20	G
85	Pt	21	H2U
85	Pt	22	A
85	Pt	32	G
85	Pt	47	G7M

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Mol	Chain	Res	Type
85	Pt	48	U
85	Pt	49	C
85	Pt	71	G
85	Pt	72	C
85	Pt	77	A

All (85) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	73	C
1	S2	127	C
1	S2	198	U
1	S2	203	G
1	S2	293	C
1	S2	370	G
1	S2	407	G
1	S2	417	C
1	S2	448	A
1	S2	500	A
1	S2	541	U
1	S2	553	U
1	S2	607	U
1	S2	868	G
1	S2	869	A
1	S2	1016	U
1	S2	1165	G
1	S2	1194	A
1	S2	1312	G
1	S2	1313	A
1	S2	1433	C
1	S2	1446	A
1	S2	1493	C
1	S2	1598	G
1	S2	1601	A
1	S2	1679	A
1	S2	1682	C
1	S2	1698	C
2	L8	51	U
2	L8	84	A
2	L8	85	U
3	L5	85	G

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Mol	Chain	Res	Type
3	L5	157	U
3	L5	158	A
3	L5	178	C
3	L5	187	U
3	L5	235	A
3	L5	278	G
3	L5	412	G
3	L5	509	A
3	L5	934	C
3	L5	955	G
3	L5	1199	G
3	L5	1214	C
3	L5	1215	C
3	L5	1268	G
3	L5	1294	A
3	L5	1359	G
3	L5	1419	G
3	L5	1613	A
3	L5	1633	G
3	L5	1677	PSU
3	L5	1698	C
3	L5	1984	A
3	L5	2042	A
3	L5	2055	G
3	L5	2259	G
3	L5	2313	A
3	L5	2470	C
3	L5	2487	G
3	L5	2587	A
3	L5	2687	U
3	L5	2696	A
3	L5	2759	G
3	L5	2903	G
3	L5	3614	G
3	L5	3672	G
3	L5	3809	G
3	L5	3876	A
3	L5	3952	A
3	L5	4049	U
3	L5	4115	G
3	L5	4452	U
3	L5	4464	A

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Mol	Chain	Res	Type
3	L5	4527	G
3	L5	4626	A
3	L5	4670	C
3	L5	4699	U
3	L5	4909	A
3	L5	4925	U
3	L5	4927	G
3	L5	5022	U
3	L5	5023	C
3	L5	5054	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3758	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.48	5 (22%)	30,36,39	2.12	10 (33%)
3	OMC	L5	2351	3	19,22,23	0.94	1 (5%)	25,31,34	0.83	1 (4%)
3	PSU	L5	3920	90,3	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
3	OMC	L5	2365	90,3	19,22,23	0.79	0	25,31,34	0.76	0
3	PSU	L5	2632	3	18,21,22	1.40	2 (11%)	21,30,33	2.00	5 (23%)
3	A2M	L5	3867	3	22,25,26	1.48	4 (18%)	30,36,39	2.03	8 (26%)
1	PSU	S2	573	1	18,21,22	1.45	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.38	2 (11%)	21,30,33	2.19	5 (23%)
3	OMG	L5	4637	3,89	23,26,27	1.28	4 (17%)	32,38,41	2.03	7 (21%)
1	OMU	S2	627	1	19,22,23	1.31	3 (15%)	25,31,34	1.99	5 (20%)
1	PSU	S2	918	1	18,21,22	1.51	3 (16%)	21,30,33	2.30	5 (23%)
1	4AC	S2	1337	1	21,24,25	1.17	2 (9%)	28,34,37	1.26	3 (10%)
3	PSU	L5	3764	3	18,21,22	1.57	4 (22%)	21,30,33	2.13	5 (23%)
1	OMC	S2	462	1	19,22,23	0.87	0	25,31,34	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3792	3	23,26,27	1.19	3 (13%)	32,38,41	2.02	6 (18%)
3	OMC	L5	4456	3	19,22,23	0.93	1 (5%)	25,31,34	1.09	2 (8%)
3	PSU	L5	4532	3	18,21,22	1.57	5 (27%)	21,30,33	2.13	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.39	4 (21%)	25,31,34	1.88	5 (20%)
3	OMC	L5	3887	3	19,22,23	0.80	0	25,31,34	0.84	0
1	OMG	S2	1447	1	23,26,27	1.24	3 (13%)	32,38,41	2.22	9 (28%)
3	OMG	L5	4196	85,3	23,26,27	1.30	4 (17%)	32,38,41	2.00	7 (21%)
1	G7M	S2	1639	85,1	23,26,27	2.43	5 (21%)	34,39,42	3.13	12 (35%)
3	PSU	L5	3853	90,3	18,21,22	1.42	4 (22%)	21,30,33	2.00	3 (14%)
3	PSU	L5	5010	3	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
1	OMU	S2	354	1	19,22,23	1.44	3 (15%)	25,31,34	2.09	6 (24%)
3	5MC	L5	3782	90,3	19,22,23	1.57	3 (15%)	26,32,35	1.16	3 (11%)
3	OMG	L5	1522	3	23,26,27	1.19	4 (17%)	32,38,41	1.97	6 (18%)
81	MLZ	Lo	53	81	8,9,10	0.78	0	4,9,11	0.66	0
3	PSU	L5	3715	3	18,21,22	1.50	3 (16%)	21,30,33	2.05	4 (19%)
3	A2M	L5	3723	3	22,25,26	1.47	4 (18%)	30,36,39	1.98	10 (33%)
3	PSU	L5	1792	90,3	18,21,22	1.55	4 (22%)	21,30,33	2.11	4 (19%)
3	OMC	L5	2422	90,3	19,22,23	0.88	0	25,31,34	1.07	2 (8%)
3	OMG	L5	4618	3	23,26,27	1.28	4 (17%)	32,38,41	2.03	7 (21%)
3	OMG	L5	1625	3	23,26,27	1.21	3 (13%)	32,38,41	2.01	6 (18%)
1	OMG	S2	644	1	23,26,27	1.28	4 (17%)	32,38,41	2.04	7 (21%)
1	A2M	S2	668	90,1	22,25,26	1.47	4 (18%)	30,36,39	2.03	10 (33%)
1	PSU	S2	1239	1	18,21,22	1.39	3 (16%)	21,30,33	2.05	3 (14%)
1	OMG	S2	867	1	23,26,27	1.22	3 (13%)	32,38,41	1.98	6 (18%)
1	MA6	S2	1851	1	23,26,27	1.44	5 (21%)	33,38,41	2.04	10 (30%)
3	PSU	L5	3637	90,3,89	18,21,22	1.51	3 (16%)	21,30,33	2.27	5 (23%)
3	PSU	L5	4299	3	18,21,22	1.40	3 (16%)	21,30,33	2.10	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.47	5 (22%)	30,36,39	2.16	10 (33%)
3	PSU	L5	3734	3	18,21,22	1.49	4 (22%)	21,30,33	2.07	3 (14%)
68	MLZ	Lb	5	68	8,9,10	0.82	0	4,9,11	0.61	0
79	M3L	Lm	98	79	10,11,12	0.37	0	9,14,16	0.10	0
85	G7M	Pt	47	85	23,26,27	1.86	2 (8%)	34,39,42	1.11	1 (2%)
1	PSU	S2	822	1	18,21,22	1.39	3 (16%)	21,30,33	2.36	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	S2	509	1	23,26,27	1.31	4 (17%)	32,38,41	2.08	6 (18%)
1	PSU	S2	1243	1	18,21,22	1.42	2 (11%)	21,30,33	2.13	4 (19%)
1	PSU	S2	572	1	18,21,22	1.44	4 (22%)	21,30,33	1.99	4 (19%)
39	V5N	LA	216	39	8,11,12	1.47	1 (12%)	8,14,16	1.81	1 (12%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	S2	651	1	18,21,22	1.40	3 (16%)	21,30,33	2.05	4 (19%)
1	PSU	S2	218	1	18,21,22	1.46	3 (16%)	21,30,33	2.16	4 (19%)
1	PSU	S2	609	1	18,21,22	1.50	4 (22%)	21,30,33	1.99	3 (14%)
3	A2M	L5	4523	90,3	22,25,26	1.44	4 (18%)	30,36,39	2.14	8 (26%)
3	PSU	L5	4636	3	18,21,22	1.57	4 (22%)	21,30,33	2.45	6 (28%)
3	PSU	L5	1781	3	18,21,22	1.43	4 (22%)	21,30,33	2.04	4 (19%)
1	PSU	S2	649	1	18,21,22	1.51	4 (22%)	21,30,33	2.12	3 (14%)
1	PSU	S2	1643	90,1	18,21,22	1.40	4 (22%)	21,30,33	2.21	5 (23%)
3	OMG	L5	3899	3	23,26,27	1.21	4 (17%)	32,38,41	2.02	6 (18%)
1	PSU	S2	681	1	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
84	4SU	At	8	90,84	18,21,22	1.86	4 (22%)	25,30,33	2.32	5 (20%)
1	MA6	S2	1850	1	23,26,27	1.47	4 (17%)	33,38,41	2.02	10 (30%)
3	PSU	L5	4569	3	18,21,22	1.50	3 (16%)	21,30,33	2.23	5 (23%)
3	PSU	L5	4420	3	18,21,22	1.37	3 (16%)	21,30,33	1.98	4 (19%)
1	PSU	S2	36	1	18,21,22	1.39	3 (16%)	21,30,33	2.14	4 (19%)
6	SAC	SA	2	6	7,8,9	3.45	2 (28%)	7,9,11	5.30	5 (71%)
3	PSU	L5	3695	3	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
3	PSU	L5	3884	3	18,21,22	1.63	4 (22%)	21,30,33	2.09	3 (14%)
3	PSU	L5	4673	3	18,21,22	1.46	3 (16%)	21,30,33	1.99	5 (23%)
1	A2M	S2	27	1	22,25,26	1.46	4 (18%)	30,36,39	2.19	9 (30%)
2	OMG	L8	75	2	23,26,27	1.18	3 (13%)	32,38,41	2.14	7 (21%)
3	PSU	L5	1677	3	18,21,22	1.57	4 (22%)	21,30,33	2.09	4 (19%)
84	MIA	At	37	84	28,31,32	2.47	7 (25%)	38,44,47	2.78	14 (36%)
1	B8N	S2	1248	1	25,29,30	0.93	1 (4%)	28,42,45	1.82	6 (21%)
1	A2M	S2	159	1	22,25,26	1.50	4 (18%)	30,36,39	1.99	9 (30%)
1	PSU	S2	1232	1	18,21,22	1.58	4 (22%)	21,30,33	2.19	4 (19%)
1	PSU	S2	1177	1	18,21,22	1.40	4 (22%)	21,30,33	2.04	3 (14%)
1	OMC	S2	517	1	19,22,23	0.92	0	25,31,34	1.00	2 (8%)
1	OMG	S2	1490	90,1	23,26,27	1.27	4 (17%)	32,38,41	2.00	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4353	3	18,21,22	1.53	4 (22%)	21,30,33	2.18	3 (14%)
3	PSU	L5	4628	3	18,21,22	1.49	4 (22%)	21,30,33	2.41	5 (23%)
1	A2M	S2	166	1	22,25,26	1.47	4 (18%)	30,36,39	2.29	8 (26%)
3	1MA	L5	1322	90,3	21,25,26	1.38	4 (19%)	30,37,40	1.70	6 (20%)
3	A2M	L5	2815	90,3	22,25,26	1.48	4 (18%)	30,36,39	1.99	7 (23%)
1	A2M	S2	484	1	22,25,26	1.48	5 (22%)	30,36,39	2.04	7 (23%)
3	A2M	L5	3760	90,3	22,25,26	1.48	5 (22%)	30,36,39	2.07	9 (30%)
1	PSU	S2	93	1	18,21,22	1.54	4 (22%)	21,30,33	2.20	4 (19%)
3	PSU	L5	2843	3	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.79	0	25,31,34	0.81	0
3	PSU	L5	4471	3	18,21,22	1.50	3 (16%)	21,30,33	1.98	5 (23%)
3	OMU	L5	2837	3	19,22,23	1.29	3 (15%)	25,31,34	1.91	5 (20%)
3	PSU	L5	4500	90,3	18,21,22	1.42	2 (11%)	21,30,33	2.09	3 (14%)
3	PSU	L5	1683	3,89	18,21,22	1.53	4 (22%)	21,30,33	1.92	3 (14%)
3	OMG	L5	3744	3	23,26,27	1.26	4 (17%)	32,38,41	2.07	7 (21%)
3	OMU	L5	3925	3	19,22,23	1.24	3 (15%)	25,31,34	1.82	5 (20%)
3	OMC	L5	2861	3	19,22,23	0.79	0	25,31,34	0.82	1 (4%)
3	OMU	L5	4498	90,3	19,22,23	1.25	3 (15%)	25,31,34	1.85	5 (20%)
1	OMU	S2	172	1	19,22,23	1.32	4 (21%)	25,31,34	2.00	6 (24%)
3	A2M	L5	3718	3	22,25,26	1.47	4 (18%)	30,36,39	1.95	10 (33%)
1	A2M	S2	576	1	22,25,26	1.53	5 (22%)	30,36,39	1.99	10 (33%)
3	PSU	L5	5001	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
52	V5N	La	39	52	8,11,12	1.39	1 (12%)	8,14,16	1.69	2 (25%)
1	PSU	S2	296	1	18,21,22	1.47	5 (27%)	21,30,33	2.16	3 (14%)
3	PSU	L5	3729	3	18,21,22	1.54	5 (27%)	21,30,33	2.19	4 (19%)
3	OMC	L5	3701	3,89	19,22,23	0.90	0	25,31,34	1.07	0
1	PSU	S2	1081	1	18,21,22	1.46	5 (27%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1367	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
1	A2M	S2	1383	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	10 (33%)
3	PSU	L5	3770	3	18,21,22	1.51	4 (22%)	21,30,33	2.24	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.38	4 (22%)	21,30,33	2.12	4 (19%)
85	H2U	Pt	21	85	18,21,22	1.06	2 (11%)	19,30,33	0.72	0
1	OMG	S2	436	1	23,26,27	1.26	3 (13%)	32,38,41	2.21	8 (25%)
3	PSU	L5	4423	3	18,21,22	1.39	3 (16%)	21,30,33	2.05	3 (14%)
84	PSU	At	39	84	18,21,22	1.51	4 (22%)	21,30,33	2.09	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	1316	3	23,26,27	1.22	3 (13%)	32,38,41	2.00	6 (18%)
1	UY1	S2	1326	90,1	19,22,23	1.38	3 (15%)	21,31,34	2.26	4 (19%)
3	PSU	L5	1779	3	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
1	PSU	S2	1056	1	18,21,22	1.46	3 (16%)	21,30,33	2.25	4 (19%)
85	OMC	Pt	33	85	19,22,23	0.92	1 (5%)	25,31,34	1.00	1 (4%)
1	OMU	S2	1804	1	19,22,23	1.27	3 (15%)	25,31,34	1.88	5 (20%)
3	OMU	L5	4227	3	19,22,23	1.26	3 (15%)	25,31,34	1.81	4 (16%)
1	PSU	S2	1174	1	18,21,22	1.51	3 (16%)	21,30,33	2.22	5 (23%)
1	OMG	S2	1328	1,89	23,26,27	1.25	3 (13%)	32,38,41	2.13	7 (21%)
3	OMG	L5	4494	3	23,26,27	1.28	4 (17%)	32,38,41	2.08	7 (21%)
3	PSU	L5	4457	3	18,21,22	1.53	4 (22%)	21,30,33	2.26	6 (28%)
1	PSU	S2	119	1	18,21,22	1.48	4 (22%)	21,30,33	2.13	4 (19%)
1	OMC	S2	174	1	19,22,23	0.86	0	25,31,34	1.00	2 (8%)
3	PSU	L5	4361	3	18,21,22	1.60	5 (27%)	21,30,33	2.19	6 (28%)
84	PSU	At	32	84	18,21,22	1.48	4 (22%)	21,30,33	2.18	4 (19%)
84	H2U	At	16	84	18,21,22	0.99	2 (11%)	19,30,33	0.82	1 (5%)
1	PSU	S2	406	1	18,21,22	1.54	5 (27%)	21,30,33	2.10	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.46	5 (22%)	30,36,39	2.11	10 (33%)
1	6MZ	S2	1832	90,1	22,25,26	1.48	5 (22%)	29,36,39	2.14	9 (31%)
1	A2M	S2	1678	1	22,25,26	1.48	4 (18%)	30,36,39	2.01	9 (30%)
3	PSU	L5	4312	3	18,21,22	1.41	4 (22%)	21,30,33	2.11	4 (19%)
3	OMC	L5	1340	3	19,22,23	0.90	0	25,31,34	0.84	0
3	OMG	L5	3944	3	23,26,27	1.25	3 (13%)	32,38,41	2.09	7 (21%)
1	PSU	S2	1004	1	18,21,22	1.39	4 (22%)	21,30,33	2.07	3 (14%)
3	A2M	L5	2787	3	22,25,26	1.45	5 (22%)	30,36,39	2.06	9 (30%)
3	OMC	L5	2804	3	19,22,23	0.81	0	25,31,34	0.79	0
3	A2M	L5	4571	3	22,25,26	1.46	3 (13%)	30,36,39	2.03	7 (23%)
1	OMU	S2	1442	90,1	19,22,23	1.27	3 (15%)	25,31,34	1.88	4 (16%)
3	OMG	L5	2364	3	23,26,27	1.18	3 (13%)	32,38,41	1.96	6 (18%)
1	OMU	S2	1288	1	19,22,23	1.32	3 (15%)	25,31,34	1.85	5 (20%)
3	PSU	L5	3762	3	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.36	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	866	1	18,21,22	1.46	3 (16%)	21,30,33	2.18	4 (19%)
1	PSU	S2	34	1	18,21,22	1.38	3 (16%)	21,30,33	2.08	4 (19%)
3	A2M	L5	400	3	22,25,26	1.46	5 (22%)	30,36,39	2.12	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5MC	L5	4447	3,89	19,22,23	1.56	3 (15%)	26,32,35	1.27	3 (11%)
3	PSU	L5	4403	3	18,21,22	1.62	5 (27%)	21,30,33	2.32	5 (23%)
87	M3L	EF	36	87	10,11,12	0.53	0	9,14,16	0.46	0
3	PSU	L5	3639	3	18,21,22	1.44	4 (22%)	21,30,33	2.14	4 (19%)
1	PSU	S2	109	1	18,21,22	1.52	4 (22%)	21,30,33	2.19	3 (14%)
3	OMC	L5	3808	3	19,22,23	0.93	0	25,31,34	1.06	1 (4%)
3	A2M	L5	1326	3	22,25,26	1.47	4 (18%)	30,36,39	2.01	7 (23%)
3	OMG	L5	2876	3	23,26,27	1.22	3 (13%)	32,38,41	2.04	6 (18%)
1	A2M	S2	99	90,1	22,25,26	1.44	4 (18%)	30,36,39	2.17	8 (26%)
1	PSU	S2	1244	1	18,21,22	1.46	3 (16%)	21,30,33	2.19	4 (19%)
84	G7M	At	46	84	23,26,27	1.90	2 (8%)	34,39,42	1.10	1 (2%)
1	PSU	S2	1347	1	18,21,22	1.50	4 (22%)	21,30,33	2.13	3 (14%)
3	PSU	L5	1582	3	18,21,22	1.52	4 (22%)	21,30,33	2.13	6 (28%)
3	PSU	L5	4293	3	18,21,22	1.44	4 (22%)	21,30,33	2.11	3 (14%)
3	PSU	L5	4531	3	18,21,22	1.43	2 (11%)	21,30,33	2.07	4 (19%)
3	OMG	L5	4228	3	23,26,27	1.19	4 (17%)	32,38,41	1.95	6 (18%)
3	PSU	L5	4442	3	18,21,22	1.55	4 (22%)	21,30,33	2.32	5 (23%)
3	OMG	L5	4623	3	23,26,27	1.22	3 (13%)	32,38,41	2.06	7 (21%)
87	M3L	EF	79	87	10,11,12	0.55	0	9,14,16	0.51	0
3	6MZ	L5	4220	3	22,25,26	1.41	4 (18%)	29,36,39	2.18	9 (31%)
66	SAC	Lr	2	66	7,8,9	3.75	2 (28%)	7,9,11	4.57	5 (71%)
87	M3L	EF	318	87	10,11,12	0.42	0	9,14,16	0.13	0
3	PSU	L5	3768	3	18,21,22	1.49	4 (22%)	21,30,33	2.06	4 (19%)
29	AME	SV	1	29	9,10,11	3.32	2 (22%)	9,11,13	3.86	3 (33%)
1	PSU	S2	815	1	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
3	OMU	L5	4306	3	19,22,23	1.28	3 (15%)	25,31,34	1.76	4 (16%)
3	A2M	L5	2363	90,3	22,25,26	1.48	5 (22%)	30,36,39	2.03	9 (30%)
3	PSU	L5	1860	3	18,21,22	1.56	4 (22%)	21,30,33	2.08	5 (23%)
40	HIC	LB	245	40	10,11,12	1.42	1 (10%)	9,14,16	1.29	2 (22%)
85	PSU	Pt	56	85	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
3	A2M	L5	3825	3	22,25,26	1.46	4 (18%)	30,36,39	2.09	10 (33%)
3	UY1	L5	3818	90,3	19,22,23	1.44	4 (21%)	21,31,34	2.00	4 (19%)
1	PSU	S2	686	1	18,21,22	1.51	4 (22%)	21,30,33	2.20	3 (14%)
1	PSU	S2	1692	1	18,21,22	1.39	4 (22%)	21,30,33	2.07	4 (19%)
3	PSU	L5	4521	90,3,89	18,21,22	1.36	2 (11%)	21,30,33	2.20	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	4620	3	19,22,23	1.40	3 (15%)	25,31,34	1.98	8 (32%)
84	H2U	At	20	84	18,21,22	1.03	2 (11%)	19,30,33	1.02	2 (10%)
3	PSU	L5	4689	3	18,21,22	1.46	3 (16%)	21,30,33	2.06	3 (14%)
2	PSU	L8	55	2	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	801	1	18,21,22	1.52	4 (22%)	21,30,33	2.00	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.78	0	25,31,34	0.98	2 (8%)
3	A2M	L5	3724	3	22,25,26	1.44	4 (18%)	30,36,39	2.05	9 (30%)
87	MLY	EF	55	87	9,10,11	0.51	0	6,11,13	0.88	0
1	OMU	S2	121	1	19,22,23	1.43	3 (15%)	25,31,34	1.90	5 (20%)
1	PSU	S2	1238	1	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
1	OMU	S2	116	1	19,22,23	1.35	3 (15%)	25,31,34	1.77	5 (20%)
3	OMG	L5	3627	3	23,26,27	1.18	4 (17%)	32,38,41	2.04	6 (18%)
3	OMC	L5	4536	3	19,22,23	0.89	0	25,31,34	1.00	0
3	OMG	L5	4392	3	23,26,27	1.30	4 (17%)	32,38,41	1.99	7 (21%)
3	UR3	L5	4530	3	19,22,23	0.89	0	26,32,35	1.86	4 (15%)
1	PSU	S2	814	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
1	A2M	S2	1031	1	22,25,26	1.49	5 (22%)	30,36,39	2.03	10 (33%)
3	PSU	L5	2508	3	18,21,22	1.40	3 (16%)	21,30,33	2.10	4 (19%)
3	A2M	L5	3785	3	22,25,26	1.43	5 (22%)	30,36,39	2.33	12 (40%)
85	4SU	Pt	8	85	18,21,22	2.07	4 (22%)	25,30,33	2.33	4 (16%)
1	A2M	S2	512	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	9 (30%)
1	A2M	S2	590	1	22,25,26	1.45	4 (18%)	30,36,39	2.10	7 (23%)
1	PSU	S2	1136	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.38	3 (16%)	21,30,33	2.12	4 (19%)
1	PSU	S2	966	1	18,21,22	1.46	2 (11%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1744	3,89	18,21,22	1.50	4 (22%)	21,30,33	2.12	3 (14%)
3	A2M	L5	2401	3	22,25,26	1.48	5 (22%)	30,36,39	2.14	9 (30%)
3	A2M	L5	1871	90,3	22,25,26	1.48	5 (22%)	30,36,39	2.13	10 (33%)
3	A2M	L5	1534	90,3	22,25,26	1.48	5 (22%)	30,36,39	2.08	7 (23%)
3	PSU	L5	4576	3	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
1	A2M	S2	468	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	9 (30%)
3	PSU	L5	3851	3	18,21,22	1.41	4 (22%)	21,30,33	2.09	4 (19%)
1	OMG	S2	683	1	23,26,27	1.21	4 (17%)	32,38,41	2.02	7 (21%)
1	4AC	S2	1842	1	21,24,25	0.98	1 (4%)	28,34,37	1.16	4 (14%)
3	PSU	L5	1536	3	18,21,22	1.42	4 (22%)	21,30,33	2.07	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1862	3	18,21,22	1.53	4 (22%)	21,30,33	2.24	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
86	5CT	5A	50	86	13,14,15	1.02	1 (7%)	8,15,17	1.14	0
1	OMC	S2	1391	1	19,22,23	0.81	0	25,31,34	0.82	0
3	OMG	L5	2424	3	23,26,27	1.32	3 (13%)	32,38,41	1.91	6 (18%)
3	OMG	L5	4499	3	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
3	OMC	L5	1881	90,3	19,22,23	0.91	0	25,31,34	1.12	2 (8%)
20	HY3	SX	62	20,89	7,8,9	1.43	1 (14%)	7,10,12	1.28	1 (14%)
1	OMC	S2	1703	90,1	19,22,23	0.78	0	25,31,34	0.75	0
2	PSU	L8	69	2,89	18,21,22	1.60	5 (27%)	21,30,33	2.40	5 (23%)
1	PSU	S2	105	1	18,21,22	1.54	4 (22%)	21,30,33	2.23	4 (19%)
3	PSU	L5	4579	3	18,21,22	1.60	6 (33%)	21,30,33	2.20	3 (14%)
1	PSU	S2	1625	1	18,21,22	1.42	3 (16%)	21,30,33	2.18	3 (14%)
1	PSU	S2	863	1	18,21,22	1.49	4 (22%)	21,30,33	2.10	4 (19%)
3	OMC	L5	3869	3	19,22,23	0.89	1 (5%)	25,31,34	1.04	0
1	OMU	S2	428	1	19,22,23	1.24	3 (15%)	25,31,34	1.93	6 (24%)
3	A2M	L5	398	3	22,25,26	1.56	4 (18%)	30,36,39	2.02	7 (23%)
2	OMU	L8	14	2,3	19,22,23	1.46	4 (21%)	25,31,34	2.04	5 (20%)
3	OMG	L5	4370	3	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
3	PSU	L5	4493	3,89	18,21,22	1.44	4 (22%)	21,30,33	2.07	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	90,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	90,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3,89	-	2/9/27/28	0/3/3/3
1	OMU	S2	627	1	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	4196	85,3	-	1/9/27/28	0/3/3/3
1	G7M	S2	1639	85,1	-	0/7/25/26	0/3/3/3
3	PSU	L5	3853	90,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	90,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
81	MLZ	Lo	53	81	-	4/7/8/10	-
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1792	90,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2422	90,3	-	3/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	3/9/27/28	0/3/3/3
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
1	A2M	S2	668	90,1	-	3/9/27/28	0/3/3/3
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1851	1	-	1/11/29/30	0/3/3/3
3	PSU	L5	3637	90,3,89	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
68	MLZ	Lb	5	68	-	3/7/8/10	-
79	M3L	Lm	98	79	-	0/9/10/12	-
85	G7M	Pt	47	85	-	0/7/25/26	0/3/3/3
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	90,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1643	90,1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
84	4SU	At	8	90,84	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	4/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
6	SAC	SA	2	6	-	2/7/8/10	-
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
2	OMG	L8	75	2	-	1/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
84	MIA	At	37	84	-	2/15/33/34	0/3/3/3
1	B8N	S2	1248	1	-	6/16/34/35	0/2/2/2
1	A2M	S2	159	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	1490	90,1	-	2/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	90,3	-	2/7/25/26	0/3/3/3
3	A2M	L5	2815	90,3	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3760	90,3	-	0/9/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4500	90,3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1683	3,89	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4498	90,3	-	0/9/27/28	0/2/2/2
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
52	V5N	La	39	52	-	0/9/10/12	0/1/1/1
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3701	3,89	-	4/9/27/28	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
85	H2U	Pt	21	85	-	5/7/38/39	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
84	PSU	At	39	84	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
1	UY1	S2	1326	90,1	-	1/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
85	OMC	Pt	33	85	-	0/9/27/28	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1174	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	1,89	-	1/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
84	PSU	At	32	84	-	0/7/25/26	0/2/2/2
84	H2U	At	16	84	-	7/7/38/39	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
1	6MZ	S2	1832	90,1	-	2/9/27/28	0/3/3/3
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	1442	90,1	-	0/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4447	3,89	-	4/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
87	M3L	EF	36	87	-	0/9/10/12	-
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
1	A2M	S2	99	90,1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
84	G7M	At	46	84	-	0/7/25/26	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
87	M3L	EF	79	87	-	3/9/10/12	-
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
66	SAC	Lr	2	66	-	3/7/8/10	-
87	M3L	EF	318	87	-	0/9/10/12	-
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	2/9/10/12	-
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	2363	90,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
85	PSU	Pt	56	85	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	90,3	-	3/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	90,3,89	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
84	H2U	At	20	84	-	1/7/38/39	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
87	MLY	EF	55	87	-	1/8/9/11	-
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
85	4SU	Pt	8	85	-	0/7/25/26	0/2/2/2
1	A2M	S2	512	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	590	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	3,89	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1871	90,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1534	90,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	3/7/25/26	0/2/2/2
86	5CT	5A	50	86	-	8/13/14/16	-
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	90,3	-	0/9/27/28	0/2/2/2
20	HY3	SX	62	20,89	-	1/1/12/14	0/1/1/1
1	OMC	S2	1703	90,1	-	0/9/27/28	0/2/2/2
2	PSU	L8	69	2,89	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	3/9/27/28	0/3/3/3
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4493	3,89	-	0/7/25/26	0/2/2/2

All (763) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	8.98	1.43	1.23
66	Lr	2	SAC	OAC-C1A	8.91	1.43	1.23
84	At	37	MIA	C2-S10	-8.67	1.68	1.75
6	SA	2	SAC	OAC-C1A	8.23	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	At	46	G7M	C8-N7	7.54	1.45	1.33
1	S2	1639	G7M	C8-N7	7.51	1.45	1.33
85	Pt	47	G7M	C8-N7	7.34	1.45	1.33
84	At	37	MIA	C13-C14	6.65	1.52	1.32
3	L5	3782	5MC	C5-C4	5.51	1.48	1.44
85	Pt	8	4SU	C4-S4	-5.43	1.59	1.68
1	S2	1639	G7M	C5-N7	-5.30	1.33	1.39
3	L5	4447	5MC	C5-C4	5.26	1.48	1.44
84	At	8	4SU	C4-S4	-4.97	1.59	1.68
3	L5	398	A2M	C5-C4	4.80	1.47	1.39
1	S2	576	A2M	C5-C4	4.73	1.47	1.39
1	S2	159	A2M	C5-C4	4.54	1.47	1.39
1	S2	1850	MA6	C5-C4	4.49	1.47	1.39
1	S2	1832	6MZ	C5-C4	4.47	1.47	1.39
3	L5	3760	A2M	C5-C4	4.47	1.47	1.39
1	S2	1851	MA6	C5-C4	4.42	1.47	1.39
1	S2	166	A2M	C5-C4	4.42	1.47	1.39
3	L5	3718	A2M	C5-C4	4.40	1.46	1.39
3	L5	3830	A2M	C5-C4	4.37	1.46	1.39
1	S2	1031	A2M	C5-C4	4.36	1.46	1.39
3	L5	400	A2M	C5-C4	4.35	1.46	1.39
1	S2	590	A2M	C5-C4	4.33	1.46	1.39
3	L5	3825	A2M	C5-C4	4.31	1.46	1.39
3	L5	1524	A2M	C5-C4	4.30	1.46	1.39
1	S2	512	A2M	C5-C4	4.29	1.46	1.39
3	L5	4571	A2M	C5-C4	4.28	1.46	1.39
3	L5	2363	A2M	C5-C4	4.26	1.46	1.39
3	L5	1534	A2M	C5-C4	4.25	1.46	1.39
3	L5	4590	A2M	C5-C4	4.25	1.46	1.39
3	L5	4523	A2M	C5-C4	4.24	1.46	1.39
3	L5	3724	A2M	C5-C4	4.24	1.46	1.39
3	L5	2815	A2M	C5-C4	4.23	1.46	1.39
1	S2	668	A2M	C5-C4	4.20	1.46	1.39
1	S2	1383	A2M	C5-C4	4.19	1.46	1.39
1	S2	468	A2M	C5-C4	4.19	1.46	1.39
3	L5	2787	A2M	C5-C4	4.18	1.46	1.39
1	S2	484	A2M	C5-C4	4.16	1.46	1.39
66	Lr	2	SAC	C1A-N	4.16	1.47	1.34
3	L5	4220	6MZ	C5-C4	4.16	1.46	1.39
84	At	37	MIA	C5-C4	4.15	1.46	1.39
3	L5	3723	A2M	C5-C4	4.15	1.46	1.39
1	S2	1678	A2M	C5-C4	4.11	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3867	A2M	C5-C4	4.10	1.46	1.39
1	S2	1639	G7M	C8-N9	4.09	1.46	1.35
1	S2	99	A2M	C5-C4	4.09	1.46	1.39
1	S2	27	A2M	C5-C4	4.07	1.46	1.39
3	L5	2401	A2M	C5-C4	4.06	1.46	1.39
3	L5	3785	A2M	C5-C4	4.05	1.46	1.39
84	At	46	G7M	C8-N9	4.02	1.46	1.35
85	Pt	8	4SU	C4-N3	-4.02	1.33	1.37
85	Pt	47	G7M	C8-N9	3.99	1.46	1.35
3	L5	1326	A2M	C5-C4	3.96	1.46	1.39
3	L5	1871	A2M	C5-C4	3.94	1.46	1.39
29	SV	1	AME	CT1-N	3.90	1.46	1.34
1	S2	1639	G7M	C5-C4	3.76	1.47	1.38
1	S2	966	PSU	C6-C5	3.75	1.39	1.35
84	At	8	4SU	C4-N3	-3.57	1.33	1.37
2	L8	69	PSU	C4-N3	-3.51	1.32	1.38
20	SX	62	HY3	C3-CA	-3.47	1.51	1.55
1	S2	918	PSU	C6-C5	3.45	1.39	1.35
1	S2	354	OMU	C4-N3	-3.45	1.32	1.38
3	L5	4471	PSU	C6-C5	3.45	1.39	1.35
39	LA	216	V5N	CG-ND1	-3.45	1.34	1.37
3	L5	4403	PSU	C4-N3	-3.44	1.32	1.38
1	S2	121	OMU	C4-N3	-3.43	1.32	1.38
3	L5	3884	PSU	C4-N3	-3.43	1.32	1.38
2	L8	14	OMU	C4-N3	-3.42	1.32	1.38
6	SA	2	SAC	C1A-N	3.42	1.45	1.34
3	L5	1677	PSU	O4'-C1'	-3.40	1.39	1.43
3	L5	1582	PSU	C4-N3	-3.39	1.32	1.38
85	Pt	8	4SU	C5-C4	-3.38	1.38	1.42
3	L5	3764	PSU	C6-C5	3.37	1.39	1.35
1	S2	815	PSU	C6-C5	3.36	1.39	1.35
3	L5	1860	PSU	C4-N3	-3.36	1.32	1.38
3	L5	4620	OMU	C4-N3	-3.35	1.32	1.38
3	L5	1683	PSU	C4-N3	-3.34	1.32	1.38
3	L5	4636	PSU	C4-N3	-3.34	1.32	1.38
1	S2	1243	PSU	C6-C5	3.33	1.39	1.35
3	L5	4457	PSU	C4-N3	-3.32	1.32	1.38
52	La	39	V5N	CG-ND1	-3.32	1.34	1.37
3	L5	4521	PSU	C6-C5	3.30	1.38	1.35
1	S2	1232	PSU	C4-N3	-3.30	1.32	1.38
3	L5	4579	PSU	C4-N3	-3.29	1.32	1.38
3	L5	1683	PSU	C6-C5	3.27	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	Pt	56	PSU	C6-C5	3.27	1.38	1.35
3	L5	3637	PSU	C4-N3	-3.27	1.32	1.38
3	L5	4673	PSU	C6-C5	3.26	1.38	1.35
1	S2	573	PSU	C4-N3	-3.26	1.32	1.38
1	S2	105	PSU	C4-N3	-3.26	1.32	1.38
3	L5	4628	PSU	C6-C5	3.26	1.38	1.35
3	L5	4361	PSU	C4-N3	-3.25	1.32	1.38
1	S2	1625	PSU	C6-C5	3.24	1.38	1.35
3	L5	1862	PSU	C4-N3	-3.23	1.32	1.38
1	S2	1337	4AC	C4-N4	-3.23	1.35	1.39
2	L8	14	OMU	C2-N3	-3.22	1.32	1.38
3	L5	3818	UY1	C4-N3	-3.22	1.32	1.38
3	L5	4569	PSU	C6-C5	3.22	1.38	1.35
3	L5	4431	PSU	C6-C5	3.21	1.38	1.35
3	L5	3734	PSU	C6-C5	3.21	1.38	1.35
84	At	39	PSU	C4-N3	-3.20	1.32	1.38
1	S2	1347	PSU	C4-N3	-3.20	1.32	1.38
1	S2	406	PSU	C4-N3	-3.20	1.32	1.38
3	L5	4532	PSU	C4-N3	-3.20	1.32	1.38
3	L5	2632	PSU	C6-C5	3.20	1.38	1.35
1	S2	1174	PSU	C6-C5	3.19	1.38	1.35
1	S2	1445	PSU	C6-C5	3.19	1.38	1.35
1	S2	1326	UY1	C4-N3	-3.18	1.32	1.38
1	S2	1174	PSU	C4-N3	-3.18	1.32	1.38
3	L5	2415	OMU	C4-N3	-3.18	1.33	1.38
3	L5	4500	PSU	C6-C5	3.18	1.38	1.35
3	L5	3637	PSU	C6-C5	3.17	1.38	1.35
1	S2	218	PSU	C4-N3	-3.16	1.32	1.38
1	S2	801	PSU	C6-C5	3.16	1.38	1.35
1	S2	1056	PSU	C6-C5	3.16	1.38	1.35
1	S2	1232	PSU	C6-C5	3.16	1.38	1.35
1	S2	509	OMG	C6-N1	-3.15	1.33	1.38
3	L5	4442	PSU	C4-N3	-3.15	1.33	1.38
1	S2	1239	PSU	C6-C5	3.15	1.38	1.35
1	S2	572	PSU	C6-C5	3.14	1.38	1.35
1	S2	866	PSU	C4-N3	-3.14	1.33	1.38
3	L5	4353	PSU	C4-N3	-3.14	1.33	1.38
1	S2	93	PSU	C4-N3	-3.13	1.33	1.38
1	S2	651	PSU	C6-C5	3.12	1.38	1.35
3	L5	3715	PSU	C4-N3	-3.12	1.33	1.38
1	S2	1056	PSU	C4-N3	-3.12	1.33	1.38
3	L5	3770	PSU	C4-N3	-3.11	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1244	PSU	C4-N3	-3.11	1.33	1.38
3	L5	4689	PSU	C4-N3	-3.11	1.33	1.38
1	S2	609	PSU	C4-N3	-3.11	1.33	1.38
3	L5	4673	PSU	C4-N3	-3.11	1.33	1.38
1	S2	649	PSU	C4-N3	-3.11	1.33	1.38
3	L5	4392	OMG	C6-N1	-3.11	1.33	1.38
3	L5	1792	PSU	C4-N3	-3.10	1.33	1.38
3	L5	2424	OMG	C6-N1	-3.10	1.33	1.38
3	L5	5010	PSU	C6-C5	3.10	1.38	1.35
1	S2	109	PSU	C4-N3	-3.10	1.33	1.38
3	L5	1744	PSU	C4-N3	-3.09	1.33	1.38
1	S2	801	PSU	C4-N3	-3.09	1.33	1.38
1	S2	36	PSU	C6-C5	3.08	1.38	1.35
3	L5	4628	PSU	C4-N3	-3.07	1.33	1.38
1	S2	686	PSU	C6-C5	3.07	1.38	1.35
1	S2	109	PSU	C6-C5	3.07	1.38	1.35
3	L5	4569	PSU	C4-N3	-3.07	1.33	1.38
1	S2	918	PSU	C4-N3	-3.06	1.33	1.38
3	L5	3768	PSU	C4-N3	-3.06	1.33	1.38
3	L5	3639	PSU	C4-N3	-3.06	1.33	1.38
1	S2	119	PSU	C4-N3	-3.05	1.33	1.38
3	L5	3758	PSU	C6-C5	3.05	1.38	1.35
3	L5	3768	PSU	C6-C5	3.05	1.38	1.35
3	L5	4423	PSU	C6-C5	3.05	1.38	1.35
2	L8	55	PSU	C6-C5	3.04	1.38	1.35
3	L5	2815	A2M	C5-N7	-3.04	1.33	1.39
86	5A	50	5CT	CB-CA	-3.03	1.49	1.53
1	S2	1238	PSU	C6-C5	3.02	1.38	1.35
1	S2	1177	PSU	C6-C5	3.02	1.38	1.35
3	L5	4493	PSU	C4-N3	-3.02	1.33	1.38
3	L5	4293	PSU	C6-C5	3.01	1.38	1.35
3	L5	1862	PSU	C6-C5	3.01	1.38	1.35
3	L5	4493	PSU	C6-C5	3.01	1.38	1.35
1	S2	681	PSU	C4-N3	-3.01	1.33	1.38
84	At	32	PSU	C4-N3	-3.01	1.33	1.38
3	L5	3920	PSU	C6-C5	3.01	1.38	1.35
1	S2	172	OMU	C4-N3	-3.01	1.33	1.38
3	L5	3844	PSU	C4-N3	-3.01	1.33	1.38
3	L5	3734	PSU	C4-N3	-3.00	1.33	1.38
1	S2	573	PSU	C6-C5	3.00	1.38	1.35
3	L5	4552	PSU	C4-N3	-3.00	1.33	1.38
3	L5	2424	OMG	C5-C4	3.00	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1536	PSU	C4-N3	-3.00	1.33	1.38
3	L5	4306	OMU	C4-N3	-3.00	1.33	1.38
3	L5	4196	OMG	C6-N1	-3.00	1.33	1.38
3	L5	4312	PSU	C4-N3	-2.99	1.33	1.38
3	L5	5001	PSU	C6-C5	2.99	1.38	1.35
1	S2	1288	OMU	C4-N3	-2.99	1.33	1.38
1	S2	34	PSU	C6-C5	2.99	1.38	1.35
3	L5	4531	PSU	C4-N3	-2.99	1.33	1.38
1	S2	121	OMU	C2-N3	-2.99	1.32	1.38
3	L5	2876	OMG	C5-C4	2.99	1.46	1.38
1	S2	863	PSU	C6-C5	2.99	1.38	1.35
3	L5	4637	OMG	C6-N1	-2.98	1.33	1.38
3	L5	1781	PSU	C6-C5	2.98	1.38	1.35
3	L5	3762	PSU	C6-C5	2.98	1.38	1.35
3	L5	4293	PSU	C4-N3	-2.98	1.33	1.38
3	L5	4471	PSU	C4-N3	-2.98	1.33	1.38
3	L5	2508	PSU	C4-N3	-2.98	1.33	1.38
1	S2	354	OMU	C2-N3	-2.97	1.32	1.38
3	L5	5001	PSU	C4-N3	-2.97	1.33	1.38
3	L5	2843	PSU	C4-N3	-2.97	1.33	1.38
1	S2	296	PSU	C4-N3	-2.96	1.33	1.38
1	S2	814	PSU	C6-C5	2.96	1.38	1.35
84	At	39	PSU	C6-C5	2.96	1.38	1.35
3	L5	1781	PSU	C4-N3	-2.96	1.33	1.38
3	L5	1779	PSU	C6-C5	2.96	1.38	1.35
3	L5	4494	OMG	C5-C4	2.96	1.46	1.38
1	S2	609	PSU	C6-C5	2.96	1.38	1.35
1	S2	863	PSU	C4-N3	-2.96	1.33	1.38
3	L5	4296	PSU	C4-N3	-2.96	1.33	1.38
1	S2	866	PSU	C6-C5	2.95	1.38	1.35
3	L5	4531	PSU	C6-C5	2.95	1.38	1.35
3	L5	1792	PSU	C6-C5	2.94	1.38	1.35
3	L5	1625	OMG	C5-C4	2.94	1.46	1.38
3	L5	4689	PSU	C6-C5	2.94	1.38	1.35
3	L5	3695	PSU	C4-N3	-2.94	1.33	1.38
3	L5	1326	A2M	C5-N7	-2.94	1.33	1.39
3	L5	3764	PSU	C4-N3	-2.94	1.33	1.38
1	S2	218	PSU	C6-C5	2.94	1.38	1.35
1	S2	36	PSU	C4-N3	-2.94	1.33	1.38
3	L5	2401	A2M	C5-N7	-2.94	1.33	1.39
3	L5	2837	OMU	C4-N3	-2.93	1.33	1.38
1	S2	1367	PSU	C6-C5	2.93	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1081	PSU	C4-N3	-2.93	1.33	1.38
1	S2	822	PSU	C6-C5	2.93	1.38	1.35
3	L5	4457	PSU	C6-C5	2.93	1.38	1.35
3	L5	4299	PSU	C6-C5	2.93	1.38	1.35
3	L5	1779	PSU	C4-N3	-2.93	1.33	1.38
3	L5	3744	OMG	C6-N1	-2.93	1.33	1.38
3	L5	3729	PSU	C4-N3	-2.93	1.33	1.38
3	L5	3792	OMG	C5-C4	2.92	1.46	1.38
3	L5	3867	A2M	C5-N7	-2.92	1.33	1.39
3	L5	1782	PSU	C4-N3	-2.92	1.33	1.38
3	L5	2876	OMG	C6-N1	-2.92	1.33	1.38
1	S2	686	PSU	C4-N3	-2.92	1.33	1.38
2	L8	75	OMG	C5-C4	2.92	1.46	1.38
3	L5	4972	PSU	C4-N3	-2.91	1.33	1.38
3	L5	4499	OMG	C5-C4	2.91	1.46	1.38
1	S2	436	OMG	C6-N1	-2.91	1.33	1.38
3	L5	1782	PSU	C6-C5	2.91	1.38	1.35
1	S2	1692	PSU	C6-C5	2.91	1.38	1.35
1	S2	1004	PSU	C6-C5	2.91	1.38	1.35
3	L5	4552	PSU	C6-C5	2.91	1.38	1.35
1	S2	572	PSU	C4-N3	-2.91	1.33	1.38
1	S2	116	OMU	C4-N3	-2.91	1.33	1.38
1	S2	484	A2M	C5-N7	-2.91	1.33	1.39
3	L5	4361	PSU	C2-N3	-2.90	1.32	1.37
3	L5	2632	PSU	C4-N3	-2.90	1.33	1.38
1	S2	93	PSU	C6-C5	2.90	1.38	1.35
3	L5	3695	PSU	C6-C5	2.90	1.38	1.35
3	L5	4576	PSU	C4-N3	-2.90	1.33	1.38
3	L5	4523	A2M	C5-N7	-2.90	1.33	1.39
3	L5	4299	PSU	C4-N3	-2.90	1.33	1.38
1	S2	644	OMG	C6-N1	-2.89	1.33	1.38
2	L8	55	PSU	C4-N3	-2.89	1.33	1.38
3	L5	3853	PSU	C4-N3	-2.89	1.33	1.38
1	S2	867	OMG	C5-C4	2.89	1.46	1.38
3	L5	3770	PSU	C6-C5	2.89	1.38	1.35
1	S2	1643	PSU	C4-N3	-2.89	1.33	1.38
1	S2	601	OMG	C5-C4	2.89	1.46	1.38
3	L5	4498	OMU	C4-N3	-2.88	1.33	1.38
3	L5	1582	PSU	C2-N3	-2.88	1.32	1.37
3	L5	3715	PSU	C6-C5	2.88	1.38	1.35
3	L5	5010	PSU	C4-N3	-2.88	1.33	1.38
1	S2	681	PSU	C6-C5	2.88	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4370	OMG	C5-C4	2.88	1.46	1.38
1	S2	814	PSU	C4-N3	-2.88	1.33	1.38
1	S2	1328	OMG	C6-N1	-2.87	1.33	1.38
3	L5	3920	PSU	C4-N3	-2.87	1.33	1.38
1	S2	627	OMU	C4-N3	-2.87	1.33	1.38
3	L5	4618	OMG	C6-N1	-2.87	1.33	1.38
3	L5	3758	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1367	PSU	C4-N3	-2.87	1.33	1.38
1	S2	1004	PSU	C4-N3	-2.87	1.33	1.38
3	L5	4420	PSU	C6-C5	2.87	1.38	1.35
1	S2	683	OMG	C5-C4	2.87	1.46	1.38
1	S2	1136	PSU	C6-C5	2.87	1.38	1.35
1	S2	1490	OMG	C6-N1	-2.86	1.33	1.38
3	L5	3851	PSU	C4-N3	-2.86	1.33	1.38
1	S2	1239	PSU	C4-N3	-2.86	1.33	1.38
3	L5	3944	OMG	C5-C4	2.85	1.46	1.38
3	L5	2843	PSU	C6-C5	2.85	1.38	1.35
1	S2	649	PSU	C6-C5	2.85	1.38	1.35
3	L5	1860	PSU	C6-C5	2.85	1.38	1.35
3	L5	3925	OMU	C4-N3	-2.85	1.33	1.38
1	S2	966	PSU	C4-N3	-2.85	1.33	1.38
1	S2	99	A2M	C5-N7	-2.85	1.33	1.39
3	L5	4447	5MC	C6-C5	2.85	1.39	1.34
1	S2	105	PSU	C6-C5	2.84	1.38	1.35
3	L5	2508	PSU	C6-C5	2.84	1.38	1.35
1	S2	1692	PSU	C4-N3	-2.84	1.33	1.38
3	L5	4494	OMG	C6-N1	-2.84	1.33	1.38
1	S2	1328	OMG	C5-C4	2.84	1.46	1.38
1	S2	1244	PSU	C6-C5	2.83	1.38	1.35
3	L5	1316	OMG	C6-N1	-2.83	1.33	1.38
3	L5	4623	OMG	C5-C4	2.83	1.46	1.38
1	S2	1177	PSU	C4-N3	-2.83	1.33	1.38
3	L5	1744	PSU	C6-C5	2.83	1.38	1.35
84	At	8	4SU	C5-C4	-2.83	1.39	1.42
1	S2	34	PSU	C4-N3	-2.83	1.33	1.38
3	L5	2839	PSU	C4-N3	-2.83	1.33	1.38
3	L5	3825	A2M	C5-N7	-2.82	1.33	1.39
3	L5	4403	PSU	C2-N3	-2.82	1.32	1.37
3	L5	2424	OMG	C5-N7	-2.82	1.33	1.39
1	S2	1447	OMG	C5-C4	2.82	1.46	1.38
1	S2	1490	OMG	C5-C4	2.82	1.46	1.38
3	L5	4227	OMU	C4-N3	-2.82	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4576	PSU	C6-C5	2.82	1.38	1.35
3	L5	4972	PSU	C6-C5	2.82	1.38	1.35
3	L5	4228	OMG	C5-C4	2.82	1.46	1.38
1	S2	651	PSU	C4-N3	-2.82	1.33	1.38
3	L5	3884	PSU	C2-N3	-2.81	1.32	1.37
3	L5	2364	OMG	C5-C4	2.81	1.46	1.38
1	S2	1804	OMU	C4-N3	-2.81	1.33	1.38
3	L5	2415	OMU	C2-N3	-2.80	1.33	1.38
85	Pt	21	H2U	C2-N3	-2.80	1.33	1.38
3	L5	4500	PSU	C4-N3	-2.80	1.33	1.38
1	S2	1238	PSU	C4-N3	-2.80	1.33	1.38
3	L5	4423	PSU	C4-N3	-2.80	1.33	1.38
3	L5	3899	OMG	C5-C4	2.80	1.46	1.38
3	L5	4361	PSU	C6-C5	2.80	1.38	1.35
3	L5	1871	A2M	C5-N7	-2.79	1.34	1.39
3	L5	3762	PSU	C4-N3	-2.79	1.33	1.38
3	L5	4353	PSU	C6-C5	2.79	1.38	1.35
3	L5	4457	PSU	C2-N3	-2.79	1.32	1.37
3	L5	3944	OMG	C6-N1	-2.79	1.33	1.38
3	L5	4571	A2M	C5-N7	-2.79	1.34	1.39
3	L5	3899	OMG	C6-N1	-2.79	1.33	1.38
1	S2	1136	PSU	C4-N3	-2.78	1.33	1.38
1	S2	644	OMG	C5-C4	2.78	1.46	1.38
1	S2	822	PSU	C4-N3	-2.78	1.33	1.38
3	L5	3729	PSU	C6-C5	2.78	1.38	1.35
1	S2	406	PSU	C6-C5	2.77	1.38	1.35
3	L5	4620	OMU	C2-N3	-2.77	1.33	1.38
3	L5	3627	OMG	C5-C4	2.77	1.46	1.38
3	L5	4618	OMG	C5-C4	2.77	1.46	1.38
3	L5	1316	OMG	C5-C4	2.77	1.46	1.38
1	S2	1081	PSU	C6-C5	2.77	1.38	1.35
3	L5	4431	PSU	C4-N3	-2.77	1.33	1.38
1	S2	815	PSU	C4-N3	-2.76	1.33	1.38
1	S2	1851	MA6	C5-C6	2.76	1.48	1.41
3	L5	1677	PSU	C4-N3	-2.76	1.33	1.38
40	LB	245	HIC	CD2-CG	2.76	1.41	1.36
1	S2	1243	PSU	C4-N3	-2.76	1.33	1.38
3	L5	3637	PSU	C2-N3	-2.76	1.32	1.37
3	L5	1522	OMG	C5-C4	2.76	1.46	1.38
3	L5	3744	OMG	C5-C4	2.76	1.46	1.38
1	S2	512	A2M	C5-N7	-2.76	1.34	1.39
1	S2	509	OMG	C5-C4	2.75	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1347	PSU	C6-C5	2.75	1.38	1.35
3	L5	1536	PSU	C6-C5	2.75	1.38	1.35
3	L5	4312	PSU	C6-C5	2.74	1.38	1.35
3	L5	1677	PSU	C6-C5	2.74	1.38	1.35
85	Pt	56	PSU	C4-N3	-2.74	1.33	1.38
3	L5	3844	PSU	C6-C5	2.73	1.38	1.35
1	S2	428	OMU	C4-N3	-2.73	1.33	1.38
1	S2	1445	PSU	C4-N3	-2.73	1.33	1.38
1	S2	1850	MA6	C5-C6	2.73	1.48	1.41
1	S2	119	PSU	C6-C5	2.73	1.38	1.35
1	S2	436	OMG	C5-C4	2.72	1.46	1.38
1	S2	1832	6MZ	C5-C6	2.72	1.48	1.41
3	L5	4521	PSU	C4-N3	-2.72	1.33	1.38
3	L5	4296	PSU	C6-C5	2.71	1.38	1.35
3	L5	1860	PSU	C2-N3	-2.71	1.33	1.37
3	L5	4590	A2M	C5-N7	-2.70	1.34	1.39
1	S2	601	OMG	C6-N1	-2.70	1.33	1.38
3	L5	1522	OMG	C6-N1	-2.69	1.33	1.38
85	Pt	8	4SU	C2-N3	-2.69	1.33	1.38
3	L5	1322	1MA	C6-N6	2.69	1.34	1.28
3	L5	3853	PSU	C6-C5	2.69	1.38	1.35
3	L5	4392	OMG	C5-C4	2.69	1.46	1.38
3	L5	1625	OMG	C6-N1	-2.68	1.33	1.38
3	L5	3884	PSU	C2-N1	-2.68	1.33	1.36
3	L5	3760	A2M	C5-C6	2.68	1.48	1.41
1	S2	1678	A2M	C5-N7	-2.68	1.34	1.39
3	L5	2364	OMG	C6-N1	-2.67	1.33	1.38
3	L5	4532	PSU	C6-C5	2.67	1.38	1.35
3	L5	4370	OMG	C6-N1	-2.66	1.33	1.38
1	S2	1643	PSU	C6-C5	2.66	1.38	1.35
3	L5	3851	PSU	C6-C5	2.66	1.38	1.35
3	L5	4623	OMG	C6-N1	-2.65	1.33	1.38
3	L5	2363	A2M	C5-N7	-2.65	1.34	1.39
3	L5	4442	PSU	C6-C5	2.64	1.38	1.35
1	S2	1639	G7M	C6-N1	-2.64	1.33	1.38
3	L5	4196	OMG	C5-C4	2.64	1.46	1.38
3	L5	3718	A2M	C5-N7	-2.64	1.34	1.39
3	L5	3627	OMG	C6-N1	-2.64	1.33	1.38
84	At	32	PSU	C6-C5	2.63	1.38	1.35
3	L5	1534	A2M	C5-N7	-2.63	1.34	1.39
3	L5	4637	OMG	C5-C4	2.63	1.45	1.38
3	L5	398	A2M	C5-C6	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4228	OMG	C6-N1	-2.63	1.33	1.38
1	S2	27	A2M	C5-N7	-2.62	1.34	1.39
3	L5	3792	OMG	C6-N1	-2.62	1.33	1.38
3	L5	3639	PSU	C6-C5	2.62	1.38	1.35
3	L5	4579	PSU	C6-C5	2.62	1.38	1.35
3	L5	1871	A2M	C4-N9	-2.62	1.32	1.37
3	L5	4636	PSU	C2-N3	-2.62	1.33	1.37
1	S2	683	OMG	C6-N1	-2.61	1.34	1.38
1	S2	801	PSU	C2-N3	-2.61	1.33	1.37
1	S2	1447	OMG	C6-N1	-2.61	1.34	1.38
3	L5	2839	PSU	C6-C5	2.61	1.38	1.35
1	S2	468	A2M	C5-N7	-2.61	1.34	1.39
3	L5	3782	5MC	C6-C5	2.61	1.38	1.34
84	At	16	H2U	C2-N3	-2.61	1.33	1.38
1	S2	509	OMG	C5-N7	-2.60	1.33	1.39
1	S2	867	OMG	C6-N1	-2.60	1.34	1.38
3	L5	3723	A2M	C5-N7	-2.60	1.34	1.39
1	S2	119	PSU	C2-N3	-2.60	1.33	1.37
1	S2	159	A2M	C5-N7	-2.60	1.34	1.39
3	L5	3724	A2M	C5-N7	-2.59	1.34	1.39
84	At	20	H2U	C2-N3	-2.59	1.33	1.38
3	L5	400	A2M	C5-N7	-2.58	1.34	1.39
3	L5	4220	6MZ	C5-N7	-2.58	1.34	1.39
3	L5	1792	PSU	C2-N3	-2.58	1.33	1.37
1	S2	1326	UY1	C6-C5	2.58	1.38	1.35
1	S2	590	A2M	C5-N7	-2.57	1.34	1.39
1	S2	1288	OMU	C2-N3	-2.57	1.33	1.38
1	S2	1383	A2M	C5-N7	-2.57	1.34	1.39
3	L5	1524	A2M	C5-N7	-2.57	1.34	1.39
3	L5	2787	A2M	C5-N7	-2.56	1.34	1.39
85	Pt	21	H2U	C4-N3	-2.56	1.33	1.37
1	S2	576	A2M	C5-C6	2.56	1.48	1.41
1	S2	1248	B8N	C6-C5	2.56	1.38	1.35
3	L5	1322	1MA	C5-C4	2.56	1.45	1.38
1	S2	1842	4AC	C4-N4	-2.55	1.36	1.39
3	L5	3764	PSU	C2-N3	-2.55	1.33	1.37
3	L5	4579	PSU	C2-N3	-2.54	1.33	1.37
3	L5	4420	PSU	C4-N3	-2.54	1.34	1.38
3	L5	4499	OMG	C6-N1	-2.53	1.34	1.38
1	S2	159	A2M	C5-C6	2.53	1.48	1.41
3	L5	1524	A2M	C5-C6	2.53	1.48	1.41
3	L5	1582	PSU	C6-C5	2.53	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L8	69	PSU	C6-C5	2.53	1.38	1.35
1	S2	576	A2M	C5-N7	-2.53	1.34	1.39
3	L5	3830	A2M	C5-N7	-2.53	1.34	1.39
3	L5	3723	A2M	C4-N9	-2.53	1.32	1.37
3	L5	4579	PSU	C2-N1	-2.53	1.33	1.36
1	S2	166	A2M	C5-C6	2.53	1.48	1.41
3	L5	4471	PSU	C2-N3	-2.52	1.33	1.37
3	L5	3782	5MC	C6-N1	-2.52	1.33	1.38
1	S2	218	PSU	C2-N3	-2.52	1.33	1.37
1	S2	105	PSU	C2-N3	-2.52	1.33	1.37
84	At	37	MIA	C5-N7	-2.52	1.34	1.39
1	S2	1031	A2M	C5-C6	2.52	1.48	1.41
1	S2	1031	A2M	C5-N7	-2.52	1.34	1.39
3	L5	1322	1MA	C5-N7	-2.51	1.34	1.39
3	L5	4227	OMU	C2-N3	-2.51	1.33	1.38
3	L5	3818	UY1	C2-N3	-2.51	1.33	1.37
3	L5	3718	A2M	C4-N9	-2.50	1.32	1.37
3	L5	2837	OMU	C2-N3	-2.50	1.33	1.38
1	S2	1442	OMU	C4-N3	-2.50	1.34	1.38
1	S2	1832	6MZ	C5-N7	-2.50	1.34	1.39
1	S2	1232	PSU	C2-N3	-2.50	1.33	1.37
3	L5	4532	PSU	C2-N3	-2.49	1.33	1.37
3	L5	3884	PSU	C6-C5	2.49	1.38	1.35
3	L5	4673	PSU	C2-N3	-2.49	1.33	1.37
3	L5	3770	PSU	C2-N3	-2.49	1.33	1.37
1	S2	166	A2M	C5-N7	-2.49	1.34	1.39
3	L5	2363	A2M	C5-C6	2.49	1.47	1.41
84	At	39	PSU	C2-N3	-2.49	1.33	1.37
3	L5	1534	A2M	C5-C6	2.49	1.47	1.41
1	S2	1490	OMG	C5-N7	-2.48	1.34	1.39
3	L5	3770	PSU	C2-N1	-2.48	1.33	1.36
1	S2	116	OMU	C5-C4	-2.48	1.38	1.43
3	L5	3830	A2M	C5-C6	2.48	1.47	1.41
1	S2	627	OMU	C2-N3	-2.48	1.33	1.38
2	L8	14	OMU	C5-C4	-2.48	1.38	1.43
3	L5	2415	OMU	C5-C4	-2.48	1.38	1.43
2	L8	69	PSU	C2-N3	-2.47	1.33	1.37
3	L5	3764	PSU	C2'-C1'	-2.47	1.50	1.53
1	S2	172	OMU	C2-N3	-2.47	1.33	1.38
1	S2	436	OMG	C5-N7	-2.47	1.34	1.39
3	L5	4498	OMU	C2-N3	-2.47	1.33	1.38
3	L5	1625	OMG	C5-N7	-2.47	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	2.46	1.38	1.35
3	L5	1322	1MA	C4-N9	-2.46	1.31	1.38
1	S2	590	A2M	C5-C6	2.46	1.47	1.41
1	S2	668	A2M	C5-C6	2.46	1.47	1.41
3	L5	3785	A2M	C5-N7	-2.45	1.34	1.39
1	S2	1347	PSU	C2-N3	-2.45	1.33	1.37
3	L5	1326	A2M	C4-N9	-2.45	1.32	1.37
3	L5	3715	PSU	C2-N3	-2.45	1.33	1.37
3	L5	4392	OMG	C5-N7	-2.45	1.34	1.39
1	S2	863	PSU	C2-N3	-2.45	1.33	1.37
3	L5	4447	5MC	C6-N1	-2.45	1.33	1.38
84	At	37	MIA	C5-C6	2.44	1.47	1.41
1	S2	1678	A2M	C5-C6	2.44	1.47	1.41
3	L5	400	A2M	C5-C6	2.44	1.47	1.41
3	L5	3785	A2M	C5-C6	2.44	1.47	1.41
3	L5	4618	OMG	C5-N7	-2.43	1.34	1.39
1	S2	609	PSU	C2-N3	-2.43	1.33	1.37
1	S2	1383	A2M	C4-N9	-2.43	1.32	1.37
3	L5	4637	OMG	C5-N7	-2.43	1.34	1.39
3	L5	1683	PSU	C2-N3	-2.43	1.33	1.37
1	S2	1804	OMU	C2-N3	-2.43	1.33	1.38
1	S2	668	A2M	C5-N7	-2.43	1.34	1.39
84	At	16	H2U	C4-N3	-2.43	1.33	1.37
1	S2	354	OMU	C5-C4	-2.43	1.38	1.43
1	S2	918	PSU	C2-N3	-2.42	1.33	1.37
1	S2	863	PSU	C2-N1	-2.42	1.33	1.36
1	S2	1625	PSU	C4-N3	-2.42	1.34	1.38
3	L5	4306	OMU	C2-N3	-2.42	1.33	1.38
1	S2	428	OMU	C2-N3	-2.42	1.33	1.38
3	L5	3825	A2M	C5-C6	2.41	1.47	1.41
3	L5	4457	PSU	C2-N1	-2.41	1.33	1.36
3	L5	4353	PSU	C2-N3	-2.41	1.33	1.37
1	S2	644	OMG	C5-N7	-2.41	1.34	1.39
3	L5	4196	OMG	C5-N7	-2.41	1.34	1.39
1	S2	649	PSU	C2-N3	-2.41	1.33	1.37
3	L5	4636	PSU	C6-C5	2.41	1.38	1.35
84	At	37	MIA	C4-N9	-2.40	1.32	1.37
3	L5	4220	6MZ	C5-C6	2.40	1.47	1.41
3	L5	3925	OMU	C2-N3	-2.40	1.33	1.38
1	S2	27	A2M	C5-C6	2.40	1.47	1.41
3	L5	2787	A2M	C5-C6	2.40	1.47	1.41
3	L5	3867	A2M	C4-N9	-2.40	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	484	A2M	C5-C6	2.40	1.47	1.41
1	S2	572	PSU	C2-N3	-2.40	1.33	1.37
3	L5	4571	A2M	C5-C6	2.40	1.47	1.41
1	S2	1678	A2M	C4-N9	-2.39	1.32	1.37
1	S2	1347	PSU	C2-N1	-2.39	1.33	1.36
1	S2	121	OMU	C5-C4	-2.39	1.38	1.43
1	S2	668	A2M	C4-N9	-2.39	1.32	1.37
3	L5	4493	PSU	C2-N3	-2.39	1.33	1.37
1	S2	1850	MA6	C5-N7	-2.39	1.34	1.39
1	S2	1383	A2M	C5-C6	2.39	1.47	1.41
1	S2	468	A2M	C4-N9	-2.39	1.32	1.37
3	L5	3792	OMG	C5-N7	-2.38	1.34	1.39
3	L5	1744	PSU	C2-N3	-2.38	1.33	1.37
3	L5	4590	A2M	C5-C6	2.38	1.47	1.41
3	L5	2815	A2M	C5-C6	2.37	1.47	1.41
3	L5	1792	PSU	C2-N1	-2.37	1.33	1.36
3	L5	398	A2M	C8-N7	2.37	1.36	1.31
1	S2	1244	PSU	C2-N3	-2.37	1.33	1.37
3	L5	4403	PSU	C6-C5	2.37	1.37	1.35
1	S2	406	PSU	C2-N3	-2.37	1.33	1.37
3	L5	4523	A2M	C5-C6	2.36	1.47	1.41
3	L5	3744	OMG	C5-N7	-2.36	1.34	1.39
3	L5	4442	PSU	C2-N3	-2.36	1.33	1.37
3	L5	4353	PSU	C2-N1	-2.36	1.33	1.36
3	L5	4403	PSU	C2-N1	-2.36	1.33	1.36
1	S2	1081	PSU	O4'-C1'	-2.36	1.40	1.43
1	S2	1174	PSU	C2-N3	-2.36	1.33	1.37
1	S2	686	PSU	C2-N1	-2.35	1.33	1.36
1	S2	1447	OMG	C5-N7	-2.35	1.34	1.39
1	S2	649	PSU	C2-N1	-2.35	1.33	1.36
1	S2	1850	MA6	C4-N9	-2.35	1.32	1.37
84	At	20	H2U	C4-N3	-2.34	1.33	1.37
3	L5	4442	PSU	C2-N1	-2.34	1.33	1.36
3	L5	3718	A2M	C5-C6	2.33	1.47	1.41
1	S2	1851	MA6	C5-N7	-2.33	1.34	1.39
3	L5	3825	A2M	C4-N9	-2.33	1.32	1.37
1	S2	1328	OMG	C5-N7	-2.33	1.34	1.39
3	L5	3760	A2M	C5-N7	-2.32	1.34	1.39
1	S2	406	PSU	C2-N1	-2.32	1.33	1.36
3	L5	3734	PSU	C2-N3	-2.32	1.33	1.37
1	S2	116	OMU	C2-N3	-2.32	1.33	1.38
1	S2	1081	PSU	C2-N3	-2.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	573	PSU	C2-N3	-2.32	1.33	1.37
3	L5	1862	PSU	C2-N3	-2.31	1.33	1.37
3	L5	4370	OMG	C5-N7	-2.31	1.34	1.39
3	L5	3729	PSU	C2-N1	-2.31	1.33	1.36
3	L5	3724	A2M	C5-C6	2.31	1.47	1.41
3	L5	3899	OMG	C5-N7	-2.31	1.34	1.39
3	L5	4590	A2M	C4-N9	-2.31	1.32	1.37
3	L5	3785	A2M	C4-N9	-2.31	1.32	1.37
3	L5	398	A2M	C5-N7	-2.31	1.34	1.39
3	L5	1316	OMG	C5-N7	-2.31	1.34	1.39
3	L5	2401	A2M	C5-C6	2.31	1.47	1.41
1	S2	296	PSU	C6-C5	2.31	1.37	1.35
2	L8	75	OMG	C6-N1	-2.31	1.34	1.38
3	L5	3639	PSU	C2-N3	-2.30	1.33	1.37
3	L5	2876	OMG	C5-N7	-2.30	1.34	1.39
1	S2	296	PSU	C2-N1	-2.30	1.33	1.36
1	S2	609	PSU	C2-N1	-2.30	1.33	1.36
3	L5	4494	OMG	C5-N7	-2.30	1.34	1.39
3	L5	2843	PSU	C2-N3	-2.29	1.33	1.37
3	L5	3729	PSU	C2'-C1'	-2.29	1.50	1.53
1	S2	512	A2M	C5-C6	2.29	1.47	1.41
3	L5	4623	OMG	C4-N9	-2.29	1.32	1.38
1	S2	93	PSU	C2-N3	-2.29	1.33	1.37
3	L5	2837	OMU	C5-C4	-2.28	1.38	1.43
1	S2	296	PSU	C2-N3	-2.28	1.33	1.37
3	L5	3723	A2M	C5-C6	2.28	1.47	1.41
3	L5	3851	PSU	C2-N3	-2.28	1.33	1.37
3	L5	3853	PSU	C2-N3	-2.28	1.33	1.37
3	L5	1536	PSU	C2-N3	-2.28	1.33	1.37
1	S2	1442	OMU	C2-N3	-2.28	1.34	1.38
2	L8	69	PSU	C2-N1	-2.28	1.33	1.36
3	L5	1860	PSU	C2-N1	-2.27	1.33	1.36
3	L5	3724	A2M	C4-N9	-2.27	1.33	1.37
1	S2	468	A2M	C5-C6	2.27	1.47	1.41
3	L5	3867	A2M	C5-C6	2.27	1.47	1.41
3	L5	3844	PSU	C2-N3	-2.26	1.33	1.37
3	L5	4532	PSU	C2'-C1'	-2.26	1.50	1.53
1	S2	1625	PSU	C2'-C1'	-2.26	1.50	1.53
3	L5	2401	A2M	C4-N9	-2.26	1.33	1.37
1	S2	109	PSU	C2-N1	-2.26	1.33	1.36
3	L5	4628	PSU	C2-N1	-2.25	1.33	1.36
1	S2	1326	UY1	C2-N3	-2.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	5001	PSU	C2-N3	-2.25	1.33	1.37
3	L5	3760	A2M	C8-N7	2.25	1.36	1.31
1	S2	1851	MA6	C4-N9	-2.25	1.33	1.37
1	S2	1442	OMU	C5-C4	-2.25	1.38	1.43
3	L5	4306	OMU	C5-C4	-2.25	1.38	1.43
3	L5	1522	OMG	C5-N7	-2.25	1.34	1.39
3	L5	2787	A2M	C4-N9	-2.24	1.33	1.37
3	L5	4532	PSU	C2-N1	-2.24	1.33	1.36
1	S2	172	OMU	C5-C4	-2.24	1.38	1.43
1	S2	627	OMU	C5-C4	-2.24	1.38	1.43
1	S2	93	PSU	C2'-C1'	-2.24	1.50	1.53
3	L5	3758	PSU	C2-N3	-2.24	1.33	1.37
3	L5	4499	OMG	C5-N7	-2.24	1.34	1.39
1	S2	1031	A2M	C4-N9	-2.24	1.33	1.37
1	S2	1643	PSU	C2-N3	-2.24	1.33	1.37
3	L5	3818	UY1	C2-N1	-2.23	1.33	1.36
1	S2	1288	OMU	C5-C4	-2.23	1.38	1.43
3	L5	4498	OMU	C5-C4	-2.23	1.38	1.43
3	L5	4361	PSU	C2-N1	-2.23	1.33	1.36
3	L5	2364	OMG	C5-N7	-2.23	1.34	1.39
1	S2	686	PSU	C2-N3	-2.23	1.33	1.37
3	L5	2839	PSU	C2-N3	-2.22	1.33	1.37
1	S2	681	PSU	C2-N3	-2.22	1.33	1.37
1	S2	814	PSU	C2-N3	-2.22	1.33	1.37
3	L5	1744	PSU	C2-N1	-2.22	1.33	1.36
1	S2	512	A2M	C4-N9	-2.22	1.33	1.37
3	L5	4689	PSU	C2-N3	-2.22	1.33	1.37
3	L5	4312	PSU	C2-N3	-2.22	1.33	1.37
1	S2	601	OMG	C5-N7	-2.22	1.34	1.39
3	L5	1779	PSU	C2-N3	-2.21	1.33	1.37
3	L5	4552	PSU	C2-N3	-2.21	1.33	1.37
3	L5	4228	OMG	C4-N9	-2.21	1.32	1.38
1	S2	159	A2M	C4-N9	-2.21	1.33	1.37
3	L5	2508	PSU	C2-N3	-2.21	1.33	1.37
3	L5	4431	PSU	C2-N3	-2.20	1.33	1.37
84	At	32	PSU	C2'-C1'	-2.20	1.50	1.53
1	S2	1643	PSU	C2-N1	-2.20	1.33	1.36
1	S2	1232	PSU	C2-N1	-2.20	1.33	1.36
3	L5	3853	PSU	C2-N1	-2.20	1.33	1.36
1	S2	822	PSU	C2-N3	-2.20	1.33	1.37
84	At	8	4SU	C2-N3	-2.20	1.34	1.38
3	L5	1326	A2M	C5-C6	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3729	PSU	C2-N3	-2.19	1.33	1.37
3	L5	3785	A2M	C8-N7	2.19	1.35	1.31
3	L5	1862	PSU	C2-N1	-2.19	1.33	1.36
3	L5	1781	PSU	C2-N3	-2.19	1.33	1.37
3	L5	4299	PSU	C2-N3	-2.19	1.33	1.37
1	S2	109	PSU	C2-N3	-2.19	1.33	1.37
3	L5	3768	PSU	C2-N3	-2.19	1.33	1.37
3	L5	4228	OMG	C5-N7	-2.19	1.34	1.39
1	S2	576	A2M	C4-N9	-2.18	1.33	1.37
1	S2	866	PSU	C2-N3	-2.18	1.33	1.37
1	S2	484	A2M	C4-N9	-2.18	1.33	1.37
85	Pt	33	OMC	C6-N1	-2.18	1.32	1.38
1	S2	99	A2M	C4-N9	-2.18	1.33	1.37
3	L5	4196	OMG	C4-N9	-2.18	1.32	1.38
3	L5	3944	OMG	C5-N7	-2.18	1.34	1.39
2	L8	69	PSU	C2'-C1'	-2.17	1.50	1.53
3	L5	3627	OMG	C5-N7	-2.17	1.34	1.39
1	S2	34	PSU	C2-N3	-2.17	1.33	1.37
3	L5	1782	PSU	C2-N3	-2.17	1.33	1.37
3	L5	2815	A2M	C4-N9	-2.17	1.33	1.37
1	S2	1692	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4620	OMU	C5-C4	-2.16	1.39	1.43
3	L5	4293	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4403	PSU	C2'-C1'	-2.16	1.50	1.53
1	S2	867	OMG	C5-N7	-2.16	1.34	1.39
3	L5	3695	PSU	C2-N3	-2.16	1.33	1.37
1	S2	1004	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4296	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4569	PSU	C2-N3	-2.16	1.33	1.37
3	L5	4618	OMG	C4-N9	-2.16	1.32	1.38
1	S2	1239	PSU	C2-N3	-2.15	1.33	1.37
3	L5	2351	OMC	C5-C4	-2.15	1.37	1.42
1	S2	105	PSU	C2-N1	-2.15	1.33	1.36
3	L5	1683	PSU	C2-N1	-2.15	1.33	1.36
84	At	32	PSU	C2-N3	-2.15	1.33	1.37
1	S2	1804	OMU	C5-C4	-2.14	1.39	1.43
3	L5	3925	OMU	C5-C4	-2.14	1.39	1.43
3	L5	3851	PSU	C2-N1	-2.14	1.33	1.36
3	L5	4392	OMG	C4-N9	-2.14	1.32	1.38
3	L5	4972	PSU	C2-N3	-2.13	1.34	1.37
1	S2	27	A2M	C4-N9	-2.13	1.33	1.37
3	L5	2363	A2M	C4-N9	-2.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3768	PSU	C2-N1	-2.12	1.33	1.36
1	S2	119	PSU	C2-N1	-2.12	1.33	1.36
3	L5	3830	A2M	C8-N7	2.12	1.35	1.31
3	L5	3920	PSU	C2-N3	-2.12	1.34	1.37
3	L5	4637	OMG	C4-N9	-2.12	1.32	1.38
84	At	39	PSU	C2-N1	-2.12	1.33	1.36
1	S2	428	OMU	C5-C4	-2.12	1.39	1.43
1	S2	1337	4AC	C7-N4	-2.12	1.32	1.37
3	L5	3639	PSU	C2-N1	-2.12	1.33	1.36
3	L5	4227	OMU	C5-C4	-2.12	1.39	1.43
3	L5	1582	PSU	C2-N1	-2.12	1.33	1.36
3	L5	4628	PSU	C2-N3	-2.12	1.34	1.37
3	L5	4579	PSU	C6-N1	-2.11	1.32	1.36
3	L5	4293	PSU	C2-N1	-2.11	1.33	1.36
1	S2	683	OMG	C5-N7	-2.11	1.34	1.39
3	L5	3734	PSU	C2-N1	-2.11	1.33	1.36
1	S2	1031	A2M	C8-N7	2.11	1.35	1.31
1	S2	509	OMG	C4-N9	-2.11	1.32	1.38
1	S2	1056	PSU	C2-N3	-2.10	1.34	1.37
1	S2	651	PSU	C2-N3	-2.10	1.34	1.37
1	S2	576	A2M	C8-N7	2.10	1.35	1.31
1	S2	406	PSU	C2'-C1'	-2.10	1.50	1.53
1	S2	644	OMG	C4-N9	-2.10	1.32	1.38
1	S2	801	PSU	C2-N1	-2.10	1.33	1.36
3	L5	3830	A2M	C4-N9	-2.09	1.33	1.37
3	L5	4420	PSU	C2-N1	-2.09	1.33	1.36
3	L5	4579	PSU	C2'-C1'	-2.09	1.50	1.53
3	L5	2401	A2M	C8-N9	-2.09	1.34	1.37
3	L5	4576	PSU	C2-N3	-2.09	1.34	1.37
3	L5	4523	A2M	C4-N9	-2.09	1.33	1.37
2	L8	55	PSU	C2-N3	-2.09	1.34	1.37
1	S2	99	A2M	C5-C6	2.08	1.46	1.41
3	L5	4590	A2M	C8-N7	2.08	1.35	1.31
3	L5	1871	A2M	C5-C6	2.08	1.46	1.41
1	S2	1367	PSU	C2-N3	-2.08	1.34	1.37
1	S2	1136	PSU	C2-N3	-2.08	1.34	1.37
3	L5	1524	A2M	C4-N9	-2.08	1.33	1.37
3	L5	4636	PSU	C2-N1	-2.08	1.34	1.36
3	L5	2787	A2M	C8-N7	2.08	1.35	1.31
3	L5	1677	PSU	C2-N3	-2.08	1.34	1.37
3	L5	400	A2M	C4-N9	-2.07	1.33	1.37
3	L5	4220	6MZ	C4-N9	-2.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	36	PSU	C2-N3	-2.07	1.34	1.37
3	L5	400	A2M	C8-N7	2.07	1.35	1.31
3	L5	3744	OMG	C4-N9	-2.07	1.32	1.38
3	L5	4493	PSU	C2-N1	-2.07	1.34	1.36
3	L5	1871	A2M	C8-N9	-2.06	1.34	1.37
3	L5	3627	OMG	C4-N9	-2.06	1.32	1.38
3	L5	2839	PSU	C2-N1	-2.06	1.34	1.36
1	S2	484	A2M	C8-N9	-2.06	1.34	1.37
3	L5	4312	PSU	C2-N1	-2.05	1.34	1.36
1	S2	572	PSU	C2-N1	-2.05	1.34	1.36
3	L5	3760	A2M	C4-N9	-2.05	1.33	1.37
2	L8	14	OMU	C6-N1	-2.05	1.33	1.38
3	L5	5010	PSU	C2-N3	-2.05	1.34	1.37
1	S2	172	OMU	C6-N1	-2.05	1.33	1.38
2	L8	75	OMG	C5-N7	-2.04	1.35	1.39
3	L5	1781	PSU	C2-N1	-2.04	1.34	1.36
3	L5	3869	OMC	C6-N1	-2.04	1.33	1.38
3	L5	1536	PSU	C2-N1	-2.04	1.34	1.36
3	L5	4361	PSU	C2'-C1'	-2.04	1.51	1.53
1	S2	1081	PSU	C2-N1	-2.04	1.34	1.36
1	S2	683	OMG	C4-N9	-2.04	1.32	1.38
1	S2	1692	PSU	C2-N1	-2.03	1.34	1.36
3	L5	1534	A2M	C4-N9	-2.03	1.33	1.37
1	S2	1238	PSU	C2-N3	-2.03	1.34	1.37
1	S2	1832	6MZ	C4-N9	-2.03	1.33	1.37
1	S2	166	A2M	C8-N7	2.03	1.35	1.31
1	S2	1177	PSU	C2-N1	-2.03	1.34	1.36
3	L5	1524	A2M	C8-N7	2.03	1.35	1.31
1	S2	1177	PSU	C2-N3	-2.03	1.34	1.37
3	L5	1522	OMG	C4-N9	-2.02	1.32	1.38
1	S2	296	PSU	C2'-C1'	-2.02	1.51	1.53
3	L5	4494	OMG	C4-N9	-2.02	1.32	1.38
1	S2	1851	MA6	C8-N7	2.02	1.35	1.31
1	S2	815	PSU	C2-N3	-2.02	1.34	1.37
3	L5	2415	OMU	C6-N1	-2.01	1.33	1.38
3	L5	2363	A2M	C8-N7	2.01	1.35	1.31
3	L5	1534	A2M	C8-N7	2.01	1.35	1.31
3	L5	4456	OMC	C6-N1	-2.01	1.33	1.38
84	At	37	MIA	C8-N7	2.00	1.35	1.31
3	L5	4423	PSU	C2-N3	-2.00	1.34	1.37
1	S2	1004	PSU	C2-N1	-2.00	1.34	1.36
1	S2	590	A2M	C4-N9	-2.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1490	OMG	C4-N9	-2.00	1.33	1.38
1	S2	1832	6MZ	C8-N7	2.00	1.35	1.31
3	L5	3899	OMG	C4-N9	-2.00	1.33	1.38

All (1167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-N	-10.15	104.04	121.98
84	At	37	MIA	C12-C13-C14	-8.54	111.69	127.01
1	S2	1639	G7M	CN7-N7-C8	-7.96	112.73	124.79
66	Lr	2	SAC	OAC-C1A-N	-7.85	108.10	121.98
3	L5	4628	PSU	N1-C2-N3	7.70	123.29	115.17
3	L5	4636	PSU	N1-C2-N3	7.53	123.11	115.17
29	SV	1	AME	OT-CT1-N	-7.48	108.76	121.98
84	At	37	MIA	C5-C4-N3	-7.45	119.33	127.18
2	L8	69	PSU	N1-C2-N3	7.38	122.95	115.17
66	Lr	2	SAC	OAC-C1A-C2A	-7.30	109.05	122.05
1	S2	1174	PSU	N1-C2-N3	7.23	122.80	115.17
1	S2	1056	PSU	N1-C2-N3	7.16	122.72	115.17
3	L5	4442	PSU	N1-C2-N3	7.13	122.69	115.17
1	S2	918	PSU	N1-C2-N3	7.10	122.66	115.17
1	S2	1232	PSU	N1-C2-N3	7.10	122.65	115.17
3	L5	4530	UR3	C4-N3-C2	-7.07	118.89	124.58
84	At	8	4SU	C4-N3-C2	-7.05	120.56	127.31
1	S2	105	PSU	N1-C2-N3	7.04	122.60	115.17
1	S2	686	PSU	N1-C2-N3	7.01	122.56	115.17
1	S2	1639	G7M	N9-C4-N3	6.98	139.90	125.95
3	L5	4403	PSU	N1-C2-N3	6.97	122.52	115.17
3	L5	1862	PSU	N1-C2-N3	6.97	122.52	115.17
1	S2	822	PSU	N1-C2-N3	6.96	122.51	115.17
3	L5	4353	PSU	N1-C2-N3	6.93	122.47	115.17
3	L5	4569	PSU	N1-C2-N3	6.92	122.47	115.17
3	L5	3637	PSU	N1-C2-N3	6.91	122.45	115.17
3	L5	4579	PSU	N1-C2-N3	6.91	122.45	115.17
1	S2	866	PSU	N1-C2-N3	6.90	122.45	115.17
29	SV	1	AME	OT-CT1-CT2	-6.90	109.76	122.05
1	S2	93	PSU	N1-C2-N3	6.88	122.43	115.17
1	S2	109	PSU	N1-C2-N3	6.87	122.42	115.17
1	S2	1639	G7M	N9-C8-N7	-6.85	95.85	112.48
1	S2	1244	PSU	N1-C2-N3	6.84	122.38	115.17
3	L5	4532	PSU	N1-C2-N3	6.83	122.38	115.17
1	S2	573	PSU	N1-C2-N3	6.80	122.34	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1243	PSU	N1-C2-N3	6.79	122.33	115.17
3	L5	3768	PSU	N1-C2-N3	6.76	122.30	115.17
6	SA	2	SAC	OAC-C1A-C2A	-6.73	110.08	122.05
1	S2	1326	UY1	N1-C2-N3	6.72	122.26	115.17
84	At	39	PSU	N1-C2-N3	6.71	122.25	115.17
3	L5	4293	PSU	N1-C2-N3	6.71	122.25	115.17
3	L5	3764	PSU	N1-C2-N3	6.71	122.25	115.17
3	L5	4361	PSU	N1-C2-N3	6.69	122.23	115.17
3	L5	3770	PSU	N1-C2-N3	6.69	122.22	115.17
84	At	32	PSU	N1-C2-N3	6.69	122.22	115.17
1	S2	36	PSU	N1-C2-N3	6.67	122.21	115.17
1	S2	815	PSU	N1-C2-N3	6.67	122.21	115.17
3	L5	1779	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	3729	PSU	N1-C2-N3	6.67	122.20	115.17
3	L5	1860	PSU	N1-C2-N3	6.67	122.20	115.17
1	S2	1347	PSU	N1-C2-N3	6.66	122.19	115.17
3	L5	2876	OMG	C5-C4-N3	-6.66	117.79	128.39
1	S2	218	PSU	N1-C2-N3	6.64	122.17	115.17
1	S2	296	PSU	N1-C2-N3	6.63	122.16	115.17
1	S2	1625	PSU	N1-C2-N3	6.62	122.16	115.17
1	S2	1367	PSU	N1-C2-N3	6.62	122.15	115.17
3	L5	4552	PSU	N1-C2-N3	6.61	122.14	115.17
3	L5	4521	PSU	N1-C2-N3	6.60	122.13	115.17
1	S2	814	PSU	N1-C2-N3	6.59	122.12	115.17
1	S2	649	PSU	N1-C2-N3	6.59	122.12	115.17
3	L5	4972	PSU	N1-C2-N3	6.58	122.11	115.17
3	L5	2424	OMG	C5-C4-N3	-6.58	117.91	128.39
3	L5	3734	PSU	N1-C2-N3	6.58	122.11	115.17
3	L5	3639	PSU	N1-C2-N3	6.57	122.10	115.17
2	L8	55	PSU	N1-C2-N3	6.57	122.10	115.17
3	L5	5010	PSU	N1-C2-N3	6.57	122.09	115.17
3	L5	2508	PSU	N1-C2-N3	6.56	122.09	115.17
3	L5	4531	PSU	N1-C2-N3	6.56	122.09	115.17
3	L5	4312	PSU	N1-C2-N3	6.55	122.08	115.17
3	L5	4576	PSU	N1-C2-N3	6.55	122.07	115.17
3	L5	3920	PSU	N1-C2-N3	6.55	122.07	115.17
3	L5	1744	PSU	N1-C2-N3	6.54	122.07	115.17
1	S2	1445	PSU	N1-C2-N3	6.52	122.05	115.17
1	S2	966	PSU	N1-C2-N3	6.52	122.05	115.17
3	L5	2843	PSU	N1-C2-N3	6.51	122.04	115.17
3	L5	3884	PSU	N1-C2-N3	6.51	122.03	115.17
1	S2	406	PSU	N1-C2-N3	6.50	122.03	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4299	PSU	N1-C2-N3	6.50	122.03	115.17
3	L5	4457	PSU	N1-C2-N3	6.50	122.03	115.17
1	S2	34	PSU	N1-C2-N3	6.50	122.03	115.17
1	S2	1639	G7M	C8-N7-C5	6.50	115.91	107.78
3	L5	1677	PSU	N1-C2-N3	6.49	122.02	115.17
85	Pt	8	4SU	C4-N3-C2	-6.49	121.09	127.31
3	L5	2839	PSU	N1-C2-N3	6.48	122.01	115.17
3	L5	4500	PSU	N1-C2-N3	6.48	122.01	115.17
3	L5	3762	PSU	N1-C2-N3	6.47	122.00	115.17
3	L5	3715	PSU	N1-C2-N3	6.47	121.99	115.17
3	L5	1792	PSU	N1-C2-N3	6.46	121.98	115.17
3	L5	4689	PSU	N1-C2-N3	6.46	121.98	115.17
1	S2	1238	PSU	N1-C2-N3	6.46	121.98	115.17
3	L5	4423	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	3844	PSU	N1-C2-N3	6.44	121.96	115.17
3	L5	3851	PSU	N1-C2-N3	6.43	121.96	115.17
1	S2	609	PSU	N1-C2-N3	6.43	121.95	115.17
1	S2	681	PSU	N1-C2-N3	6.43	121.95	115.17
3	L5	4493	PSU	N1-C2-N3	6.42	121.94	115.17
3	L5	4296	PSU	N1-C2-N3	6.40	121.92	115.17
1	S2	1328	OMG	C5-C4-N3	-6.40	118.21	128.39
1	S2	651	PSU	N1-C2-N3	6.39	121.91	115.17
1	S2	1177	PSU	N1-C2-N3	6.38	121.90	115.17
3	L5	1536	PSU	N1-C2-N3	6.38	121.90	115.17
3	L5	3758	PSU	N1-C2-N3	6.38	121.89	115.17
1	S2	1081	PSU	N1-C2-N3	6.37	121.89	115.17
3	L5	1781	PSU	N1-C2-N3	6.36	121.88	115.17
1	S2	1004	PSU	N1-C2-N3	6.35	121.87	115.17
3	L5	1625	OMG	C5-C4-N3	-6.34	118.29	128.39
85	Pt	56	PSU	N1-C2-N3	6.34	121.86	115.17
85	Pt	8	4SU	C5-C4-N3	6.34	120.65	114.75
1	S2	436	OMG	C5-C4-N3	-6.34	118.31	128.39
3	L5	1782	PSU	N1-C2-N3	6.34	121.85	115.17
3	L5	3792	OMG	C5-C4-N3	-6.33	118.32	128.39
1	S2	1692	PSU	N1-C2-N3	6.32	121.84	115.17
3	L5	1582	PSU	N1-C2-N3	6.32	121.84	115.17
1	S2	1239	PSU	N1-C2-N3	6.32	121.83	115.17
3	L5	3695	PSU	N1-C2-N3	6.31	121.82	115.17
3	L5	5001	PSU	N1-C2-N3	6.31	121.82	115.17
3	L5	4673	PSU	N1-C2-N3	6.30	121.81	115.17
1	S2	863	PSU	N1-C2-N3	6.30	121.81	115.17
3	L5	1683	PSU	N1-C2-N3	6.28	121.80	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4471	PSU	N1-C2-N3	6.25	121.77	115.17
1	S2	1136	PSU	N1-C2-N3	6.24	121.75	115.17
3	L5	2632	PSU	N1-C2-N3	6.22	121.73	115.17
1	S2	1490	OMG	C5-C4-N3	-6.19	118.53	128.39
3	L5	3818	UY1	N1-C2-N3	6.19	121.70	115.17
1	S2	801	PSU	N1-C2-N3	6.19	121.69	115.17
1	S2	1447	OMG	C5-C4-N3	-6.18	118.56	128.39
3	L5	4370	OMG	C5-C4-N3	-6.18	118.56	128.39
3	L5	3853	PSU	N1-C2-N3	6.17	121.67	115.17
3	L5	4431	PSU	N1-C2-N3	6.15	121.66	115.17
1	S2	166	A2M	C5-C4-N3	-6.15	118.24	126.72
1	S2	509	OMG	C5-C4-N3	-6.14	118.62	128.39
1	S2	119	PSU	N1-C2-N3	6.11	121.62	115.17
2	L8	75	OMG	C5-C4-N3	-6.10	118.68	128.39
1	S2	867	OMG	C5-C4-N3	-6.09	118.70	128.39
1	S2	590	A2M	C5-C4-N3	-6.08	118.34	126.72
3	L5	4392	OMG	C5-C4-N3	-6.08	118.71	128.39
3	L5	1316	OMG	C5-C4-N3	-6.08	118.72	128.39
3	L5	4523	A2M	C5-C4-N3	-6.08	118.35	126.72
3	L5	3899	OMG	C5-C4-N3	-6.06	118.74	128.39
3	L5	3744	OMG	C5-C4-N3	-6.06	118.75	128.39
3	L5	4420	PSU	N1-C2-N3	6.04	121.54	115.17
1	S2	644	OMG	C5-C4-N3	-6.03	118.80	128.39
3	L5	4637	OMG	C5-C4-N3	-6.01	118.83	128.39
3	L5	4196	OMG	C5-C4-N3	-6.00	118.83	128.39
1	S2	601	OMG	C5-C4-N3	-6.00	118.85	128.39
1	S2	484	A2M	C5-C4-N3	-5.97	118.50	126.72
3	L5	1524	A2M	C5-C4-N3	-5.96	118.51	126.72
3	L5	2364	OMG	C5-C4-N3	-5.95	118.92	128.39
3	L5	4571	A2M	C5-C4-N3	-5.93	118.55	126.72
84	At	8	4SU	C5-C4-N3	5.93	120.27	114.75
3	L5	2401	A2M	C5-C4-N3	-5.91	118.58	126.72
3	L5	4618	OMG	C5-C4-N3	-5.90	118.99	128.39
1	S2	27	A2M	C5-C4-N3	-5.90	118.59	126.72
3	L5	4220	6MZ	C5-C4-N3	-5.90	118.59	126.72
3	L5	4494	OMG	C5-C4-N3	-5.90	119.01	128.39
3	L5	2815	A2M	C5-C4-N3	-5.89	118.61	126.72
1	S2	99	A2M	C5-C4-N3	-5.89	118.61	126.72
3	L5	2363	A2M	C5-C4-N3	-5.88	118.62	126.72
1	S2	1643	PSU	N1-C2-N3	5.88	121.37	115.17
84	At	37	MIA	N3-C4-N9	5.87	134.44	126.99
3	L5	4499	OMG	C5-C4-N3	-5.86	119.06	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3627	OMG	C5-C4-N3	-5.84	119.10	128.39
1	S2	572	PSU	N1-C2-N3	5.83	121.31	115.17
3	L5	3944	OMG	C5-C4-N3	-5.83	119.12	128.39
3	L5	1522	OMG	C5-C4-N3	-5.82	119.13	128.39
3	L5	1534	A2M	C5-C4-N3	-5.80	118.72	126.72
3	L5	3867	A2M	C5-C4-N3	-5.80	118.73	126.72
3	L5	398	A2M	C5-C4-N3	-5.78	118.76	126.72
3	L5	2787	A2M	C5-C4-N3	-5.77	118.77	126.72
1	S2	1832	6MZ	C5-C4-N3	-5.75	118.80	126.72
1	S2	1447	OMG	C2-N3-C4	5.73	122.17	112.30
3	L5	400	A2M	C5-C4-N3	-5.72	118.84	126.72
1	S2	1639	G7M	C5-C4-N3	-5.72	117.35	128.15
1	S2	683	OMG	C5-C4-N3	-5.70	119.31	128.39
1	S2	512	A2M	C5-C4-N3	-5.66	118.93	126.72
1	S2	1678	A2M	C5-C4-N3	-5.65	118.93	126.72
3	L5	3830	A2M	C5-C4-N3	-5.65	118.94	126.72
1	S2	159	A2M	C5-C4-N3	-5.62	118.98	126.72
3	L5	1326	A2M	C5-C4-N3	-5.59	119.03	126.72
1	S2	1031	A2M	C5-C4-N3	-5.58	119.03	126.72
3	L5	3760	A2M	C5-C4-N3	-5.56	119.06	126.72
3	L5	4590	A2M	C5-C4-N3	-5.50	119.14	126.72
3	L5	4228	OMG	C5-C4-N3	-5.50	119.64	128.39
3	L5	3785	A2M	C5-C4-N3	-5.48	119.17	126.72
3	L5	3724	A2M	C5-C4-N3	-5.47	119.19	126.72
3	L5	4623	OMG	C5-C4-N3	-5.46	119.70	128.39
1	S2	1248	B8N	C4-N3-C2	-5.40	118.97	125.62
3	L5	3825	A2M	C5-C4-N3	-5.39	119.30	126.72
2	L8	75	OMG	C2-N3-C4	5.38	121.56	112.30
1	S2	468	A2M	C5-C4-N3	-5.36	119.33	126.72
1	S2	1383	A2M	C5-C4-N3	-5.36	119.34	126.72
1	S2	436	OMG	C2-N3-C4	5.36	121.53	112.30
1	S2	1851	MA6	C5-C4-N3	-5.36	119.34	126.72
3	L5	1871	A2M	C5-C4-N3	-5.32	119.39	126.72
2	L8	14	OMU	C4-N3-C2	-5.30	120.03	126.61
1	S2	576	A2M	C5-C4-N3	-5.24	119.50	126.72
1	S2	627	OMU	C4-N3-C2	-5.19	120.17	126.61
1	S2	668	A2M	C5-C4-N3	-5.18	119.58	126.72
1	S2	867	OMG	C2-N3-C4	5.17	121.20	112.30
1	S2	1328	OMG	C2-N3-C4	5.17	121.20	112.30
3	L5	4196	OMG	C2-N3-C4	5.17	121.20	112.30
3	L5	3723	A2M	C5-C4-N3	-5.17	119.60	126.72
3	L5	4392	OMG	C2-N3-C4	5.16	121.19	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3744	OMG	C2-N3-C4	5.16	121.18	112.30
3	L5	2876	OMG	C2-N3-C4	5.15	121.17	112.30
3	L5	3792	OMG	C2-N3-C4	5.14	121.16	112.30
1	S2	683	OMG	C2-N3-C4	5.12	121.12	112.30
3	L5	4370	OMG	C2-N3-C4	5.10	121.08	112.30
3	L5	3627	OMG	C2-N3-C4	5.09	121.07	112.30
1	S2	601	OMG	C2-N3-C4	5.08	121.05	112.30
1	S2	1850	MA6	C5-C4-N3	-5.08	119.72	126.72
3	L5	3899	OMG	C2-N3-C4	5.07	121.03	112.30
1	S2	1490	OMG	C2-N3-C4	5.06	121.02	112.30
3	L5	2837	OMU	C4-N3-C2	-5.03	120.36	126.61
3	L5	3718	A2M	C5-C4-N3	-5.03	119.79	126.72
1	S2	99	A2M	N3-C4-N9	5.03	135.72	127.17
1	S2	1804	OMU	C4-N3-C2	-5.02	120.38	126.61
3	L5	4499	OMG	C2-N3-C4	5.01	120.93	112.30
3	L5	4618	OMG	C2-N3-C4	5.01	120.93	112.30
1	S2	354	OMU	C4-N3-C2	-5.00	120.40	126.61
3	L5	2364	OMG	C2-N3-C4	5.00	120.92	112.30
3	L5	1522	OMG	C2-N3-C4	5.00	120.92	112.30
3	L5	4498	OMU	C4-N3-C2	-5.00	120.41	126.61
1	S2	644	OMG	C2-N3-C4	4.99	120.90	112.30
3	L5	1625	OMG	C2-N3-C4	4.99	120.89	112.30
3	L5	2876	OMG	N9-C4-N3	4.99	135.92	125.95
3	L5	4623	OMG	C2-N3-C4	4.97	120.86	112.30
3	L5	1316	OMG	C2-N3-C4	4.97	120.85	112.30
3	L5	3944	OMG	C2-N3-C4	4.95	120.83	112.30
3	L5	1625	OMG	N9-C4-N3	4.95	135.85	125.95
1	S2	590	A2M	N3-C4-N9	4.95	135.58	127.17
3	L5	4571	A2M	N3-C4-N9	4.95	135.58	127.17
3	L5	2424	OMG	N9-C4-N3	4.93	135.82	125.95
84	At	37	MIA	C11-S10-C2	-4.93	98.55	102.25
3	L5	3867	A2M	N3-C4-N9	4.93	135.55	127.17
3	L5	4636	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L5	4523	A2M	N3-C4-N9	4.91	135.53	127.17
1	S2	166	A2M	N3-C4-N9	4.91	135.52	127.17
3	L5	4494	OMG	C2-N3-C4	4.91	120.76	112.30
3	L5	4637	OMG	C2-N3-C4	4.91	120.75	112.30
3	L5	3925	OMU	C4-N3-C2	-4.90	120.53	126.61
1	S2	172	OMU	C4-N3-C2	-4.90	120.53	126.61
3	L5	4227	OMU	C4-N3-C2	-4.90	120.53	126.61
3	L5	3637	PSU	C4-N3-C2	-4.88	119.65	126.37
3	L5	2815	A2M	N3-C4-N9	4.88	135.46	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	428	OMU	C4-N3-C2	-4.86	120.58	126.61
3	L5	3792	OMG	N9-C4-N3	4.84	135.62	125.95
3	L5	4228	OMG	C2-N3-C4	4.82	120.61	112.30
1	S2	436	OMG	N9-C4-N3	4.82	135.59	125.95
3	L5	4220	6MZ	N3-C4-N9	4.81	135.35	127.17
6	SA	2	SAC	C-CA-N	-4.81	100.22	109.50
1	S2	1326	UY1	C4-N3-C2	-4.79	119.78	126.37
1	S2	1442	OMU	C4-N3-C2	-4.78	120.68	126.61
1	S2	509	OMG	C2-N3-C4	4.77	120.52	112.30
3	L5	1524	A2M	N3-C4-N9	4.75	135.25	127.17
3	L5	2401	A2M	N3-C4-N9	4.75	135.25	127.17
3	L5	2415	OMU	C4-N3-C2	-4.75	120.72	126.61
3	L5	2424	OMG	C2-N3-C4	4.75	120.48	112.30
1	S2	484	A2M	N3-C4-N9	4.71	135.18	127.17
3	L5	4620	OMU	N3-C2-N1	4.67	120.97	114.89
3	L5	1322	1MA	C5-C4-N3	-4.66	120.41	127.27
2	L8	14	OMU	C5-C4-N3	4.65	121.32	114.80
3	L5	4628	PSU	O2-C2-N1	-4.65	117.99	122.79
3	L5	1534	A2M	N3-C4-N9	4.65	135.07	127.17
3	L5	1326	A2M	N3-C4-N9	4.63	135.04	127.17
1	S2	1244	PSU	C4-N3-C2	-4.62	120.00	126.37
3	L5	400	A2M	N3-C4-N9	4.62	135.02	127.17
84	At	32	PSU	C4-N3-C2	-4.61	120.02	126.37
1	S2	218	PSU	C4-N3-C2	-4.61	120.02	126.37
1	S2	27	A2M	N3-C4-N9	4.61	135.00	127.17
3	L5	4370	OMG	N9-C4-N3	4.60	135.16	125.95
3	L5	2363	A2M	N3-C4-N9	4.60	134.99	127.17
3	L5	1582	PSU	C4-N3-C2	-4.60	120.04	126.37
2	L8	75	OMG	N9-C4-N3	4.60	135.15	125.95
1	S2	512	A2M	N3-C4-N9	4.60	134.98	127.17
3	L5	3785	A2M	O4'-C1'-N9	4.59	116.91	108.09
1	S2	105	PSU	C4-N3-C2	-4.59	120.04	126.37
1	S2	1056	PSU	C4-N3-C2	-4.57	120.07	126.37
1	S2	1328	OMG	N9-C4-N3	4.57	135.09	125.95
1	S2	93	PSU	C4-N3-C2	-4.56	120.09	126.37
1	S2	867	OMG	N9-C4-N3	4.56	135.06	125.95
1	S2	509	OMG	N9-C4-N3	4.54	135.02	125.95
3	L5	4442	PSU	C4-N3-C2	-4.53	120.13	126.37
2	L8	69	PSU	C4-N3-C2	-4.53	120.14	126.37
3	L5	4196	OMG	N9-C4-N3	4.52	135.00	125.95
1	S2	681	PSU	C4-N3-C2	-4.52	120.15	126.37
3	L5	4637	OMG	N9-C4-N3	4.52	134.99	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	121	OMU	C4-N3-C2	-4.51	121.02	126.61
3	L5	3830	A2M	N3-C4-N9	4.51	134.83	127.17
85	Pt	47	G7M	N9-C8-N7	-4.51	101.54	112.48
1	S2	121	OMU	N3-C2-N1	4.49	120.73	114.89
1	S2	1678	A2M	N3-C4-N9	4.48	134.79	127.17
1	S2	822	PSU	C4-N3-C2	-4.48	120.20	126.37
3	L5	1316	OMG	N9-C4-N3	4.48	134.91	125.95
3	L5	3639	PSU	C4-N3-C2	-4.48	120.20	126.37
3	L5	2364	OMG	N9-C4-N3	4.48	134.91	125.95
3	L5	2787	A2M	N3-C4-N9	4.48	134.78	127.17
3	L5	3830	A2M	C2'-C1'-N9	-4.47	106.40	113.75
3	L5	4494	OMG	N9-C4-N3	4.47	134.88	125.95
3	L5	3899	OMG	N9-C4-N3	4.46	134.88	125.95
3	L5	4403	PSU	C4-N3-C2	-4.46	120.23	126.37
3	L5	4306	OMU	C4-N3-C2	-4.45	121.09	126.61
3	L5	4628	PSU	C4-N3-C2	-4.44	120.25	126.37
1	S2	354	OMU	N3-C2-N1	4.44	120.67	114.89
1	S2	644	OMG	N9-C4-N3	4.43	134.82	125.95
1	S2	1639	G7M	C8-N9-C4	4.43	118.07	107.09
1	S2	1832	6MZ	N3-C4-N9	4.43	134.69	127.17
3	L5	3760	A2M	N3-C4-N9	4.42	134.69	127.17
29	SV	1	AME	CT2-CT1-N	-4.42	108.78	116.12
3	L5	4498	OMU	N3-C2-N1	4.42	120.64	114.89
3	L5	2843	PSU	C4-N3-C2	-4.41	120.29	126.37
3	L5	1862	PSU	C4-N3-C2	-4.41	120.29	126.37
1	S2	36	PSU	C4-N3-C2	-4.41	120.29	126.37
1	S2	1850	MA6	C2-N1-C6	4.41	122.60	111.83
1	S2	1639	G7M	C2-N3-C4	4.41	119.89	112.30
3	L5	1322	1MA	C2-N3-C4	4.41	121.17	112.53
3	L5	4532	PSU	C4-N3-C2	-4.41	120.30	126.37
84	At	46	G7M	N9-C8-N7	-4.40	101.80	112.48
1	S2	296	PSU	O2-C2-N1	-4.40	118.26	122.79
1	S2	1031	A2M	N3-C4-N9	4.39	134.64	127.17
1	S2	1625	PSU	C4-N3-C2	-4.39	120.32	126.37
85	Pt	8	4SU	C5-C4-S4	-4.39	119.29	124.31
1	S2	601	OMG	N9-C4-N3	4.39	134.73	125.95
3	L5	5001	PSU	C4-N3-C2	-4.39	120.33	126.37
1	S2	296	PSU	C4-N3-C2	-4.39	120.33	126.37
3	L5	4972	PSU	C4-N3-C2	-4.39	120.33	126.37
1	S2	119	PSU	C4-N3-C2	-4.38	120.33	126.37
1	S2	1490	OMG	N9-C4-N3	4.38	134.72	125.95
3	L5	398	A2M	N3-C4-N9	4.38	134.62	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1288	OMU	C4-N3-C2	-4.38	121.17	126.61
3	L5	4296	PSU	C4-N3-C2	-4.38	120.34	126.37
1	S2	166	A2M	C2'-C1'-N9	-4.38	106.55	113.75
1	S2	814	PSU	C4-N3-C2	-4.37	120.35	126.37
1	S2	866	PSU	C4-N3-C2	-4.37	120.35	126.37
3	L5	4590	A2M	N3-C4-N9	4.37	134.60	127.17
2	L8	14	OMU	N3-C2-N1	4.37	120.58	114.89
3	L5	2837	OMU	N3-C2-N1	4.37	120.58	114.89
3	L5	1871	A2M	N3-C4-N9	4.37	134.59	127.17
3	L5	4457	PSU	C4-N3-C2	-4.37	120.36	126.37
3	L5	1677	PSU	C4-N3-C2	-4.36	120.37	126.37
3	L5	3920	PSU	C4-N3-C2	-4.36	120.37	126.37
3	L5	3724	A2M	N3-C4-N9	4.35	134.57	127.17
3	L5	1779	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	4353	PSU	C4-N3-C2	-4.35	120.38	126.37
1	S2	468	A2M	N3-C4-N9	4.35	134.56	127.17
1	S2	159	A2M	N3-C4-N9	4.34	134.55	127.17
3	L5	4361	PSU	C4-N3-C2	-4.34	120.40	126.37
1	S2	1367	PSU	C4-N3-C2	-4.33	120.40	126.37
3	L5	2839	PSU	C4-N3-C2	-4.33	120.41	126.37
3	L5	4576	PSU	C4-N3-C2	-4.33	120.41	126.37
3	L5	2508	PSU	C4-N3-C2	-4.33	120.41	126.37
3	L5	3844	PSU	C4-N3-C2	-4.32	120.42	126.37
3	L5	4312	PSU	C4-N3-C2	-4.32	120.42	126.37
1	S2	172	OMU	N3-C2-N1	4.31	120.50	114.89
1	S2	1851	MA6	C2-N1-C6	4.30	122.34	111.83
3	L5	3785	A2M	N3-C4-N9	4.30	134.48	127.17
1	S2	1243	PSU	C4-N3-C2	-4.30	120.45	126.37
2	L8	55	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	34	PSU	C4-N3-C2	-4.30	120.45	126.37
1	S2	683	OMG	N9-C4-N3	4.29	134.54	125.95
3	L5	4552	PSU	C4-N3-C2	-4.29	120.46	126.37
1	S2	1288	OMU	N3-C2-N1	4.29	120.47	114.89
1	S2	1643	PSU	C4-N3-C2	-4.29	120.46	126.37
3	L5	3925	OMU	N3-C2-N1	4.29	120.47	114.89
1	S2	627	OMU	N3-C2-N1	4.29	120.47	114.89
3	L5	3770	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	4521	PSU	C4-N3-C2	-4.28	120.47	126.37
1	S2	686	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	3758	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	3851	PSU	C4-N3-C2	-4.28	120.47	126.37
3	L5	1782	PSU	C4-N3-C2	-4.28	120.48	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	C4-N3-C2	-4.28	120.48	126.37
3	L5	4499	OMG	N9-C4-N3	4.28	134.51	125.95
3	L5	4299	PSU	C4-N3-C2	-4.28	120.48	126.37
1	S2	1804	OMU	N3-C2-N1	4.28	120.46	114.89
3	L5	4431	PSU	C4-N3-C2	-4.27	120.48	126.37
3	L5	3818	UY1	C4-N3-C2	-4.27	120.48	126.37
3	L5	3723	A2M	N3-C4-N9	4.27	134.43	127.17
1	S2	1692	PSU	C4-N3-C2	-4.27	120.49	126.37
3	L5	1862	PSU	O2-C2-N1	-4.27	118.39	122.79
3	L5	3744	OMG	N9-C4-N3	4.26	134.48	125.95
3	L5	4392	OMG	N9-C4-N3	4.26	134.48	125.95
1	S2	354	OMU	C5-C4-N3	4.26	120.77	114.80
1	S2	918	PSU	C4-N3-C2	-4.25	120.51	126.37
1	S2	1239	PSU	C4-N3-C2	-4.25	120.52	126.37
3	L5	1536	PSU	C4-N3-C2	-4.24	120.53	126.37
1	S2	1238	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	4493	PSU	C4-N3-C2	-4.24	120.53	126.37
1	S2	1347	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	3944	OMG	N9-C4-N3	4.24	134.42	125.95
1	S2	651	PSU	C4-N3-C2	-4.23	120.55	126.37
3	L5	3729	PSU	C4-N3-C2	-4.22	120.55	126.37
3	L5	1744	PSU	C4-N3-C2	-4.22	120.56	126.37
1	S2	436	OMG	C2'-C1'-N9	-4.22	106.23	114.24
1	S2	815	PSU	C4-N3-C2	-4.21	120.57	126.37
3	L5	4618	OMG	N9-C4-N3	4.21	134.36	125.95
3	L5	4227	OMU	N3-C2-N1	4.20	120.36	114.89
3	L5	4579	PSU	C4-N3-C2	-4.20	120.58	126.37
84	At	8	4SU	C5-C4-S4	-4.20	119.51	124.31
3	L5	3627	OMG	N9-C4-N3	4.20	134.35	125.95
3	L5	3944	OMG	C2'-C1'-N9	-4.20	106.27	114.24
3	L5	4569	PSU	C4-N3-C2	-4.20	120.59	126.37
3	L5	3825	A2M	N3-C4-N9	4.19	134.30	127.17
1	S2	686	PSU	O2-C2-N1	-4.19	118.47	122.79
1	S2	1232	PSU	C4-N3-C2	-4.19	120.59	126.37
3	L5	2415	OMU	N3-C2-N1	4.19	120.35	114.89
3	L5	3762	PSU	C4-N3-C2	-4.19	120.60	126.37
84	At	39	PSU	C4-N3-C2	-4.19	120.60	126.37
1	S2	1004	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	4531	PSU	C4-N3-C2	-4.18	120.61	126.37
1	S2	1445	PSU	C4-N3-C2	-4.18	120.61	126.37
3	L5	1522	OMG	N9-C4-N3	4.18	134.31	125.95
1	S2	668	A2M	N3-C4-N9	4.17	134.26	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	8	4SU	N3-C2-N1	4.17	120.32	114.89
1	S2	1081	PSU	C4-N3-C2	-4.17	120.63	126.37
3	L5	4500	PSU	C4-N3-C2	-4.17	120.63	126.37
85	Pt	56	PSU	C4-N3-C2	-4.16	120.64	126.37
1	S2	1442	OMU	C5-C4-N3	4.16	120.63	114.80
3	L5	4306	OMU	N3-C2-N1	4.16	120.30	114.89
3	L5	4423	PSU	C4-N3-C2	-4.15	120.66	126.37
1	S2	1174	PSU	C4-N3-C2	-4.15	120.66	126.37
3	L5	4293	PSU	C4-N3-C2	-4.14	120.66	126.37
3	L5	1781	PSU	C4-N3-C2	-4.14	120.66	126.37
1	S2	109	PSU	O2-C2-N1	-4.14	118.52	122.79
1	S2	627	OMU	C5-C4-N3	4.14	120.60	114.80
1	S2	1625	PSU	O2-C2-N1	-4.14	118.52	122.79
3	L5	2415	OMU	C5-C4-N3	4.14	120.59	114.80
1	S2	649	PSU	C4-N3-C2	-4.14	120.67	126.37
3	L5	4447	5MC	C5-C6-N1	-4.13	118.82	123.31
1	S2	109	PSU	C4-N3-C2	-4.13	120.68	126.37
3	L5	3695	PSU	C4-N3-C2	-4.13	120.68	126.37
1	S2	1383	A2M	N3-C4-N9	4.13	134.19	127.17
1	S2	1177	PSU	C4-N3-C2	-4.12	120.69	126.37
1	S2	1447	OMG	N9-C4-N3	4.12	134.20	125.95
2	L8	69	PSU	O2-C2-N1	-4.12	118.54	122.79
3	L5	4620	OMU	C4-N3-C2	-4.11	121.51	126.61
1	S2	1639	G7M	C1'-N9-C8	-4.11	112.86	126.74
3	L5	3729	PSU	O2-C2-N1	-4.11	118.55	122.79
1	S2	1136	PSU	C4-N3-C2	-4.11	120.72	126.37
1	S2	573	PSU	C4-N3-C2	-4.09	120.74	126.37
3	L5	3734	PSU	C4-N3-C2	-4.09	120.74	126.37
3	L5	1860	PSU	C4-N3-C2	-4.08	120.74	126.37
1	S2	428	OMU	N3-C2-N1	4.08	120.20	114.89
3	L5	4442	PSU	O2-C2-N1	-4.08	118.58	122.79
1	S2	1804	OMU	C5-C4-N3	4.06	120.49	114.80
3	L5	3715	PSU	C4-N3-C2	-4.06	120.78	126.37
1	S2	116	OMU	N3-C2-N1	4.05	120.17	114.89
84	At	37	MIA	C15-C14-C13	-4.05	110.49	122.66
1	S2	822	PSU	O2-C2-N1	-4.05	118.61	122.79
3	L5	1792	PSU	C4-N3-C2	-4.04	120.81	126.37
3	L5	2839	PSU	O2-C2-N1	-4.04	118.63	122.79
39	LA	216	V5N	CD2-CG-ND1	4.03	111.19	105.76
1	S2	1851	MA6	N3-C4-N9	4.03	134.02	127.17
1	S2	863	PSU	C4-N3-C2	-4.03	120.82	126.37
3	L5	4228	OMG	N9-C4-N3	4.02	133.99	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4623	OMG	C6-C5-N7	4.02	137.60	130.29
1	S2	1248	B8N	C31-N3-C4	4.01	122.86	117.18
1	S2	509	OMG	C2'-C1'-N9	-4.00	106.64	114.24
3	L5	3853	PSU	C4-N3-C2	-4.00	120.86	126.37
3	L5	4227	OMU	C5-C4-N3	3.99	120.39	114.80
3	L5	3925	OMU	C5-C4-N3	3.98	120.38	114.80
1	S2	572	PSU	C4-N3-C2	-3.98	120.88	126.37
3	L5	4579	PSU	O2-C2-N1	-3.98	118.68	122.79
1	S2	1850	MA6	N3-C4-N9	3.98	133.94	127.17
3	L5	2837	OMU	C5-C4-N3	3.98	120.37	114.80
1	S2	428	OMU	C5-C4-N3	3.98	120.37	114.80
1	S2	576	A2M	C2'-C1'-N9	-3.98	107.21	113.75
3	L5	4353	PSU	O2-C2-N1	-3.97	118.69	122.79
3	L5	2632	PSU	C4-N3-C2	-3.97	120.90	126.37
84	At	37	MIA	C16-C14-C13	-3.97	110.74	122.66
1	S2	121	OMU	C5-C4-N3	3.94	120.32	114.80
3	L5	1744	PSU	O2-C2-N1	-3.94	118.73	122.79
3	L5	3762	PSU	O2-C2-N1	-3.94	118.73	122.79
3	L5	4500	PSU	O2-C2-N1	-3.93	118.73	122.79
1	S2	166	A2M	C2-N3-C4	3.93	121.44	111.83
3	L5	3718	A2M	N3-C4-N9	3.93	133.85	127.17
3	L5	4673	PSU	C4-N3-C2	-3.93	120.96	126.37
3	L5	4689	PSU	C4-N3-C2	-3.92	120.98	126.37
1	S2	1442	OMU	N3-C2-N1	3.91	119.98	114.89
1	S2	866	PSU	O2-C2-N1	-3.91	118.76	122.79
3	L5	3770	PSU	O2-C2-N1	-3.90	118.76	122.79
1	S2	576	A2M	N3-C4-N9	3.90	133.80	127.17
1	S2	649	PSU	O2-C2-N1	-3.90	118.77	122.79
1	S2	172	OMU	C5-C4-N3	3.89	120.25	114.80
3	L5	4498	OMU	C5-C4-N3	3.89	120.25	114.80
3	L5	4471	PSU	C4-N3-C2	-3.89	121.01	126.37
1	S2	590	A2M	C2-N3-C4	3.89	121.34	111.83
1	S2	1851	MA6	C4-C5-N7	-3.89	106.14	110.58
3	L5	4494	OMG	C2'-C1'-N9	-3.89	106.87	114.24
1	S2	99	A2M	C2'-C1'-N9	-3.86	107.39	113.75
3	L5	3884	PSU	C4-N3-C2	-3.85	121.06	126.37
3	L5	4431	PSU	O2-C2-N1	-3.85	118.81	122.79
3	L5	4576	PSU	O2-C2-N1	-3.85	118.82	122.79
1	S2	512	A2M	C2'-C1'-N9	-3.84	107.43	113.75
84	At	32	PSU	O2-C2-N1	-3.84	118.83	122.79
1	S2	1056	PSU	O2-C2-N1	-3.84	118.83	122.79
1	S2	801	PSU	C4-N3-C2	-3.83	121.10	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3920	PSU	O2-C2-N1	-3.82	118.85	122.79
3	L5	3768	PSU	C4-N3-C2	-3.82	121.11	126.37
1	S2	1850	MA6	C4-C5-N7	-3.82	106.22	110.58
3	L5	4299	PSU	O2-C2-N1	-3.81	118.86	122.79
1	S2	27	A2M	C2-N3-C4	3.81	121.13	111.83
3	L5	4623	OMG	N9-C4-N3	3.81	133.57	125.95
1	S2	1832	6MZ	C4-C5-N7	-3.81	106.23	110.58
1	S2	1383	A2M	C2'-C1'-N9	-3.80	107.50	113.75
3	L5	4420	PSU	O2-C2-N1	-3.80	118.87	122.79
3	L5	4590	A2M	C2'-C1'-N9	-3.80	107.50	113.75
3	L5	2401	A2M	C2-N3-C4	3.79	121.09	111.83
3	L5	4220	6MZ	C2-N3-C4	3.79	121.09	111.83
3	L5	4293	PSU	O2-C2-N1	-3.79	118.88	122.79
3	L5	4569	PSU	O2-C2-N1	-3.78	118.89	122.79
3	L5	4531	PSU	O2-C2-N1	-3.78	118.89	122.79
1	S2	1248	B8N	N3-C2-N1	3.78	121.34	116.72
1	S2	354	OMU	C2'-C1'-N1	-3.77	107.09	114.24
1	S2	1643	PSU	O2-C2-N1	-3.76	118.91	122.79
1	S2	99	A2M	C2-N3-C4	3.76	121.02	111.83
1	S2	966	PSU	C4-N3-C2	-3.76	121.19	126.37
1	S2	1136	PSU	O2-C2-N1	-3.76	118.91	122.79
1	S2	1004	PSU	O2-C2-N1	-3.75	118.92	122.79
3	L5	1524	A2M	C2-N3-C4	3.75	121.00	111.83
1	S2	406	PSU	C4-N3-C2	-3.75	121.21	126.37
1	S2	966	PSU	O2-C2-N1	-3.74	118.93	122.79
3	L5	3639	PSU	O2-C2-N1	-3.74	118.93	122.79
3	L5	4552	PSU	O2-C2-N1	-3.74	118.93	122.79
3	L5	3851	PSU	O2-C2-N1	-3.74	118.93	122.79
1	S2	1288	OMU	C5-C4-N3	3.74	120.04	114.80
1	S2	815	PSU	O2-C2-N1	-3.74	118.93	122.79
3	L5	4403	PSU	O2-C2-N1	-3.73	118.94	122.79
3	L5	2363	A2M	C2-N3-C4	3.73	120.95	111.83
3	L5	4521	PSU	O2-C2-N1	-3.73	118.94	122.79
1	S2	1337	4AC	N4-C4-N3	3.73	119.92	113.87
3	L5	1871	A2M	N3-C2-N1	-3.73	122.94	128.58
1	S2	484	A2M	C2-N3-C4	3.72	120.92	111.83
1	S2	918	PSU	O2-C2-N1	-3.72	118.95	122.79
3	L5	3785	A2M	C2-N3-C4	3.72	120.91	111.83
1	S2	1692	PSU	O2-C2-N1	-3.71	118.96	122.79
1	S2	1243	PSU	O2-C2-N1	-3.71	118.96	122.79
1	S2	1445	PSU	O2-C2-N1	-3.71	118.96	122.79
3	L5	4420	PSU	C4-N3-C2	-3.70	121.27	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1832	6MZ	C2-N3-C4	3.70	120.87	111.83
3	L5	3844	PSU	O2-C2-N1	-3.70	118.97	122.79
3	L5	4306	OMU	C5-C4-N3	3.70	119.98	114.80
1	S2	1447	OMG	C6-C5-N7	3.69	137.01	130.29
1	S2	576	A2M	C4-C5-N7	-3.69	106.36	110.58
1	S2	27	A2M	C2'-C1'-N9	-3.69	107.68	113.75
3	L5	1677	PSU	O2-C2-N1	-3.69	118.99	122.79
1	S2	1326	UY1	O2-C2-N1	-3.68	118.99	122.79
3	L5	4523	A2M	C2-N3-C4	3.68	120.83	111.83
3	L5	4590	A2M	C2-N3-C4	3.68	120.83	111.83
3	L5	2815	A2M	C2-N3-C4	3.68	120.83	111.83
85	Pt	8	4SU	N3-C2-N1	3.68	119.68	114.89
1	S2	1367	PSU	O2-C2-N1	-3.68	118.99	122.79
1	S2	1238	PSU	O2-C2-N1	-3.68	119.00	122.79
3	L5	4532	PSU	O2-C2-N1	-3.68	119.00	122.79
3	L5	1871	A2M	C2'-C1'-N9	-3.68	107.70	113.75
1	S2	1347	PSU	O2-C2-N1	-3.68	119.00	122.79
1	S2	1832	6MZ	C6-C5-N7	3.67	136.44	132.43
3	L5	2787	A2M	C2-N3-C4	3.67	120.81	111.83
3	L5	4972	PSU	O2-C2-N1	-3.67	119.01	122.79
1	S2	1639	G7M	CN7-N7-C5	3.66	131.37	126.80
1	S2	468	A2M	C2'-C1'-N9	-3.66	107.73	113.75
3	L5	1782	PSU	O2-C2-N1	-3.65	119.02	122.79
3	L5	1534	A2M	C2-N3-C4	3.65	120.75	111.83
1	S2	1678	A2M	C2-N3-C4	3.65	120.75	111.83
1	S2	668	A2M	C4-C5-N7	-3.65	106.41	110.58
3	L5	3825	A2M	C2-N3-C4	3.65	120.74	111.83
84	At	37	MIA	C6-C5-N7	3.65	136.41	132.43
3	L5	1871	A2M	C2-N3-C4	3.65	120.74	111.83
3	L5	3825	A2M	N3-C2-N1	-3.65	123.06	128.58
3	L5	4228	OMG	C6-C5-N7	3.65	136.92	130.29
3	L5	4636	PSU	O2-C2-N1	-3.64	119.03	122.79
1	S2	1177	PSU	O2-C2-N1	-3.64	119.03	122.79
3	L5	3764	PSU	C4-N3-C2	-3.64	121.35	126.37
3	L5	3724	A2M	C2-N3-C4	3.64	120.71	111.83
3	L5	398	A2M	C2-N3-C4	3.63	120.70	111.83
3	L5	1326	A2M	C2-N3-C4	3.63	120.70	111.83
3	L5	3734	PSU	O2-C2-N1	-3.63	119.04	122.79
3	L5	3830	A2M	C2-N3-C4	3.63	120.70	111.83
1	S2	609	PSU	O2-C2-N1	-3.63	119.05	122.79
3	L5	1792	PSU	O2-C2-N1	-3.63	119.05	122.79
3	L5	4590	A2M	N3-C2-N1	-3.62	123.11	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	Pt	56	PSU	O2-C2-N1	-3.62	119.06	122.79
1	S2	918	PSU	C3'-C2'-C1'	3.62	105.96	101.69
1	S2	863	PSU	O2-C2-N1	-3.62	119.06	122.79
3	L5	4423	PSU	O2-C2-N1	-3.62	119.06	122.79
1	S2	116	OMU	C4-N3-C2	-3.62	122.12	126.61
1	S2	36	PSU	O2-C2-N1	-3.61	119.07	122.79
1	S2	512	A2M	C2-N3-C4	3.61	120.64	111.83
3	L5	3627	OMG	C6-C5-N7	3.60	136.84	130.29
3	L5	1536	PSU	O2-C2-N1	-3.60	119.08	122.79
3	L5	3853	PSU	O2-C2-N1	-3.60	119.08	122.79
3	L5	4689	PSU	O2-C2-N1	-3.60	119.08	122.79
3	L5	3760	A2M	C2-N3-C4	3.60	120.61	111.83
3	L5	3695	PSU	O2-C2-N1	-3.60	119.08	122.79
1	S2	609	PSU	C4-N3-C2	-3.59	121.42	126.37
3	L5	400	A2M	C2-N3-C4	3.58	120.58	111.83
3	L5	4220	6MZ	C9-N6-C6	-3.57	119.54	122.85
1	S2	1851	MA6	C2-N3-C4	3.57	120.55	111.83
3	L5	400	A2M	C2'-C1'-N9	-3.57	107.88	113.75
1	S2	1031	A2M	C2-N3-C4	3.57	120.54	111.83
2	L8	55	PSU	O2-C2-N1	-3.57	119.11	122.79
1	S2	406	PSU	O2-C2-N1	-3.56	119.11	122.79
3	L5	4312	PSU	O2-C2-N1	-3.56	119.11	122.79
1	S2	1442	OMU	O4-C4-C5	-3.56	119.02	125.16
1	S2	814	PSU	O2-C2-N1	-3.56	119.12	122.79
3	L5	1683	PSU	C4-N3-C2	-3.56	121.47	126.37
3	L5	1779	PSU	O2-C2-N1	-3.56	119.12	122.79
3	L5	4571	A2M	C2-N3-C4	3.56	120.52	111.83
1	S2	822	PSU	C3'-C2'-C1'	3.56	105.88	101.69
1	S2	99	A2M	N3-C2-N1	-3.55	123.20	128.58
1	S2	159	A2M	C4-C5-N7	-3.55	106.52	110.58
3	L5	2363	A2M	C4-C5-N7	-3.55	106.53	110.58
3	L5	1781	PSU	O2-C2-N1	-3.54	119.14	122.79
3	L5	4403	PSU	C3'-C2'-C1'	3.54	105.86	101.69
3	L5	3867	A2M	C2-N3-C4	3.54	120.47	111.83
3	L5	3723	A2M	C2-N3-C4	3.53	120.46	111.83
3	L5	3944	OMG	C6-C5-N7	3.53	136.71	130.29
1	S2	1328	OMG	C2'-C1'-N9	-3.52	107.55	114.24
1	S2	1081	PSU	O2-C2-N1	-3.52	119.16	122.79
3	L5	2787	A2M	C4-C5-N7	-3.52	106.56	110.58
3	L5	2508	PSU	O2-C2-N1	-3.51	119.17	122.79
3	L5	3782	5MC	C5-C6-N1	-3.51	119.50	123.31
3	L5	5010	PSU	O2-C2-N1	-3.51	119.17	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1174	PSU	O2-C2-N1	-3.51	119.17	122.79
3	L5	3785	A2M	C4-C5-N7	-3.51	106.57	110.58
3	L5	4296	PSU	O2-C2-N1	-3.50	119.17	122.79
1	S2	468	A2M	C2-N3-C4	3.50	120.38	111.83
3	L5	3758	PSU	O2-C2-N1	-3.49	119.19	122.79
3	L5	2401	A2M	N3-C2-N1	-3.49	123.30	128.58
1	S2	93	PSU	O2-C2-N1	-3.49	119.19	122.79
1	S2	1383	A2M	C2-N3-C4	3.49	120.35	111.83
3	L5	3724	A2M	N3-C2-N1	-3.49	123.31	128.58
3	L5	1522	OMG	C6-C5-N7	3.48	136.62	130.29
1	S2	484	A2M	C4-C5-N7	-3.48	106.61	110.58
3	L5	3723	A2M	N3-C2-N1	-3.47	123.33	128.58
3	L5	4392	OMG	C6-C5-N7	3.47	136.61	130.29
1	S2	1031	A2M	C4-C5-N7	-3.47	106.61	110.58
1	S2	105	PSU	O2-C2-N1	-3.46	119.22	122.79
1	S2	27	A2M	C4-C5-N7	-3.46	106.63	110.58
1	S2	590	A2M	N3-C2-N1	-3.45	123.36	128.58
3	L5	3785	A2M	N3-C2-N1	-3.45	123.36	128.58
3	L5	2843	PSU	O2-C2-N1	-3.45	119.23	122.79
1	S2	1678	A2M	C4-C5-N7	-3.45	106.64	110.58
3	L5	1524	A2M	C4-C5-N7	-3.45	106.64	110.58
1	S2	27	A2M	N3-C2-N1	-3.45	123.37	128.58
3	L5	4499	OMG	C6-C5-N7	3.43	136.53	130.29
3	L5	4618	OMG	C6-C5-N7	3.43	136.53	130.29
1	S2	683	OMG	C6-C5-N7	3.42	136.52	130.29
66	Lr	2	SAC	CB-CA-C	-3.42	103.83	111.35
3	L5	3760	A2M	C4-C5-N7	-3.42	106.67	110.58
3	L5	3744	OMG	C6-C5-N7	3.42	136.51	130.29
3	L5	400	A2M	C4-C5-N7	-3.41	106.68	110.58
1	S2	601	OMG	C6-C5-N7	3.41	136.50	130.29
1	S2	1850	MA6	C2-N3-C4	3.41	120.16	111.83
2	L8	75	OMG	C2'-C1'-N9	-3.40	107.78	114.24
1	S2	668	A2M	C2-N3-C4	3.40	120.14	111.83
3	L5	4457	PSU	C6-C5-C4	-3.40	115.88	118.17
1	S2	681	PSU	O2-C2-N1	-3.40	119.28	122.79
1	S2	1383	A2M	C4-C5-N7	-3.40	106.70	110.58
3	L5	1534	A2M	C4-C5-N7	-3.40	106.70	110.58
3	L5	398	A2M	C4-C5-N7	-3.39	106.70	110.58
1	S2	34	PSU	O2-C2-N1	-3.39	119.29	122.79
1	S2	651	PSU	O2-C2-N1	-3.38	119.30	122.79
1	S2	468	A2M	N3-C2-N1	-3.38	123.46	128.58
3	L5	398	A2M	N3-C2-N1	-3.38	123.47	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1244	PSU	O2-C2-N1	-3.38	119.30	122.79
1	S2	159	A2M	C2-N3-C4	3.38	120.08	111.83
6	SA	2	SAC	C2A-C1A-N	-3.37	110.52	116.12
84	At	37	MIA	C4-C5-N7	-3.36	106.73	110.58
1	S2	1832	6MZ	N1-C2-N3	-3.36	123.50	128.58
1	S2	512	A2M	N3-C2-N1	-3.35	123.51	128.58
52	La	39	V5N	CD2-CG-ND1	3.35	110.27	105.76
3	L5	4220	6MZ	N1-C2-N3	-3.35	123.52	128.58
1	S2	166	A2M	N3-C2-N1	-3.35	123.52	128.58
3	L5	1326	A2M	N3-C2-N1	-3.34	123.52	128.58
3	L5	4494	OMG	C6-C5-N7	3.34	136.37	130.29
3	L5	3884	PSU	O2-C2-N1	-3.34	119.35	122.79
3	L5	3830	A2M	C4-C5-N7	-3.33	106.77	110.58
2	L8	75	OMG	C6-C5-N7	3.33	136.35	130.29
1	S2	119	PSU	O2-C2-N1	-3.33	119.35	122.79
1	S2	590	A2M	C4-C5-N7	-3.33	106.78	110.58
3	L5	3830	A2M	N3-C2-N1	-3.32	123.55	128.58
84	At	39	PSU	O2-C2-N1	-3.32	119.36	122.79
66	Lr	2	SAC	C2A-C1A-N	-3.32	110.61	116.12
1	S2	1490	OMG	C6-C5-N7	3.32	136.33	130.29
1	S2	1678	A2M	N3-C2-N1	-3.31	123.57	128.58
1	S2	1851	MA6	N1-C2-N3	-3.31	123.58	128.58
3	L5	3899	OMG	C6-C5-N7	3.30	136.29	130.29
1	S2	1239	PSU	O2-C2-N1	-3.30	119.39	122.79
3	L5	3818	UY1	O2-C2-N1	-3.29	119.40	122.79
3	L5	4637	OMG	C2'-C1'-N9	-3.29	108.00	114.24
3	L5	4523	A2M	C4-C5-N7	-3.28	106.83	110.58
3	L5	4196	OMG	C6-C5-N7	3.28	136.26	130.29
1	S2	668	A2M	C4-N9-C8	3.27	109.17	105.74
1	S2	166	A2M	C4-C5-N7	-3.27	106.84	110.58
1	S2	1328	OMG	C6-C5-N7	3.27	136.24	130.29
3	L5	3724	A2M	C2'-C1'-N9	-3.27	108.37	113.75
3	L5	3760	A2M	N3-C2-N1	-3.27	123.64	128.58
3	L5	4620	OMU	C5-C4-N3	3.26	119.37	114.80
3	L5	3825	A2M	C4-C5-N7	-3.26	106.85	110.58
3	L5	4530	UR3	C5-C4-N3	3.26	119.33	115.04
3	L5	4618	OMG	C2'-C1'-N9	-3.26	108.06	114.24
3	L5	2787	A2M	N3-C2-N1	-3.25	123.66	128.58
3	L5	2364	OMG	C6-C5-N7	3.25	136.20	130.29
1	S2	1850	MA6	N1-C2-N3	-3.25	123.67	128.58
1	S2	576	A2M	C2-N3-C4	3.24	119.73	111.83
3	L5	2401	A2M	C4-C5-N7	-3.23	106.88	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1031	A2M	N3-C2-N1	-3.23	123.69	128.58
1	S2	436	OMG	C6-C5-N7	3.23	136.16	130.29
3	L5	3718	A2M	C4-C5-N7	-3.22	106.90	110.58
3	L5	1316	OMG	C6-C5-N7	3.22	136.15	130.29
1	S2	627	OMU	O4-C4-C5	-3.22	119.61	125.16
1	S2	867	OMG	C6-C5-N7	3.22	136.14	130.29
1	S2	1383	A2M	N3-C2-N1	-3.21	123.72	128.58
1	S2	1643	PSU	C3'-C2'-C1'	3.21	105.48	101.69
1	S2	1232	PSU	O2-C2-N1	-3.21	119.48	122.79
3	L5	3744	OMG	C2'-C1'-N9	-3.21	108.16	114.24
1	S2	683	OMG	C2'-C1'-N9	-3.20	108.16	114.24
1	S2	218	PSU	O2-C2-N1	-3.20	119.49	122.79
84	At	37	MIA	C2-N3-C4	3.20	120.67	112.29
3	L5	3715	PSU	O2-C2-N1	-3.19	119.50	122.79
3	L5	4590	A2M	C4-C5-N7	-3.19	106.94	110.58
1	S2	1445	PSU	C3'-C2'-C1'	3.18	105.44	101.69
3	L5	1534	A2M	N3-C2-N1	-3.18	123.77	128.58
3	L5	2363	A2M	N3-C2-N1	-3.18	123.77	128.58
3	L5	3718	A2M	C2-N3-C4	3.18	119.59	111.83
3	L5	4623	OMG	C2'-C1'-N9	-3.18	108.21	114.24
3	L5	4370	OMG	C6-C5-N7	3.18	136.07	130.29
3	L5	4442	PSU	C3'-C2'-C1'	3.18	105.44	101.69
3	L5	3825	A2M	C2'-C1'-N9	-3.17	108.53	113.75
1	S2	668	A2M	N3-C2-N1	-3.17	123.78	128.58
3	L5	2837	OMU	O4-C4-C5	-3.17	119.70	125.16
3	L5	2815	A2M	N3-C2-N1	-3.17	123.79	128.58
1	S2	484	A2M	N3-C2-N1	-3.16	123.80	128.58
3	L5	4521	PSU	C3'-C2'-C1'	3.16	105.41	101.69
1	S2	512	A2M	C4-C5-N7	-3.16	106.97	110.58
1	S2	1804	OMU	O4-C4-C5	-3.15	119.72	125.16
3	L5	4637	OMG	C6-C5-N7	3.15	136.02	130.29
1	S2	644	OMG	C6-C5-N7	3.15	136.01	130.29
3	L5	3768	PSU	O2-C2-N1	-3.14	119.55	122.79
1	S2	116	OMU	C5-C4-N3	3.14	119.20	114.80
3	L5	4220	6MZ	C4-C5-N7	-3.13	107.01	110.58
3	L5	1322	1MA	N9-C4-N3	3.12	134.02	126.90
3	L5	1524	A2M	N3-C2-N1	-3.12	123.86	128.58
3	L5	4361	PSU	O2-C2-N1	-3.12	119.57	122.79
3	L5	2415	OMU	O4-C4-C5	-3.12	119.79	125.16
3	L5	2632	PSU	O2-C2-N1	-3.12	119.58	122.79
3	L5	400	A2M	N3-C2-N1	-3.12	123.87	128.58
1	S2	468	A2M	C4-C5-N7	-3.11	107.03	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3764	PSU	O2-C2-N1	-3.10	119.59	122.79
1	S2	573	PSU	O2-C2-N1	-3.09	119.60	122.79
3	L5	3718	A2M	C2'-C1'-N9	-3.09	108.67	113.75
3	L5	1860	PSU	O2-C2-N1	-3.09	119.61	122.79
3	L5	4498	OMU	O4-C4-C5	-3.08	119.85	125.16
3	L5	3785	A2M	C4-N9-C8	3.07	108.97	105.74
3	L5	4523	A2M	N3-C2-N1	-3.07	123.93	128.58
2	L8	14	OMU	O4-C4-C5	-3.07	119.86	125.16
3	L5	4493	PSU	O2-C2-N1	-3.06	119.63	122.79
3	L5	4571	A2M	N3-C2-N1	-3.06	123.95	128.58
3	L5	4306	OMU	O4-C4-C5	-3.06	119.89	125.16
3	L5	4227	OMU	O4-C4-C5	-3.05	119.89	125.16
1	S2	509	OMG	C6-C5-N7	3.04	135.83	130.29
3	L5	4571	A2M	C4-C5-N7	-3.03	107.11	110.58
1	S2	428	OMU	O4-C4-C5	-3.03	119.94	125.16
3	L5	4636	PSU	C5-C6-N1	-3.03	117.94	122.14
3	L5	5001	PSU	O2-C2-N1	-3.02	119.67	122.79
1	S2	1842	4AC	C6-C5-C4	3.02	120.64	117.00
3	L5	3925	OMU	O4-C4-C5	-3.02	119.96	125.16
1	S2	1850	MA6	C4-N9-C8	3.01	108.90	105.74
1	S2	572	PSU	O2-C2-N1	-3.00	119.69	122.79
3	L5	1871	A2M	C4-C5-N7	-3.00	107.15	110.58
3	L5	4457	PSU	O2-C2-N1	-3.00	119.70	122.79
3	L5	2815	A2M	C4-C5-N7	-2.99	107.16	110.58
1	S2	172	OMU	O4-C4-C5	-2.99	120.01	125.16
3	L5	4220	6MZ	C6-C5-N7	2.98	135.68	132.43
1	S2	644	OMG	C2'-C1'-N9	-2.97	108.60	114.24
84	At	37	MIA	C4-N9-C8	2.97	108.86	105.74
2	L8	69	PSU	C3'-C2'-C1'	2.97	105.19	101.69
3	L5	3724	A2M	C4-C5-N7	-2.97	107.19	110.58
3	L5	3808	OMC	O2-C2-N3	-2.97	117.65	122.33
40	LB	245	HIC	NE2-CE1-ND1	-2.95	111.53	112.66
3	L5	3867	A2M	N3-C2-N1	-2.95	124.12	128.58
3	L5	4457	PSU	C3'-C2'-C1'	2.95	105.17	101.69
3	L5	3723	A2M	C4-C5-N7	-2.95	107.21	110.58
1	S2	354	OMU	O4-C4-C5	-2.94	120.09	125.16
3	L5	3723	A2M	C4-N9-C8	2.93	108.82	105.74
1	S2	119	PSU	C6-C5-C4	-2.93	116.19	118.17
3	L5	4620	OMU	C2'-C1'-N1	-2.93	108.68	114.24
1	S2	1643	PSU	C6-C5-C4	-2.92	116.20	118.17
1	S2	1288	OMU	O4-C4-C5	-2.92	120.12	125.16
3	L5	1683	PSU	O2-C2-N1	-2.91	119.79	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3792	OMG	C6-C5-N7	2.90	135.56	130.29
3	L5	4523	A2M	C2'-C1'-N9	-2.89	108.99	113.75
3	L5	2876	OMG	C6-C5-N7	2.89	135.55	130.29
1	S2	863	PSU	C6-C5-C4	-2.89	116.22	118.17
3	L5	2401	A2M	C2'-C1'-N9	-2.89	109.00	113.75
2	L8	14	OMU	C2'-C1'-N1	-2.88	108.77	114.24
3	L5	1871	A2M	C4-N9-C8	2.88	108.76	105.74
3	L5	3718	A2M	N3-C2-N1	-2.87	124.23	128.58
3	L5	1326	A2M	C4-C5-N7	-2.87	107.30	110.58
1	S2	116	OMU	O4-C4-C5	-2.87	120.21	125.16
1	S2	966	PSU	C3'-C2'-C1'	2.86	105.07	101.69
3	L5	4447	5MC	C5-C4-N3	-2.86	118.82	121.75
1	S2	1639	G7M	O6-C6-C5	-2.86	121.63	128.01
3	L5	3760	A2M	C4-N9-C8	2.84	108.72	105.74
3	L5	3770	PSU	C3'-C2'-C1'	2.83	105.03	101.69
3	L5	400	A2M	C4-N9-C8	2.83	108.71	105.74
1	S2	172	OMU	O2'-C2'-C1'	2.83	114.35	108.99
3	L5	1625	OMG	C6-C5-N7	2.82	135.42	130.29
1	S2	1288	OMU	C2'-C1'-N1	-2.81	108.90	114.24
6	SA	2	SAC	CB-CA-C	-2.81	105.16	111.35
1	S2	468	A2M	C4-N9-C8	2.81	108.69	105.74
1	S2	1248	B8N	C1'-C5-C4	2.80	121.85	117.61
3	L5	3867	A2M	C4-N9-C8	2.80	108.68	105.74
1	S2	99	A2M	C4-N9-C8	2.79	108.67	105.74
1	S2	1678	A2M	C4-N9-C8	2.79	108.67	105.74
3	L5	4623	OMG	C4-C5-N7	-2.76	106.30	110.67
1	S2	1031	A2M	C4-N9-C8	2.75	108.62	105.74
3	L5	3867	A2M	C4-C5-N7	-2.75	107.44	110.58
1	S2	159	A2M	N3-C2-N1	-2.74	124.44	128.58
1	S2	1832	6MZ	C5-N7-C8	2.74	107.75	103.45
3	L5	3782	5MC	C5-C4-N3	-2.74	118.95	121.75
1	S2	99	A2M	C4-C5-N7	-2.73	107.47	110.58
3	L5	1524	A2M	C4-N9-C8	2.72	108.60	105.74
1	S2	572	PSU	C6-C5-C4	-2.72	116.34	118.17
3	L5	3637	PSU	C5-C6-N1	-2.72	118.36	122.14
3	L5	4220	6MZ	C4-N9-C8	2.72	108.59	105.74
1	S2	576	A2M	N3-C2-N1	-2.72	124.47	128.58
1	S2	801	PSU	O2-C2-N1	-2.71	119.99	122.79
1	S2	93	PSU	C5-C6-N1	-2.71	118.38	122.14
1	S2	668	A2M	C5-N7-C8	2.71	107.71	103.45
1	S2	1328	OMG	C4-C5-N7	-2.71	106.38	110.67
1	S2	1326	UY1	C5-C6-N1	-2.70	118.39	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C4-N9-C8	2.70	108.57	105.74
1	S2	590	A2M	C4-N9-C8	2.70	108.57	105.74
1	S2	1851	MA6	C5-N7-C8	2.69	107.69	103.45
3	L5	2787	A2M	C4-N9-C8	2.69	108.56	105.74
1	S2	1850	MA6	C5-N7-C8	2.69	107.68	103.45
1	S2	1447	OMG	C4-C5-N7	-2.69	106.41	110.67
3	L5	3637	PSU	O2-C2-N1	-2.68	120.03	122.79
1	S2	1851	MA6	C4-N9-C8	2.68	108.55	105.74
3	L5	3627	OMG	C4-C5-N7	-2.67	106.43	110.67
3	L5	4620	OMU	O4'-C4'-C3'	-2.66	99.88	105.15
1	S2	1244	PSU	C5-C6-N1	-2.66	118.45	122.14
3	L5	1534	A2M	C4-N9-C8	2.66	108.53	105.74
3	L5	4590	A2M	C4-N9-C8	2.65	108.52	105.74
1	S2	116	OMU	C6-N1-C2	-2.64	117.78	121.00
3	L5	1582	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L5	2422	OMC	O2-C2-N3	-2.64	118.18	122.33
3	L5	4499	OMG	C4-C5-N7	-2.63	106.50	110.67
84	At	32	PSU	C5-C6-N1	-2.63	118.49	122.14
1	S2	627	OMU	O2-C2-N1	-2.62	119.39	122.80
3	L5	3785	A2M	C4'-O4'-C1'	-2.62	103.69	109.47
1	S2	1490	OMG	C4-C5-N7	-2.61	106.53	110.67
1	S2	1031	A2M	C2'-C1'-N9	-2.61	109.46	113.75
1	S2	121	OMU	O4-C4-C5	-2.61	120.67	125.16
3	L5	2363	A2M	C4-N9-C8	2.60	108.47	105.74
3	L5	2363	A2M	C5-N7-C8	2.60	107.54	103.45
3	L5	4471	PSU	O2-C2-N1	-2.58	120.12	122.79
3	L5	1524	A2M	C5-N7-C8	2.58	107.51	103.45
3	L5	1326	A2M	C4-N9-C8	2.58	108.45	105.74
1	S2	484	A2M	C5-N7-C8	2.58	107.50	103.45
3	L5	3785	A2M	C5-N7-C8	2.57	107.50	103.45
1	S2	601	OMG	C4-C5-N7	-2.57	106.59	110.67
2	L8	69	PSU	C5-C6-N1	-2.57	118.57	122.14
3	L5	2401	A2M	C4-N9-C8	2.57	108.44	105.74
1	S2	1842	4AC	N4-C4-N3	2.57	118.03	113.87
3	L5	400	A2M	C5-N7-C8	2.56	107.48	103.45
3	L5	3944	OMG	C4-C5-N7	-2.56	106.61	110.67
3	L5	4618	OMG	C4-C5-N7	-2.56	106.62	110.67
1	S2	1383	A2M	C4-N9-C8	2.56	108.42	105.74
3	L5	4523	A2M	C5-N7-C8	2.56	107.47	103.45
1	S2	1832	6MZ	C4-N9-C8	2.55	108.42	105.74
3	L5	4628	PSU	C3'-C2'-C1'	2.55	104.69	101.69
1	S2	1248	B8N	C3'-C2'-C1'	2.54	104.69	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	512	A2M	C4-N9-C8	2.54	108.40	105.74
3	L5	4673	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	3764	PSU	C3'-C2'-C1'	2.54	104.68	101.69
1	S2	27	A2M	C5-N7-C8	2.54	107.44	103.45
3	L5	2787	A2M	C5-N7-C8	2.53	107.43	103.45
3	L5	4228	OMG	C4-C5-N7	-2.53	106.66	110.67
3	L5	4456	OMC	C2'-C1'-N1	-2.52	109.45	114.24
3	L5	3899	OMG	C4-C5-N7	-2.52	106.67	110.67
3	L5	1316	OMG	C4-C5-N7	-2.52	106.67	110.67
1	S2	1678	A2M	C5-N7-C8	2.52	107.41	103.45
2	L8	75	OMG	O6-C6-C5	-2.52	119.88	126.53
3	L5	1522	OMG	C4-C5-N7	-2.52	106.68	110.67
3	L5	1534	A2M	C5-N7-C8	2.52	107.40	103.45
3	L5	3744	OMG	C4-C5-N7	-2.51	106.69	110.67
3	L5	4530	UR3	C6-N1-C2	-2.51	119.75	121.80
3	L5	4392	OMG	C4-C5-N7	-2.51	106.69	110.67
1	S2	27	A2M	C4-N9-C8	2.50	108.37	105.74
3	L5	1322	1MA	N1-C2-N3	-2.50	123.02	126.00
3	L5	4530	UR3	C3U-N3-C4	2.50	121.33	117.87
3	L5	2876	OMG	C4-C5-N7	-2.50	106.71	110.67
3	L5	3760	A2M	C5-N7-C8	2.49	107.37	103.45
3	L5	4370	OMG	C4-C5-N7	-2.49	106.73	110.67
1	S2	590	A2M	C5-N7-C8	2.48	107.35	103.45
1	S2	1447	OMG	O4'-C1'-N9	2.48	113.97	108.36
84	At	37	MIA	C5-N7-C8	2.47	107.34	103.45
3	L5	3830	A2M	C5-N7-C8	2.47	107.34	103.45
3	L5	4498	OMU	O2-C2-N1	-2.47	119.58	122.80
1	S2	1031	A2M	C5-N7-C8	2.46	107.32	103.45
1	S2	1842	4AC	C5-C4-N3	-2.46	118.75	122.60
1	S2	484	A2M	C4-N9-C8	2.46	108.32	105.74
2	L8	75	OMG	C4-C5-N7	-2.46	106.78	110.67
3	L5	3637	PSU	O2-C2-N3	-2.45	117.51	121.86
3	L5	3818	UY1	C5-C6-N1	-2.44	118.75	122.14
3	L5	4571	A2M	C5-N7-C8	2.44	107.28	103.45
1	S2	166	A2M	C5-N7-C8	2.44	107.28	103.45
3	L5	3825	A2M	C5-N7-C8	2.44	107.28	103.45
52	La	39	V5N	O-C-CA	-2.43	118.51	124.77
1	S2	159	A2M	C2'-C1'-N9	-2.43	109.76	113.75
1	S2	1243	PSU	C5-C6-N1	-2.42	118.78	122.14
1	S2	509	OMG	C4-C5-N7	-2.42	106.83	110.67
3	L5	1881	OMC	C2'-C1'-N1	2.42	118.83	114.24
3	L5	2401	A2M	C5-N7-C8	2.41	107.24	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4523	A2M	C4-N9-C8	2.41	108.27	105.74
1	S2	681	PSU	C5-C6-N1	-2.41	118.80	122.14
1	S2	436	OMG	C4-C5-N7	-2.40	106.86	110.67
3	L5	3825	A2M	C2-N1-C6	2.40	122.68	118.73
1	S2	462	OMC	C2'-C1'-N1	-2.40	109.68	114.24
3	L5	3792	OMG	O6-C6-C5	-2.40	120.21	126.53
84	At	20	H2U	C5-C6-N1	-2.40	104.27	111.52
1	S2	867	OMG	C4-C5-N7	-2.39	106.88	110.67
1	S2	668	A2M	N9-C8-N7	-2.39	110.54	113.94
3	L5	3724	A2M	C4-N9-C8	2.39	108.25	105.74
3	L5	4296	PSU	C5-C6-N1	-2.39	118.82	122.14
3	L5	1779	PSU	C5-C6-N1	-2.39	118.82	122.14
3	L5	2364	OMG	C4-C5-N7	-2.39	106.89	110.67
3	L5	5001	PSU	C5-C6-N1	-2.38	118.83	122.14
1	S2	1056	PSU	C5-C6-N1	-2.38	118.83	122.14
3	L5	1582	PSU	C5-C6-N1	-2.38	118.83	122.14
1	S2	644	OMG	C4-C5-N7	-2.38	106.90	110.67
3	L5	4620	OMU	C6-N1-C2	-2.38	118.11	121.00
3	L5	4220	6MZ	C5-N7-C8	2.38	107.18	103.45
3	L5	3785	A2M	C6-C5-N7	2.37	136.67	132.09
3	L5	2815	A2M	C4-N9-C8	2.37	108.23	105.74
3	L5	3841	OMC	O2-C2-N3	-2.37	118.60	122.33
3	L5	4431	PSU	C6-C5-C4	-2.37	116.58	118.17
1	S2	668	A2M	C6-C5-N7	2.36	136.65	132.09
1	S2	159	A2M	C5-N7-C8	2.36	107.17	103.45
3	L5	3729	PSU	C3'-C2'-C1'	2.36	104.48	101.69
1	S2	683	OMG	C4-C5-N7	-2.36	106.93	110.67
3	L5	3718	A2M	C2-N1-C6	2.36	122.61	118.73
1	S2	1383	A2M	C5-N7-C8	2.36	107.16	103.45
1	S2	166	A2M	C4-N9-C8	2.35	108.21	105.74
3	L5	4494	OMG	C4-C5-N7	-2.35	106.95	110.67
66	Lr	2	SAC	C-CA-N	2.35	114.03	109.50
3	L5	3785	A2M	N9-C8-N7	-2.34	110.61	113.94
3	L5	1625	OMG	C4-C5-N7	-2.34	106.96	110.67
3	L5	4590	A2M	C5-N7-C8	2.34	107.13	103.45
3	L5	4590	A2M	C2-N1-C6	2.34	122.57	118.73
3	L5	4637	OMG	C4-C5-N7	-2.34	106.96	110.67
1	S2	1337	4AC	C6-C5-C4	2.34	119.81	117.00
3	L5	4571	A2M	C4-N9-C8	2.33	108.19	105.74
3	L5	2843	PSU	C5-C6-N1	-2.33	118.90	122.14
3	L5	2422	OMC	C2'-C1'-N1	-2.33	109.81	114.24
3	L5	3825	A2M	C4-N9-C8	2.33	108.19	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1871	A2M	C2-N1-C6	2.33	122.55	118.73
3	L5	3782	5MC	O2-C2-N3	-2.32	118.67	122.33
1	S2	121	OMU	C2'-C1'-N1	-2.32	109.84	114.24
3	L5	3718	A2M	C4-N9-C8	2.32	108.17	105.74
3	L5	1677	PSU	C5-C6-N1	-2.32	118.92	122.14
3	L5	2424	OMG	C6-C5-N7	2.32	134.51	130.29
3	L5	3792	OMG	C4-C5-N7	-2.32	107.00	110.67
3	L5	4972	PSU	C5-C6-N1	-2.32	118.92	122.14
1	S2	1174	PSU	C5-C6-N1	-2.31	118.93	122.14
3	L5	2815	A2M	C5-N7-C8	2.31	107.08	103.45
3	L5	2364	OMG	O6-C6-C5	-2.30	120.45	126.53
3	L5	1625	OMG	O6-C6-C5	-2.30	120.47	126.53
1	S2	436	OMG	O6-C6-C5	-2.29	120.47	126.53
3	L5	1322	1MA	C6-C5-N7	2.29	136.21	132.16
3	L5	4420	PSU	O4'-C1'-C2'	2.29	108.32	105.15
3	L5	1316	OMG	O6-C6-C5	-2.29	120.48	126.53
1	S2	512	A2M	C5-N7-C8	2.29	107.05	103.45
3	L5	4312	PSU	C5-C6-N1	-2.29	118.96	122.14
1	S2	576	A2M	C5-N7-C8	2.29	107.05	103.45
1	S2	1851	MA6	C6-C5-N7	2.29	137.09	133.43
84	At	16	H2U	C5-C6-N1	-2.28	104.61	111.52
3	L5	3639	PSU	C5-C6-N1	-2.28	118.97	122.14
3	L5	4403	PSU	C5-C6-N1	-2.28	118.97	122.14
1	S2	517	OMC	C2'-C1'-N1	-2.28	109.91	114.24
1	S2	517	OMC	O2-C2-N3	-2.28	118.74	122.33
3	L5	4636	PSU	C3'-C2'-C1'	2.27	104.37	101.69
1	S2	468	A2M	C5-N7-C8	2.27	107.02	103.45
3	L5	4196	OMG	O6-C6-C5	-2.27	120.54	126.53
84	At	37	MIA	C2-N1-C6	2.27	121.85	117.54
3	L5	4361	PSU	C3'-C2'-C1'	2.27	104.36	101.69
1	S2	174	OMC	C2'-C1'-N1	-2.26	109.94	114.24
3	L5	3851	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	4521	PSU	C5-C6-N1	-2.26	119.00	122.14
3	L5	398	A2M	C2-N1-C6	2.26	122.44	118.73
3	L5	4637	OMG	O6-C6-C5	-2.26	120.57	126.53
3	L5	2508	PSU	C5-C6-N1	-2.26	119.00	122.14
1	S2	644	OMG	O6-C6-C5	-2.25	120.58	126.53
3	L5	3844	PSU	C5-C6-N1	-2.25	119.01	122.14
1	S2	1232	PSU	O2-C2-N3	-2.25	117.86	121.86
3	L5	4636	PSU	O2-C2-N3	-2.25	117.86	121.86
3	L5	4532	PSU	C5-C6-N1	-2.25	119.01	122.14
3	L5	4196	OMG	C4-C5-N7	-2.25	107.10	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	814	PSU	C5-C6-N1	-2.25	119.02	122.14
1	S2	1850	MA6	C6-C5-N7	2.24	137.02	133.43
1	S2	34	PSU	C5-C6-N1	-2.24	119.03	122.14
1	S2	918	PSU	C5-C6-N1	-2.24	119.03	122.14
1	S2	867	OMG	O6-C6-C5	-2.24	120.63	126.53
1	S2	1490	OMG	C2'-C1'-N9	-2.24	109.99	114.24
1	S2	36	PSU	C5-C6-N1	-2.23	119.04	122.14
3	L5	4569	PSU	C5-C6-N1	-2.23	119.04	122.14
2	L8	55	PSU	C5-C6-N1	-2.23	119.05	122.14
3	L5	3758	PSU	C5-C6-N1	-2.23	119.05	122.14
3	L5	4442	PSU	C5-C6-N1	-2.23	119.05	122.14
84	At	8	4SU	O2-C2-N1	-2.22	119.90	122.80
1	S2	218	PSU	C5-C6-N1	-2.22	119.05	122.14
3	L5	1524	A2M	C2'-C1'-N9	-2.22	110.10	113.75
3	L5	4620	OMU	O4-C4-C5	-2.22	121.33	125.16
3	L5	4228	OMG	O6-C6-C5	-2.22	120.68	126.53
3	L5	3627	OMG	O6-C6-C5	-2.21	120.69	126.53
3	L5	2837	OMU	O2-C2-N1	-2.21	119.92	122.80
1	S2	651	PSU	C5-C6-N1	-2.21	119.07	122.14
1	S2	576	A2M	C2-N1-C6	2.21	122.36	118.73
3	L5	1322	1MA	C4-C5-N7	-2.21	107.17	110.67
1	S2	159	A2M	C4-N9-C8	2.21	108.06	105.74
3	L5	3920	PSU	C5-C6-N1	-2.20	119.08	122.14
3	L5	3723	A2M	C2'-C1'-N9	-2.20	110.13	113.75
3	L5	4531	PSU	C5-C6-N1	-2.19	119.10	122.14
3	L5	398	A2M	C5-N7-C8	2.19	106.89	103.45
3	L5	2415	OMU	C1'-N1-C2	2.19	121.52	117.59
3	L5	1522	OMG	O6-C6-C5	-2.19	120.76	126.53
3	L5	1326	A2M	C5-N7-C8	2.19	106.89	103.45
84	At	37	MIA	N9-C8-N7	-2.19	110.84	113.94
3	L5	2861	OMC	O2-C2-N3	-2.18	118.89	122.33
1	S2	1447	OMG	O6-C6-C5	-2.18	120.77	126.53
3	L5	4456	OMC	O2-C2-N3	-2.18	118.89	122.33
1	S2	99	A2M	C5-N7-C8	2.18	106.87	103.45
85	Pt	56	PSU	C5-C6-N1	-2.18	119.12	122.14
3	L5	1881	OMC	O2'-C2'-C1'	2.18	113.12	108.99
3	L5	4569	PSU	C2'-C3'-C4'	-2.18	98.41	102.61
3	L5	4576	PSU	C5-C6-N1	-2.17	119.12	122.14
3	L5	1782	PSU	C5-C6-N1	-2.17	119.12	122.14
1	S2	866	PSU	C5-C6-N1	-2.17	119.13	122.14
3	L5	4673	PSU	O2-C2-N3	-2.17	118.01	121.86
3	L5	3899	OMG	O6-C6-C5	-2.17	120.82	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1031	A2M	C6-C5-N7	2.16	136.26	132.09
1	S2	1850	MA6	N9-C8-N7	-2.16	110.87	113.94
3	L5	4493	PSU	C6-C5-C4	-2.16	116.72	118.17
3	L5	3744	OMG	O6-C6-C5	-2.16	120.83	126.53
3	L5	3718	A2M	C5-N7-C8	2.16	106.84	103.45
3	L5	3825	A2M	C6-C5-N7	2.16	136.25	132.09
1	S2	1174	PSU	O2-C2-N3	-2.16	118.03	121.86
3	L5	3723	A2M	C5-N7-C8	2.15	106.83	103.45
1	S2	468	A2M	C2-N1-C6	2.15	122.26	118.73
3	L5	4623	OMG	O6-C6-C5	-2.15	120.86	126.53
1	S2	1367	PSU	C5-C6-N1	-2.15	119.16	122.14
3	L5	1871	A2M	C5-N7-C8	2.15	106.83	103.45
1	S2	601	OMG	O6-C6-C5	-2.15	120.86	126.53
3	L5	2424	OMG	O6-C6-C5	-2.15	120.86	126.53
3	L5	1792	PSU	C6-C5-C4	-2.15	116.72	118.17
1	S2	1238	PSU	C5-C6-N1	-2.15	119.16	122.14
3	L5	2632	PSU	C3'-C2'-C1'	2.14	104.22	101.69
1	S2	573	PSU	O2-C2-N3	-2.14	118.06	121.86
1	S2	1490	OMG	O6-C6-C5	-2.14	120.88	126.53
3	L5	3770	PSU	C6-C5-C4	-2.14	116.73	118.17
85	Pt	33	OMC	O2-C2-N3	-2.14	118.95	122.33
3	L5	2363	A2M	C6-C5-N7	2.14	136.22	132.09
3	L5	4494	OMG	O6-C6-C5	-2.14	120.89	126.53
3	L5	1871	A2M	C6-C5-N7	2.14	136.21	132.09
3	L5	4370	OMG	O6-C6-C5	-2.14	120.89	126.53
1	S2	576	A2M	C6-C5-N7	2.14	136.21	132.09
3	L5	3867	A2M	C5-N7-C8	2.14	106.81	103.45
3	L5	3724	A2M	C5-N7-C8	2.13	106.80	103.45
1	S2	1383	A2M	C6-C5-N7	2.13	136.20	132.09
3	L5	3760	A2M	C6-C5-N7	2.13	136.19	132.09
1	S2	1678	A2M	C6-C5-N7	2.13	136.19	132.09
1	S2	1832	6MZ	C2-N1-C6	2.13	122.29	115.24
3	L5	2632	PSU	C6-C5-C4	-2.13	116.74	118.17
1	S2	512	A2M	C2-N1-C6	2.12	122.22	118.73
3	L5	4590	A2M	C6-C5-N7	2.12	136.19	132.09
3	L5	4552	PSU	C5-C6-N1	-2.12	119.19	122.14
3	L5	4618	OMG	O6-C6-C5	-2.12	120.93	126.53
3	L5	4361	PSU	C5-C6-N1	-2.12	119.19	122.14
3	L5	5010	PSU	C5-C6-N1	-2.12	119.19	122.14
3	L5	3785	A2M	O4'-C1'-C2'	-2.12	102.94	106.59
3	L5	1582	PSU	O2-C2-N3	-2.12	118.09	121.86
1	S2	406	PSU	O2'-C2'-C1'	-2.12	106.18	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1692	PSU	C5-C6-N1	-2.12	119.20	122.14
3	L5	4620	OMU	O2-C2-N3	-2.12	117.58	121.49
1	S2	1081	PSU	C5-C6-N1	-2.11	119.21	122.14
3	L5	2839	PSU	C5-C6-N1	-2.11	119.21	122.14
3	L5	4471	PSU	O2-C2-N3	-2.11	118.11	121.86
1	S2	668	A2M	C2-N1-C6	2.11	122.20	118.73
1	S2	27	A2M	C6-C5-N7	2.11	136.16	132.09
1	S2	428	OMU	O2-C2-N1	-2.10	120.06	122.80
3	L5	3723	A2M	C2-N1-C6	2.10	122.18	118.73
1	S2	354	OMU	O2-C2-N1	-2.10	120.06	122.80
3	L5	2424	OMG	C4-C5-N7	-2.10	107.34	110.67
1	S2	683	OMG	O6-C6-C5	-2.10	121.00	126.53
1	S2	174	OMC	O2-C2-N3	-2.09	119.03	122.33
20	SX	62	HY3	O-C-CA	-2.09	119.33	124.86
3	L5	2787	A2M	C6-C5-N7	2.09	136.12	132.09
1	S2	1639	G7M	C5-C6-N1	2.09	116.16	111.84
3	L5	3768	PSU	O2-C2-N3	-2.09	118.15	121.86
1	S2	1445	PSU	C5-C6-N1	-2.09	119.24	122.14
3	L5	3841	OMC	C2'-C1'-N1	-2.09	110.28	114.24
1	S2	172	OMU	O2-C2-N1	-2.09	120.08	122.80
3	L5	4499	OMG	O6-C6-C5	-2.09	121.03	126.53
84	At	39	PSU	C5-C6-N1	-2.09	119.25	122.14
1	S2	1248	B8N	O2-C2-N3	-2.08	119.18	121.98
1	S2	1851	MA6	N9-C8-N7	-2.08	110.98	113.94
1	S2	1383	A2M	C2-N1-C6	2.08	122.15	118.73
3	L5	3764	PSU	O2-C2-N3	-2.08	118.16	121.86
1	S2	576	A2M	C4-N9-C8	2.08	107.92	105.74
3	L5	2787	A2M	N9-C8-N7	-2.08	110.99	113.94
3	L5	3760	A2M	N9-C8-N7	-2.08	110.99	113.94
3	L5	400	A2M	N9-C8-N7	-2.07	110.99	113.94
3	L5	3925	OMU	O2-C2-N1	-2.07	120.10	122.80
1	S2	1328	OMG	O6-C6-C5	-2.07	121.06	126.53
1	S2	801	PSU	C6-C5-C4	-2.07	116.78	118.17
3	L5	3715	PSU	C5-C6-N1	-2.07	119.27	122.14
84	At	37	MIA	N3-C2-N1	-2.07	123.22	127.00
1	S2	105	PSU	O2-C2-N3	-2.07	118.18	121.86
1	S2	1447	OMG	C4'-O4'-C1'	-2.07	104.90	109.47
3	L5	1860	PSU	O2-C2-N3	-2.07	118.19	121.86
1	S2	1678	A2M	N9-C8-N7	-2.06	111.01	113.94
1	S2	1804	OMU	O2-C2-N1	-2.06	120.11	122.80
1	S2	1447	OMG	C2'-C1'-N9	-2.06	110.33	114.24
3	L5	1524	A2M	N9-C8-N7	-2.06	111.01	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4361	PSU	O2-C2-N3	-2.06	118.20	121.86
3	L5	1860	PSU	C5-C6-N1	-2.06	119.28	122.14
40	LB	245	HIC	CB-CG-CD2	-2.06	124.99	129.96
1	S2	436	OMG	C5-C6-N1	2.06	118.49	113.25
3	L5	3830	A2M	C6-C5-N7	2.06	136.05	132.09
3	L5	4299	PSU	C5-C6-N1	-2.05	119.29	122.14
3	L5	4392	OMG	O6-C6-C5	-2.05	121.11	126.53
1	S2	159	A2M	C6-C5-N7	2.05	136.05	132.09
3	L5	1536	PSU	C5-C6-N1	-2.05	119.29	122.14
3	L5	1582	PSU	C3'-C2'-C1'	2.05	104.11	101.69
3	L5	4628	PSU	C6-N1-C2	-2.05	120.79	122.69
3	L5	1524	A2M	C6-C5-N7	2.05	136.04	132.09
1	S2	1842	4AC	O7-C7-N4	2.05	125.12	121.90
3	L5	4447	5MC	O2-C2-N3	-2.05	119.11	122.33
3	L5	4392	OMG	C5-C6-N1	2.04	118.45	113.25
3	L5	3944	OMG	O6-C6-C5	-2.04	121.16	126.53
3	L5	1781	PSU	C5-C6-N1	-2.03	119.32	122.14
3	L5	1862	PSU	C5-C6-N1	-2.03	119.32	122.14
84	At	20	H2U	O2-C2-N1	-2.03	120.66	123.10
1	S2	428	OMU	C2'-C1'-N1	-2.03	110.39	114.24
3	L5	2401	A2M	C2-N1-C6	2.03	122.06	118.73
3	L5	3867	A2M	C3'-C2'-C1'	2.03	106.69	102.81
1	S2	1337	4AC	C3'-C2'-C1'	2.02	105.29	101.46
3	L5	2351	OMC	O2-C2-N3	-2.02	119.14	122.33
3	L5	3723	A2M	C6-C5-N7	2.02	135.99	132.09
3	L5	2876	OMG	O6-C6-C5	-2.02	121.20	126.53
3	L5	3724	A2M	C2-N1-C6	2.02	122.05	118.73
3	L5	2363	A2M	N9-C8-N7	-2.02	111.07	113.94
1	S2	822	PSU	C5-C6-N1	-2.02	119.34	122.14
3	L5	4457	PSU	O2-C2-N3	-2.02	118.28	121.86
1	S2	1639	G7M	C3'-C2'-C1'	2.02	105.28	101.46
3	L5	4196	OMG	C5-C6-N1	2.01	118.38	113.25
1	S2	815	PSU	C5-C6-N1	-2.01	119.35	122.14
3	L5	3830	A2M	N9-C8-N7	-2.01	111.09	113.94
3	L5	3762	PSU	C5-C6-N1	-2.01	119.35	122.14
1	S2	1136	PSU	O4'-C1'-C2'	2.00	107.92	105.15
3	L5	4471	PSU	C5-C6-N1	-2.00	119.36	122.14
1	S2	1031	A2M	C2-N1-C6	2.00	122.02	118.73
3	L5	4673	PSU	C6-C5-C4	-2.00	116.82	118.17
3	L5	3718	A2M	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
2	L8	75	OMG	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA
6	SA	2	SAC	C-CA-CB-OG
66	Lr	2	SAC	C2A-C1A-N-CA
81	Lo	53	MLZ	C-CA-CB-CG
84	At	16	H2U	O4'-C4'-C5'-O5'
84	At	16	H2U	C3'-C4'-C5'-O5'
84	At	16	H2U	O4'-C1'-N1-C2
84	At	16	H2U	O4'-C1'-N1-C6
84	At	37	MIA	C12-C13-C14-C15
84	At	37	MIA	C12-C13-C14-C16
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	174	OMC	C1'-C2'-O2'-CM2
1	S2	462	OMC	C1'-C2'-O2'-CM2
1	S2	484	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	867	OMG	C1'-C2'-O2'-CM2
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1248	B8N	C31-C32-C33-N34
1	S2	1288	OMU	O4'-C4'-C5'-O5'
1	S2	1328	OMG	C1'-C2'-O2'-CM2
1	S2	1337	4AC	N3-C4-N4-C7
1	S2	1337	4AC	C5-C4-N4-C7
1	S2	1447	OMG	C1'-C2'-O2'-CM2
1	S2	1490	OMG	C1'-C2'-O2'-CM2
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C2'-C1'-C5-C4
3	L5	4420	PSU	C2'-C1'-C5-C6
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4456	OMC	C1'-C2'-O2'-CM2
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4569	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4618	OMG	C1'-C2'-O2'-CM2
3	L5	4620	OMU	C1'-C2'-O2'-CM2
3	L5	4637	OMG	C1'-C2'-O2'-CM2
39	LA	216	V5N	O-C-CA-CB
68	Lb	5	MLZ	N-CA-CB-CG
68	Lb	5	MLZ	C-CA-CB-CG
68	Lb	5	MLZ	O-C-CA-CB
86	5A	50	5CT	NZ-C1-C2-C3
86	5A	50	5CT	NZ-C1-C2-O1
86	5A	50	5CT	C1-C2-C3-C4
86	5A	50	5CT	O1-C2-C3-C4
86	5A	50	5CT	C2-C3-C4-N1
29	SV	1	AME	OT-CT1-N-CA
85	Pt	21	H2U	O4'-C4'-C5'-O5'
85	Pt	21	H2U	C3'-C4'-C5'-O5'
1	S2	576	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	O4'-C4'-C5'-O5'
3	L5	4306	OMU	C3'-C4'-C5'-O5'
3	L5	4420	PSU	C3'-C4'-C5'-O5'
66	Lr	2	SAC	OAC-C1A-N-CA
1	S2	512	A2M	O4'-C4'-C5'-O5'
1	S2	1288	OMU	C3'-C4'-C5'-O5'
3	L5	4532	PSU	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
1	S2	590	A2M	C3'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	4569	PSU	C3'-C4'-C5'-O5'
84	At	16	H2U	C2'-C1'-N1-C6
29	SV	1	AME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
1	S2	590	A2M	O4'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
3	L5	3944	OMG	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C2
1	S2	576	A2M	O4'-C4'-C5'-O5'
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3844	PSU	O4'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4306	OMU	O4'-C4'-C5'-O5'
1	S2	1248	B8N	C32-C33-C34-O36
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
81	Lo	53	MLZ	CG-CD-CE-NZ
1	S2	1248	B8N	C32-C33-C34-O35
3	L5	4447	5MC	C2'-C1'-N1-C2
1	S2	512	A2M	C3'-C4'-C5'-O5'
66	Lr	2	SAC	C-CA-CB-OG
81	Lo	53	MLZ	CA-CB-CG-CD
3	L5	2422	OMC	C3'-C4'-C5'-O5'
1	S2	1288	OMU	C1'-C2'-O2'-CM2
3	L5	3718	A2M	C1'-C2'-O2'-CM'
20	SX	62	HY3	O-C-CA-C3
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	3944	OMG	O4'-C4'-C5'-O5'
1	S2	1248	B8N	C31-C32-C33-C34
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
1	S2	1248	B8N	N34-C33-C34-O36
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
84	At	16	H2U	C2'-C1'-N1-C2
86	5A	50	5CT	C-CA-CB-CG
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	1625	OMG	C3'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
1	S2	428	OMU	C2'-C1'-N1-C6
87	EF	79	M3L	CD-CE-NZ-CM1
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	4447	5MC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
81	Lo	53	MLZ	N-CA-CB-CG
3	L5	3729	PSU	O4'-C4'-C5'-O5'
87	EF	79	M3L	CD-CE-NZ-CM3
85	Pt	21	H2U	C4'-C5'-O5'-P
87	EF	79	M3L	CD-CE-NZ-CM2
1	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
1	S2	627	OMU	C2'-C1'-N1-C6
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	4500	PSU	O4'-C1'-C5-C4
3	L5	1326	A2M	C3'-C4'-C5'-O5'
84	At	16	H2U	C4'-C5'-O5'-P
87	EF	55	MLY	CD-CE-NZ-CH1
1	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
1	S2	1248	B8N	N34-C33-C34-O35
86	5A	50	5CT	CD-CE-NZ-C1
85	Pt	21	H2U	C2'-C1'-N1-C6
3	L5	1322	1MA	C2'-C1'-N9-C4
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	398	A2M	C3'-C4'-C5'-O5'
3	L5	3844	PSU	C3'-C4'-C5'-O5'
1	S2	627	OMU	O4'-C1'-N1-C6
85	Pt	21	H2U	C2'-C1'-N1-C2
1	S2	428	OMU	O4'-C1'-N1-C6
3	L5	1322	1MA	C2'-C1'-N9-C8
1	S2	99	A2M	C1'-C2'-O2'-CM'
1	S2	468	A2M	C1'-C2'-O2'-CM'
1	S2	1383	A2M	C1'-C2'-O2'-CM'
3	L5	3830	A2M	C1'-C2'-O2'-CM'
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4532	PSU	C3'-C4'-C5'-O5'
3	L5	4637	OMG	O4'-C4'-C5'-O5'
84	At	20	H2U	C3'-C4'-C5'-O5'
1	S2	1326	UY1	C2'-C1'-C5-C6
1	S2	627	OMU	O4'-C1'-N1-C2
1	S2	428	OMU	O4'-C1'-N1-C2
1	S2	668	A2M	C2'-C1'-N9-C8
3	L5	3887	OMC	C4'-C5'-O5'-P
1	S2	428	OMU	C2'-C1'-N1-C2
1	S2	627	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
86	5A	50	5CT	N-CA-CB-CG

There are no ring outliers.

90 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2351	OMC	1	0
3	L5	2632	PSU	1	0
3	L5	3867	A2M	2	0
1	S2	573	PSU	1	0
1	S2	1445	PSU	3	0
3	L5	4637	OMG	1	0
1	S2	627	OMU	1	0
1	S2	1337	4AC	2	0
3	L5	3764	PSU	1	0
3	L5	2415	OMU	1	0
3	L5	3887	OMC	1	0
1	S2	1447	OMG	2	0
3	L5	4196	OMG	1	0
1	S2	1639	G7M	1	0
3	L5	3723	A2M	1	0
3	L5	2422	OMC	1	0
1	S2	644	OMG	1	0
1	S2	1239	PSU	1	0
1	S2	867	OMG	1	0
1	S2	509	OMG	3	0
1	S2	572	PSU	1	0
1	S2	601	OMG	1	0
3	L5	4523	A2M	1	0
1	S2	1643	PSU	1	0
3	L5	3899	OMG	1	0
1	S2	681	PSU	1	0
1	S2	1850	MA6	1	0
3	L5	4569	PSU	1	0
1	S2	36	PSU	1	0
3	L5	3884	PSU	1	0
1	S2	27	A2M	1	0
2	L8	75	OMG	1	0
84	At	37	MIA	1	0
1	S2	1232	PSU	2	0
1	S2	1177	PSU	1	0
1	S2	1490	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2815	A2M	2	0
1	S2	484	A2M	1	0
1	S2	93	PSU	2	0
3	L5	3925	OMU	1	0
3	L5	2861	OMC	1	0
3	L5	3718	A2M	3	0
1	S2	576	A2M	2	0
3	L5	5001	PSU	1	0
3	L5	3701	OMC	1	0
3	L5	2839	PSU	1	0
85	Pt	21	H2U	1	0
1	S2	1174	PSU	1	0
1	S2	1328	OMG	2	0
1	S2	174	OMC	1	0
84	At	16	H2U	1	0
1	S2	1678	A2M	1	0
3	L5	1340	OMC	2	0
3	L5	2787	A2M	1	0
3	L5	2364	OMG	2	0
1	S2	1288	OMU	1	0
3	L5	4447	5MC	1	0
3	L5	1326	A2M	1	0
3	L5	2876	OMG	1	0
1	S2	99	A2M	1	0
3	L5	4531	PSU	1	0
87	EF	79	M3L	2	0
66	Lr	2	SAC	1	0
3	L5	2363	A2M	2	0
3	L5	3818	UY1	1	0
3	L5	4521	PSU	1	0
3	L5	4620	OMU	1	0
3	L5	4689	PSU	1	0
3	L5	3724	A2M	1	0
1	S2	121	OMU	1	0
1	S2	116	OMU	3	0
3	L5	3627	OMG	1	0
3	L5	4536	OMC	1	0
3	L5	4392	OMG	1	0
3	L5	4530	UR3	1	0
1	S2	1031	A2M	1	0
3	L5	3785	A2M	1	0
1	S2	1136	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1871	A2M	1	0
3	L5	1536	PSU	1	0
86	5A	50	5CT	5	0
3	L5	2424	OMG	1	0
3	L5	1881	OMC	3	0
2	L8	69	PSU	1	0
3	L5	4579	PSU	2	0
1	S2	1625	PSU	1	0
1	S2	428	OMU	1	0
3	L5	398	A2M	1	0
2	L8	14	OMU	1	0
3	L5	4370	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 486 are monoatomic - leaving 24 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	$\# Z > 2$
88	SPD	S2	1901	-	9,9,9	0.16	0	8,8,8	0.26	0
88	SPD	L5	5103	-	9,9,9	0.33	0	8,8,8	0.93	0
88	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.92	0
92	PUT	L5	5113	-	5,5,5	0.10	0	4,4,4	0.12	0
92	PUT	L5	5115	-	5,5,5	0.14	0	4,4,4	0.23	0
88	SPD	L5	5104	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPD	L5	5106	-	9,9,9	0.31	0	8,8,8	0.89	0
92	PUT	L5	5112	-	5,5,5	0.15	0	4,4,4	0.26	0
88	SPD	L5	5108	-	9,9,9	0.15	0	8,8,8	0.24	0
98	ZIY	EF	502	-	81,82,82	1.02	4 (4%)	111,117,117	1.42	14 (12%)
93	3H3	L5	5119	-	34,34,34	3.30	13 (38%)	36,45,45	3.67	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5102	-	9,9,9	0.31	0	8,8,8	0.89	0
91	ANM	L5	5101	89	20,20,20	1.19	1 (5%)	24,27,27	1.42	3 (12%)
92	PUT	L5	5111	-	5,5,5	0.08	0	4,4,4	0.16	0
88	SPD	L5	5107	-	9,9,9	0.18	0	8,8,8	0.40	0
92	PUT	L5	5116	-	5,5,5	0.09	0	4,4,4	0.13	0
92	PUT	L5	5118	-	5,5,5	0.16	0	4,4,4	0.25	0
96	MET	Pt	78	85	6,7,8	0.54	0	2,7,9	1.23	0
97	GSP	EF	501	90	33,34,34	1.90	3 (9%)	47,54,54	1.71	9 (19%)
92	PUT	L5	5114	-	5,5,5	0.13	0	4,4,4	0.20	0
88	SPD	L5	5110	-	9,9,9	0.33	0	8,8,8	0.89	0
92	PUT	L5	5117	-	5,5,5	0.14	0	4,4,4	0.21	0
88	SPD	L5	5109	-	9,9,9	0.32	0	8,8,8	0.90	0
95	PHE	At	77	84	10,11,12	0.33	0	8,13,15	0.71	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
88	SPD	S2	1901	-	-	3/7/7/7	-
88	SPD	L5	5103	-	-	3/7/7/7	-
88	SPD	L5	5105	-	-	2/7/7/7	-
92	PUT	L5	5113	-	-	0/3/3/3	-
92	PUT	L5	5115	-	-	0/3/3/3	-
88	SPD	L5	5104	-	-	3/7/7/7	-
88	SPD	L5	5106	-	-	0/7/7/7	-
92	PUT	L5	5112	-	-	0/3/3/3	-
88	SPD	L5	5108	-	-	2/7/7/7	-
98	ZIY	EF	502	-	-	11/120/140/140	0/3/4/4
93	3H3	L5	5119	-	-	15/39/51/51	0/1/2/2
88	SPD	L5	5102	-	-	0/7/7/7	-
91	ANM	L5	5101	89	-	0/10/23/23	0/2/2/2
92	PUT	L5	5111	-	-	1/3/3/3	-
88	SPD	L5	5107	-	-	2/7/7/7	-
92	PUT	L5	5116	-	-	0/3/3/3	-
92	PUT	L5	5118	-	-	1/3/3/3	-
96	MET	Pt	78	85	-	0/5/6/8	-
97	GSP	EF	501	90	-	0/21/38/38	0/3/3/3
92	PUT	L5	5114	-	-	1/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5110	-	-	2/7/7/7	-
92	PUT	L5	5117	-	-	3/3/3/3	-
88	SPD	L5	5109	-	-	1/7/7/7	-
95	PHE	At	77	84	-	2/5/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	EF	501	GSP	PG-S1G	-9.47	1.70	1.90
93	L5	5119	3H3	C13-C12	8.92	1.53	1.33
93	L5	5119	3H3	O3-C22	7.71	1.38	1.23
93	L5	5119	3H3	O4-C23	7.27	1.37	1.23
93	L5	5119	3H3	C23-N	6.66	1.48	1.37
93	L5	5119	3H3	C22-N	5.57	1.46	1.37
93	L5	5119	3H3	C3-C2	5.54	1.54	1.33
98	EF	502	ZIY	C72-C71	-4.71	1.32	1.51
91	L5	5101	ANM	O2-C5	4.56	1.45	1.35
93	L5	5119	3H3	C19-C20	3.39	1.58	1.53
93	L5	5119	3H3	O1-C11	-3.10	1.39	1.44
93	L5	5119	3H3	C4-C3	2.82	1.53	1.44
98	EF	502	ZIY	C54-C55	-2.47	1.50	1.53
93	L5	5119	3H3	O-C10	-2.31	1.16	1.21
93	L5	5119	3H3	O1-C10	2.26	1.39	1.34
93	L5	5119	3H3	C24-C20	-2.19	1.49	1.53
93	L5	5119	3H3	O2-C16	-2.17	1.18	1.21
98	EF	502	ZIY	C45-C47	2.08	1.55	1.52
98	EF	502	ZIY	C53-C54	2.07	1.56	1.53
97	EF	501	GSP	C2-N3	2.03	1.38	1.33
97	EF	501	GSP	C5-N7	-2.00	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	L5	5119	3H3	O3-C22-N	-10.23	104.53	120.30
93	L5	5119	3H3	C22-N-C23	-9.59	114.32	125.87
93	L5	5119	3H3	O4-C23-N	-8.79	106.74	120.30
98	EF	502	ZIY	O33-C75-C74	6.82	126.71	118.96
93	L5	5119	3H3	O3-C22-C21	-6.57	110.09	122.62
93	L5	5119	3H3	C15-C14-C13	-5.99	104.99	110.73
93	L5	5119	3H3	O4-C23-C24	-5.20	112.71	122.62
97	EF	501	GSP	C5-C4-N3	-5.02	120.41	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	EF	501	GSP	C2-N3-C4	4.61	120.23	112.30
91	L5	5101	ANM	O2-C5-C6	4.42	118.96	111.09
98	EF	502	ZIY	O35-C79-C01	3.64	118.37	110.80
97	EF	501	GSP	PB-O3B-PG	-3.64	119.85	133.17
93	L5	5119	3H3	C25-C12-C13	-3.60	114.33	123.56
93	L5	5119	3H3	C21-C22-N	-3.39	111.81	115.92
98	EF	502	ZIY	C70-C69-N17	3.33	124.94	118.87
97	EF	501	GSP	N9-C4-N3	3.20	132.34	125.95
93	L5	5119	3H3	C11-C12-C13	-3.17	108.62	119.78
98	EF	502	ZIY	C36-N05-C30	-3.05	107.23	112.01
97	EF	501	GSP	C2-N1-C6	-3.01	119.66	125.11
93	L5	5119	3H3	C7-C8-C9	-2.97	119.74	125.92
93	L5	5119	3H3	O1-C10-C9	2.92	117.74	111.39
98	EF	502	ZIY	C30-C28-N02	2.79	123.94	118.87
98	EF	502	ZIY	C45-C44-N08	2.73	119.67	116.13
93	L5	5119	3H3	C4-C3-C2	-2.73	106.04	124.25
98	EF	502	ZIY	C73-N20-C70	-2.72	107.74	112.01
91	L5	5101	ANM	C2-O2-C5	-2.70	113.52	117.72
93	L5	5119	3H3	C8-C9-C10	-2.69	116.36	122.78
97	EF	501	GSP	N9-C8-N7	-2.62	108.55	113.40
97	EF	501	GSP	C5-C6-N1	2.56	119.76	113.25
97	EF	501	GSP	C8-N7-C5	2.45	108.62	104.26
97	EF	501	GSP	O6-C6-C5	-2.43	120.11	126.53
93	L5	5119	3H3	C1-C2-C3	-2.42	121.11	126.11
91	L5	5101	ANM	O2-C5-O3	-2.37	118.41	122.99
98	EF	502	ZIY	O37-C79-C01	-2.32	119.34	124.46
98	EF	502	ZIY	C77-O35-C79	2.26	120.90	117.55
98	EF	502	ZIY	O29-C69-C70	-2.26	115.56	120.28
93	L5	5119	3H3	C6-C7-C8	-2.25	107.07	112.73
98	EF	502	ZIY	C71-C70-C69	2.24	115.22	110.83
93	L5	5119	3H3	C24-C23-N	-2.19	113.26	115.92
98	EF	502	ZIY	C32-C30-C28	-2.18	106.55	110.83
93	L5	5119	3H3	C25-C12-C11	-2.14	111.72	115.96
93	L5	5119	3H3	C19-C18-C17	-2.07	108.74	112.96
98	EF	502	ZIY	C53-C54-C55	-2.04	110.19	113.00
98	EF	502	ZIY	C71-C72-C73	2.02	110.52	104.90

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	S2	1901	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
93	L5	5119	3H3	C2-C1-C11-O1
93	L5	5119	3H3	C2-C1-C11-C12
93	L5	5119	3H3	C-C1-C11-O1
93	L5	5119	3H3	C-C1-C11-C12
93	L5	5119	3H3	C1-C11-O1-C10
93	L5	5119	3H3	C12-C11-O1-C10
93	L5	5119	3H3	C9-C10-O1-C11
93	L5	5119	3H3	C12-C13-C14-C16
93	L5	5119	3H3	C25-C12-C13-C14
93	L5	5119	3H3	C1-C11-C12-C25
98	EF	502	ZIY	C47-C48-O18-C52
98	EF	502	ZIY	C62-C63-C64-C65
98	EF	502	ZIY	N20-C74-C75-O33
98	EF	502	ZIY	O31-C74-C75-O33
98	EF	502	ZIY	C22-C14-O03-C19
98	EF	502	ZIY	C13-C14-O03-C19
93	L5	5119	3H3	O-C10-O1-C11
93	L5	5119	3H3	C2-C3-C4-C5
88	L5	5103	SPD	C3-C4-C5-N6
88	L5	5104	SPD	C3-C4-C5-N6
98	EF	502	ZIY	N17-C63-C64-C65
98	EF	502	ZIY	C49-C48-O18-C52
93	L5	5119	3H3	O1-C10-C9-C8
88	L5	5110	SPD	C3-C4-C5-N6
92	L5	5117	PUT	C1-C2-C3-C4
92	L5	5118	PUT	C1-C2-C3-C4
88	L5	5103	SPD	C8-C7-N6-C5
88	S2	1901	SPD	C3-C4-C5-N6
88	L5	5108	SPD	N6-C7-C8-C9
95	At	77	PHE	CA-CB-CG-CD2
95	At	77	PHE	CA-CB-CG-CD1
93	L5	5119	3H3	O-C10-C9-C8
92	L5	5117	PUT	N1-C1-C2-C3
88	L5	5109	SPD	C2-C3-C4-C5
88	L5	5104	SPD	C2-C3-C4-C5
88	L5	5107	SPD	N6-C7-C8-C9
98	EF	502	ZIY	C63-C64-C65-C66
88	L5	5105	SPD	C8-C7-N6-C5
88	L5	5108	SPD	N1-C2-C3-C4
88	L5	5105	SPD	N6-C7-C8-C9
88	L5	5107	SPD	C8-C7-N6-C5
92	L5	5111	PUT	C2-C3-C4-N2

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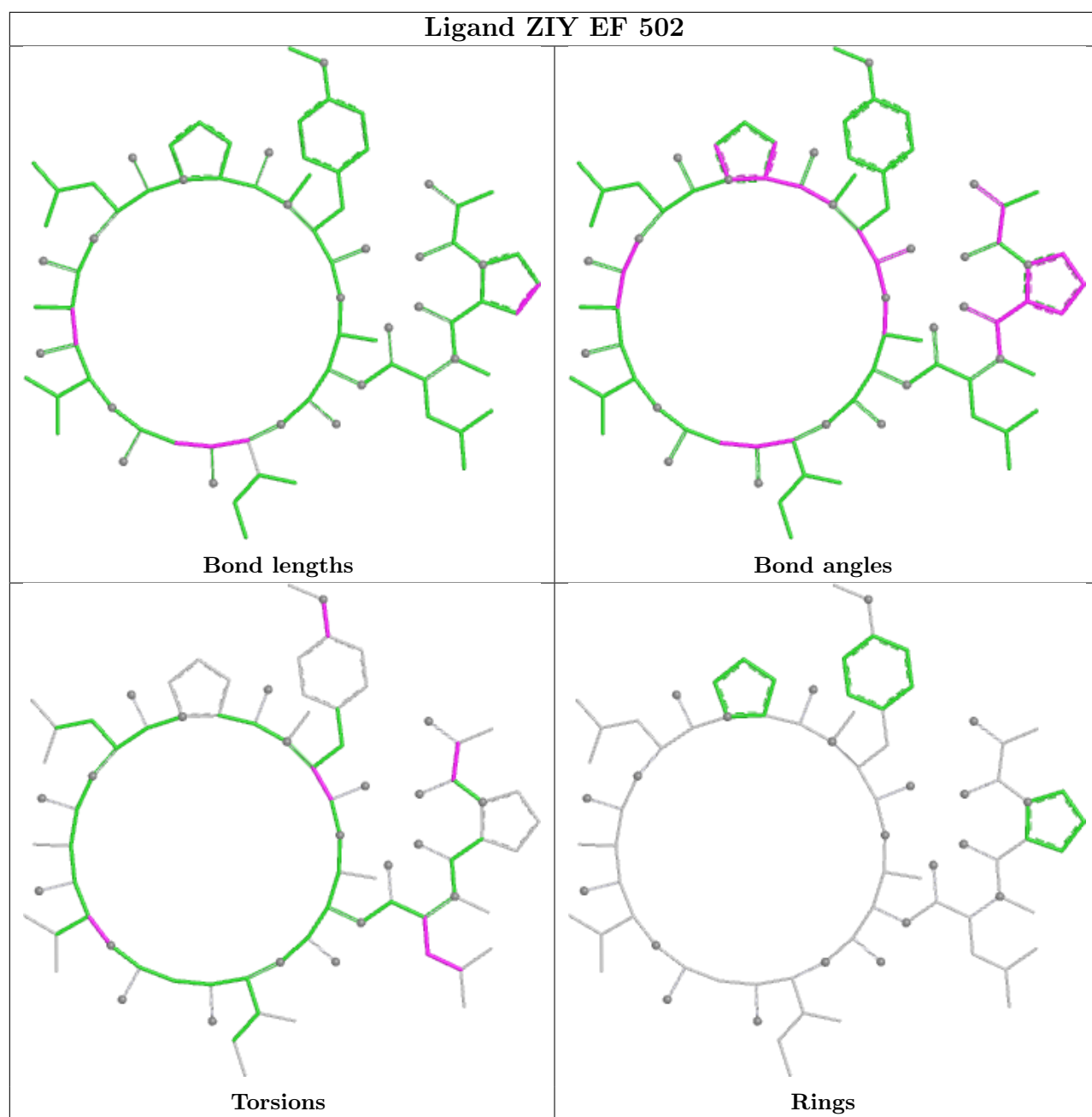
Mol	Chain	Res	Type	Atoms
98	EF	502	ZIY	C63-C64-C65-C67
88	L5	5104	SPD	C8-C7-N6-C5
88	L5	5103	SPD	C2-C3-C4-C5
88	L5	5110	SPD	N6-C7-C8-C9
92	L5	5114	PUT	C2-C3-C4-N2
92	L5	5117	PUT	C2-C3-C4-N2
88	S2	1901	SPD	C8-C7-N6-C5
93	L5	5119	3H3	C12-C13-C14-C15
98	EF	502	ZIY	N02-C01-C79-O35

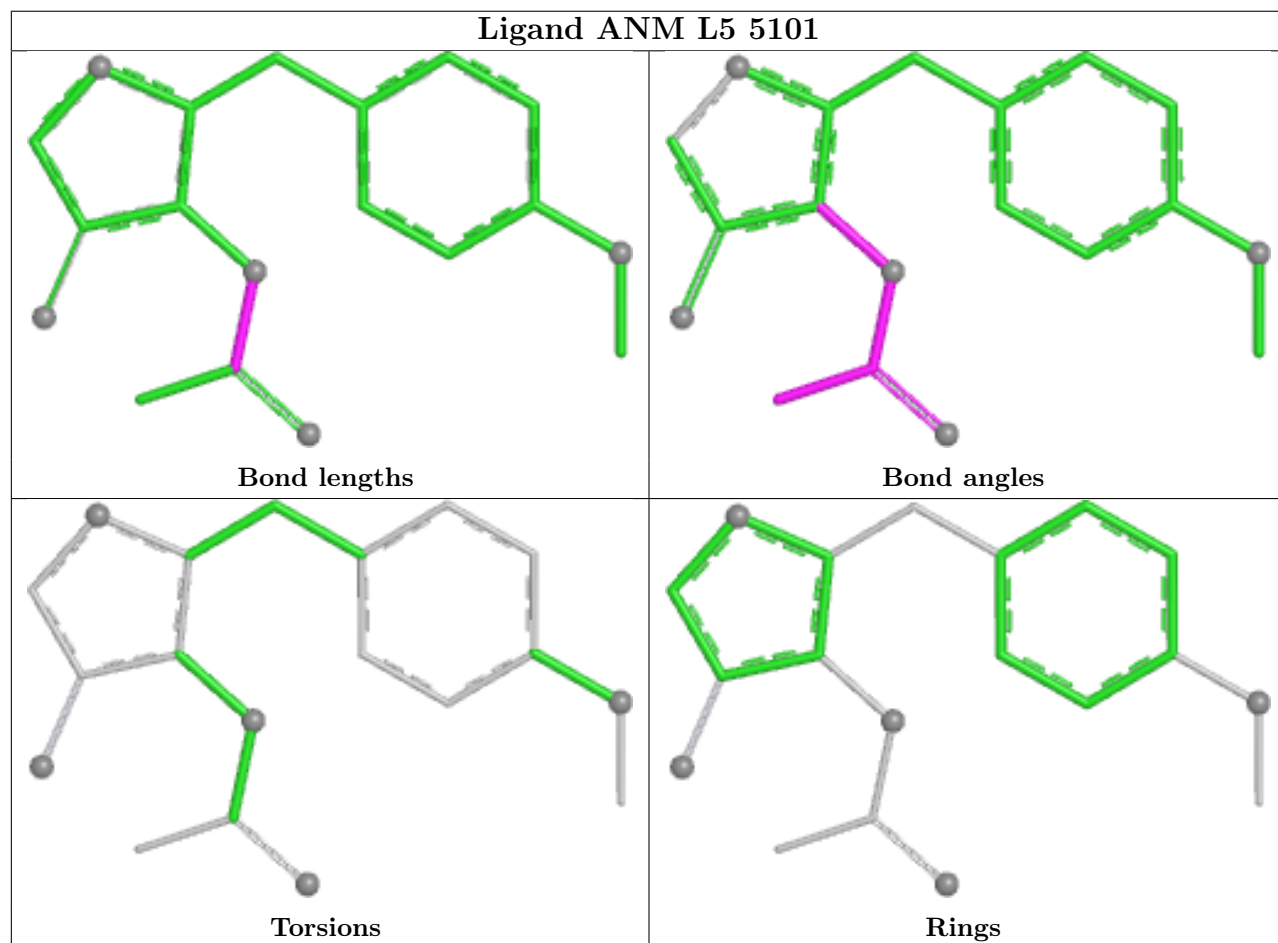
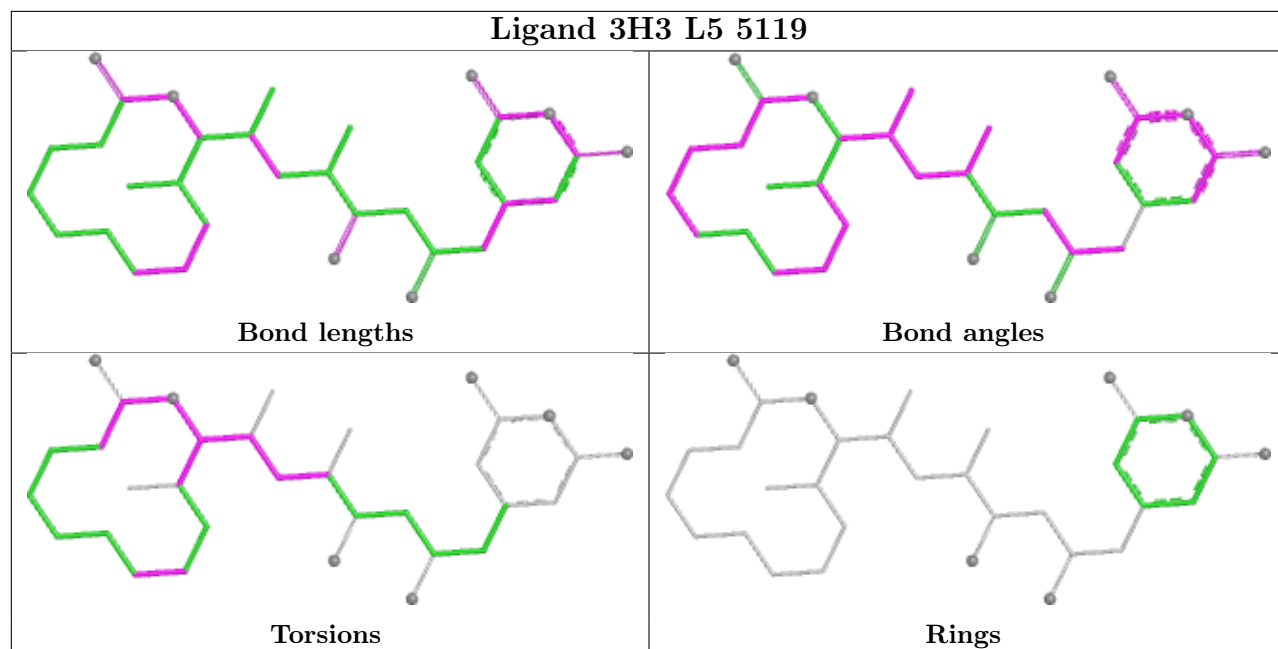
There are no ring outliers.

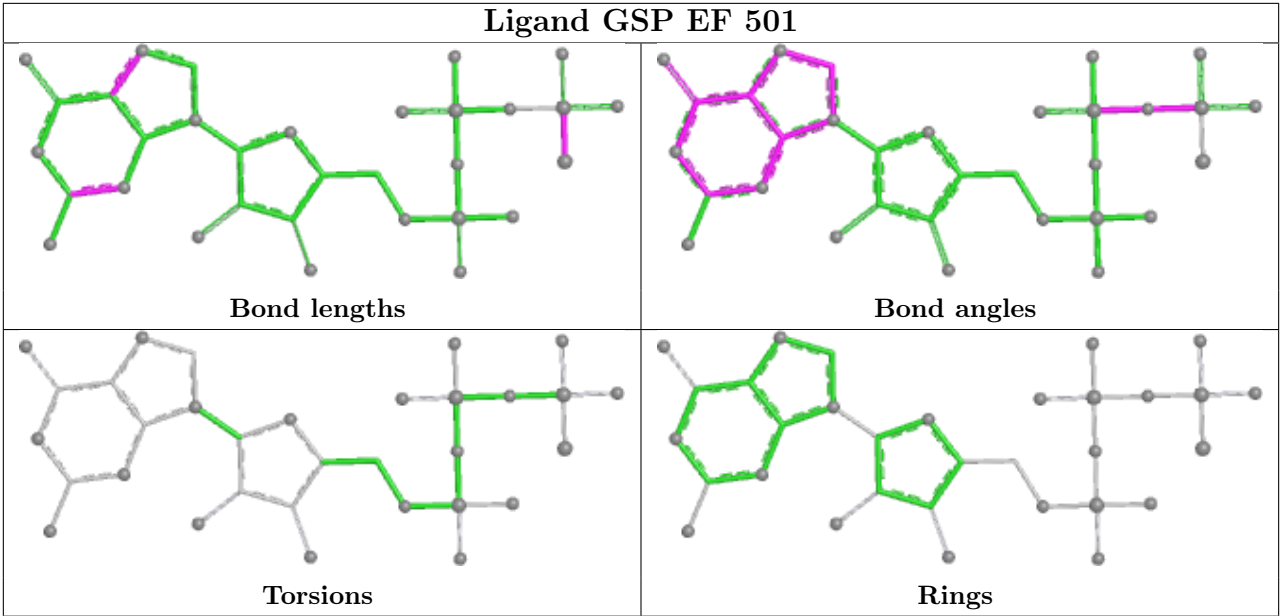
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5108	SPD	1	0
93	L5	5119	3H3	13	0
88	L5	5110	SPD	2	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
3	L5	12
1	S2	5
44	LE	2
68	Lb	1
64	LW	1
25	SL	1
5	SB	1
54	LI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	34.19
1	LE	76:ALA	C	88:VAL	N	25.47
1	S2	739:C	O3'	799:U	P	22.94
1	L5	1706:A	O3'	1719:A	P	19.41
1	LW	64:SER	C	71:ARG	N	19.29
1	L5	989:U	O3'	1064:G	P	17.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	130:G	O3'	139:C	P	16.19
1	S2	1761:U	O3'	1771:G	P	15.77
1	L5	4776:G	O3'	4858:C	P	15.69
1	L5	760:G	O3'	903:C	P	15.45
1	L5	1220:G	O3'	1234:G	P	14.67
1	L5	518:G	O3'	643:C	P	14.01
1	L5	2910:G	O3'	3584:C	P	13.51
1	SL	23:VAL	C	32:LYS	N	13.49
1	SB	10:THR	C	21:VAL	N	12.53
1	L5	2113:G	O3'	2249:C	P	12.42
1	L5	3977:C	O3'	4034:G	P	12.10
1	S2	698:G	O3'	730:C	P	11.58
1	L5	499:G	O3'	503:C	P	9.06
1	LI	104:SER	C	113:THR	N	8.85
1	S2	225:G	O3'	287:U	P	6.79
1	LE	221:LYS	C	238:GLU	N	6.36
1	L5	1101:C	O3'	1168:G	P	5.88
1	L5	2543:A	O3'	2547:G	P	5.84

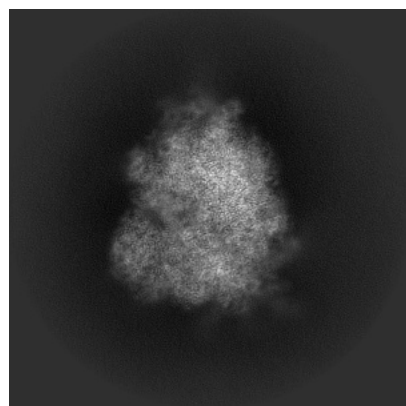
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29758. These allow visual inspection of the internal detail of the map and identification of artifacts.

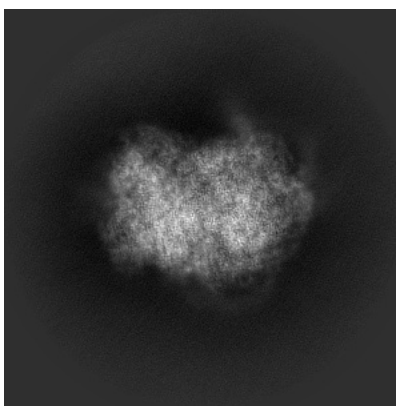
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

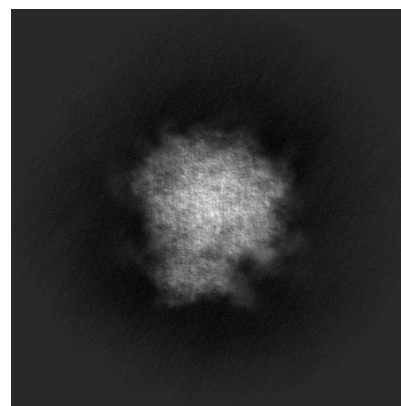
6.1.1 Primary map



X

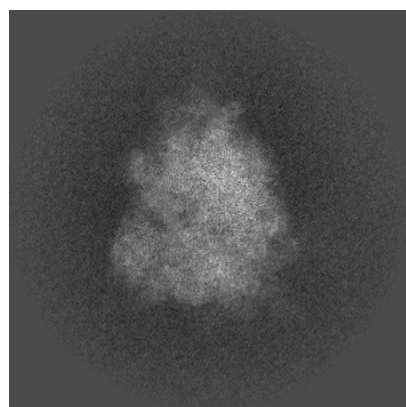


Y

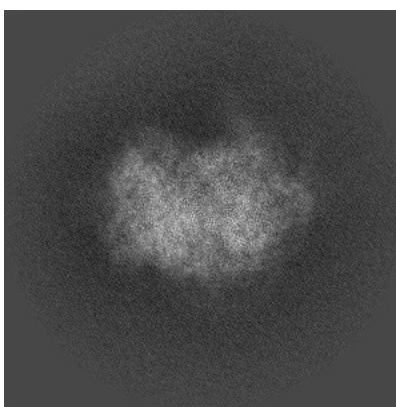


Z

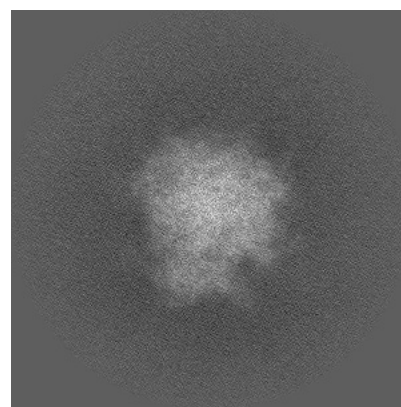
6.1.2 Raw map



X



Y

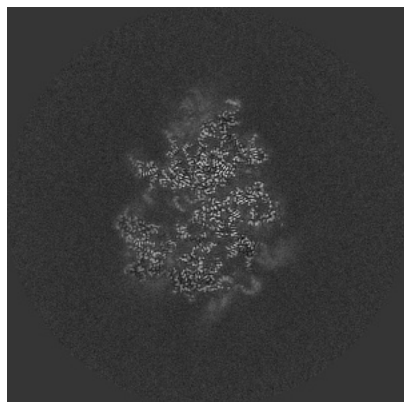


Z

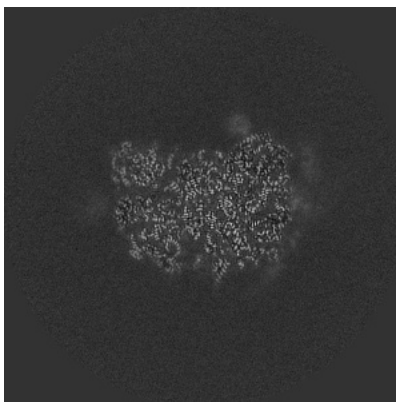
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

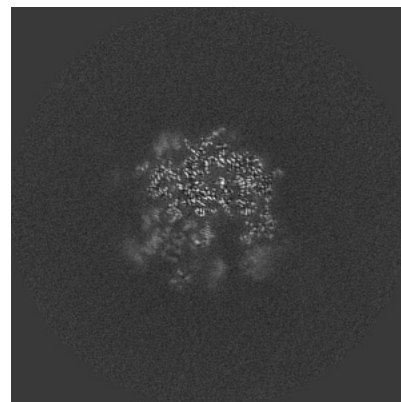
6.2.1 Primary map



X Index: 320

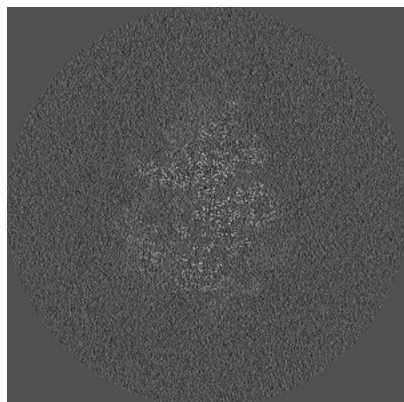


Y Index: 320

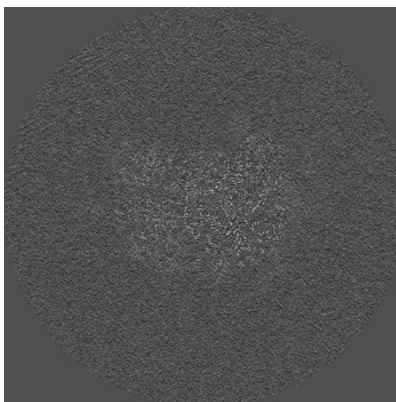


Z Index: 320

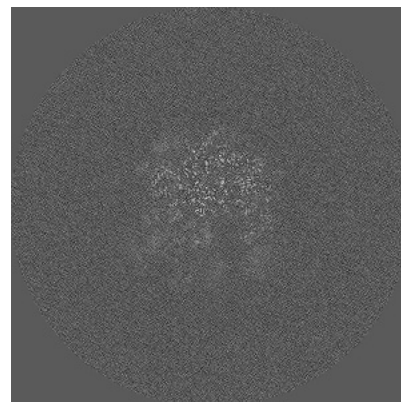
6.2.2 Raw map



X Index: 320



Y Index: 320

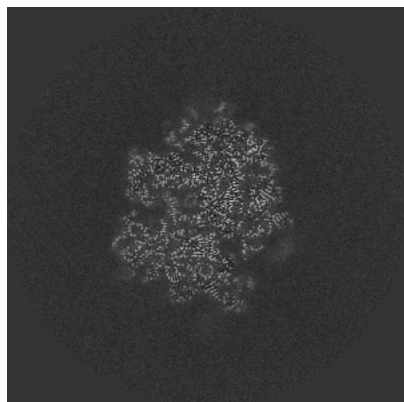


Z Index: 320

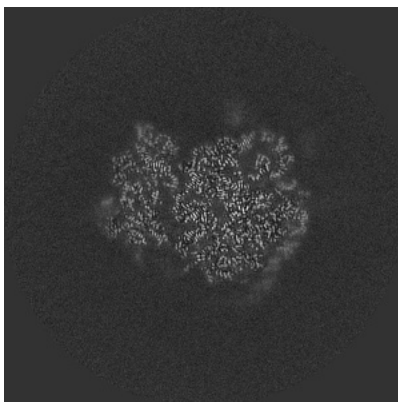
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

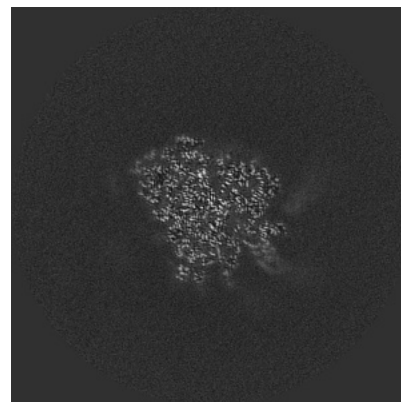
6.3.1 Primary map



X Index: 297

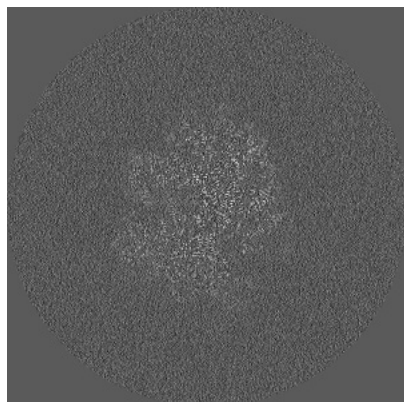


Y Index: 342

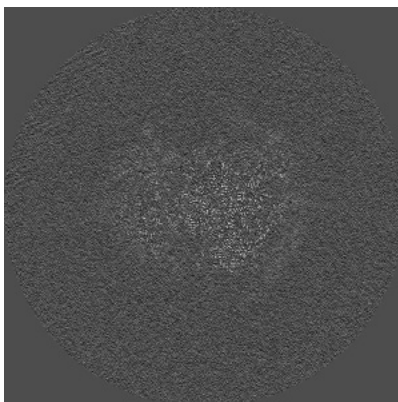


Z Index: 362

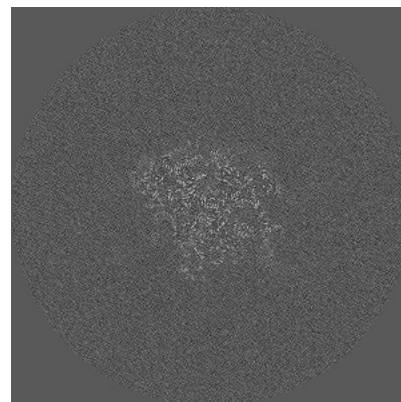
6.3.2 Raw map



X Index: 297



Y Index: 332

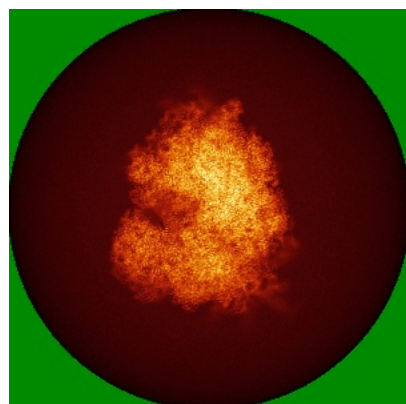


Z Index: 353

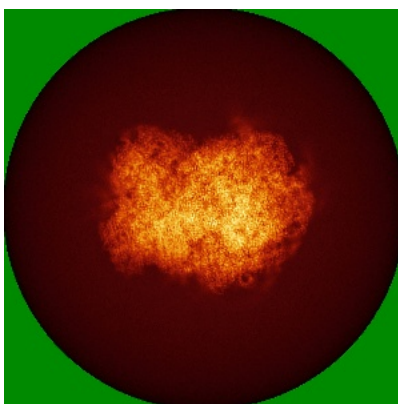
The images above show the largest variance slices of the map in three orthogonal directions.

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

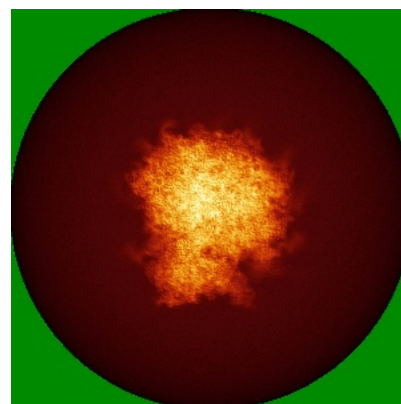
6.4.1 Primary map



X

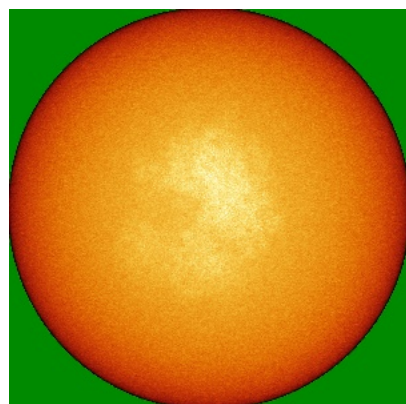


Y

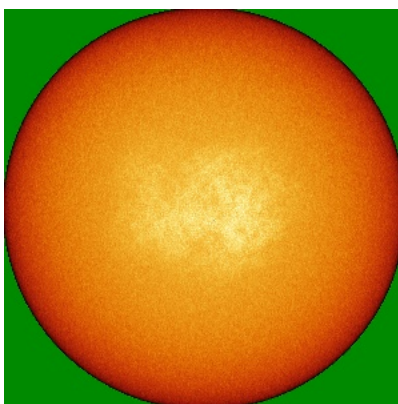


Z

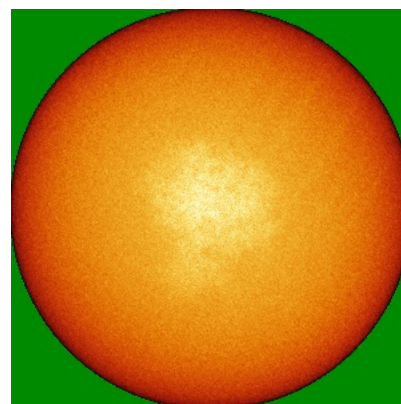
6.4.2 Raw map



X



Y

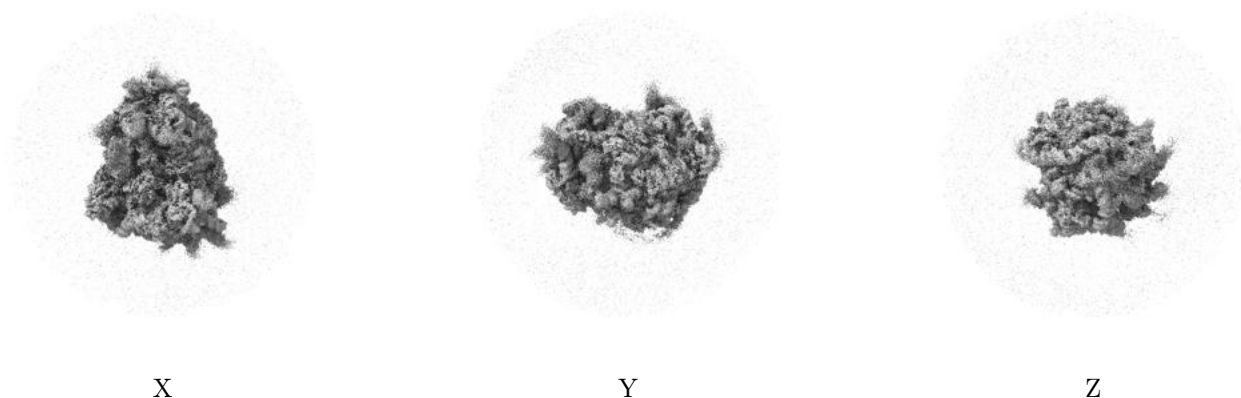


Z

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

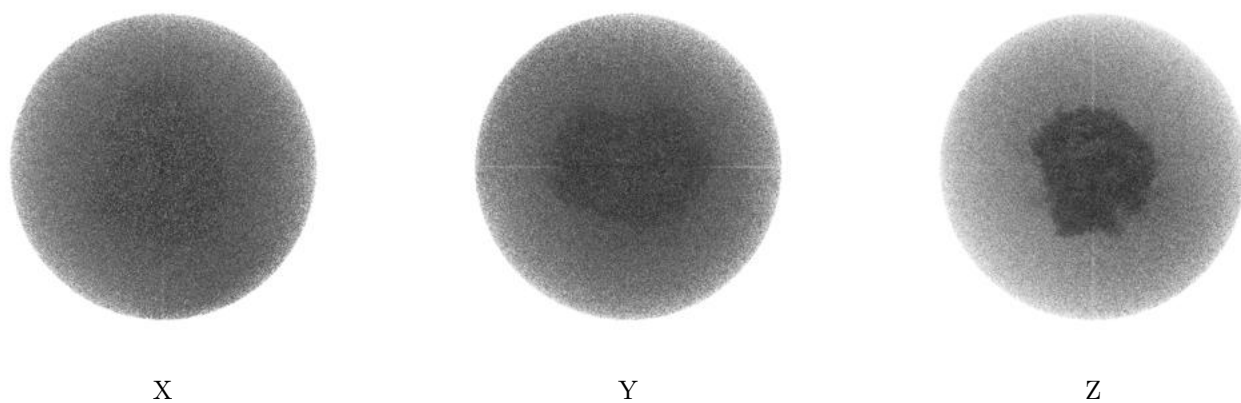
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

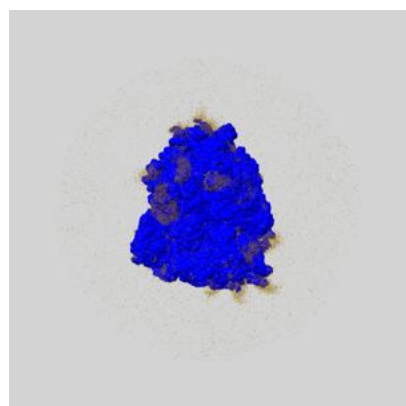
6.6 Mask visualisation [i](#)

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

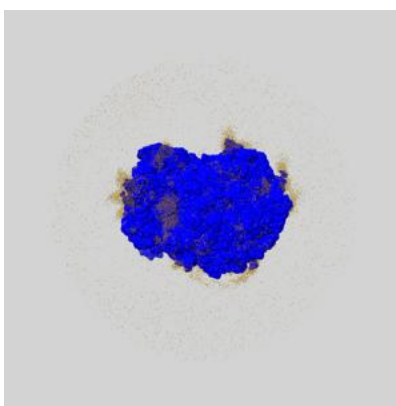
A mask typically either:

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

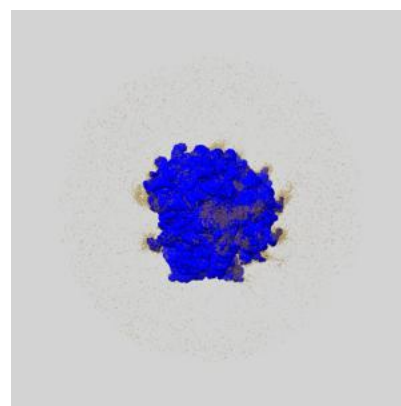
6.6.1 emd_29758_msk_1.map [i](#)



X



Y

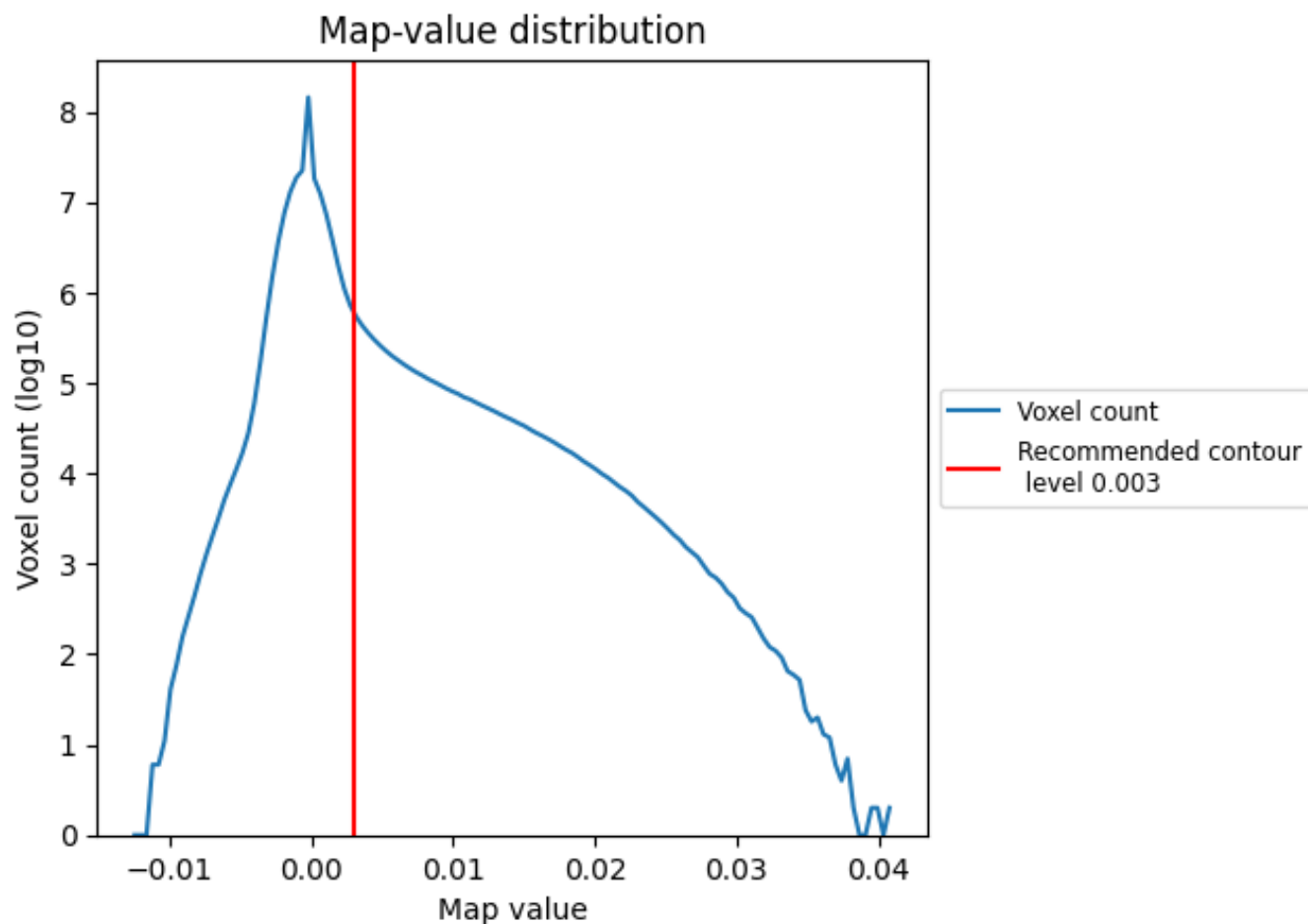


Z

7 Map analysis [i](#)

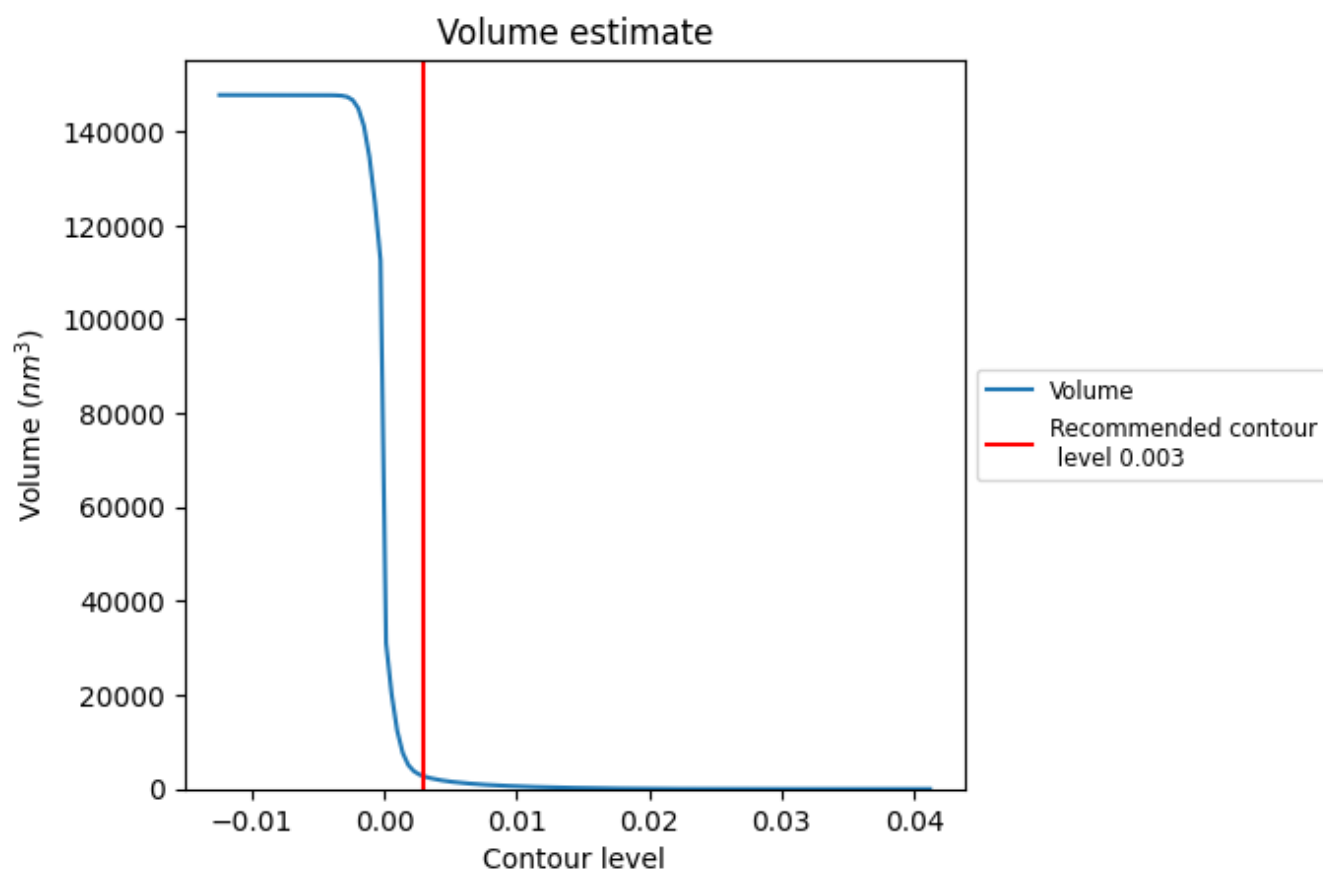
This section contains the results of statistical analysis of the map.

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.

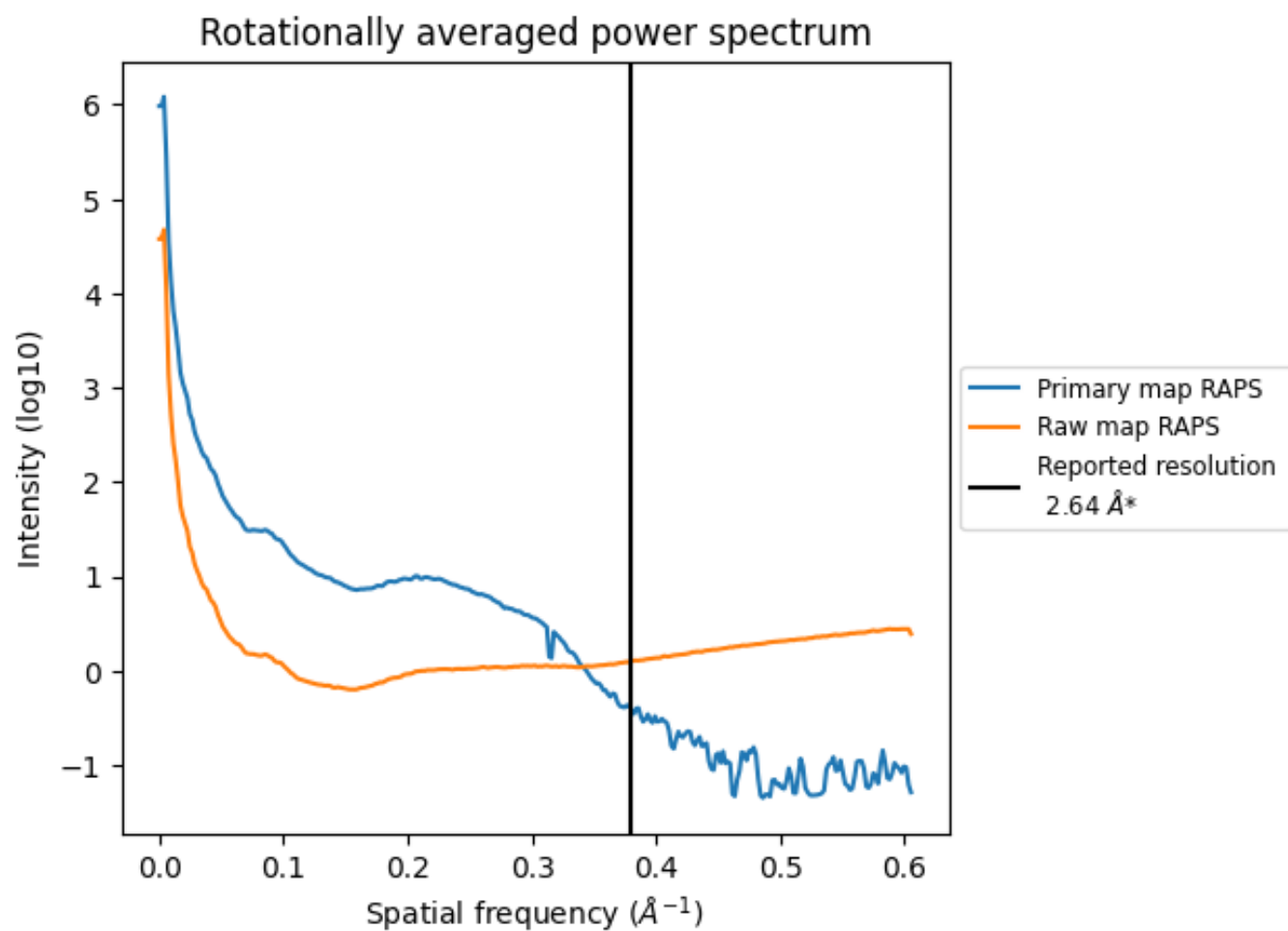
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2694 nm^3 ; this corresponds to an approximate mass of 2433 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 ⓘ

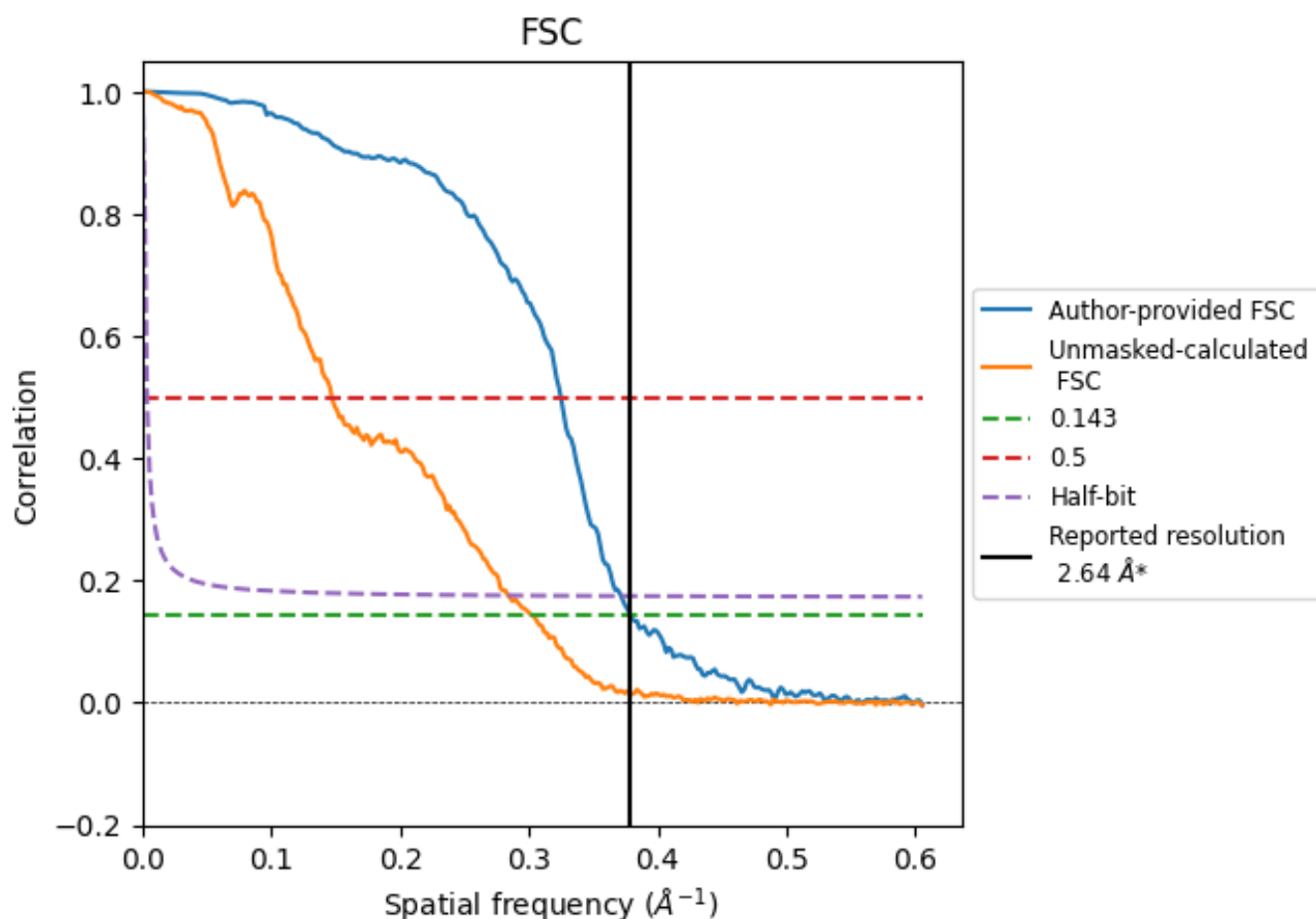


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

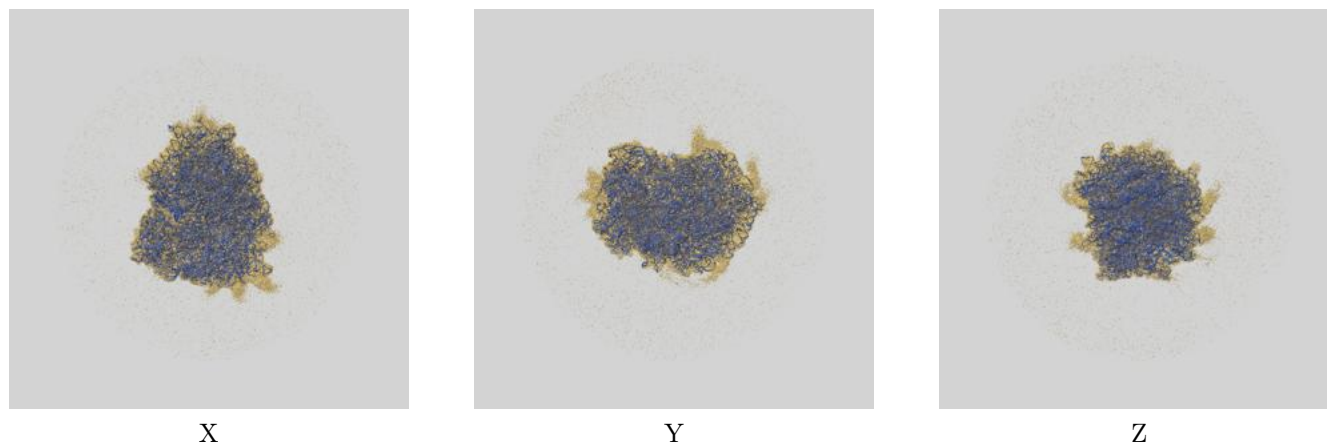
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	3.08	2.69
Unmasked-calculated*	3.30	6.79	3.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.64 by more than 10 %

9 Map-model fit [i](#)

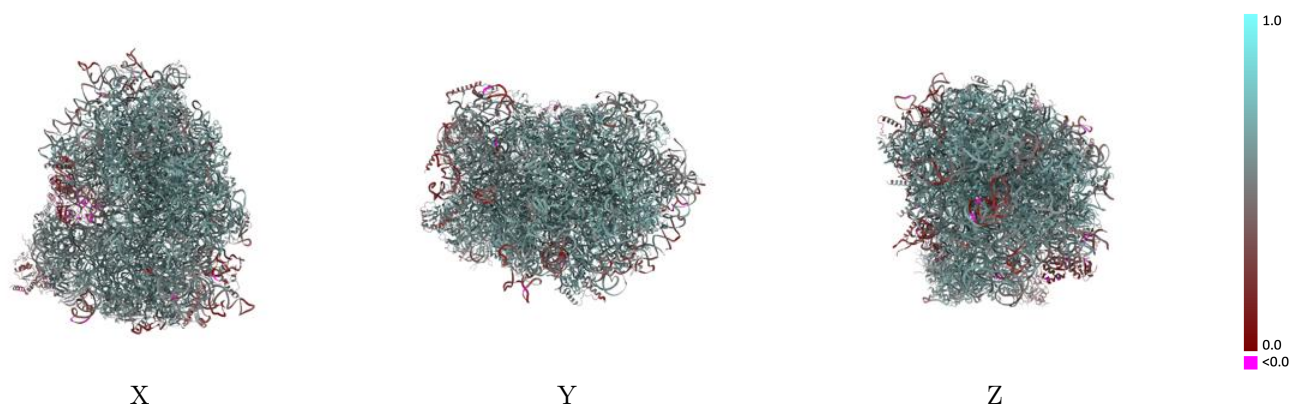
This section contains information regarding the fit between EMDB map EMD-29758 and PDB model 8G5Z. Per-residue inclusion information can be found in section [3](#) on page [30](#).

9.1 Map-model overlay [i](#)



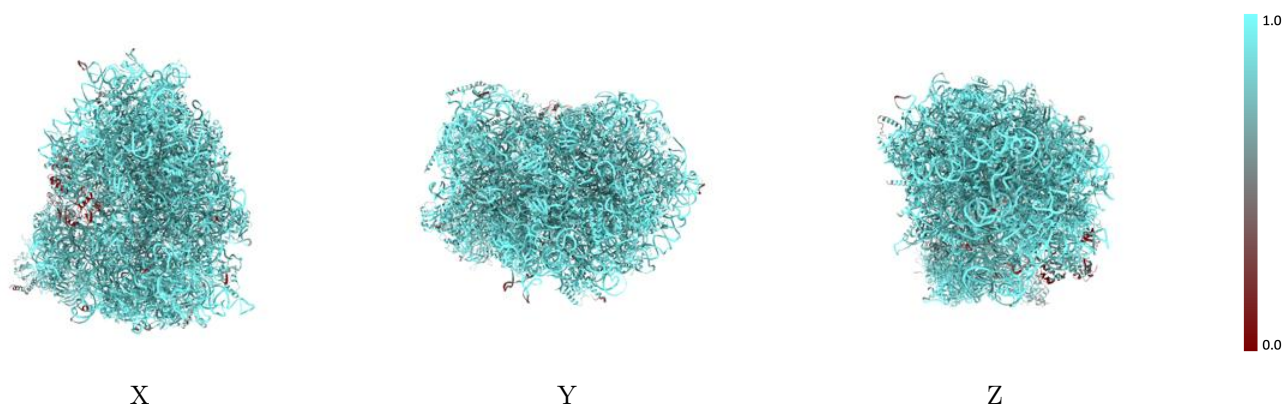
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



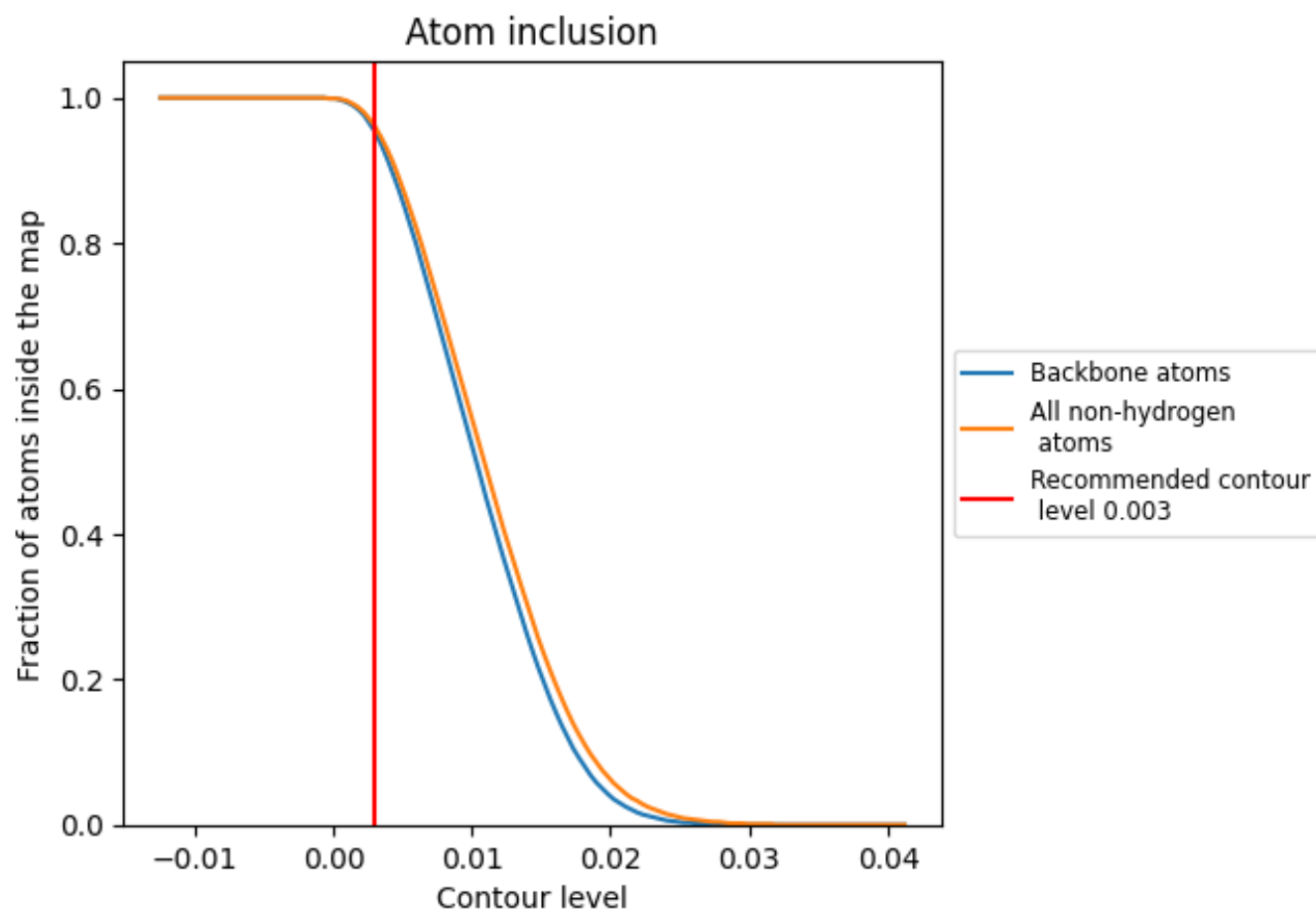
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9620	 0.5700
5A	 0.8440	 0.4390
At	 0.9700	 0.5310
EF	 0.9250	 0.5690
L5	 0.9830	 0.5750
L7	 0.9970	 0.6250
L8	 0.9960	 0.6030
LA	 0.9900	 0.6470
LB	 0.9700	 0.6270
LC	 0.9780	 0.6290
LD	 0.9680	 0.5930
LE	 0.9790	 0.5990
LF	 0.9870	 0.6290
LG	 0.9160	 0.5540
LH	 0.9680	 0.6000
LI	 0.9740	 0.6120
LJ	 0.9610	 0.5820
LK	 0.3550	 0.1790
LL	 0.9610	 0.6000
LM	 0.9780	 0.6140
LN	 0.9980	 0.6530
LO	 0.9720	 0.6230
LP	 0.9840	 0.6410
LQ	 0.9880	 0.6460
LR	 0.9440	 0.5810
LS	 0.9910	 0.6310
LT	 0.9710	 0.6210
LU	 0.9320	 0.5290
LV	 0.9780	 0.6320
LW	 0.8580	 0.4970
LX	 0.9770	 0.6140
LY	 0.9720	 0.6090
LZ	 0.9740	 0.6040
La	 0.9870	 0.6480
Lb	 0.9110	 0.5510



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Chain	Atom inclusion	Q-score
Lc	 0.9610	 0.6060
Ld	 0.9580	 0.5980
Le	 0.9900	 0.6490
Lf	 0.9890	 0.6450
Lg	 0.9590	 0.6160
Lh	 0.9800	 0.6120
Li	 0.9500	 0.5750
Lj	 1.0000	 0.6550
Lk	 0.9320	 0.5500
Ll	 0.9830	 0.6180
Lm	 0.9670	 0.6120
Ln	 0.9770	 0.6260
Lo	 0.9810	 0.6190
Lp	 0.9710	 0.6260
Lq	 0.4000	 0.2120
Lr	 0.9880	 0.6340
Lz	 0.7110	 0.2890
Pt	 0.9900	 0.5610
S2	 0.9880	 0.5600
SA	 0.9580	 0.5850
SB	 0.9530	 0.5880
SC	 0.9650	 0.5940
SD	 0.9420	 0.5460
SE	 0.9580	 0.5560
SF	 0.9620	 0.5730
SG	 0.9310	 0.5150
SH	 0.9020	 0.5190
SI	 0.9500	 0.5490
SJ	 0.9300	 0.5170
SK	 0.9490	 0.5330
SL	 0.9640	 0.5850
SM	 0.6490	 0.3020
SN	 0.9750	 0.6070
SO	 0.9610	 0.5990
SP	 0.9250	 0.5330
SQ	 0.9620	 0.5770
SR	 0.9100	 0.5300
SS	 0.9480	 0.5560
ST	 0.9620	 0.5680
SU	 0.9040	 0.5130
SV	 0.9700	 0.5880
SW	 0.9830	 0.6160

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Chain	Atom inclusion	Q-score
SX	 0.9770	 0.6120
SY	 0.9030	 0.5040
SZ	 0.8810	 0.5360
Sa	 0.9820	 0.6060
Sb	 0.9530	 0.5750
Sc	 0.9090	 0.5370
Sd	 0.9840	 0.5970
Se	 0.9340	 0.5140
Sf	 0.7830	 0.3820
Sg	 0.9050	 0.5040
mR	 0.9570	 0.5310