



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 11:39 pm BST

PDB ID : 9H6I / pdb_00009h6i
EMDB ID : EMD-51899
Title : Structure of the Arabidopsis thaliana 80S ribosome in complex with P- and E-site tRNAs, mRNA, and thermospermine
Authors : Faille, A.; Warren, A.J.
Deposited on : 2024-10-24
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

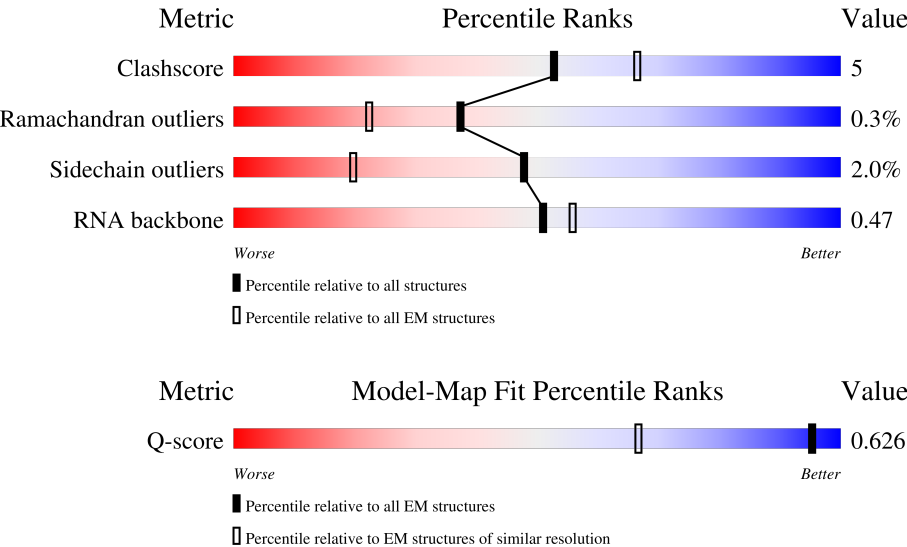
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	2	76	43% 71% 21% 8%
1	W2	76	62% 67% 28% ..
2	3	164	11% 55% 35% 7% ..

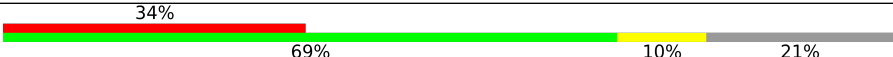
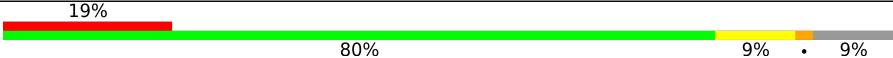
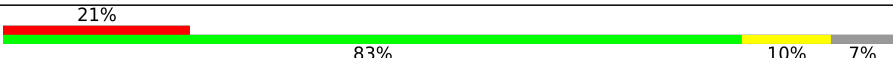
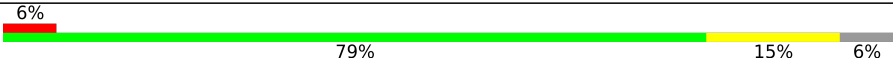
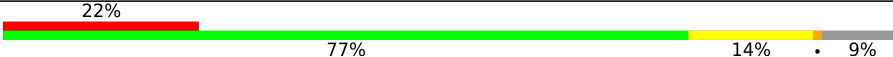
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A	3385	
4	C3	121	
5	BC	25	
6	BM	176	
7	BO	146	
8	AR	83	
9	AU	119	
10	Ma	131	
11	Ia	194	
12	AE	130	
13	AX	112	
14	AP	135	
15	Ja	262	
16	Ea	204	
17	AL	217	
18	Va	142	
19	Ka	133	
20	AW	112	
21	BD	105	
22	BS	389	
23	AM	164	
24	AC	284	
25	BI	140	
26	AH	134	
27	BT	406	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	AV	133	
29	AD	207	
30	AJ	187	
31	BQ	258	
32	BH	206	
33	Da	151	
34	BK	301	
35	AT	112	
36	Pa	62	
37	BP	123	
38	BN	154	
39	BG	256	
40	Fa	120	
41	Ha	146	
42	BU	182	
43	BR	247	
44	Xa	160	
45	BV	262	
46	BJ	221	
47	AO	164	
48	BW	82	
49	AK	214	
50	Na	86	
51	AB	197	
52	BF	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	AA	250	
54	AG	206	
55	Ga	128	
56	BA	51	
57	AF	146	
58	Wa	152	
59	Ta	249	
60	AZ	69	
61	BE	92	
62	Za	298	
63	AQ	143	
64	Oa	64	
65	Ua	150	
66	Ya	150	
67	BB	141	
68	AN	124	
69	Ra	190	
70	BL	143	
71	La	108	
72	Aa	222	
73	AY	95	
74	Ca	56	
75	h1	1805	
76	B1	12	
77	Ba	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	AI	177	49% 42% 10% 48%
79	L3	23	87% 100%

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 208167 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 Transfer RNA Phe (GAA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	76	Total	C	N	O	P	0	0
			1630	726	298	530	76		
1	W2	76	Total	C	N	O	P	0	0
			1629	726	298	529	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	162	Total	C	N	O	P	0	0
			3453	1544	617	1130	162		

- Molecule 3 is a RNA chain called Ribosomal RNA 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	3149	Total	C	N	O	P	0	0
			67505	30153	12264	21939	3149		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	119	Total	C	N	O	P	0	0
			2536	1132	454	831	119		

- Molecule 5 is a protein called Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BM	155	Total	C	N	O	S	0	0
			1246	774	247	221	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BO	125	Total	C	N	O	S	0	0
			1030	637	211	179	3		

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AR	51	Total	C	N	O	S	0	0
			425	258	100	66	1		

- Molecule 9 is a protein called Large ribosomal subunit protein eL31y.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AU	109	Total	C	N	O	S	0	0
			888	558	168	160	2		

- Molecule 10 is a protein called Small ribosomal subunit protein eS26y.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ma	98	Total	C	N	O	S	0	0
			789	485	166	132	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ia	190	Total	C	N	O	S	0	0
			1512	961	270	275	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8z/uS8w.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	129	Total	C	N	O	S	0	0
			1033	660	188	180	5		

- Molecule 13 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AX	97	Total	C	N	O	S	0	0
			786	492	166	126	2		

- Molecule 14 is a protein called Large ribosomal subunit protein eL27x.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AP	134	Total	C	N	O	S	0	0
			1092	706	200	183	3		

- Molecule 15 is a protein called Small ribosomal subunit protein eS4x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ja	258	Total	C	N	O	S	0	0
			2074	1325	386	357	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ea	203	Total	C	N	O	S	0	0
			1705	1065	358	279	3		

- Molecule 17 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AL	175	Total	C	N	O	S	0	0
			1485	960	273	244	8		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12y.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Va	139	Total	C	N	O	S	0	0
			1082	689	207	183	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS24y.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ka	120	Total	C	N	O	S	0	0
			986	627	191	165	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL33y.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AW	111	Total	C	N	O	S	0	0
			901	568	174	155	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BD	97	Total	C	N	O	S	0	0
			792	497	158	132	5		

- Molecule 22 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	386	Total	C	N	O	S	0	0
			3111	1981	581	532	17		

- Molecule 23 is a protein called Large ribosomal subunit protein eL21z/eL21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	163	Total	C	N	O	S	0	0
			1307	827	254	222	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS5y/uS5u/uS5v.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AC	215	Total	C	N	O	S	0	0
			1672	1075	300	290	7		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BI	131	Total	C	N	O	S	0	0
			986	624	183	171	8		

- Molecule 26 is a protein called Large ribosomal subunit protein eL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AH	128	Total	C	N	O	S	0	0
			1042	665	194	179	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	393	Total	C	N	O	S	0	0
			3056	1934	573	535	14		

- Molecule 28 is a protein called Large ribosomal subunit protein eL32z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AV	126	Total	C	N	O	S	0	0
			1028	649	204	171	4		

- Molecule 29 is a protein called Small ribosomal subunit protein uS7y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	184	Total	C	N	O	S	0	0
			1454	912	275	261	6		

- Molecule 30 is a protein called Large ribosomal subunit protein eL18x.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AJ	186	Total	C	N	O	S	0	0
			1468	932	283	249	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BQ	245	Total	C	N	O	S	0	0
			1877	1175	379	316	7		

- Molecule 32 is a protein called Large ribosomal subunit protein uL13y.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	205	Total	C	N	O	S	0	0
			1636	1038	314	273	11		

- Molecule 33 is a protein called Small ribosomal subunit protein uS15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Da	149	Total	C	N	O	S	0	0
			1190	759	223	206	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BK	281	Total	C	N	O	S	0	0
			2277	1441	418	414	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AT	94	Total	C	N	O	S	0	0
			720	457	127	131	5		

- Molecule 36 is a protein called Small ribosomal subunit protein eS30z/eS30y/eS30x.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Pa	49	Total	C	N	O	0	0
			389	236	92	61		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	120	Total	C	N	O	S	0	0
			975	617	191	166	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	117	Total	C	N	O	S	0	0
			955	615	170	168	2		

- Molecule 39 is a protein called Large ribosomal subunit protein eL8y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	234	Total	C	N	O	S	0	0
			1874	1207	339	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Fa	111	Total	C	N	O	S	0	0
			896	560	187	148	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ha	145	Total	C	N	O	S	0	0
			1156	744	225	184	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	169	Total	C	N	O	S	0	0
			1366	863	254	242	7		

- Molecule 43 is a protein called Ribosomal protein L30/L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	232	Total	C	N	O	S	0	0
			1898	1221	348	325	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Xa	146	Total	C	N	O	S	0	0
			1163	742	224	192	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS1y.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BV	212	Total	C	N	O	S	0	0
			1718	1087	313	310	8		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BJ	207	Total	C	N	O	S	0	0
			1653	1047	327	268	11		

- Molecule 47 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AO	62	Total	C	N	O	S	0	0
			528	343	100	81	4		

- Molecule 48 is a protein called Small ribosomal subunit protein eS21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	73	Total	C	N	O	S	0	0
			568	355	104	107	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AK	178	Total	C	N	O	S	0	0
			1480	920	308	241	11		

- Molecule 50 is a protein called Small ribosomal subunit protein eS27y.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	83	Total	C	N	O	S	0	0
			647	405	118	117	7		

- Molecule 51 is a protein called Small ribosomal subunit protein uS4y.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AB	180	Total	C	N	O	S	0	0
			1514	953	303	254	4		

- Molecule 52 is a protein called Large ribosomal subunit protein eL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1491	966	273	250	2		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	208	Total	C	N	O	S	0	0
			1625	1031	296	290	8		

- Molecule 54 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	203	Total	C	N	O	S	0	0
			1648	1041	326	277	4		

- Molecule 55 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ga	52	Total	C	N	O	S	0	0
			433	271	89	66	7		

- Molecule 56 is a protein called Large ribosomal subunit protein eL39z/eL39x.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BA	50	Total	C	N	O	S	0	0
			444	282	97	63	2		

- Molecule 57 is a protein called Small ribosomal subunit protein uS9z.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	138	Total	C	N	O	S	0	0
			1113	708	213	187	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS13z/uS13y/uS13x.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Wa	139	Total	C	N	O	S	0	0
			1136	709	224	198	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ta	225	Total	C	N	O	S	0	0
			1795	1123	354	310	8		

- Molecule 60 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AZ	68	Total	C	N	O	S	0	0
			562	359	103	98	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL43y.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BE	90	Total	C	N	O	S	0	0
			702	441	135	120	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Za	198	Total	C	N	O	S	0	0
			1575	1000	283	279	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL28z.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AQ	136	Total	C	N	O	S	0	0
			1056	667	197	190	2		

- Molecule 64 is a protein called Small ribosomal subunit protein eS28x.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Oa	59	Total	C	N	O	S	0	0
			471	289	96	84	2		

- Molecule 65 is a protein called Small ribosomal subunit protein uS11y.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ua	127	Total	C	N	O	S	0	0
			962	591	189	177	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS19y.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ya	129	Total	C	N	O	S	0	0
			1024	657	190	172	5		

- Molecule 67 is a protein called Small ribosomal subunit protein eS17w.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BB	119	Total	C	N	O	S	0	0
			955	597	175	178	5		

- Molecule 68 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	99	Total	C	N	O	S	0	0
			808	517	143	146	2		

- Molecule 69 is a protein called Small ribosomal subunit protein eS7x.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ra	184	Total	C	N	O	S	0	0
			1506	955	275	270	6		

- Molecule 70 is a protein called Small ribosomal subunit protein eS19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BL	136	Total	C	N	O	S	0	0
			1064	673	202	186	3		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25w.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	La	71	Total	C	N	O	S	0	0
			562	354	105	99	4		

- Molecule 72 is a protein called Small ribosomal subunit protein eS8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aa	185	Total	C	N	O	S	0	0
			1494	928	296	266	4		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AY	87	Total	C	N	O	S	0	0
			705	429	157	113	6		

- Molecule 74 is a protein called Small ribosomal subunit protein uS14z/uS14y/uS14x.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ca	55	Total	C	N	O	S	0	0
			440	273	91	71	5		

- Molecule 75 is a RNA chain called Ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h1	1612	Total	C	N	O	P	0	0
			34449	15422	6154	11261	1612		

- Molecule 76 is a RNA chain called Messenger RNA (poly-U).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	B1	12	Total	C	N	O	P	0	0
			240	108	24	96	12		

- Molecule 77 is a protein called Small ribosomal subunit protein uS10y.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ba	101	Total	C	N	O	S	0	0
			799	505	149	142	3		

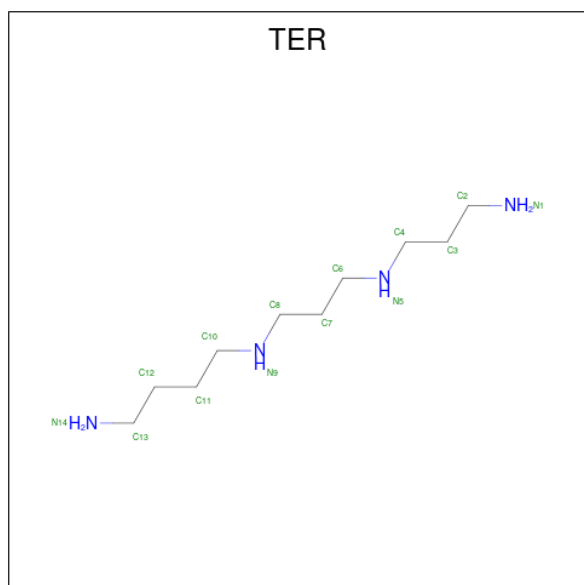
- Molecule 78 is a protein called Small ribosomal subunit protein eS10z.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AI	92	Total	C	N	O	S	0	0
			779	514	127	133	5		

- Molecule 79 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	L3	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 80 is N-(3-AMINO-PROPYL)-N-(5-AMINOPROPYL)-1,4-DIAMINOBUTANE (CCD ID: TER) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
80	3	1	Total	C	N	0
			14	10	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
80	3	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	A	1	Total	C	N	0
			14	10	4	
80	h1	1	Total	C	N	0
			14	10	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
80	h1	1	Total	C	N	0
			14	10	4	
80	h1	1	Total	C	N	0
			14	10	4	
80	h1	1	Total	C	N	0
			14	10	4	
80	h1	1	Total	C	N	0
			14	10	4	
80	h1	1	Total	C	N	0
			14	10	4	

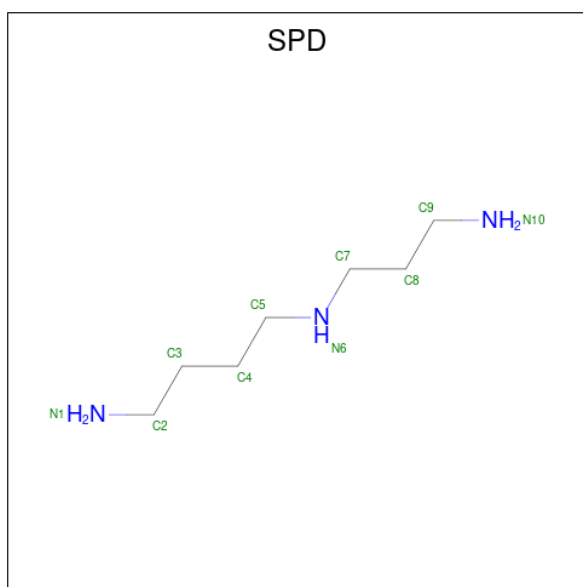
- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	3	4	Total	Mg	0
			4	4	
81	A	193	Total	Mg	0
			193	193	
81	C3	4	Total	Mg	0
			4	4	
81	BM	1	Total	Mg	0
			1	1	
81	Ma	1	Total	Mg	0
			1	1	
81	BS	3	Total	Mg	0
			3	3	
81	AC	1	Total	Mg	0
			1	1	
81	BI	1	Total	Mg	0
			1	1	
81	Da	1	Total	Mg	0
			1	1	
81	BR	1	Total	Mg	0
			1	1	
81	Wa	1	Total	Mg	0
			1	1	
81	Ta	1	Total	Mg	0
			1	1	
81	AY	1	Total	Mg	0
			1	1	
81	h1	76	Total	Mg	0
			76	76	

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

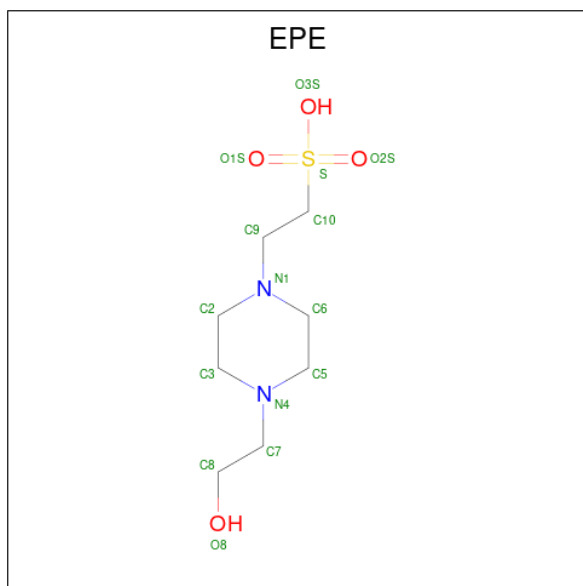
Mol	Chain	Residues	Atoms		AltConf
82	3	3	Total 3	K 3	0
82	A	125	Total 125	K 125	0
82	C3	1	Total 1	K 1	0
82	BM	2	Total 2	K 2	0
82	AR	1	Total 1	K 1	0
82	Ea	1	Total 1	K 1	0
82	Va	1	Total 1	K 1	0
82	BD	1	Total 1	K 1	0
82	BS	2	Total 2	K 2	0
82	AV	1	Total 1	K 1	0
82	AD	1	Total 1	K 1	0
82	AJ	1	Total 1	K 1	0
82	BQ	2	Total 2	K 2	0
82	Fa	1	Total 1	K 1	0
82	BJ	1	Total 1	K 1	0
82	AG	1	Total 1	K 1	0
82	Wa	1	Total 1	K 1	0
82	Ua	1	Total 1	K 1	0
82	Ca	1	Total 1	K 1	0
82	h1	39	Total 39	K 39	0

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
83	A	1	Total	C	N	0
			10	7	3	

- Molecule 84 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					AltConf
84	A	1	Total	C	N	O	S	0
			15	8	2	4	1	

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

Mol	Chain	Residues	Atoms		AltConf
85	Ma	1	Total 1	Zn 1	0
85	BD	1	Total 1	Zn 1	0
85	Ga	1	Total 1	Zn 1	0
85	BE	1	Total 1	Zn 1	0
85	AY	1	Total 1	Zn 1	0
85	Ca	1	Total 1	Zn 1	0

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	2	4	Total 4	O 4	0
86	3	288	Total 288	O 288	0
86	A	6924	Total 6924	O 6924	0
86	C3	153	Total 153	O 153	0
86	BC	13	Total 13	O 13	0
86	BM	62	Total 62	O 62	0
86	BO	33	Total 33	O 33	0
86	AR	44	Total 44	O 44	0
86	AU	30	Total 30	O 30	0
86	Ma	24	Total 24	O 24	0
86	Ia	20	Total 20	O 20	0
86	AE	17	Total 17	O 17	0
86	AX	24	Total 24	O 24	0
86	AP	14	Total 14	O 14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	Ja	13	Total 13	O 13	0
86	Ea	135	Total 135	O 135	0
86	AL	58	Total 58	O 58	0
86	Va	23	Total 23	O 23	0
86	AW	52	Total 52	O 52	0
86	BD	63	Total 63	O 63	0
86	BS	153	Total 153	O 153	0
86	AM	69	Total 69	O 69	0
86	AC	14	Total 14	O 14	0
86	BI	39	Total 39	O 39	0
86	AH	22	Total 22	O 22	0
86	BT	131	Total 131	O 131	0
86	AV	67	Total 67	O 67	0
86	AD	4	Total 4	O 4	0
86	AJ	111	Total 111	O 111	0
86	BQ	126	Total 126	O 126	0
86	BH	85	Total 85	O 85	0
86	Da	15	Total 15	O 15	0
86	BK	66	Total 66	O 66	0
86	AT	7	Total 7	O 7	0
86	Pa	2	Total 2	O 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	BP	21	Total 21	O 21	0
86	BN	27	Total 27	O 27	0
86	BG	32	Total 32	O 32	0
86	Fa	61	Total 61	O 61	0
86	Ha	85	Total 85	O 85	0
86	BU	5	Total 5	O 5	0
86	BR	68	Total 68	O 68	0
86	Xa	13	Total 13	O 13	0
86	BV	11	Total 11	O 11	0
86	BJ	31	Total 31	O 31	0
86	AO	19	Total 19	O 19	0
86	AK	45	Total 45	O 45	0
86	Na	2	Total 2	O 2	0
86	AB	5	Total 5	O 5	0
86	BF	13	Total 13	O 13	0
86	AA	1	Total 1	O 1	0
86	AG	77	Total 77	O 77	0
86	Ga	9	Total 9	O 9	0
86	BA	21	Total 21	O 21	0
86	AF	4	Total 4	O 4	0
86	Ta	6	Total 6	O 6	0

Continued on next page...

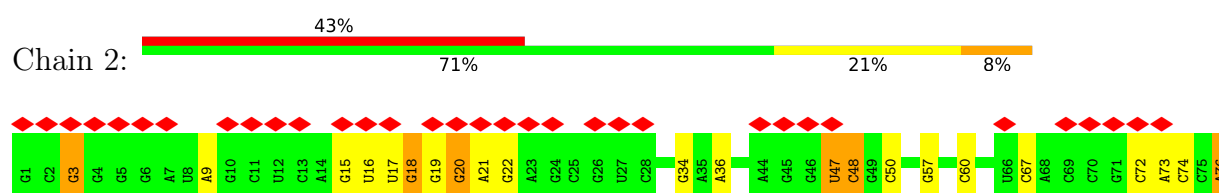
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	AZ	4	Total 4	O 4	0
86	BE	32	Total 32	O 32	0
86	Za	1	Total 1	O 1	0
86	AQ	3	Total 3	O 3	0
86	Oa	3	Total 3	O 3	0
86	Ua	22	Total 22	O 22	0
86	Ya	1	Total 1	O 1	0
86	BL	2	Total 2	O 2	0
86	Aa	6	Total 6	O 6	0
86	AY	69	Total 69	O 69	0
86	Ca	1	Total 1	O 1	0
86	h1	1264	Total 1264	O 1264	0
86	B1	18	Total 18	O 18	0
86	W2	21	Total 21	O 21	0
86	Ba	1	Total 1	O 1	0

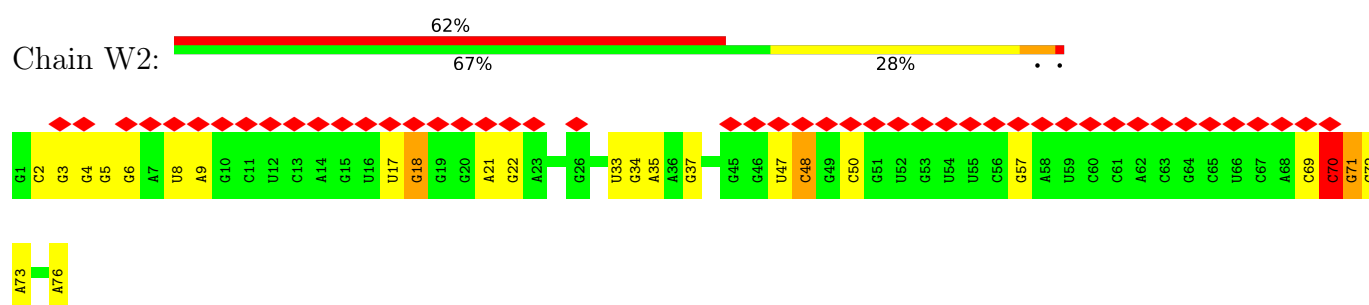
3 Residue-property plots

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

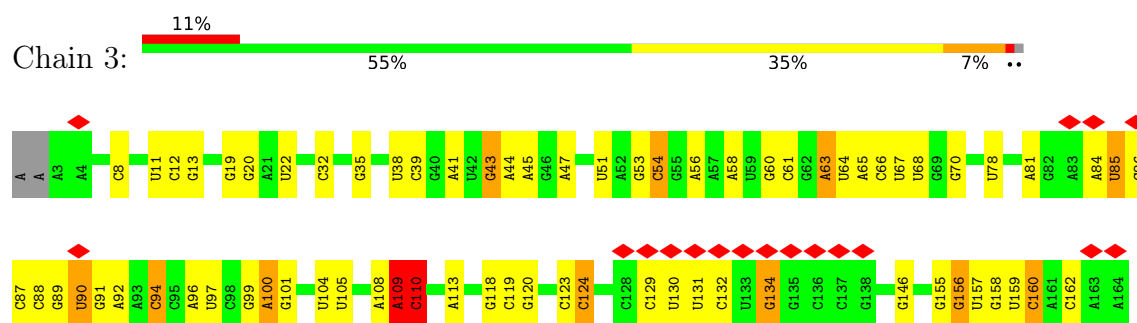
- Molecule 1: Transfer RNA Phe (GAA)



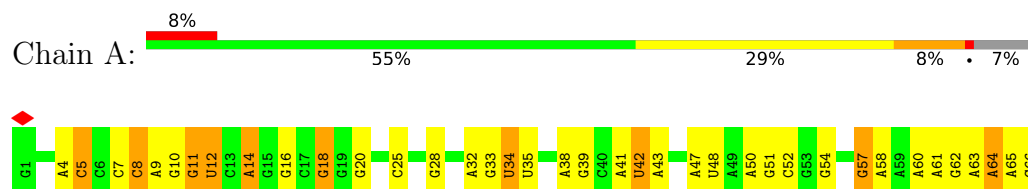
- Molecule 1: Transfer RNA Phe (GAA)

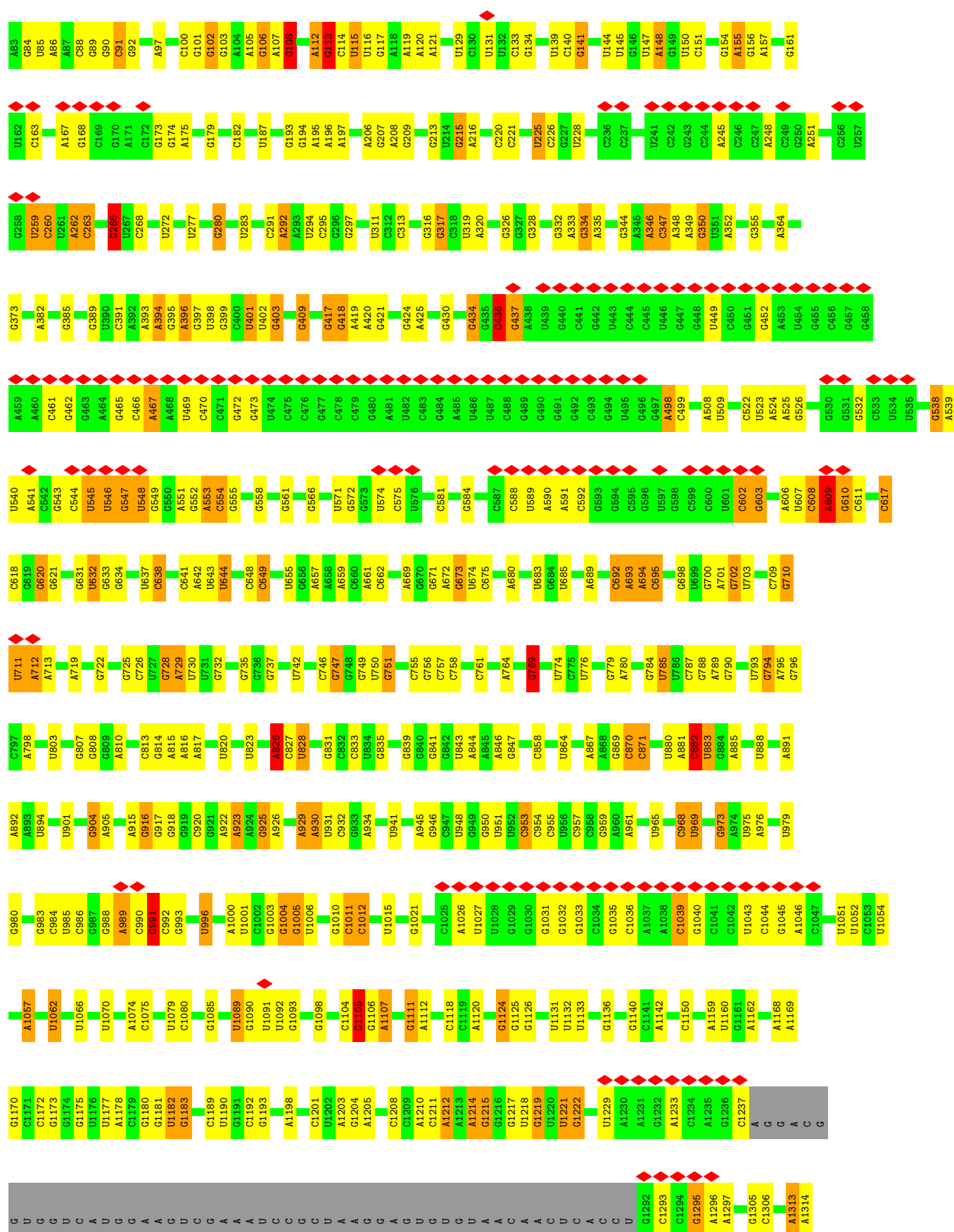


- Molecule 2: Ribosomal RNA 5.8S

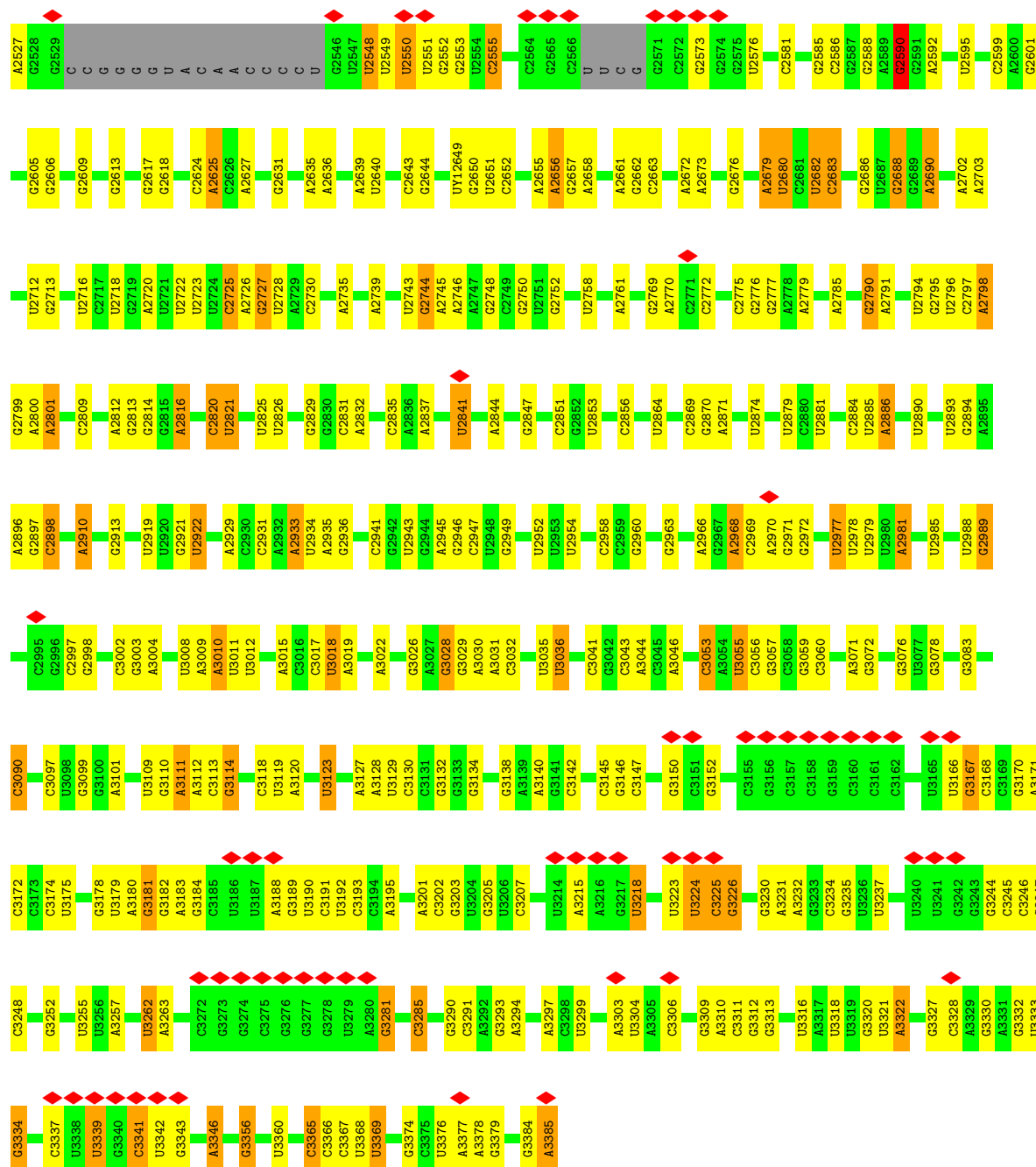


- Molecule 3: Ribosomal RNA 25S



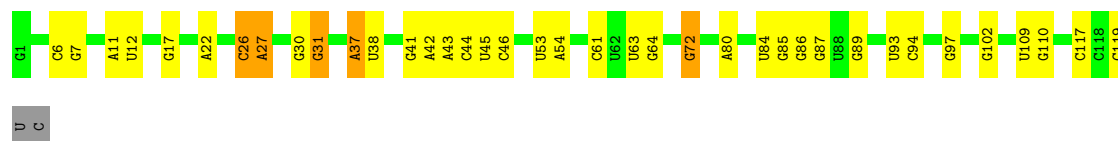




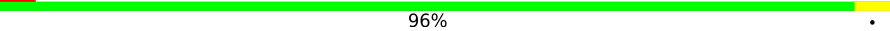


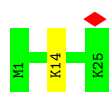
• Molecule 4: Ribosomal RNA 5S

Chain C3: 67% 27% . .



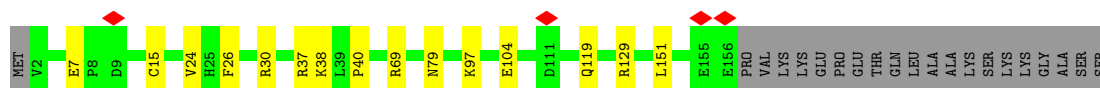
• Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v

Chain BC:  96%



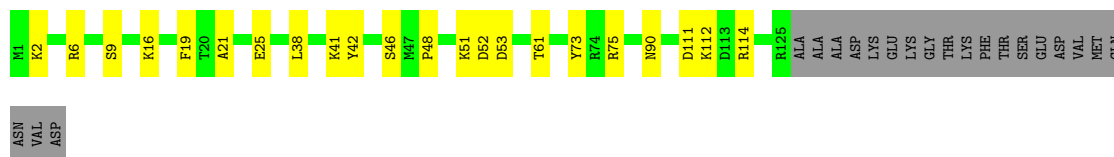
- Molecule 6: Large ribosomal subunit protein uL22z

Chain BM:  80% 9% 12%



- Molecule 7: Large ribosomal subunit protein uL24z

Chain BO:  71% 15% 14%



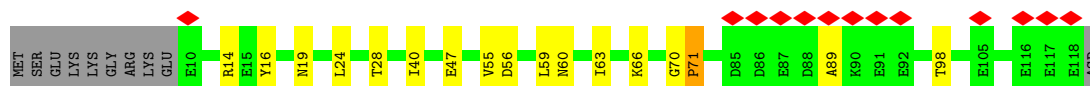
- Molecule 8: 60S ribosomal protein L29

Chain AR:  51% 10% 39%



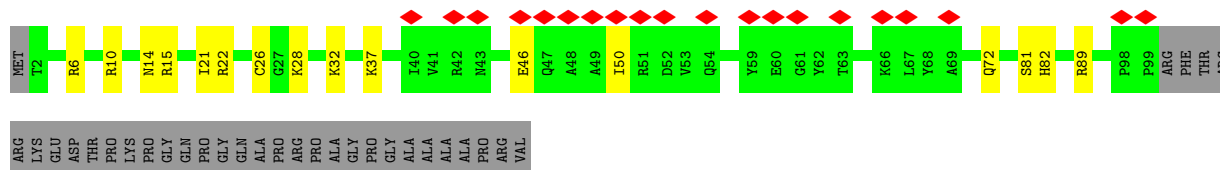
- Molecule 9: Large ribosomal subunit protein eL31y

Chain AU:  11% 77% 13% 8%

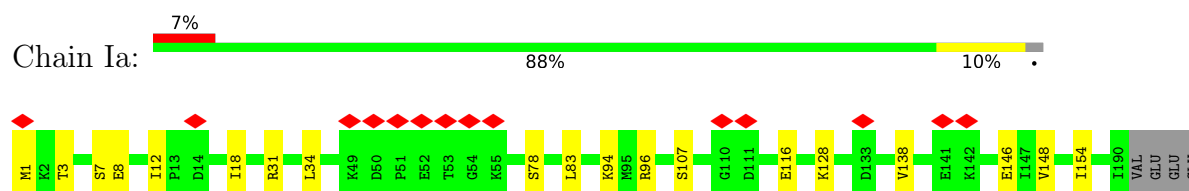


- Molecule 10: Small ribosomal subunit protein eS26y

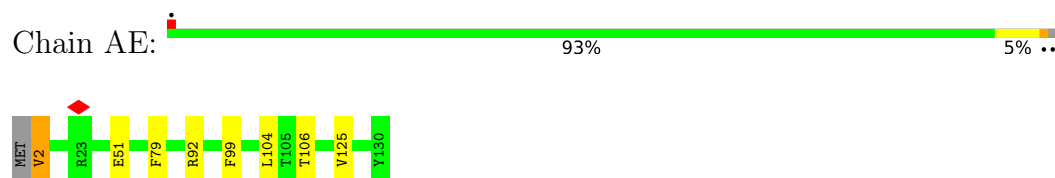
Chain Ma:  15% 63% 12% 25%



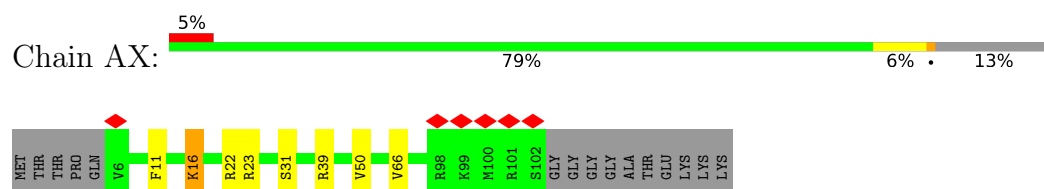
- Molecule 11: Large ribosomal subunit protein uL6z/uL6y



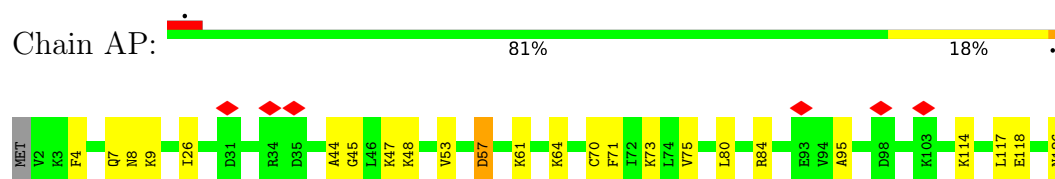
- Molecule 12: Small ribosomal subunit protein uS8z/uS8w



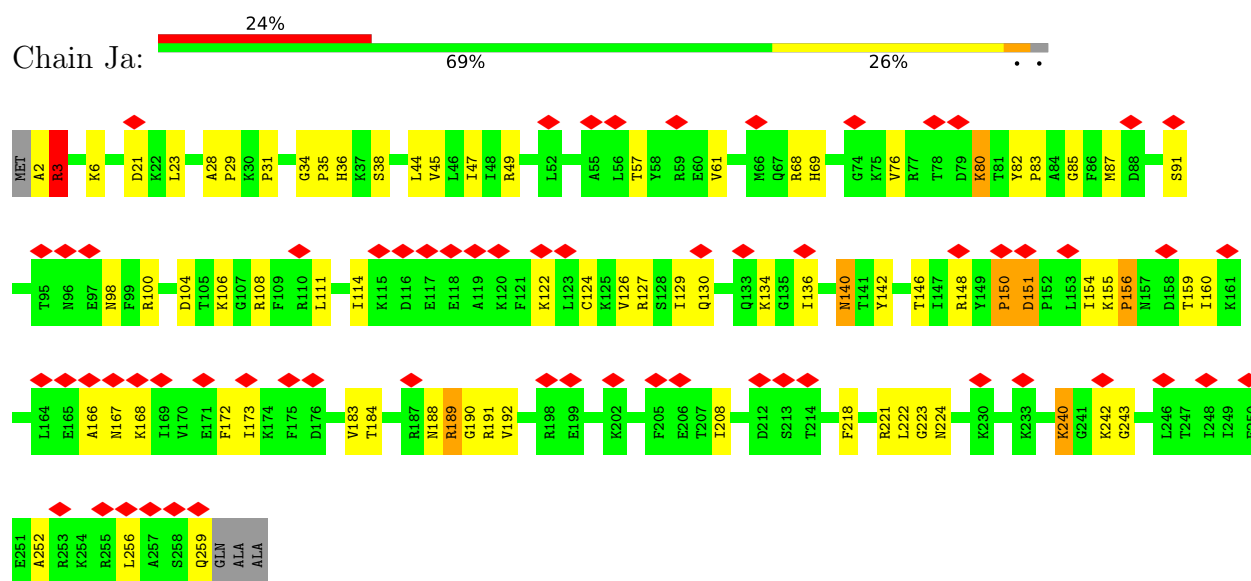
- Molecule 13: Large ribosomal subunit protein eL36y



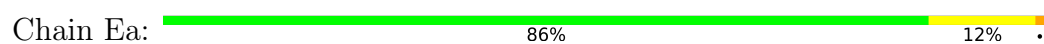
- Molecule 14: Large ribosomal subunit protein eL27x



- Molecule 15: Small ribosomal subunit protein eS4x

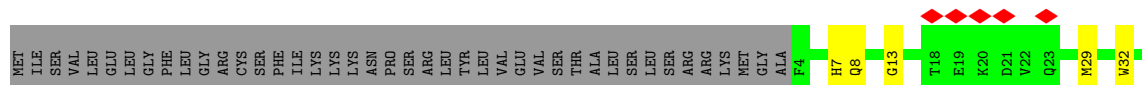


- Molecule 16: Large ribosomal subunit protein eL15z

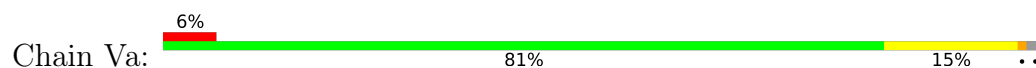




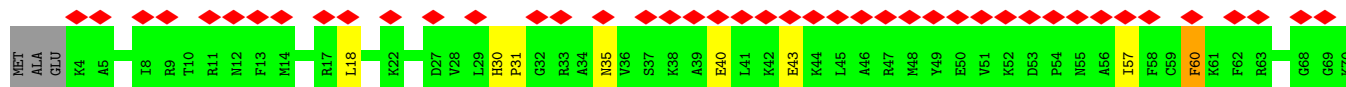
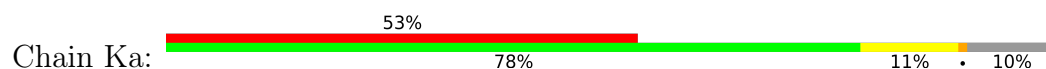
- Molecule 17: Ribosomal protein L18ae/LX family protein



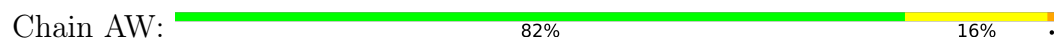
- Molecule 18: Small ribosomal subunit protein uS12y



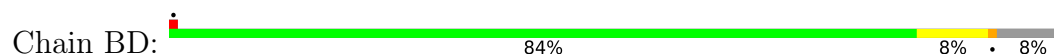
- Molecule 19: Small ribosomal subunit protein eS24y



- Molecule 20: Large ribosomal subunit protein eL33y

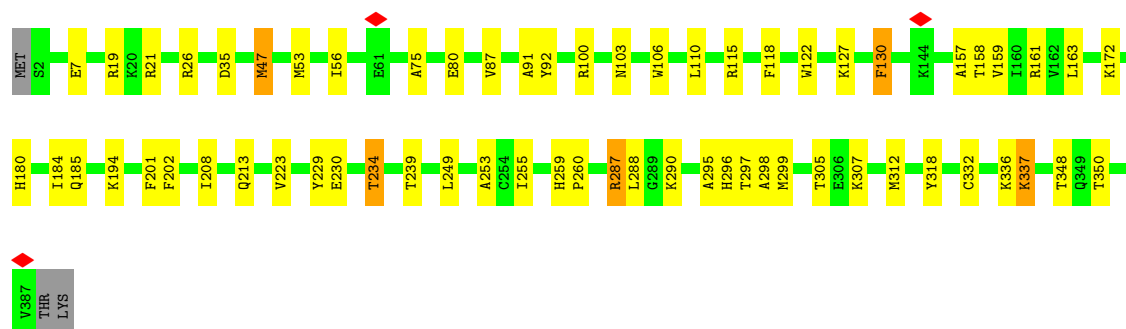


- Molecule 21: Large ribosomal subunit protein eL42z/eL42y



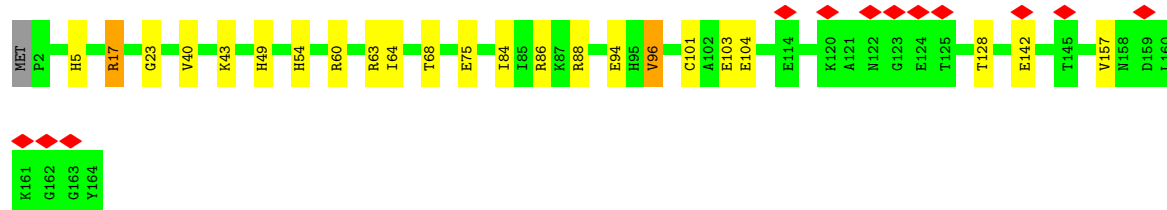
- Molecule 22: Large ribosomal subunit protein uL3z

Chain BS:  83% 15% ..



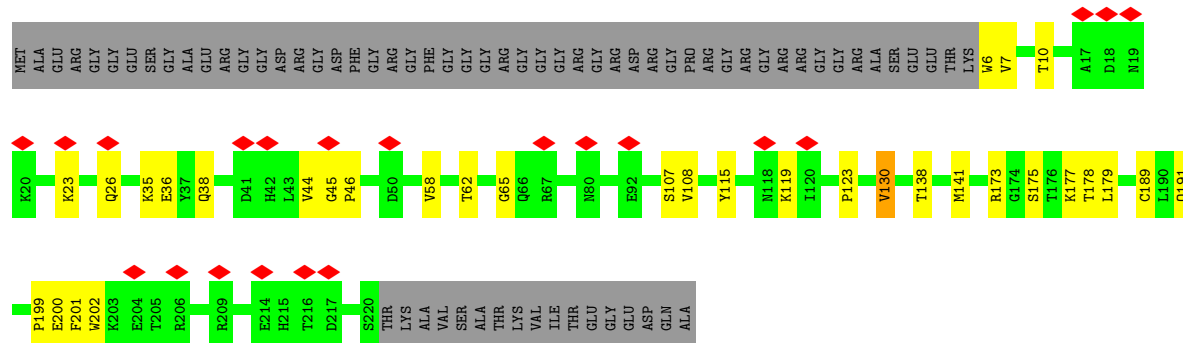
- Molecule 23: Large ribosomal subunit protein eL21z/eL21y

Chain AM:  7% 85% 13% ..



- Molecule 24: Small ribosomal subunit protein uS5y/uS5u/uS5v

Chain AC:  7% 64% 11% 24%



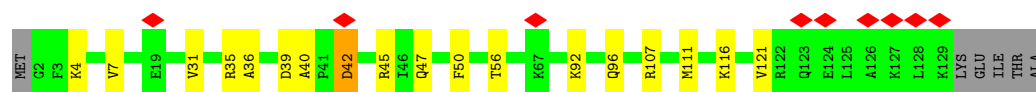
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI:  74% 19% 6%

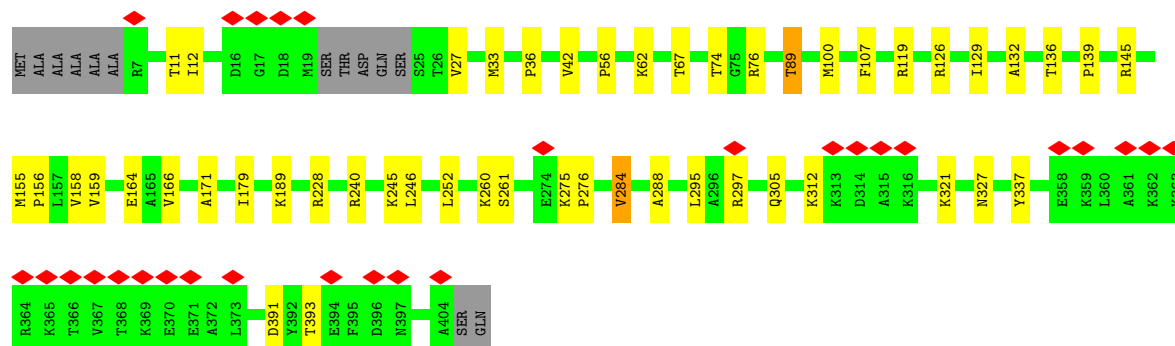
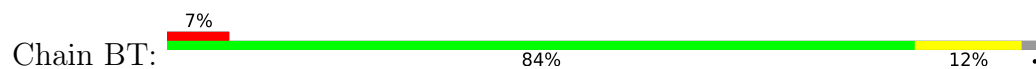


- Molecule 26: Large ribosomal subunit protein eL14y

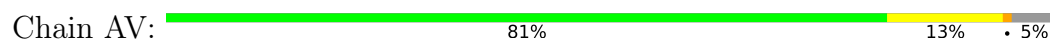
Chain AH:  7% 82% 13% ..



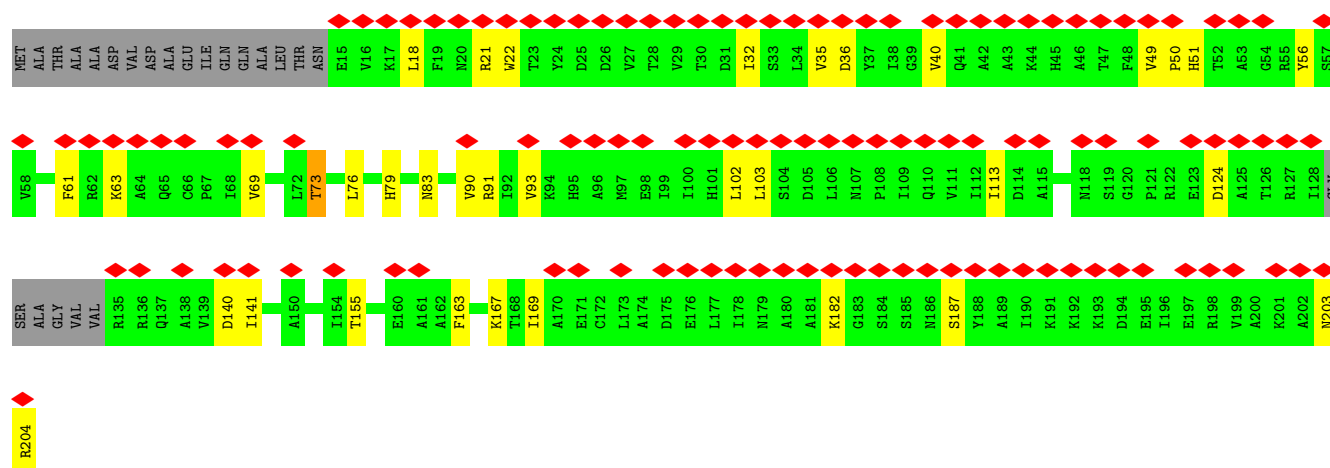
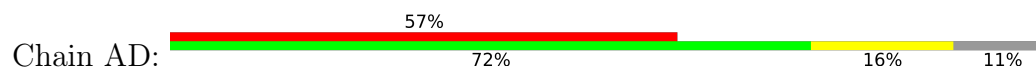
- Molecule 27: Large ribosomal subunit protein uL4z



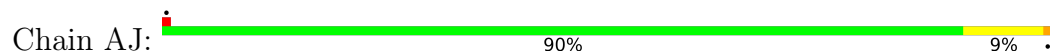
- Molecule 28: Large ribosomal subunit protein eL32z

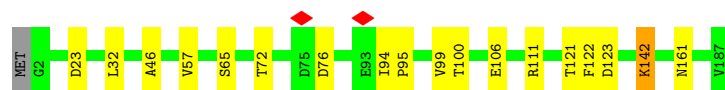


- Molecule 29: Small ribosomal subunit protein uS7y



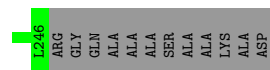
- Molecule 30: Large ribosomal subunit protein eL18x





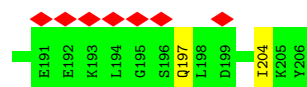
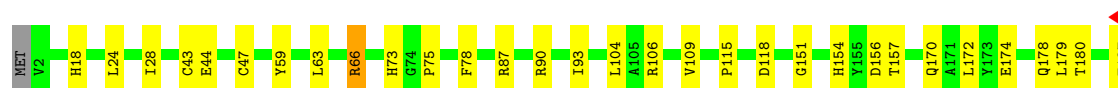
- Molecule 31: Large ribosomal subunit protein uL2z

Chain BQ: 83% 11% • 5%



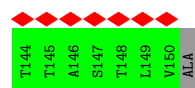
- Molecule 32: Large ribosomal subunit protein uL13y

Chain BH: 83% 16%



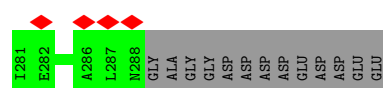
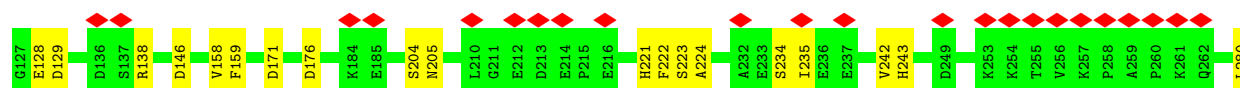
- Molecule 33: Small ribosomal subunit protein uS15y

Chain Da: 20% 90% 8% ••



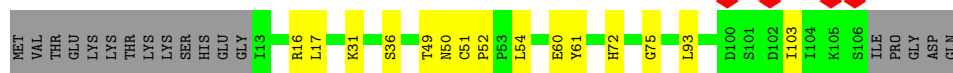
- Molecule 34: Large ribosomal subunit protein uL18z

Chain BK: 10% 78% 15% • 7%



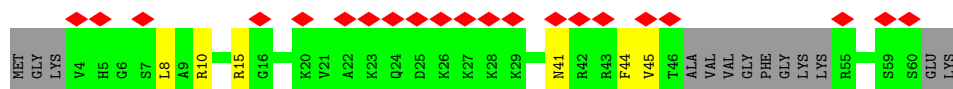
- Molecule 35: Large ribosomal subunit protein eL30y

Chain AT: 



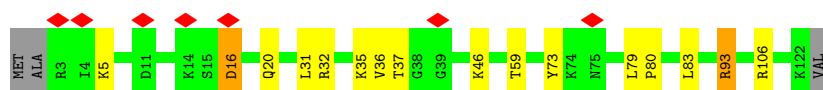
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x

Chain Pa: 



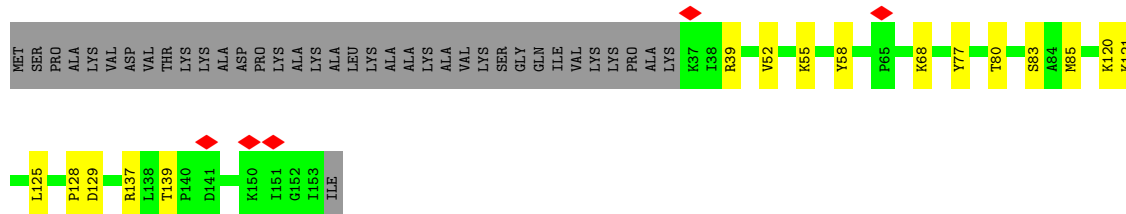
- Molecule 37: Large ribosomal subunit protein uL29x

Chain BP: 



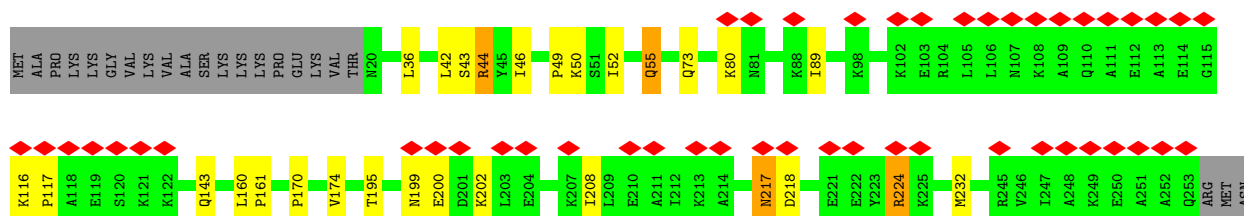
- Molecule 38: Large ribosomal subunit protein uL23y

Chain BN: 



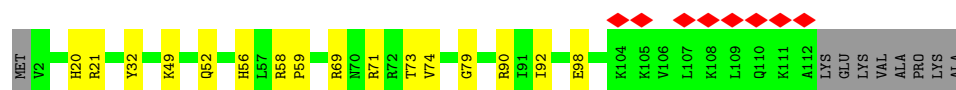
- Molecule 39: Large ribosomal subunit protein eL8y

Chain BG: 



- Molecule 40: Large ribosomal subunit protein eL34z

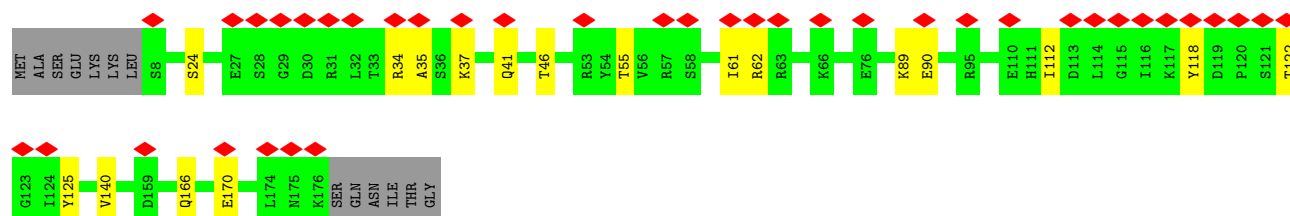
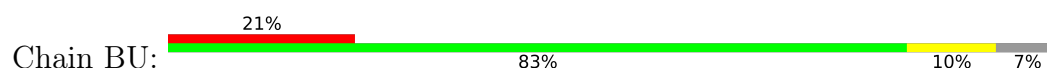
Chain Fa: 



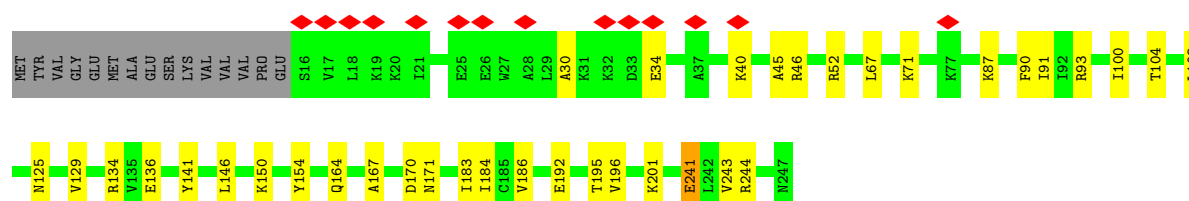
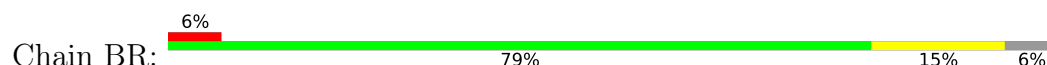
- Molecule 41: Large ribosomal subunit protein uL15x



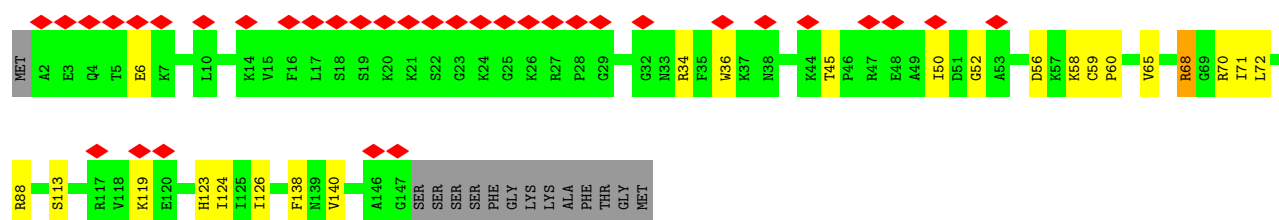
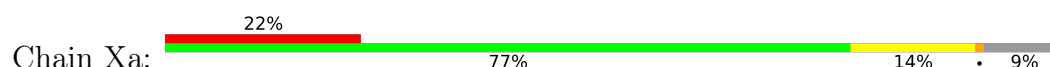
- Molecule 42: Large ribosomal subunit protein uL5z



- Molecule 43: Ribosomal protein L30/L7 family protein

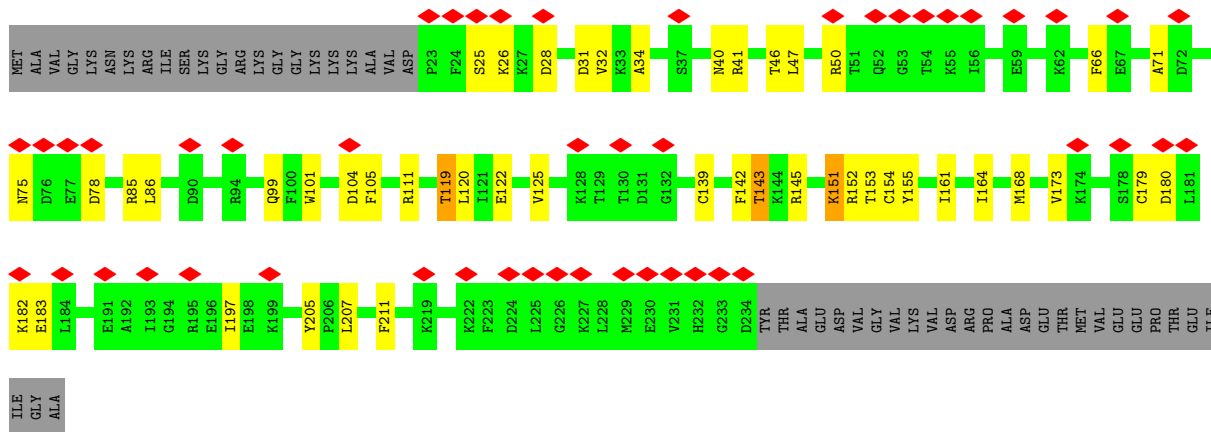


- Molecule 44: Small ribosomal subunit protein uS17z

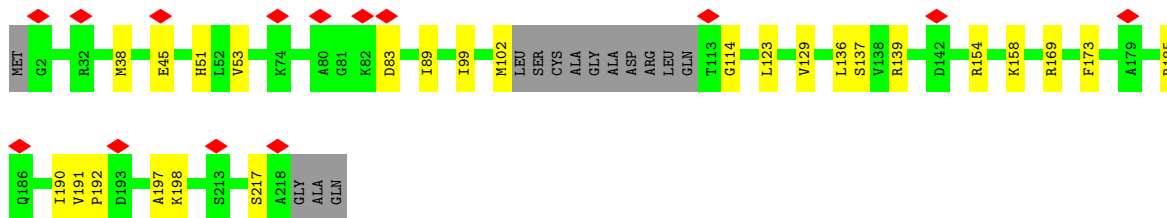
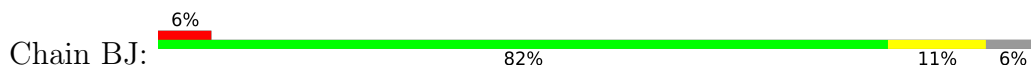


- Molecule 45: Small ribosomal subunit protein eS1y

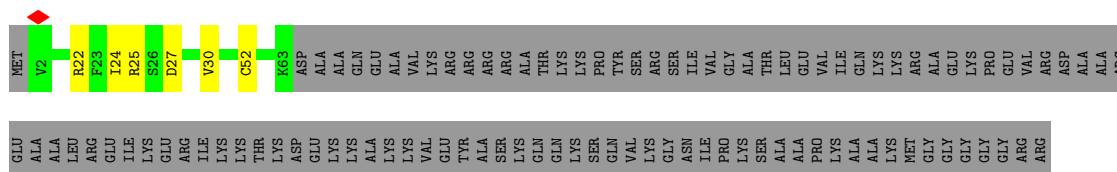




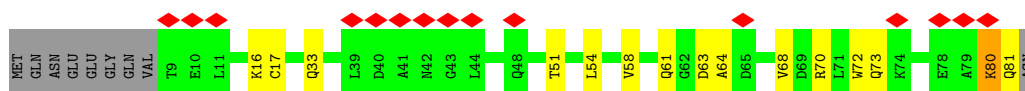
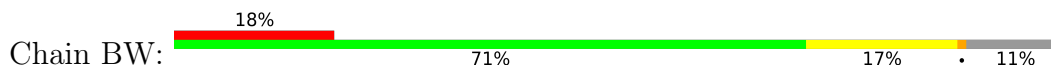
- Molecule 46: Large ribosomal subunit protein uL16y



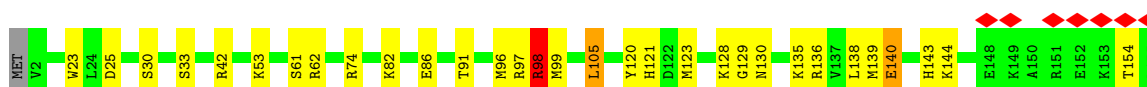
- Molecule 47: Large ribosomal subunit protein eL24z



- Molecule 48: Small ribosomal subunit protein eS21y

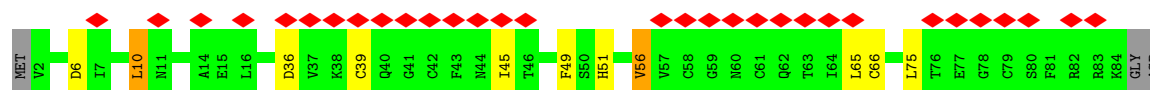
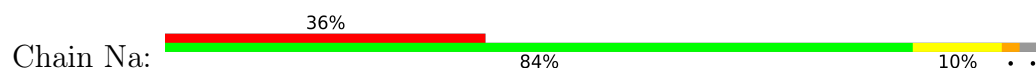


- Molecule 49: Large ribosomal subunit protein eL19x

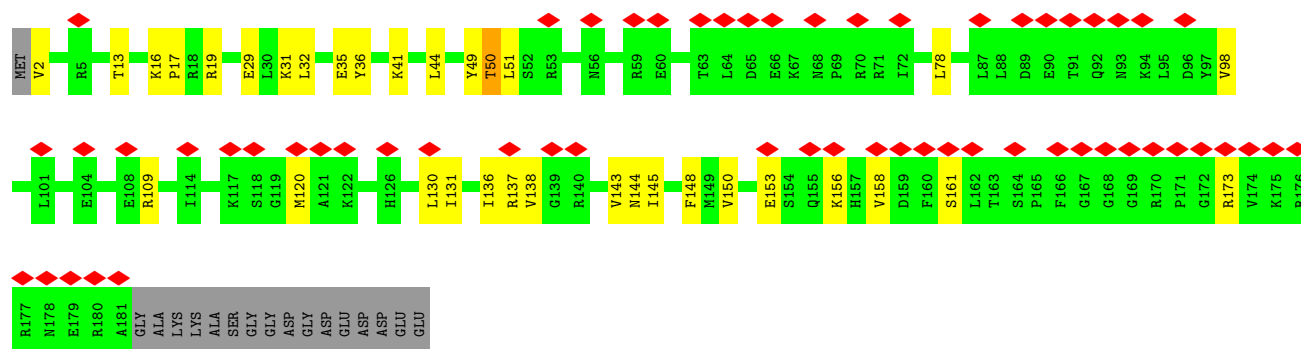
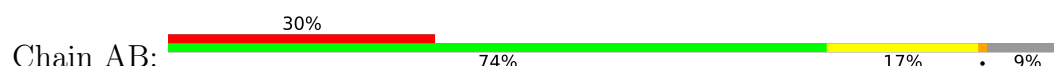




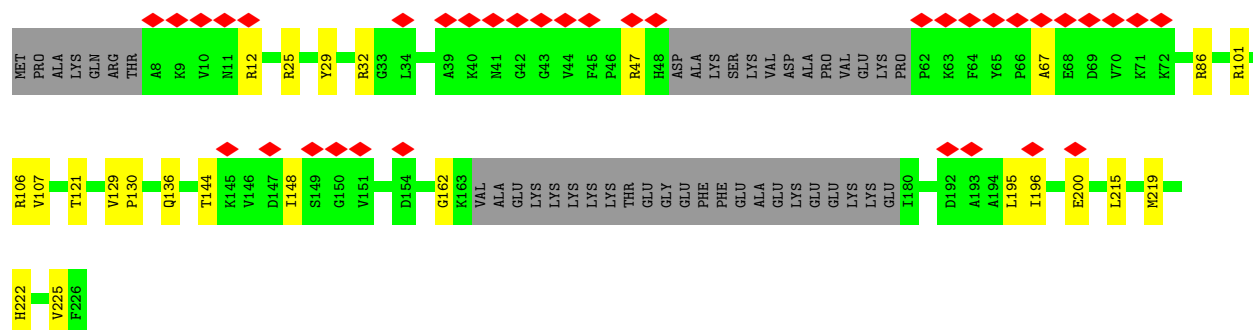
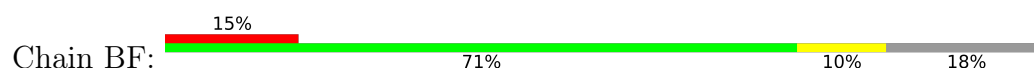
- Molecule 50: Small ribosomal subunit protein eS27y



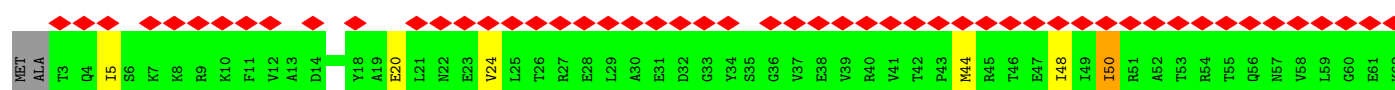
- Molecule 51: Small ribosomal subunit protein uS4y

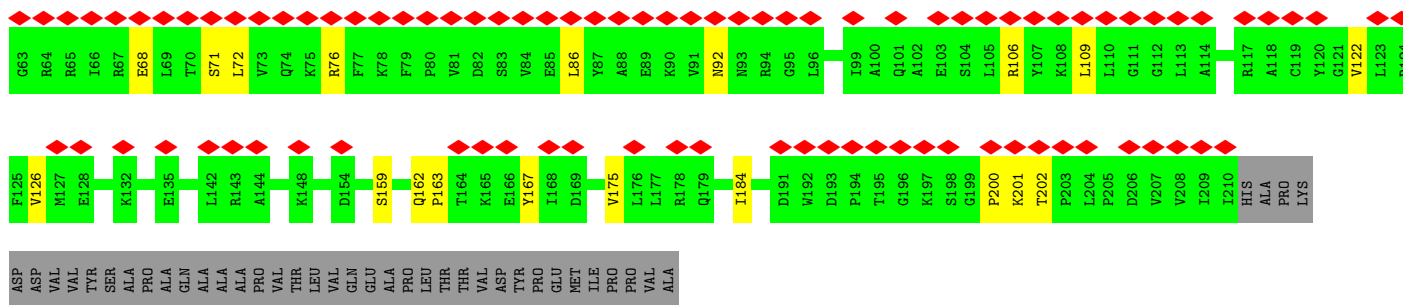


- Molecule 52: Large ribosomal subunit protein eL6y

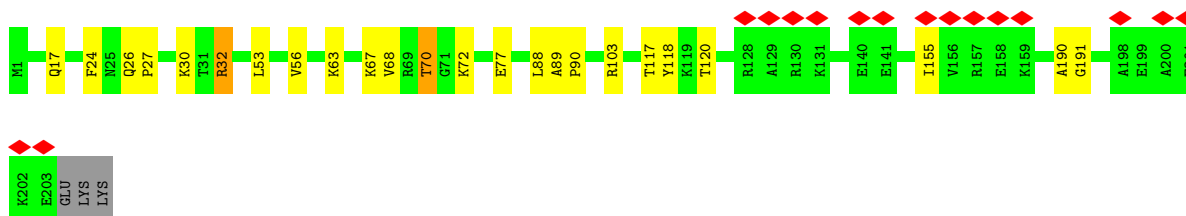
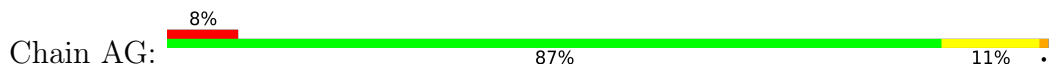


- Molecule 53: Small ribosomal subunit protein uS3z

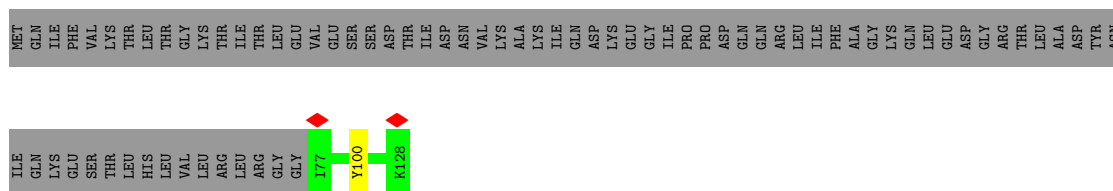




- Molecule 54: Large ribosomal subunit protein eL13z



- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein

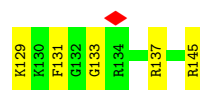


- Molecule 56: Large ribosomal subunit protein eL39z/eL39x

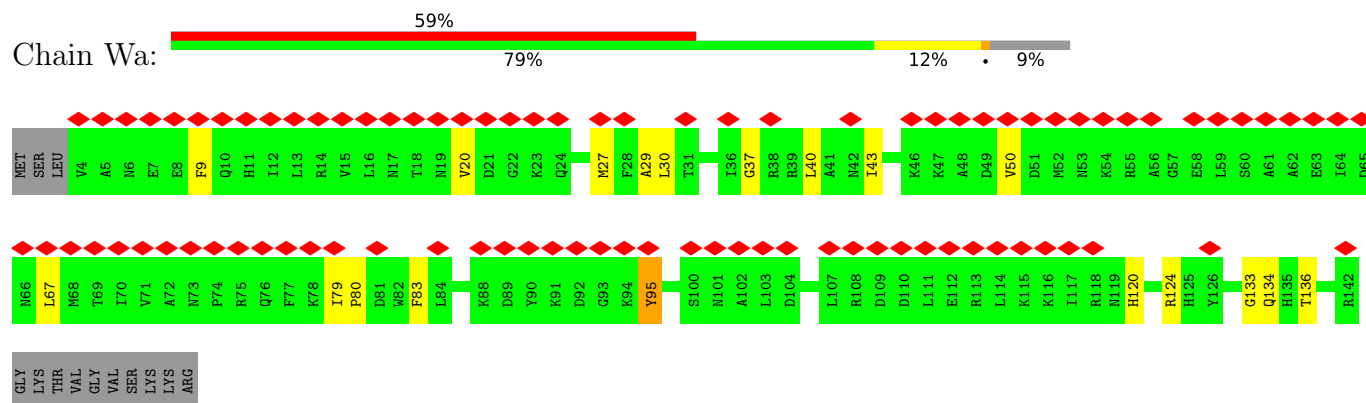


- Molecule 57: Small ribosomal subunit protein uS9z

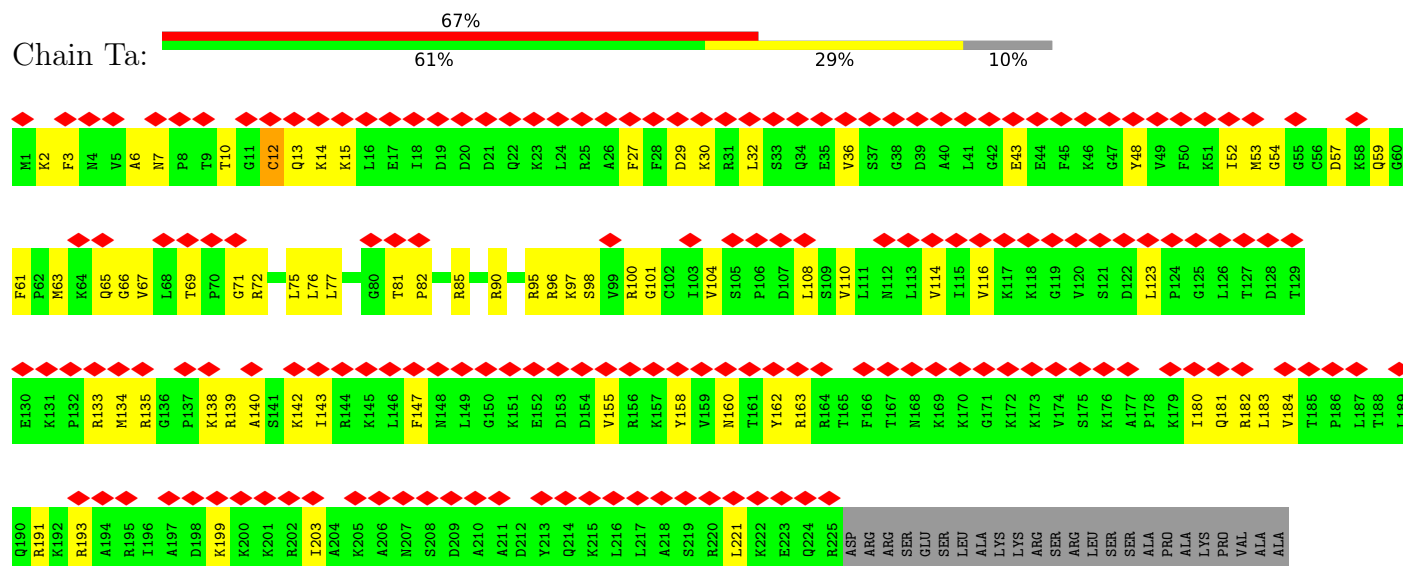




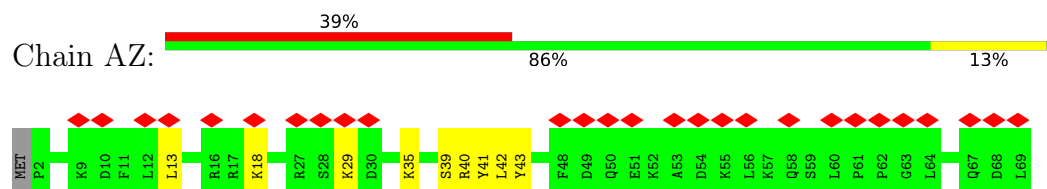
- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x



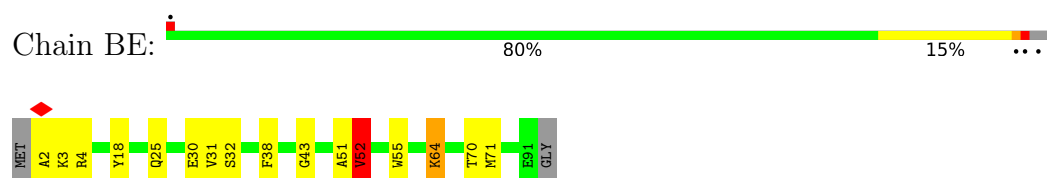
- Molecule 59: Small ribosomal subunit protein eS6y



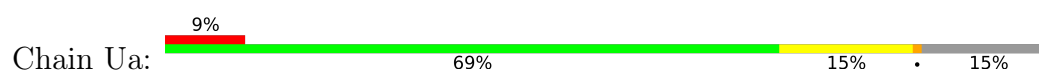
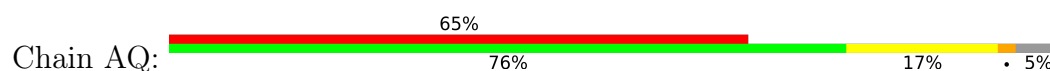
- Molecule 60: Large ribosomal subunit protein eL38z/eL38y

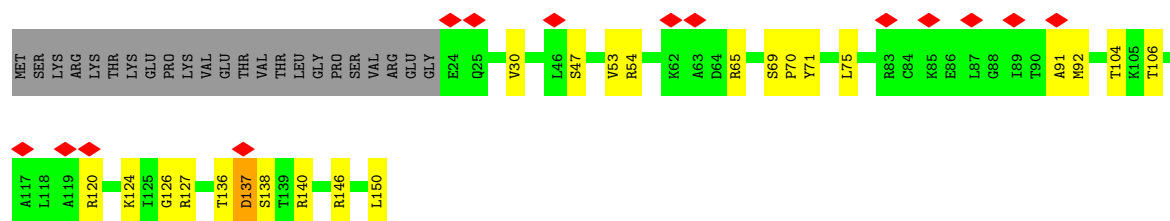


- Molecule 61: Large ribosomal subunit protein eL43y

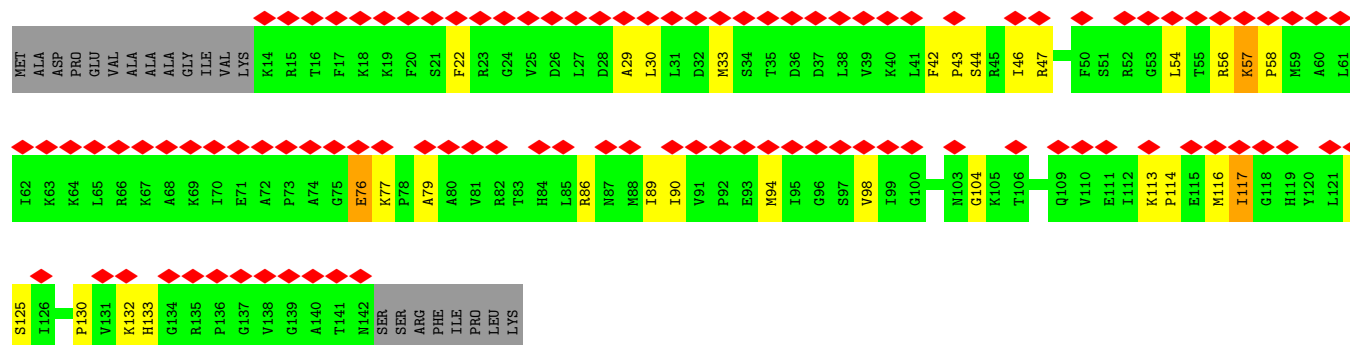


Chain Za:

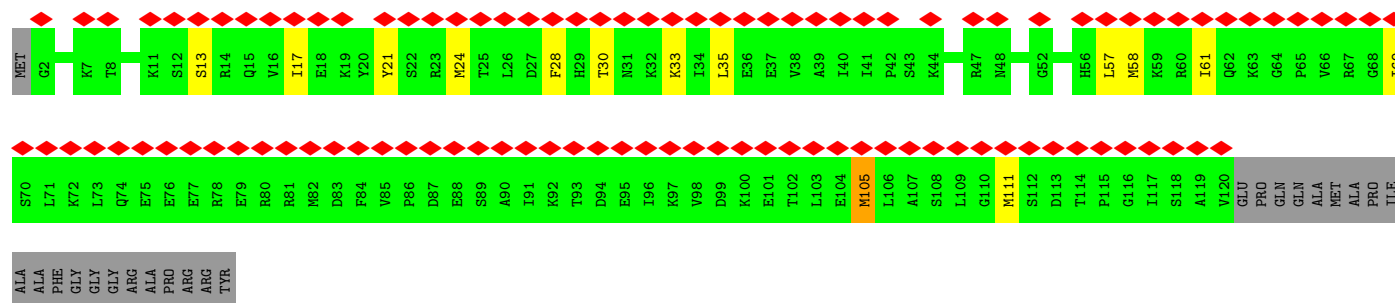
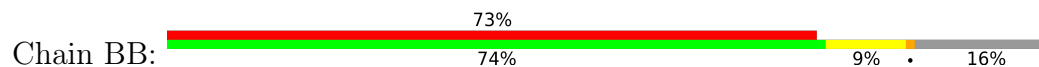




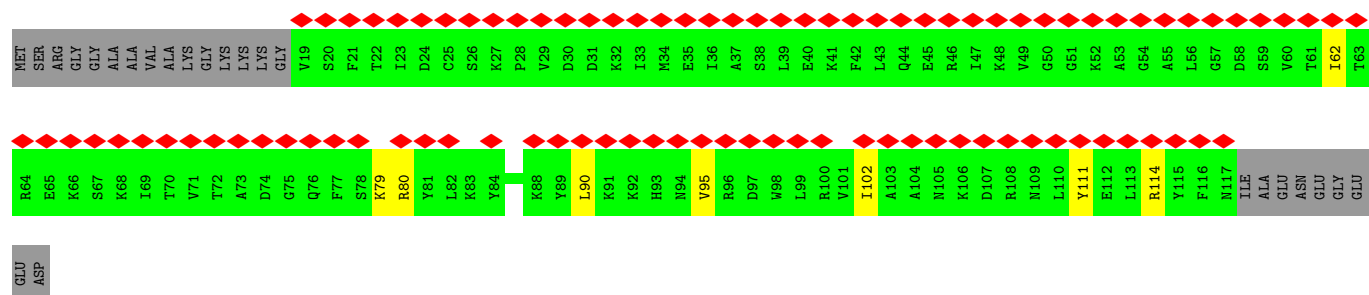
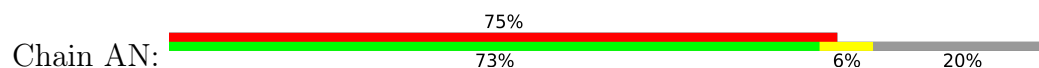
- Molecule 66: Small ribosomal subunit protein uS19y



- Molecule 67: Small ribosomal subunit protein eS17w



- Molecule 68: Large ribosomal subunit protein eL22z

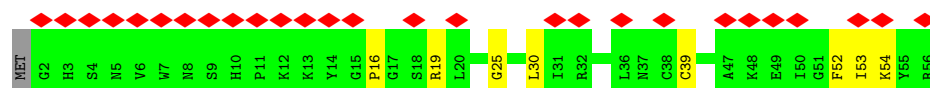
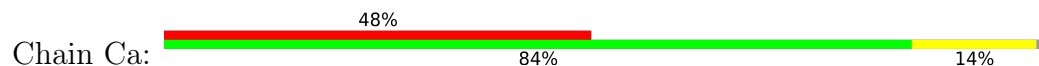


- Molecule 69: Small ribosomal subunit protein eS7x

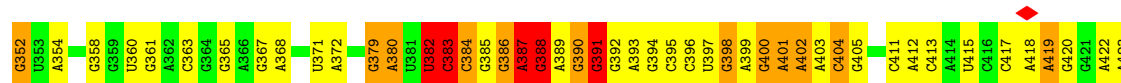
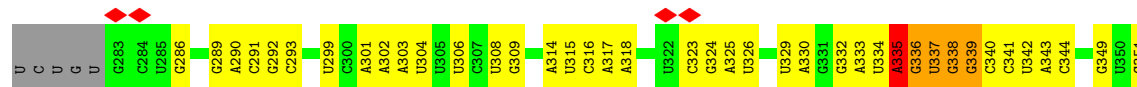
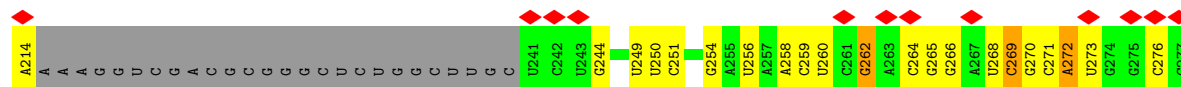
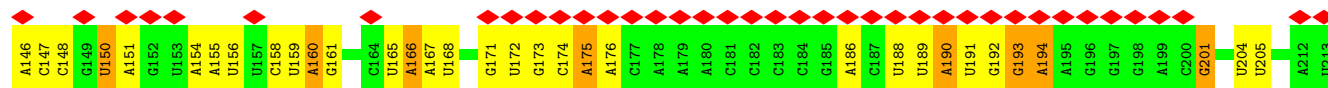
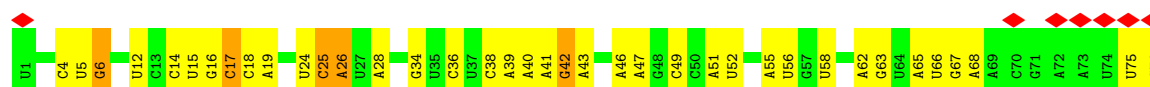
- Molecule 73: Large ribosomal subunit protein eL37z



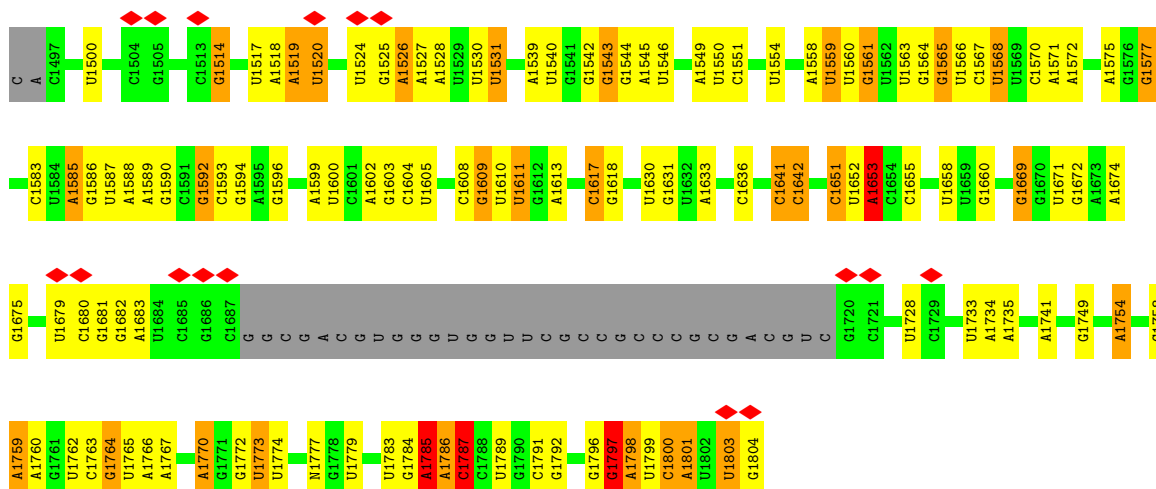
- Molecule 74: Small ribosomal subunit protein uS14z/uS14y/uS14x



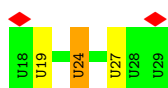
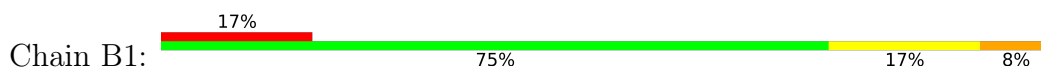
- Molecule 75: Ribosomal RNA 18S



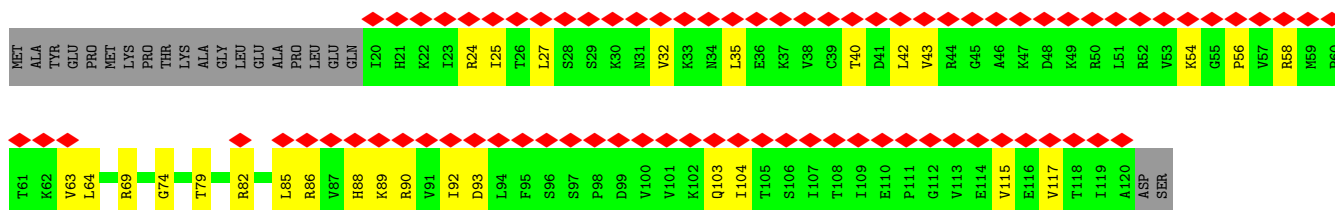




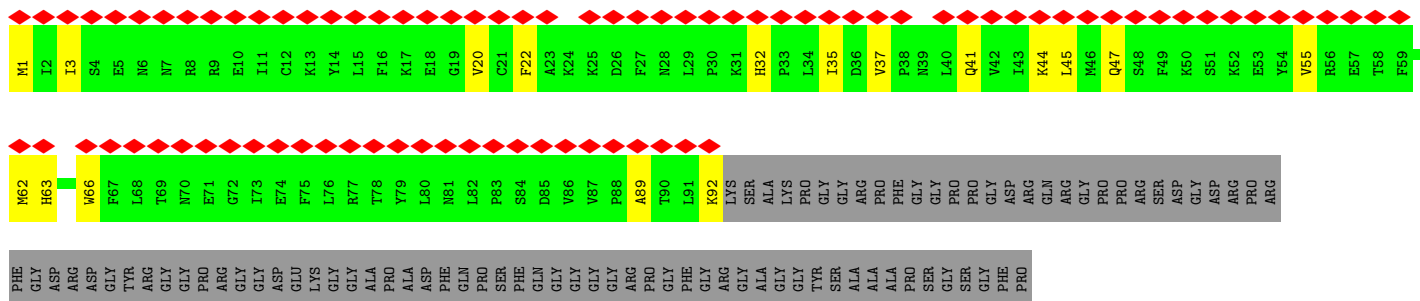
• Molecule 76: Messenger RNA (poly-U)



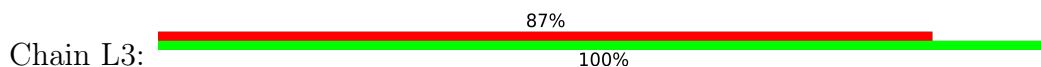
• Molecule 77: Small ribosomal subunit protein uS10y



• Molecule 78: Small ribosomal subunit protein eS10z



• Molecule 79: Nascent polypeptide



X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24
----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.337	Depositor
Minimum map value	-3.463	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	497.4, 497.4, 497.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TER, UR3, OMU, 4AC, MA6, K, OMG, MLY, C4J, MG, UY1, OMC, A2M, 1MG, HIC, 5MC, ZN, EPE, SPD, PSU, 6MZ, 1MA, G7M

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	2	0.56	0/1823	0.89	2/2840 (0.1%)
1	W2	0.56	0/1822	0.91	4/2840 (0.1%)
2	3	0.60	0/3713	1.21	26/5784 (0.4%)
3	A	0.61	12/72568 (0.0%)	1.23	573/113188 (0.5%)
4	C3	0.57	0/2834	1.19	18/4415 (0.4%)
5	BC	0.71	0/238	1.24	0/302
6	BM	0.77	0/1269	1.20	3/1705 (0.2%)
7	BO	0.65	0/1042	1.11	3/1390 (0.2%)
8	AR	0.76	0/435	1.22	0/577
9	AU	0.69	0/900	1.18	2/1202 (0.2%)
10	Ma	0.52	0/804	0.94	0/1081
11	Ia	0.56	0/1533	0.96	0/2050
12	AE	0.56	0/1051	1.05	0/1406
13	AX	0.63	0/793	1.10	1/1047 (0.1%)
14	AP	0.56	0/1110	1.09	0/1477
15	Ja	0.48	0/2116	0.98	0/2841
16	Ea	0.83	0/1743	1.29	4/2335 (0.2%)
17	AL	0.68	0/1523	1.19	5/2042 (0.2%)
18	Va	0.56	0/1100	0.99	0/1465
19	Ka	0.46	0/1001	0.91	0/1329
20	AW	0.74	0/921	1.18	2/1234 (0.2%)
21	BD	0.70	0/806	1.15	2/1065 (0.2%)
22	BS	0.71	1/3165 (0.0%)	1.16	8/4238 (0.2%)
23	AM	0.68	0/1335	1.17	3/1789 (0.2%)
24	AC	0.54	0/1709	0.97	0/2310
25	BI	0.74	0/1002	1.21	3/1347 (0.2%)
26	AH	0.55	0/1054	1.00	1/1408 (0.1%)
27	BT	0.71	0/3112	1.13	4/4187 (0.1%)
28	AV	0.72	0/1045	1.18	3/1399 (0.2%)
29	AD	0.46	0/1473	0.94	0/1985
30	AJ	0.74	0/1492	1.15	2/1995 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BQ	0.78	0/1921	1.19	4/2584 (0.2%)
32	BH	0.74	0/1664	1.15	3/2224 (0.1%)
33	Da	0.56	0/1214	1.00	0/1630
34	BK	0.57	0/2321	1.05	2/3119 (0.1%)
35	AT	0.62	0/731	1.00	0/982
36	Pa	0.51	0/394	0.97	0/519
37	BP	0.59	0/984	1.06	0/1306
38	BN	0.59	0/972	1.11	2/1309 (0.2%)
39	BG	0.57	0/1908	1.05	2/2561 (0.1%)
40	Fa	0.76	0/909	1.18	0/1214
41	Ha	0.79	0/1187	1.28	8/1584 (0.5%)
42	BU	0.47	0/1388	0.91	0/1858
43	BR	0.67	0/1931	1.17	6/2584 (0.2%)
44	Xa	0.53	0/1189	0.93	0/1590
45	BV	0.48	0/1746	1.00	3/2341 (0.1%)
46	BJ	0.58	0/1691	1.00	0/2263
47	AO	0.64	0/541	1.00	0/718
48	BW	0.50	0/577	0.91	0/777
49	AK	0.71	0/1499	1.12	4/1975 (0.2%)
50	Na	0.48	0/657	0.95	0/883
51	AB	0.46	0/1540	0.93	0/2061
52	BF	0.55	0/1521	1.00	0/2040
53	AA	0.46	0/1647	0.91	0/2212
54	AG	0.65	0/1680	1.12	3/2251 (0.1%)
55	Ga	0.59	0/428	1.06	0/564
56	BA	0.74	0/456	1.20	0/603
57	AF	0.47	0/1133	0.92	0/1513
58	Wa	0.45	0/1152	0.92	0/1541
59	Ta	0.47	0/1819	0.97	1/2422 (0.0%)
60	AZ	0.55	0/570	1.06	0/758
61	BE	0.70	0/711	1.28	5/942 (0.5%)
62	Za	0.47	0/1609	0.94	1/2173 (0.0%)
63	AQ	0.50	0/1070	0.97	0/1436
64	Oa	0.46	0/474	0.87	0/632
65	Ua	0.52	0/974	0.98	0/1305
66	Ya	0.47	0/1044	0.92	0/1398
67	BB	0.46	0/965	0.94	0/1287
68	AN	0.45	0/820	0.88	0/1097
69	Ra	0.45	0/1530	0.95	1/2052 (0.0%)
70	BL	0.47	0/1086	0.90	0/1459
71	La	0.46	0/568	0.89	0/762
72	Aa	0.48	0/1517	0.91	0/2027
73	AY	0.82	0/717	1.25	2/951 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Ca	0.51	0/450	0.88	0/598
75	h1	0.58	12/36567 (0.0%)	1.07	174/56975 (0.3%)
76	B1	0.61	0/263	1.04	1/404 (0.2%)
77	Ba	0.46	0/809	0.92	0/1090
78	AI	0.45	0/801	0.93	0/1082
All	All	0.60	25/205877 (0.0%)	1.13	891/301929 (0.3%)

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
3	A	0	16
6	BM	0	1
7	BO	0	1
9	AU	0	1
10	Ma	0	3
11	Ia	0	1
12	AE	0	1
15	Ja	0	1
16	Ea	0	4
17	AL	0	1
19	Ka	0	1
21	BD	0	1
22	BS	0	3
23	AM	0	3
27	BT	0	1
28	AV	0	2
29	AD	0	1
31	BQ	0	1
32	BH	0	1
33	Da	0	1
34	BK	0	4
37	BP	0	1
39	BG	0	1
40	Fa	0	1
41	Ha	0	1
43	BR	0	1
49	AK	0	4
52	BF	0	1
54	AG	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
56	BA	0	1
63	AQ	0	1
69	Ra	0	1
72	Aa	0	2
73	AY	0	3
All	All	0	68

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2279	A2M	O3'-P	6.00	1.62	1.56
75	h1	422	A2M	O3'-P	5.76	1.62	1.56
3	A	2218	A2M	O3'-P	5.71	1.61	1.56
3	A	2124	A2M	O3'-P	5.58	1.61	1.56
75	h1	438	A2M	O3'-P	5.47	1.61	1.56
75	h1	1381	OMU	O3'-P	5.46	1.61	1.56
3	A	2359	A2M	O3'-P	5.39	1.61	1.56
3	A	2945	A2M	O3'-P	5.32	1.61	1.56
3	A	1142	A2M	O3'-P	5.30	1.61	1.56
3	A	48	OMU	O3'-P	5.30	1.61	1.56
22	BS	21	ARG	NE-CZ	-5.28	1.27	1.33
75	h1	1575	A2M	O3'-P	5.27	1.61	1.56
3	A	2254	A2M	O3'-P	5.22	1.61	1.56
3	A	1646	1MG	O3'-P	5.21	1.61	1.56
3	A	2716	OMU	O3'-P	5.19	1.61	1.56
75	h1	1261	OMU	O3'-P	5.15	1.61	1.56
3	A	2408	OMU	O3'-P	5.15	1.61	1.56
75	h1	975	A2M	O3'-P	5.13	1.61	1.56
75	h1	28	A2M	O3'-P	5.12	1.61	1.56
75	h1	123	OMU	O3'-P	5.12	1.61	1.56
75	h1	580	OMU	O3'-P	5.11	1.61	1.56
75	h1	1270	OMU	O3'-P	5.10	1.61	1.56
75	h1	1263	OMU	O3'-P	5.10	1.61	1.56
3	A	2933	A2M	O3'-P	5.06	1.61	1.56
75	h1	1232	OMU	O3'-P	5.03	1.61	1.56

All (891) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	325	A	O3'-P-O5'	-13.53	83.71	104.00
75	h1	382	U	O3'-P-O5'	-12.32	85.51	104.00
4	C3	37	A	O3'-P-O5'	-12.10	85.85	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2672	A	O3'-P-O5'	-11.62	86.57	104.00
3	A	206	A	C4'-C3'-O3'	-11.51	95.74	113.00
3	A	1111	G	O3'-P-O5'	-11.13	87.30	104.00
3	A	2712	U	O3'-P-O5'	-11.08	87.38	104.00
3	A	2113	C	O3'-P-O5'	-10.86	87.71	104.00
3	A	1739	C	O3'-P-O5'	-10.63	88.05	104.00
75	h1	1313	A	O3'-P-O5'	-10.52	88.22	104.00
75	h1	1797	G	O3'-P-O5'	-10.50	88.25	104.00
3	A	1644	G	C2'-C3'-O3'	-10.04	98.64	113.70
75	h1	1653	A	O3'-P-O5'	-9.88	89.17	104.00
4	C3	72	G	O3'-P-O5'	-9.81	89.29	104.00
3	A	991	G	O3'-P-O5'	-9.76	89.36	104.00
27	BT	89	THR	OG1-CB-CG2	-9.73	89.85	109.30
3	A	206	A	O3'-P-O5'	-9.69	89.47	104.00
3	A	1111	G	C2'-C3'-O3'	-9.61	99.29	113.70
3	A	554	C	C2'-C3'-O3'	9.59	128.08	113.70
3	A	1588	A	O3'-P-O5'	-9.43	89.86	104.00
3	A	2332	U	O5'-P-OP2	-9.43	79.71	108.00
3	A	425	A	O3'-P-O5'	-9.40	89.90	104.00
75	h1	1172	A	C2'-C3'-O3'	-9.26	99.81	113.70
75	h1	1288	A	O3'-P-O5'	-9.23	90.15	104.00
75	h1	435	C	C2'-C3'-O3'	-9.21	99.89	113.70
75	h1	386	G	O3'-P-O5'	-9.19	90.22	104.00
25	BI	48	ARG	N-CA-CB	-9.14	97.67	111.56
2	3	41	A	C3'-C2'-O2'	-9.13	100.91	114.60
3	A	538	G	O3'-P-O5'	-9.01	90.48	104.00
75	h1	99	U	O3'-P-O5'	-8.95	90.57	104.00
3	A	1944	U	O3'-P-O5'	-8.89	90.66	104.00
3	A	2702	A	O3'-P-O5'	-8.82	90.77	104.00
3	A	1118	C	O3'-P-O5'	-8.72	90.92	104.00
3	A	2897	G	O3'-P-O5'	-8.71	90.94	104.00
28	AV	42	ARG	CB-CA-C	-8.68	96.10	110.85
3	A	864	U	O3'-P-O5'	-8.67	91.00	104.00
3	A	1384	G	O3'-P-O5'	-8.66	91.01	104.00
75	h1	387	A	O4'-C4'-C3'	-8.66	95.34	104.00
3	A	671	G	O3'-P-O5'	-8.61	91.08	104.00
3	A	156	G	O3'-P-O5'	-8.61	91.09	104.00
3	A	1930	G	O3'-P-O5'	-8.57	91.14	104.00
2	3	101	G	O3'-P-O5'	-8.55	91.17	104.00
3	A	2625	A	O3'-P-O5'	-8.55	91.17	104.00
75	h1	371	U	O3'-P-O5'	-8.51	91.24	104.00
3	A	2511	U	O3'-P-O5'	-8.47	91.29	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	922	A	O3'-P-O5'	-8.44	91.34	104.00
3	A	2365	A	O3'-P-O5'	-8.38	91.43	104.00
3	A	2745	A	O3'-P-O5'	-8.37	91.44	104.00
3	A	3035	U	O3'-P-O5'	-8.33	91.50	104.00
75	h1	1081	U	O3'-P-O5'	-8.26	91.61	104.00
3	A	3083	G	O3'-P-O5'	-8.24	91.65	104.00
75	h1	1114	A	O3'-P-O5'	-8.21	91.68	104.00
3	A	3090	C	O3'-P-O5'	-8.21	91.68	104.00
3	A	1879	C	O3'-P-O5'	-8.19	91.71	104.00
3	A	2372	C	C1'-C2'-O2'	-8.18	99.52	111.80
3	A	3360	U	O3'-P-O5'	-8.16	91.75	104.00
3	A	1566	A	O3'-P-O5'	-8.15	91.78	104.00
75	h1	942	A	O3'-P-O5'	-8.14	91.78	104.00
3	A	554	C	O3'-P-O5'	-8.14	91.79	104.00
41	Ha	26	ARG	CD-NE-CZ	8.09	135.72	124.40
3	A	3009	A	O3'-P-O5'	8.08	116.12	104.00
3	A	10	G	O3'-P-O5'	-8.05	91.92	104.00
75	h1	1032	U	O3'-P-O5'	-8.05	91.92	104.00
3	A	945	A2M	O3'-P-O5'	-8.00	88.80	104.00
75	h1	977	G	O3'-P-O5'	-7.99	92.02	104.00
3	A	85	U	O3'-P-O5'	-7.95	92.07	104.00
3	A	698	G	O3'-P-O5'	-7.93	92.11	104.00
3	A	725	G	O3'-P-O5'	7.92	115.88	104.00
75	h1	951	C	O3'-P-O5'	-7.89	92.17	104.00
3	A	2640	U	O3'-P-O5'	-7.88	92.17	104.00
3	A	1410	G	O3'-P-O5'	-7.87	92.19	104.00
3	A	11	G	P-O5'-C5'	-7.86	109.11	120.90
3	A	3309	G	C2'-C3'-O3'	-7.84	101.94	113.70
3	A	3101	A	O3'-P-O5'	-7.79	92.31	104.00
3	A	553	A	O3'-P-O5'	-7.79	92.32	104.00
3	A	1533	A	O3'-P-O5'	-7.77	92.35	104.00
3	A	108	G	O3'-P-O5'	-7.72	92.42	104.00
3	A	814	OMG	O3'-P-O5'	-7.72	92.42	104.00
3	A	3130	C	O3'-P-O5'	-7.71	92.44	104.00
3	A	1931	G	O3'-P-O5'	-7.69	92.46	104.00
3	A	1882	U	O3'-P-O5'	-7.68	92.47	104.00
3	A	291	C	O3'-P-O5'	7.68	115.51	104.00
4	C3	27	A	O3'-P-O5'	-7.67	92.50	104.00
3	A	2775	C	C2'-C3'-O3'	-7.66	102.21	113.70
3	A	1606	A	C1'-C2'-O2'	-7.66	100.32	111.80
75	h1	402	A	C3'-C2'-O2'	-7.65	103.12	114.60
3	A	2165	U	O3'-P-O5'	-7.62	92.57	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1005	U	O3'-P-O5'	-7.58	92.63	104.00
75	h1	400	G	O5'-P-OP2	-7.54	85.38	108.00
3	A	2267	U	O3'-P-O5'	-7.54	92.69	104.00
75	h1	98	C	O3'-P-O5'	-7.54	92.69	104.00
3	A	3019	A	O3'-P-O5'	-7.53	92.71	104.00
3	A	1738	U	C2'-C3'-O3'	-7.52	102.42	113.70
3	A	2599	C	C2'-C3'-O3'	-7.52	102.42	113.70
2	3	100	A	O3'-P-O5'	-7.51	92.74	104.00
3	A	882	C	C2'-C3'-O3'	-7.47	102.49	113.70
3	A	2183	G	O3'-P-O5'	-7.47	92.80	104.00
75	h1	1765	U	O3'-P-O5'	-7.46	92.81	104.00
3	A	2988	U	C2'-C3'-O3'	-7.46	102.51	113.70
41	Ha	67	LYS	CB-CA-C	-7.45	98.02	110.68
3	A	266	G	O3'-P-O5'	-7.43	92.85	104.00
3	A	566	G	O3'-P-O5'	-7.42	92.88	104.00
3	A	1339	U	O3'-P-O5'	-7.41	92.89	104.00
3	A	882	C	C4'-C3'-O3'	7.39	124.09	113.00
61	BE	25	GLN	CB-CA-C	-7.39	99.27	110.88
2	3	156	G	O3'-P-O5'	-7.37	92.95	104.00
3	A	985	U	O3'-P-O5'	-7.35	92.98	104.00
75	h1	959	PSU	O3'-P-O5'	-7.33	93.01	104.00
75	h1	892	C	O3'-P-O5'	-7.31	93.03	104.00
75	h1	426	C	O3'-P-O5'	-7.28	93.08	104.00
3	A	1377	G	O3'-P-O5'	-7.28	93.09	104.00
75	h1	18	C	O3'-P-O5'	-7.27	93.09	104.00
3	A	2114	G	C4'-C3'-O3'	-7.27	102.10	113.00
3	A	3004	A	C2'-C3'-O3'	-7.26	102.81	113.70
75	h1	1089	A	O3'-P-O5'	-7.26	93.11	104.00
3	A	1427	A	O3'-P-O5'	-7.24	93.15	104.00
3	A	3333	U	O3'-P-O5'	-7.23	93.15	104.00
3	A	2512	U	O3'-P-O5'	-7.23	93.16	104.00
3	A	2398	G	C2'-C3'-O3'	-7.21	102.88	113.70
75	h1	1129	C	C2'-C3'-O3'	-7.20	102.90	113.70
3	A	1950	G	O3'-P-O5'	-7.18	93.23	104.00
3	A	350	G	O3'-P-O5'	-7.18	93.24	104.00
39	BG	73	GLN	CB-CA-C	-7.15	96.19	110.42
2	3	65	A	O3'-P-O5'	-7.14	93.28	104.00
3	A	1876	G	O3'-P-O5'	-7.13	93.30	104.00
75	h1	1468	C	O3'-P-O5'	-7.13	93.31	104.00
4	C3	61	C	O3'-P-O5'	-7.10	93.35	104.00
30	AJ	122	PHE	CA-CB-CG	-7.10	106.70	113.80
3	A	1603	A	C4'-C3'-O3'	-7.08	102.37	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1177	U	C3'-C2'-O2'	7.07	121.31	110.70
75	h1	1012	C	O3'-P-O5'	-7.07	93.40	104.00
3	A	1482	G	O3'-P-O5'	-7.06	93.40	104.00
3	A	3029	G	O3'-P-O5'	-7.06	93.42	104.00
3	A	2226	A	O3'-P-O5'	-7.05	93.42	104.00
4	C3	44	C	O3'-P-O5'	-7.05	93.43	104.00
75	h1	382	U	C2'-C3'-O3'	7.04	120.06	109.50
1	W2	73	A	O3'-P-O5'	-7.04	93.44	104.00
3	A	870	C	C2'-C3'-O3'	-7.03	103.15	113.70
3	A	1336	A	O3'-P-O5'	-7.02	93.47	104.00
2	3	92	A	C2'-C3'-O3'	-7.02	103.17	113.70
3	A	14	A	O3'-P-O5'	-7.02	93.48	104.00
3	A	729	A	O5'-P-OP2	-7.01	86.97	108.00
3	A	1182	U	O3'-P-O5'	-7.01	93.48	104.00
3	A	1519	C	C1'-C2'-O2'	-6.99	97.92	108.40
75	h1	4	C	O3'-P-O5'	-6.98	93.53	104.00
75	h1	1111	G	O3'-P-O5'	-6.98	93.53	104.00
75	h1	1420	A	O3'-P-O5'	-6.97	93.54	104.00
75	h1	1023	C	C2'-C3'-O3'	-6.97	103.25	113.70
3	A	617	C	O3'-P-O5'	-6.96	93.56	104.00
3	A	2331	C	O3'-P-O5'	6.96	114.44	104.00
3	A	2686	G	C1'-C2'-O2'	6.95	118.82	108.40
3	A	2796	U	O3'-P-O5'	-6.93	93.60	104.00
3	A	3207	C	C2'-C3'-O3'	-6.92	103.32	113.70
3	A	2825	PSU	O3'-P-O5'	-6.91	93.63	104.00
75	h1	166	A	O3'-P-O5'	-6.90	93.64	104.00
3	A	1340	A	O3'-P-O5'	-6.90	93.65	104.00
23	AM	68	THR	CA-CB-OG1	6.90	119.95	109.60
3	A	2988	U	O3'-P-O5'	-6.90	93.65	104.00
3	A	1660	C	C2'-C3'-O3'	-6.89	103.37	113.70
3	A	953	C	C1'-C2'-O2'	-6.88	98.07	108.40
3	A	2722	U	O3'-P-O5'	-6.88	93.68	104.00
3	A	1006	U	O3'-P-O5'	-6.87	93.69	104.00
3	A	2890	U	C2'-C3'-O3'	-6.87	103.39	113.70
75	h1	1269	G	C4'-C3'-O3'	-6.87	102.69	113.00
3	A	1712	U	C2'-C3'-O3'	-6.87	103.40	113.70
3	A	1395	C	O3'-P-O5'	-6.86	93.71	104.00
75	h1	19	A	O3'-P-O5'	-6.85	93.72	104.00
39	BG	55	GLN	CB-CA-C	-6.85	99.37	110.74
3	A	2798	A	O3'-P-O5'	-6.84	93.73	104.00
75	h1	872	A	O3'-P-O5'	-6.84	93.74	104.00
2	3	58	A	C2'-C3'-O3'	-6.84	103.45	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PSU	O3'-P-O5'	-6.83	93.75	104.00
4	C3	30	G	O3'-P-O5'	-6.83	93.75	104.00
75	h1	337	PSU	O3'-P-O5'	-6.82	93.77	104.00
3	A	3138	G	O3'-P-O5'	-6.80	93.79	104.00
3	A	72	A	O3'-P-O5'	-6.77	93.84	104.00
3	A	1341	U	C1'-C2'-O2'	-6.77	101.64	111.80
49	AK	91	THR	CA-CB-OG1	-6.77	99.44	109.60
3	A	2640	U	C2'-C3'-O3'	-6.76	103.56	113.70
3	A	728	G	O3'-P-O5'	6.74	114.11	104.00
75	h1	1145	U	O3'-P-O5'	-6.73	93.90	104.00
3	A	295	C	O3'-P-O5'	-6.73	93.90	104.00
3	A	1413	G	C1'-C2'-O2'	6.73	118.50	108.40
3	A	67	U	O3'-P-O5'	-6.73	93.91	104.00
3	A	823	U	O3'-P-O5'	-6.72	93.91	104.00
3	A	9	A	O3'-P-O5'	-6.71	93.93	104.00
3	A	54	G	O3'-P-O5'	-6.71	93.94	104.00
16	Ea	131	GLU	CB-CG-CD	6.70	123.99	112.60
3	A	2820	C	O3'-P-O5'	-6.69	93.96	104.00
3	A	1205	A	O3'-P-O5'	-6.68	93.97	104.00
3	A	979	U	C3'-C2'-O2'	6.68	120.72	110.70
3	A	2725	C	O3'-P-O5'	-6.68	93.98	104.00
3	A	1465	A	O3'-P-O5'	-6.67	93.99	104.00
3	A	2332	U	O5'-P-OP1	6.67	128.01	108.00
3	A	961	A	C4'-C3'-O3'	-6.66	103.01	113.00
3	A	346	A	O3'-P-O5'	-6.66	94.02	104.00
3	A	1638	A	C1'-C2'-O2'	6.64	118.36	108.40
75	h1	1600	U	O3'-P-O5'	-6.63	94.05	104.00
1	W2	70	C	C2'-C3'-O3'	6.63	123.64	113.70
4	C3	87	G	O3'-P-O5'	-6.61	94.09	104.00
75	h1	1568	U	O3'-P-O5'	-6.60	94.09	104.00
3	A	1326	U	C2'-C3'-O3'	6.60	119.41	109.50
16	Ea	50	ARG	N-CA-CB	-6.60	100.05	110.22
4	C3	26	C	O3'-P-O5'	-6.60	94.10	104.00
3	A	1370	U	O3'-P-O5'	-6.59	94.11	104.00
3	A	3262	U	C2'-C3'-O3'	6.59	119.39	109.50
3	A	91	C	O3'-P-O5'	6.59	113.88	104.00
3	A	1478	OMC	O3'-P-O5'	-6.59	94.12	104.00
3	A	701	A	O3'-P-O5'	6.58	113.87	104.00
13	AX	16	LYS	N-CA-CB	-6.58	99.37	110.49
75	h1	889	U	C4'-C3'-O3'	-6.58	103.13	113.00
3	A	347	C	C2'-C3'-O3'	6.57	119.36	109.50
3	A	1429	C	C2'-C3'-O3'	-6.57	103.85	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BS	47	MET	CG-SD-CE	-6.56	86.47	100.90
75	h1	1116	U	O3'-P-O5'	-6.55	94.17	104.00
3	A	1665	G	C2'-C3'-O3'	-6.55	103.88	113.70
61	BE	64	LYS	N-CA-CB	-6.54	99.42	111.13
3	A	1698	C	C2'-C3'-O3'	-6.54	103.89	113.70
3	A	2142	A	O3'-P-O5'	-6.54	94.19	104.00
27	BT	107	PHE	CB-CA-C	-6.53	98.49	109.65
75	h1	1196	C	O3'-P-O5'	-6.52	94.22	104.00
3	A	1159	A	C2'-C3'-O3'	-6.52	103.92	113.70
75	h1	958	G	C3'-C2'-O2'	6.51	120.46	110.70
3	A	1860	A	C4'-C3'-O3'	6.50	119.16	109.40
3	A	1105	G	O3'-P-O5'	-6.49	94.26	104.00
3	A	729	A	O5'-P-OP1	6.49	127.46	108.00
3	A	620	G	O3'-P-O5'	-6.48	94.28	104.00
3	A	1477	A	C2'-C3'-O3'	-6.48	103.98	113.70
75	h1	800	G	O3'-P-O5'	-6.48	94.29	104.00
1	W2	2	C	O3'-P-O5'	-6.47	94.29	104.00
3	A	892	A	O3'-P-O5'	-6.46	94.31	104.00
3	A	2237	G	O3'-P-O5'	-6.46	94.31	104.00
3	A	871	C	O3'-P-O5'	-6.45	94.32	104.00
3	A	643	U	O3'-P-O5'	-6.45	94.33	104.00
75	h1	1792	G	C4'-C3'-C2'	-6.45	96.15	102.60
75	h1	36	C	O3'-P-O5'	-6.45	94.33	104.00
3	A	402	U	C2'-C3'-O3'	-6.44	104.04	113.70
3	A	1830	C	O3'-P-O5'	-6.44	94.34	104.00
3	A	1313	A	C1'-O4'-C4'	-6.43	103.27	109.70
75	h1	1596	G	O3'-P-O5'	-6.43	94.35	104.00
3	A	1222	G	O3'-P-O5'	-6.43	94.36	104.00
3	A	609	A	C4'-C3'-O3'	6.42	119.04	109.40
3	A	498	A	O3'-P-O5'	-6.42	94.37	104.00
3	A	1519	C	C4'-C3'-O3'	-6.42	103.37	113.00
3	A	816	A2M	OP2-P-O3'	6.42	119.32	105.20
3	A	2981	A	C4'-C3'-O3'	-6.42	103.38	113.00
28	AV	103	THR	CA-CB-OG1	-6.42	99.98	109.60
3	A	1661	G	O3'-P-O5'	-6.41	94.39	104.00
2	3	104	U	O3'-P-O5'	-6.41	94.39	104.00
3	A	8	C	C4'-C3'-O3'	-6.40	103.40	113.00
3	A	1748	G	C1'-C2'-O2'	6.39	117.99	108.40
3	A	2162	C	O3'-P-O5'	6.39	113.59	104.00
31	BQ	72	GLN	CB-CA-C	6.39	120.77	110.16
3	A	292	A	O5'-P-OP1	-6.38	88.84	108.00
3	A	2154	G	C3'-C2'-O2'	6.38	120.28	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BK	159	PHE	CA-CB-CG	-6.38	107.42	113.80
3	A	1394	U	C2'-C3'-O3'	-6.38	104.13	113.70
3	A	1124	G	C4'-C3'-O3'	-6.38	103.43	113.00
3	A	1926	U	O3'-P-O5'	-6.38	94.44	104.00
22	BS	180	HIS	CA-CB-CG	-6.38	107.42	113.80
9	AU	71	PRO	CB-CA-C	-6.37	105.40	111.39
3	A	2998	G	C4'-C3'-C2'	-6.37	96.23	102.60
3	A	88	C	O3'-P-O5'	-6.37	94.45	104.00
3	A	2919	U	C1'-C2'-O2'	6.36	117.94	108.40
73	AY	63	ARG	CB-CA-C	-6.35	97.42	110.38
22	BS	229	TYR	N-CA-CB	-6.35	100.39	109.85
3	A	930	A	O3'-P-O5'	-6.34	94.49	104.00
3	A	1456	G	O3'-P-O5'	-6.33	94.50	104.00
3	A	953	C	C3'-C2'-O2'	6.33	120.19	110.70
3	A	810	A	C1'-C2'-O2'	-6.32	102.32	111.80
3	A	64	A	O3'-P-O5'	-6.31	94.53	104.00
3	A	571	U	O3'-P-O5'	-6.31	94.53	104.00
3	A	2812	A	O3'-P-O5'	-6.31	94.53	104.00
3	A	1746	C	O3'-P-O5'	-6.31	94.54	104.00
3	A	1582	A	O3'-P-O5'	-6.31	94.54	104.00
3	A	951	U	O3'-P-O5'	-6.31	94.54	104.00
1	W2	72	C	O3'-P-O5'	-6.30	94.55	104.00
3	A	1605	A	O3'-P-O5'	-6.30	94.56	104.00
3	A	2377	U	O3'-P-O5'	6.30	113.44	104.00
75	h1	1592	G	O3'-P-O5'	-6.29	94.56	104.00
3	A	2936	G	C1'-C2'-O2'	6.29	117.83	108.40
3	A	1667	G	C3'-C2'-O2'	6.28	120.12	110.70
9	AU	28	THR	CA-CB-OG1	-6.28	100.18	109.60
75	h1	390	OMG	O3'-P-O5'	6.27	113.41	104.00
3	A	683	U	O3'-P-O5'	6.27	113.40	104.00
3	A	761	C	C4'-C3'-O3'	-6.27	103.60	113.00
3	A	225	U	O3'-P-O5'	-6.26	94.61	104.00
3	A	260	C	O3'-P-O5'	-6.26	94.61	104.00
3	A	1425	G	C2'-C3'-O3'	-6.26	104.32	113.70
3	A	554	C	C3'-C2'-C1'	-6.25	95.05	101.30
3	A	788	G	O3'-P-O5'	-6.24	94.64	104.00
3	A	3346	A	O3'-P-O5'	-6.24	94.64	104.00
3	A	1711	C	O3'-P-O5'	-6.24	94.64	104.00
3	A	3327	G	O3'-P-O5'	-6.23	94.65	104.00
3	A	2972	G	C4'-C3'-C2'	-6.22	96.38	102.60
3	A	3008	U	O3'-P-O5'	-6.22	94.67	104.00
3	A	1498	A	C4'-C3'-O3'	-6.22	103.67	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BI	65	VAL	N-CA-CB	-6.22	103.91	111.00
3	A	1709	C	C2'-C3'-O3'	-6.21	104.38	113.70
3	A	700	G	C4'-C3'-O3'	-6.21	103.69	113.00
30	AJ	100	THR	CA-CB-OG1	-6.21	100.29	109.60
3	A	2794	U	C3'-C2'-O2'	6.20	120.00	110.70
75	h1	1092	A	O3'-P-O5'	-6.20	94.69	104.00
3	A	3322	A	O3'-P-O5'	-6.19	94.71	104.00
3	A	1874	C	O3'-P-O5'	-6.19	94.71	104.00
3	A	1711	C	C1'-C2'-O2'	-6.19	99.12	108.40
75	h1	977	G	C2'-C3'-O3'	-6.19	104.42	113.70
3	A	66	C	O3'-P-O5'	-6.18	94.73	104.00
3	A	2997	C	O3'-P-O5'	6.18	113.27	104.00
75	h1	523	A	O3'-P-O5'	-6.18	94.73	104.00
75	h1	1431	OMG	O3'-P-O5'	-6.17	94.75	104.00
75	h1	97	G	C1'-C2'-O2'	6.16	117.64	108.40
75	h1	991	C	O3'-P-O5'	-6.16	94.76	104.00
3	A	1627	G	O3'-P-O5'	-6.16	94.77	104.00
75	h1	114	U	O3'-P-O5'	-6.15	94.77	104.00
75	h1	452	U	O3'-P-O5'	-6.14	94.80	104.00
75	h1	1545	A	O3'-P-O5'	-6.14	94.80	104.00
75	h1	1633	A	O3'-P-O5'	-6.14	94.79	104.00
3	A	1670	C	O3'-P-O5'	-6.13	94.80	104.00
3	A	649	C	O3'-P-O5'	-6.13	94.81	104.00
3	A	925	G	C2'-C3'-O3'	-6.13	104.51	113.70
69	Ra	140	ARG	CB-CA-C	-6.13	103.06	111.51
41	Ha	26	ARG	NE-CZ-NH2	-6.12	113.69	119.20
3	A	1724	A	C2'-C3'-O3'	-6.12	104.51	113.70
3	A	1504	U	C2'-C3'-O3'	-6.12	104.53	113.70
3	A	332	G	O3'-P-O5'	-6.12	94.83	104.00
3	A	1890	OMU	O3'-P-O5'	-6.12	92.38	104.00
75	h1	585	C	O3'-P-O5'	-6.09	94.87	104.00
75	h1	145	A	O3'-P-O5'	-6.08	94.87	104.00
3	A	916	G	O4'-C1'-C2'	-6.08	99.72	105.80
3	A	2192	G	C4'-C3'-O3'	-6.08	103.89	113.00
3	A	526	G	C3'-C2'-O2'	6.07	119.81	110.70
43	BR	46	ARG	N-CA-CB	6.07	119.05	110.12
75	h1	1167	A	C1'-C2'-O2'	6.07	117.50	108.40
4	C3	45	U	C2'-C3'-O3'	-6.07	104.60	113.70
3	A	1755	C	C1'-C2'-O2'	-6.06	99.31	108.40
75	h1	1586	G	O3'-P-O5'	-6.06	94.92	104.00
3	A	1567	U	O3'-P-O5'	-6.05	94.92	104.00
3	A	1192	C	O3'-P-O5'	-6.05	94.93	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1221	U	C4'-C3'-O3'	-6.04	103.93	113.00
3	A	1841	A	O3'-P-O5'	-6.04	94.93	104.00
3	A	103	G	C1'-C2'-O2'	6.04	117.46	108.40
3	A	1178	A	C4'-C3'-O3'	-6.04	103.94	113.00
31	BQ	147	ARG	CB-CA-C	6.04	119.50	109.53
3	A	151	C	O3'-P-O5'	-6.04	94.94	104.00
43	BR	244	ARG	CB-CA-C	-6.04	100.76	110.79
3	A	1556	A	C4'-C3'-O3'	-6.04	103.94	113.00
3	A	106	G	C1'-C2'-O2'	-6.03	99.36	108.40
27	BT	11	THR	CA-CB-OG1	-6.02	100.56	109.60
3	A	2109	G	C2'-C3'-O3'	-6.02	104.68	113.70
75	h1	391	G	C4'-C3'-O3'	-6.02	103.98	113.00
3	A	1689	U	O3'-P-O5'	-6.01	94.98	104.00
3	A	3002	C	C2'-C3'-O3'	-6.01	104.68	113.70
3	A	57	G	O5'-P-OP2	-6.01	89.97	108.00
7	BO	19	PHE	CA-CB-CG	-6.01	107.79	113.80
3	A	147	U	O3'-P-O5'	-6.01	94.99	104.00
73	AY	3	LYS	CB-CA-C	-6.00	98.47	110.42
75	h1	1489	G	O3'-P-O5'	-6.00	95.00	104.00
3	A	313	C	O3'-P-O5'	-6.00	95.00	104.00
75	h1	612	G	C4'-C3'-O3'	-6.00	104.00	113.00
3	A	1737	G	O3'-P-O5'	-6.00	95.00	104.00
3	A	1214	A	C2'-C3'-O3'	-6.00	104.71	113.70
6	BM	40	PRO	CB-CA-C	-5.99	103.56	111.23
3	A	2831	C	C4'-C3'-O3'	-5.99	104.02	113.00
20	AW	50	LYS	N-CA-CB	5.99	118.85	109.69
3	A	3003	G	C4'-C3'-O3'	-5.99	104.02	113.00
3	A	1557	A	C4'-C3'-O3'	-5.98	104.03	113.00
3	A	2390	C	C2'-C3'-O3'	-5.98	104.73	113.70
75	h1	1762	U	O3'-P-O5'	-5.98	95.03	104.00
75	h1	625	A	O3'-P-O5'	-5.98	95.03	104.00
3	A	119	A	O3'-P-O5'	-5.97	95.04	104.00
75	h1	383	C	OP1-P-O3'	5.97	125.92	108.00
3	A	1748	G	O3'-P-O5'	-5.96	95.05	104.00
3	A	2401	G	O3'-P-O5'	-5.96	95.06	104.00
2	3	105	U	O3'-P-O5'	-5.95	95.07	104.00
75	h1	1485	C	O3'-P-O5'	-5.95	95.08	104.00
3	A	268	C	O3'-P-O5'	5.95	112.92	104.00
3	A	1873	U	C4'-C3'-C2'	-5.95	96.65	102.60
3	A	2397	A	O3'-P-O5'	-5.95	95.08	104.00
3	A	1215	G	O3'-P-O5'	-5.94	95.08	104.00
2	3	109	A	O3'-P-O5'	-5.94	95.09	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	692	C	O3'-P-O5'	-5.94	95.09	104.00
3	A	364	A	O3'-P-O5'	-5.94	95.09	104.00
75	h1	1422	G	O3'-P-O5'	-5.94	95.09	104.00
3	A	2590	G	O3'-P-O5'	-5.93	95.10	104.00
4	C3	41	G	O3'-P-O5'	-5.93	95.10	104.00
3	A	1054	PSU	O3'-P-O5'	-5.93	95.10	104.00
3	A	108	G	O5'-P-OP2	-5.93	90.21	108.00
3	A	2631	G	C2'-C3'-O3'	-5.92	104.81	113.70
75	h1	1100	U	C4'-C3'-O3'	5.92	118.29	109.40
3	A	18	G	C4'-C3'-O3'	-5.92	104.12	113.00
3	A	2725	C	C4'-C3'-O3'	-5.92	104.12	113.00
3	A	1472	PSU	O3'-P-O5'	-5.92	95.13	104.00
75	h1	1558	A	O3'-P-O5'	-5.91	95.14	104.00
3	A	526	G	O3'-P-O5'	-5.91	95.14	104.00
3	A	1052	U	O3'-P-O5'	-5.91	95.14	104.00
75	h1	966	U	C2'-C3'-O3'	-5.90	104.85	113.70
75	h1	92	G	P-O5'-C5'	-5.90	112.05	120.90
3	A	344	G	C4'-C3'-O3'	-5.89	104.16	113.00
3	A	2437	A	O3'-P-O5'	-5.89	95.16	104.00
3	A	3044	A	O3'-P-O5'	-5.89	95.16	104.00
3	A	1637	A	O3'-P-O5'	-5.89	95.17	104.00
75	h1	1787	C	O5'-P-OP2	-5.89	90.33	108.00
41	Ha	2	THR	CA-CB-OG1	-5.89	100.77	109.60
3	A	996	U	C4'-C3'-O3'	-5.88	104.17	113.00
3	A	385	G	O3'-P-O5'	-5.88	95.18	104.00
75	h1	957	U	C2'-C3'-O3'	-5.88	104.88	113.70
75	h1	1013	U	O3'-P-O5'	-5.88	95.18	104.00
3	A	215	G	O3'-P-O5'	-5.87	95.19	104.00
3	A	1642	U	C4'-C3'-O3'	-5.87	104.19	113.00
75	h1	624	A	C4'-C3'-O3'	5.87	118.20	109.40
3	A	1120	A	C4'-C3'-C2'	-5.86	96.74	102.60
4	C3	17	G	O3'-P-O5'	-5.86	95.21	104.00
49	AK	98	ARG	CB-CG-CD	-5.86	97.83	111.30
3	A	2673	A	O3'-P-O5'	-5.85	95.22	104.00
75	h1	1525	G	O3'-P-O5'	-5.85	95.22	104.00
3	A	1180	G	O3'-P-O5'	-5.85	95.23	104.00
3	A	2413	C	C3'-C2'-O2'	5.85	119.47	110.70
3	A	1712	U	O3'-P-O5'	-5.84	95.24	104.00
3	A	662	C	C1'-C2'-O2'	-5.84	99.64	108.40
2	3	94	C	C2'-C3'-O3'	5.84	118.25	109.50
3	A	725	G	C2'-C3'-O3'	-5.84	104.94	113.70
3	A	2813	G	C4'-C3'-O3'	-5.83	104.25	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AL	144	PHE	CA-CB-CG	-5.83	107.97	113.80
3	A	2274	G	C4'-C3'-O3'	-5.83	104.26	113.00
3	A	1795	C	C3'-C2'-O2'	-5.82	105.87	114.60
3	A	3246	C	O3'-P-O5'	-5.82	95.28	104.00
3	A	1490	A	C1'-C2'-O2'	-5.81	103.08	111.80
3	A	558	G	O3'-P-O5'	-5.81	95.29	104.00
7	BO	73	TYR	N-CA-CB	-5.81	102.73	110.57
3	A	2954	PSU	O3'-P-O5'	-5.80	95.30	104.00
75	h1	349	G	O3'-P-O5'	-5.80	95.30	104.00
75	h1	752	PSU	O3'-P-O5'	-5.80	95.30	104.00
75	h1	398	G	C4'-C3'-C2'	-5.79	96.81	102.60
3	A	632	U	O3'-P-O5'	-5.79	95.31	104.00
3	A	2374	G	C2'-C3'-O3'	-5.79	105.01	113.70
3	A	2353	G	O3'-P-O5'	-5.79	95.32	104.00
3	A	3374	G	O3'-P-O5'	-5.78	95.33	104.00
3	A	1333	G	C4'-C3'-O3'	-5.78	104.33	113.00
3	A	2785	A	C4'-C3'-O3'	-5.78	104.33	113.00
3	A	1943	C	O3'-P-O5'	-5.78	95.33	104.00
49	AK	140	GLU	N-CA-CB	5.76	118.58	109.82
3	A	1204	G	C2'-C3'-O3'	-5.75	105.07	113.70
3	A	1376	A2M	O3'-P-O5'	-5.75	93.07	104.00
59	Ta	29	ASP	CA-CB-CG	5.75	118.35	112.60
75	h1	1083	U	O3'-P-O5'	-5.75	95.38	104.00
75	h1	867	G	O3'-P-O5'	-5.74	95.39	104.00
3	A	195	A	C4'-C3'-O3'	-5.74	104.39	113.00
3	A	794	G	O3'-P-O5'	-5.73	95.40	104.00
75	h1	315	U	C2'-C3'-O3'	5.73	118.10	109.50
3	A	417	G	O3'-P-O5'	-5.73	95.41	104.00
3	A	1834	C	O3'-P-O5'	-5.73	95.41	104.00
3	A	2727	G	C1'-O4'-C4'	-5.73	103.97	109.70
43	BR	244	ARG	N-CA-CB	5.73	118.55	110.12
75	h1	1164	A	O3'-P-O5'	-5.73	95.41	104.00
3	A	3365	C	C2'-C3'-O3'	-5.73	105.11	113.70
3	A	808	G	C4'-C3'-O3'	-5.72	104.42	113.00
3	A	2116	A	C3'-C2'-O2'	5.72	119.28	110.70
1	2	67	C	O3'-P-O5'	-5.70	95.45	104.00
3	A	1833	U	O3'-P-O5'	-5.70	95.45	104.00
22	BS	213	GLN	CB-CA-C	-5.70	99.02	110.30
3	A	554	C	C4'-C3'-C2'	-5.70	96.90	102.60
2	3	61	C	O3'-P-O5'	5.69	112.53	104.00
75	h1	1113	G	O3'-P-O5'	-5.69	95.47	104.00
3	A	1340	A	C4'-C3'-O3'	-5.68	104.48	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1351	U	C2'-C3'-O3'	-5.68	105.18	113.70
3	A	1093	G	C4'-C3'-O3'	-5.68	104.48	113.00
21	BD	83	ARG	N-CA-CB	-5.68	100.26	110.37
75	h1	970	C	C4'-C3'-O3'	-5.68	104.49	113.00
75	h1	1070	C	O3'-P-O5'	-5.67	95.49	104.00
3	A	644	U	O3'-P-O5'	-5.67	95.49	104.00
75	h1	956	A	O3'-P-O5'	-5.67	95.50	104.00
75	h1	1138	A	O3'-P-O5'	5.66	112.49	104.00
3	A	1862	G	C3'-C2'-O2'	5.66	119.19	110.70
75	h1	91	C	O3'-P-O5'	-5.66	95.51	104.00
3	A	2521	A	C1'-C2'-O2'	-5.66	103.32	111.80
49	AK	86	GLU	CB-CA-C	-5.65	101.40	110.79
2	3	45	A	C3'-C2'-O2'	5.65	119.18	110.70
3	A	1675	G	C4'-C3'-O3'	-5.65	104.52	113.00
3	A	3293	G	C4'-C3'-O3'	-5.65	104.52	113.00
3	A	3378	A	O3'-P-O5'	-5.65	95.52	104.00
41	Ha	26	ARG	CG-CD-NE	-5.65	99.57	112.00
3	A	1594	G	C4'-C3'-O3'	-5.64	104.53	113.00
3	A	816	A2M	O3'-P-O5'	-5.64	93.28	104.00
3	A	1550	G	C2'-C3'-O3'	-5.64	105.25	113.70
75	h1	1294	U	O3'-P-O5'	-5.64	95.54	104.00
3	A	3285	C	C2'-C3'-O3'	-5.63	105.25	113.70
3	A	196	A	P-O5'-C5'	-5.63	112.46	120.90
3	A	703	U	C4'-C3'-O3'	-5.63	104.56	113.00
3	A	280	G	C4'-C3'-O3'	-5.63	104.56	113.00
3	A	1535	U	C4'-C3'-O3'	5.63	117.84	109.40
17	AL	82	ARG	N-CA-CB	-5.62	101.04	110.83
3	A	11	G	C5'-C4'-C3'	-5.62	107.57	116.00
3	A	669	A	C1'-C2'-O2'	5.62	116.83	108.40
4	C3	6	C	O3'-P-O5'	-5.62	95.57	104.00
3	A	259	U	O3'-P-O5'	-5.62	95.57	104.00
3	A	2790	OMG	O3'-P-O5'	-5.62	95.58	104.00
3	A	764	A	C2'-C3'-O3'	-5.62	105.28	113.70
75	h1	352	G	C2'-C3'-O3'	5.62	117.92	109.50
75	h1	379	G	C4'-C3'-C2'	-5.62	96.98	102.60
3	A	2683	C	O3'-P-O5'	-5.61	95.58	104.00
34	BK	13	PHE	CA-CB-CG	-5.61	108.19	113.80
75	h1	930	A	O3'-P-O5'	-5.61	95.58	104.00
3	A	3053	C	P-O5'-C5'	-5.61	112.49	120.90
75	h1	435	C	O3'-P-O5'	-5.60	95.60	104.00
3	A	2682	U	O3'-P-O5'	-5.60	95.60	104.00
75	h1	861	U	O3'-P-O5'	-5.60	95.60	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2832	A	C1'-C2'-O2'	5.59	116.79	108.40
45	BV	119	THR	CA-CB-OG1	-5.59	101.21	109.60
75	h1	1779	U	C4'-C3'-O3'	-5.59	104.61	113.00
22	BS	223	VAL	N-CA-CB	-5.59	103.64	111.25
3	A	820	U	O3'-P-O5'	-5.59	95.62	104.00
3	A	34	PSU	O3'-P-O5'	-5.58	95.62	104.00
3	A	1747	U	OP1-P-O3'	5.58	124.74	108.00
32	BH	44	GLU	N-CA-CB	5.58	119.81	110.32
3	A	1193	G	O3'-P-O5'	-5.58	95.64	104.00
3	A	1725	G	C4'-C3'-O3'	-5.58	104.64	113.00
3	A	39	G	C2'-C3'-O3'	-5.57	105.34	113.70
3	A	2936	G	O3'-P-O5'	-5.57	95.64	104.00
3	A	263	C	O3'-P-O5'	-5.57	95.65	104.00
75	h1	1467	G	O3'-P-O5'	-5.57	95.65	104.00
3	A	1697	A	C3'-C2'-O2'	5.56	119.05	110.70
3	A	1414	C	C2'-C3'-O3'	-5.56	105.36	113.70
3	A	294	U	C1'-C2'-O2'	-5.56	103.47	111.80
3	A	1911	A	C2'-C3'-O3'	-5.55	105.37	113.70
75	h1	1432	G	O3'-P-O5'	-5.55	95.67	104.00
3	A	1887	C	O3'-P-O5'	-5.55	95.67	104.00
3	A	3043	C	O3'-P-O5'	-5.55	95.67	104.00
75	h1	119	U	O3'-P-O5'	-5.55	95.68	104.00
3	A	638	C	O3'-P-O5'	-5.55	95.68	104.00
3	A	920	C	C3'-C2'-O2'	5.54	119.01	110.70
3	A	1866	A	C4'-C3'-O3'	-5.54	104.69	113.00
3	A	2978	U	O3'-P-O5'	-5.54	95.69	104.00
75	h1	1651	C	C2'-C3'-O3'	-5.54	105.39	113.70
3	A	1531	U	C1'-C2'-O2'	-5.54	103.50	111.80
3	A	915	A	C1'-C2'-O2'	-5.54	103.50	111.80
3	A	3356	G	C2'-C3'-O3'	-5.54	105.40	113.70
3	A	2929	A	O3'-P-O5'	5.53	112.30	104.00
75	h1	18	C	C2'-C3'-O3'	-5.53	105.41	113.70
3	A	112	A	O3'-P-O5'	-5.53	95.71	104.00
3	A	3060	C	C2'-C3'-O3'	-5.53	105.41	113.70
2	3	19	G	C4'-C3'-O3'	-5.53	104.71	113.00
3	A	297	G	C1'-C2'-O2'	5.52	116.69	108.40
3	A	88	C	C2'-C3'-O3'	-5.52	105.42	113.70
2	3	43	G	C1'-C2'-O2'	-5.52	103.52	111.80
3	A	1159	A	O3'-P-O5'	5.52	112.28	104.00
32	BH	115	PRO	N-CA-CB	5.52	106.28	103.19
3	A	1428	G	O3'-P-O5'	-5.52	95.73	104.00
3	A	1840	C	OP2-P-O3'	-5.52	91.45	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	101	G	O3'-P-O5'	-5.51	95.73	104.00
75	h1	49	C	O3'-P-O5'	-5.51	95.73	104.00
3	A	1839	U	C4'-C3'-O3'	-5.51	104.73	113.00
3	A	316	G	O3'-P-O5'	-5.51	95.74	104.00
3	A	1107	A	C1'-C2'-O2'	5.51	116.66	108.40
16	Ea	124	ASP	CA-CB-CG	5.51	118.11	112.60
75	h1	963	C	O3'-P-O5'	5.51	112.26	104.00
3	A	713	A	C4'-C3'-C2'	-5.50	97.10	102.60
61	BE	52	VAL	N-CA-CB	5.50	117.32	110.05
3	A	1333	G	O3'-P-O5'	-5.50	95.75	104.00
75	h1	1119	G	O3'-P-O5'	-5.50	95.75	104.00
3	A	2639	A2M	OP2-P-O3'	5.50	117.30	105.20
3	A	2199	G	C1'-C2'-O2'	5.50	116.64	108.40
3	A	1536	C	C2'-C3'-O3'	-5.49	105.46	113.70
43	BR	104	THR	CA-CB-OG1	-5.49	101.36	109.60
3	A	813	C	C4'-C3'-C2'	-5.49	97.11	102.60
3	A	1706	C	O3'-P-O5'	-5.49	95.77	104.00
3	A	1861	A	C3'-C2'-O2'	5.49	118.93	110.70
75	h1	988	G	O3'-P-O5'	-5.49	95.77	104.00
3	A	954	C	C3'-C2'-O2'	5.49	118.93	110.70
3	A	2183	G	C4'-C3'-C2'	-5.49	97.11	102.60
38	BN	139	THR	CA-CB-OG1	-5.49	101.37	109.60
3	A	316	G	C1'-C2'-O2'	5.48	116.62	108.40
3	A	1909	C	O3'-P-O5'	-5.48	95.78	104.00
3	A	2609	G	C4'-C3'-C2'	-5.48	97.12	102.60
75	h1	1460	C	O3'-P-O5'	-5.48	95.78	104.00
3	A	1656	A	C3'-C2'-O2'	-5.48	106.38	114.60
3	A	2998	G	O5'-P-OP2	-5.48	91.56	108.00
17	AL	7	HIS	CA-CB-CG	-5.48	108.32	113.80
75	h1	1749	G	C4'-C3'-O3'	-5.48	104.79	113.00
3	A	1879	C	C2'-C3'-O3'	-5.47	105.49	113.70
3	A	2966	A	C4'-C3'-O3'	-5.47	104.80	113.00
3	A	749	G	C1'-C2'-O2'	5.47	116.60	108.40
3	A	2625	A	C4'-C3'-O3'	-5.47	104.80	113.00
4	C3	80	A	C1'-C2'-O2'	5.46	116.60	108.40
3	A	957	C	O3'-P-O5'	-5.46	95.81	104.00
3	A	2977	U	C3'-C2'-C1'	-5.46	96.04	101.50
3	A	82	U	O3'-P-O5'	-5.46	95.81	104.00
3	A	3053	C	O3'-P-O5'	-5.46	95.81	104.00
75	h1	567	C	O3'-P-O5'	-5.46	95.81	104.00
75	h1	1203	A	O3'-P-O5'	-5.46	95.82	104.00
45	BV	104	ASP	CA-CB-CG	5.45	118.05	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	C	O3'-P-O5'	-5.45	95.83	104.00
3	A	1005	G	C1'-C2'-O2'	-5.45	103.62	111.80
3	A	1528	G	C1'-C2'-O2'	5.45	116.58	108.40
3	A	2125	A	C1'-C2'-O2'	5.45	116.58	108.40
3	A	2130	A	C2'-C3'-O3'	5.45	121.88	113.70
2	3	156	G	C4'-C3'-O3'	-5.45	104.83	113.00
75	h1	1674	A	C1'-C2'-O2'	5.45	116.57	108.40
3	A	1793	C	C2'-C3'-O3'	-5.44	105.53	113.70
75	h1	1159	C	C3'-C2'-O2'	-5.44	106.44	114.60
3	A	508	A	C4'-C3'-C2'	-5.44	97.16	102.60
75	h1	1586	G	C3'-C2'-C1'	-5.44	96.06	101.50
75	h1	1642	C	C4'-C3'-O3'	-5.44	104.84	113.00
3	A	692	C	C4'-C3'-O3'	-5.44	104.84	113.00
3	A	1160	U	C4'-C3'-O3'	-5.44	104.84	113.00
3	A	2588	G	C1'-C2'-O2'	5.44	116.56	108.40
75	h1	1658	U	O3'-P-O5'	-5.43	95.85	104.00
75	h1	17	C	O5'-P-OP2	-5.43	91.70	108.00
3	A	1847	G	C3'-C2'-O2'	5.43	118.85	110.70
3	A	1937	G	C1'-C2'-O2'	5.43	116.54	108.40
3	A	2426	C	O3'-P-O5'	5.43	112.14	104.00
6	BM	69	ARG	CD-NE-CZ	-5.43	116.80	124.40
3	A	1445	U	C4'-C3'-O3'	-5.43	104.86	113.00
3	A	2243	C	C4'-C3'-O3'	-5.43	104.86	113.00
3	A	2342	U	C4'-C3'-O3'	-5.42	104.86	113.00
75	h1	388	G	O5'-P-OP1	5.42	124.26	108.00
3	A	695	C	C2'-C3'-O3'	-5.42	105.57	113.70
3	A	272	U	C4'-C3'-C2'	-5.42	97.18	102.60
3	A	2853	PSU	O3'-P-O5'	-5.42	95.87	104.00
3	A	1626	C	C3'-C2'-O2'	5.42	118.83	110.70
3	A	2690	A	C1'-C2'-O2'	5.42	116.52	108.40
3	A	155	A	C1'-C2'-O2'	5.41	116.52	108.40
75	h1	860	A	O3'-P-O5'	-5.41	95.89	104.00
3	A	89	G	C1'-C2'-O2'	5.41	116.51	108.40
3	A	2931	C	C4'-C3'-O3'	-5.41	104.89	113.00
3	A	3015	A	O3'-P-O5'	-5.40	95.89	104.00
75	h1	1006	A	O3'-P-O5'	-5.40	95.90	104.00
21	BD	28	TYR	CB-CA-C	-5.40	100.42	109.65
3	A	1217	G	O3'-P-O5'	-5.40	95.90	104.00
75	h1	864	A	C2'-C3'-O3'	5.40	117.60	109.50
3	A	2624	C	O3'-P-O5'	-5.39	95.91	104.00
75	h1	1282	G	O3'-P-O5'	-5.39	95.91	104.00
3	A	807	G	C4'-C3'-O3'	-5.39	104.91	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	929	A	C3'-C2'-O2'	-5.39	106.51	114.60
3	A	2378	U	O3'-P-O5'	-5.39	95.92	104.00
4	C3	86	G	C4'-C3'-O3'	-5.39	104.92	113.00
2	3	54	C	C4'-C3'-C2'	-5.38	97.22	102.60
3	A	1796	U	C1'-C2'-O2'	-5.38	103.72	111.80
3	A	2801	A	O3'-P-O5'	-5.38	95.93	104.00
75	h1	12	U	C3'-C2'-O2'	5.38	118.77	110.70
75	h1	1583	C	C3'-C2'-O2'	5.38	118.77	110.70
3	A	2750	G	C4'-C3'-O3'	-5.38	104.94	113.00
75	h1	1758	G	O3'-P-O5'	-5.38	95.93	104.00
2	3	119	C	O3'-P-O5'	-5.38	95.94	104.00
3	A	1323	G	O3'-P-O5'	5.37	112.06	104.00
2	3	63	A	C3'-C2'-O2'	-5.37	106.54	114.60
3	A	3127	A	O3'-P-O5'	-5.37	95.94	104.00
3	A	1000	A	C4'-C3'-C2'	-5.37	97.23	102.60
3	A	1820	C	O3'-P-O5'	-5.37	95.95	104.00
3	A	2522	A	O3'-P-O5'	-5.37	95.95	104.00
3	A	2821	U	O3'-P-O5'	-5.37	95.95	104.00
17	AL	121	PRO	CB-CA-C	-5.37	103.79	111.62
3	A	554	C	C3'-C2'-O2'	5.36	118.75	110.70
3	A	973	G	C4'-C3'-C2'	-5.36	97.24	102.60
31	BQ	72	GLN	N-CA-CB	-5.36	102.29	110.65
75	h1	1036	G	C4'-C3'-C2'	-5.36	97.24	102.60
75	h1	173	G	O3'-P-O5'	-5.36	95.97	104.00
75	h1	423	A	O3'-P-O5'	-5.36	95.97	104.00
3	A	1739	C	C3'-C2'-O2'	5.35	118.73	110.70
3	A	1755	C	C3'-C2'-O2'	5.35	118.72	110.70
3	A	761	C	C3'-C2'-O2'	5.35	118.72	110.70
3	A	2856	C	C2'-C3'-O3'	-5.35	105.68	113.70
3	A	1098	G	C3'-C2'-O2'	5.34	118.71	110.70
3	A	82	U	C4'-C3'-O3'	-5.34	105.00	113.00
3	A	2513	A	C2'-C3'-O3'	-5.34	105.70	113.70
75	h1	877	G	O3'-P-O5'	-5.34	96.00	104.00
75	h1	748	U	O3'-P-O5'	-5.33	96.00	104.00
75	h1	804	G	O3'-P-O5'	-5.33	96.00	104.00
2	3	110	C	O3'-P-O5'	-5.33	96.01	104.00
3	A	2829	G	C2'-C3'-O3'	-5.33	105.71	113.70
7	BO	16	LYS	CB-CA-C	-5.32	101.95	110.79
3	A	1736	G	C3'-C2'-O2'	5.32	118.68	110.70
75	h1	92	G	O3'-P-O5'	-5.32	96.02	104.00
3	A	1539	U	C4'-C3'-O3'	-5.32	105.02	113.00
3	A	758	C	O3'-P-O5'	-5.32	96.02	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	BR	243	VAL	N-CA-CB	5.32	117.12	110.47
41	Ha	145	THR	CA-CB-OG1	-5.32	101.63	109.60
3	A	1865	G	C4'-C3'-O3'	-5.31	105.03	113.00
3	A	194	G	C2'-C3'-O3'	-5.31	105.73	113.70
3	A	3376	U	O3'-P-O5'	-5.31	96.03	104.00
3	A	52	C	O3'-P-O5'	-5.31	96.04	104.00
3	A	673	G	C1'-C2'-O2'	-5.30	103.84	111.80
3	A	3041	C	C4'-C3'-C2'	-5.30	97.30	102.60
3	A	409	G	C2'-C3'-O3'	-5.30	105.75	113.70
4	C3	46	C	O3'-P-O5'	-5.30	96.05	104.00
3	A	382	A	O3'-P-O5'	-5.30	96.05	104.00
3	A	1374	U	C2'-C3'-O3'	-5.30	105.75	113.70
3	A	1443	G	C1'-C2'-O2'	-5.30	103.85	111.80
3	A	226	C	O3'-P-O5'	-5.30	96.06	104.00
3	A	3110	G	C2'-C3'-O3'	-5.30	105.75	113.70
3	A	769	G	O3'-P-O5'	-5.29	96.06	104.00
3	A	1863	G	C2'-C3'-O3'	-5.29	105.76	113.70
75	h1	1122	C	O3'-P-O5'	5.29	111.94	104.00
3	A	737	G	C4'-C3'-O3'	-5.29	105.06	113.00
3	A	2881	U	C4'-C3'-C2'	-5.29	97.31	102.60
3	A	32	A	O3'-P-O5'	-5.29	96.06	104.00
75	h1	379	G	C2'-C3'-O3'	5.29	121.64	113.70
75	h1	1759	A	C4'-C3'-O3'	-5.29	105.07	113.00
3	A	2894	G	C2'-C3'-O3'	-5.29	105.77	113.70
3	A	1752	G	O4'-C1'-C2'	-5.28	100.52	105.80
3	A	2152	U	C4'-C3'-C2'	-5.28	97.32	102.60
3	A	1949	G	C4'-C3'-O3'	-5.28	105.08	113.00
3	A	1170	G	C2'-C3'-O3'	-5.28	105.78	113.70
76	B1	24	U	C2'-C3'-O3'	5.28	117.41	109.50
75	h1	1565	G	O3'-P-O5'	-5.27	96.09	104.00
3	A	1890	OMU	OP2-P-O3'	5.27	116.80	105.20
3	A	2727	G	O4'-C1'-N9	5.27	116.11	108.20
75	h1	1765	U	C1'-C2'-O2'	-5.27	103.90	111.80
3	A	141	G	O3'-P-O5'	-5.26	96.10	104.00
3	A	703	U	O3'-P-O5'	-5.26	96.10	104.00
3	A	1695	U	OP2-P-O3'	5.26	123.80	108.00
3	A	968	C	C2'-C3'-O3'	-5.26	105.81	113.70
3	A	115	U	O3'-P-O5'	-5.26	96.11	104.00
3	A	2758	U	C4'-C3'-O3'	-5.26	105.11	113.00
3	A	2952	UR3	O3'-P-O5'	-5.26	94.01	104.00
54	AG	70	THR	CA-CB-OG1	-5.25	101.72	109.60
41	Ha	53	PHE	CA-CB-CG	-5.25	108.55	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1103	G	C4'-C3'-C2'	-5.25	97.35	102.60
3	A	1494	G	C2'-C3'-O3'	-5.25	105.83	113.70
3	A	3145	C	C3'-C2'-O2'	5.24	118.56	110.70
3	A	953	C	C2'-C3'-O3'	-5.24	105.84	113.70
3	A	1411	G	C4'-C3'-O3'	-5.24	105.14	113.00
3	A	904	G	O3'-P-O5'	-5.24	96.14	104.00
3	A	2821	U	C2'-C3'-O3'	-5.24	105.84	113.70
62	Za	134	ASP	CA-CB-CG	5.24	117.84	112.60
75	h1	635	U	C3'-C2'-O2'	5.23	118.55	110.70
3	A	348	A	O3'-P-O5'	-5.23	96.16	104.00
22	BS	130	PHE	CA-CB-CG	-5.23	108.57	113.80
75	h1	1474	A	O3'-P-O5'	-5.23	96.16	104.00
3	A	3112	A	C4'-C3'-O3'	-5.22	105.16	113.00
3	A	2307	A	O3'-P-O5'	5.22	111.83	104.00
75	h1	757	G	C2'-C3'-O3'	-5.22	105.87	113.70
23	AM	49	HIS	CA-CB-CG	-5.22	108.58	113.80
2	3	51	U	C2'-C3'-O3'	-5.22	105.88	113.70
3	A	1798	G	C4'-C3'-O3'	-5.22	105.17	113.00
3	A	2374	G	N9-C1'-C2'	5.22	119.82	112.00
3	A	922	A	C2'-C3'-O3'	-5.21	105.88	113.70
3	A	2382	A	O3'-P-O5'	5.21	111.82	104.00
32	BH	66	ARG	N-CA-CB	-5.21	102.11	110.77
75	h1	875	C	C4'-C3'-O3'	-5.21	105.18	113.00
75	h1	1801	A	O3'-P-O5'	-5.21	96.18	104.00
2	3	96	A	C2'-C3'-O3'	-5.21	105.88	113.70
6	BM	119	GLN	N-CA-CB	-5.21	101.80	111.13
75	h1	939	G	C4'-C3'-O3'	-5.21	105.18	113.00
38	BN	137	ARG	CB-CA-C	-5.21	101.26	109.80
75	h1	1204	A	O3'-P-O5'	-5.21	96.19	104.00
3	A	2436	A	O3'-P-O5'	-5.21	96.19	104.00
3	A	2985	U	O3'-P-O5'	-5.21	96.19	104.00
3	A	2661	A	C2'-C3'-O3'	-5.21	105.89	113.70
75	h1	330	A	O3'-P-O5'	-5.21	96.19	104.00
75	h1	998	G	O3'-P-O5'	-5.20	96.20	104.00
3	A	1609	C	O3'-P-O5'	-5.20	96.21	104.00
75	h1	335	A	O3'-P-O5'	-5.20	96.21	104.00
3	A	182	C	O3'-P-O5'	-5.19	96.21	104.00
3	A	1839	U	O3'-P-O5'	5.19	111.78	104.00
22	BS	239	THR	CA-CB-OG1	-5.19	101.82	109.60
3	A	436	C	O3'-P-O5'	-5.19	96.22	104.00
3	A	1444	A	C4'-C3'-O3'	-5.19	105.22	113.00
3	A	1208	C	O3'-P-O5'	-5.18	96.23	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	328	G	C2'-C3'-O3'	-5.18	105.93	113.70
3	A	1860	A	O4'-C1'-N9	5.18	115.97	108.20
3	A	1365	A	O3'-P-O5'	-5.17	96.24	104.00
3	A	2949	G	O3'-P-O5'	-5.17	96.24	104.00
75	h1	4	C	C4'-C3'-O3'	-5.17	105.24	113.00
75	h1	1291	PSU	O3'-P-O5'	-5.17	96.24	104.00
3	A	1849	A	C3'-C2'-O2'	-5.17	106.84	114.60
3	A	2968	A	C2'-C3'-O3'	-5.17	105.95	113.70
20	AW	95	PRO	O-C-N	-5.17	118.72	121.15
28	AV	80	THR	CA-CB-OG1	-5.17	101.85	109.60
3	A	33	G	C4'-C3'-C2'	-5.17	97.43	102.60
3	A	1462	A	O3'-P-O5'	5.17	111.75	104.00
3	A	2658	A	C4'-C3'-C2'	-5.17	97.43	102.60
3	A	2395	A	C2'-C3'-O3'	-5.17	105.95	113.70
3	A	1329	G	O3'-P-O5'	-5.16	96.25	104.00
3	A	2105	A	O3'-P-O5'	-5.16	96.25	104.00
75	h1	358	G	OP1-P-O3'	5.16	123.49	108.00
3	A	1005	G	O3'-P-O5'	-5.16	96.26	104.00
3	A	2260	A	C1'-C2'-O2'	5.16	116.14	108.40
4	C3	37	A	C3'-C2'-O2'	5.16	118.44	110.70
3	A	215	G	O5'-P-OP1	5.16	123.46	108.00
3	A	102	G	C4'-C3'-O3'	-5.15	105.27	113.00
3	A	2398	G	O3'-P-O5'	-5.15	96.27	104.00
3	A	1840	C	OP1-P-O3'	5.15	123.45	108.00
17	AL	160	PRO	N-CA-CB	5.15	105.90	103.22
41	Ha	34	ASN	CA-CB-CG	-5.15	107.45	112.60
3	A	2357	C	C2'-C3'-O3'	-5.14	105.99	113.70
4	C3	97	G	C4'-C3'-C2'	-5.14	97.46	102.60
3	A	2100	C	C1'-O4'-C4'	-5.14	104.56	109.70
3	A	2375	G	O3'-P-O5'	5.13	111.70	104.00
23	AM	96	VAL	N-CA-CB	-5.13	103.84	112.47
3	A	2176	A	O3'-P-O5'	-5.13	96.30	104.00
3	A	251	A	O3'-P-O5'	-5.13	96.30	104.00
2	3	13	G	O3'-P-O5'	-5.13	96.31	104.00
3	A	2275	C	C4'-C3'-O3'	-5.13	105.31	113.00
3	A	1880	G	C4'-C3'-O3'	-5.13	105.31	113.00
3	A	2306	C	O3'-P-O5'	-5.13	96.31	104.00
75	h1	1295	G	O3'-P-O5'	-5.12	96.31	104.00
3	A	2576	U	O3'-P-O5'	-5.12	96.32	104.00
2	3	60	G	O3'-P-O5'	-5.12	96.32	104.00
75	h1	1108	G	C1'-C2'-O2'	-5.12	100.72	108.40
61	BE	30	GLU	N-CA-CB	5.12	117.74	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	334	G	O3'-P-O5'	5.12	111.67	104.00
3	A	751	G	O3'-P-O5'	-5.11	96.33	104.00
3	A	1561	G	O3'-P-O5'	-5.11	96.33	104.00
75	h1	1115	G	O3'-P-O5'	-5.11	96.33	104.00
3	A	50	A	C4'-C3'-C2'	-5.11	97.49	102.60
75	h1	339	G	O3'-P-O5'	-5.11	96.33	104.00
3	A	1740	C	C2'-C3'-O3'	-5.11	106.04	113.70
3	A	2170	A	C3'-C2'-O2'	5.11	118.36	110.70
3	A	389	G	O3'-P-O5'	-5.11	96.34	104.00
75	h1	62	A	O3'-P-O5'	-5.11	96.34	104.00
3	A	2394	G	C4'-C3'-O3'	-5.11	105.34	113.00
61	BE	25	GLN	N-CA-CB	5.11	117.41	110.01
3	A	317	G	P-O5'-C5'	-5.10	113.25	120.90
3	A	86	A	O3'-P-O5'	5.10	111.65	104.00
3	A	3123	U	C4'-C3'-C2'	-5.10	97.50	102.60
54	AG	72	LYS	N-CA-CB	5.10	117.56	110.07
2	3	8	C	C2'-C3'-O3'	-5.10	106.06	113.70
3	A	787	C	C2'-C3'-O3'	-5.10	106.06	113.70
3	A	1182	U	C3'-C2'-O2'	5.10	118.34	110.70
3	A	60	A	O3'-P-O5'	-5.09	96.36	104.00
3	A	319	U	O3'-P-O5'	5.09	111.64	104.00
3	A	1362	G	O3'-P-O5'	-5.09	96.36	104.00
75	h1	1120	G	O3'-P-O5'	-5.09	96.36	104.00
4	C3	31	G	O3'-P-O5'	-5.09	96.36	104.00
3	A	215	G	O5'-P-OP2	-5.09	92.74	108.00
3	A	1221	U	C3'-C2'-O2'	5.09	118.33	110.70
3	A	1561	G	C4'-C3'-O3'	5.09	117.03	109.40
3	A	2118	A	C2'-C3'-O3'	-5.08	106.07	113.70
3	A	2408	OMU	OP1-P-O3'	5.08	116.38	105.20
75	h1	98	C	C3'-C2'-O2'	5.08	118.33	110.70
3	A	1851	C	C1'-C2'-O2'	-5.08	104.18	111.80
3	A	2601	G	C1'-C2'-O2'	5.08	116.02	108.40
3	A	1529	G	C4'-C3'-C2'	-5.08	97.52	102.60
3	A	113	G	O4'-C1'-N9	5.08	115.82	108.20
3	A	2135	U	O3'-P-O5'	-5.08	96.39	104.00
3	A	2329	C	O5'-P-OP2	-5.08	92.78	108.00
3	A	3036	U	O3'-P-O5'	-5.07	96.39	104.00
3	A	1089	U	O3'-P-O5'	-5.07	96.39	104.00
3	A	702	G	C2'-C3'-O3'	-5.07	106.10	113.70
3	A	1150	C	C2'-C3'-O3'	-5.07	106.10	113.70
3	A	1482	G	C4'-C3'-C2'	-5.07	97.53	102.60
3	A	1172	C	C1'-C2'-O2'	5.07	116.00	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1274	G	O3'-P-O5'	-5.07	96.40	104.00
3	A	20	G	C3'-C2'-O2'	5.06	118.30	110.70
25	BI	48	ARG	CG-CD-NE	-5.06	100.86	112.00
75	h1	941	A	C4'-C3'-C2'	-5.06	97.54	102.60
3	A	1181	G	C2'-C3'-O3'	-5.06	106.11	113.70
3	A	2293	A	N9-C1'-C2'	5.06	119.59	112.00
3	A	3281	G	C1'-C2'-O2'	5.06	115.99	108.40
54	AG	24	PHE	CA-CB-CG	-5.06	108.74	113.80
3	A	2779	A	O3'-P-O5'	-5.05	96.42	104.00
26	AH	56	THR	CA-CB-OG1	-5.05	102.02	109.60
3	A	1447	U	C4'-C3'-O3'	-5.05	105.42	113.00
3	A	1748	G	C2'-C3'-O3'	-5.05	106.12	113.70
3	A	1842	U	O3'-P-O5'	5.04	111.57	104.00
3	A	1592	G	O3'-P-O5'	5.04	111.56	104.00
3	A	1335	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	2	3	G	O3'-P-O5'	-5.04	96.44	104.00
3	A	2246	C	O3'-P-O5'	-5.04	96.44	104.00
3	A	347	C	P-O5'-C5'	-5.04	113.35	120.90
27	BT	189	LYS	CB-CA-C	-5.04	101.31	110.63
75	h1	891	U	O3'-P-O5'	-5.04	96.44	104.00
75	h1	988	G	C2'-C3'-O3'	-5.04	106.15	113.70
75	h1	1211	C	O3'-P-O5'	-5.04	96.45	104.00
3	A	403	G	O4'-C1'-N9	5.03	115.75	108.20
3	A	2617	G	C2'-C3'-O3'	5.03	117.05	109.50
43	BR	136	GLU	N-CA-CB	-5.03	102.63	110.43
2	3	118	G	C4'-C3'-O3'	-5.03	105.45	113.00
3	A	1797	U	C1'-C2'-O2'	-5.03	104.25	111.80
31	BQ	226	ARG	CB-CA-C	-5.03	100.73	109.64
3	A	3028	G	C4'-C3'-C2'	-5.03	97.57	102.60
3	A	1589	A	O5'-P-OP2	5.03	123.08	108.00
16	Ea	105	ARG	CA-CB-CG	-5.02	104.05	114.10
3	A	1594	G	O3'-P-O5'	-5.02	96.47	104.00
45	BV	151	LYS	CB-CA-C	-5.02	101.61	109.70
3	A	655	U	O3'-P-O5'	-5.02	96.47	104.00
75	h1	961	U	O3'-P-O5'	-5.02	96.47	104.00
3	A	3142	C	C4'-C3'-C2'	-5.02	97.58	102.60
3	A	722	G	C1'-C2'-O2'	5.01	115.92	108.40
3	A	950	G	C2'-C3'-O3'	-5.01	106.18	113.70
3	A	3127	A	C4'-C3'-C2'	-5.01	97.59	102.60
75	h1	975	A2M	OP1-P-O3'	5.01	116.22	105.20
75	h1	1653	A	C1'-C2'-O2'	5.01	115.92	108.40
3	A	961	A	C3'-C2'-O2'	5.01	118.21	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1864	U	C1'-C2'-O2'	5.01	115.91	108.40
22	BS	234	THR	CA-CB-OG1	-5.01	102.09	109.60
3	A	100	C	C2'-C3'-O3'	-5.01	106.19	113.70
75	h1	124	G	O3'-P-O5'	-5.00	96.49	104.00
3	A	2369	G	C3'-C2'-O2'	5.00	118.20	110.70
3	A	3018	U	O3'-P-O5'	5.00	111.50	104.00

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1004	G	Sidechain
3	A	113	G	Sidechain
3	A	1136	G	Sidechain
3	A	1413	G	Sidechain
3	A	1860	A	Sidechain
3	A	193	G	Sidechain
3	A	2130	A	Sidechain
3	A	2293	A	Sidechain
3	A	2303	G	Sidechain
3	A	2374	G	Sidechain
3	A	2744	G	Sidechain
3	A	2963	G	Sidechain
3	A	355	G	Sidechain
3	A	403	G	Sidechain
3	A	815	A	Sidechain
3	A	92	G	Sidechain
29	AD	79	HIS	Peptide
12	AE	92	ARG	Sidechain
54	AG	32	ARG	Sidechain
49	AK	62	ARG	Sidechain
49	AK	74	ARG	Sidechain
49	AK	97	ARG	Sidechain
49	AK	98	ARG	Sidechain
17	AL	97	ARG	Sidechain
23	AM	17	ARG	Sidechain
23	AM	60	ARG	Sidechain
23	AM	63	ARG	Sidechain
63	AQ	24	PHE	Peptide
9	AU	14	ARG	Sidechain
28	AV	25	ARG	Sidechain
28	AV	65	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
73	AY	12	ARG	Sidechain
73	AY	21	ARG	Sidechain
73	AY	33	ARG	Sidechain
72	Aa	25	ARG	Sidechain
72	Aa	50	ARG	Sidechain
56	BA	30	ARG	Sidechain
21	BD	42	ARG	Sidechain
52	BF	106	ARG	Sidechain
39	BG	44	ARG	Sidechain
32	BH	106	ARG	Sidechain
34	BK	23	ARG	Sidechain
34	BK	24	ARG	Sidechain
34	BK	33	ARG	Sidechain
34	BK	54	ARG	Sidechain
6	BM	129	ARG	Sidechain
7	BO	6	ARG	Sidechain
37	BP	93	ARG	Sidechain
31	BQ	30	ARG	Sidechain
43	BR	134	ARG	Sidechain
22	BS	19	ARG	Sidechain
22	BS	287	ARG	Sidechain
22	BS	7	GLU	Peptide
27	BT	145	ARG	Sidechain
33	Da	121	ARG	Sidechain
16	Ea	143	ARG	Sidechain
16	Ea	185	ARG	Sidechain
16	Ea	41	ARG	Sidechain
16	Ea	96	ARG	Sidechain
40	Fa	90	ARG	Sidechain
41	Ha	26	ARG	Sidechain
11	Ia	31	ARG	Sidechain
15	Ja	49	ARG	Sidechain
19	Ka	120	ARG	Sidechain
10	Ma	15	ARG	Sidechain
10	Ma	22	ARG	Sidechain
10	Ma	6	ARG	Sidechain
69	Ra	131	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1630	0	822	11	0
1	W2	1629	0	823	14	0
2	3	3453	0	1754	36	0
3	A	67505	0	34100	433	0
4	C3	2536	0	1284	9	0
5	BC	237	0	289	1	0
6	BM	1246	0	1264	6	0
7	BO	1030	0	1110	12	0
8	AR	425	0	440	8	0
9	AU	888	0	933	11	0
10	Ma	789	0	810	10	0
11	Ia	1512	0	1598	9	0
12	AE	1033	0	1070	7	0
13	AX	786	0	888	6	0
14	AP	1092	0	1182	21	0
15	Ja	2074	0	2180	68	0
16	Ea	1705	0	1765	22	0
17	AL	1485	0	1547	16	0
18	Va	1082	0	1153	19	0
19	Ka	986	0	1053	9	0
20	AW	901	0	926	13	0
21	BD	792	0	843	4	0
22	BS	3111	0	3221	39	0
23	AM	1307	0	1359	14	0
24	AC	1672	0	1748	19	0
25	BI	986	0	1048	21	0
26	AH	1042	0	1119	12	0
27	BT	3056	0	3214	40	0
28	AV	1028	0	1105	15	0
29	AD	1454	0	1512	27	0
30	AJ	1468	0	1577	13	0
31	BQ	1877	0	1922	22	0
32	BH	1636	0	1752	22	0
33	Da	1190	0	1273	6	0
34	BK	2277	0	2311	28	0
35	AT	720	0	754	10	0
36	Pa	389	0	419	4	0
37	BP	975	0	1100	12	0
38	BN	955	0	1037	12	0
39	BG	1874	0	2015	22	0
40	Fa	896	0	975	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	Ha	1156	0	1207	9	0
42	BU	1366	0	1407	10	0
43	BR	1898	0	2005	19	0
44	Xa	1163	0	1222	14	0
45	BV	1718	0	1774	28	0
46	BJ	1653	0	1707	13	0
47	AO	528	0	557	6	0
48	BW	568	0	566	9	0
49	AK	1480	0	1610	23	0
50	Na	647	0	663	8	0
51	AB	1514	0	1576	23	0
52	BF	1491	0	1596	16	0
53	AA	1625	0	1718	17	0
54	AG	1648	0	1755	17	0
55	Ga	433	0	475	1	0
56	BA	444	0	477	3	0
57	AF	1113	0	1169	31	0
58	Wa	1136	0	1177	14	0
59	Ta	1795	0	1920	56	0
60	AZ	562	0	606	4	0
61	BE	702	0	741	12	0
62	Za	1575	0	1578	33	0
63	AQ	1056	0	1128	17	0
64	Oa	471	0	497	13	0
65	Ua	962	0	994	23	0
66	Ya	1024	0	1090	18	0
67	BB	955	0	1012	12	0
68	AN	808	0	845	5	0
69	Ra	1506	0	1571	19	0
70	BL	1064	0	1097	9	0
71	La	562	0	599	15	0
72	Aa	1494	0	1538	29	0
73	AY	705	0	725	20	0
74	Ca	440	0	431	7	0
75	h1	34449	0	17386	392	0
76	B1	240	0	120	3	0
77	Ba	799	0	868	22	0
78	AI	779	0	790	15	0
79	L3	115	0	32	0	0
80	3	28	0	52	1	0
80	A	266	0	494	18	0
80	h1	84	0	156	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	3	4	0	0	0	0
81	A	193	0	0	0	0
81	AC	1	0	0	0	0
81	AY	1	0	0	0	0
81	BI	1	0	0	0	0
81	BM	1	0	0	0	0
81	BR	1	0	0	0	0
81	BS	3	0	0	0	0
81	C3	4	0	0	0	0
81	Da	1	0	0	0	0
81	Ma	1	0	0	0	0
81	Ta	1	0	0	0	0
81	Wa	1	0	0	0	0
81	h1	76	0	0	0	0
82	3	3	0	0	0	0
82	A	125	0	0	0	0
82	AD	1	0	0	0	0
82	AG	1	0	0	0	0
82	AJ	1	0	0	0	0
82	AR	1	0	0	0	0
82	AV	1	0	0	0	0
82	BD	1	0	0	0	0
82	BJ	1	0	0	0	0
82	BM	2	0	0	0	0
82	BQ	2	0	0	0	0
82	BS	2	0	0	0	0
82	C3	1	0	0	0	0
82	Ca	1	0	0	0	0
82	Ea	1	0	0	0	0
82	Fa	1	0	0	0	0
82	Ua	1	0	0	0	0
82	Va	1	0	0	0	0
82	Wa	1	0	0	0	0
82	h1	39	0	0	0	0
83	A	10	0	19	1	0
84	A	15	0	18	2	0
85	AY	1	0	0	0	0
85	BD	1	0	0	0	0
85	BE	1	0	0	0	0
85	Ca	1	0	0	0	0
85	Ga	1	0	0	0	0
85	Ma	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	2	4	0	0	0	0
86	3	288	0	0	14	0
86	A	6924	0	0	164	0
86	AA	1	0	0	0	0
86	AB	5	0	0	0	0
86	AC	14	0	0	1	0
86	AD	4	0	0	2	0
86	AE	17	0	0	0	0
86	AF	4	0	0	1	0
86	AG	77	0	0	3	0
86	AH	22	0	0	0	0
86	AJ	111	0	0	3	0
86	AK	45	0	0	5	0
86	AL	58	0	0	3	0
86	AM	69	0	0	2	0
86	AO	19	0	0	0	0
86	AP	14	0	0	3	0
86	AQ	3	0	0	0	0
86	AR	44	0	0	1	0
86	AT	7	0	0	1	0
86	AU	30	0	0	3	0
86	AV	67	0	0	3	0
86	AW	52	0	0	2	0
86	AX	24	0	0	1	0
86	AY	69	0	0	8	0
86	AZ	4	0	0	0	0
86	Aa	6	0	0	2	0
86	B1	18	0	0	0	0
86	BA	21	0	0	0	0
86	BC	13	0	0	1	0
86	BD	63	0	0	1	0
86	BE	32	0	0	1	0
86	BF	13	0	0	0	0
86	BG	32	0	0	3	0
86	BH	85	0	0	2	0
86	BI	39	0	0	0	0
86	BJ	31	0	0	1	0
86	BK	66	0	0	1	0
86	BL	2	0	0	0	0
86	BM	62	0	0	0	0
86	BN	27	0	0	1	0
86	BO	33	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	BP	21	0	0	0	0
86	BQ	126	0	0	3	0
86	BR	68	0	0	4	0
86	BS	153	0	0	3	0
86	BT	131	0	0	5	0
86	BU	5	0	0	0	0
86	BV	11	0	0	0	0
86	Ba	1	0	0	0	0
86	C3	153	0	0	4	0
86	Ca	1	0	0	0	0
86	Da	15	0	0	0	0
86	Ea	135	0	0	4	0
86	Fa	61	0	0	1	0
86	Ga	9	0	0	0	0
86	Ha	85	0	0	0	0
86	Ia	20	0	0	0	0
86	Ja	13	0	0	2	0
86	Ma	24	0	0	2	0
86	Na	2	0	0	0	0
86	Oa	3	0	0	1	0
86	Pa	2	0	0	0	0
86	Ta	6	0	0	5	0
86	Ua	22	0	0	0	0
86	Va	23	0	0	3	0
86	W2	21	0	0	3	0
86	Xa	13	0	0	1	0
86	Ya	1	0	0	1	0
86	Za	1	0	0	0	0
86	h1	1264	0	0	80	0
All	All	208167	0	146263	1816	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 (1816) 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)
73:AY:76:THR:O	73:AY:77:CYS:N	1.59	1.33
31:BQ:102:LEU:HG	86:BQ:516:HOH:O	1.04	1.18
75:h1:1784:G:H3'	75:h1:1785:MA6:P	1.84	1.16
75:h1:389:A:N7	86:h1:2102:HOH:O	1.85	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1491:A:N7	86:A:3801:HOH:O	1.89	1.06
17:AL:29:MET:SD	86:AM:260:HOH:O	2.14	1.05
49:AK:121:HIS:ND1	86:AK:301:HOH:O	1.91	1.04
39:BG:232:MET:SD	86:BG:327:HOH:O	2.14	1.03
2:3:81:A:N7	86:3:301:HOH:O	1.93	1.01
59:Ta:72:ARG:NH2	75:h1:420:G:O2'	1.96	0.99
73:AY:8:PHE:CD1	86:AY:360:HOH:O	2.15	0.97
75:h1:428:G:OP2	86:h1:2101:HOH:O	1.82	0.97
8:AR:19:ASN:O	8:AR:20:GLY:O	1.82	0.97
4:C3:119:C:O3'	86:C3:301:HOH:O	1.86	0.94
76:B1:24:U:H3	1:W2:34:G:H1	1.14	0.94
3:A:1354:G:N7	86:A:3812:HOH:O	2.01	0.94
3:A:847:G:O6	61:BE:4:ARG:NH2	2.02	0.93
78:AI:1:MET:HE1	78:AI:41:GLN:HA	1.51	0.92
3:A:3184:G:H1	3:A:3190:U:H3	1.18	0.91
65:Ua:137:ASP:HA	86:h1:3197:HOH:O	1.69	0.91
25:BI:90:ARG:CZ	25:BI:96:MET:HE1	2.02	0.90
73:AY:76:THR:O	73:AY:77:CYS:CA	2.20	0.90
11:Ia:3:THR:HA	17:AL:143:GLN:HE22	1.37	0.90
3:A:693:A:N3	86:A:3814:HOH:O	2.04	0.89
53:AA:72:LEU:HD21	78:AI:20:VAL:HG21	1.54	0.89
3:A:28:G:H5''	16:Ea:172:ARG:HD3	1.55	0.89
43:BR:241:GLU:OE1	86:BR:401:HOH:O	1.89	0.89
44:Xa:6:GLU:OE1	75:h1:329:U:O2'	1.90	0.88
3:A:1183:G:OP1	86:A:3802:HOH:O	1.90	0.88
75:h1:1175:C:OP1	86:h1:2103:HOH:O	1.90	0.88
3:A:3226:G:H1	3:A:3237:U:H3	1.22	0.87
75:h1:390:OMG:OP1	86:h1:2104:HOH:O	1.92	0.87
3:A:2837:A:OP1	46:BJ:154:ARG:NH2	2.07	0.87
3:A:3071:A:N3	86:A:3816:HOH:O	2.05	0.87
3:A:844:A:N1	86:A:3823:HOH:O	2.09	0.86
3:A:62:G:OP1	16:Ea:185:ARG:NH1	2.08	0.86
3:A:756:G:N7	86:A:3820:HOH:O	2.07	0.85
3:A:991:G:N1	3:A:1111:G:H2'	1.92	0.85
30:AJ:161:ASN:HB2	86:AJ:391:HOH:O	1.75	0.85
1:2:18:G:H2'	1:2:57:G:N2	1.91	0.85
59:Ta:181:GLN:NE2	75:h1:65:A:OP1	2.09	0.85
75:h1:42:G:N7	86:h1:2119:HOH:O	2.09	0.85
57:AF:116:ARG:NH2	86:AF:201:HOH:O	2.10	0.85
3:A:1492:G:O5'	86:A:3805:HOH:O	1.96	0.84
3:A:1537:G:OP2	86:A:3804:HOH:O	1.94	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A:6621:HOH:O	16:Ea:169:LYS:HE2	1.78	0.83
75:h1:1655:C:OP1	86:h1:2106:HOH:O	1.96	0.83
3:A:2590:G:N7	86:A:3826:HOH:O	2.09	0.83
3:A:923:A:OP2	86:A:3806:HOH:O	1.96	0.83
75:h1:309:G:O6	86:h1:2105:HOH:O	1.95	0.83
29:AD:169:ILE:HD12	75:h1:1476:U:C5	2.14	0.82
22:BS:26:ARG:HD2	22:BS:47:MET:HE1	1.60	0.82
3:A:2522:A:N3	86:A:3830:HOH:O	2.11	0.82
1:2:18:G:H2'	1:2:57:G:H22	1.42	0.82
3:A:1880:G:N7	86:A:3828:HOH:O	2.10	0.82
3:A:401:U:P	86:A:3811:HOH:O	2.37	0.82
3:A:1522:G:OP2	86:A:3807:HOH:O	1.98	0.82
3:A:742:U:H3	3:A:747:G:H1	1.28	0.82
3:A:1951:G:OP2	49:AK:135:LYS:NZ	2.13	0.82
3:A:991:G:H1	3:A:1111:G:H2'	1.45	0.81
65:Ua:137:ASP:OD1	65:Ua:137:ASP:C	2.23	0.81
75:h1:361:G:N3	86:h1:2122:HOH:O	2.12	0.81
3:A:3297:A:N7	86:A:3832:HOH:O	2.14	0.81
22:BS:26:ARG:CD	22:BS:47:MET:HE1	2.11	0.81
2:3:94:C:O3'	86:3:302:HOH:O	1.98	0.81
3:A:3059:G:N7	86:A:3831:HOH:O	2.14	0.81
3:A:3182:G:H1	3:A:3192:U:H3	1.25	0.81
46:BJ:51:HIS:ND1	46:BJ:137:SER:OG	2.14	0.81
3:A:320:A:OP1	86:A:3808:HOH:O	1.99	0.80
10:Ma:32:LYS:NZ	86:Ma:301:HOH:O	1.95	0.80
3:A:1739:C:O2'	40:Fa:52:GLN:OE1	2.00	0.80
75:h1:24:U:O3'	86:h1:2108:HOH:O	2.00	0.80
25:BI:112:MET:HE1	25:BI:117:ILE:HD11	1.62	0.80
3:A:1525:C:OP2	86:A:3809:HOH:O	2.00	0.79
32:BH:43:CYS:SG	32:BH:109:VAL:CG1	2.70	0.79
75:h1:351:G:OP2	86:h1:2107:HOH:O	2.00	0.79
3:A:1808:A:N7	86:A:3840:HOH:O	2.15	0.79
3:A:401:U:O5'	86:A:3811:HOH:O	2.00	0.79
75:h1:985:G:N7	86:h1:2129:HOH:O	2.16	0.79
3:A:3218:U:O4	3:A:3245:C:N3	2.16	0.78
72:Aa:31:ARG:NH1	75:h1:334:U:OP1	2.14	0.78
3:A:710:G:N7	86:A:3844:HOH:O	2.16	0.78
3:A:3134:G:OP1	86:A:3810:HOH:O	2.00	0.78
3:A:28:G:C5'	16:Ea:172:ARG:HD3	2.13	0.78
3:A:334:G:N7	86:A:3833:HOH:O	2.14	0.77
65:Ua:137:ASP:OD1	65:Ua:138:SER:N	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:117:U:H2'	75:h1:118:U:C6	2.19	0.77
59:Ta:65:GLN:HE22	75:h1:1683:A:H2'	1.50	0.77
59:Ta:7:ASN:HB3	59:Ta:12:CYS:SG	2.25	0.76
3:A:352:A:N1	27:BT:89:THR:HG22	2.01	0.76
75:h1:1286:U:OP2	86:h1:2110:HOH:O	2.03	0.76
73:AY:8:PHE:CE1	86:AY:360:HOH:O	2.38	0.76
3:A:3118:C:OP2	80:A:3416:TER:N14	2.19	0.76
43:BR:183:ILE:HD11	43:BR:192:GLU:HG3	1.67	0.75
75:h1:390:OMG:OP2	86:h1:2111:HOH:O	2.03	0.75
75:h1:438:A2M:O2'	86:h1:2112:HOH:O	2.04	0.75
3:A:817:A:N7	86:A:3859:HOH:O	2.20	0.75
3:A:1806:G:N7	86:A:3854:HOH:O	2.19	0.75
86:A:9843:HOH:O	16:Ea:193:LYS:HD3	1.86	0.75
53:AA:48:ILE:HB	53:AA:86:LEU:HD23	1.69	0.74
3:A:18:G:N7	86:A:3853:HOH:O	2.18	0.74
3:A:1306:C:OP2	86:A:3813:HOH:O	2.03	0.74
75:h1:451:C:OP1	86:h1:2109:HOH:O	2.03	0.74
3:A:1881:A:N7	86:A:3858:HOH:O	2.20	0.74
3:A:2387:C:OP2	86:A:3817:HOH:O	2.05	0.74
3:A:3167:G:N7	86:A:3863:HOH:O	2.20	0.74
75:h1:1059:U:H3'	75:h1:1060:U:C5'	2.18	0.74
3:A:2119:A:N1	86:A:3867:HOH:O	2.21	0.74
75:h1:1800:C:OP2	86:h1:2113:HOH:O	2.05	0.74
3:A:1305:G:N7	86:A:3862:HOH:O	2.20	0.73
9:AU:16:TYR:CZ	9:AU:47:GLU:HG2	2.23	0.73
72:Aa:22:ARG:HB3	75:h1:387:A:H5'	1.70	0.73
3:A:3330:G:O2'	86:A:3819:HOH:O	2.06	0.73
72:Aa:171:CYS:SG	72:Aa:172:ILE:O	2.45	0.73
3:A:3201:A:OP2	86:A:3818:HOH:O	2.06	0.73
3:A:1605:A:N7	86:A:3869:HOH:O	2.21	0.73
3:A:757:C:O2'	86:A:3815:HOH:O	2.04	0.73
3:A:1353:G:N7	86:A:3874:HOH:O	2.21	0.73
75:h1:1587:U:OP1	86:h1:2114:HOH:O	2.06	0.73
14:AP:75:VAL:HG11	14:AP:80:LEU:HD21	1.71	0.72
3:A:2595:U:H5	86:A:7825:HOH:O	1.72	0.72
20:AW:54:MET:HE1	20:AW:88:ALA:HB1	1.69	0.72
3:A:2841:U:H2'	3:A:2841:U:O2	1.88	0.72
27:BT:12:ILE:HD11	27:BT:27:VAL:HG23	1.71	0.71
3:A:904:G:O5'	86:A:3821:HOH:O	2.08	0.71
3:A:1212:A:N3	86:A:3879:HOH:O	2.22	0.71
15:Ja:21:ASP:OD1	75:h1:776:C:OP1	2.06	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:428:G:OP2	86:h1:2116:HOH:O	2.07	0.71
3:A:609:A:N6	52:BF:25:ARG:O	2.24	0.71
75:h1:393:A:N3	86:h1:2148:HOH:O	2.23	0.71
75:h1:594:A:O2'	75:h1:598:C:OP1	2.06	0.71
75:h1:401:A:N1	86:h1:2149:HOH:O	2.23	0.71
3:A:1343:C:OP2	86:A:3824:HOH:O	2.09	0.71
39:BG:170:PRO:HA	39:BG:217:ASN:HD21	1.55	0.71
75:h1:39:A:C8	86:h1:2272:HOH:O	2.43	0.71
3:A:3030:A:N1	86:A:3895:HOH:O	2.24	0.71
75:h1:385:G:N7	86:h1:2151:HOH:O	2.24	0.71
3:A:8:C:OP2	86:A:3825:HOH:O	2.09	0.71
75:h1:1296:G:N7	86:h1:2150:HOH:O	2.24	0.70
1:W2:37:G:O6	86:W2:101:HOH:O	2.09	0.70
3:A:1792:G:N7	86:A:3894:HOH:O	2.24	0.70
75:h1:931:A:N7	86:h1:2152:HOH:O	2.24	0.70
75:h1:1641:OMC:O2	75:h1:1767:6MZ:N1	2.24	0.70
12:AE:2:VAL:N	75:h1:1035:C:HO2'	1.89	0.70
3:A:1089:U:O2	34:BK:138:ARG:NH2	2.24	0.70
3:A:3078:G:N7	86:A:3891:HOH:O	2.23	0.70
4:C3:72:G:N3	86:C3:303:HOH:O	2.24	0.70
13:AX:31:SER:HB3	86:AX:224:HOH:O	1.92	0.70
75:h1:1385:A:H1'	77:Ba:58:ARG:HD2	1.73	0.70
3:A:3174:C:N4	32:BH:172:LEU:HD13	2.07	0.70
3:A:584:G:N7	52:BF:32:ARG:NH2	2.39	0.70
74:Ca:25:GLY:HA3	78:AI:62:MET:HE3	1.73	0.70
2:3:81:A:C5	86:3:301:HOH:O	2.40	0.70
75:h1:1784:G:C3'	75:h1:1785:MA6:P	2.74	0.70
3:A:7:C:H3'	86:A:3825:HOH:O	1.91	0.70
75:h1:1172:A:H2'	75:h1:1173:G:C8	2.26	0.70
3:A:3046:A:O4'	86:A:3822:HOH:O	2.09	0.70
75:h1:386:G:OP2	86:h1:2120:HOH:O	2.10	0.70
59:Ta:90:ARG:HD3	86:Ta:401:HOH:O	1.92	0.69
2:3:120:G:N7	86:3:307:HOH:O	2.26	0.69
3:A:2680:U:H1'	42:BU:24:SER:OG	1.91	0.69
52:BF:86:ARG:NH2	52:BF:136:GLN:O	2.25	0.69
75:h1:986:G:N7	86:h1:2153:HOH:O	2.25	0.69
86:A:4184:HOH:O	16:Ea:170:LYS:HE3	1.92	0.69
3:A:2739:A:N7	86:A:3911:HOH:O	2.25	0.69
3:A:2896:A:N7	86:A:3898:HOH:O	2.24	0.69
75:h1:1201:G:OP1	86:h1:2118:HOH:O	2.09	0.69
75:h1:465:U:H2'	75:h1:466:A2M:H8	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2735:A:N7	86:A:3902:HOH:O	2.24	0.69
75:h1:389:A:OP1	86:h1:2117:HOH:O	2.08	0.69
51:AB:29:GLU:HB2	51:AB:44:LEU:CD2	2.22	0.69
3:A:108:G:N3	86:A:3922:HOH:O	2.26	0.69
11:Ia:12:ILE:HD13	11:Ia:18:ILE:HG21	1.75	0.69
34:BK:22:ARG:HB3	34:BK:28:THR:HG22	1.75	0.69
86:Ta:403:HOH:O	75:h1:159:U:C2	2.44	0.69
3:A:72:A:OP2	13:AX:22:ARG:NH2	2.25	0.69
3:A:867:A:N1	86:A:3905:HOH:O	2.24	0.69
3:A:2244:G:N7	86:A:3917:HOH:O	2.26	0.69
15:Ja:6:LYS:HB3	86:h1:2934:HOH:O	1.91	0.69
18:Va:15:ARG:NH2	18:Va:18:ILE:HG21	2.07	0.69
12:AE:51:GLU:HG3	69:Ra:141:THR:O	1.93	0.68
2:3:113:A:N1	86:3:305:HOH:O	2.25	0.68
33:Da:38:CYS:SG	33:Da:78:HIS:ND1	2.65	0.68
75:h1:1034:C:OP2	86:h1:2121:HOH:O	2.11	0.68
3:A:1214:A:O3'	86:A:3827:HOH:O	2.10	0.68
16:Ea:15:GLN:NE2	86:Ea:403:HOH:O	2.25	0.68
66:Ya:86:ARG:NH2	66:Ya:125:SER:O	2.26	0.68
72:Aa:46:ARG:HB3	72:Aa:56:TRP:CZ3	2.28	0.68
3:A:401:U:OP2	86:A:3811:HOH:O	2.12	0.68
2:3:124:C:N3	86:3:309:HOH:O	2.27	0.68
22:BS:110:LEU:O	22:BS:115:ARG:NH1	2.26	0.68
69:Ra:64:TYR:HA	69:Ra:96:VAL:O	1.94	0.67
3:A:1515:G:OP2	86:A:3829:HOH:O	2.11	0.67
75:h1:96:G:N7	86:h1:2158:HOH:O	2.26	0.67
75:h1:146:A:N6	75:h1:165:U:O2	2.28	0.67
19:Ka:35:ASN:OD1	75:h1:523:A:O2'	2.13	0.67
75:h1:1295:G:N7	86:h1:2164:HOH:O	2.28	0.67
15:Ja:122:LYS:NZ	15:Ja:124:CYS:SG	2.68	0.67
2:3:110:C:OP2	86:3:303:HOH:O	2.13	0.66
3:A:1057:A:H5'	86:BJ:414:HOH:O	1.94	0.66
42:BU:112:ILE:HD11	42:BU:118:TYR:HA	1.76	0.66
20:AW:45:GLU:OE1	52:BF:222:HIS:NE2	2.27	0.66
23:AM:5:HIS:ND1	86:AM:201:HOH:O	2.27	0.66
49:AK:170:ARG:HH12	75:h1:817:A:H2'	1.59	0.66
75:h1:462:A:OP1	86:h1:2125:HOH:O	2.14	0.66
15:Ja:3:ARG:HB3	75:h1:94:A:H1'	1.78	0.66
59:Ta:65:GLN:NE2	75:h1:1683:A:H2'	2.10	0.66
3:A:611:C:O2'	52:BF:47:ARG:O	2.13	0.66
3:A:3111:A:OP1	11:Ia:78:SER:OG	2.06	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1215:G:N7	86:A:3964:HOH:O	2.29	0.66
75:h1:799:A2M:O2'	86:h1:2127:HOH:O	2.15	0.66
75:h1:1590:G:H1	75:h1:1610:U:H3	1.43	0.66
32:BH:43:CYS:SG	32:BH:109:VAL:HG13	2.35	0.65
73:AY:76:THR:C	73:AY:77:CYS:N	2.52	0.65
3:A:789:A:OP2	30:AJ:161:ASN:ND2	2.29	0.65
3:A:841:G:N7	86:A:3943:HOH:O	2.28	0.65
83:A:3401:SPD:H31	41:Ha:38:MET:HE1	1.79	0.65
17:AL:154:VAL:HA	17:AL:178:MET:HE3	1.78	0.65
34:BK:22:ARG:HB3	34:BK:28:THR:CG2	2.26	0.65
3:A:3318:U:OP2	86:A:3839:HOH:O	2.15	0.65
75:h1:367:G:C2	75:h1:368:A:C8	2.84	0.65
75:h1:1652:U:H2'	75:h1:1653:A:C8	2.30	0.65
43:BR:170:ASP:OD1	43:BR:171:ASN:N	2.29	0.65
3:A:3072:G:N7	86:A:3979:HOH:O	2.30	0.65
25:BI:40:ILE:O	25:BI:41:SER:HB3	1.95	0.65
15:Ja:34:GLY:O	86:Ja:301:HOH:O	2.14	0.65
63:AQ:3:THR:O	63:AQ:4:VAL:HG22	1.97	0.65
3:A:735:G:N7	86:A:3955:HOH:O	2.29	0.65
69:Ra:115:ARG:O	69:Ra:118:THR:OG1	2.07	0.65
3:A:2748:G:N7	86:A:3939:HOH:O	2.27	0.65
46:BJ:38:MET:HG2	46:BJ:83:ASP:HA	1.79	0.65
75:h1:1048:G:N7	86:h1:2163:HOH:O	2.28	0.65
75:h1:427:A:OP1	86:h1:2126:HOH:O	2.14	0.64
3:A:25:C:OP2	86:A:3835:HOH:O	2.15	0.64
75:h1:302:A:H2'	75:h1:303:A:C8	2.32	0.64
75:h1:1764:G:OP2	86:h1:2128:HOH:O	2.15	0.64
3:A:2981:A:N7	80:A:3414:TER:H41	2.12	0.64
20:AW:18:ILE:HD11	20:AW:103:VAL:HG13	1.79	0.64
59:Ta:104:VAL:HG13	59:Ta:108:LEU:HD22	1.79	0.64
75:h1:869:G:H1	75:h1:961:U:H3	1.45	0.64
3:A:102:G:OP1	86:A:3838:HOH:O	2.15	0.64
3:A:2164:C:OP1	86:A:3834:HOH:O	2.14	0.64
75:h1:1679:U:H3	75:h1:1728:U:H3	1.45	0.64
3:A:320:A:N3	86:A:3975:HOH:O	2.30	0.64
43:BR:91:ILE:N	43:BR:91:ILE:HD12	2.12	0.64
86:A:8185:HOH:O	38:BN:121:LYS:HD3	1.98	0.64
13:AX:50:VAL:HA	39:BG:224:ARG:HH12	1.63	0.64
3:A:1446:OMC:HM23	27:BT:100:MET:HG3	1.80	0.64
3:A:1631:G:N7	14:AP:48:LYS:NZ	2.46	0.64
27:BT:76:ARG:NH1	86:BT:501:HOH:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AK:143:HIS:O	49:AK:144:LYS:C	2.41	0.64
49:AK:42:ARG:NH1	86:AK:302:HOH:O	2.20	0.64
49:AK:170:ARG:NH2	75:h1:819:G:N7	2.46	0.64
57:AF:145:ARG:NH2	1:W2:33:U:OP2	2.31	0.64
72:Aa:56:TRP:HB2	72:Aa:179:CYS:O	1.98	0.64
3:A:784:G:H3'	86:A:4535:HOH:O	1.97	0.63
3:A:2234:OMG:H4'	1:W2:71:G:OP1	1.97	0.63
3:A:51:G:OP1	86:A:3841:HOH:O	2.15	0.63
3:A:61:A:OP1	16:Ea:172:ARG:NH2	2.31	0.63
3:A:208:A:H4'	3:A:209:G:OP2	1.97	0.63
65:Ua:30:VAL:HB	65:Ua:92:MET:HE2	1.80	0.63
75:h1:342:U:H2'	75:h1:343:A:C8	2.34	0.63
2:3:70:G:N7	86:3:311:HOH:O	2.30	0.63
3:A:1222:G:OP2	86:A:3842:HOH:O	2.15	0.63
57:AF:129:LYS:NZ	57:AF:133:GLY:O	2.31	0.63
45:BV:143:THR:HG23	45:BV:205:TYR:CE1	2.34	0.63
74:Ca:53:ILE:C	74:Ca:54:LYS:N	2.57	0.63
2:3:81:A:N6	86:3:301:HOH:O	2.15	0.63
3:A:2304:C:O2'	3:A:2305:G:OP2	2.16	0.63
32:BH:154:HIS:ND1	86:BH:303:HOH:O	2.31	0.63
45:BV:168:MET:HA	45:BV:197:ILE:HD12	1.79	0.63
43:BR:90:PHE:C	43:BR:91:ILE:HD12	2.24	0.63
59:Ta:193:ARG:NH2	75:h1:286:G:N7	2.45	0.63
72:Aa:181:ARG:HD3	86:Aa:305:HOH:O	1.99	0.63
45:BV:119:THR:HG21	45:BV:161:ILE:HD11	1.81	0.63
3:A:1003:G:H5''	23:AM:43:LYS:HE2	1.81	0.62
15:Ja:2:ALA:N	86:Ja:302:HOH:O	2.31	0.62
31:BQ:221:HIS:ND1	86:BQ:401:HOH:O	1.88	0.62
15:Ja:3:ARG:HG3	15:Ja:3:ARG:HH11	1.64	0.62
59:Ta:155:VAL:HG21	59:Ta:180:ILE:HD12	1.80	0.62
75:h1:1386:G:OP1	77:Ba:88:HIS:ND1	2.29	0.62
65:Ua:137:ASP:OD2	75:h1:928:C:O2	2.17	0.62
38:BN:80:THR:HA	38:BN:85:MET:HE3	1.80	0.62
3:A:1219:G:N7	86:A:3995:HOH:O	2.31	0.62
59:Ta:85:ARG:NH1	86:Ta:403:HOH:O	2.31	0.62
4:C3:12:U:C2	86:C3:358:HOH:O	2.51	0.62
19:Ka:85:LYS:HE3	19:Ka:98:LEU:HB3	1.82	0.62
75:h1:1171:G:C2	75:h1:1172:A:C8	2.87	0.62
75:h1:1608:C:H2'	75:h1:1609:G:C8	2.34	0.62
2:3:162:C:OP2	39:BG:80:LYS:NZ	2.26	0.62
25:BI:90:ARG:NH1	25:BI:96:MET:HE1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3224:U:H2'	3:A:3225:C:O4'	2.00	0.62
48:BW:80:LYS:O	48:BW:81:GLN:C	2.43	0.62
75:h1:428:G:C2	75:h1:429:C:C5	2.87	0.62
15:Ja:106:LYS:NZ	75:h1:791:G:OP1	2.32	0.62
22:BS:249:LEU:O	86:BS:501:HOH:O	2.16	0.62
66:Ya:114:PRO:O	66:Ya:117:ILE:HG12	2.00	0.62
3:A:649:C:OP2	86:A:3843:HOH:O	2.16	0.62
3:A:694:A:N6	86:A:4042:HOH:O	2.33	0.62
42:BU:34:ARG:HD2	42:BU:122:THR:HA	1.81	0.62
3:A:588:C:H2'	3:A:589:U:H2'	1.81	0.61
78:AI:44:LYS:HA	78:AI:47:GLN:HG2	1.80	0.61
28:AV:88:MET:HG3	63:AQ:41:THR:HA	1.82	0.61
32:BH:59:TYR:OH	32:BH:78:PHE:O	2.17	0.61
57:AF:50:ILE:HD11	57:AF:83:ILE:HG21	1.81	0.61
67:BB:30:THR:O	67:BB:33:LYS:HG3	1.99	0.61
75:h1:440:A:H1'	75:h1:468:PSU:O4	2.00	0.61
43:BR:154:TYR:CE1	43:BR:186:VAL:HG11	2.35	0.61
75:h1:939:G:N7	86:h1:2178:HOH:O	2.31	0.61
3:A:2205:A:H2'	3:A:2206:A:O4'	2.00	0.61
59:Ta:76:LEU:HA	59:Ta:95:ARG:O	2.00	0.61
5:BC:14:LYS:HD2	86:BC:109:HOH:O	2.00	0.61
46:BJ:139:ARG:HB2	46:BJ:173:PHE:CE1	2.35	0.61
80:A:3420:TER:N14	86:A:3999:HOH:O	2.31	0.61
29:AD:163:PHE:O	75:h1:1475:C:OP2	2.19	0.61
67:BB:58:MET:HE2	67:BB:58:MET:HA	1.82	0.61
3:A:1198:A:N1	3:A:1325:U:O2'	2.34	0.61
3:A:710:G:H5''	3:A:711:U:C5	2.36	0.61
3:A:3183:A:H61	3:A:3191:C:H42	1.47	0.61
34:BK:22:ARG:CB	34:BK:28:THR:CG2	2.79	0.61
15:Ja:127:ARG:HB2	15:Ja:140:ASN:HB2	1.82	0.60
29:AD:103:LEU:HD21	71:La:60:LEU:HD22	1.83	0.60
73:AY:64:MET:HE3	73:AY:67:LEU:HD23	1.82	0.60
3:A:1695:U:O2'	3:A:1750:A:N1	2.34	0.60
3:A:2730:C:N3	86:A:4002:HOH:O	2.31	0.60
3:A:1493:A:OP2	86:A:3845:HOH:O	2.16	0.60
29:AD:204:ARG:HH22	65:Ua:70:PRO:HD2	1.64	0.60
1:W2:70:C:H2'	1:W2:71:G:C8	2.37	0.60
75:h1:342:U:H2'	75:h1:343:A:H8	1.66	0.60
3:A:796:G:N7	86:A:4012:HOH:O	2.32	0.60
3:A:1105:G:OP1	23:AM:128:THR:OG1	2.18	0.60
34:BK:70:ALA:N	86:BK:401:HOH:O	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AK:163:ARG:NH2	75:h1:817:A:O5'	2.34	0.60
75:h1:1764:G:N7	86:h1:2177:HOH:O	2.31	0.60
45:BV:25:SER:O	45:BV:50:ARG:NH2	2.34	0.60
14:AP:26:ILE:HD13	14:AP:95:ALA:HB3	1.83	0.60
72:Aa:108:ALA:HB3	72:Aa:109:PRO:HD3	1.83	0.60
65:Ua:136:THR:HG23	75:h1:887:U:H1'	1.82	0.60
57:AF:92:VAL:HG22	57:AF:107:ILE:CD1	2.31	0.60
65:Ua:137:ASP:HB2	75:h1:929:G:H4'	1.82	0.60
15:Ja:29:PRO:HD3	75:h1:450:C:H5'	1.84	0.59
28:AV:25:ARG:NE	86:AV:302:HOH:O	2.33	0.59
59:Ta:57:ASP:HB3	59:Ta:100:ARG:HD2	1.84	0.59
66:Ya:46:ILE:HG23	66:Ya:89:ILE:HD13	1.82	0.59
3:A:397:G:N7	86:A:4008:HOH:O	2.31	0.59
3:A:424:G:H22	3:A:644:U:H3	1.50	0.59
3:A:2183:G:O2'	3:A:2312:PSU:OP2	2.20	0.59
8:AR:19:ASN:C	8:AR:20:GLY:O	2.44	0.59
27:BT:33:MET:CE	27:BT:156:PRO:HG3	2.32	0.59
48:BW:54:LEU:HD13	48:BW:64:ALA:HB1	1.84	0.59
31:BQ:30:ARG:NH1	31:BQ:72:GLN:OE1	2.34	0.59
57:AF:47:ARG:O	57:AF:50:ILE:HG22	2.02	0.59
62:Za:55:LEU:HA	62:Za:58:THR:HG23	1.83	0.59
63:AQ:71:ALA:HB1	63:AQ:85:VAL:HG13	1.85	0.59
72:Aa:75:ARG:HH12	72:Aa:113:TRP:CD1	2.20	0.59
3:A:420:A:N3	86:A:4006:HOH:O	2.31	0.59
3:A:2548:U:H5	31:BQ:40:TYR:O	1.85	0.59
75:h1:58:U:O4	86:h1:2123:HOH:O	2.13	0.59
3:A:880:U:OP2	86:A:3847:HOH:O	2.17	0.59
3:A:891:A:N1	86:A:4019:HOH:O	2.32	0.59
3:A:996:U:O4	86:A:3848:HOH:O	2.17	0.59
20:AW:18:ILE:HD11	20:AW:103:VAL:CG1	2.33	0.59
27:BT:36:PRO:HB3	27:BT:288:ALA:HB2	1.83	0.59
32:BH:90:ARG:HG3	32:BH:104:LEU:HD11	1.83	0.59
77:Ba:85:LEU:HD23	77:Ba:85:LEU:C	2.27	0.59
26:AH:35:ARG:HD2	26:AH:47:GLN:OE1	2.02	0.59
45:BV:120:LEU:HD21	45:BV:122:GLU:HG3	1.85	0.59
73:AY:11:ARG:NE	86:AY:301:HOH:O	1.81	0.59
3:A:263:C:OP2	86:A:3849:HOH:O	2.17	0.59
3:A:3053:C:O2'	3:A:3055:U:OP2	2.20	0.58
27:BT:129:ILE:HD11	27:BT:246:LEU:HD12	1.85	0.58
75:h1:607:A:N7	86:h1:2183:HOH:O	2.32	0.58
7:BO:48:PRO:HD2	86:BO:201:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:3:ARG:HG3	15:Ja:3:ARG:NH1	2.16	0.58
25:BI:33:GLY:HA3	25:BI:69:LYS:HD3	1.85	0.58
25:BI:112:MET:HE3	25:BI:132:ILE:HA	1.85	0.58
62:Za:159:ARG:HG2	62:Za:160:PHE:CD2	2.38	0.58
4:C3:63:U:H1'	34:BK:280:LEU:HD11	1.84	0.58
15:Ja:104:ASP:O	15:Ja:190:GLY:HA3	2.04	0.58
25:BI:96:MET:HE2	47:AO:22:ARG:HH11	1.68	0.58
48:BW:70:ARG:NH1	50:Na:6:ASP:OD1	2.34	0.58
75:h1:323:C:N4	75:h1:1669:G:OP1	2.35	0.58
1:2:20:G:N3	1:2:20:G:H3'	2.18	0.58
3:A:1814:G:H2'	3:A:1815:A:O4'	2.03	0.58
75:h1:97:G:O6	86:h1:2131:HOH:O	2.17	0.58
24:AC:191:GLN:HG2	86:AC:402:HOH:O	2.02	0.58
59:Ta:61:PHE:CE2	59:Ta:98:SER:HB2	2.38	0.58
75:h1:382:U:OP1	86:h1:2130:HOH:O	2.17	0.58
75:h1:559:G:N7	86:h1:2184:HOH:O	2.32	0.58
3:A:1627:G:N3	86:A:4018:HOH:O	2.32	0.58
75:h1:425:G:O6	86:h1:2124:HOH:O	2.14	0.58
59:Ta:180:ILE:HG21	59:Ta:183:LEU:HD22	1.85	0.58
75:h1:1559:U:O2'	75:h1:1560:U:H2'	2.04	0.58
3:A:213:G:N7	80:A:3418:TER:H122	2.19	0.57
3:A:710:G:H5''	3:A:711:U:H5	1.69	0.57
3:A:793:U:OP2	86:A:3846:HOH:O	2.16	0.57
8:AR:23:LYS:HD3	23:AM:84:ILE:HD12	1.86	0.57
37:BP:80:PRO:HD2	37:BP:83:LEU:HD12	1.86	0.57
45:BV:120:LEU:HD23	45:BV:120:LEU:C	2.28	0.57
3:A:2399:A:H1'	86:A:4131:HOH:O	2.04	0.57
72:Aa:25:ARG:O	86:Aa:301:HOH:O	2.17	0.57
75:h1:76:C:O2'	75:h1:77:A:O4'	2.18	0.57
3:A:2720:A:N7	86:A:4033:HOH:O	2.33	0.57
44:Xa:58:LYS:O	44:Xa:65:VAL:HG11	2.04	0.57
86:A:5105:HOH:O	54:AG:17:GLN:CD	2.47	0.57
75:h1:87:A:C2	75:h1:88:C:C5	2.93	0.57
75:h1:204:U:H2'	75:h1:205:U:H6	1.70	0.57
57:AF:137:ARG:NH1	75:h1:1585:A:OP1	2.28	0.57
1:2:18:G:C2'	1:2:57:G:N2	2.67	0.57
24:AC:35:LYS:NZ	62:Za:113:THR:O	2.31	0.57
32:BH:18:HIS:HA	32:BH:47:CYS:SG	2.44	0.57
57:AF:99:VAL:HG12	57:AF:100:ASP:H	1.69	0.57
75:h1:428:G:C2	75:h1:429:C:C6	2.92	0.57
75:h1:944:C:H2'	86:h1:2779:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A:6921:HOH:O	54:AG:30:LYS:HE3	2.03	0.57
29:AD:91:ARG:NH2	75:h1:1530:U:OP1	2.38	0.57
43:BR:201:LYS:NZ	86:BR:402:HOH:O	1.97	0.57
52:BF:148:ILE:HG22	52:BF:195:LEU:CD2	2.35	0.57
3:A:393:A:O2'	3:A:396:A:OP1	2.21	0.57
24:AC:178:THR:HG21	75:h1:14:C:OP2	2.05	0.57
62:Za:67:ARG:HA	62:Za:189:MET:HE1	1.87	0.57
75:h1:1059:U:H3'	75:h1:1060:U:H5''	1.86	0.57
75:h1:389:A:O2'	86:h1:2115:HOH:O	2.06	0.56
37:BP:37:THR:O	37:BP:37:THR:HG22	2.05	0.56
3:A:280:G:N1	86:A:3997:HOH:O	2.31	0.56
3:A:1491:A:N3	3:A:1491:A:O2'	2.31	0.56
3:A:1705:C:OP2	86:A:3851:HOH:O	2.18	0.56
3:A:1722:U:OP1	86:A:3850:HOH:O	2.18	0.56
3:A:2137:A:HO2'	73:AY:2:GLY:N	2.03	0.56
3:A:2280:U:O2	3:A:2308:U:H4'	2.04	0.56
3:A:2969:C:OP1	80:A:3421:TER:H112	2.05	0.56
17:AL:154:VAL:HG23	17:AL:155:PHE:CD2	2.40	0.56
18:Va:67:LYS:HD2	36:Pa:8:LEU:HD23	1.87	0.56
26:AH:107:ARG:NH2	52:BF:225:VAL:O	2.38	0.56
65:Ua:150:LEU:HB2	75:h1:1773:U:O2	2.05	0.56
67:BB:13:SER:O	67:BB:17:ILE:HG12	2.04	0.56
11:Ia:116:GLU:HG2	11:Ia:128:LYS:HG2	1.86	0.56
24:AC:175:SER:O	24:AC:178:THR:HG22	2.05	0.56
28:AV:36:PRO:HB3	86:AV:365:HOH:O	2.05	0.56
33:Da:15:ALA:O	75:h1:960:U:H5'	2.05	0.56
44:Xa:59:CYS:SG	44:Xa:60:PRO:HD2	2.46	0.56
45:BV:111:ARG:NH2	75:h1:931:A:N3	2.54	0.56
57:AF:145:ARG:NH1	1:W2:35:A:OP2	2.39	0.56
63:AQ:24:PHE:O	63:AQ:29:SER:OG	2.20	0.56
77:Ba:42:LEU:HD23	77:Ba:104:ILE:HG22	1.88	0.56
15:Ja:69:HIS:CD2	19:Ka:18:LEU:HD12	2.40	0.56
25:BI:112:MET:CE	25:BI:117:ILE:HD11	2.35	0.56
39:BG:232:MET:CE	86:BG:327:HOH:O	2.49	0.56
75:h1:1482:A:C2	75:h1:1531:PSU:C4	2.94	0.56
3:A:418:G:O6	32:BH:73:HIS:HE1	1.89	0.56
3:A:1840:C:H5''	3:A:1841:A:O5'	2.06	0.56
58:Wa:20:VAL:HG13	58:Wa:29:ALA:HB1	1.88	0.56
59:Ta:139:ARG:O	59:Ta:143:ILE:HG22	2.06	0.56
73:AY:8:PHE:CG	86:AY:360:HOH:O	2.51	0.56
75:h1:96:G:HO2'	75:h1:462:A:HO2'	1.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:335:A:C6	75:h1:336:G:C6	2.94	0.56
2:3:155:OMG:HM22	39:BG:52:ILE:CD1	2.36	0.56
75:h1:1177:G:OP1	86:h1:2133:HOH:O	2.18	0.56
1:2:15:G:H2'	1:2:16:U:C2	2.41	0.56
58:Wa:40:LEU:HA	58:Wa:43:ILE:HG22	1.88	0.55
72:Aa:50:ARG:CB	75:h1:335:A:H5'	2.36	0.55
3:A:1201:C:H2'	86:A:8760:HOH:O	2.04	0.55
3:A:1572:C:H42	3:A:1576:A:H61	1.53	0.55
3:A:2527:A:C2	3:A:2581:C:N3	2.74	0.55
80:A:3418:TER:H132	86:A:8605:HOH:O	2.06	0.55
14:AP:4:PHE:O	14:AP:9:LYS:HD3	2.06	0.55
3:A:750:U:O4	3:A:751:G:C6	2.59	0.55
3:A:1566:A:C8	39:BG:49:PRO:HB3	2.41	0.55
16:Ea:10:LEU:HD22	86:Ea:527:HOH:O	2.06	0.55
29:AD:204:ARG:NH2	65:Ua:69:SER:OG	2.39	0.55
72:Aa:58:ALA:HB2	72:Aa:180:GLY:HA2	1.88	0.55
9:AU:71:PRO:HD2	86:AU:206:HOH:O	2.06	0.55
45:BV:139:CYS:SG	45:BV:168:MET:HE3	2.46	0.55
59:Ta:3:PHE:O	59:Ta:15:LYS:HA	2.06	0.55
75:h1:129:U:H3'	75:h1:130:A:H5'	1.88	0.55
75:h1:388:G:OP2	86:h1:2136:HOH:O	2.18	0.55
3:A:2968:A:N7	31:BQ:215:ASN:ND2	2.54	0.55
7:BO:53:ASP:OD1	7:BO:114:ARG:NH1	2.32	0.55
22:BS:80:GLU:OE1	22:BS:318:TYR:OH	2.20	0.55
31:BQ:206:PRO:HG3	31:BQ:213:GLY:HA3	1.89	0.55
75:h1:249:U:OP1	86:h1:2132:HOH:O	2.18	0.55
3:A:1335:G:H2'	3:A:1336:A:O4'	2.07	0.55
3:A:1644:G:OP2	40:Fa:69:ARG:NH1	2.37	0.55
59:Ta:142:LYS:NZ	75:h1:166:A:OP2	2.24	0.55
3:A:1936:G:O6	80:A:3411:TER:H41	2.07	0.55
48:BW:54:LEU:HD11	48:BW:68:VAL:CG2	2.37	0.55
71:La:56:PRO:HB3	71:La:89:VAL:HG13	1.89	0.55
75:h1:82:G:OP2	75:h1:82:G:H8	1.90	0.55
75:h1:343:A:H2'	75:h1:344:C:C6	2.42	0.55
3:A:1813:C:OP2	14:AP:61:LYS:HE2	2.07	0.55
26:AH:92:LYS:O	26:AH:96:GLN:HG3	2.06	0.55
50:Na:56:VAL:HG12	50:Na:66:CYS:HB2	1.89	0.55
75:h1:1421:G:O2'	75:h1:1422:G:H5'	2.07	0.55
3:A:826:A2M:HM'3	3:A:929:A:C4	2.42	0.55
3:A:2679:A:N3	42:BU:61:ILE:HD11	2.22	0.55
86:A:4843:HOH:O	38:BN:83:SER:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:87:MET:CE	15:Ja:100:ARG:HD3	2.36	0.55
71:La:88:GLY:O	71:La:90:ILE:N	2.39	0.55
75:h1:1111:G:N7	86:h1:2191:HOH:O	2.33	0.55
3:A:1795:C:H5'	61:BE:52:VAL:HG13	1.89	0.54
3:A:2115:G:N3	3:A:2115:G:H5'	2.23	0.54
9:AU:16:TYR:OH	9:AU:47:GLU:HG2	2.07	0.54
18:Va:121:VAL:HG12	18:Va:129:LEU:HD11	1.89	0.54
38:BN:85:MET:HA	38:BN:85:MET:HE2	1.89	0.54
48:BW:33:GLN:HE21	48:BW:51:THR:HG21	1.73	0.54
65:Ua:150:LEU:HD12	75:h1:1789:U:OP1	2.06	0.54
72:Aa:67:SER:O	72:Aa:186:ILE:HG12	2.07	0.54
75:h1:1554:U:O2'	75:h1:1599:A:N3	2.39	0.54
3:A:1818:G:H2'	3:A:1819:C:C6	2.42	0.54
23:AM:103:GLU:HG3	23:AM:104:GLU:N	2.23	0.54
20:AW:15:ARG:O	20:AW:38:GLU:HG2	2.07	0.54
75:h1:259:C:H2'	75:h1:260:U:H6	1.73	0.54
29:AD:69:VAL:O	29:AD:73:THR:HG23	2.07	0.54
62:Za:16:GLU:HB2	67:BB:111:MET:SD	2.47	0.54
73:AY:76:THR:O	73:AY:77:CYS:CB	2.55	0.54
75:h1:139:U:H4'	75:h1:140:C:O5'	2.06	0.54
13:AX:11:PHE:CD1	41:Ha:125:LYS:HD3	2.42	0.54
59:Ta:69:THR:O	59:Ta:101:GLY:HA3	2.08	0.54
75:h1:404:C:O2	86:h1:2137:HOH:O	2.18	0.54
3:A:11:G:H5'	3:A:12:U:OP2	2.07	0.54
3:A:317:G:O6	86:A:3852:HOH:O	2.18	0.54
3:A:1012:C:O2	3:A:1012:C:O4'	2.24	0.54
4:C3:93:U:H2'	4:C3:94:C:C6	2.42	0.54
15:Ja:36:HIS:CD2	15:Ja:85:GLY:HA3	2.43	0.54
15:Ja:87:MET:HE3	15:Ja:100:ARG:HD3	1.88	0.54
39:BG:89:ILE:HD12	39:BG:208:ILE:HD12	1.89	0.54
65:Ua:136:THR:O	65:Ua:137:ASP:HB3	2.08	0.54
66:Ya:42:PHE:O	66:Ya:47:ARG:NH1	2.41	0.54
3:A:266:G:H5'	16:Ea:14:LYS:HE2	1.88	0.54
44:Xa:126:ILE:HG23	44:Xa:138:PHE:HB3	1.90	0.54
64:Oa:11:VAL:HG21	64:Oa:36:PHE:HE1	1.73	0.54
72:Aa:50:ARG:HB3	75:h1:335:A:H5'	1.89	0.54
3:A:522:C:C4	3:A:525:A:H4'	2.43	0.54
3:A:2551:U:H5'	86:A:7686:HOH:O	2.08	0.54
22:BS:26:ARG:CG	22:BS:47:MET:HE1	2.38	0.54
38:BN:55:LYS:CG	38:BN:55:LYS:O	2.56	0.54
62:Za:21:MET:HE1	62:Za:180:TRP:CZ3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:379:G:O2'	75:h1:380:A:OP2	2.23	0.54
2:3:156:G:N2	39:BG:55:GLN:OE1	2.38	0.54
3:A:144:OMU:HM22	3:A:145:U:OP1	2.07	0.54
3:A:2497:U:O2	3:A:2497:U:O4'	2.26	0.54
54:AG:63:LYS:NZ	86:AG:407:HOH:O	2.41	0.54
58:Wa:50:VAL:HG21	58:Wa:67:LEU:HD21	1.90	0.54
3:A:1815:A:H1'	3:A:1818:G:H21	1.73	0.54
12:AE:79:PHE:CD1	18:Va:7:MET:HE1	2.43	0.54
75:h1:522:A:H2'	75:h1:523:A:C8	2.43	0.54
57:AF:71:VAL:HG13	57:AF:83:ILE:HD11	1.88	0.53
69:Ra:52:MET:HE2	69:Ra:62:VAL:HG21	1.89	0.53
77:Ba:54:LYS:HB2	77:Ba:93:ASP:HB2	1.90	0.53
3:A:1425:G:OP1	80:A:3410:TER:N14	2.41	0.53
17:AL:150:LYS:HA	26:AH:7:VAL:O	2.08	0.53
45:BV:32:VAL:CG2	45:BV:46:THR:HG23	2.38	0.53
49:AK:135:LYS:O	49:AK:136:ARG:C	2.49	0.53
53:AA:106:ARG:HG2	53:AA:175:VAL:HG22	1.89	0.53
59:Ta:30:LYS:O	59:Ta:104:VAL:HG23	2.07	0.53
63:AQ:94:PHE:N	63:AQ:95:PRO:HD2	2.23	0.53
3:A:1229:U:O2'	3:A:1296:A:N1	2.41	0.53
29:AD:169:ILE:CD1	75:h1:1476:U:C5	2.89	0.53
13:AX:23:ARG:NH2	54:AG:77:GLU:OE2	2.42	0.53
51:AB:2:VAL:N	75:h1:463:G:OP1	2.41	0.53
58:Wa:30:LEU:HD11	58:Wa:67:LEU:HD13	1.91	0.53
75:h1:1289:G:O6	86:h1:2134:HOH:O	2.18	0.53
3:A:1575:A:H2'	3:A:1576:A:O4'	2.08	0.53
12:AE:106:THR:O	75:h1:807:A:H1'	2.09	0.53
29:AD:61:PHE:CE2	64:Oa:46:ARG:HG3	2.43	0.53
59:Ta:75:LEU:O	59:Ta:96:ARG:HA	2.08	0.53
73:AY:70:VAL:N	73:AY:71:PRO:CD	2.71	0.53
75:h1:447:A:H1'	75:h1:527:A:H5'	1.91	0.53
30:AJ:94:ILE:HD11	30:AJ:111:ARG:CZ	2.39	0.53
45:BV:66:PHE:CE2	65:Ua:47:SER:HB3	2.43	0.53
53:AA:50:ILE:C	53:AA:50:ILE:HD12	2.34	0.53
71:La:51:LEU:HD21	71:La:84:LEU:HD11	1.91	0.53
73:AY:39:TYR:CD1	73:AY:40:PRO:HA	2.44	0.53
3:A:1354:G:O6	86:A:3836:HOH:O	2.15	0.53
22:BS:122:TRP:CE2	22:BS:127:LYS:HE3	2.44	0.53
3:A:116:U:C2'	3:A:117:G:H5'	2.39	0.53
29:AD:21:ARG:HG2	29:AD:22:TRP:CZ2	2.44	0.53
44:Xa:126:ILE:HD13	44:Xa:140:VAL:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BW:72:TRP:HD1	62:Za:64:MET:HE2	1.74	0.53
51:AB:131:ILE:O	51:AB:144:ASN:HA	2.09	0.53
75:h1:417:C:O2'	75:h1:420:G:O6	2.22	0.53
3:A:2156:G:N7	31:BQ:152:SER:OG	2.34	0.53
75:h1:884:U:H3	75:h1:946:U:H3	1.56	0.53
75:h1:1474:A:C2	75:h1:1542:G:H4'	2.44	0.53
3:A:2680:U:H1'	42:BU:24:SER:HG	1.73	0.52
3:A:3178:G:N2	86:A:4052:HOH:O	2.34	0.52
9:AU:16:TYR:OH	9:AU:47:GLU:CG	2.56	0.52
17:AL:51:LYS:O	17:AL:53:VAL:HG23	2.10	0.52
22:BS:184:ILE:HD12	86:BS:652:HOH:O	2.09	0.52
59:Ta:203:ILE:HD11	75:h1:128:G:N1	2.24	0.52
75:h1:1302:PSU:OP1	86:h1:2138:HOH:O	2.19	0.52
3:A:112:A:H2'	3:A:113:G:O4'	2.09	0.52
3:A:1609:C:O2'	86:A:3855:HOH:O	2.19	0.52
6:BM:30:ARG:HD3	6:BM:30:ARG:C	2.34	0.52
31:BQ:137:ILE:HD11	31:BQ:149:LYS:HB2	1.92	0.52
59:Ta:135:ARG:NH2	75:h1:147:C:O2	2.42	0.52
77:Ba:35:LEU:HD11	77:Ba:90:ARG:CG	2.39	0.52
3:A:462:G:H5'	63:AQ:74:LYS:HE3	1.90	0.52
28:AV:87:MET:HE3	28:AV:88:MET:HE3	1.91	0.52
51:AB:137:ARG:HD3	51:AB:161:SER:HA	1.91	0.52
75:h1:433:C:H2'	75:h1:434:G:O4'	2.09	0.52
75:h1:547:A:C6	75:h1:596:A:C8	2.98	0.52
75:h1:627:C:O2	75:h1:975:A2M:N1	2.42	0.52
3:A:1893:A:N3	86:A:4049:HOH:O	2.34	0.52
29:AD:203:ASN:O	29:AD:204:ARG:HG2	2.08	0.52
69:Ra:45:TYR:OH	69:Ra:68:ARG:NH2	2.40	0.52
75:h1:1318:C:H2'	75:h1:1319:G:O4'	2.09	0.52
57:AF:131:PHE:CE1	77:Ba:79:THR:HA	2.44	0.52
78:AI:32:HIS:HB3	78:AI:35:ILE:O	2.09	0.52
3:A:1827:G:H5''	60:AZ:39:SER:OG	2.08	0.52
3:A:2688:G:N3	3:A:2688:G:H2'	2.25	0.52
24:AC:23:LYS:HB2	24:AC:26:GLN:HG3	1.91	0.52
18:Va:26:GLN:OE1	86:Va:301:HOH:O	2.18	0.52
28:AV:44:ARG:NH1	28:AV:44:ARG:HG2	2.24	0.52
3:A:2896:A:H2'	3:A:2898:C:H5''	1.91	0.52
37:BP:73:TYR:HB3	37:BP:79:LEU:HD22	1.92	0.52
45:BV:28:ASP:OD1	45:BV:50:ARG:NH1	2.42	0.52
53:AA:109:LEU:HD12	53:AA:184:ILE:HD11	1.92	0.52
75:h1:451:C:C2	75:h1:460:G:N2	2.78	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3257:A:C2	52:BF:162:GLY:O	2.63	0.52
32:BH:87:ARG:HB3	86:BH:381:HOH:O	2.09	0.52
35:AT:16:ARG:HB3	35:AT:103:ILE:HG12	1.90	0.52
57:AF:96:GLN:HG3	57:AF:104:LYS:HG3	1.92	0.52
75:h1:1774:U:OP2	86:h1:2139:HOH:O	2.19	0.52
3:A:1564:U:H2'	84:A:3402:EPE:H52	1.91	0.52
3:A:2149:G:O2'	3:A:2187:U:OP1	2.16	0.52
3:A:2682:U:H2'	3:A:2683:C:C6	2.44	0.52
3:A:2847:G:OP1	55:Ga:100:TYR:OH	2.26	0.52
15:Ja:108:ARG:NH2	75:h1:791:G:OP2	2.36	0.52
18:Va:4:THR:HG21	86:h1:3126:HOH:O	2.10	0.52
73:AY:11:ARG:NH2	86:AY:301:HOH:O	2.42	0.52
75:h1:758:A:O2'	75:h1:759:A:O4'	2.28	0.52
2:3:110:C:H2'	2:3:110:C:O5'	2.10	0.51
3:A:976:A:OP1	41:Ha:47:LYS:NZ	2.43	0.51
22:BS:103:ASN:N	22:BS:103:ASN:OD1	2.40	0.51
34:BK:119:TYR:OH	34:BK:138:ARG:O	2.27	0.51
62:Za:126:LEU:HD12	62:Za:146:ILE:HG21	1.91	0.51
64:Oa:57:GLU:OE1	65:Ua:120:ARG:NE	2.41	0.51
75:h1:763:A:C2	75:h1:794:A2M:C2	2.93	0.51
3:A:105:A:H2'	3:A:106:G:O4'	2.10	0.51
3:A:3384:G:H21	3:A:3385:A:H62	1.58	0.51
10:Ma:26:CYS:SG	10:Ma:28:LYS:HB2	2.51	0.51
66:Ya:44:SER:OG	75:h1:1551:C:H3'	2.09	0.51
74:Ca:52:PHE:CD1	77:Ba:85:LEU:HB2	2.46	0.51
75:h1:1412:G:N2	75:h1:1414:A:H3'	2.25	0.51
2:3:130:U:O4'	2:3:130:U:O2	2.29	0.51
3:A:692:C:OP2	86:A:3857:HOH:O	2.19	0.51
30:AJ:121:THR:OG1	30:AJ:123:ASP:OD1	2.29	0.51
35:AT:93:LEU:C	35:AT:93:LEU:HD12	2.35	0.51
75:h1:204:U:H2'	75:h1:205:U:C6	2.45	0.51
75:h1:395:C:H2'	75:h1:396:C:C6	2.46	0.51
75:h1:781:C:O2	75:h1:783:A:N7	2.43	0.51
34:BK:81:HIS:ND1	34:BK:81:HIS:C	2.68	0.51
3:A:65:A:OP2	86:A:3856:HOH:O	2.19	0.51
3:A:2527:A:C2	3:A:2581:C:C2	2.98	0.51
3:A:3316:U:H5''	22:BS:312:MET:HE2	1.91	0.51
17:AL:42:LYS:O	17:AL:45:TYR:HB3	2.11	0.51
20:AW:19:LEU:HD11	20:AW:36:GLN:HB2	1.91	0.51
29:AD:51:HIS:O	57:AF:81:TYR:OH	2.29	0.51
73:AY:11:ARG:CZ	86:AY:301:HOH:O	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:593:A:H2'	75:h1:594:A:C8	2.45	0.51
1:W2:47:U:O2'	1:W2:50:C:OP1	2.26	0.51
3:A:144:OMU:OP1	3:A:145:U:O2'	2.26	0.51
3:A:1610:C:P	86:A:4459:HOH:O	2.67	0.51
86:A:9791:HOH:O	20:AW:89:LYS:HD2	2.10	0.51
29:AD:40:VAL:HG11	29:AD:113:ILE:HD11	1.92	0.51
43:BR:125:ASN:OD1	43:BR:125:ASN:C	2.54	0.51
49:AK:105:LEU:HD12	49:AK:138:LEU:HD23	1.93	0.51
75:h1:926:G:N7	86:h1:2194:HOH:O	2.34	0.51
75:h1:1134:A:H2'	75:h1:1135:C:O4'	2.10	0.51
3:A:3369:U:H3'	86:A:4689:HOH:O	2.11	0.51
22:BS:287:ARG:NH1	22:BS:297:THR:O	2.43	0.51
69:Ra:155:LEU:O	69:Ra:187:PRO:HD2	2.11	0.51
3:A:602:C:H4'	3:A:603:G:O5'	2.11	0.51
49:AK:130:ASN:HA	86:AK:313:HOH:O	2.09	0.51
75:h1:390:OMG:O2'	86:h1:2135:HOH:O	2.18	0.51
75:h1:886:G:H2'	75:h1:887:U:C6	2.46	0.51
3:A:67:U:H5'	86:A:5892:HOH:O	2.11	0.51
3:A:1317:G:C2	3:A:1318:A:C2	2.99	0.51
22:BS:35:ASP:OD2	22:BS:194:LYS:NZ	2.34	0.51
28:AV:89:HIS:NE2	63:AQ:41:THR:O	2.43	0.51
51:AB:120:MET:HE1	51:AB:158:VAL:HG12	1.92	0.51
59:Ta:48:TYR:CE2	59:Ta:123:LEU:HD23	2.46	0.51
59:Ta:140:ALA:HA	59:Ta:180:ILE:HD11	1.92	0.51
75:h1:758:A:C2	75:h1:759:A:C4	2.99	0.51
3:A:2884:C:O2'	3:A:2885:U:H5'	2.11	0.51
39:BG:89:ILE:CD1	39:BG:208:ILE:HD12	2.41	0.51
70:BL:23:LEU:HD22	70:BL:111:MET:HE1	1.93	0.51
78:AI:1:MET:HE2	78:AI:44:LYS:HB2	1.92	0.51
3:A:694:A:H5''	27:BT:119:ARG:HD2	1.92	0.50
10:Ma:37:LYS:HG2	10:Ma:72:GLN:HG2	1.92	0.50
33:Da:62:GLN:O	33:Da:63:VAL:C	2.54	0.50
42:BU:55:THR:HG23	42:BU:62:ARG:HA	1.93	0.50
52:BF:67:ALA:HA	63:AQ:120:ALA:HB1	1.93	0.50
52:BF:107:VAL:HG11	52:BF:129:VAL:HG11	1.93	0.50
61:BE:51:ALA:O	61:BE:52:VAL:C	2.53	0.50
62:Za:62:LEU:HD23	62:Za:182:LEU:HD23	1.92	0.50
75:h1:262:G:C2	75:h1:264:C:C4	2.99	0.50
75:h1:1477:G:H2'	75:h1:1478:A:C8	2.46	0.50
3:A:2454:A:H2'	3:A:2454:A:N3	2.26	0.50
10:Ma:14:ASN:HB2	75:h1:1076:C:O2'	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BQ:226:ARG:NH2	31:BQ:233:GLN:OE1	2.44	0.50
61:BE:71:MET:HE1	86:BE:215:HOH:O	2.09	0.50
10:Ma:46:GLU:O	10:Ma:50:ILE:HG13	2.12	0.50
20:AW:89:LYS:HE3	86:AW:229:HOH:O	2.10	0.50
28:AV:85:LEU:HD21	63:AQ:35:LYS:HG2	1.93	0.50
75:h1:1567:C:H2'	75:h1:1568:U:O4'	2.12	0.50
75:h1:1571:A:C2	75:h1:1572:A:C4	2.99	0.50
53:AA:68:GLU:O	53:AA:71:SER:OG	2.23	0.50
75:h1:749:A:H62	75:h1:806:G:H21	1.58	0.50
15:Ja:34:GLY:HA3	15:Ja:83:PRO:HG3	1.93	0.50
22:BS:87:VAL:HB	22:BS:110:LEU:HD22	1.93	0.50
34:BK:83:LEU:N	34:BK:84:PRO:CD	2.74	0.50
41:Ha:2:THR:HG22	41:Ha:4:ARG:HG2	1.94	0.50
64:Oa:37:ILE:CD1	64:Oa:39:ARG:HD3	2.41	0.50
65:Ua:146:ARG:HB2	65:Ua:150:LEU:HD22	1.93	0.50
75:h1:15:U:H2'	75:h1:16:G:O4'	2.11	0.50
3:A:694:A:H61	3:A:798:A:H5''	1.77	0.50
3:A:1536:C:H6	3:A:1536:C:H5'	1.76	0.50
22:BS:106:TRP:CH2	22:BS:163:LEU:HD13	2.46	0.50
51:AB:109:ARG:NH2	51:AB:150:VAL:O	2.45	0.50
72:Aa:109:PRO:C	72:Aa:111:LYS:H	2.20	0.50
75:h1:1339:C:H1'	75:h1:1413:A:C4	2.46	0.50
3:A:1183:G:P	86:A:3802:HOH:O	2.64	0.50
14:AP:114:LYS:HE3	14:AP:118:GLU:OE2	2.11	0.50
15:Ja:129:ILE:HD11	15:Ja:154:ILE:HG22	1.93	0.50
15:Ja:136:ILE:HD13	15:Ja:148:ARG:NH2	2.25	0.50
75:h1:1679:U:H2'	75:h1:1680:C:O4'	2.12	0.50
1:W2:37:G:N1	86:W2:101:HOH:O	2.39	0.50
77:Ba:35:LEU:HD11	77:Ba:90:ARG:HG2	1.94	0.50
3:A:835:G:N7	86:A:4080:HOH:O	2.35	0.50
3:A:988:G:H4'	3:A:989:A:C4	2.46	0.50
3:A:1564:U:O2	39:BG:50:LYS:NZ	2.44	0.50
51:AB:29:GLU:HB2	51:AB:44:LEU:HD23	1.92	0.50
3:A:1639:C:O2'	3:A:1640:G:H5'	2.12	0.50
9:AU:40:ILE:CD1	9:AU:63:ILE:HD11	2.42	0.50
2:3:146:G:N7	86:3:316:HOH:O	2.34	0.49
3:A:352:A:N1	27:BT:89:THR:CG2	2.73	0.49
15:Ja:129:ILE:HG22	75:h1:244:OMG:HM21	1.93	0.49
22:BS:26:ARG:HG3	22:BS:47:MET:CE	2.42	0.49
27:BT:164:GLU:OE2	27:BT:261:SER:OG	2.29	0.49
41:Ha:44:LEU:C	41:Ha:44:LEU:HD23	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ra:52:MET:CE	69:Ra:62:VAL:HG21	2.42	0.49
75:h1:292:G:C2	75:h1:293:C:C5	3.00	0.49
3:A:2113:C:H5''	86:A:3972:HOH:O	2.11	0.49
40:Fa:21:ARG:HD2	86:Fa:303:HOH:O	2.12	0.49
64:Oa:22:GLN:OE1	86:Oa:101:HOH:O	2.20	0.49
75:h1:343:A:H2'	75:h1:344:C:H6	1.76	0.49
75:h1:365:G:N7	86:h1:2197:HOH:O	2.35	0.49
3:A:1814:G:N7	14:AP:64:LYS:HE2	2.27	0.49
20:AW:83:SER:OG	86:AW:201:HOH:O	2.20	0.49
34:BK:171:ASP:C	34:BK:171:ASP:OD1	2.53	0.49
53:AA:76:ARG:NH2	78:AI:63:HIS:CE1	2.80	0.49
3:A:693:A:N6	3:A:709:C:H2'	2.27	0.49
3:A:3181:G:O6	26:AH:4:LYS:NZ	2.43	0.49
65:Ua:54:ARG:NH1	75:h1:918:U:O2	2.46	0.49
71:La:51:LEU:C	71:La:51:LEU:HD23	2.37	0.49
3:A:2191:U:H5''	3:A:2192:G:H5'	1.95	0.49
8:AR:33:ARG:HD3	86:AR:241:HOH:O	2.11	0.49
17:AL:8:GLN:NE2	86:AL:211:HOH:O	2.45	0.49
39:BG:43:SER:HA	39:BG:46:ILE:HD12	1.94	0.49
77:Ba:25:ILE:HD11	77:Ba:115:VAL:CG1	2.42	0.49
3:A:712:A:O2'	54:AG:67:LYS:HE2	2.13	0.49
38:BN:128:PRO:HB2	56:BA:17:MET:HE1	1.95	0.49
66:Ya:113:LYS:O	66:Ya:116:MET:HG2	2.13	0.49
67:BB:28:PHE:CE2	75:h1:1392:C:H6	2.31	0.49
1:2:76:A:P	80:A:3421:TER:H101	2.52	0.49
3:A:1398:U:H2'	86:A:4552:HOH:O	2.12	0.49
20:AW:112:ILE:OXT	52:BF:86:ARG:NH1	2.45	0.49
24:AC:7:VAL:HG13	24:AC:7:VAL:O	2.12	0.49
57:AF:22:THR:HG21	57:AF:67:MET:HE3	1.93	0.49
86:Ta:403:HOH:O	75:h1:159:U:N1	2.44	0.49
67:BB:105:MET:C	67:BB:105:MET:SD	2.96	0.49
69:Ra:107:LYS:NZ	75:h1:747:U:OP2	2.44	0.49
3:A:466:C:O2'	3:A:467:A:O4'	2.30	0.49
3:A:1469:A:H5'	9:AU:55:VAL:O	2.12	0.49
3:A:1551:G:N7	86:A:4069:HOH:O	2.34	0.49
46:BJ:190:ILE:HA	46:BJ:198:LYS:O	2.12	0.49
59:Ta:199:LYS:O	59:Ta:203:ILE:HG22	2.13	0.49
72:Aa:56:TRP:HB2	72:Aa:179:CYS:C	2.38	0.49
72:Aa:157:SER:O	72:Aa:160:GLU:HG2	2.13	0.49
3:A:157:A:C2	3:A:260:C:O2	2.65	0.49
15:Ja:208:ILE:HD12	15:Ja:222:LEU:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ea:35:SER:HA	16:Ea:65:ARG:HG2	1.95	0.49
26:AH:42:ASP:OD1	26:AH:42:ASP:N	2.45	0.49
66:Ya:22:PHE:HB3	66:Ya:30:LEU:HD11	1.94	0.49
75:h1:39:A:N9	86:h1:2272:HOH:O	2.45	0.49
75:h1:1360:G:OP2	75:h1:1363:A:N6	2.46	0.49
1:2:16:U:H2'	1:2:60:C:O2	2.12	0.49
3:A:941:U:H3'	86:A:7090:HOH:O	2.13	0.49
3:A:2130:A:H5'	86:A:6603:HOH:O	2.12	0.49
3:A:2275:C:OP2	86:A:3861:HOH:O	2.20	0.49
14:AP:57:ASP:OD1	14:AP:61:LYS:CB	2.61	0.49
23:AM:94:GLU:OE1	23:AM:94:GLU:N	2.39	0.49
25:BI:89:ARG:HD2	25:BI:95:PHE:CZ	2.48	0.49
31:BQ:91:GLY:O	31:BQ:102:LEU:HD23	2.13	0.49
68:AN:90:LEU:HD23	68:AN:95:VAL:HG23	1.94	0.49
2:3:44:A:P	86:3:370:HOH:O	2.71	0.48
2:3:81:A:C6	86:3:301:HOH:O	2.55	0.48
2:3:90:U:O2'	37:BP:5:LYS:NZ	2.45	0.48
3:A:793:U:O2'	30:AJ:65:SER:OG	2.25	0.48
3:A:959:G:H5'	3:A:980:G:OP1	2.12	0.48
34:BK:223:SER:OG	34:BK:224:ALA:N	2.45	0.48
35:AT:60:GLU:OE1	35:AT:72:HIS:NE2	2.36	0.48
60:AZ:40:ARG:HD3	60:AZ:41:TYR:CE2	2.48	0.48
75:h1:128:G:OP1	75:h1:201:G:O2'	2.30	0.48
3:A:391:C:N3	3:A:394:A:OP2	2.46	0.48
3:A:984:C:O2'	30:AJ:142:LYS:NZ	2.45	0.48
3:A:1396:G:N7	86:A:4090:HOH:O	2.35	0.48
3:A:3011:U:H2'	3:A:3012:U:C6	2.48	0.48
86:A:6835:HOH:O	34:BK:15:ARG:HD3	2.13	0.48
9:AU:24:LEU:HB2	86:AU:228:HOH:O	2.13	0.48
24:AC:130:VAL:HG23	24:AC:141:MET:HB2	1.95	0.48
43:BR:91:ILE:N	43:BR:91:ILE:CD1	2.76	0.48
50:Na:66:CYS:SG	50:Na:75:LEU:HD23	2.53	0.48
52:BF:121:THR:HA	52:BF:130:PRO:O	2.13	0.48
59:Ta:191:ARG:NH2	75:h1:270:G:N7	2.60	0.48
69:Ra:51:HIS:NE2	69:Ra:59:LYS:HD3	2.28	0.48
2:3:110:C:O5'	2:3:110:C:C2'	2.62	0.48
15:Ja:29:PRO:HD3	75:h1:450:C:OP1	2.12	0.48
15:Ja:221:ARG:NH2	75:h1:756:A:O4'	2.47	0.48
27:BT:166:VAL:HG13	27:BT:171:ALA:CB	2.43	0.48
38:BN:125:LEU:C	38:BN:125:LEU:HD12	2.38	0.48
51:AB:130:LEU:HB3	51:AB:136:ILE:CD1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:56:LEU:HD11	57:AF:114:TYR:CD2	2.48	0.48
75:h1:151:A:C2	75:h1:160:A:C6	3.01	0.48
3:A:584:G:OP2	52:BF:12:ARG:NH2	2.34	0.48
3:A:2522:A:H1'	86:A:3830:HOH:O	2.12	0.48
10:Ma:21:ILE:HD12	10:Ma:21:ILE:C	2.39	0.48
15:Ja:29:PRO:CD	75:h1:450:C:H5'	2.42	0.48
44:Xa:36:TRP:CG	44:Xa:50:ILE:HG12	2.48	0.48
54:AG:103:ARG:NH1	86:AG:403:HOH:O	2.30	0.48
75:h1:1016:U:H5''	75:h1:1017:C:OP2	2.13	0.48
2:3:43:G:O2'	2:3:109:A:N1	2.42	0.48
3:A:472:G:H2'	3:A:473:G:C8	2.49	0.48
25:BI:22:VAL:O	25:BI:23:ALA:HB3	2.13	0.48
32:BH:118:ASP:OD1	32:BH:118:ASP:N	2.41	0.48
34:BK:50:ARG:NH1	34:BK:146:ASP:OD2	2.40	0.48
44:Xa:70:ARG:NH1	75:h1:306:U:O2	2.31	0.48
57:AF:80:VAL:O	57:AF:84:ARG:HG3	2.14	0.48
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HG3	1.95	0.48
75:h1:779:G:N2	75:h1:787:U:C2	2.82	0.48
3:A:2820:C:C4	3:A:2821:U:C5	3.01	0.48
10:Ma:32:LYS:O	10:Ma:37:LYS:NZ	2.46	0.48
15:Ja:148:ARG:HD3	75:h1:126:U:H5'	1.95	0.48
17:AL:13:GLY:HA3	86:AL:214:HOH:O	2.14	0.48
43:BR:52:ARG:HH21	43:BR:184:ILE:HG12	1.78	0.48
75:h1:1110:G:O2'	75:h1:1139:A:N1	2.36	0.48
2:3:68:U:HO2'	37:BP:59:THR:HG1	1.60	0.48
3:A:608:C:C4	52:BF:29:TYR:CD2	3.02	0.48
3:A:2391:G:H4'	22:BS:255:ILE:HD13	1.95	0.48
34:BK:9:SER:O	34:BK:12:TYR:HB3	2.14	0.48
49:AK:53:LYS:NZ	86:AK:303:HOH:O	2.43	0.48
51:AB:16:LYS:HB3	51:AB:17:PRO:HD2	1.95	0.48
59:Ta:6:ALA:O	59:Ta:114:VAL:HA	2.12	0.48
7:BO:41:LYS:HE3	7:BO:42:TYR:CZ	2.49	0.48
15:Ja:183:VAL:HB	15:Ja:188:ASN:O	2.13	0.48
19:Ka:30:HIS:N	19:Ka:31:PRO:CD	2.77	0.48
21:BD:25:VAL:HG22	21:BD:72:LEU:HD22	1.94	0.48
45:BV:105:PHE:HZ	45:BV:211:PHE:CG	2.32	0.48
66:Ya:43:PRO:HD2	66:Ya:46:ILE:HD12	1.95	0.48
75:h1:390:OMG:N7	86:h1:2201:HOH:O	2.35	0.48
1:W2:47:U:O2'	1:W2:48:C:H5''	2.14	0.48
27:BT:33:MET:HE3	27:BT:156:PRO:HG3	1.95	0.48
29:AD:32:ILE:HA	29:AD:35:VAL:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BV:143:THR:HG22	45:BV:154:CYS:SG	2.54	0.48
45:BV:180:ASP:C	45:BV:180:ASP:OD1	2.57	0.48
59:Ta:66:GLY:HA2	75:h1:1683:A:H1'	1.96	0.48
75:h1:465:U:H2'	75:h1:466:A2M:C8	2.43	0.48
3:A:641:C:O2'	3:A:642:A:H5'	2.14	0.48
3:A:1576:A:H2'	3:A:1577:C:C6	2.49	0.48
24:AC:177:LYS:HD2	75:h1:6:G:OP2	2.13	0.48
34:BK:22:ARG:HB2	34:BK:28:THR:CG2	2.43	0.48
54:AG:26:GLN:HB3	54:AG:27:PRO:HD3	1.95	0.48
57:AF:23:HIS:O	57:AF:67:MET:O	2.32	0.48
75:h1:574:C:H6	75:h1:574:C:O5'	1.97	0.48
75:h1:1542:G:C6	75:h1:1543:G:C4	3.01	0.48
3:A:989:A:N3	3:A:991:G:H1'	2.29	0.47
14:AP:57:ASP:OD1	14:AP:61:LYS:HD2	2.14	0.47
24:AC:10:THR:OG1	24:AC:36:GLU:OE2	2.18	0.47
67:BB:21:TYR:HA	67:BB:24:MET:HE3	1.95	0.47
75:h1:419:A:H5'	75:h1:420:G:C8	2.49	0.47
3:A:28:G:H5'	16:Ea:172:ARG:HD3	1.95	0.47
15:Ja:29:PRO:HD3	75:h1:450:C:C5'	2.43	0.47
21:BD:23:HIS:HA	21:BD:73:GLN:O	2.14	0.47
25:BI:122:GLY:HA2	25:BI:140:VAL:O	2.13	0.47
69:Ra:47:ASN:O	69:Ra:48:GLN:O	2.31	0.47
75:h1:1046:C:H4'	86:h1:2196:HOH:O	2.14	0.47
75:h1:1203:A:H1'	75:h1:1208:PSU:O2	2.15	0.47
75:h1:1230:G:N2	75:h1:1256:G:O2'	2.42	0.47
3:A:4:A:H2'	3:A:5:C:O4'	2.13	0.47
31:BQ:65:HIS:CE1	31:BQ:68:ARG:HG3	2.48	0.47
32:BH:73:HIS:O	32:BH:73:HIS:ND1	2.48	0.47
35:AT:49:THR:HG23	35:AT:75:GLY:H	1.78	0.47
46:BJ:89:ILE:HD13	46:BJ:136:LEU:CD2	2.44	0.47
54:AG:117:THR:O	54:AG:120:THR:HB	2.14	0.47
74:Ca:16:PRO:HD2	75:h1:1206:C:N3	2.29	0.47
75:h1:448:A:C5	75:h1:449:PSU:N1	2.82	0.47
75:h1:615:G:H4'	75:h1:616:C:OP1	2.14	0.47
75:h1:1566:U:H2'	75:h1:1567:C:C6	2.50	0.47
1:2:36:A:O2'	75:h1:1760:A:N1	2.44	0.47
2:3:64:U:H4'	86:3:339:HOH:O	2.14	0.47
14:AP:84:ARG:HG2	35:AT:61:TYR:OH	2.15	0.47
22:BS:230:GLU:CD	22:BS:234:THR:HB	2.40	0.47
31:BQ:179:MET:HE1	31:BQ:185:ALA:HA	1.97	0.47
53:AA:44:MET:CG	53:AA:44:MET:O	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:75:GLY:H	57:AF:78:SER:HG	1.62	0.47
75:h1:259:C:H2'	75:h1:260:U:C6	2.49	0.47
75:h1:521:C:C4	75:h1:536:A:C8	3.02	0.47
75:h1:1296:G:O6	86:h1:2141:HOH:O	2.20	0.47
75:h1:1350:G:H2'	75:h1:1351:C:C6	2.49	0.47
3:A:2826:U:H2'	3:A:2826:U:O2	2.13	0.47
86:A:9799:HOH:O	8:AR:10:HIS:HD2	1.96	0.47
15:Ja:45:VAL:HG22	15:Ja:80:LYS:HB2	1.96	0.47
25:BI:96:MET:HE2	47:AO:22:ARG:NH1	2.29	0.47
29:AD:76:LEU:O	86:AD:401:HOH:O	2.20	0.47
42:BU:166:GLN:O	42:BU:170:GLU:HA	2.14	0.47
62:Za:94:PHE:CE2	62:Za:182:LEU:HD12	2.49	0.47
71:La:70:MET:HB2	71:La:72:ILE:HD12	1.97	0.47
72:Aa:172:ILE:HG22	72:Aa:173:SER:N	2.30	0.47
75:h1:154:A:H2'	75:h1:155:A:O4'	2.14	0.47
75:h1:979:A:H2'	75:h1:980:A:O4'	2.15	0.47
3:A:769:G:N2	3:A:779:G:O2'	2.45	0.47
15:Ja:106:LYS:HD2	15:Ja:108:ARG:NH2	2.30	0.47
45:BV:179:CYS:HB3	45:BV:183:GLU:HB2	1.96	0.47
57:AF:97:LYS:HG3	57:AF:98:TYR:CD1	2.50	0.47
75:h1:120:G:OP2	75:h1:121:PSU:N1	2.39	0.47
75:h1:778:A2M:N1	75:h1:789:U:C2	2.83	0.47
75:h1:1339:C:H1'	75:h1:1413:A:C5	2.50	0.47
75:h1:1766:A:O2'	75:h1:1787:C:H5'	2.15	0.47
1:2:34:G:H1	76:B1:27:U:H3	1.63	0.47
2:3:85:U:O3'	2:3:87:C:OP2	2.32	0.47
3:A:1338:C:H2'	3:A:1339:U:O4'	2.15	0.47
3:A:1709:C:OP1	40:Fa:49:LYS:NZ	2.45	0.47
3:A:2726:A:N1	86:A:4091:HOH:O	2.35	0.47
4:C3:102:G:H5''	4:C3:102:G:N3	2.29	0.47
12:AE:104:LEU:HD23	12:AE:125:VAL:HA	1.97	0.47
27:BT:33:MET:CE	27:BT:156:PRO:CG	2.92	0.47
29:AD:73:THR:HG22	29:AD:93:VAL:HG21	1.97	0.47
31:BQ:226:ARG:NH1	31:BQ:228:ASP:OD1	2.43	0.47
45:BV:86:LEU:HA	45:BV:99:GLN:O	2.15	0.47
54:AG:89:ALA:HB3	54:AG:90:PRO:HD3	1.97	0.47
58:Wa:133:GLY:HA3	75:h1:1561:G:H5''	1.97	0.47
62:Za:22:MET:HE3	62:Za:55:LEU:HG	1.97	0.47
75:h1:268:U:H2'	75:h1:269:C:H6	1.80	0.47
75:h1:352:G:C8	75:h1:354:A:N1	2.82	0.47
75:h1:1118:PSU:H2'	75:h1:1119:G:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:AI:55:VAL:HG21	78:AI:66:TRP:HB3	1.95	0.47
3:A:2285:C:C5	3:A:2296:U:C2	3.02	0.47
22:BS:92:TYR:HB2	22:BS:159:VAL:HB	1.96	0.47
22:BS:299:MET:HG2	22:BS:305:THR:O	2.15	0.47
27:BT:245:LYS:CD	86:BT:628:HOH:O	2.63	0.47
28:AV:126:ARG:O	28:AV:127:LEU:HD23	2.15	0.47
58:Wa:95:TYR:CD1	58:Wa:95:TYR:N	2.83	0.47
59:Ta:2:LYS:HB2	59:Ta:110:VAL:HG22	1.97	0.47
59:Ta:221:LEU:C	59:Ta:221:LEU:HD12	2.40	0.47
75:h1:612:G:OP1	86:h1:2140:HOH:O	2.20	0.47
3:A:1617:G:H2'	3:A:1618:G:O4'	2.14	0.47
3:A:3071:A:H1'	86:A:3816:HOH:O	2.13	0.47
3:A:3366:C:H2'	3:A:3367:C:H6	1.80	0.47
52:BF:196:ILE:O	52:BF:200:GLU:HG2	2.14	0.47
62:Za:169:ASN:O	62:Za:175:ILE:HD11	2.14	0.47
66:Ya:133:HIS:HB3	75:h1:1463:A:N7	2.29	0.47
3:A:148:A:N3	86:A:4108:HOH:O	2.36	0.47
3:A:1949:G:P	49:AK:136:ARG:HH21	2.38	0.47
22:BS:287:ARG:HD3	22:BS:295:ALA:O	2.14	0.47
62:Za:182:LEU:O	62:Za:186:VAL:HG23	2.15	0.47
75:h1:161:G:H5''	75:h1:161:G:N3	2.30	0.47
3:A:1043:U:H2'	3:A:1044:C:C6	2.49	0.46
86:A:4544:HOH:O	27:BT:74:THR:HG21	2.15	0.46
18:Va:121:VAL:HG12	18:Va:129:LEU:CD1	2.45	0.46
32:BH:172:LEU:C	32:BH:172:LEU:HD23	2.40	0.46
66:Ya:56:ARG:O	66:Ya:57:LYS:HB2	2.14	0.46
66:Ya:130:PRO:HA	86:Ya:201:HOH:O	2.15	0.46
69:Ra:19:CYS:O	69:Ra:23:VAL:HG23	2.14	0.46
75:h1:1733:U:H2'	75:h1:1734:A:O4'	2.15	0.46
3:A:116:U:C5	3:A:117:G:C6	3.03	0.46
3:A:572:G:C2	3:A:620:G:H2'	2.50	0.46
4:C3:26:C:N3	86:C3:306:HOH:O	2.35	0.46
27:BT:166:VAL:HG13	27:BT:171:ALA:HB3	1.96	0.46
27:BT:245:LYS:HG3	86:BT:628:HOH:O	2.15	0.46
37:BP:36:VAL:HG11	38:BN:77:TYR:CD1	2.50	0.46
43:BR:91:ILE:HG13	43:BR:141:TYR:HB3	1.96	0.46
59:Ta:57:ASP:CB	59:Ta:100:ARG:HD2	2.45	0.46
67:BB:58:MET:O	67:BB:61:ILE:HG22	2.15	0.46
75:h1:444:C:N3	75:h1:445:C:C5	2.84	0.46
3:A:1376:A2M:C2	3:A:1377:G:C4	2.99	0.46
10:Ma:10:ARG:HA	86:Ma:310:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:29:PRO:O	15:Ja:31:PRO:HD3	2.15	0.46
24:AC:200:GLU:OE1	24:AC:201:PHE:CD1	2.69	0.46
33:Da:62:GLN:O	33:Da:65:SER:N	2.46	0.46
58:Wa:134:GLN:NE2	75:h1:1546:U:OP1	2.47	0.46
62:Za:43:PHE:CE2	67:BB:105:MET:HA	2.51	0.46
63:AQ:58:THR:HB	63:AQ:71:ALA:HB3	1.98	0.46
75:h1:614:U:OP2	75:h1:615:G:O2'	2.33	0.46
1:2:47:U:H3'	1:2:48:C:C5'	2.46	0.46
3:A:1794:C:O2'	3:A:1796:U:OP2	2.29	0.46
3:A:3232:A:OP2	86:A:3868:HOH:O	2.21	0.46
18:Va:121:VAL:CG1	18:Va:129:LEU:HD11	2.45	0.46
24:AC:179:LEU:HD23	24:AC:179:LEU:C	2.40	0.46
32:BH:24:LEU:O	32:BH:28:ILE:HG12	2.16	0.46
34:BK:65:VAL:CG1	34:BK:72:ASP:HB3	2.44	0.46
75:h1:1588:A:H2'	75:h1:1589:A:O4'	2.16	0.46
10:Ma:81:SER:O	10:Ma:82:HIS:HB2	2.15	0.46
15:Ja:148:ARG:CD	75:h1:126:U:H5'	2.46	0.46
17:AL:44:TRP:CH2	86:AL:214:HOH:O	2.68	0.46
23:AM:17:ARG:NH2	23:AM:23:GLY:O	2.48	0.46
35:AT:50:ASN:HB3	86:AT:204:HOH:O	2.15	0.46
44:Xa:60:PRO:HD2	44:Xa:113:SER:HG	1.81	0.46
45:BV:143:THR:HG21	45:BV:154:CYS:O	2.15	0.46
49:AK:23:TRP:CH2	49:AK:25:ASP:HA	2.51	0.46
59:Ta:147:PHE:HD2	59:Ta:158:TYR:HB3	1.81	0.46
62:Za:112:PHE:CE2	62:Za:126:LEU:HD11	2.50	0.46
64:Oa:14:MET:HE1	64:Oa:27:ARG:N	2.31	0.46
66:Ya:90:ILE:HA	66:Ya:94:MET:HE2	1.97	0.46
75:h1:795:C:H3'	75:h1:796:A:C8	2.50	0.46
75:h1:1544:G:N2	75:h1:1570:C:H1'	2.31	0.46
2:3:159:U:H2'	2:3:160:C:O4'	2.15	0.46
3:A:1661:G:N7	86:A:4104:HOH:O	2.36	0.46
3:A:2212:A2M:H8	3:A:2212:A2M:O5'	2.16	0.46
3:A:2725:C:N3	86:A:4102:HOH:O	2.36	0.46
3:A:3174:C:N4	32:BH:172:LEU:CD1	2.78	0.46
80:A:3405:TER:H32	16:Ea:81:TYR:CE2	2.50	0.46
15:Ja:45:VAL:HG23	15:Ja:80:LYS:O	2.15	0.46
15:Ja:160:ILE:HD13	15:Ja:172:PHE:HB3	1.97	0.46
28:AV:10:VAL:HG22	28:AV:64:THR:HB	1.96	0.46
34:BK:146:ASP:C	34:BK:146:ASP:OD1	2.59	0.46
62:Za:73:GLU:N	62:Za:73:GLU:OE1	2.48	0.46
65:Ua:71:TYR:CE1	65:Ua:75:LEU:HD21	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:175:A:H4'	75:h1:176:A:H5''	1.96	0.46
75:h1:302:A:H2'	75:h1:303:A:H8	1.76	0.46
75:h1:1001:C:O2'	75:h1:1003:G:N7	2.48	0.46
77:Ba:63:VAL:HG12	77:Ba:86:ARG:HG2	1.98	0.46
14:AP:75:VAL:HG11	14:AP:80:LEU:CD2	2.42	0.46
15:Ja:159:THR:HG22	15:Ja:173:ILE:HB	1.97	0.46
15:Ja:192:VAL:HG23	15:Ja:243:GLY:HA3	1.97	0.46
27:BT:159:VAL:HG11	27:BT:179:ILE:HG21	1.98	0.46
35:AT:51:CYS:O	35:AT:52:PRO:C	2.57	0.46
44:XA:88:ARG:NH1	86:XA:201:HOH:O	2.35	0.46
48:BW:72:TRP:CD1	62:ZA:64:MET:HE2	2.50	0.46
50:Na:56:VAL:HG13	50:Na:65:LEU:HB2	1.97	0.46
59:Ta:162:TYR:O	59:Ta:163:ARG:C	2.59	0.46
62:ZA:43:PHE:CD2	62:ZA:44:LYS:HG2	2.50	0.46
75:h1:515:U:H2'	75:h1:516:G:C8	2.51	0.46
3:A:831:G:N7	86:A:4111:HOH:O	2.36	0.46
3:A:880:U:P	86:A:3847:HOH:O	2.72	0.46
3:A:3111:A:OP1	11:Ia:78:SER:CB	2.64	0.46
4:C3:37:A:O2'	4:C3:43:A:N1	2.46	0.46
15:Ja:28:ALA:O	15:Ja:29:PRO:C	2.59	0.46
22:BS:161:ARG:HG2	22:BS:185:GLN:HA	1.96	0.46
25:BI:75:LYS:HD2	25:BI:77:LEU:HD21	1.98	0.46
30:AJ:23:ASP:OD1	30:AJ:23:ASP:C	2.57	0.46
57:AF:49:LYS:HB3	57:AF:84:ARG:HD2	1.98	0.46
64:Oa:17:THR:O	64:Oa:21:GLY:HA2	2.16	0.46
3:A:2555:C:N3	86:A:4113:HOH:O	2.36	0.46
3:A:2723:U:H4'	23:AM:54:HIS:CD2	2.51	0.46
3:A:3285:C:P	86:A:4342:HOH:O	2.73	0.46
80:A:3414:TER:H41	80:A:3414:TER:HN11	1.59	0.46
15:Ja:166:ALA:O	15:Ja:167:ASN:C	2.58	0.46
16:Ea:108:ARG:NH1	86:Ea:408:HOH:O	2.42	0.46
22:BS:26:ARG:HG3	22:BS:47:MET:HE1	1.97	0.46
24:AC:45:GLY:N	24:AC:46:PRO:HD2	2.30	0.46
25:BI:89:ARG:HB2	25:BI:95:PHE:CE2	2.50	0.46
25:BI:112:MET:HE1	25:BI:117:ILE:CD1	2.39	0.46
32:BH:172:LEU:HD23	32:BH:172:LEU:O	2.16	0.46
51:AB:29:GLU:HG3	51:AB:41:LYS:HD3	1.97	0.46
3:A:931:U:OP1	73:AY:3:LYS:HE2	2.16	0.46
3:A:1728:G:N7	86:A:4096:HOH:O	2.35	0.46
6:BM:15:CYS:SG	6:BM:151:LEU:HB2	2.56	0.46
34:BK:83:LEU:HD13	34:BK:88:LEU:HD23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AB:145:ILE:HG21	75:h1:771:C:O2	2.16	0.46
3:A:72:A:C8	3:A:72:A:H5''	2.51	0.45
22:BS:290:LYS:O	22:BS:296:HIS:HB2	2.16	0.45
63:AQ:111:ARG:NH2	63:AQ:113:ASP:OD2	2.43	0.45
74:Ca:19:ARG:NH2	75:h1:1599:A:OP1	2.47	0.45
15:Ja:155:LYS:HB3	15:Ja:156:PRO:HD2	1.97	0.45
37:BP:31:LEU:HD21	37:BP:46:LYS:HE3	1.98	0.45
57:AF:30:LEU:HG	57:AF:66:ASN:HD22	1.81	0.45
61:BE:55:TRP:CZ2	61:BE:70:THR:C	2.95	0.45
68:AN:62:ILE:HD12	68:AN:62:ILE:N	2.31	0.45
70:BL:115:ASP:OD2	70:BL:125:THR:HG22	2.15	0.45
75:h1:51:A:C6	75:h1:52:U:C2	3.04	0.45
75:h1:341:C:C2	75:h1:342:U:C5	3.03	0.45
3:A:333:A:O2'	3:A:334:G:H5'	2.16	0.45
14:AP:73:LYS:HA	86:AP:211:HOH:O	2.15	0.45
51:AB:153:GLU:O	51:AB:156:LYS:NZ	2.49	0.45
60:AZ:13:LEU:HD23	60:AZ:13:LEU:HA	1.87	0.45
75:h1:453:G:N2	75:h1:458:G:C4	2.84	0.45
75:h1:1641:OMC:H2'	75:h1:1642:C:O4'	2.16	0.45
3:A:63:A:OP1	16:Ea:177:LYS:NZ	2.35	0.45
3:A:2307:A:N3	3:A:2960:G:O2'	2.43	0.45
15:Ja:35:PRO:HD2	15:Ja:83:PRO:HG2	1.99	0.45
31:BQ:228:ASP:O	31:BQ:229:ALA:C	2.59	0.45
58:Wa:43:ILE:HG12	70:BL:37:ILE:HD13	1.97	0.45
72:Aa:39:SER:HB3	72:Aa:60:ARG:HG2	1.97	0.45
75:h1:1115:G:C6	80:h1:1903:TER:H61	2.51	0.45
75:h1:1526:A:H2'	75:h1:1527:A:C8	2.51	0.45
77:Ba:40:THR:HA	77:Ba:43:VAL:HG12	1.97	0.45
2:3:11:U:H2'	2:3:12:C:C6	2.52	0.45
3:A:1233:A:OP2	3:A:1295:G:N2	2.49	0.45
3:A:2851:C:N3	46:BJ:158:LYS:NZ	2.63	0.45
86:A:3868:HOH:O	22:BS:100:ARG:NH2	2.40	0.45
27:BT:42:VAL:HG21	27:BT:252:LEU:HD21	1.97	0.45
28:AV:118:VAL:O	86:AV:301:HOH:O	2.21	0.45
46:BJ:190:ILE:CG2	46:BJ:197:ALA:HB1	2.46	0.45
51:AB:138:VAL:HG12	51:AB:143:VAL:HG21	1.99	0.45
75:h1:1797:G:H4'	75:h1:1798:A:OP1	2.15	0.45
17:AL:75:LYS:N	17:AL:75:LYS:HD2	2.32	0.45
24:AC:115:TYR:OH	24:AC:123:PRO:HD3	2.17	0.45
30:AJ:161:ASN:CB	86:AJ:391:HOH:O	2.47	0.45
39:BG:217:ASN:ND2	86:BG:302:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Fa:56:HIS:CD2	40:Fa:56:HIS:N	2.81	0.45
49:AK:98:ARG:O	49:AK:99:MET:C	2.60	0.45
59:Ta:180:ILE:HG12	59:Ta:181:GLN:N	2.32	0.45
69:Ra:54:ILE:HD13	69:Ra:169:THR:HA	1.99	0.45
70:BL:15:PHE:CD1	70:BL:15:PHE:C	2.93	0.45
73:AY:11:ARG:NH2	86:AY:304:HOH:O	2.49	0.45
77:Ba:69:ARG:NH2	77:Ba:74:GLY:O	2.50	0.45
3:A:2422:A:H2'	3:A:2423:G:O4'	2.16	0.45
7:BO:111:ASP:O	7:BO:112:LYS:C	2.57	0.45
13:AX:39:ARG:NH2	16:Ea:2:GLY:O	2.49	0.45
14:AP:7:GLN:HG2	14:AP:8:ASN:ND2	2.32	0.45
34:BK:62:ALA:O	34:BK:105:LEU:HD13	2.17	0.45
46:BJ:185:ARG:NH1	46:BJ:192:PRO:HD3	2.32	0.45
50:Na:39:CYS:SG	50:Na:65:LEU:HD22	2.56	0.45
69:Ra:44:LEU:HD11	69:Ra:76:ILE:CD1	2.47	0.45
75:h1:141:G:H2'	75:h1:142:G:C8	2.51	0.45
75:h1:452:U:O2	75:h1:459:G:N2	2.49	0.45
3:A:472:G:H2'	3:A:473:G:H8	1.81	0.45
3:A:633:G:OP1	20:AW:64:LYS:HG3	2.17	0.45
3:A:1359:A:O4'	27:BT:305:GLN:HG3	2.17	0.45
9:AU:56:ASP:HB2	9:AU:98:THR:HG22	1.98	0.45
15:Ja:98:ASN:C	15:Ja:114:ILE:HG22	2.42	0.45
29:AD:76:LEU:HD23	29:AD:155:THR:HG23	1.99	0.45
44:Xa:68:ARG:CD	75:h1:114:U:H5'	2.47	0.45
49:AK:30:SER:O	49:AK:33:SER:OG	2.33	0.45
62:Za:28:HIS:HB3	62:Za:55:LEU:HD22	1.98	0.45
68:AN:102:ILE:HD12	68:AN:114:ARG:HG3	1.98	0.45
75:h1:389:A:H5''	86:h1:3264:HOH:O	2.17	0.45
2:3:56:A:OP1	56:BA:21:ARG:NH1	2.45	0.45
3:A:436:C:O3'	3:A:437:G:H8	2.00	0.45
3:A:498:A:H2'	3:A:499:C:O4'	2.17	0.45
3:A:973:G:H5'	41:Ha:29:PRO:HB2	1.98	0.45
3:A:2265:C:H2'	3:A:2266:U:C6	2.52	0.45
3:A:2266:U:H2'	3:A:2267:U:H2'	1.97	0.45
27:BT:12:ILE:HD11	27:BT:27:VAL:CG2	2.42	0.45
59:Ta:32:LEU:HD11	59:Ta:54:GLY:HA2	1.99	0.45
61:BE:31:VAL:O	61:BE:32:SER:C	2.59	0.45
75:h1:394:G:OP1	75:h1:1733:U:O2'	2.32	0.45
75:h1:915:G:O3'	75:h1:916:A:H8	2.00	0.45
3:A:1169:A:H5''	3:A:1342:A:OP1	2.17	0.45
22:BS:298:ALA:HB3	22:BS:307:LYS:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:896:G:H1	75:h1:918:U:H3	1.65	0.45
76:B1:24:U:O4	1:W2:34:G:O6	2.34	0.45
3:A:881:A:N3	86:A:4106:HOH:O	2.36	0.44
7:BO:48:PRO:CD	86:BO:201:HOH:O	2.64	0.44
17:AL:39:ALA:O	17:AL:40:LYS:C	2.59	0.44
24:AC:173:ARG:HD3	75:h1:1098:U:O4	2.16	0.44
25:BI:13:LYS:HD3	25:BI:128:LEU:HD11	1.98	0.44
41:Ha:120:PHE:HE1	41:Ha:122:VAL:CG2	2.29	0.44
45:BV:145:ARG:NH2	45:BV:151:LYS:O	2.50	0.44
46:BJ:102:MET:HE1	46:BJ:114:GLY:O	2.17	0.44
57:AF:96:GLN:CG	57:AF:104:LYS:HG3	2.47	0.44
59:Ta:182:ARG:NH1	75:h1:140:C:C5	2.85	0.44
62:Za:36:TYR:CD1	75:h1:1041:G:H4'	2.52	0.44
72:Aa:49:VAL:HG11	72:Aa:55:LYS:HG3	1.99	0.44
3:A:1592:G:P	86:A:4937:HOH:O	2.75	0.44
3:A:2100:C:C2	3:A:2101:U:C5	3.06	0.44
3:A:2652:C:O2'	3:A:2656:A:N1	2.47	0.44
15:Ja:240:LYS:O	15:Ja:242:LYS:NZ	2.50	0.44
22:BS:201:PHE:O	22:BS:202:PHE:C	2.59	0.44
54:AG:27:PRO:HD2	86:AG:414:HOH:O	2.17	0.44
59:Ta:67:VAL:HB	59:Ta:101:GLY:HA2	1.99	0.44
59:Ta:134:MET:HE1	75:h1:148:C:O4'	2.16	0.44
62:Za:70:VAL:HG11	62:Za:189:MET:CE	2.47	0.44
75:h1:290:A:C5	75:h1:291:C:C5	3.05	0.44
75:h1:1651:C:H2'	75:h1:1652:U:C6	2.53	0.44
78:AI:89:ALA:HA	78:AI:92:LYS:HD3	1.99	0.44
2:3:35:G:OP1	54:AG:32:ARG:HD3	2.18	0.44
3:A:320:A:P	86:A:3808:HOH:O	2.72	0.44
3:A:544:C:C2'	3:A:545:U:H5'	2.47	0.44
14:AP:47:LYS:NZ	86:AP:203:HOH:O	2.49	0.44
15:Ja:150:PRO:O	15:Ja:151:ASP:HB2	2.16	0.44
18:Va:26:GLN:O	18:Va:27:TYR:C	2.61	0.44
26:AH:36:ALA:HB2	26:AH:50:PHE:CE1	2.52	0.44
26:AH:39:ASP:OD2	26:AH:45:ARG:HG3	2.17	0.44
59:Ta:163:ARG:NH2	75:h1:80:C:OP1	2.50	0.44
75:h1:1491:G:H3'	75:h1:1518:A:H61	1.82	0.44
3:A:674:U:H2'	3:A:675:OMC:C6	2.52	0.44
3:A:1222:G:N7	86:A:4127:HOH:O	2.36	0.44
3:A:1557:A:N6	86:A:3803:HOH:O	1.90	0.44
3:A:1567:U:O4	3:A:1580:G:O2'	2.29	0.44
3:A:2522:A:C6	31:BQ:67:PHE:CE1	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BM:7:GLU:OE2	6:BM:7:GLU:HA	2.17	0.44
26:AH:39:ASP:OD1	26:AH:40:ALA:N	2.51	0.44
28:AV:44:ARG:HG2	28:AV:44:ARG:HH11	1.81	0.44
33:Da:114:ARG:HA	33:Da:114:ARG:HD3	1.76	0.44
54:AG:53:LEU:HD22	54:AG:118:TYR:CG	2.52	0.44
65:Ua:65:ARG:NH1	75:h1:907:A:OP1	2.50	0.44
75:h1:171:G:C2	75:h1:172:U:C2	3.06	0.44
3:A:3312:G:O2'	3:A:3313:G:H5'	2.16	0.44
3:A:3321:U:C5	47:AO:52:CYS:HB2	2.53	0.44
22:BS:56:ILE:HD12	22:BS:56:ILE:C	2.43	0.44
22:BS:118:PHE:CE2	22:BS:130:PHE:HE2	2.36	0.44
22:BS:336:LYS:O	22:BS:337:LYS:HB2	2.17	0.44
39:BG:199:ASN:HA	39:BG:202:LYS:HE2	1.99	0.44
50:Na:49:PHE:CE2	50:Na:51:HIS:HB2	2.53	0.44
57:AF:31:ILE:HG22	57:AF:67:MET:HG3	1.99	0.44
59:Ta:48:TYR:CZ	59:Ta:123:LEU:HD23	2.53	0.44
61:BE:2:ALA:O	61:BE:3:LYS:HB3	2.16	0.44
72:Aa:25:ARG:HB2	72:Aa:28:GLU:HG2	2.00	0.44
73:AY:25:ARG:HD2	73:AY:25:ARG:O	2.17	0.44
75:h1:43:A:O2'	75:h1:100:C:OP1	2.30	0.44
75:h1:1605:U:H6	75:h1:1605:U:O5'	2.01	0.44
78:AI:1:MET:HE3	78:AI:3:ILE:HD11	1.99	0.44
3:A:1173:G:N3	86:A:4125:HOH:O	2.36	0.44
3:A:1954:G:H2'	3:A:2091:A:H61	1.83	0.44
15:Ja:44:LEU:HD23	15:Ja:47:ILE:HD12	1.99	0.44
16:Ea:26:ARG:O	16:Ea:27:CYS:C	2.58	0.44
19:Ka:40:GLU:O	19:Ka:43:GLU:HG2	2.17	0.44
30:AJ:76:ASP:OD1	30:AJ:76:ASP:N	2.47	0.44
39:BG:170:PRO:HA	39:BG:217:ASN:ND2	2.27	0.44
49:AK:129:GLY:O	49:AK:130:ASN:HB3	2.18	0.44
51:AB:130:LEU:HB3	51:AB:136:ILE:HD13	1.99	0.44
62:Za:136:GLN:N	62:Za:137:PRO:CD	2.81	0.44
68:AN:79:LYS:HG2	68:AN:111:TYR:CE2	2.52	0.44
73:AY:65:ARG:HD3	86:AY:323:HOH:O	2.16	0.44
75:h1:79:A:H2'	75:h1:80:C:C6	2.51	0.44
75:h1:101:A:OP2	75:h1:101:A:H3'	2.17	0.44
75:h1:291:C:C2	75:h1:292:G:C8	3.05	0.44
75:h1:763:A:N6	75:h1:764:G:C2	2.86	0.44
75:h1:1088:A:H2'	75:h1:1089:A:C8	2.53	0.44
75:h1:1324:C:H2'	75:h1:1325:G:O4'	2.18	0.44
77:Ba:64:LEU:HD12	77:Ba:64:LEU:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:420:A:H2'	3:A:421:G:O4'	2.18	0.44
3:A:2841:U:O2	3:A:2841:U:C2'	2.60	0.44
3:A:2879:PSU:O4	22:BS:253:ALA:HB3	2.17	0.44
22:BS:259:HIS:HA	22:BS:260:PRO:C	2.42	0.44
25:BI:112:MET:CE	25:BI:132:ILE:HA	2.46	0.44
53:AA:162:GLN:HB3	53:AA:163:PRO:HD3	2.00	0.44
58:Wa:83:PHE:CE2	70:BL:37:ILE:HD11	2.52	0.44
62:Za:29:LEU:O	62:Za:168:ASN:HB2	2.17	0.44
71:La:55:ALA:N	71:La:56:PRO:HD2	2.32	0.44
75:h1:1549:A:H2'	75:h1:1550:U:O4'	2.18	0.44
75:h1:1604:C:H1'	86:h1:2621:HOH:O	2.18	0.44
3:A:1686:U:H2'	3:A:1688:U:H1'	1.99	0.44
3:A:1819:C:H2'	3:A:1820:C:O4'	2.18	0.44
3:A:2744:G:O2'	3:A:2746:A:N7	2.39	0.44
15:Ja:184:THR:C	15:Ja:189:ARG:HG3	2.43	0.44
27:BT:321:LYS:HD2	43:BR:167:ALA:HB1	1.98	0.44
31:BQ:181:LYS:NZ	86:BQ:403:HOH:O	2.40	0.44
35:AT:54:LEU:HD11	40:Fa:92:ILE:HG22	1.99	0.44
43:BR:30:ALA:O	43:BR:34:GLU:HG2	2.18	0.44
52:BF:215:LEU:HD23	52:BF:219:MET:HE2	1.99	0.44
56:BA:21:ARG:HB2	56:BA:22:PRO:HD2	2.00	0.44
63:AQ:10:TRP:O	63:AQ:14:LYS:HB2	2.18	0.44
72:Aa:51:GLY:HA2	75:h1:399:A:O3'	2.18	0.44
75:h1:25:C:P	86:h1:2108:HOH:O	2.74	0.44
75:h1:383:C:C2	75:h1:384:C:C5	3.06	0.44
75:h1:1192:C4J:C6	75:h1:1192:C4J:C4'	2.95	0.44
78:AI:1:MET:CE	78:AI:44:LYS:HB2	2.48	0.44
2:3:156:G:O2'	2:3:158:G:OP1	2.29	0.44
3:A:728:G:H5''	86:A:5139:HOH:O	2.18	0.44
3:A:955:C:H6	3:A:955:C:O5'	2.01	0.44
3:A:1348:C:H5'	86:A:8877:HOH:O	2.18	0.44
3:A:3119:U:H1'	3:A:3120:A:H5''	2.00	0.44
15:Ja:21:ASP:OD1	15:Ja:23:LEU:N	2.51	0.44
15:Ja:126:VAL:HG12	15:Ja:156:PRO:O	2.17	0.44
18:Va:124:VAL:O	18:Va:127:VAL:N	2.47	0.44
28:AV:87:MET:CE	28:AV:88:MET:HE3	2.48	0.44
30:AJ:46:ALA:HB3	86:AJ:315:HOH:O	2.17	0.44
43:BR:93:ARG:CZ	43:BR:108:LEU:HD13	2.47	0.44
44:Xa:60:PRO:HD2	44:Xa:113:SER:OG	2.18	0.44
45:BV:125:VAL:HG21	45:BV:173:VAL:CG2	2.48	0.44
50:Na:36:ASP:HB3	50:Na:45:ILE:HG12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AA:20:GLU:O	53:AA:24:VAL:HG23	2.17	0.44
65:Ua:104:THR:HG22	65:Ua:106:THR:H	1.83	0.44
66:Ya:104:GLY:O	75:h1:1212:A:H1'	2.17	0.44
3:A:174:G:H2'	3:A:175:A:O4'	2.18	0.43
3:A:409:G:H5'	6:BM:26:PHE:HZ	1.83	0.43
3:A:1620:A:H2'	3:A:1621:C:O4'	2.18	0.43
11:Ia:34:LEU:HB3	11:Ia:83:LEU:HD22	2.00	0.43
15:Ja:252:ALA:O	15:Ja:256:LEU:HG	2.18	0.43
17:AL:8:GLN:HB2	17:AL:32:TRP:CH2	2.53	0.43
22:BS:158:THR:HG23	86:BS:640:HOH:O	2.17	0.43
29:AD:124:ASP:HB2	29:AD:141:ILE:HD11	1.99	0.43
31:BQ:122:ASP:C	31:BQ:122:ASP:OD1	2.61	0.43
57:AF:52:GLU:N	57:AF:53:PRO:CD	2.81	0.43
61:BE:3:LYS:HG3	61:BE:4:ARG:HG3	2.00	0.43
62:Za:114:ASN:HB3	62:Za:117:GLN:HB2	2.00	0.43
67:BB:24:MET:HE1	67:BB:58:MET:HE3	1.99	0.43
3:A:1324:C:OP2	86:A:3871:HOH:O	2.21	0.43
3:A:1397:C:OP1	28:AV:105:LYS:NZ	2.46	0.43
3:A:1738:U:H2'	3:A:1739:C:O4'	2.18	0.43
8:AR:24:PRO:HG2	23:AM:86:ARG:CZ	2.48	0.43
15:Ja:240:LYS:HB2	75:h1:788:C:C2	2.53	0.43
18:Va:38:LYS:HB3	18:Va:39:PRO:CD	2.48	0.43
25:BI:25:THR:HA	25:BI:37:LEU:O	2.17	0.43
28:AV:87:MET:HE3	28:AV:88:MET:CE	2.48	0.43
43:BR:87:LYS:HB3	43:BR:196:VAL:HG21	2.00	0.43
46:BJ:51:HIS:CE1	46:BJ:137:SER:HG	2.27	0.43
53:AA:76:ARG:HA	78:AI:22:PHE:CZ	2.52	0.43
71:La:72:ILE:HG23	71:La:76:LEU:HD23	2.00	0.43
75:h1:872:A:H2'	75:h1:873:G:C8	2.54	0.43
3:A:43:A:OP1	86:A:3866:HOH:O	2.21	0.43
3:A:262:A:H4'	3:A:263:C:OP2	2.18	0.43
29:AD:140:ASP:O	64:Oa:41:VAL:HA	2.18	0.43
34:BK:129:ASP:OD2	34:BK:176:ASP:HB3	2.17	0.43
53:AA:167:TYR:CE1	53:AA:200:PRO:HG2	2.53	0.43
57:AF:50:ILE:CD1	57:AF:83:ILE:HG21	2.48	0.43
62:Za:69:ILE:HG23	62:Za:78:ILE:HD13	1.99	0.43
72:Aa:156:ASP:HB3	72:Aa:159:ILE:HD12	2.00	0.43
75:h1:428:G:N3	75:h1:429:C:C6	2.87	0.43
75:h1:1527:A:H2'	75:h1:1528:A:C8	2.53	0.43
3:A:617:C:O2'	27:BT:327:ASN:OD1	2.34	0.43
3:A:882:C:H3'	3:A:883:U:H4'	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1636:C:N3	3:A:1711:C:O2'	2.52	0.43
3:A:2526:G:H2'	3:A:2527:A:O4'	2.17	0.43
3:A:3036:U:O2	25:BI:12:ASN:ND2	2.51	0.43
23:AM:40:VAL:HG11	23:AM:64:ILE:HD11	2.00	0.43
29:AD:90:VAL:HG11	57:AF:45:ILE:HG21	1.99	0.43
29:AD:102:LEU:HD11	71:La:93:VAL:HG21	2.00	0.43
44:Xa:34:ARG:HH21	44:Xa:52:GLY:C	2.26	0.43
45:BV:34:ALA:O	45:BV:41:ARG:HD2	2.18	0.43
66:Ya:76:GLU:O	66:Ya:77:LYS:C	2.61	0.43
75:h1:564:G:N7	86:h1:2204:HOH:O	2.36	0.43
75:h1:803:U:H2'	75:h1:804:G:C8	2.53	0.43
75:h1:935:C:C4	75:h1:1078:C:H4'	2.54	0.43
75:h1:1293:G:H2'	75:h1:1294:U:C6	2.53	0.43
75:h1:1327:A2M:HM'3	75:h1:1327:A2M:H1'	1.88	0.43
3:A:1079:U:H2'	3:A:1080:C:C6	2.53	0.43
3:A:1800:A:H2'	3:A:1801:A:C8	2.53	0.43
3:A:3341:C:H4'	3:A:3342:U:H3'	2.00	0.43
7:BO:53:ASP:CG	7:BO:114:ARG:HH12	2.24	0.43
11:Ia:7:SER:O	11:Ia:8:GLU:HG3	2.18	0.43
53:AA:159:SER:N	75:h1:1329:G:OP1	2.48	0.43
53:AA:200:PRO:O	53:AA:202:THR:N	2.51	0.43
61:BE:64:LYS:CD	61:BE:71:MET:HE2	2.49	0.43
75:h1:1125:A:H2'	75:h1:1126:A:C8	2.54	0.43
3:A:843:U:H2'	3:A:844:A:O4'	2.18	0.43
3:A:991:G:C6	3:A:1111:G:H2'	2.54	0.43
3:A:1124:G:N3	3:A:1124:G:H2'	2.34	0.43
18:Va:3:LYS:HB3	86:Va:306:HOH:O	2.19	0.43
18:Va:3:LYS:N	86:Va:307:HOH:O	2.50	0.43
26:AH:121:VAL:HG22	32:BH:187:GLU:HA	2.00	0.43
46:BJ:99:ILE:HG22	46:BJ:123:LEU:HB2	2.01	0.43
64:Oa:44:PRO:HB3	75:h1:1617:C:OP2	2.18	0.43
70:BL:31:LEU:HB3	70:BL:35:THR:HG21	2.00	0.43
75:h1:314:A:C2	75:h1:317:A:C8	3.06	0.43
75:h1:522:A:C6	75:h1:523:A:C6	3.07	0.43
75:h1:1472:A:H2'	75:h1:1473:C:C6	2.53	0.43
75:h1:1542:G:C6	75:h1:1543:G:C5	3.07	0.43
86:3:338:HOH:O	80:A:3406:TER:H31	2.18	0.43
3:A:461:C:O2'	63:AQ:86:ASN:OD1	2.36	0.43
3:A:710:G:N2	86:A:3864:HOH:O	2.20	0.43
3:A:827:C:H2'	3:A:828:PSU:O4'	2.19	0.43
3:A:847:G:C6	61:BE:4:ARG:NH2	2.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1070:U:O2	23:AM:101:CYS:HB2	2.18	0.43
3:A:1125:G:N7	86:A:4128:HOH:O	2.37	0.43
3:A:2886:A:H2'	3:A:2886:A:N3	2.34	0.43
45:BV:71:ALA:HB3	65:Ua:127:ARG:NH2	2.34	0.43
71:La:60:LEU:HD23	71:La:65:ILE:HD11	2.01	0.43
72:Aa:68:TRP:CD2	72:Aa:71:GLU:HG2	2.52	0.43
75:h1:612:G:OP2	86:h1:2143:HOH:O	2.21	0.43
75:h1:1348:U:OP2	77:Ba:24:ARG:NH2	2.51	0.43
77:Ba:25:ILE:HD11	77:Ba:115:VAL:HG12	2.01	0.43
86:A:5105:HOH:O	54:AG:17:GLN:HG3	2.17	0.43
14:AP:70:CYS:SG	14:AP:117:LEU:HD12	2.59	0.43
15:Ja:47:ILE:HG23	15:Ja:111:LEU:HD11	2.00	0.43
35:AT:17:LEU:HD23	35:AT:17:LEU:HA	1.91	0.43
43:BR:67:LEU:O	43:BR:71:LYS:HG3	2.19	0.43
49:AK:139:MET:O	49:AK:140:GLU:C	2.62	0.43
75:h1:397:U:H2'	75:h1:398:G:O4'	2.18	0.43
75:h1:1384:U:H1'	75:h1:1519:A:N6	2.34	0.43
3:A:2154:G:N7	86:A:4135:HOH:O	2.37	0.43
3:A:3310:A:N6	3:A:3311:C:C4	2.87	0.43
86:A:9863:HOH:O	27:BT:67:THR:HG22	2.18	0.43
15:Ja:146:THR:CG2	75:h1:125:A:H1'	2.49	0.43
25:BI:140:VAL:HG11	47:AO:24:ILE:HG12	2.00	0.43
40:Fa:71:ARG:HD2	40:Fa:71:ARG:HA	1.85	0.43
48:BW:54:LEU:HD11	48:BW:68:VAL:HG23	1.99	0.43
59:Ta:134:MET:HE1	75:h1:148:C:C1'	2.49	0.43
70:BL:66:TYR:CD1	70:BL:66:TYR:C	2.96	0.43
71:La:90:ILE:HG22	71:La:104:ARG:HA	2.01	0.43
3:A:2451:U:N3	3:A:2453:U:OP1	2.52	0.43
15:Ja:3:ARG:O	75:h1:400:G:O2'	2.33	0.43
15:Ja:34:GLY:HA3	15:Ja:83:PRO:CG	2.48	0.43
15:Ja:127:ARG:HG2	15:Ja:142:TYR:CZ	2.54	0.43
27:BT:321:LYS:NZ	86:BR:403:HOH:O	2.51	0.43
31:BQ:179:MET:O	31:BQ:180:LEU:HB2	2.18	0.43
37:BP:106:ARG:HB2	37:BP:106:ARG:CZ	2.49	0.43
60:AZ:35:LYS:HA	60:AZ:43:TYR:O	2.19	0.43
75:h1:143:A:H2'	75:h1:144:U:C6	2.54	0.43
75:h1:1777:4AC:O7	75:h1:1777:4AC:H5	2.19	0.43
1:2:47:U:H2'	1:2:50:C:OP1	2.19	0.42
2:3:32:C:H4'	27:BT:56:PRO:HG2	2.00	0.42
3:A:16:G:OP2	38:BN:58:TYR:OH	2.28	0.42
3:A:391:C:O2'	3:A:393:A:N7	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:469:U:H2'	3:A:470:C:C6	2.53	0.42
3:A:1611:G:H2'	3:A:1612:G:O4'	2.19	0.42
3:A:2814:OMG:HM21	3:A:2816:A:H2'	2.01	0.42
86:A:7383:HOH:O	27:BT:62:LYS:HE2	2.18	0.42
11:Ia:96:ARG:HD2	11:Ia:146:GLU:HG3	2.01	0.42
15:Ja:134:LYS:N	75:h1:254:G:OP1	2.49	0.42
15:Ja:191:ARG:CZ	15:Ja:218:PHE:CD2	3.02	0.42
16:Ea:167:GLU:OE1	16:Ea:167:GLU:HA	2.19	0.42
25:BI:62:MET:HE3	25:BI:76:VAL:HG12	2.00	0.42
27:BT:240:ARG:HD3	86:BT:585:HOH:O	2.18	0.42
37:BP:93:ARG:HG2	37:BP:93:ARG:HH11	1.84	0.42
53:AA:162:GLN:N	53:AA:163:PRO:CD	2.82	0.42
57:AF:42:GLN:HB2	57:AF:43:PRO:HD3	1.99	0.42
58:Wa:120:HIS:CE1	58:Wa:124:ARG:HD2	2.53	0.42
75:h1:1671:U:H2'	75:h1:1672:G:O4'	2.18	0.42
3:A:139:U:H2'	3:A:140:C:C6	2.54	0.42
3:A:1431:G:OP1	80:A:3419:TER:H71	2.19	0.42
3:A:2550:U:H5''	86:A:5766:HOH:O	2.18	0.42
24:AC:199:PRO:HA	24:AC:202:TRP:CD1	2.54	0.42
27:BT:295:LEU:HD11	30:AJ:32:LEU:HB2	2.01	0.42
49:AK:120:TYR:O	49:AK:121:HIS:C	2.60	0.42
54:AG:88:LEU:O	54:AG:89:ALA:C	2.62	0.42
59:Ta:77:LEU:HD12	59:Ta:97:LYS:HB2	2.00	0.42
64:Oa:14:MET:HE3	64:Oa:38:MET:SD	2.59	0.42
66:Ya:86:ARG:HB3	66:Ya:122:ALA:HB2	2.00	0.42
75:h1:464:G:C5	75:h1:465:U:C5	3.06	0.42
75:h1:997:C:O2'	75:h1:998:G:H5'	2.18	0.42
75:h1:1118:PSU:H2'	75:h1:1119:G:H8	1.82	0.42
77:Ba:25:ILE:CG2	77:Ba:92:ILE:HB	2.49	0.42
3:A:225:U:H6	3:A:225:U:O5'	2.02	0.42
3:A:1221:U:H3'	86:A:3842:HOH:O	2.19	0.42
3:A:1337:C:O2'	20:AW:81:GLY:HA2	2.19	0.42
3:A:1754:G:C6	3:A:1755:C:C4	3.07	0.42
3:A:2359:A2M:HM'3	3:A:2359:A2M:H1'	1.78	0.42
15:Ja:68:ARG:HB3	15:Ja:76:VAL:HG11	2.01	0.42
18:Va:133:PHE:O	36:Pa:15:ARG:NH2	2.49	0.42
19:Ka:57:ILE:HG12	19:Ka:77:ILE:HG13	2.01	0.42
19:Ka:71:SER:OG	19:Ka:72:SER:N	2.52	0.42
27:BT:126:ARG:O	27:BT:129:ILE:HG22	2.19	0.42
37:BP:106:ARG:NH1	37:BP:106:ARG:CB	2.82	0.42
40:Fa:69:ARG:O	40:Fa:73:THR:HG23	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AB:35:GLU:HG2	51:AB:36:TYR:CD2	2.54	0.42
63:AQ:13:VAL:O	63:AQ:14:LYS:C	2.63	0.42
69:Ra:141:THR:HG22	69:Ra:142:ARG:N	2.35	0.42
73:AY:51:VAL:O	73:AY:55:ARG:HG3	2.18	0.42
75:h1:1065:G:C5	75:h1:1066:A:N7	2.87	0.42
2:3:155:OMG:HM23	2:3:155:OMG:H1'	1.90	0.42
3:A:1572:C:H2'	3:A:1573:U:O4'	2.19	0.42
3:A:2682:U:H2'	3:A:2683:C:H6	1.83	0.42
3:A:3010:A:N7	86:A:4133:HOH:O	2.37	0.42
15:Ja:108:ARG:H	15:Ja:108:ARG:HG2	1.69	0.42
27:BT:12:ILE:HG13	27:BT:260:LYS:HE2	2.02	0.42
49:AK:123:MET:HE2	49:AK:123:MET:HA	2.00	0.42
54:AG:89:ALA:HB3	54:AG:90:PRO:CD	2.49	0.42
59:Ta:96:ARG:HH22	75:h1:1675:G:P	2.42	0.42
75:h1:390:OMG:P	86:h1:2104:HOH:O	2.70	0.42
75:h1:1564:G:C2	75:h1:1565:G:C8	3.08	0.42
77:Ba:32:VAL:HG22	77:Ba:88:HIS:CE1	2.55	0.42
2:3:123:C:H2'	2:3:124:C:O4'	2.19	0.42
3:A:785:PSU:OP2	8:AR:41:ARG:NH1	2.52	0.42
3:A:1910:A:O5'	3:A:1910:A:H8	2.03	0.42
3:A:2662:G:H2'	3:A:2663:C:O4'	2.19	0.42
4:C3:11:A:O2'	4:C3:12:U:H3'	2.19	0.42
6:BM:37:ARG:O	6:BM:38:LYS:HB2	2.19	0.42
17:AL:116:HIS:O	17:AL:117:ARG:C	2.63	0.42
23:AM:142:GLU:OE1	23:AM:142:GLU:HA	2.20	0.42
39:BG:36:LEU:HD23	39:BG:36:LEU:HA	1.96	0.42
51:AB:32:LEU:HD13	51:AB:44:LEU:HD11	2.01	0.42
51:AB:136:ILE:N	51:AB:136:ILE:HD12	2.35	0.42
69:Ra:81:VAL:O	69:Ra:85:GLU:HB2	2.18	0.42
71:La:79:ARG:HD3	71:La:82:ARG:HH12	1.84	0.42
72:Aa:103:VAL:HG22	72:Aa:170:ALA:O	2.20	0.42
75:h1:778:A2M:C6	75:h1:789:U:N3	2.82	0.42
78:AI:45:LEU:O	78:AI:45:LEU:HD12	2.20	0.42
3:A:1722:U:O4	49:AK:128:LYS:NZ	2.51	0.42
3:A:3017:C:H2'	3:A:3018:U:O4'	2.20	0.42
7:BO:75:ARG:HD2	86:BO:231:HOH:O	2.18	0.42
38:BN:120:LYS:HE2	86:BN:208:HOH:O	2.19	0.42
45:BV:142:PHE:CD1	45:BV:142:PHE:N	2.88	0.42
49:AK:42:ARG:HD3	86:AK:302:HOH:O	2.19	0.42
54:AG:190:ALA:O	54:AG:191:GLY:C	2.63	0.42
62:Za:80:VAL:HG12	62:Za:91:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ya:54:LEU:HD12	66:Ya:58:PRO:HG3	2.00	0.42
75:h1:777:A:C4	75:h1:790:G:N2	2.87	0.42
75:h1:1295:G:O2'	75:h1:1322:A:N1	2.50	0.42
75:h1:1766:A:H1'	75:h1:1787:C:H5'	2.01	0.42
3:A:437:G:O6	3:A:634:G:H1'	2.19	0.42
80:A:3404:TER:H81	86:A:9079:HOH:O	2.18	0.42
29:AD:51:HIS:O	29:AD:51:HIS:ND1	2.47	0.42
31:BQ:133:TYR:CD1	31:BQ:133:TYR:C	2.98	0.42
32:BH:179:LEU:O	32:BH:179:LEU:HD23	2.20	0.42
59:Ta:27:PHE:CD1	59:Ta:36:VAL:HG21	2.54	0.42
59:Ta:138:LYS:HE2	75:h1:66:U:OP1	2.20	0.42
69:Ra:68:ARG:HD2	69:Ra:69:LEU:HG	2.02	0.42
72:Aa:4:SER:OG	72:Aa:24:LYS:HD3	2.20	0.42
75:h1:201:G:C2	75:h1:265:G:N3	2.88	0.42
75:h1:785:G:C2	75:h1:786:C:C2	3.08	0.42
75:h1:1274:G:O6	75:h1:1433:U:H2'	2.19	0.42
75:h1:1276:A:C2	75:h1:1277:U:H1'	2.55	0.42
21:BD:35:LEU:HA	21:BD:40:LYS:HG2	2.02	0.42
42:BU:89:LYS:O	42:BU:90:GLU:CB	2.67	0.42
62:Za:58:THR:HG22	62:Za:166:PRO:HG2	2.02	0.42
64:Oa:58:ARG:HB3	64:Oa:58:ARG:NH1	2.35	0.42
77:Ba:35:LEU:HD11	77:Ba:90:ARG:HG3	2.01	0.42
77:Ba:85:LEU:C	77:Ba:85:LEU:CD2	2.91	0.42
3:A:803:OMU:H6	3:A:803:OMU:O5'	2.20	0.42
3:A:1571:G:H2'	3:A:1572:C:C6	2.55	0.42
3:A:1805:C:H2'	3:A:1806:G:O4'	2.19	0.42
3:A:2347:U:H5'	3:A:2389:OMG:OP1	2.20	0.42
3:A:2377:U:OP1	80:A:3417:TER:H41	2.19	0.42
15:Ja:155:LYS:HD3	15:Ja:155:LYS:HA	1.83	0.42
22:BS:53:MET:HE2	22:BS:75:ALA:HB1	2.02	0.42
36:Pa:44:PHE:CD2	51:AB:31:LYS:HG3	2.55	0.42
42:BU:35:ALA:HB2	42:BU:125:TYR:CE1	2.55	0.42
44:Xa:123:HIS:O	44:Xa:124:ILE:HD12	2.19	0.42
48:BW:16:LYS:O	48:BW:17:CYS:C	2.63	0.42
59:Ta:76:LEU:N	86:Ta:402:HOH:O	2.23	0.42
59:Ta:81:THR:HB	59:Ta:82:PRO:HD2	2.02	0.42
75:h1:1107:C:H2'	86:h1:2884:HOH:O	2.19	0.42
75:h1:1148:A:H2'	75:h1:1149:C:O4'	2.20	0.42
75:h1:1342:G:C6	75:h1:1343:C:C5	3.08	0.42
75:h1:1500:U:C4	75:h1:1514:G:C2	3.08	0.42
75:h1:1763:C:H2'	75:h1:1764:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:680:A:N7	86:A:4137:HOH:O	2.37	0.42
3:A:1740:C:O2'	3:A:1741:A:H5'	2.20	0.42
3:A:2270:G:N3	3:A:2270:G:H2'	2.35	0.42
3:A:2427:G:H2'	3:A:2428:A:C8	2.55	0.42
3:A:2627:A:H1'	3:A:2797:C:C2	2.55	0.42
16:Ea:63:ARG:HD3	86:Ea:419:HOH:O	2.20	0.42
22:BS:118:PHE:CE2	22:BS:130:PHE:CE2	3.08	0.42
23:AM:157:VAL:HG21	46:BJ:169:ARG:CZ	2.50	0.42
26:AH:116:LYS:HE3	32:BH:197:GLN:OE1	2.19	0.42
27:BT:275:LYS:HE3	27:BT:276:PRO:O	2.19	0.42
27:BT:391:ASP:OD1	27:BT:393:THR:HG23	2.20	0.42
34:BK:126:THR:HG22	34:BK:128:GLU:H	1.84	0.42
39:BG:160:LEU:HB3	39:BG:161:PRO:HD3	2.02	0.42
51:AB:148:PHE:CZ	75:h1:768:G:C6	3.07	0.42
75:h1:427:A:H2'	86:h1:2116:HOH:O	2.20	0.42
75:h1:1754:A2M:HM'3	75:h1:1754:A2M:H1'	1.88	0.42
77:Ba:27:LEU:O	77:Ba:89:LYS:HA	2.20	0.42
3:A:833:C:O2'	3:A:1543:A:N3	2.47	0.41
3:A:1552:G:H5'	84:A:3402:EPE:H62	2.02	0.41
3:A:1750:A:H8	3:A:1750:A:OP1	2.03	0.41
3:A:2507:U:H2'	3:A:2508:U:O4'	2.19	0.41
14:AP:45:GLY:HA3	14:AP:71:PHE:CZ	2.55	0.41
15:Ja:222:LEU:O	15:Ja:224:ASN:N	2.53	0.41
40:Fa:20:HIS:CE1	40:Fa:32:TYR:CE1	3.08	0.41
72:Aa:139:SER:HB2	75:h1:188:U:O4	2.20	0.41
3:A:1660:C:O2'	3:A:1661:G:H5'	2.20	0.41
3:A:1729:G:N3	3:A:1729:G:H5'	2.35	0.41
3:A:2399:A:N3	86:A:4131:HOH:O	2.37	0.41
80:A:3418:TER:H101	86:A:7629:HOH:O	2.20	0.41
14:AP:26:ILE:HD11	14:AP:44:ALA:HB2	2.02	0.41
15:Ja:108:ARG:NH2	75:h1:791:G:P	2.93	0.41
51:AB:13:THR:O	51:AB:49:TYR:CD2	2.72	0.41
57:AF:69:ILE:HG21	57:AF:83:ILE:HD12	2.03	0.41
62:Za:180:TRP:CD2	62:Za:203:VAL:HG22	2.55	0.41
75:h1:299:U:O2'	86:h1:2142:HOH:O	2.21	0.41
75:h1:338:G:P	86:h1:2162:HOH:O	2.79	0.41
2:3:12:C:OP1	80:A:3412:TER:H42	2.19	0.41
3:A:280:G:H3'	3:A:280:G:N3	2.35	0.41
24:AC:44:VAL:C	24:AC:46:PRO:HD2	2.45	0.41
38:BN:129:ASP:OD1	38:BN:129:ASP:C	2.64	0.41
45:BV:164:ILE:HD13	45:BV:207:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AB:78:LEU:HD21	51:AB:98:VAL:HG11	2.02	0.41
57:AF:30:LEU:HD12	57:AF:30:LEU:O	2.21	0.41
58:Wa:37:GLY:HA3	75:h1:1568:U:OP1	2.20	0.41
62:Za:167:ALA:HB1	62:Za:178:LEU:HD11	2.02	0.41
75:h1:46:A:N6	75:h1:435:C:H4'	2.36	0.41
75:h1:336:G:H2'	75:h1:337:PSU:H6	1.85	0.41
75:h1:617:A:N1	75:h1:1107:C:O2	2.53	0.41
75:h1:1172:A:O2'	75:h1:1572:A:N3	2.49	0.41
75:h1:1353:A:H2'	75:h1:1354:C:O4'	2.20	0.41
3:A:434:G:O4'	3:A:436:C:H2'	2.21	0.41
3:A:452:G:H4'	63:AQ:96:ARG:HH12	1.86	0.41
3:A:1360:G:N7	3:A:1363:C:N4	2.61	0.41
3:A:1714:G:O6	35:AT:31:LYS:HE3	2.21	0.41
3:A:2989:G:OP2	86:A:3873:HOH:O	2.21	0.41
3:A:3046:A:H3'	86:A:8868:HOH:O	2.20	0.41
86:A:6621:HOH:O	16:Ea:169:LYS:CE	2.52	0.41
6:BM:79:ASN:C	6:BM:79:ASN:OD1	2.64	0.41
10:Ma:89:ARG:NH1	75:h1:1090:U:OP1	2.52	0.41
14:AP:53:VAL:HA	86:AP:208:HOH:O	2.20	0.41
15:Ja:80:LYS:H	15:Ja:80:LYS:HD3	1.85	0.41
16:Ea:65:ARG:HD2	16:Ea:127:TYR:CD1	2.55	0.41
16:Ea:176:GLY:O	16:Ea:185:ARG:NH2	2.53	0.41
18:Va:15:ARG:HH21	18:Va:18:ILE:HG21	1.83	0.41
20:AW:42:THR:OG1	20:AW:45:GLU:HG3	2.21	0.41
24:AC:107:SER:O	24:AC:108:VAL:C	2.64	0.41
29:AD:182:LYS:HE2	29:AD:182:LYS:N	2.34	0.41
32:BH:156:ASP:O	32:BH:157:THR:C	2.61	0.41
33:Da:46:THR:OG1	33:Da:49:GLN:HG3	2.20	0.41
45:BV:85:ARG:O	45:BV:101:TRP:N	2.46	0.41
51:AB:173:ARG:HD2	75:h1:539:G:C6	2.56	0.41
58:Wa:83:PHE:CD2	70:BL:37:ILE:HD11	2.56	0.41
62:Za:43:PHE:HD2	62:Za:44:LYS:HG2	1.85	0.41
75:h1:40:A:H2'	75:h1:41:A:O4'	2.20	0.41
75:h1:1801:A:O5'	75:h1:1801:A:H8	2.04	0.41
77:Ba:56:PRO:HA	77:Ba:92:ILE:HG12	2.02	0.41
2:3:155:OMG:HM22	39:BG:52:ILE:HD11	2.02	0.41
3:A:2913:G:O2'	3:A:2933:A2M:N1	2.52	0.41
3:A:3022:A:C2	3:A:3030:A:C4	3.09	0.41
12:AE:99:PHE:O	12:AE:99:PHE:CD1	2.74	0.41
19:Ka:84:ALA:O	19:Ka:88:GLU:HB2	2.21	0.41
59:Ta:13:GLN:HG3	75:h1:150:U:OP1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:133:ARG:O	59:Ta:134:MET:HB3	2.21	0.41
65:Ua:91:ALA:HA	65:Ua:124:LYS:O	2.21	0.41
75:h1:603:A:H2'	75:h1:604:PSU:O4'	2.21	0.41
75:h1:1152:A:O2'	75:h1:1770:A:N7	2.52	0.41
3:A:547:G:O2'	3:A:548:U:P	2.79	0.41
3:A:551:A:H2'	3:A:553:A:O4'	2.20	0.41
3:A:1678:G:O6	68:AN:80:ARG:NH2	2.54	0.41
3:A:1932:A:OP1	86:A:3876:HOH:O	2.22	0.41
3:A:2826:U:O2	3:A:2826:U:C2'	2.67	0.41
3:A:3334:G:H5''	3:A:3334:G:H8	1.85	0.41
80:A:3408:TER:H61	80:A:3408:TER:H31	1.84	0.41
12:AE:79:PHE:HD1	18:Va:7:MET:HE1	1.85	0.41
19:Ka:60:PHE:O	75:h1:525:C:OP1	2.38	0.41
24:AC:62:THR:OG1	24:AC:65:GLY:O	2.19	0.41
31:BQ:94:ALA:O	31:BQ:102:LEU:HD21	2.21	0.41
37:BP:16:ASP:N	37:BP:16:ASP:OD1	2.54	0.41
43:BR:45:ALA:HB2	86:BR:450:HOH:O	2.19	0.41
53:AA:44:MET:O	53:AA:44:MET:HG2	2.21	0.41
57:AF:113:ARG:HH11	57:AF:113:ARG:HB3	1.84	0.41
59:Ta:32:LEU:HD13	59:Ta:63:MET:SD	2.61	0.41
62:Za:158:MET:O	62:Za:159:ARG:C	2.63	0.41
65:Ua:140:ARG:NH2	75:h1:1791:C:OP1	2.53	0.41
72:Aa:140:ASN:HB3	75:h1:190:A:C2	2.56	0.41
75:h1:63:G:H4'	75:h1:168:U:C5	2.56	0.41
75:h1:383:C:C2'	75:h1:384:C:O5'	2.68	0.41
75:h1:411:C:N4	75:h1:412:A:N6	2.68	0.41
75:h1:792:A:H2'	75:h1:792:A:N3	2.35	0.41
75:h1:1180:G:N3	86:h1:2208:HOH:O	2.37	0.41
75:h1:1461:G:O2'	75:h1:1462:C:OP1	2.28	0.41
78:AI:20:VAL:HG23	78:AI:66:TRP:O	2.21	0.41
3:A:7:C:H2'	3:A:8:C:O4'	2.21	0.41
3:A:1917:A:H5'	49:AK:82:LYS:O	2.21	0.41
3:A:2790:OMG:HM23	3:A:2790:OMG:H1'	1.91	0.41
7:BO:90:ASN:OD1	7:BO:90:ASN:C	2.64	0.41
9:AU:19:ASN:OD1	9:AU:19:ASN:C	2.64	0.41
9:AU:70:GLY:HA2	86:AU:206:HOH:O	2.21	0.41
14:AP:26:ILE:CD1	14:AP:95:ALA:HB3	2.50	0.41
18:Va:43:SER:OG	18:Va:75:LYS:NZ	2.53	0.41
18:Va:124:VAL:O	18:Va:125:SER:C	2.63	0.41
34:BK:204:SER:O	34:BK:205:ASN:C	2.62	0.41
34:BK:221:HIS:CD2	34:BK:222:PHE:CE2	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AG:56:VAL:HG22	54:AG:155:ILE:HG12	2.02	0.41
59:Ta:160:ASN:HA	59:Ta:163:ARG:CG	2.50	0.41
66:Ya:29:ALA:O	66:Ya:33:MET:HB2	2.21	0.41
69:Ra:99:ARG:CZ	69:Ra:125:ALA:HB1	2.51	0.41
71:La:81:ILE:HG21	71:La:102:TYR:CE1	2.56	0.41
75:h1:26:A:N1	75:h1:602:UY1:N3	2.68	0.41
75:h1:95:PSU:H2'	75:h1:96:G:O4'	2.21	0.41
3:A:466:C:O2'	3:A:467:A:O5'	2.38	0.41
3:A:1175:G:H5'	86:A:8825:HOH:O	2.21	0.41
3:A:2522:A:C5	31:BQ:67:PHE:CE1	3.08	0.41
3:A:3132:G:H5'	32:BH:151:GLY:HA3	2.02	0.41
7:BO:21:ALA:HB1	7:BO:25:GLU:HB2	2.03	0.41
18:Va:17:ARG:O	18:Va:21:ARG:HG3	2.21	0.41
27:BT:12:ILE:HD12	27:BT:158:VAL:HG11	2.03	0.41
27:BT:245:LYS:CG	86:BT:628:HOH:O	2.69	0.41
31:BQ:189:TYR:O	31:BQ:190:ARG:C	2.64	0.41
59:Ta:3:PHE:CZ	59:Ta:27:PHE:CE2	3.08	0.41
74:Ca:53:ILE:C	74:Ca:54:LYS:CA	2.94	0.41
75:h1:193:G:O2'	75:h1:194:A:H8	2.04	0.41
75:h1:332:G:C4	75:h1:333:A:C8	3.09	0.41
75:h1:865:C:H5''	86:h1:2637:HOH:O	2.20	0.41
75:h1:1458:G:C2	75:h1:1459:C:C2	3.09	0.41
3:A:948:U:OP2	41:Ha:26:ARG:NH2	2.40	0.41
3:A:1903:A:H2'	3:A:1903:A:N3	2.35	0.41
3:A:2553:G:N1	40:Fa:98:GLU:OE2	2.46	0.41
11:Ia:94:LYS:HG2	11:Ia:148:VAL:HG22	2.03	0.41
15:Ja:57:THR:O	15:Ja:61:VAL:HG23	2.21	0.41
17:AL:74:ILE:CD1	26:AH:31:VAL:HG22	2.51	0.41
21:BD:42:ARG:HD2	86:BD:331:HOH:O	2.20	0.41
22:BS:348:THR:HG22	22:BS:350:THR:HG23	2.02	0.41
27:BT:337:TYR:O	27:BT:337:TYR:CG	2.73	0.41
86:AD:402:HOH:O	75:h1:1475:C:H2'	2.21	0.41
34:BK:234:SER:O	34:BK:235:ILE:C	2.64	0.41
38:BN:39:ARG:HD3	39:BG:43:SER:HB3	2.02	0.41
43:BR:195:THR:O	43:BR:196:VAL:C	2.62	0.41
45:BV:26:LYS:O	45:BV:50:ARG:HG3	2.21	0.41
47:AO:24:ILE:HG13	47:AO:30:VAL:HG22	2.02	0.41
47:AO:25:ARG:HB3	47:AO:27:ASP:OD1	2.20	0.41
58:Wa:79:ILE:HA	58:Wa:80:PRO:HD3	1.96	0.41
59:Ta:36:VAL:HG23	59:Ta:52:ILE:HD11	2.02	0.41
59:Ta:155:VAL:HA	59:Ta:158:TYR:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Za:62:LEU:CD2	62:Za:182:LEU:HD23	2.51	0.41
62:Za:115:GLN:OE1	62:Za:116:MET:HE2	2.21	0.41
63:AQ:20:LEU:HD13	63:AQ:44:HIS:CE1	2.55	0.41
64:Oa:10:VAL:HG12	64:Oa:47:GLU:HA	2.02	0.41
67:BB:28:PHE:CE2	75:h1:1392:C:C6	3.08	0.41
71:La:84:LEU:HD22	71:La:89:VAL:HG11	2.03	0.41
75:h1:963:C:OP2	86:h1:2144:HOH:O	2.22	0.41
75:h1:1320:U:H2'	75:h1:1321:U:O4'	2.20	0.41
75:h1:1680:C:H2'	75:h1:1681:G:O4'	2.20	0.41
2:3:108:A:C8	2:3:109:A:C8	3.09	0.41
3:A:609:A:H4'	3:A:610:G:O5'	2.21	0.41
3:A:1010:G:H2'	3:A:1011:C:O4'	2.20	0.41
3:A:1373:A:H2'	3:A:1374:U:O4'	2.21	0.41
3:A:1478:OMC:N3	3:A:1517:OMC:N3	2.69	0.41
3:A:1517:OMC:HM23	3:A:1517:OMC:H1'	1.92	0.41
3:A:3031:A:O2'	3:A:3032:C:H5'	2.20	0.41
15:Ja:2:ALA:O	15:Ja:3:ARG:HB2	2.21	0.41
15:Ja:44:LEU:CD1	15:Ja:82:TYR:HB3	2.51	0.41
17:AL:83:TYR:CD2	17:AL:118:VAL:HG21	2.56	0.41
24:AC:6:TRP:CD1	24:AC:38:GLN:HE21	2.39	0.41
27:BT:284:VAL:HG21	30:AJ:106:GLU:HG3	2.01	0.41
34:BK:242:VAL:O	34:BK:243:HIS:C	2.64	0.41
45:BV:153:THR:HG21	45:BV:155:TYR:CE2	2.56	0.41
61:BE:38:PHE:CZ	61:BE:43:GLY:HA2	2.55	0.41
66:Ya:133:HIS:HB3	75:h1:1463:A:C8	2.56	0.41
67:BB:57:LEU:HD22	67:BB:69:ILE:HD11	2.02	0.41
69:Ra:19:CYS:HA	69:Ra:22:GLN:OE1	2.21	0.41
75:h1:97:G:C6	86:h1:2131:HOH:O	2.74	0.41
75:h1:335:A:C2'	75:h1:336:G:O5'	2.69	0.41
75:h1:379:G:HO2'	75:h1:380:A:P	2.44	0.41
75:h1:390:OMG:C2	75:h1:391:G:C8	3.09	0.41
75:h1:1202:G:C2	75:h1:1602:A:C8	3.09	0.41
75:h1:1593:C:H2'	75:h1:1594:G:H8	1.86	0.41
78:AI:35:ILE:HG22	78:AI:37:VAL:HG23	2.03	0.41
2:3:110:C:OP1	80:3:201:TER:H81	2.21	0.40
3:A:1169:A:O2'	3:A:1376:A2M:H5'	2.21	0.40
3:A:1846:C:O2	73:AY:9:GLY:HA2	2.20	0.40
3:A:1880:G:N3	3:A:1880:G:H3'	2.36	0.40
3:A:2417:A:H2'	3:A:2418:C:C6	2.56	0.40
3:A:3113:C:H4'	3:A:3114:G:OP2	2.21	0.40
3:A:3337:C:O2'	3:A:3339:U:OP2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BK:94:ASN:OD1	34:BK:94:ASN:C	2.65	0.40
49:AK:96:MET:HE3	49:AK:96:MET:HB2	1.74	0.40
61:BE:64:LYS:HD3	61:BE:71:MET:HE2	2.01	0.40
64:Oa:23:VAL:HG12	64:Oa:24:THR:N	2.35	0.40
75:h1:1031:A:OP2	86:h1:2145:HOH:O	2.22	0.40
75:h1:1117:A:C2	75:h1:1132:A:C4	3.09	0.40
75:h1:1391:A:C2	75:h1:1415:G:C4	3.08	0.40
75:h1:1631:G:H5''	75:h1:1798:A:OP2	2.22	0.40
1:W2:18:G:O2'	1:W2:57:G:N2	2.51	0.40
2:3:130:U:O2'	2:3:134:G:N2	2.55	0.40
3:A:522:C:C5	3:A:525:A:H4'	2.56	0.40
3:A:3146:G:H2'	3:A:3147:C:O4'	2.21	0.40
22:BS:208:ILE:O	22:BS:208:ILE:HG13	2.21	0.40
23:AM:75:GLU:HG2	23:AM:88:ARG:HG2	2.03	0.40
27:BT:132:ALA:O	27:BT:136:THR:HG23	2.21	0.40
27:BT:139:PRO:HG3	27:BT:155:MET:HG3	2.02	0.40
29:AD:56:TYR:HB3	29:AD:63:LYS:HA	2.03	0.40
29:AD:167:LYS:HA	71:La:64:SER:OG	2.20	0.40
34:BK:42:ASN:OD1	34:BK:42:ASN:N	2.55	0.40
39:BG:143:GLN:NE2	39:BG:195:THR:O	2.54	0.40
45:BV:40:ASN:OD1	45:BV:75:ASN:HB2	2.21	0.40
57:AF:67:MET:HE2	57:AF:87:ILE:HG23	2.03	0.40
74:Ca:30:LEU:HA	74:Ca:39:CYS:HA	2.03	0.40
75:h1:268:U:H2'	75:h1:269:C:C6	2.55	0.40
75:h1:1486:A:H2'	75:h1:1487:A:C8	2.56	0.40
3:A:34:PSU:H5'	3:A:35:U:OP2	2.22	0.40
3:A:436:C:O2'	3:A:437:G:H2'	2.22	0.40
3:A:465:G:O6	63:AQ:76:LYS:NZ	2.48	0.40
3:A:1039:C:H2'	3:A:1040:G:C8	2.57	0.40
3:A:1356:G:H5''	27:BT:312:LYS:HD2	2.03	0.40
3:A:2618:OMG:H1'	3:A:2618:OMG:HM23	1.84	0.40
7:BO:51:LYS:O	7:BO:52:ASP:HB2	2.20	0.40
9:AU:59:LEU:O	9:AU:60:ASN:C	2.64	0.40
14:AP:126:ASN:O	14:AP:127:ARG:C	2.64	0.40
29:AD:18:LEU:HD11	29:AD:50:PRO:HD3	2.02	0.40
34:BK:105:LEU:O	34:BK:106:ALA:C	2.64	0.40
39:BG:42:LEU:O	39:BG:44:ARG:N	2.54	0.40
42:BU:37:LYS:O	42:BU:41:GLN:HG3	2.20	0.40
43:BR:146:LEU:HD11	43:BR:150:LYS:HE3	2.04	0.40
44:Xa:71:ILE:O	44:Xa:72:LEU:HD23	2.21	0.40
51:AB:50:THR:O	51:AB:51:LEU:C	2.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Ua:137:ASP:CG	75:h1:928:C:O2	2.65	0.40
69:Ra:126:MET:CE	69:Ra:177:LEU:HB3	2.51	0.40
75:h1:193:G:C4	75:h1:194:A:C8	3.10	0.40
75:h1:342:U:C2	75:h1:343:A:N7	2.89	0.40
75:h1:578:G:H4'	75:h1:582:A:C4	2.56	0.40
75:h1:1432:G:C5	75:h1:1433:U:C4	3.10	0.40
1:W2:37:G:C6	86:W2:101:HOH:O	2.58	0.40
3:A:545:U:O2'	3:A:546:U:P	2.79	0.40
3:A:1032:G:C6	3:A:1033:G:C6	3.10	0.40
14:AP:57:ASP:OD1	14:AP:61:LYS:HB3	2.20	0.40
15:Ja:2:ALA:O	75:h1:95:PSU:OP1	2.40	0.40
15:Ja:31:PRO:HB2	15:Ja:38:SER:OG	2.21	0.40
15:Ja:136:ILE:HD13	15:Ja:148:ARG:HH21	1.86	0.40
22:BS:91:ALA:HB1	22:BS:157:ALA:HB2	2.04	0.40
28:AV:100:ASN:OD1	28:AV:100:ASN:N	2.51	0.40
30:AJ:94:ILE:HA	30:AJ:95:PRO:HD2	1.93	0.40
32:BH:63:LEU:HA	32:BH:63:LEU:HD23	1.83	0.40
32:BH:66:ARG:HA	32:BH:75:PRO:HD2	2.03	0.40
36:Pa:41:ASN:O	36:Pa:45:VAL:HB	2.22	0.40
37:BP:32:ARG:O	37:BP:35:LYS:N	2.54	0.40
39:BG:200:GLU:OE1	39:BG:200:GLU:N	2.46	0.40
40:Fa:74:VAL:O	40:Fa:79:GLY:HA3	2.21	0.40
41:Ha:23:GLY:O	41:Ha:24:LYS:HB2	2.20	0.40
45:BV:152:ARG:HB3	75:h1:1803:U:N3	2.37	0.40
50:Na:10:LEU:HD13	50:Na:10:LEU:HA	1.96	0.40
58:Wa:27:MET:HE2	58:Wa:27:MET:HB3	1.98	0.40
59:Ta:71:GLY:HA2	59:Ta:100:ARG:NH2	2.36	0.40
59:Ta:138:LYS:CE	75:h1:66:U:OP1	2.70	0.40
72:Aa:74:THR:OG1	75:h1:258:A:H1'	2.21	0.40
75:h1:778:A2M:C2	75:h1:789:U:O2	2.70	0.40
75:h1:778:A2M:C2	75:h1:789:U:C2	3.05	0.40
75:h1:1378:G:H2'	75:h1:1379:C:O4'	2.21	0.40
75:h1:1421:G:HO2'	75:h1:1422:G:H5'	1.86	0.40
75:h1:1543:G:C6	75:h1:1544:G:N1	2.89	0.40
75:h1:1571:A:C2	75:h1:1572:A:C5	3.09	0.40
1:W2:69:C:H2'	1:W2:70:C:O4'	2.21	0.40
1:W2:70:C:O2'	1:W2:71:G:OP1	2.28	0.40
3:A:2769:G:C6	3:A:2770:A:N6	2.89	0.40
3:A:3368:U:OP1	22:BS:172:LYS:NZ	2.47	0.40
7:BO:2:LYS:HD2	7:BO:2:LYS:C	2.47	0.40
7:BO:38:LEU:HD23	7:BO:38:LEU:HA	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AR:35:MET:HB2	8:AR:40:LEU:HD11	2.03	0.40
29:AD:83:ASN:ND2	75:h1:1589:A:O2'	2.44	0.40
53:AA:122:VAL:O	53:AA:126:VAL:HG23	2.21	0.40
70:BL:134:GLN:HB3	70:BL:138:ARG:NH2	2.37	0.40
75:h1:166:A:O2'	75:h1:167:A:H5'	2.22	0.40
75:h1:271:C:H2'	75:h1:272:A:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BC	23/25 (92%)	23 (100%)	0	0	100	100
6	BM	153/176 (87%)	148 (97%)	5 (3%)	0	100	100
7	BO	123/146 (84%)	117 (95%)	6 (5%)	0	100	100
8	AR	49/83 (59%)	46 (94%)	2 (4%)	1 (2%)	6	4
9	AU	107/119 (90%)	104 (97%)	2 (2%)	1 (1%)	14	14
10	Ma	96/131 (73%)	91 (95%)	5 (5%)	0	100	100
11	Ia	188/194 (97%)	185 (98%)	3 (2%)	0	100	100
12	AE	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
13	AX	95/112 (85%)	91 (96%)	3 (3%)	1 (1%)	11	10
14	AP	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
15	Ja	256/262 (98%)	228 (89%)	24 (9%)	4 (2%)	7	6
16	Ea	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
17	AL	173/217 (80%)	166 (96%)	7 (4%)	0	100	100
18	Va	137/142 (96%)	129 (94%)	7 (5%)	1 (1%)	18	19
19	Ka	118/133 (89%)	108 (92%)	10 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AW	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
21	BD	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
22	BS	383/389 (98%)	375 (98%)	7 (2%)	1 (0%)	36	42
23	AM	161/164 (98%)	155 (96%)	6 (4%)	0	100	100
24	AC	213/284 (75%)	207 (97%)	6 (3%)	0	100	100
25	BI	129/140 (92%)	122 (95%)	6 (5%)	1 (1%)	16	16
26	AH	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
27	BT	389/406 (96%)	376 (97%)	12 (3%)	1 (0%)	36	42
28	AV	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
29	AD	180/207 (87%)	170 (94%)	10 (6%)	0	100	100
30	AJ	184/187 (98%)	178 (97%)	6 (3%)	0	100	100
31	BQ	243/258 (94%)	228 (94%)	14 (6%)	1 (0%)	30	34
32	BH	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
33	Da	147/151 (97%)	138 (94%)	8 (5%)	1 (1%)	18	19
34	BK	279/301 (93%)	269 (96%)	10 (4%)	0	100	100
35	AT	92/112 (82%)	89 (97%)	3 (3%)	0	100	100
36	Pa	45/62 (73%)	41 (91%)	4 (9%)	0	100	100
37	BP	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
38	BN	115/154 (75%)	110 (96%)	5 (4%)	0	100	100
39	BG	232/256 (91%)	221 (95%)	9 (4%)	2 (1%)	14	14
40	Fa	109/120 (91%)	106 (97%)	3 (3%)	0	100	100
41	Ha	143/146 (98%)	134 (94%)	8 (6%)	1 (1%)	18	19
42	BU	167/182 (92%)	161 (96%)	6 (4%)	0	100	100
43	BR	230/247 (93%)	221 (96%)	9 (4%)	0	100	100
44	Xa	144/160 (90%)	132 (92%)	11 (8%)	1 (1%)	18	19
45	BV	210/262 (80%)	196 (93%)	13 (6%)	1 (0%)	24	27
46	BJ	203/221 (92%)	193 (95%)	10 (5%)	0	100	100
47	AO	60/164 (37%)	58 (97%)	2 (3%)	0	100	100
48	BW	71/82 (87%)	66 (93%)	4 (6%)	1 (1%)	9	7
49	AK	176/214 (82%)	172 (98%)	4 (2%)	0	100	100
50	Na	81/86 (94%)	69 (85%)	12 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	AB	178/197 (90%)	172 (97%)	6 (3%)	0	100	100
52	BF	184/233 (79%)	172 (94%)	12 (6%)	0	100	100
53	AA	206/250 (82%)	183 (89%)	21 (10%)	2 (1%)	12	11
54	AG	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
55	Ga	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
56	BA	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
57	AF	136/146 (93%)	119 (88%)	17 (12%)	0	100	100
58	Wa	137/152 (90%)	126 (92%)	11 (8%)	0	100	100
59	Ta	223/249 (90%)	196 (88%)	26 (12%)	1 (0%)	30	34
60	AZ	66/69 (96%)	57 (86%)	8 (12%)	1 (2%)	8	6
61	BE	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	11	10
62	Za	196/298 (66%)	186 (95%)	10 (5%)	0	100	100
63	AQ	134/143 (94%)	116 (87%)	17 (13%)	1 (1%)	18	19
64	Oa	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
65	Ua	125/150 (83%)	116 (93%)	8 (6%)	1 (1%)	16	16
66	Ya	127/150 (85%)	113 (89%)	11 (9%)	3 (2%)	4	3
67	BB	117/141 (83%)	106 (91%)	11 (9%)	0	100	100
68	AN	97/124 (78%)	85 (88%)	12 (12%)	0	100	100
69	Ra	182/190 (96%)	160 (88%)	20 (11%)	2 (1%)	11	10
70	BL	134/143 (94%)	127 (95%)	7 (5%)	0	100	100
71	La	69/108 (64%)	67 (97%)	1 (1%)	1 (1%)	9	7
72	Aa	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
73	AY	83/95 (87%)	79 (95%)	3 (4%)	1 (1%)	10	8
74	Ca	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
77	Ba	99/122 (81%)	96 (97%)	3 (3%)	0	100	100
78	AI	90/177 (51%)	86 (96%)	4 (4%)	0	100	100
All	All	10397/11933 (87%)	9827 (94%)	537 (5%)	33 (0%)	37	42

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AR	20	GLY
15	Ja	151	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	Ya	57	LYS
39	BG	218	ASP
44	Xa	56	ASP
69	Ra	48	GLN
45	BV	47	LEU
48	BW	80	LYS
59	Ta	14	LYS
66	Ya	79	ALA
13	AX	16	LYS
25	BI	41	SER
31	BQ	29	PHE
33	Da	63	VAL
61	BE	18	TYR
66	Ya	76	GLU
9	AU	89	ALA
15	Ja	150	PRO
15	Ja	223	GLY
18	Va	86	ASN
27	BT	228	ARG
53	AA	5	ILE
53	AA	201	LYS
60	AZ	29	LYS
73	AY	87	ARG
15	Ja	3	ARG
22	BS	337	LYS
63	AQ	21	VAL
41	Ha	15	VAL
71	La	89	VAL
39	BG	117	PRO
65	Ua	126	GLY
69	Ra	8	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BC	24/24 (100%)	24 (100%)	0	100	100
6	BM	131/148 (88%)	128 (98%)	3 (2%)	44	59
7	BO	116/133 (87%)	113 (97%)	3 (3%)	40	55
8	AR	44/71 (62%)	44 (100%)	0	100	100
9	AU	96/105 (91%)	95 (99%)	1 (1%)	68	81
10	Ma	87/110 (79%)	87 (100%)	0	100	100
11	Ia	171/175 (98%)	167 (98%)	4 (2%)	44	59
12	AE	111/112 (99%)	110 (99%)	1 (1%)	70	84
13	AX	84/94 (89%)	83 (99%)	1 (1%)	63	78
14	AP	116/117 (99%)	115 (99%)	1 (1%)	70	84
15	Ja	225/227 (99%)	215 (96%)	10 (4%)	25	34
16	Ea	179/180 (99%)	178 (99%)	1 (1%)	78	89
17	AL	161/198 (81%)	158 (98%)	3 (2%)	50	66
18	Va	111/114 (97%)	106 (96%)	5 (4%)	24	33
19	Ka	104/114 (91%)	103 (99%)	1 (1%)	68	81
20	AW	97/98 (99%)	94 (97%)	3 (3%)	35	48
21	BD	87/93 (94%)	87 (100%)	0	100	100
22	BS	326/329 (99%)	324 (99%)	2 (1%)	78	89
23	AM	137/138 (99%)	136 (99%)	1 (1%)	76	87
24	AC	183/225 (81%)	178 (97%)	5 (3%)	39	53
25	BI	104/110 (94%)	103 (99%)	1 (1%)	68	81
26	AH	112/117 (96%)	110 (98%)	2 (2%)	51	68
27	BT	323/331 (98%)	321 (99%)	2 (1%)	78	89
28	AV	114/121 (94%)	114 (100%)	0	100	100
29	AD	156/171 (91%)	152 (97%)	4 (3%)	40	55
30	AJ	157/158 (99%)	153 (98%)	4 (2%)	42	56
31	BQ	191/197 (97%)	189 (99%)	2 (1%)	68	81
32	BH	176/177 (99%)	170 (97%)	6 (3%)	32	44
33	Da	132/133 (99%)	129 (98%)	3 (2%)	44	59
34	BK	238/254 (94%)	233 (98%)	5 (2%)	47	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	AT	81/97 (84%)	80 (99%)	1 (1%)	63	78
36	Pa	40/49 (82%)	39 (98%)	1 (2%)	42	56
37	BP	108/110 (98%)	106 (98%)	2 (2%)	50	66
38	BN	108/136 (79%)	106 (98%)	2 (2%)	50	66
39	BG	200/219 (91%)	196 (98%)	4 (2%)	48	64
40	Fa	97/104 (93%)	95 (98%)	2 (2%)	47	63
41	Ha	120/121 (99%)	119 (99%)	1 (1%)	73	85
42	BU	147/158 (93%)	145 (99%)	2 (1%)	59	75
43	BR	199/212 (94%)	194 (98%)	5 (2%)	42	56
44	Xa	124/135 (92%)	121 (98%)	3 (2%)	43	58
45	BV	187/226 (83%)	183 (98%)	4 (2%)	47	63
46	BJ	170/179 (95%)	165 (97%)	5 (3%)	37	51
47	AO	58/137 (42%)	58 (100%)	0	100	100
48	BW	60/68 (88%)	56 (93%)	4 (7%)	15	17
49	AK	158/181 (87%)	155 (98%)	3 (2%)	50	66
50	Na	76/78 (97%)	74 (97%)	2 (3%)	40	55
51	AB	161/172 (94%)	159 (99%)	2 (1%)	63	78
52	BF	157/194 (81%)	155 (99%)	2 (1%)	61	76
53	AA	174/207 (84%)	172 (99%)	2 (1%)	65	79
54	AG	174/177 (98%)	172 (99%)	2 (1%)	65	79
55	Ga	47/114 (41%)	47 (100%)	0	100	100
56	BA	47/48 (98%)	47 (100%)	0	100	100
57	AF	117/123 (95%)	115 (98%)	2 (2%)	53	69
58	Wa	121/132 (92%)	118 (98%)	3 (2%)	42	56
59	Ta	193/213 (91%)	186 (96%)	7 (4%)	31	42
60	AZ	64/65 (98%)	62 (97%)	2 (3%)	35	48
61	BE	72/73 (99%)	71 (99%)	1 (1%)	59	75
62	Za	166/228 (73%)	160 (96%)	6 (4%)	31	42
63	AQ	116/122 (95%)	111 (96%)	5 (4%)	26	35
64	Oa	52/57 (91%)	48 (92%)	4 (8%)	12	13
65	Ua	100/121 (83%)	98 (98%)	2 (2%)	48	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	Ya	110/126 (87%)	107 (97%)	3 (3%)	39	53
67	BB	108/122 (88%)	106 (98%)	2 (2%)	50	66
68	AN	88/104 (85%)	88 (100%)	0	100	100
69	Ra	165/169 (98%)	156 (94%)	9 (6%)	19	24
70	BL	110/113 (97%)	109 (99%)	1 (1%)	70	84
71	La	61/92 (66%)	60 (98%)	1 (2%)	55	71
72	Aa	158/183 (86%)	155 (98%)	3 (2%)	50	66
73	AY	73/78 (94%)	71 (97%)	2 (3%)	39	53
74	Ca	47/48 (98%)	47 (100%)	0	100	100
77	Ba	93/110 (84%)	90 (97%)	3 (3%)	34	47
78	AI	87/139 (63%)	87 (100%)	0	100	100
All	All	9087/10114 (90%)	8908 (98%)	179 (2%)	48	64

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BM	24	VAL
6	BM	97	LYS
6	BM	104	GLU
7	BO	9	SER
7	BO	46	SER
7	BO	61	THR
9	AU	66	LYS
11	Ia	1	MET
11	Ia	107	SER
11	Ia	138	VAL
11	Ia	154	ILE
12	AE	2	VAL
13	AX	66	VAL
14	AP	57	ASP
15	Ja	3	ARG
15	Ja	80	LYS
15	Ja	91	SER
15	Ja	130	GLN
15	Ja	140	ASN
15	Ja	156	PRO
15	Ja	168	LYS
15	Ja	189	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	Ja	240	LYS
15	Ja	259	GLN
16	Ea	27	CYS
17	AL	47	LEU
17	AL	141	THR
17	AL	147	SER
18	Va	4	THR
18	Va	93	ILE
18	Va	104	PHE
18	Va	122	VAL
18	Va	124	VAL
19	Ka	60	PHE
20	AW	2	VAL
20	AW	64	LYS
20	AW	102	ARG
22	BS	288	LEU
22	BS	332	CYS
23	AM	96	VAL
24	AC	58	VAL
24	AC	119	LYS
24	AC	130	VAL
24	AC	138	THR
24	AC	189	CYS
25	BI	109	LYS
26	AH	42	ASP
26	AH	111	MET
27	BT	284	VAL
27	BT	297	ARG
29	AD	36	ASP
29	AD	49	VAL
29	AD	73	THR
29	AD	187	SER
30	AJ	57	VAL
30	AJ	72	THR
30	AJ	99	VAL
30	AJ	142	LYS
31	BQ	154	SER
31	BQ	208	GLU
32	BH	93	ILE
32	BH	170	GLN
32	BH	174	GLU
32	BH	178	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	BH	180	THR
32	BH	204	ILE
33	Da	6	SER
33	Da	31	GLN
33	Da	58	HIS
34	BK	28	THR
34	BK	77	SER
34	BK	81	HIS
34	BK	101	THR
34	BK	158	VAL
35	AT	36	SER
36	Pa	10	ARG
37	BP	16	ASP
37	BP	20	GLN
38	BN	52	VAL
38	BN	68	LYS
39	BG	116	LYS
39	BG	174	VAL
39	BG	217	ASN
39	BG	224	ARG
40	Fa	58	ARG
40	Fa	59	PRO
41	Ha	60	TYR
42	BU	46	THR
42	BU	140	VAL
43	BR	40	LYS
43	BR	100	ILE
43	BR	129	VAL
43	BR	164	GLN
43	BR	241	GLU
44	Xa	45	THR
44	Xa	68	ARG
44	Xa	119	LYS
45	BV	31	ASP
45	BV	78	ASP
45	BV	143	THR
45	BV	182	LYS
46	BJ	45	GLU
46	BJ	53	VAL
46	BJ	129	VAL
46	BJ	191	VAL
46	BJ	217	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	BW	58	VAL
48	BW	61	GLN
48	BW	63	ASP
48	BW	73	GLN
49	AK	61	SER
49	AK	105	LEU
49	AK	154	THR
50	Na	10	LEU
50	Na	56	VAL
51	AB	19	ARG
51	AB	50	THR
52	BF	101	ARG
52	BF	144	THR
53	AA	50	ILE
53	AA	92	ASN
54	AG	68	VAL
54	AG	70	THR
57	AF	24	CYS
57	AF	42	GLN
58	Wa	9	PHE
58	Wa	95	TYR
58	Wa	136	THR
59	Ta	10	THR
59	Ta	12	CYS
59	Ta	43	GLU
59	Ta	53	MET
59	Ta	59	GLN
59	Ta	116	VAL
59	Ta	184	VAL
60	AZ	18	LYS
60	AZ	42	LEU
61	BE	52	VAL
62	Za	28	HIS
62	Za	58	THR
62	Za	76	GLN
62	Za	126	LEU
62	Za	128	LEU
62	Za	181	LEU
63	AQ	4	VAL
63	AQ	19	PHE
63	AQ	21	VAL
63	AQ	36	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	AQ	39	ASN
64	Oa	26	VAL
64	Oa	28	VAL
64	Oa	55	GLU
64	Oa	62	ARG
65	Ua	53	VAL
65	Ua	137	ASP
66	Ya	98	VAL
66	Ya	117	ILE
66	Ya	132	LYS
67	BB	35	LEU
67	BB	105	MET
69	Ra	12	LYS
69	Ra	38	LYS
69	Ra	47	ASN
69	Ra	52	MET
69	Ra	63	ILE
69	Ra	87	LYS
69	Ra	127	LEU
69	Ra	130	VAL
69	Ra	181	ASP
70	BL	66	TYR
71	La	41	VAL
72	Aa	46	ARG
72	Aa	92	VAL
72	Aa	187	LEU
73	AY	33	ARG
73	AY	40	PRO
77	Ba	82	ARG
77	Ba	103	GLN
77	Ba	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
7	BO	18	HIS
14	AP	8	ASN
15	Ja	36	HIS
15	Ja	130	GLN
15	Ja	140	ASN
15	Ja	209	HIS
15	Ja	259	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Ea	153	ASN
17	AL	10	GLN
17	AL	59	GLN
17	AL	143	GLN
18	Va	96	ASN
20	AW	36	GLN
21	BD	23	HIS
22	BS	109	HIS
22	BS	149	GLN
22	BS	317	HIS
23	AM	54	HIS
24	AC	42	HIS
24	AC	161	GLN
27	BT	43	ASN
29	AD	137	GLN
31	BQ	21	HIS
32	BH	68	ASN
32	BH	73	HIS
32	BH	178	GLN
33	Da	105	ASN
34	BK	196	ASN
36	Pa	39	GLN
37	BP	20	GLN
39	BG	143	GLN
39	BG	149	HIS
40	Fa	19	GLN
41	Ha	94	ASN
42	BU	22	ASN
43	BR	65	ASN
43	BR	118	ASN
43	BR	162	ASN
43	BR	163	HIS
43	BR	224	ASN
45	BV	95	ASN
46	BJ	73	ASN
46	BJ	210	GLN
48	BW	33	GLN
50	Na	40	GLN
51	AB	3	ASN
51	AB	112	GLN
51	AB	125	HIS
53	AA	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	AG	147	GLN
57	AF	66	ASN
57	AF	76	HIS
58	Wa	19	ASN
58	Wa	66	ASN
59	Ta	65	GLN
59	Ta	148	ASN
62	Za	96	GLN
67	BB	15	GLN
68	AN	44	GLN
70	BL	109	GLN
72	Aa	20	GLN
74	Ca	5	ASN
77	Ba	21	HIS
77	Ba	103	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	75/76 (98%)	13 (17%)	1 (1%)
1	W2	75/76 (98%)	14 (18%)	1 (1%)
2	3	161/164 (98%)	24 (14%)	4 (2%)
3	A	3143/3385 (92%)	456 (14%)	59 (1%)
4	C3	118/121 (97%)	14 (11%)	2 (1%)
75	h1	1604/1805 (88%)	269 (16%)	0
76	B1	11/12 (91%)	1 (9%)	0
All	All	5187/5639 (91%)	791 (15%)	67 (1%)

All (791) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	G
1	2	9	A
1	2	17	U
1	2	18	G
1	2	20	G
1	2	21	A
1	2	22	G
1	2	47	U
1	2	48	C
1	2	72	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	73	A
1	2	74	C
1	2	76	A
2	3	38	U
2	3	39	C
2	3	53	G
2	3	63	A
2	3	66	C
2	3	67	U
2	3	84	A
2	3	85	U
2	3	86	C
2	3	88	C
2	3	89	G
2	3	90	U
2	3	91	G
2	3	99	G
2	3	100	A
2	3	109	A
2	3	110	C
2	3	124	C
2	3	129	C
2	3	131	U
2	3	132	C
2	3	134	G
2	3	157	U
2	3	160	C
3	A	5	C
3	A	12	U
3	A	14	A
3	A	38	A
3	A	41	A
3	A	42	PSU
3	A	47	A
3	A	57	G
3	A	58	A
3	A	64	A
3	A	72	A
3	A	84	G
3	A	90	G
3	A	97	A
3	A	107	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	108	G
3	A	114	C
3	A	115	U
3	A	120	A
3	A	121	A
3	A	129	U
3	A	131	U
3	A	133	C
3	A	134	G
3	A	141	G
3	A	148	A
3	A	154	G
3	A	155	A
3	A	161	G
3	A	163	C
3	A	167	A
3	A	168	G
3	A	173	G
3	A	179	G
3	A	187	U
3	A	197	A
3	A	207	G
3	A	215	G
3	A	216	A
3	A	221	C
3	A	245	A
3	A	248	A
3	A	259	U
3	A	262	A
3	A	266	G
3	A	283	U
3	A	292	A
3	A	326	G
3	A	335	A
3	A	346	A
3	A	347	C
3	A	349	A
3	A	350	G
3	A	373	G
3	A	395	G
3	A	396	A
3	A	398	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	399	G
3	A	401	U
3	A	417	G
3	A	418	G
3	A	419	A
3	A	430	G
3	A	434	G
3	A	436	C
3	A	437	G
3	A	449	U
3	A	467	A
3	A	523	U
3	A	524	A
3	A	532	G
3	A	538	G
3	A	539	A
3	A	540	U
3	A	541	A
3	A	543	G
3	A	545	U
3	A	546	U
3	A	547	G
3	A	548	U
3	A	549	G
3	A	552	G
3	A	554	C
3	A	555	G
3	A	561	G
3	A	574	U
3	A	575	C
3	A	581	C
3	A	590	A
3	A	591	A
3	A	592	C
3	A	602	C
3	A	603	G
3	A	606	A
3	A	607	U
3	A	608	C
3	A	609	A
3	A	610	G
3	A	618	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	621	G
3	A	631	G
3	A	632	U
3	A	637	U
3	A	638	C
3	A	648	C
3	A	661	A2M
3	A	672	A
3	A	673	G
3	A	689	A
3	A	693	A
3	A	694	A
3	A	695	C
3	A	702	G
3	A	710	G
3	A	711	U
3	A	712	A
3	A	719	A
3	A	726	C
3	A	729	A
3	A	730	U
3	A	732	G
3	A	746	C
3	A	747	G
3	A	769	G
3	A	774	U
3	A	776	U
3	A	780	A
3	A	790	G
3	A	794	G
3	A	795	A
3	A	826	A2M
3	A	839	G
3	A	846	A
3	A	858	C
3	A	870	C
3	A	871	C
3	A	883	U
3	A	888	U
3	A	916	G
3	A	917	OMG
3	A	918	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	923	A
3	A	925	G
3	A	926	A
3	A	930	A
3	A	932	C
3	A	934	A
3	A	946	G
3	A	953	C
3	A	968	C
3	A	969	PSU
3	A	983	G
3	A	986	C
3	A	989	A
3	A	990	C
3	A	991	G
3	A	992	C
3	A	993	G
3	A	1004	G
3	A	1005	G
3	A	1011	C
3	A	1012	C
3	A	1021	G
3	A	1027	U
3	A	1031	G
3	A	1035	G
3	A	1036	C
3	A	1039	C
3	A	1045	G
3	A	1046	A
3	A	1051	U
3	A	1057	A
3	A	1062	PSU
3	A	1074	A
3	A	1075	C
3	A	1085	G
3	A	1090	G
3	A	1091	U
3	A	1092	U
3	A	1104	C
3	A	1105	G
3	A	1106	G
3	A	1107	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1112	A
3	A	1126	G
3	A	1140	G
3	A	1162	A
3	A	1168	A
3	A	1183	G
3	A	1189	C
3	A	1190	U
3	A	1203	A
3	A	1210	A
3	A	1211	C
3	A	1212	A
3	A	1219	G
3	A	1237	C
3	A	1293	C
3	A	1295	G
3	A	1297	A
3	A	1313	A
3	A	1314	A
3	A	1315	U
3	A	1317	G
3	A	1319	U
3	A	1326	U
3	A	1327	A
3	A	1341	U
3	A	1358	A
3	A	1359	A
3	A	1360	G
3	A	1361	A
3	A	1362	G
3	A	1363	C
3	A	1364	C
3	A	1408	A
3	A	1428	G
3	A	1443	G
3	A	1446	OMC
3	A	1455	A
3	A	1460	C
3	A	1461	A
3	A	1484	A
3	A	1490	A
3	A	1492	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1511	G
3	A	1517	OMC
3	A	1536	C
3	A	1537	G
3	A	1542	U
3	A	1545	G
3	A	1564	U
3	A	1569	G
3	A	1575	A
3	A	1576	A
3	A	1581	A
3	A	1588	A
3	A	1589	A
3	A	1590	A
3	A	1594	G
3	A	1643	A
3	A	1645	G
3	A	1657	C
3	A	1725	G
3	A	1744	G
3	A	1751	A
3	A	1752	G
3	A	1765	C
3	A	1766	G
3	A	1768	G
3	A	1799	A
3	A	1816	G
3	A	1817	U
3	A	1818	G
3	A	1823	U
3	A	1844	A
3	A	1845	OMC
3	A	1848	OMC
3	A	1849	A
3	A	1868	C
3	A	1880	G
3	A	1881	A
3	A	1882	U
3	A	1908	G
3	A	2091	A
3	A	2092	A
3	A	2101	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2110	G
3	A	2111	OMU
3	A	2121	G
3	A	2130	A
3	A	2139	U
3	A	2157	A
3	A	2196	A
3	A	2208	G
3	A	2226	A
3	A	2230	A
3	A	2247	G
3	A	2254	A2M
3	A	2256	PSU
3	A	2271	G
3	A	2277	A
3	A	2278	A
3	A	2279	A2M
3	A	2305	G
3	A	2306	C
3	A	2308	U
3	A	2311	A
3	A	2313	G
3	A	2332	U
3	A	2333	G
3	A	2334	U
3	A	2370	A
3	A	2371	A
3	A	2372	C
3	A	2373	G
3	A	2390	C
3	A	2391	G
3	A	2395	A
3	A	2398	G
3	A	2399	A
3	A	2400	A
3	A	2401	G
3	A	2402	A
3	A	2409	U
3	A	2410	G
3	A	2433	G
3	A	2443	U
3	A	2446	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2450	G
3	A	2451	U
3	A	2452	G
3	A	2453	U
3	A	2454	A
3	A	2455	G
3	A	2457	A
3	A	2458	U
3	A	2459	A
3	A	2460	A
3	A	2461	G
3	A	2492	A
3	A	2495	U
3	A	2496	U
3	A	2497	U
3	A	2498	A
3	A	2499	A
3	A	2506	U
3	A	2512	U
3	A	2513	A
3	A	2520	G
3	A	2548	U
3	A	2549	U
3	A	2550	U
3	A	2552	G
3	A	2555	C
3	A	2573	G
3	A	2586	C
3	A	2590	G
3	A	2592	A
3	A	2605	G
3	A	2606	G
3	A	2613	G
3	A	2625	A
3	A	2635	A
3	A	2636	A
3	A	2643	C
3	A	2644	G
3	A	2651	U
3	A	2655	A
3	A	2656	A
3	A	2657	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2676	G
3	A	2679	A
3	A	2680	U
3	A	2688	G
3	A	2690	A
3	A	2703	A
3	A	2713	G
3	A	2718	U
3	A	2728	U
3	A	2752	G
3	A	2761	A
3	A	2772	C
3	A	2776	G
3	A	2777	G
3	A	2791	A
3	A	2795	G
3	A	2798	A
3	A	2799	G
3	A	2800	A
3	A	2801	A
3	A	2809	C
3	A	2816	A
3	A	2841	U
3	A	2844	A
3	A	2870	G
3	A	2874	U
3	A	2886	A
3	A	2898	C
3	A	2910	A2M
3	A	2922	PSU
3	A	2934	U
3	A	2935	A
3	A	2941	C
3	A	2946	G
3	A	2970	A
3	A	2971	G
3	A	2979	U
3	A	2989	G
3	A	3010	A
3	A	3026	G
3	A	3028	G
3	A	3055	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	3056	C
3	A	3057	G
3	A	3076	G
3	A	3090	C
3	A	3099	G
3	A	3111	A
3	A	3114	G
3	A	3123	U
3	A	3128	A
3	A	3129	U
3	A	3140	A
3	A	3150	G
3	A	3152	G
3	A	3166	U
3	A	3167	G
3	A	3168	C
3	A	3170	G
3	A	3172	C
3	A	3175	U
3	A	3179	U
3	A	3180	A
3	A	3181	G
3	A	3188	A
3	A	3189	G
3	A	3195	A
3	A	3202	C
3	A	3203	G
3	A	3205	G
3	A	3215	A
3	A	3218	U
3	A	3223	U
3	A	3224	U
3	A	3225	C
3	A	3226	G
3	A	3230	G
3	A	3231	A
3	A	3234	C
3	A	3235	G
3	A	3244	G
3	A	3248	C
3	A	3252	G
3	A	3262	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	3263	A
3	A	3281	G
3	A	3291	C
3	A	3294	A
3	A	3303	A
3	A	3304	U
3	A	3306	C
3	A	3322	A
3	A	3328	C
3	A	3332	G
3	A	3334	G
3	A	3339	U
3	A	3341	C
3	A	3343	G
3	A	3346	A
3	A	3356	G
3	A	3365	C
3	A	3369	U
3	A	3377	A
3	A	3379	G
3	A	3385	A
4	C3	7	G
4	C3	22	A
4	C3	27	A
4	C3	31	G
4	C3	38	U
4	C3	42	A
4	C3	53	U
4	C3	54	A
4	C3	64	G
4	C3	84	U
4	C3	85	G
4	C3	89	G
4	C3	110	G
4	C3	117	C
75	h1	5	U
75	h1	6	G
75	h1	17	C
75	h1	25	C
75	h1	26	A
75	h1	34	G
75	h1	42	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	47	A
75	h1	55	A
75	h1	56	U
75	h1	67	G
75	h1	68	A
75	h1	75	U
75	h1	82	G
75	h1	84	G
75	h1	105	A
75	h1	115	A
75	h1	123	OMU
75	h1	127	G
75	h1	128	G
75	h1	129	U
75	h1	130	A
75	h1	132	C
75	h1	133	U
75	h1	135	C
75	h1	136	U
75	h1	139	U
75	h1	140	C
75	h1	143	A
75	h1	150	U
75	h1	156	U
75	h1	158	C
75	h1	160	A
75	h1	174	C
75	h1	175	A
75	h1	186	A
75	h1	189	U
75	h1	190	A
75	h1	191	U
75	h1	192	G
75	h1	193	G
75	h1	194	A
75	h1	201	G
75	h1	214	A
75	h1	250	U
75	h1	251	C
75	h1	262	G
75	h1	266	G
75	h1	269	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	272	A
75	h1	273	U
75	h1	276	C
75	h1	289	G
75	h1	301	A
75	h1	316	C
75	h1	318	A
75	h1	324	G
75	h1	326	U
75	h1	335	A
75	h1	336	G
75	h1	338	G
75	h1	339	G
75	h1	340	C
75	h1	363	C
75	h1	372	A
75	h1	380	A
75	h1	382	U
75	h1	383	C
75	h1	384	C
75	h1	387	A
75	h1	388	G
75	h1	391	G
75	h1	392	G
75	h1	401	A
75	h1	402	A
75	h1	403	A
75	h1	404	C
75	h1	405	G
75	h1	413	C
75	h1	418	A
75	h1	419	A
75	h1	424	G
75	h1	426	C
75	h1	427	A
75	h1	428	G
75	h1	436	G
75	h1	441	U
75	h1	446	C
75	h1	460	G
75	h1	466	A2M
75	h1	470	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	479	A
75	h1	488	G
75	h1	503	U
75	h1	505	G
75	h1	509	U
75	h1	512	G
75	h1	521	C
75	h1	536	A
75	h1	540	A
75	h1	542	G
75	h1	544	U
75	h1	559	G
75	h1	560	U
75	h1	561	C
75	h1	563	G
75	h1	567	C
75	h1	578	G
75	h1	580	OMU
75	h1	581	A
75	h1	583	PSU
75	h1	584	U
75	h1	594	A
75	h1	596	A
75	h1	597	OMG
75	h1	608	A
75	h1	621	A2M
75	h1	622	A
75	h1	624	A
75	h1	625	A
75	h1	636	G
75	h1	641	U
75	h1	758	A
75	h1	759	A
75	h1	768	G
75	h1	769	C
75	h1	778	A2M
75	h1	783	A
75	h1	784	C
75	h1	785	G
75	h1	789	U
75	h1	792	A
75	h1	815	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	816	U
75	h1	817	A
75	h1	830	U
75	h1	831	A
75	h1	833	U
75	h1	854	G
75	h1	857	A
75	h1	861	U
75	h1	864	A
75	h1	865	C
75	h1	877	G
75	h1	878	G
75	h1	887	U
75	h1	934	A
75	h1	936	U
75	h1	946	U
75	h1	961	U
75	h1	966	U
75	h1	967	A
75	h1	977	G
75	h1	989	C
75	h1	1005	U
75	h1	1006	A
75	h1	1027	A
75	h1	1029	C
75	h1	1040	A
75	h1	1054	G
75	h1	1060	U
75	h1	1061	A
75	h1	1063	A
75	h1	1082	A
75	h1	1088	A
75	h1	1093	A
75	h1	1098	U
75	h1	1110	G
75	h1	1115	G
75	h1	1120	G
75	h1	1139	A
75	h1	1141	G
75	h1	1147	G
75	h1	1159	C
75	h1	1160	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	1168	G
75	h1	1173	G
75	h1	1186	U
75	h1	1192	C4J
75	h1	1193	C
75	h1	1195	A
75	h1	1197	A
75	h1	1200	G
75	h1	1201	G
75	h1	1203	A
75	h1	1214	G
75	h1	1218	A
75	h1	1219	G
75	h1	1232	OMU
75	h1	1239	A
75	h1	1244	G
75	h1	1245	A
75	h1	1246	G
75	h1	1247	C
75	h1	1252	U
75	h1	1257	A
75	h1	1259	U
75	h1	1266	G
75	h1	1270	OMU
75	h1	1289	G
75	h1	1315	U
75	h1	1316	U
75	h1	1322	A
75	h1	1342	G
75	h1	1348	U
75	h1	1362	C
75	h1	1363	A
75	h1	1364	U
75	h1	1373	G
75	h1	1375	C
75	h1	1391	A
75	h1	1393	U
75	h1	1394	A
75	h1	1401	U
75	h1	1402	U
75	h1	1416	U
75	h1	1417	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	1418	U
75	h1	1423	C
75	h1	1430	A
75	h1	1431	OMG
75	h1	1435	U
75	h1	1438	G
75	h1	1449	A
75	h1	1462	C
75	h1	1463	A
75	h1	1474	A
75	h1	1514	G
75	h1	1517	U
75	h1	1519	A
75	h1	1520	PSU
75	h1	1524	U
75	h1	1526	A
75	h1	1539	A
75	h1	1540	U
75	h1	1543	G
75	h1	1559	U
75	h1	1561	G
75	h1	1577	G7M
75	h1	1585	A
75	h1	1592	G
75	h1	1603	G
75	h1	1609	G
75	h1	1611	PSU
75	h1	1613	A
75	h1	1617	C
75	h1	1618	G
75	h1	1636	C
75	h1	1653	A
75	h1	1660	G
75	h1	1669	G
75	h1	1682	G
75	h1	1735	A
75	h1	1741	A
75	h1	1759	A
75	h1	1764	G
75	h1	1770	A
75	h1	1772	G
75	h1	1773	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	1785	MA6
75	h1	1786	MA6
75	h1	1787	C
75	h1	1796	G
75	h1	1797	G
75	h1	1798	A
75	h1	1799	U
75	h1	1800	C
75	h1	1803	U
75	h1	1804	G
76	B1	19	U
1	W2	3	G
1	W2	4	G
1	W2	5	G
1	W2	6	G
1	W2	8	U
1	W2	9	A
1	W2	17	U
1	W2	18	G
1	W2	21	A
1	W2	22	G
1	W2	48	C
1	W2	70	C
1	W2	71	G
1	W2	76	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	19	G
2	3	20	G
2	3	54	C
2	3	99	G
2	3	109	A
3	A	91	C
3	A	220	C
3	A	394	A
3	A	547	G
3	A	554	C
3	A	591	A
3	A	602	C
3	A	609	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	637	U
3	A	659	A
3	A	693	A
3	A	869	G
3	A	882	C
3	A	905	A
3	A	917	OMG
3	A	925	G
3	A	990	C
3	A	992	C
3	A	1004	G
3	A	1011	C
3	A	1026	A
3	A	1182	U
3	A	1218	U
3	A	1313	A
3	A	1377	G
3	A	1460	C
3	A	1476	A
3	A	1536	C
3	A	1606	A
3	A	1743	C
3	A	1843	A
3	A	1848	OMC
3	A	2143	A
3	A	2157	A
3	A	2304	C
3	A	2370	A
3	A	2372	C
3	A	2390	C
3	A	2398	G
3	A	2496	U
3	A	2585	G
3	A	2643	C
3	A	2655	A
3	A	2703	A
3	A	2713	G
3	A	2727	G
3	A	2871	A
3	A	3055	U
3	A	3097	C
3	A	3167	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	3171	A
3	A	3179	U
3	A	3193	C
3	A	3225	C
3	A	3230	G
3	A	3247	G
3	A	3255	U
3	A	3303	A
3	A	3320	G
4	C3	84	U
4	C3	109	U
1	W2	70	C

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

216 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	A	1681	3	18,21,22	0.93	1 (5%)	22,30,33	1.23	3 (13%)
3	OMU	A	44	82,3	19,22,23	0.64	0	26,31,34	0.80	0
75	PSU	h1	360	75	18,21,22	0.72	1 (5%)	22,30,33	0.87	0
75	4AC	h1	1281	75	21,24,25	0.48	0	29,34,37	0.67	0
75	UY1	h1	602	75	19,22,23	0.96	1 (5%)	22,31,34	0.82	0
3	PSU	A	34	3	18,21,22	1.04	2 (11%)	22,30,33	1.16	3 (13%)
3	PSU	A	2134	3	18,21,22	0.99	1 (5%)	22,30,33	1.10	1 (4%)
3	OMU	A	2716	3	19,22,23	0.47	0	26,31,34	0.81	1 (3%)
75	PSU	h1	1104	75	18,21,22	0.92	1 (5%)	22,30,33	0.99	1 (4%)
2	PSU	3	78	2	18,21,22	0.91	1 (5%)	22,30,33	0.71	0
75	PSU	h1	605	75	18,21,22	1.07	2 (11%)	22,30,33	1.13	3 (13%)
75	PSU	h1	1188	75	18,21,22	0.86	1 (5%)	22,30,33	0.84	1 (4%)
75	PSU	h1	256	75	18,21,22	0.96	1 (5%)	22,30,33	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	A	1376	3,81	22,25,26	0.30	0	31,36,39	0.73	0
75	A2M	h1	438	75	22,25,26	0.28	0	31,36,39	0.56	0
3	A2M	A	2218	3	22,25,26	0.21	0	31,36,39	0.57	0
75	A2M	h1	799	75	22,25,26	0.30	0	31,36,39	0.69	0
3	OMC	A	2835	3	19,22,23	0.31	0	26,31,34	0.68	1 (3%)
3	PSU	A	1054	3	18,21,22	0.78	1 (5%)	22,30,33	1.02	3 (13%)
3	OMG	A	2393	3,81	23,26,27	0.51	0	33,38,41	0.78	0
3	OMC	A	2958	3	19,22,23	0.58	0	26,31,34	0.71	1 (3%)
75	PSU	h1	121	75	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
3	PSU	A	2864	3	18,21,22	1.02	2 (11%)	22,30,33	0.85	0
3	1MG	A	1646	3	22,26,27	0.70	1 (4%)	33,39,42	0.63	0
3	OMU	A	2734	3,81	19,22,23	0.53	0	26,31,34	0.75	0
75	PSU	h1	752	75	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
3	UY1	A	2649	3	19,22,23	0.82	1 (5%)	22,31,34	0.98	0
75	PSU	h1	583	75	18,21,22	0.91	1 (5%)	22,30,33	0.75	0
3	OMC	A	1848	3,81	19,22,23	0.57	0	26,31,34	0.88	1 (3%)
3	A2M	A	2359	3	22,25,26	0.43	0	31,36,39	0.70	0
3	PSU	A	2743	3	18,21,22	0.92	1 (5%)	22,30,33	1.10	2 (9%)
3	A2M	A	2319	3	22,25,26	0.37	0	31,36,39	0.67	0
3	OMG	A	2814	3	23,26,27	0.52	0	33,38,41	0.56	0
75	A2M	h1	422	75	22,25,26	0.20	0	31,36,39	0.65	0
75	G7M	h1	1577	75,1	23,26,27	0.77	1 (4%)	35,39,42	0.59	1 (2%)
3	OMG	A	3290	3,81	23,26,27	0.48	0	33,38,41	0.79	2 (6%)
3	PSU	A	150	82,3	18,21,22	1.04	2 (11%)	22,30,33	0.64	0
3	A2M	A	1142	3	22,25,26	0.39	0	31,36,39	0.65	0
3	PSU	A	2825	82,3	18,21,22	1.04	1 (5%)	22,30,33	0.90	0
3	PSU	A	975	82,3	18,21,22	1.35	3 (16%)	22,30,33	1.03	1 (4%)
75	A2M	h1	543	75	22,25,26	0.21	0	31,36,39	0.63	0
75	PSU	h1	604	75	18,21,22	0.88	1 (5%)	22,30,33	0.87	1 (4%)
75	PSU	h1	1483	75	18,21,22	0.93	1 (5%)	22,30,33	0.54	0
3	PSU	A	1062	82,3	18,21,22	0.79	1 (5%)	22,30,33	1.01	1 (4%)
75	PSU	h1	304	75	18,21,22	1.10	1 (5%)	22,30,33	0.89	0
75	A2M	h1	162	75	22,25,26	0.19	0	31,36,39	0.52	0
3	OMG	A	2234	3	23,26,27	0.42	0	33,38,41	0.66	1 (3%)
3	PSU	A	965	3	18,21,22	0.91	1 (5%)	22,30,33	1.04	2 (9%)
3	PSU	A	894	3	18,21,22	1.22	2 (11%)	22,30,33	0.97	0
3	PSU	A	509	3	18,21,22	1.07	1 (5%)	22,30,33	0.99	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	1306	75	18,21,22	0.80	1 (5%)	22,30,33	0.75	0
75	PSU	h1	1563	75	18,21,22	0.87	1 (5%)	22,30,33	0.69	0
75	A2M	h1	1327	75	22,25,26	0.20	0	31,36,39	0.65	1 (3%)
75	PSU	h1	1182	75	18,21,22	0.98	1 (5%)	22,30,33	0.79	1 (4%)
75	PSU	h1	1520	75	18,21,22	0.94	1 (5%)	22,30,33	0.65	0
2	OMG	3	79	2	23,26,27	0.32	0	33,38,41	0.54	0
75	OMG	h1	1272	75,82	23,26,27	0.30	0	33,38,41	0.52	0
3	1MA	A	657	3,81	21,25,26	0.55	0	31,37,40	0.98	1 (3%)
75	A2M	h1	621	75,81	22,25,26	0.38	0	31,36,39	0.78	2 (6%)
3	PSU	A	828	3	18,21,22	1.18	2 (11%)	22,30,33	1.19	3 (13%)
75	PSU	h1	762	75	18,21,22	0.89	1 (5%)	22,30,33	0.76	0
3	PSU	A	2922	3	18,21,22	0.99	1 (5%)	22,30,33	1.03	1 (4%)
3	PSU	A	228	3	18,21,22	0.88	1 (5%)	22,30,33	0.69	0
75	PSU	h1	95	75	18,21,22	0.98	1 (5%)	22,30,33	0.95	1 (4%)
3	OMG	A	1853	3	23,26,27	0.55	0	33,38,41	0.97	2 (6%)
75	PSU	h1	308	75	18,21,22	1.06	1 (5%)	22,30,33	1.12	2 (9%)
75	OMG	h1	1431	75,81	23,26,27	0.34	0	33,38,41	0.56	0
3	OMC	A	2681	3	19,22,23	0.28	0	26,31,34	0.71	0
3	PSU	A	1132	3	18,21,22	0.85	1 (5%)	22,30,33	0.97	1 (4%)
75	MA6	h1	1786	75	23,26,27	0.32	0	34,38,41	0.77	1 (2%)
3	PSU	A	2252	3	18,21,22	0.84	1 (5%)	22,30,33	0.93	1 (4%)
22	HIC	BS	246	22	10,11,12	0.51	0	8,14,16	0.68	0
75	OMC	h1	1216	75	19,22,23	0.31	0	26,31,34	0.51	0
75	PSU	h1	948	75	18,21,22	0.91	1 (5%)	22,30,33	0.60	0
3	OMG	A	2921	3	23,26,27	0.37	0	33,38,41	0.69	1 (3%)
3	OMU	A	48	3	19,22,23	0.59	0	26,31,34	0.64	0
3	A2M	A	2254	3	22,25,26	0.22	0	31,36,39	0.49	0
75	PSU	h1	959	75,82	18,21,22	1.02	1 (5%)	22,30,33	0.82	0
3	PSU	A	3109	3	18,21,22	0.84	1 (5%)	22,30,33	0.81	1 (4%)
75	PSU	h1	1000	75	18,21,22	0.84	1 (5%)	22,30,33	0.72	0
75	PSU	h1	1215	75	18,21,22	0.94	1 (5%)	22,30,33	0.65	0
75	OMC	h1	471	75	19,22,23	0.32	0	26,31,34	0.60	0
75	A2M	h1	28	75,81	22,25,26	0.24	0	31,36,39	0.58	0
3	PSU	A	2430	3	18,21,22	0.82	1 (5%)	22,30,33	0.98	0
75	OMU	h1	123	75	19,22,23	0.27	0	26,31,34	0.79	2 (7%)
75	OMG	h1	390	75	23,26,27	0.32	0	33,38,41	0.62	1 (3%)
75	PSU	h1	1291	75	18,21,22	0.90	1 (5%)	22,30,33	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	A	1845	3	19,22,23	0.88	1 (5%)	26,31,34	0.89	1 (3%)
3	OMG	A	2286	3	23,26,27	0.34	0	33,38,41	0.42	0
3	OMG	A	2916	3	23,26,27	0.47	0	33,38,41	0.53	0
3	A2M	A	2639	3	22,25,26	0.38	0	31,36,39	0.62	0
3	PSU	A	1015	82,3	18,21,22	0.97	1 (5%)	22,30,33	0.82	0
3	OMC	A	2335	3	19,22,23	0.70	0	26,31,34	0.69	0
75	PSU	h1	1208	75	18,21,22	0.98	1 (5%)	22,30,33	0.71	0
3	A2M	A	826	82,3,81	22,25,26	0.45	0	31,36,39	0.89	1 (3%)
3	OMU	A	2408	82,3	19,22,23	0.43	0	26,31,34	0.76	0
3	OMG	A	2790	3	23,26,27	0.30	0	33,38,41	0.54	0
3	A2M	A	2324	3	22,25,26	0.37	0	31,36,39	0.74	1 (3%)
3	A2M	A	2945	3,81	22,25,26	0.39	0	31,36,39	0.82	1 (3%)
75	A2M	h1	1754	75	22,25,26	0.20	0	31,36,39	0.63	1 (3%)
3	A2M	A	2212	3,81	22,25,26	0.40	0	31,36,39	0.65	0
3	OMU	A	1066	3	19,22,23	0.37	0	26,31,34	0.83	1 (3%)
75	PSU	h1	337	75,82	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
3	PSU	A	2264	3	18,21,22	0.91	1 (5%)	22,30,33	0.61	0
3	PSU	A	42	82,3	18,21,22	1.21	3 (16%)	22,30,33	1.03	1 (4%)
3	PSU	A	2209	3	18,21,22	0.85	1 (5%)	22,30,33	0.70	0
3	OMU	A	2920	82,3	19,22,23	0.47	0	26,31,34	0.53	0
3	PSU	A	2974	3	18,21,22	0.92	0	22,30,33	1.05	0
3	OMC	A	2195	82,3	19,22,23	0.59	0	26,31,34	0.82	1 (3%)
3	PSU	A	1480	3	18,21,22	1.01	1 (5%)	22,30,33	0.75	1 (4%)
75	OMU	h1	1381	75	19,22,23	0.22	0	26,31,34	0.52	0
3	A2M	A	1458	3,81	22,25,26	0.63	0	31,36,39	0.84	0
3	A2M	A	885	3	22,25,26	0.55	0	31,36,39	0.82	1 (3%)
3	A2M	A	2910	3	22,25,26	0.40	0	31,36,39	0.75	1 (3%)
3	PSU	A	2256	3	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
3	PSU	A	901	82,3	18,21,22	1.07	2 (11%)	22,30,33	0.87	0
3	OMC	A	1446	3	19,22,23	0.52	0	26,31,34	0.97	1 (3%)
3	OMC	A	1478	3	19,22,23	0.44	0	26,31,34	0.49	0
3	PSU	A	277	3	18,21,22	1.38	4 (22%)	22,30,33	1.03	2 (9%)
75	PSU	h1	449	75,82	18,21,22	0.91	1 (5%)	22,30,33	0.93	1 (4%)
2	PSU	3	22	2,3	18,21,22	1.03	2 (11%)	22,30,33	0.93	1 (4%)
75	OMU	h1	1263	75	19,22,23	0.25	0	26,31,34	0.41	0
2	A2M	3	47	2	22,25,26	0.38	0	31,36,39	0.94	2 (6%)
75	OMG	h1	597	75	23,26,27	0.33	0	33,38,41	0.67	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	OMU	h1	1232	75	19,22,23	0.24	0	26,31,34	0.37	0
3	OMU	A	2419	3	19,22,23	0.57	0	26,31,34	0.97	1 (3%)
3	A2M	A	816	3	22,25,26	0.50	0	31,36,39	1.04	2 (6%)
3	OMC	A	2291	3	19,22,23	0.38	0	26,31,34	0.82	1 (3%)
75	A2M	h1	778	75	22,25,26	0.20	0	31,36,39	0.48	0
75	OMC	h1	38	75	19,22,23	0.28	0	26,31,34	0.58	1 (3%)
3	PSU	A	2943	82,3,81	18,21,22	0.97	1 (5%)	22,30,33	1.13	2 (9%)
75	OMU	h1	1270	75,81	19,22,23	0.25	0	26,31,34	0.75	1 (3%)
75	OMU	h1	580	75	19,22,23	0.18	0	26,31,34	0.43	0
75	PSU	h1	1302	75	18,21,22	0.82	1 (5%)	22,30,33	0.83	0
3	PSU	A	1131	3	18,21,22	1.01	1 (5%)	22,30,33	0.93	1 (4%)
3	OMU	A	2882	3	19,22,23	0.40	0	26,31,34	0.55	0
75	PSU	h1	1118	75	18,21,22	0.93	1 (5%)	22,30,33	0.86	0
3	OMU	A	3299	3	19,22,23	0.49	0	26,31,34	0.75	1 (3%)
3	PSU	A	2258	3	18,21,22	0.82	1 (5%)	22,30,33	0.84	0
3	5MC	A	2276	3,81	18,22,23	0.46	0	26,32,35	0.90	1 (3%)
3	PSU	A	685	3	18,21,22	1.22	2 (11%)	22,30,33	1.05	4 (18%)
3	PSU	A	2414	3,81	18,21,22	1.03	2 (11%)	22,30,33	1.03	2 (9%)
3	OMG	A	2618	3,1	23,26,27	0.30	0	33,38,41	0.57	0
3	OMC	A	1517	3,81	19,22,23	0.59	0	26,31,34	0.96	1 (3%)
3	OMG	A	2792	3	23,26,27	0.41	0	33,38,41	0.60	0
3	OMC	A	2947	3	19,22,23	0.47	0	26,31,34	0.68	1 (3%)
3	UR3	A	2952	82,3	19,22,23	0.63	0	26,32,35	0.80	0
75	OMG	h1	244	75	23,26,27	0.32	0	33,38,41	0.42	0
3	PSU	A	311	82,3	18,21,22	1.12	1 (5%)	22,30,33	1.21	3 (13%)
3	PSU	A	2853	3	18,21,22	0.80	1 (5%)	22,30,33	0.96	1 (4%)
75	6MZ	h1	1767	75,82,81	22,25,26	0.52	0	30,36,39	0.73	0
75	PSU	h1	1531	75	18,21,22	0.93	1 (5%)	22,30,33	0.58	0
75	PSU	h1	761	75	18,21,22	0.91	1 (5%)	22,30,33	0.81	0
75	A2M	h1	1575	75	22,25,26	0.25	0	31,36,39	0.55	0
3	OMC	A	1858	3	19,22,23	0.79	0	26,31,34	1.07	2 (7%)
3	PSU	A	2132	82,3	18,21,22	1.03	1 (5%)	22,30,33	1.05	2 (9%)
3	OMU	A	803	3	19,22,23	0.36	0	26,31,34	0.85	0
75	PSU	h1	606	75	18,21,22	1.06	1 (5%)	22,30,33	0.77	0
75	PSU	h1	1176	75	18,21,22	0.83	1 (5%)	22,30,33	0.76	0
3	PSU	A	785	3	18,21,22	1.10	2 (11%)	22,30,33	1.06	2 (9%)
3	OMG	A	2389	3	23,26,27	0.44	0	33,38,41	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	A2M	h1	466	75	22,25,26	0.20	0	31,36,39	0.60	1 (3%)
55	MLY	Ga	113	55	9,10,11	0.49	0	6,11,13	0.45	0
75	PSU	h1	415	75	18,21,22	0.89	1 (5%)	22,30,33	0.68	0
3	OMG	A	814	3	23,26,27	0.46	0	33,38,41	0.56	1 (3%)
3	PSU	A	1133	3	18,21,22	0.91	1 (5%)	22,30,33	1.10	2 (9%)
75	OMU	h1	1010	75	19,22,23	0.26	0	26,31,34	0.64	0
3	OMC	A	675	3	19,22,23	0.53	0	26,31,34	0.61	0
3	PSU	A	2312	82,3	18,21,22	0.88	1 (5%)	22,30,33	0.93	1 (4%)
3	PSU	A	2316	3,81	18,21,22	0.93	1 (5%)	22,30,33	0.72	0
75	A2M	h1	794	75	22,25,26	0.18	0	31,36,39	0.67	1 (3%)
3	A2M	A	2933	3	22,25,26	0.40	0	31,36,39	0.94	1 (3%)
75	PSU	h1	1025	75	18,21,22	0.91	1 (5%)	22,30,33	1.09	1 (4%)
75	PSU	h1	808	75	18,21,22	0.99	1 (5%)	22,30,33	0.76	0
75	PSU	h1	1630	75	18,21,22	0.89	1 (5%)	22,30,33	0.99	0
3	PSU	A	1472	3	18,21,22	0.84	1 (5%)	22,30,33	0.81	0
3	A2M	A	945	3	22,25,26	0.43	0	31,36,39	1.38	3 (9%)
75	OMU	h1	1445	75	19,22,23	0.25	0	26,31,34	0.42	0
75	PSU	h1	634	75	18,21,22	0.95	2 (11%)	22,30,33	1.25	2 (9%)
3	PSU	A	2262	3	18,21,22	0.80	1 (5%)	22,30,33	0.82	0
3	OMU	A	2345	3	19,22,23	0.40	0	26,31,34	0.49	0
3	PSU	A	2879	3	18,21,22	0.73	0	22,30,33	1.05	0
75	PSU	h1	103	75,82	18,21,22	0.92	1 (5%)	22,30,33	0.97	1 (4%)
3	A2M	A	2124	3	22,25,26	0.41	0	31,36,39	0.87	2 (6%)
3	PSU	A	2189	82,3	18,21,22	0.69	1 (5%)	22,30,33	1.08	2 (9%)
75	OMC	h1	416	75	19,22,23	0.24	0	26,31,34	0.53	0
3	OMG	A	2122	3	23,26,27	0.49	0	33,38,41	0.69	0
3	OMG	A	2407	82,3	23,26,27	0.47	0	33,38,41	0.75	1 (3%)
3	OMU	A	676	3	19,22,23	0.50	0	26,31,34	0.84	0
3	OMC	A	2878	3	19,22,23	0.46	0	26,31,34	0.51	0
3	PSU	A	2954	3	18,21,22	0.81	1 (5%)	22,30,33	0.82	1 (4%)
75	OMU	h1	1261	75	19,22,23	0.23	0	26,31,34	0.42	0
3	OMC	A	2363	3	19,22,23	0.49	0	26,31,34	0.62	0
3	5MC	A	2869	82,3	18,22,23	0.54	0	26,32,35	1.21	2 (7%)
3	PSU	A	2893	3	18,21,22	0.92	1 (5%)	22,30,33	0.76	0
3	PSU	A	1001	3	18,21,22	0.99	1 (5%)	22,30,33	0.87	1 (4%)
3	A2M	A	2279	3	22,25,26	0.46	0	31,36,39	1.04	1 (3%)
75	4AC	h1	1777	75	21,24,25	0.55	0	29,34,37	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	1783	75	18,21,22	0.95	2 (11%)	22,30,33	0.86	1 (4%)
75	MA6	h1	1785	75	23,26,27	0.28	0	34,38,41	0.73	1 (2%)
75	C4J	h1	1192	75	24,29,30	0.92	1 (4%)	29,42,45	1.13	1 (3%)
2	PSU	3	97	2,82	18,21,22	0.90	1 (5%)	22,30,33	0.82	0
3	OMU	A	144	82,3	19,22,23	0.42	0	26,31,34	0.73	0
75	PSU	h1	1611	75	18,21,22	0.89	1 (5%)	22,30,33	0.91	1 (4%)
75	OMU	h1	613	75	19,22,23	0.30	0	26,31,34	0.50	0
75	PSU	h1	468	75	18,21,22	0.85	1 (5%)	22,30,33	0.72	0
75	A2M	h1	975	75	22,25,26	0.26	0	31,36,39	0.71	1 (3%)
75	OMC	h1	1641	75,81	19,22,23	0.40	0	26,31,34	0.83	1 (3%)
3	A2M	A	661	3	22,25,26	0.53	0	31,36,39	0.74	0
3	PSU	A	969	3	18,21,22	0.84	1 (5%)	22,30,33	1.19	3 (13%)
3	OMU	A	1890	3	19,22,23	0.63	0	26,31,34	1.27	2 (7%)
3	OMG	A	917	82,3	23,26,27	0.36	0	33,38,41	0.53	0
3	OMG	A	1459	3,81	23,26,27	0.50	0	33,38,41	0.75	1 (3%)
3	OMU	A	2111	3	19,22,23	0.24	0	26,31,34	0.56	0
2	OMG	3	155	2,3	23,26,27	0.44	0	33,38,41	0.41	0
3	OMG	A	2650	3	23,26,27	0.43	0	33,38,41	1.03	1 (3%)

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	A	1681	3	-	0/7/25/26	0/2/2/2
3	OMU	A	44	82,3	-	0/9/27/28	0/2/2/2
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
75	UY1	h1	602	75	-	0/9/27/28	0/2/2/2
3	PSU	A	34	3	-	1/7/25/26	0/2/2/2
3	PSU	A	2134	3	-	0/7/25/26	0/2/2/2
3	OMU	A	2716	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
2	PSU	3	78	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1188	75	-	1/7/25/26	0/2/2/2
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
3	A2M	A	1376	3,81	-	0/9/27/28	0/3/3/3
75	A2M	h1	438	75	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	A	2218	3	-	0/9/27/28	0/3/3/3
75	A2M	h1	799	75	-	1/9/27/28	0/3/3/3
3	OMC	A	2835	3	-	0/9/27/28	0/2/2/2
3	PSU	A	1054	3	-	0/7/25/26	0/2/2/2
3	OMG	A	2393	3,81	-	0/9/27/28	0/3/3/3
3	OMC	A	2958	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	121	75	-	0/7/25/26	0/2/2/2
3	PSU	A	2864	3	-	0/7/25/26	0/2/2/2
3	1MG	A	1646	3	-	0/7/25/26	0/3/3/3
3	OMU	A	2734	3,81	-	0/9/27/28	0/2/2/2
75	PSU	h1	752	75	-	2/7/25/26	0/2/2/2
3	UY1	A	2649	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	583	75	-	3/7/25/26	0/2/2/2
3	OMC	A	1848	3,81	-	0/9/27/28	0/2/2/2
3	A2M	A	2359	3	-	0/9/27/28	0/3/3/3
3	PSU	A	2743	3	-	0/7/25/26	0/2/2/2
3	A2M	A	2319	3	-	0/9/27/28	0/3/3/3
3	OMG	A	2814	3	-	0/9/27/28	0/3/3/3
75	A2M	h1	422	75	-	2/9/27/28	0/3/3/3
75	G7M	h1	1577	75,1	-	0/7/25/26	0/3/3/3
3	OMG	A	3290	3,81	-	0/9/27/28	0/3/3/3
3	PSU	A	150	82,3	-	0/7/25/26	0/2/2/2
3	A2M	A	1142	3	-	0/9/27/28	0/3/3/3
3	PSU	A	2825	82,3	-	0/7/25/26	0/2/2/2
3	PSU	A	975	82,3	-	0/7/25/26	0/2/2/2
75	A2M	h1	543	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1483	75	-	0/7/25/26	0/2/2/2
3	PSU	A	1062	82,3	-	2/7/25/26	0/2/2/2
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	162	75	-	1/9/27/28	0/3/3/3
3	OMG	A	2234	3	-	0/9/27/28	0/3/3/3
3	PSU	A	965	3	-	0/7/25/26	0/2/2/2
3	PSU	A	894	3	-	0/7/25/26	0/2/2/2
3	PSU	A	509	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	1306	75	-	3/7/25/26	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	1327	75	-	1/9/27/28	0/3/3/3
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1520	75	-	5/7/25/26	0/2/2/2
2	OMG	3	79	2	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	OMG	h1	1272	75,82	-	0/9/27/28	0/3/3/3
3	1MA	A	657	3,81	-	1/7/25/26	0/3/3/3
75	A2M	h1	621	75,81	-	2/9/27/28	0/3/3/3
3	PSU	A	828	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2
3	PSU	A	2922	3	-	1/7/25/26	0/2/2/2
3	PSU	A	228	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	95	75	-	0/7/25/26	0/2/2/2
3	OMG	A	1853	3	-	0/9/27/28	0/3/3/3
75	PSU	h1	308	75	-	0/7/25/26	0/2/2/2
75	OMG	h1	1431	75,81	-	1/9/27/28	0/3/3/3
3	OMC	A	2681	3	-	0/9/27/28	0/2/2/2
3	PSU	A	1132	3	-	0/7/25/26	0/2/2/2
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
3	PSU	A	2252	3	-	0/7/25/26	0/2/2/2
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
75	OMC	h1	1216	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
3	OMG	A	2921	3	-	1/9/27/28	0/3/3/3
3	OMU	A	48	3	-	0/9/27/28	0/2/2/2
3	A2M	A	2254	3	-	0/9/27/28	0/3/3/3
75	PSU	h1	959	75,82	-	0/7/25/26	0/2/2/2
3	PSU	A	3109	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2
75	OMC	h1	471	75	-	0/9/27/28	0/2/2/2
75	A2M	h1	28	75,81	-	0/9/27/28	0/3/3/3
3	PSU	A	2430	3	-	0/7/25/26	0/2/2/2
75	OMU	h1	123	75	-	2/9/27/28	0/2/2/2
75	OMG	h1	390	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
3	OMC	A	1845	3	-	0/9/27/28	0/2/2/2
3	OMG	A	2286	3	-	0/9/27/28	0/3/3/3
3	OMG	A	2916	3	-	1/9/27/28	0/3/3/3
3	A2M	A	2639	3	-	0/9/27/28	0/3/3/3
3	PSU	A	1015	82,3	-	0/7/25/26	0/2/2/2
3	OMC	A	2335	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	1208	75	-	0/7/25/26	0/2/2/2
3	A2M	A	826	82,3,81	-	2/9/27/28	0/3/3/3
3	OMU	A	2408	82,3	-	0/9/27/28	0/2/2/2
3	OMG	A	2790	3	-	0/9/27/28	0/3/3/3
3	A2M	A	2324	3	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	A	2945	3,81	-	0/9/27/28	0/3/3/3
75	A2M	h1	1754	75	-	1/9/27/28	0/3/3/3
3	A2M	A	2212	3,81	-	0/9/27/28	0/3/3/3
3	OMU	A	1066	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	337	75,82	-	0/7/25/26	0/2/2/2
3	PSU	A	2264	3	-	0/7/25/26	0/2/2/2
3	PSU	A	42	82,3	-	0/7/25/26	0/2/2/2
3	PSU	A	2209	3	-	0/7/25/26	0/2/2/2
3	OMU	A	2920	82,3	-	0/9/27/28	0/2/2/2
3	PSU	A	2974	3	-	0/7/25/26	0/2/2/2
3	OMC	A	2195	82,3	-	4/9/27/28	0/2/2/2
3	PSU	A	1480	3	-	0/7/25/26	0/2/2/2
75	OMU	h1	1381	75	-	0/9/27/28	0/2/2/2
3	A2M	A	1458	3,81	-	0/9/27/28	0/3/3/3
3	A2M	A	885	3	-	0/9/27/28	0/3/3/3
3	A2M	A	2910	3	-	5/9/27/28	0/3/3/3
3	PSU	A	2256	3	-	2/7/25/26	0/2/2/2
3	PSU	A	901	82,3	-	0/7/25/26	0/2/2/2
3	OMC	A	1446	3	-	1/9/27/28	0/2/2/2
3	OMC	A	1478	3	-	1/9/27/28	0/2/2/2
3	PSU	A	277	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	449	75,82	-	0/7/25/26	0/2/2/2
2	PSU	3	22	2,3	-	0/7/25/26	0/2/2/2
75	OMU	h1	1263	75	-	0/9/27/28	0/2/2/2
2	A2M	3	47	2	-	0/9/27/28	0/3/3/3
75	OMG	h1	597	75	-	3/9/27/28	0/3/3/3
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
3	OMU	A	2419	3	-	0/9/27/28	0/2/2/2
3	A2M	A	816	3	-	0/9/27/28	0/3/3/3
3	OMC	A	2291	3	-	0/9/27/28	0/2/2/2
75	A2M	h1	778	75	-	2/9/27/28	0/3/3/3
75	OMC	h1	38	75	-	0/9/27/28	0/2/2/2
3	PSU	A	2943	82,3,81	-	0/7/25/26	0/2/2/2
75	OMU	h1	1270	75,81	-	2/9/27/28	0/2/2/2
75	OMU	h1	580	75	-	5/9/27/28	0/2/2/2
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
3	PSU	A	1131	3	-	0/7/25/26	0/2/2/2
3	OMU	A	2882	3	-	1/9/27/28	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
3	OMU	A	3299	3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	A	2258	3	-	0/7/25/26	0/2/2/2
3	5MC	A	2276	3,81	-	0/7/25/26	0/2/2/2
3	PSU	A	685	3	-	0/7/25/26	0/2/2/2
3	PSU	A	2414	3,81	-	0/7/25/26	0/2/2/2
3	OMG	A	2618	3,1	-	0/9/27/28	0/3/3/3
3	OMC	A	1517	3,81	-	3/9/27/28	0/2/2/2
3	OMG	A	2792	3	-	0/9/27/28	0/3/3/3
3	OMC	A	2947	3	-	0/9/27/28	0/2/2/2
3	UR3	A	2952	82,3	-	0/7/25/26	0/2/2/2
75	OMG	h1	244	75	-	0/9/27/28	0/3/3/3
3	PSU	A	311	82,3	-	0/7/25/26	0/2/2/2
3	PSU	A	2853	3	-	0/7/25/26	0/2/2/2
75	6MZ	h1	1767	75,82,81	-	0/9/27/28	0/3/3/3
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
3	OMC	A	1858	3	-	0/9/27/28	0/2/2/2
3	PSU	A	2132	82,3	-	0/7/25/26	0/2/2/2
3	OMU	A	803	3	-	0/9/27/28	0/2/2/2
75	PSU	h1	606	75	-	1/7/25/26	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
3	PSU	A	785	3	-	1/7/25/26	0/2/2/2
3	OMG	A	2389	3	-	0/9/27/28	0/3/3/3
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
55	MLY	Ga	113	55	-	0/8/9/11	-
75	PSU	h1	415	75	-	1/7/25/26	0/2/2/2
3	OMG	A	814	3	-	0/9/27/28	0/3/3/3
3	PSU	A	1133	3	-	0/7/25/26	0/2/2/2
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
3	OMC	A	675	3	-	0/9/27/28	0/2/2/2
3	PSU	A	2312	82,3	-	1/7/25/26	0/2/2/2
3	PSU	A	2316	3,81	-	0/7/25/26	0/2/2/2
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3
3	A2M	A	2933	3	-	0/9/27/28	0/3/3/3
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	808	75	-	1/7/25/26	0/2/2/2
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
3	PSU	A	1472	3	-	0/7/25/26	0/2/2/2
3	A2M	A	945	3	-	0/9/27/28	0/3/3/3
75	OMU	h1	1445	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
3	PSU	A	2262	3	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	A	2345	3	-	0/9/27/28	0/2/2/2
3	PSU	A	2879	3	-	0/7/25/26	0/2/2/2
75	PSU	h1	103	75,82	-	2/7/25/26	0/2/2/2
3	A2M	A	2124	3	-	1/9/27/28	0/3/3/3
3	PSU	A	2189	82,3	-	0/7/25/26	0/2/2/2
75	OMC	h1	416	75	-	0/9/27/28	0/2/2/2
3	OMG	A	2122	3	-	0/9/27/28	0/3/3/3
3	OMG	A	2407	82,3	-	0/9/27/28	0/3/3/3
3	OMU	A	676	3	-	0/9/27/28	0/2/2/2
3	OMC	A	2878	3	-	0/9/27/28	0/2/2/2
3	PSU	A	2954	3	-	0/7/25/26	0/2/2/2
75	OMU	h1	1261	75	-	0/9/27/28	0/2/2/2
3	OMC	A	2363	3	-	0/9/27/28	0/2/2/2
3	5MC	A	2869	82,3	-	4/7/25/26	0/2/2/2
3	PSU	A	2893	3	-	0/7/25/26	0/2/2/2
3	PSU	A	1001	3	-	0/7/25/26	0/2/2/2
3	A2M	A	2279	3	-	1/9/27/28	0/3/3/3
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
75	PSU	h1	1783	75	-	1/7/25/26	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
75	C4J	h1	1192	75	-	3/16/34/35	0/2/2/2
2	PSU	3	97	2,82	-	0/7/25/26	0/2/2/2
3	OMU	A	144	82,3	-	2/9/27/28	0/2/2/2
75	PSU	h1	1611	75	-	2/7/25/26	0/2/2/2
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	468	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
75	OMC	h1	1641	75,81	-	1/9/27/28	0/2/2/2
3	A2M	A	661	3	-	1/9/27/28	0/3/3/3
3	PSU	A	969	3	-	1/7/25/26	0/2/2/2
3	OMU	A	1890	3	-	0/9/27/28	0/2/2/2
3	OMG	A	917	82,3	-	1/9/27/28	0/3/3/3
3	OMG	A	1459	3,81	-	0/9/27/28	0/3/3/3
3	OMU	A	2111	3	-	2/9/27/28	0/2/2/2
2	OMG	3	155	2,3	-	0/9/27/28	0/3/3/3
3	OMG	A	2650	3	-	1/9/27/28	0/3/3/3

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	304	PSU	C6-C5	4.05	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	1182	PSU	C6-C5	3.87	1.39	1.35
75	h1	959	PSU	C6-C5	3.80	1.39	1.35
75	h1	256	PSU	C6-C5	3.79	1.39	1.35
75	h1	606	PSU	C6-C5	3.76	1.39	1.35
3	A	2825	PSU	C6-C5	3.75	1.39	1.35
75	h1	1215	PSU	C6-C5	3.73	1.39	1.35
75	h1	1531	PSU	C6-C5	3.70	1.39	1.35
75	h1	308	PSU	C6-C5	3.70	1.39	1.35
75	h1	95	PSU	C6-C5	3.69	1.39	1.35
75	h1	1520	PSU	C6-C5	3.63	1.39	1.35
3	A	2922	PSU	C6-C5	3.62	1.39	1.35
75	h1	1208	PSU	C6-C5	3.62	1.39	1.35
75	h1	1483	PSU	C6-C5	3.60	1.39	1.35
3	A	785	PSU	C6-C5	3.59	1.39	1.35
3	A	1015	PSU	C6-C5	3.51	1.39	1.35
75	h1	583	PSU	C6-C5	3.48	1.39	1.35
75	h1	1563	PSU	C6-C5	3.48	1.39	1.35
75	h1	121	PSU	C6-C5	3.48	1.39	1.35
3	A	901	PSU	C6-C5	3.47	1.39	1.35
3	A	277	PSU	C4-C5	-3.47	1.34	1.44
3	A	311	PSU	C6-C5	3.44	1.39	1.35
75	h1	415	PSU	C6-C5	3.44	1.39	1.35
75	h1	449	PSU	C6-C5	3.43	1.39	1.35
75	h1	808	PSU	C6-C5	3.42	1.39	1.35
3	A	1001	PSU	C6-C5	3.39	1.39	1.35
75	h1	762	PSU	C6-C5	3.35	1.39	1.35
75	h1	948	PSU	C6-C5	3.35	1.39	1.35
75	h1	605	PSU	C6-C5	3.33	1.39	1.35
75	h1	752	PSU	C6-C5	3.33	1.39	1.35
3	A	509	PSU	C6-C5	3.32	1.39	1.35
75	h1	468	PSU	C6-C5	3.29	1.39	1.35
75	h1	1176	PSU	C6-C5	3.29	1.39	1.35
3	A	2264	PSU	C6-C5	3.28	1.39	1.35
3	A	1480	PSU	C6-C5	3.28	1.39	1.35
75	h1	1188	PSU	C6-C5	3.27	1.39	1.35
3	A	2256	PSU	C6-C5	3.27	1.39	1.35
3	A	2316	PSU	C6-C5	3.27	1.39	1.35
75	h1	1291	PSU	C6-C5	3.26	1.39	1.35
75	h1	1611	PSU	C6-C5	3.26	1.39	1.35
75	h1	1000	PSU	C6-C5	3.25	1.39	1.35
3	A	685	PSU	C6-C5	3.25	1.39	1.35
3	A	975	PSU	C6-C5	3.25	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	1192	C4J	C6-C5	3.23	1.39	1.34
75	h1	602	UY1	C6-C5	3.21	1.39	1.35
2	3	78	PSU	C6-C5	3.20	1.39	1.35
3	A	42	PSU	C6-C5	3.20	1.39	1.35
3	A	277	PSU	C6-C5	3.17	1.39	1.35
3	A	2864	PSU	C6-C5	3.16	1.39	1.35
3	A	228	PSU	C6-C5	3.14	1.39	1.35
3	A	1681	PSU	C6-C5	3.12	1.39	1.35
75	h1	337	PSU	C6-C5	3.10	1.38	1.35
75	h1	1118	PSU	C6-C5	3.08	1.38	1.35
3	A	2209	PSU	C6-C5	3.07	1.38	1.35
3	A	34	PSU	C6-C5	3.05	1.38	1.35
2	3	97	PSU	C6-C5	3.02	1.38	1.35
3	A	1131	PSU	C6-C5	3.01	1.38	1.35
75	h1	761	PSU	C6-C5	2.98	1.38	1.35
75	h1	1783	PSU	C6-C5	2.97	1.38	1.35
75	h1	1630	PSU	C6-C5	2.97	1.38	1.35
3	A	2262	PSU	C6-C5	2.96	1.38	1.35
3	A	1472	PSU	C6-C5	2.96	1.38	1.35
3	A	2134	PSU	C6-C5	2.95	1.38	1.35
3	A	150	PSU	C6-C5	2.94	1.38	1.35
3	A	1062	PSU	C6-C5	2.93	1.38	1.35
75	h1	103	PSU	C6-C5	2.92	1.38	1.35
3	A	2258	PSU	C6-C5	2.88	1.38	1.35
3	A	828	PSU	C6-C5	2.87	1.38	1.35
75	h1	604	PSU	C6-C5	2.86	1.38	1.35
3	A	2312	PSU	C6-C5	2.85	1.38	1.35
3	A	894	PSU	C4-C5	-2.83	1.36	1.44
3	A	894	PSU	C6-C5	2.83	1.38	1.35
2	3	22	PSU	C6-C5	2.81	1.38	1.35
3	A	2252	PSU	C6-C5	2.80	1.38	1.35
3	A	685	PSU	C4-C5	-2.77	1.36	1.44
3	A	2893	PSU	C6-C5	2.77	1.38	1.35
3	A	2132	PSU	C6-C5	2.76	1.38	1.35
75	h1	1025	PSU	C6-C5	2.76	1.38	1.35
3	A	2853	PSU	C6-C5	2.75	1.38	1.35
3	A	1132	PSU	C6-C5	2.74	1.38	1.35
75	h1	1104	PSU	C6-C5	2.68	1.38	1.35
3	A	2430	PSU	C6-C5	2.66	1.38	1.35
75	h1	605	PSU	C4-C5	-2.65	1.36	1.44
75	h1	1306	PSU	C6-C5	2.65	1.38	1.35
75	h1	1577	G7M	C8-N7	2.64	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1054	PSU	C6-C5	2.62	1.38	1.35
3	A	3109	PSU	C6-C5	2.62	1.38	1.35
75	h1	1302	PSU	C6-C5	2.59	1.38	1.35
75	h1	634	PSU	C6-C5	2.57	1.38	1.35
3	A	2649	UY1	C6-C5	2.52	1.38	1.35
3	A	2743	PSU	C6-C5	2.49	1.38	1.35
3	A	965	PSU	C6-C5	2.49	1.38	1.35
3	A	150	PSU	C4-C5	-2.48	1.37	1.44
3	A	2954	PSU	C6-C5	2.44	1.38	1.35
75	h1	360	PSU	C6-C5	2.42	1.38	1.35
3	A	42	PSU	O4-C4	-2.41	1.19	1.23
3	A	1646	1MG	C5-C6	-2.41	1.39	1.45
3	A	1133	PSU	C6-C5	2.38	1.38	1.35
3	A	2414	PSU	C6-C5	2.35	1.38	1.35
3	A	975	PSU	C4-C5	-2.33	1.37	1.44
3	A	975	PSU	C4-N3	-2.24	1.34	1.38
3	A	2943	PSU	C6-C5	2.23	1.37	1.35
3	A	969	PSU	C6-C5	2.22	1.37	1.35
3	A	277	PSU	C4-N3	-2.22	1.34	1.38
3	A	1845	OMC	O5'-C5'	-2.22	1.39	1.44
3	A	2189	PSU	C6-C5	2.22	1.37	1.35
75	h1	1783	PSU	C4-C5	-2.21	1.37	1.44
75	h1	634	PSU	C4-C5	-2.21	1.37	1.44
3	A	785	PSU	C4-C5	-2.18	1.37	1.44
2	3	22	PSU	C4-C5	-2.18	1.38	1.44
3	A	42	PSU	C4-C5	-2.17	1.38	1.44
3	A	2864	PSU	O5'-C5'	-2.13	1.39	1.44
3	A	277	PSU	O4-C4	-2.06	1.19	1.23
3	A	901	PSU	C4-C5	-2.04	1.38	1.44
3	A	828	PSU	O4-C4	2.02	1.27	1.23
3	A	34	PSU	C4-C5	-2.01	1.38	1.44
3	A	2414	PSU	C4-C5	-2.00	1.38	1.44

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	945	A2M	O2'-C2'-C1'	-5.81	97.75	109.08
3	A	2650	OMG	O2'-C2'-C1'	-4.42	100.45	109.08
75	h1	634	PSU	C6-C5-C4	4.03	121.02	118.20
3	A	1890	OMU	O2'-C2'-C1'	3.53	115.96	109.08
75	h1	1192	C4J	O4'-C1'-C2'	-3.40	100.35	105.14
3	A	1858	OMC	O3'-C3'-C2'	-3.32	101.75	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1025	PSU	C3'-C2'-C1'	3.30	105.48	101.64
3	A	2291	OMC	C2'-C1'-N1	-3.16	108.08	114.22
3	A	2716	OMU	O2'-C2'-C1'	3.16	115.25	109.08
3	A	828	PSU	C6-C5-C4	3.14	120.39	118.20
3	A	2910	A2M	O3'-C3'-C4'	-3.12	102.03	111.05
3	A	1681	PSU	C6-C5-C4	3.11	120.37	118.20
3	A	1517	OMC	O2'-C2'-C1'	3.07	115.06	109.08
75	h1	975	A2M	O2'-C2'-C1'	3.00	114.92	109.08
75	h1	1327	A2M	O2'-C2'-C1'	2.98	114.88	109.08
3	A	1848	OMC	O2'-C2'-C1'	-2.95	103.33	109.08
3	A	2922	PSU	C6-C5-C4	2.92	120.24	118.20
75	h1	1785	MA6	C2-N1-C6	2.90	118.61	111.75
3	A	2869	5MC	C1'-N1-C6	2.90	125.95	121.12
75	h1	605	PSU	C6-C5-C4	2.90	120.22	118.20
3	A	2134	PSU	C5-C6-N1	-2.89	117.78	122.11
3	A	1133	PSU	C6-C5-C4	2.88	120.21	118.20
3	A	1890	OMU	C2'-C1'-N1	-2.88	108.64	114.22
75	h1	1786	MA6	C2-N1-C6	2.88	118.55	111.75
3	A	2279	A2M	O4'-C1'-N9	2.84	113.66	108.06
75	h1	597	OMG	O2'-C2'-C1'	2.84	114.62	109.08
75	h1	794	A2M	O2'-C2'-C1'	2.79	114.52	109.08
3	A	2252	PSU	C2'-C3'-C4'	-2.72	97.36	102.64
3	A	2853	PSU	C2'-C3'-C4'	-2.71	97.38	102.64
75	h1	1641	OMC	O2'-C2'-C1'	2.70	114.36	109.08
3	A	2933	A2M	O2'-C2'-C1'	2.70	114.35	109.08
3	A	2869	5MC	C5-C6-N1	-2.69	120.57	123.34
3	A	1858	OMC	C2'-C1'-N1	-2.69	109.01	114.22
3	A	1446	OMC	O2'-C2'-C1'	-2.68	103.86	109.08
3	A	2407	OMG	O2'-C2'-C1'	-2.67	103.88	109.08
3	A	1131	PSU	C2'-C3'-C4'	-2.60	97.60	102.64
3	A	2419	OMU	O2'-C2'-C1'	-2.56	104.09	109.08
75	h1	1270	OMU	C2'-C1'-N1	2.54	119.15	114.22
3	A	2132	PSU	C4-N3-C2	-2.54	122.68	126.34
3	A	945	A2M	C2'-C1'-N9	2.52	117.78	113.53
3	A	1133	PSU	C2'-C3'-C4'	-2.51	97.76	102.64
75	h1	621	A2M	O2'-C2'-C1'	2.51	113.97	109.08
3	A	969	PSU	C6-C5-C4	2.48	119.93	118.20
3	A	2943	PSU	C5-C6-N1	-2.48	118.39	122.11
3	A	2276	5MC	C5-C6-N1	-2.48	120.79	123.34
75	h1	1104	PSU	C2'-C3'-C4'	-2.48	97.83	102.64
3	A	2921	OMG	C2'-C1'-N9	-2.46	109.44	114.22
75	h1	634	PSU	C5-C6-N1	-2.46	118.42	122.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	605	PSU	C5-C6-N1	-2.44	118.44	122.11
3	A	1132	PSU	C2'-C3'-C4'	-2.44	97.90	102.64
3	A	311	PSU	O2'-C2'-C3'	2.43	119.67	111.82
3	A	1681	PSU	C5-C6-N1	-2.43	118.47	122.11
75	h1	1754	A2M	O2'-C2'-C1'	2.41	113.78	109.08
3	A	969	PSU	C3'-C2'-C1'	2.41	104.44	101.64
75	h1	1783	PSU	C6-C5-C4	2.40	119.88	118.20
3	A	3290	OMG	C3'-C2'-C1'	-2.40	98.37	102.89
3	A	2189	PSU	C4-N3-C2	-2.37	122.92	126.34
3	A	311	PSU	C2'-C3'-C4'	-2.37	98.04	102.64
3	A	945	A2M	O3'-C3'-C4'	-2.37	104.21	111.05
3	A	685	PSU	C6-C5-C4	2.35	119.84	118.20
75	h1	103	PSU	C2'-C3'-C4'	-2.34	98.10	102.64
3	A	2124	A2M	O2'-C2'-C1'	-2.34	104.52	109.08
3	A	2743	PSU	C4-N3-C2	-2.34	122.97	126.34
3	A	311	PSU	O2'-C2'-C1'	-2.33	105.67	111.23
2	3	47	A2M	O3'-C3'-C2'	2.33	117.79	111.17
3	A	814	OMG	C2'-C1'-N9	-2.33	109.71	114.22
3	A	2234	OMG	C2'-C1'-N9	-2.32	109.72	114.22
3	A	828	PSU	C5-C6-N1	-2.31	118.64	122.11
3	A	2324	A2M	O2'-C2'-C1'	2.30	113.57	109.08
3	A	885	A2M	O3'-C3'-C2'	-2.30	104.63	111.17
3	A	1459	OMG	O3'-C3'-C2'	2.30	117.70	111.17
3	A	685	PSU	C5-C6-N1	-2.30	118.66	122.11
3	A	785	PSU	C3'-C2'-C1'	2.27	104.28	101.64
3	A	3109	PSU	C2'-C3'-C4'	-2.27	98.24	102.64
3	A	816	A2M	C1'-N9-C8	-2.25	122.05	127.14
75	h1	38	OMC	O2'-C2'-C1'	2.24	113.45	109.08
3	A	2414	PSU	O2'-C2'-C3'	2.24	119.07	111.82
3	A	3290	OMG	O4'-C1'-N9	2.24	113.48	108.36
3	A	277	PSU	C5-C6-N1	-2.23	118.77	122.11
3	A	2743	PSU	C5-C6-N1	-2.22	118.78	122.11
2	3	47	A2M	C2'-C1'-N9	-2.22	109.80	113.53
3	A	42	PSU	C2'-C3'-C4'	-2.21	98.35	102.64
75	h1	95	PSU	C5-C6-N1	-2.21	118.79	122.11
3	A	826	A2M	O4'-C1'-N9	-2.21	103.70	108.06
3	A	816	A2M	C2'-C1'-N9	-2.20	109.83	113.53
75	h1	466	A2M	O2'-C2'-C1'	2.19	113.36	109.08
75	h1	390	OMG	C2'-C1'-N9	-2.19	109.97	114.22
3	A	785	PSU	O2'-C2'-C1'	2.19	116.46	111.23
3	A	2124	A2M	O3'-C3'-C2'	2.19	117.39	111.17
75	h1	1182	PSU	C2'-C3'-C4'	-2.19	98.39	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	1611	PSU	C2'-C3'-C4'	-2.18	98.40	102.64
3	A	2414	PSU	O2'-C2'-C1'	-2.18	106.03	111.23
3	A	2958	OMC	O4'-C4'-C3'	-2.18	100.80	105.11
3	A	1062	PSU	C2'-C3'-C4'	-2.18	98.40	102.64
3	A	1054	PSU	C5-C6-N1	-2.18	118.84	122.11
2	3	22	PSU	C6-C5-C4	2.17	119.72	118.20
75	h1	604	PSU	C2'-C3'-C4'	-2.16	98.44	102.64
3	A	34	PSU	C4-N3-C2	-2.15	123.24	126.34
3	A	2943	PSU	C4-N3-C2	-2.14	123.25	126.34
3	A	1480	PSU	C2'-C3'-C4'	-2.14	98.49	102.64
75	h1	123	OMU	O4'-C4'-C3'	-2.14	100.89	105.11
3	A	2954	PSU	C2'-C3'-C4'	-2.14	98.49	102.64
3	A	2189	PSU	C5-C6-N1	-2.12	118.92	122.11
3	A	828	PSU	C4-N3-C2	-2.12	123.28	126.34
3	A	509	PSU	O3'-C3'-C4'	-2.12	104.93	111.05
3	A	1845	OMC	O3'-C3'-C2'	2.11	117.17	111.17
3	A	1001	PSU	C5-C6-N1	-2.11	118.94	122.11
75	h1	449	PSU	C3'-C2'-C1'	2.11	104.10	101.64
3	A	2947	OMC	O3'-C3'-C2'	2.11	117.15	111.17
75	h1	256	PSU	C2'-C3'-C4'	-2.10	98.57	102.64
3	A	975	PSU	C5-C6-N1	-2.09	118.98	122.11
3	A	2945	A2M	C2'-C1'-N9	-2.09	110.02	113.53
3	A	34	PSU	C3'-C2'-C1'	-2.09	99.21	101.64
3	A	3299	OMU	O3'-C3'-C4'	-2.08	105.04	111.05
75	h1	1188	PSU	C2'-C3'-C4'	-2.07	98.61	102.64
3	A	965	PSU	C4-N3-C2	-2.07	123.35	126.34
3	A	2195	OMC	C3'-C2'-C1'	-2.06	99.01	102.89
3	A	1066	OMU	C2'-C1'-N1	-2.06	110.22	114.22
3	A	965	PSU	C2'-C3'-C4'	-2.06	98.64	102.64
3	A	1853	OMG	C1'-N9-C4	2.06	132.61	126.50
75	h1	605	PSU	C4-N3-C2	-2.06	123.38	126.34
3	A	2132	PSU	N1-C2-N3	2.06	117.46	115.13
75	h1	1577	G7M	N9-C8-N7	-2.05	107.15	112.21
3	A	657	1MA	O4'-C1'-N9	-2.04	103.69	108.36
75	h1	308	PSU	C5-C6-N1	-2.04	119.04	122.11
3	A	1054	PSU	C2'-C3'-C4'	-2.04	98.68	102.64
75	h1	621	A2M	O4'-C1'-N9	-2.03	104.06	108.06
3	A	969	PSU	C5-C6-N1	-2.03	119.06	122.11
3	A	1054	PSU	C4-N3-C2	-2.03	123.42	126.34
3	A	277	PSU	C4-N3-C2	-2.03	123.42	126.34
3	A	1853	OMG	C1'-N9-C8	-2.02	120.93	126.70
3	A	34	PSU	C6-C5-C4	2.02	119.61	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	PSU	C2'-C3'-C4'	-2.02	98.72	102.64
3	A	685	PSU	C4-N3-C2	-2.02	123.43	126.34
75	h1	308	PSU	O2'-C2'-C3'	2.01	118.33	111.82
3	A	1681	PSU	O2'-C2'-C3'	2.01	118.31	111.82
3	A	685	PSU	C2'-C3'-C4'	-2.01	98.75	102.64
75	h1	123	OMU	O3'-C3'-C2'	2.00	116.86	111.17
3	A	2312	PSU	C6-C5-C4	2.00	119.60	118.20
3	A	2835	OMC	O3'-C3'-C4'	-2.00	105.26	111.05

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	785	PSU	C2'-C1'-C5-C4
3	A	1062	PSU	O4'-C4'-C5'-O5'
3	A	1517	OMC	C1'-C2'-O2'-CM2
3	A	2111	OMU	C3'-C4'-C5'-O5'
3	A	2111	OMU	O4'-C4'-C5'-O5'
3	A	2195	OMC	C2'-C1'-N1-C2
3	A	2195	OMC	C2'-C1'-N1-C6
3	A	2882	OMU	C1'-C2'-O2'-CM2
3	A	2910	A2M	O4'-C4'-C5'-O5'
75	h1	123	OMU	C3'-C4'-C5'-O5'
75	h1	123	OMU	O4'-C4'-C5'-O5'
75	h1	162	A2M	C1'-C2'-O2'-CM'
75	h1	580	OMU	O4'-C4'-C5'-O5'
75	h1	597	OMG	O4'-C4'-C5'-O5'
75	h1	597	OMG	C3'-C4'-C5'-O5'
75	h1	621	A2M	C1'-C2'-O2'-CM'
75	h1	778	A2M	O4'-C4'-C5'-O5'
75	h1	778	A2M	C3'-C4'-C5'-O5'
75	h1	794	A2M	C1'-C2'-O2'-CM'
75	h1	1232	OMU	C3'-C4'-C5'-O5'
75	h1	1232	OMU	O4'-C4'-C5'-O5'
75	h1	1306	PSU	C2'-C1'-C5-C4
75	h1	1327	A2M	C1'-C2'-O2'-CM'
75	h1	1520	PSU	C2'-C1'-C5-C4
75	h1	1520	PSU	O4'-C1'-C5-C4
75	h1	1520	PSU	C2'-C1'-C5-C6
75	h1	1641	OMC	C1'-C2'-O2'-CM2
75	h1	1754	A2M	C1'-C2'-O2'-CM'
3	A	1062	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2256	PSU	O4'-C4'-C5'-O5'
75	h1	466	A2M	O4'-C4'-C5'-O5'
75	h1	1192	C4J	C3'-C4'-C5'-O5'
75	h1	1192	C4J	O4'-C4'-C5'-O5'
75	h1	1270	OMU	O4'-C4'-C5'-O5'
3	A	1517	OMC	C3'-C4'-C5'-O5'
3	A	2256	PSU	C3'-C4'-C5'-O5'
3	A	2910	A2M	C3'-C4'-C5'-O5'
75	h1	466	A2M	C3'-C4'-C5'-O5'
75	h1	583	PSU	C3'-C4'-C5'-O5'
75	h1	583	PSU	O4'-C4'-C5'-O5'
75	h1	1270	OMU	C3'-C4'-C5'-O5'
75	h1	1611	PSU	O4'-C4'-C5'-O5'
3	A	2650	OMG	C3'-C2'-O2'-CM2
75	h1	1192	C4J	C4'-C5'-O5'-P
3	A	1517	OMC	O4'-C4'-C5'-O5'
75	h1	103	PSU	O4'-C4'-C5'-O5'
3	A	144	OMU	C3'-C2'-O2'-CM2
75	h1	422	A2M	O4'-C4'-C5'-O5'
3	A	2922	PSU	C4'-C5'-O5'-P
3	A	2869	5MC	C2'-C1'-N1-C6
75	h1	1611	PSU	C3'-C4'-C5'-O5'
3	A	2312	PSU	C4'-C5'-O5'-P
3	A	2910	A2M	C2'-C1'-N9-C8
3	A	2921	OMG	C3'-C2'-O2'-CM2
3	A	2195	OMC	O4'-C1'-N1-C6
75	h1	580	OMU	C2'-C1'-N1-C6
3	A	2195	OMC	O4'-C1'-N1-C2
3	A	34	PSU	O4'-C4'-C5'-O5'
75	h1	1188	PSU	O4'-C4'-C5'-O5'
3	A	2869	5MC	O4'-C1'-N1-C6
75	h1	580	OMU	O4'-C1'-N1-C6
3	A	917	OMG	C3'-C2'-O2'-CM2
3	A	661	A2M	C4'-C5'-O5'-P
75	h1	597	OMG	C4'-C5'-O5'-P
75	h1	1786	MA6	C4'-C5'-O5'-P
3	A	144	OMU	O4'-C4'-C5'-O5'
75	h1	621	A2M	O4'-C4'-C5'-O5'
3	A	2910	A2M	C2'-C1'-N9-C4
75	h1	1431	OMG	C4'-C5'-O5'-P
3	A	2869	5MC	O4'-C1'-N1-C2
3	A	969	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	h1	415	PSU	O4'-C1'-C5-C4
75	h1	752	PSU	O4'-C1'-C5-C4
75	h1	808	PSU	O4'-C1'-C5-C4
75	h1	1306	PSU	O4'-C1'-C5-C4
3	A	2124	A2M	C3'-C2'-O2'-CM'
3	A	2869	5MC	C2'-C1'-N1-C2
3	A	657	1MA	C2'-C1'-N9-C8
75	h1	580	OMU	O4'-C1'-N1-C2
3	A	826	A2M	C4'-C5'-O5'-P
75	h1	422	A2M	C3'-C4'-C5'-O5'
75	h1	799	A2M	O4'-C4'-C5'-O5'
75	h1	1783	PSU	O4'-C4'-C5'-O5'
3	A	1446	OMC	O4'-C4'-C5'-O5'
75	h1	1520	PSU	O4'-C4'-C5'-O5'
75	h1	583	PSU	O4'-C1'-C5-C6
75	h1	752	PSU	O4'-C1'-C5-C6
75	h1	1306	PSU	O4'-C1'-C5-C6
75	h1	1520	PSU	O4'-C1'-C5-C6
3	A	826	A2M	O4'-C4'-C5'-O5'
3	A	2279	A2M	O4'-C4'-C5'-O5'
75	h1	103	PSU	C3'-C4'-C5'-O5'
75	h1	580	OMU	C2'-C1'-N1-C2
3	A	2916	OMG	C3'-C2'-O2'-CM2
75	h1	606	PSU	O4'-C4'-C5'-O5'
3	A	1478	OMC	O4'-C1'-N1-C6
3	A	2910	A2M	O4'-C1'-N9-C8

There are no ring outliers.

48 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	h1	602	UY1	1	0
3	A	34	PSU	1	0
3	A	1376	A2M	2	0
75	h1	438	A2M	1	0
75	h1	799	A2M	1	0
75	h1	121	PSU	1	0
3	A	2359	A2M	1	0
3	A	2814	OMG	1	0
75	h1	604	PSU	1	0
3	A	2234	OMG	1	0
75	h1	1327	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	828	PSU	1	0
75	h1	95	PSU	2	0
75	h1	390	OMG	6	0
75	h1	1208	PSU	1	0
3	A	826	A2M	1	0
3	A	2790	OMG	1	0
75	h1	1754	A2M	1	0
3	A	2212	A2M	1	0
75	h1	337	PSU	1	0
3	A	1446	OMC	1	0
3	A	1478	OMC	1	0
75	h1	449	PSU	1	0
75	h1	778	A2M	4	0
75	h1	1302	PSU	1	0
75	h1	1118	PSU	2	0
3	A	2618	OMG	1	0
3	A	1517	OMC	2	0
75	h1	244	OMG	1	0
75	h1	1767	6MZ	1	0
75	h1	1531	PSU	1	0
3	A	803	OMU	1	0
3	A	785	PSU	1	0
3	A	2389	OMG	1	0
75	h1	466	A2M	2	0
3	A	675	OMC	1	0
3	A	2312	PSU	1	0
75	h1	794	A2M	1	0
3	A	2933	A2M	1	0
3	A	2879	PSU	1	0
75	h1	1777	4AC	1	0
75	h1	1785	MA6	2	0
75	h1	1192	C4J	1	0
3	A	144	OMU	2	0
75	h1	468	PSU	1	0
75	h1	975	A2M	1	0
75	h1	1641	OMC	2	0
2	3	155	OMG	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 511 ligands modelled in this entry, 482 are monoatomic - leaving 29 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	$\# Z > 2$
80	TER	A	3408	-	13,13,13	0.28	0	12,12,12	0.45	0
80	TER	A	3409	-	13,13,13	0.22	0	12,12,12	0.33	0
80	TER	A	3405	-	13,13,13	0.24	0	12,12,12	0.28	0
80	TER	A	3407	-	13,13,13	0.33	0	12,12,12	0.56	0
80	TER	A	3417	-	13,13,13	0.18	0	12,12,12	0.34	0
80	TER	A	3419	-	13,13,13	0.18	0	12,12,12	0.27	0
80	TER	A	3413	-	13,13,13	0.19	0	12,12,12	0.44	0
84	EPE	A	3402	-	15,15,15	0.81	1 (6%)	18,20,20	0.78	0
80	TER	h1	1904	-	13,13,13	0.20	0	12,12,12	0.37	0
80	TER	A	3406	-	13,13,13	0.26	0	12,12,12	0.55	0
80	TER	A	3415	-	13,13,13	0.19	0	12,12,12	0.35	0
80	TER	A	3412	-	13,13,13	0.16	0	12,12,12	0.36	0
80	TER	A	3421	-	13,13,13	0.21	0	12,12,12	0.31	0
80	TER	A	3404	-	13,13,13	0.24	0	12,12,12	0.30	0
80	TER	A	3410	-	13,13,13	0.20	0	12,12,12	0.23	0
80	TER	A	3411	-	13,13,13	0.21	0	12,12,12	0.22	0
80	TER	A	3403	-	13,13,13	0.30	0	12,12,12	0.69	1 (8%)
80	TER	h1	1906	-	13,13,13	0.19	0	12,12,12	0.24	0
80	TER	A	3420	-	13,13,13	0.50	0	12,12,12	0.65	0
83	SPD	A	3401	-	9,9,9	0.37	0	8,8,8	0.81	0
80	TER	A	3418	-	13,13,13	0.21	0	12,12,12	0.24	0
80	TER	3	202	-	13,13,13	0.21	0	12,12,12	0.32	0
80	TER	h1	1903	-	13,13,13	0.17	0	12,12,12	0.20	0
80	TER	h1	1905	-	13,13,13	0.21	0	12,12,12	0.22	0
80	TER	h1	1901	-	13,13,13	0.27	0	12,12,12	0.47	0
80	TER	A	3414	-	13,13,13	0.28	0	12,12,12	0.25	0
80	TER	A	3416	-	13,13,13	0.14	0	12,12,12	0.21	0
80	TER	h1	1902	-	13,13,13	0.16	0	12,12,12	0.26	0
80	TER	3	201	-	13,13,13	0.32	0	12,12,12	0.37	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
80	TER	A	3408	-	-	6/11/11/11	-
80	TER	A	3409	-	-	5/11/11/11	-
80	TER	A	3405	-	-	6/11/11/11	-
80	TER	A	3407	-	-	5/11/11/11	-
80	TER	A	3417	-	-	7/11/11/11	-
80	TER	A	3419	-	-	3/11/11/11	-
80	TER	A	3413	-	-	3/11/11/11	-
84	EPE	A	3402	-	-	3/9/19/19	0/1/1/1
80	TER	h1	1904	-	-	7/11/11/11	-
80	TER	A	3406	-	-	5/11/11/11	-
80	TER	A	3415	-	-	6/11/11/11	-
80	TER	A	3412	-	-	4/11/11/11	-
80	TER	A	3421	-	-	7/11/11/11	-
80	TER	A	3404	-	-	3/11/11/11	-
80	TER	A	3410	-	-	6/11/11/11	-
80	TER	A	3411	-	-	6/11/11/11	-
80	TER	A	3403	-	-	1/11/11/11	-
80	TER	h1	1906	-	-	7/11/11/11	-
80	TER	A	3420	-	-	3/11/11/11	-
83	SPD	A	3401	-	-	2/7/7/7	-
80	TER	A	3418	-	-	7/11/11/11	-
80	TER	3	202	-	-	7/11/11/11	-
80	TER	h1	1903	-	-	5/11/11/11	-
80	TER	h1	1905	-	-	6/11/11/11	-
80	TER	h1	1901	-	-	6/11/11/11	-
80	TER	A	3414	-	-	4/11/11/11	-
80	TER	A	3416	-	-	5/11/11/11	-
80	TER	h1	1902	-	-	9/11/11/11	-
80	TER	3	201	-	-	4/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	A	3402	EPE	O3S-S	2.45	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A	3403	TER	C10-N9-C8	-2.09	103.58	113.45

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	A	3408	TER	C3-C4-N5-C6
80	A	3419	TER	N1-C2-C3-C4
80	h1	1903	TER	C6-C7-C8-N9
80	h1	1904	TER	N1-C2-C3-C4
80	h1	1904	TER	C7-C8-N9-C10
84	A	3402	EPE	C10-C9-N1-C6
84	A	3402	EPE	C8-C7-N4-C5
80	h1	1902	TER	C10-C11-C12-C13
80	A	3408	TER	C6-C7-C8-N9
80	A	3415	TER	C6-C7-C8-N9
80	3	202	TER	N9-C10-C11-C12
80	h1	1901	TER	N9-C10-C11-C12
80	A	3409	TER	N9-C10-C11-C12
80	3	201	TER	N5-C6-C7-C8
80	A	3407	TER	C2-C3-C4-N5
80	A	3414	TER	C2-C3-C4-N5
80	A	3414	TER	N5-C6-C7-C8
80	h1	1906	TER	N9-C10-C11-C12
80	A	3416	TER	N9-C10-C11-C12
80	3	202	TER	C2-C3-C4-N5
80	h1	1905	TER	N5-C6-C7-C8
80	A	3406	TER	N9-C10-C11-C12
80	h1	1902	TER	N9-C10-C11-C12
80	A	3418	TER	N9-C10-C11-C12
80	A	3405	TER	N5-C6-C7-C8
80	A	3406	TER	N5-C6-C7-C8
80	A	3409	TER	N5-C6-C7-C8
80	A	3420	TER	C2-C3-C4-N5
80	h1	1902	TER	N5-C6-C7-C8
80	h1	1905	TER	C6-C7-C8-N9
80	A	3409	TER	C7-C8-N9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
80	A	3421	TER	C7-C6-N5-C4
80	A	3421	TER	N9-C10-C11-C12
80	A	3405	TER	C6-C7-C8-N9
80	A	3411	TER	C2-C3-C4-N5
80	A	3417	TER	C2-C3-C4-N5
80	h1	1901	TER	C2-C3-C4-N5
83	A	3401	SPD	N6-C7-C8-C9
80	h1	1903	TER	N9-C10-C11-C12
80	A	3412	TER	N5-C6-C7-C8
80	A	3415	TER	C2-C3-C4-N5
80	A	3421	TER	N5-C6-C7-C8
80	A	3417	TER	N9-C10-C11-C12
80	A	3407	TER	C7-C8-N9-C10
80	A	3411	TER	C7-C6-N5-C4
80	A	3418	TER	C3-C4-N5-C6
80	h1	1901	TER	C11-C10-N9-C8
80	h1	1902	TER	C11-C10-N9-C8
80	A	3412	TER	C2-C3-C4-N5
80	A	3411	TER	C6-C7-C8-N9
80	A	3417	TER	N5-C6-C7-C8
80	h1	1901	TER	C6-C7-C8-N9
80	h1	1905	TER	C2-C3-C4-N5
80	h1	1902	TER	C3-C4-N5-C6
80	A	3410	TER	C11-C12-C13-N14
80	A	3408	TER	C10-C11-C12-C13
80	A	3408	TER	C7-C8-N9-C10
80	A	3410	TER	C7-C6-N5-C4
80	A	3417	TER	C7-C6-N5-C4
80	A	3417	TER	C11-C10-N9-C8
80	A	3405	TER	N9-C10-C11-C12
80	h1	1902	TER	C6-C7-C8-N9
80	h1	1901	TER	N1-C2-C3-C4
80	h1	1903	TER	N1-C2-C3-C4
80	A	3418	TER	C10-C11-C12-C13
80	A	3417	TER	C3-C4-N5-C6
80	A	3405	TER	C11-C12-C13-N14
80	3	202	TER	C10-C11-C12-C13
80	A	3413	TER	C10-C11-C12-C13
80	h1	1904	TER	C10-C11-C12-C13
80	A	3417	TER	C10-C11-C12-C13
80	h1	1905	TER	C10-C11-C12-C13
80	h1	1904	TER	N9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
80	h1	1903	TER	C10-C11-C12-C13
80	A	3404	TER	N5-C6-C7-C8
80	A	3419	TER	C10-C11-C12-C13
80	h1	1906	TER	N5-C6-C7-C8
80	A	3415	TER	C7-C8-N9-C10
80	h1	1906	TER	C11-C12-C13-N14
80	A	3410	TER	C10-C11-C12-C13
80	A	3420	TER	C10-C11-C12-C13
80	A	3404	TER	C6-C7-C8-N9
80	A	3410	TER	N5-C6-C7-C8
80	h1	1904	TER	C7-C6-N5-C4
80	h1	1906	TER	C10-C11-C12-C13
80	A	3413	TER	N5-C6-C7-C8
80	A	3405	TER	C11-C10-N9-C8
80	A	3411	TER	C11-C10-N9-C8
80	A	3414	TER	N1-C2-C3-C4
80	h1	1902	TER	N1-C2-C3-C4
80	3	201	TER	C7-C6-N5-C4
80	A	3413	TER	C11-C10-N9-C8
80	A	3415	TER	C11-C12-C13-N14
80	A	3407	TER	C10-C11-C12-C13
80	A	3415	TER	C10-C11-C12-C13
80	A	3409	TER	C2-C3-C4-N5
80	A	3412	TER	C6-C7-C8-N9
84	A	3402	EPE	C8-C7-N4-C3
80	h1	1901	TER	C10-C11-C12-C13
80	A	3418	TER	C11-C12-C13-N14
80	A	3421	TER	C11-C12-C13-N14
80	A	3418	TER	C6-C7-C8-N9
80	3	202	TER	C3-C4-N5-C6
80	A	3406	TER	C7-C6-N5-C4
80	h1	1905	TER	C11-C10-N9-C8
80	A	3408	TER	N9-C10-C11-C12
80	3	202	TER	C7-C8-N9-C10
80	A	3405	TER	C7-C8-N9-C10
80	A	3403	TER	C3-C4-N5-C6
80	h1	1902	TER	C7-C8-N9-C10
80	A	3404	TER	C10-C11-C12-C13
80	3	202	TER	C7-C6-N5-C4
80	A	3414	TER	C7-C6-N5-C4
80	A	3416	TER	C7-C8-N9-C10
80	h1	1906	TER	C3-C4-N5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
80	h1	1906	TER	C11-C10-N9-C8
80	A	3407	TER	C11-C12-C13-N14
80	h1	1905	TER	N9-C10-C11-C12
80	A	3409	TER	C6-C7-C8-N9
80	A	3419	TER	C3-C4-N5-C6
80	A	3411	TER	C7-C8-N9-C10
80	A	3412	TER	C3-C4-N5-C6
80	A	3415	TER	C11-C10-N9-C8
80	h1	1904	TER	C11-C12-C13-N14
80	h1	1902	TER	C7-C6-N5-C4
80	h1	1903	TER	C7-C6-N5-C4
80	A	3406	TER	C10-C11-C12-C13
80	A	3416	TER	C2-C3-C4-N5
80	A	3407	TER	N1-C2-C3-C4
80	A	3421	TER	N1-C2-C3-C4
83	A	3401	SPD	C7-C8-C9-N10
80	3	201	TER	C11-C10-N9-C8
80	A	3406	TER	C3-C4-N5-C6
80	A	3410	TER	C7-C8-N9-C10
80	A	3418	TER	C7-C6-N5-C4
80	A	3418	TER	C7-C8-N9-C10
80	A	3421	TER	C3-C4-N5-C6
80	h1	1904	TER	C3-C4-N5-C6
80	A	3410	TER	C6-C7-C8-N9
80	A	3416	TER	C10-C11-C12-C13
80	A	3420	TER	C3-C4-N5-C6
80	A	3421	TER	C7-C8-N9-C10
80	h1	1906	TER	C7-C6-N5-C4
80	3	202	TER	C11-C12-C13-N14
80	A	3408	TER	C11-C12-C13-N14
80	A	3416	TER	N5-C6-C7-C8
80	3	201	TER	C6-C7-C8-N9
80	A	3411	TER	N9-C10-C11-C12

There are no ring outliers.

18 monomers are involved in 23 short contacts:

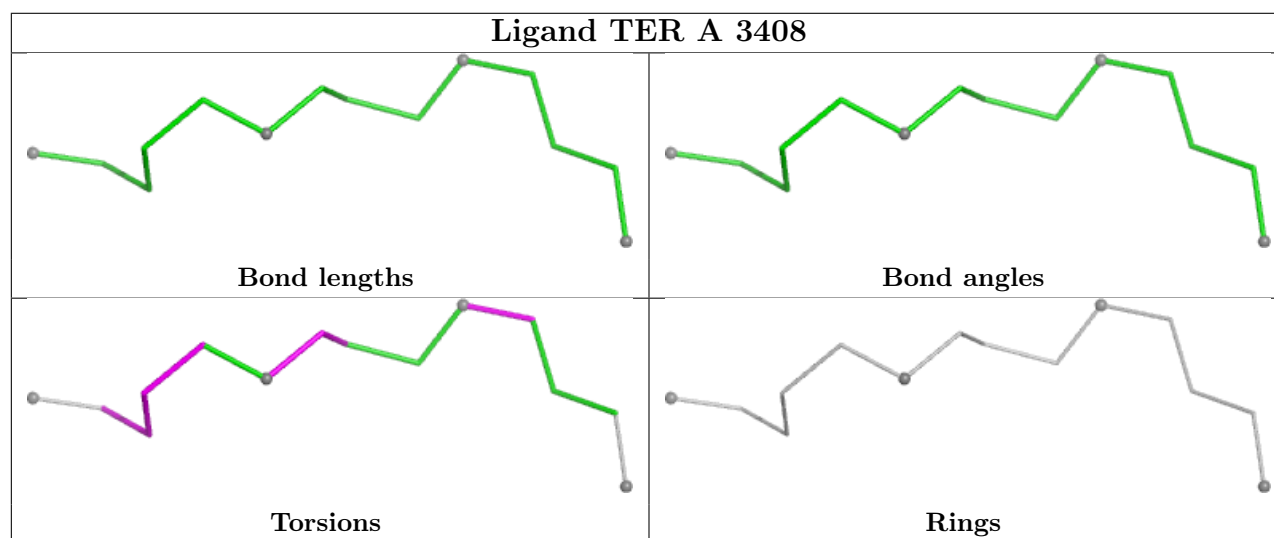
Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	A	3408	TER	1	0
80	A	3405	TER	1	0
80	A	3417	TER	1	0
80	A	3419	TER	1	0

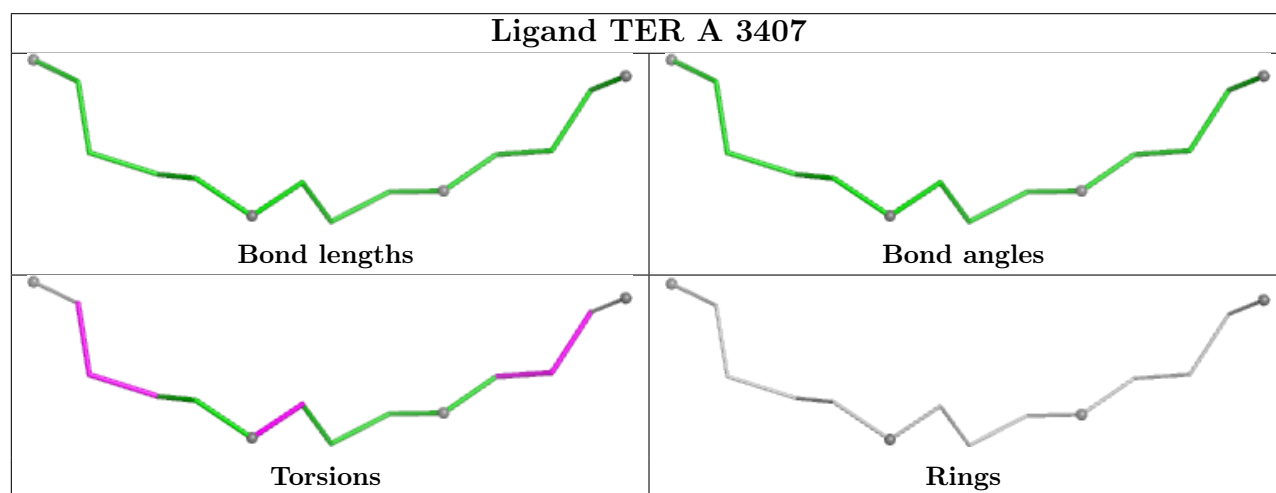
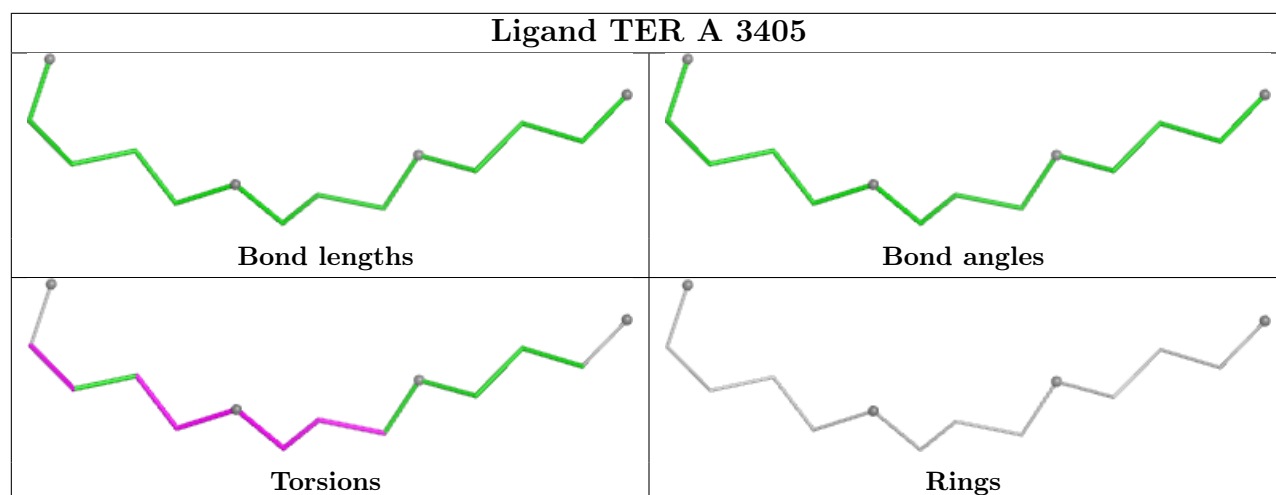
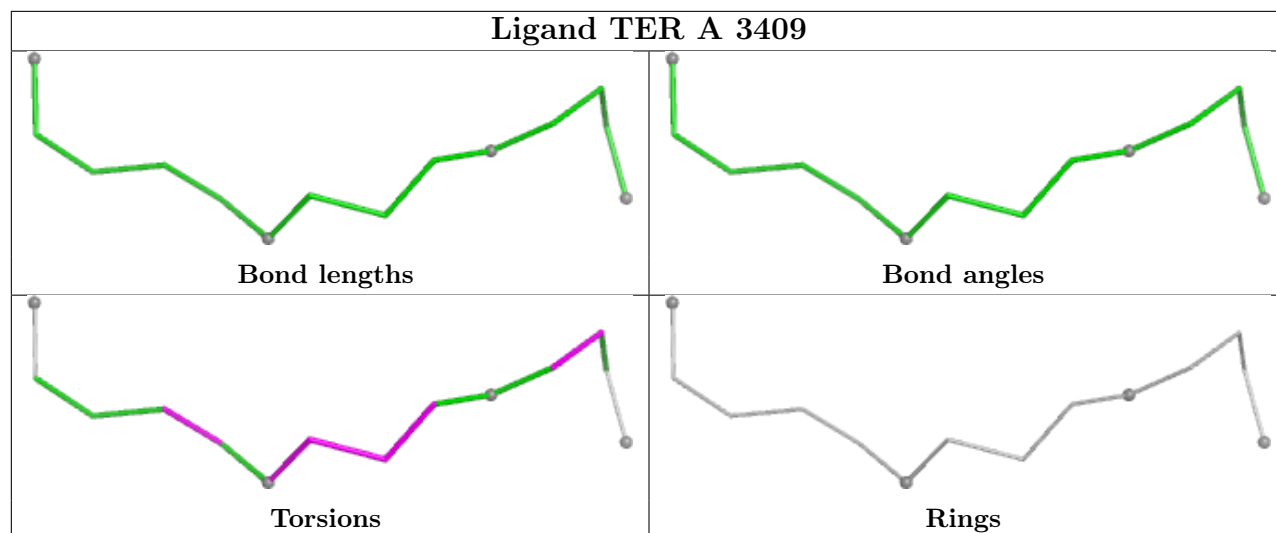
Continued on next page...

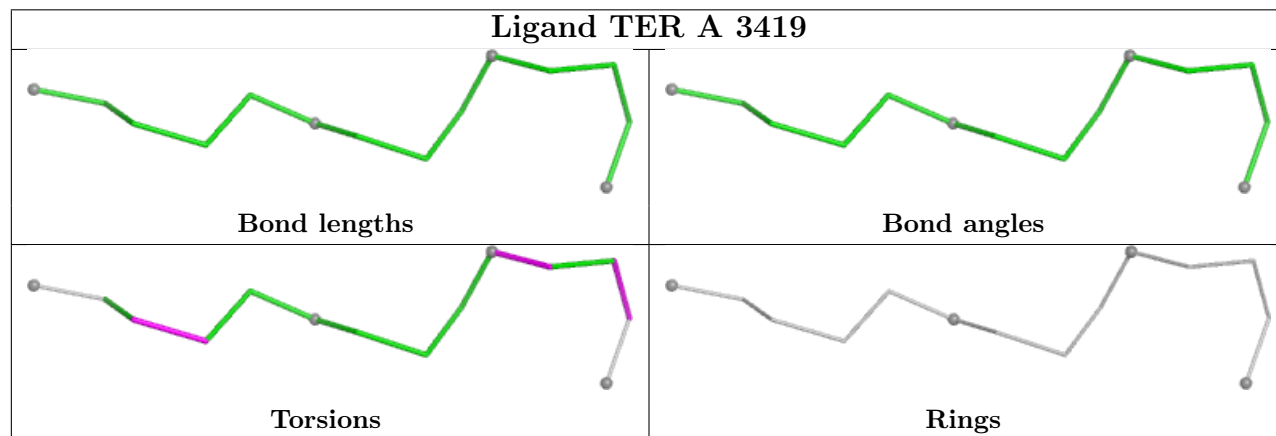
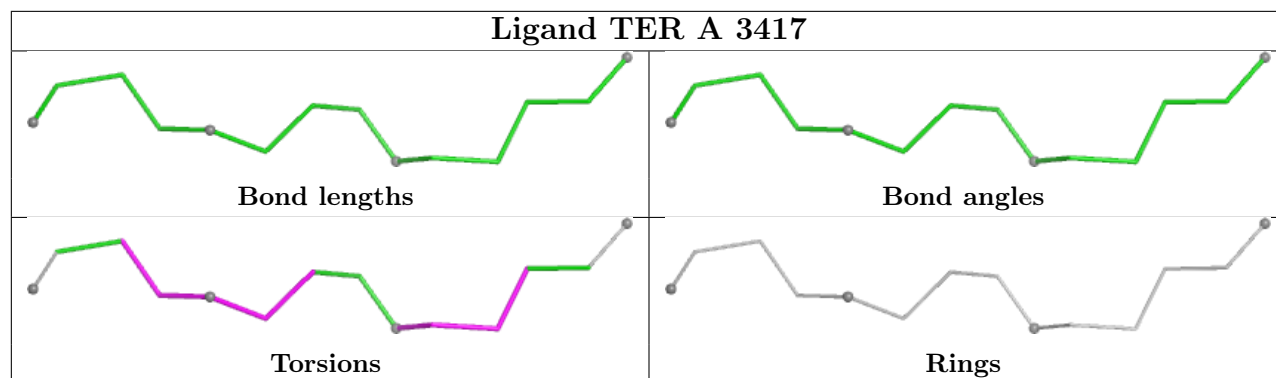
Continued from previous page...

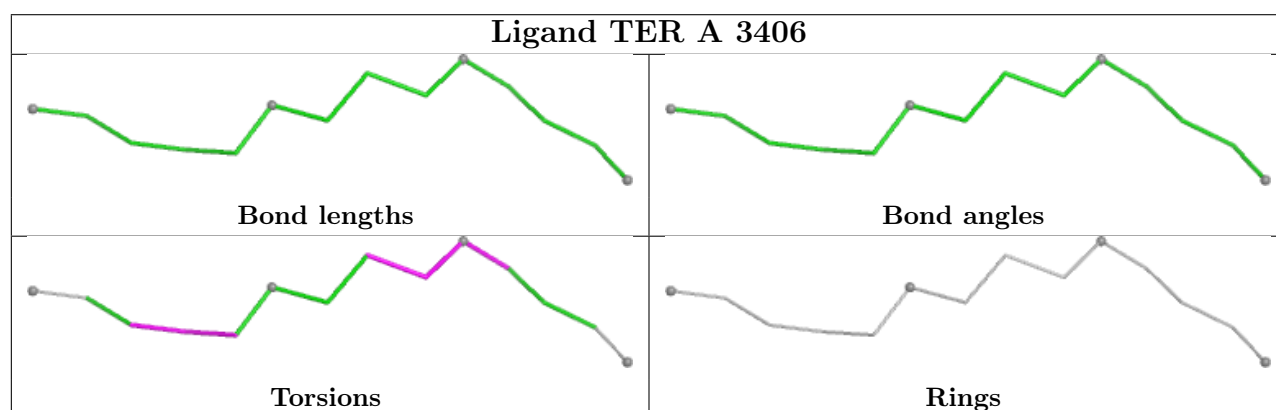
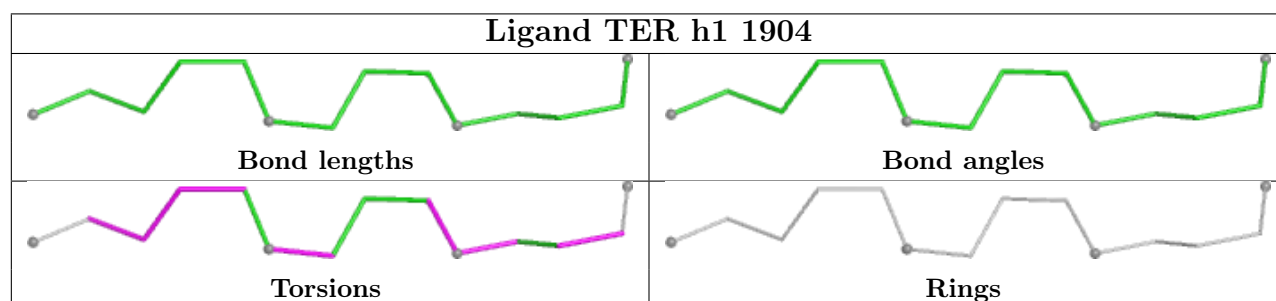
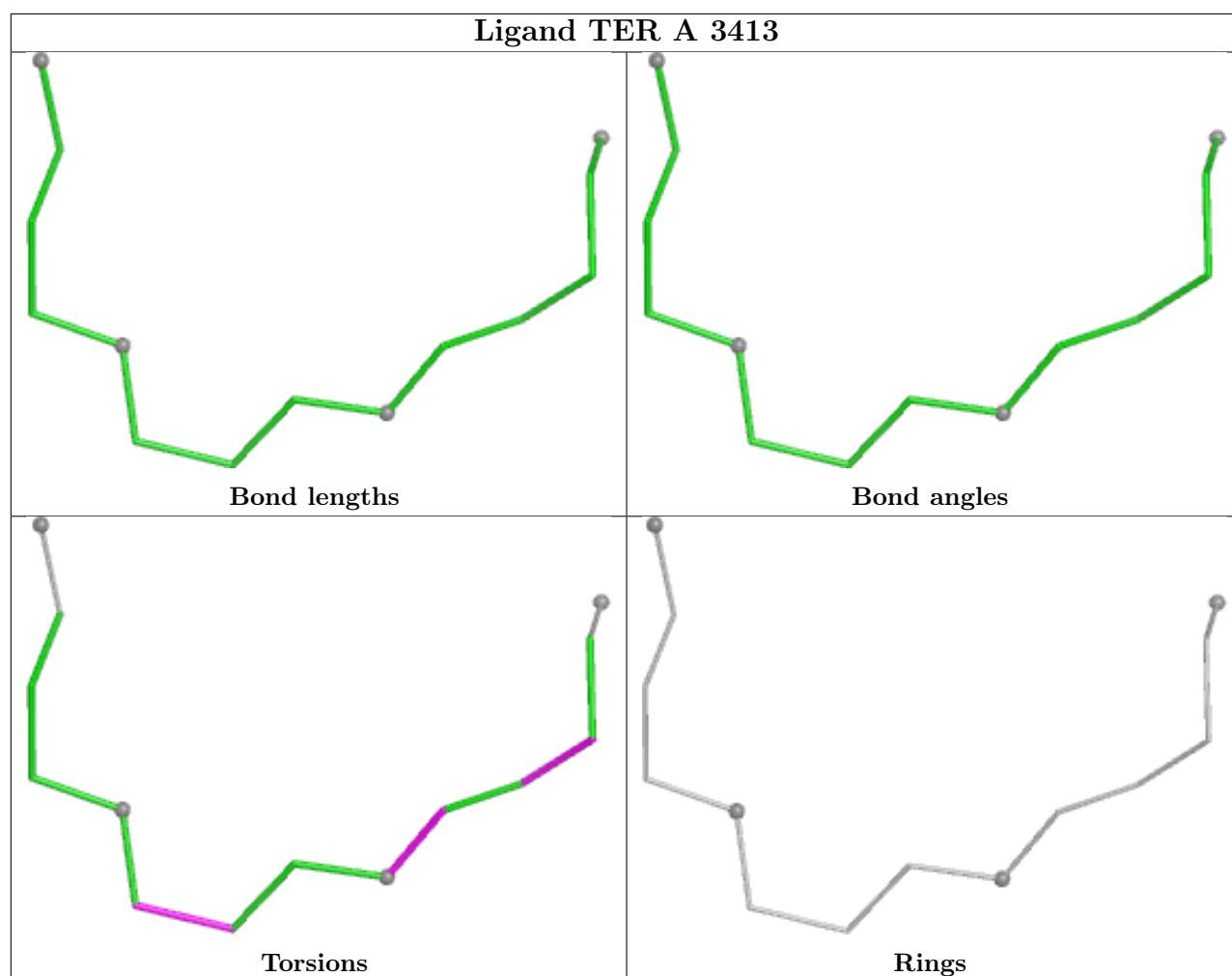
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	3402	EPE	2	0
80	A	3406	TER	1	0
80	A	3412	TER	1	0
80	A	3421	TER	2	0
80	A	3404	TER	1	0
80	A	3410	TER	1	0
80	A	3411	TER	1	0
80	A	3420	TER	1	0
83	A	3401	SPD	1	0
80	A	3418	TER	3	0
80	h1	1903	TER	1	0
80	A	3414	TER	2	0
80	A	3416	TER	1	0
80	3	201	TER	1	0

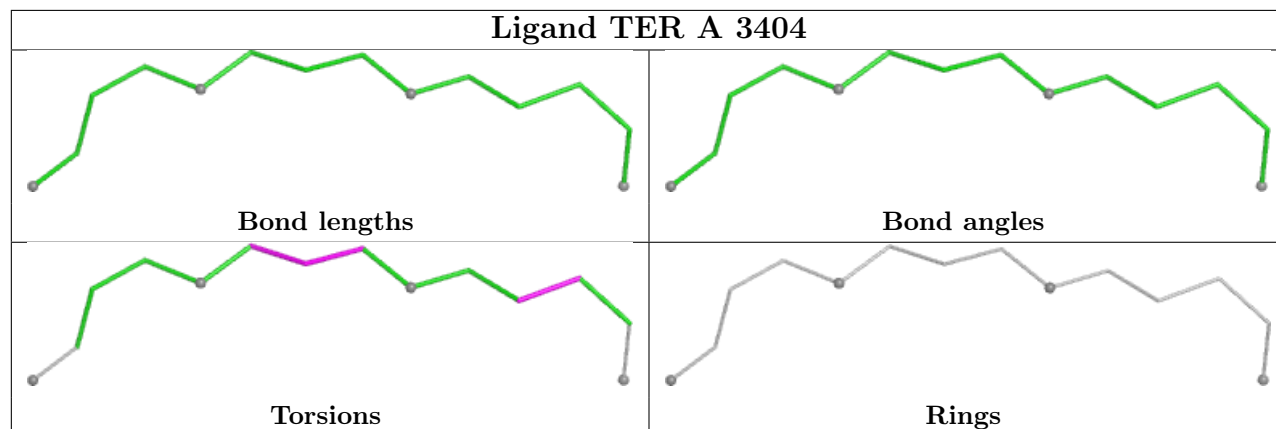
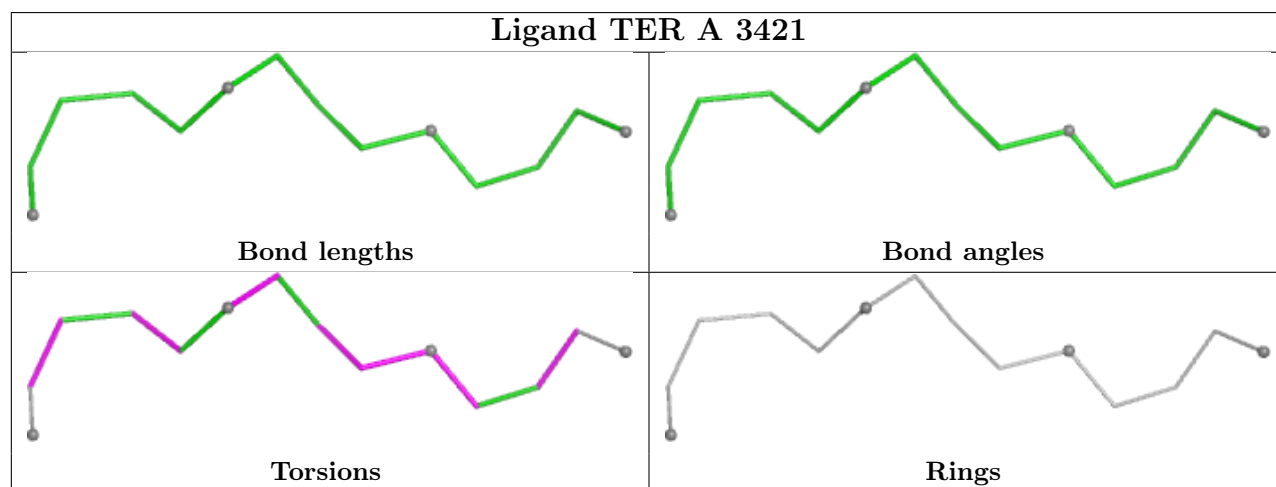
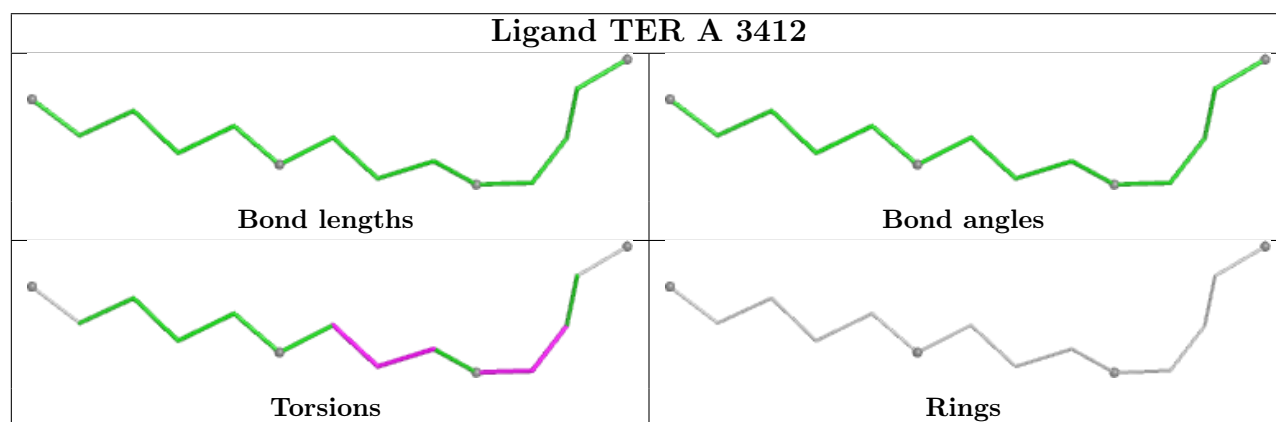
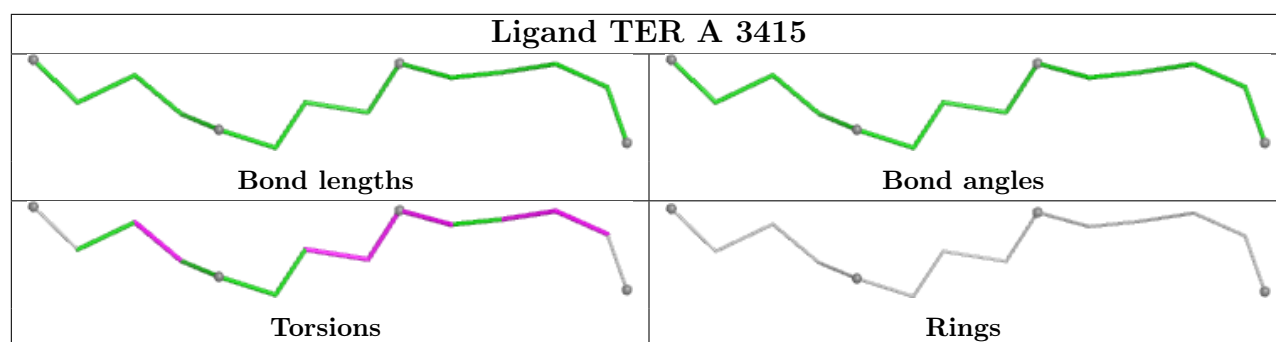
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

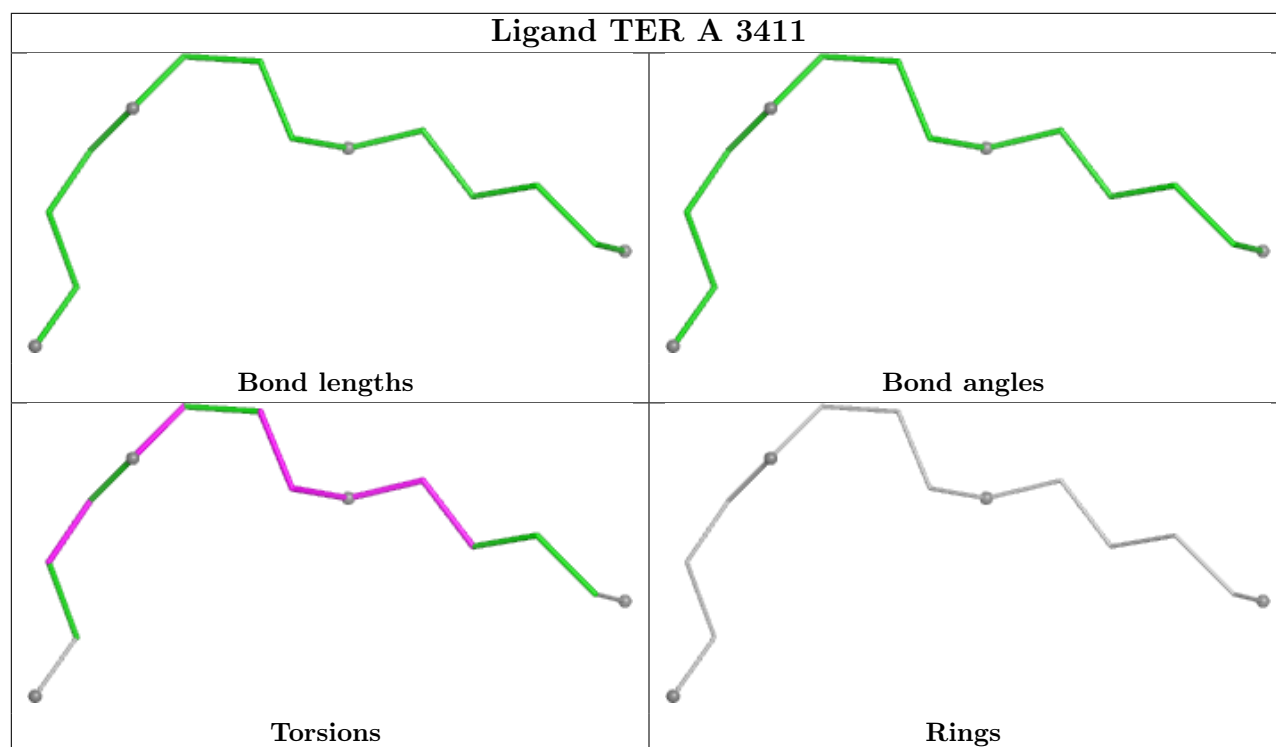
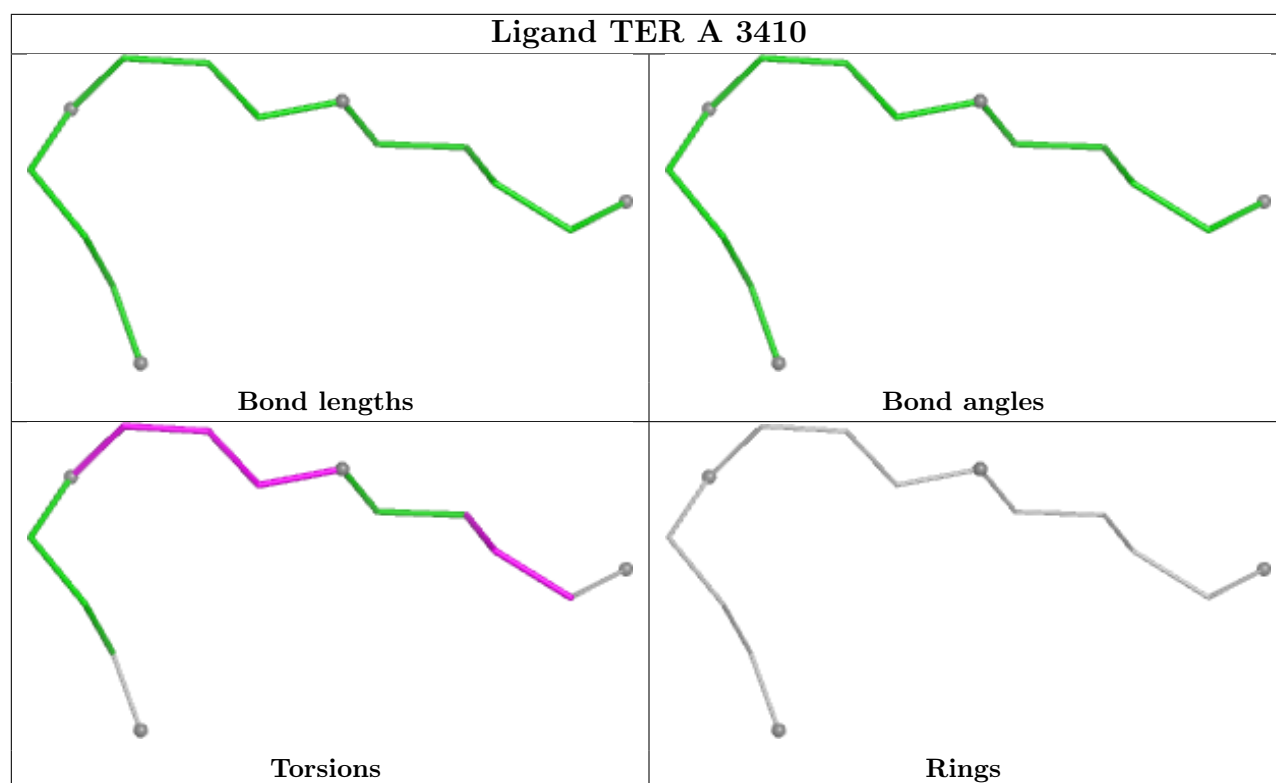


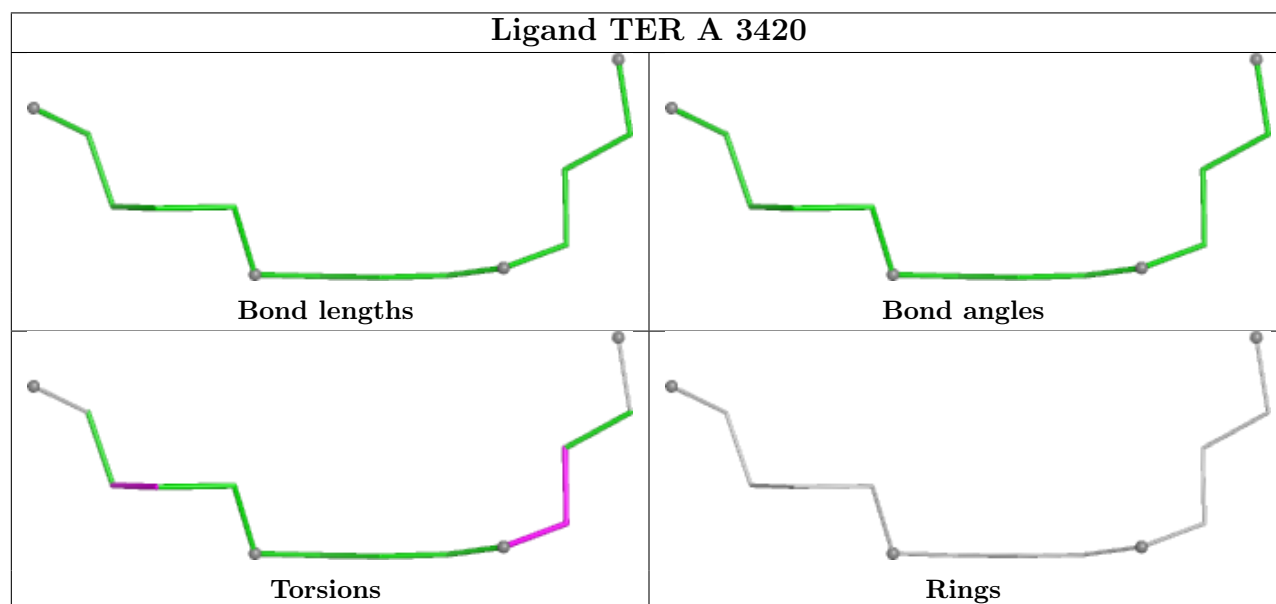
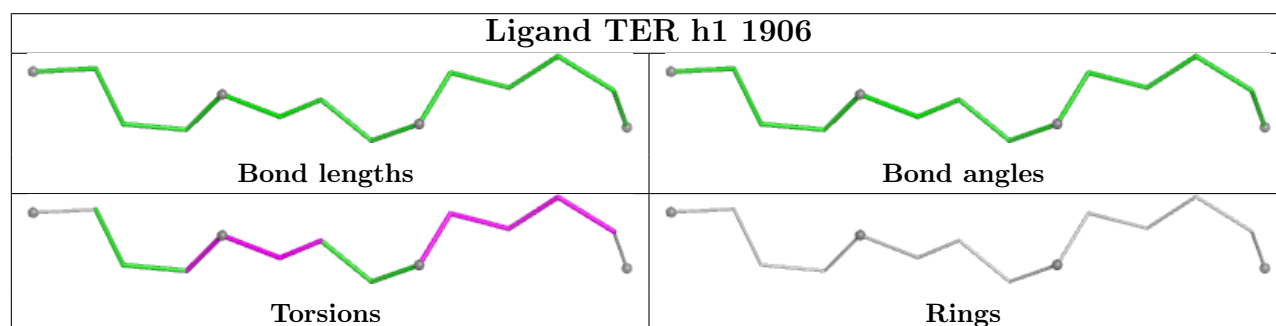
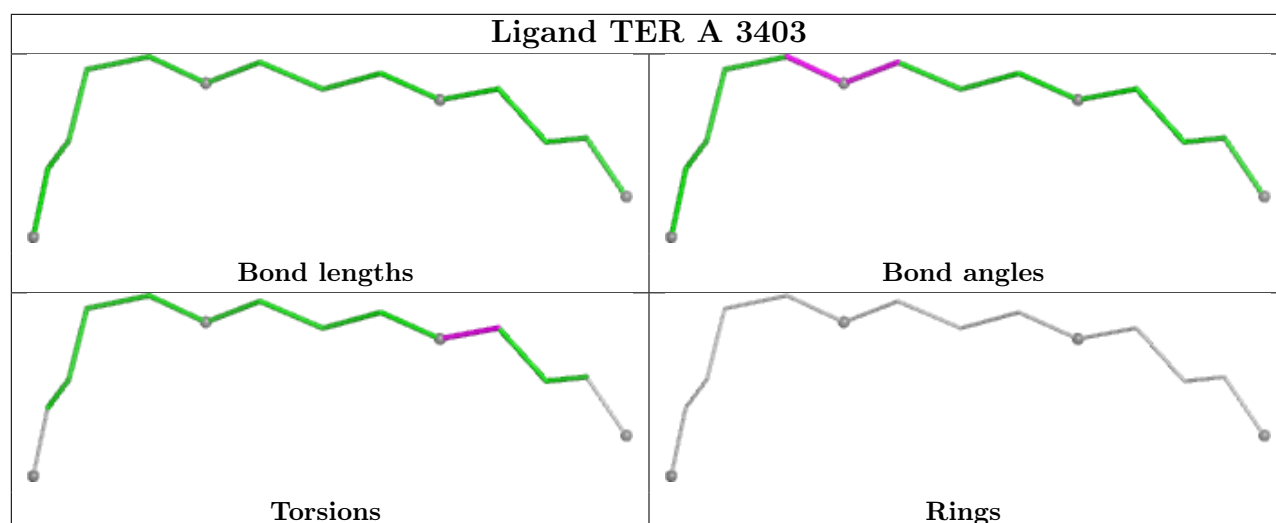


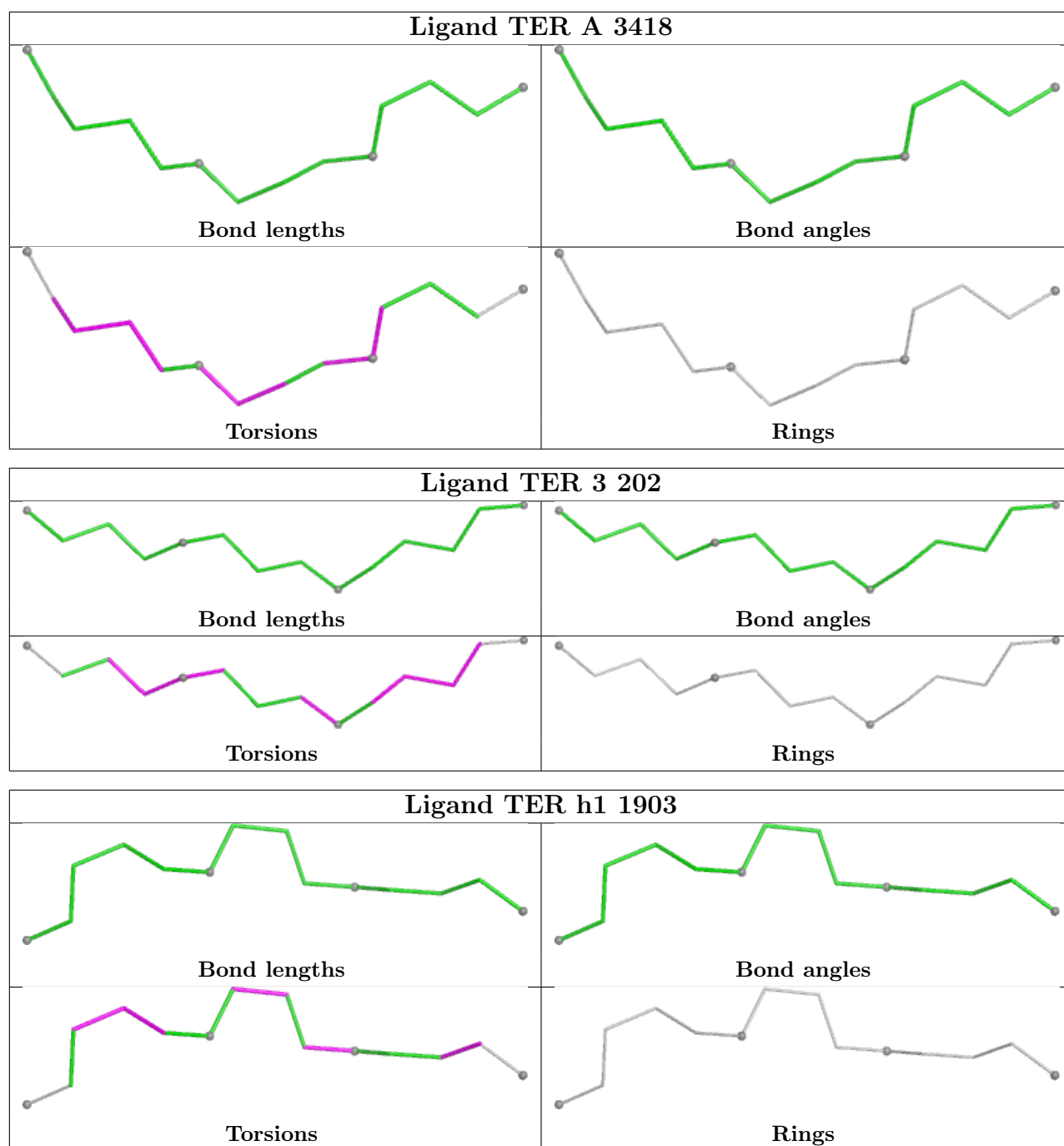


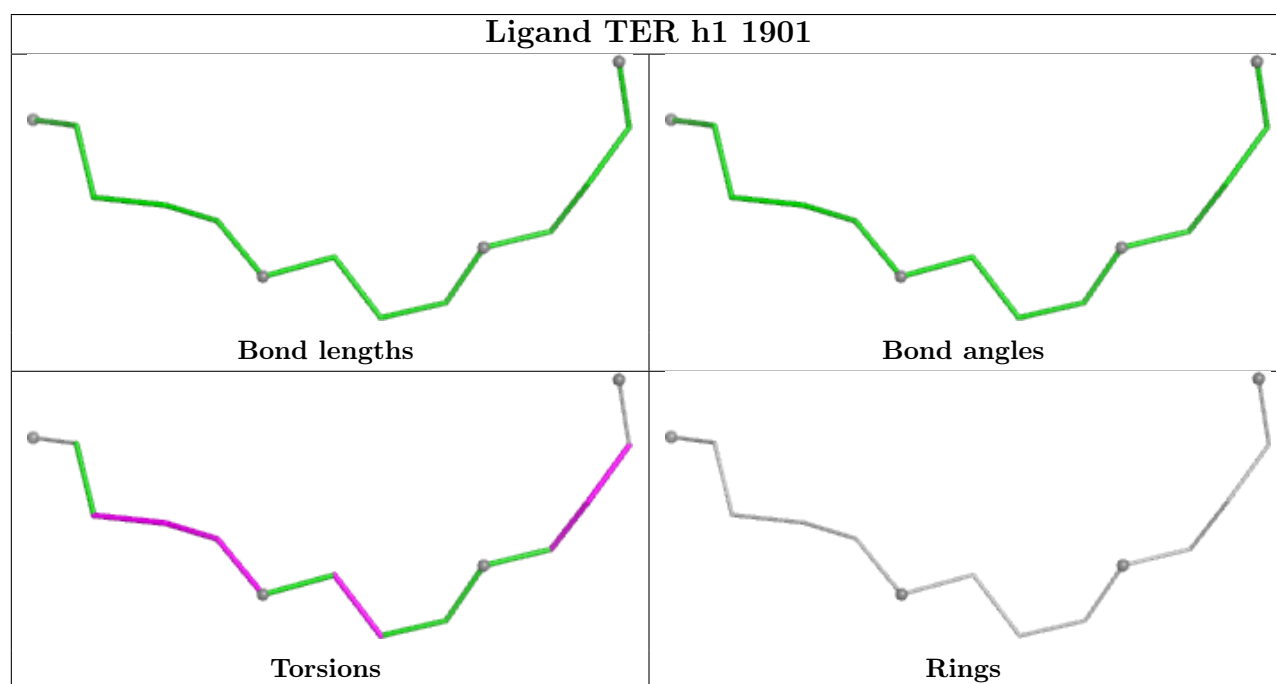
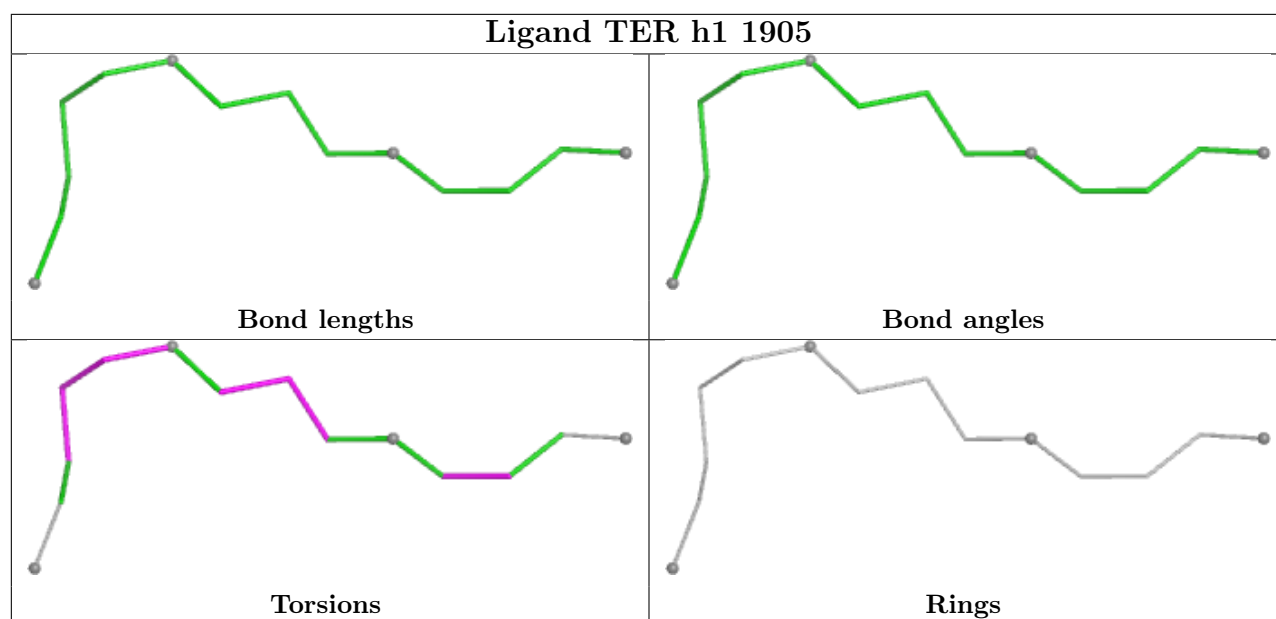


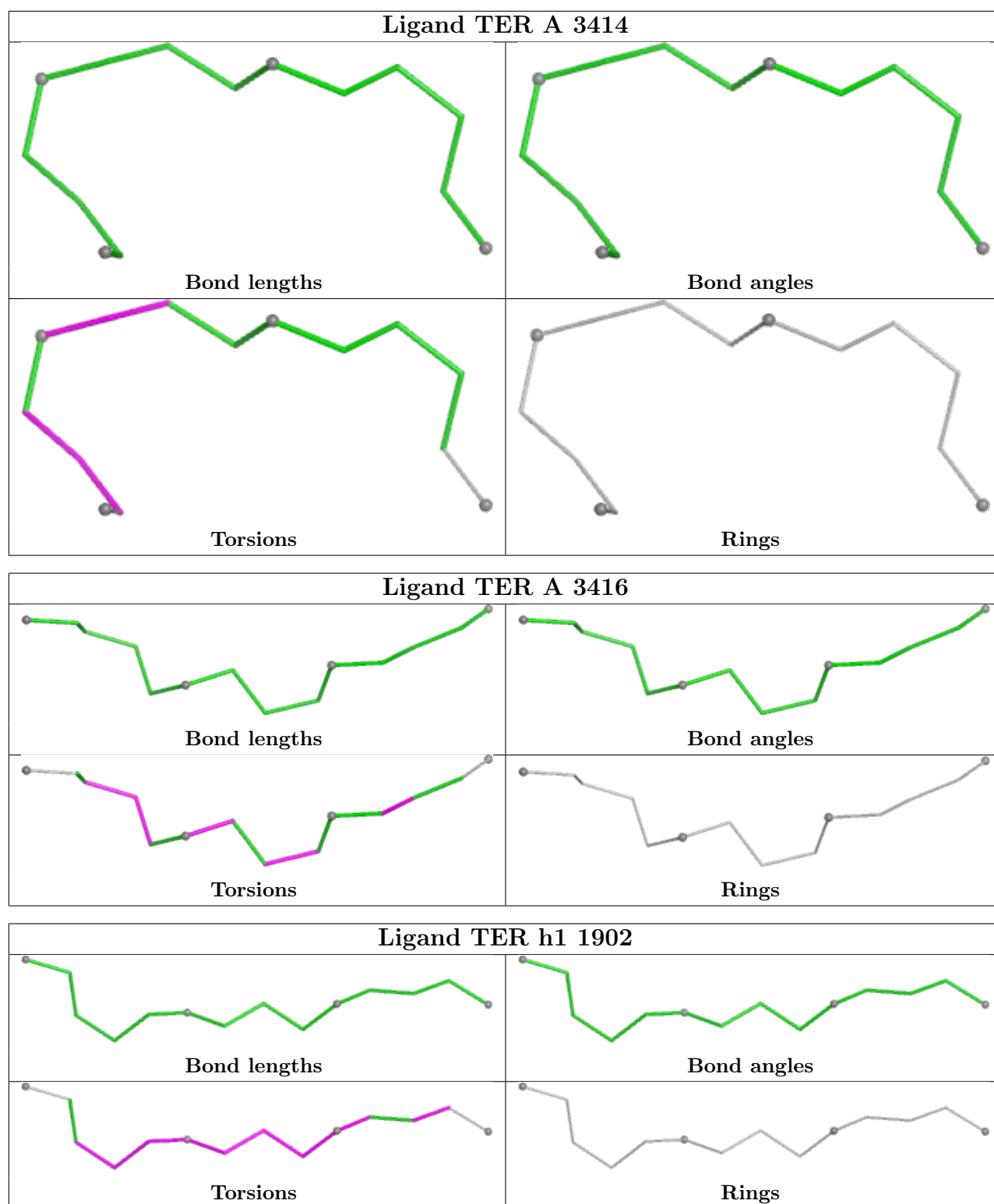


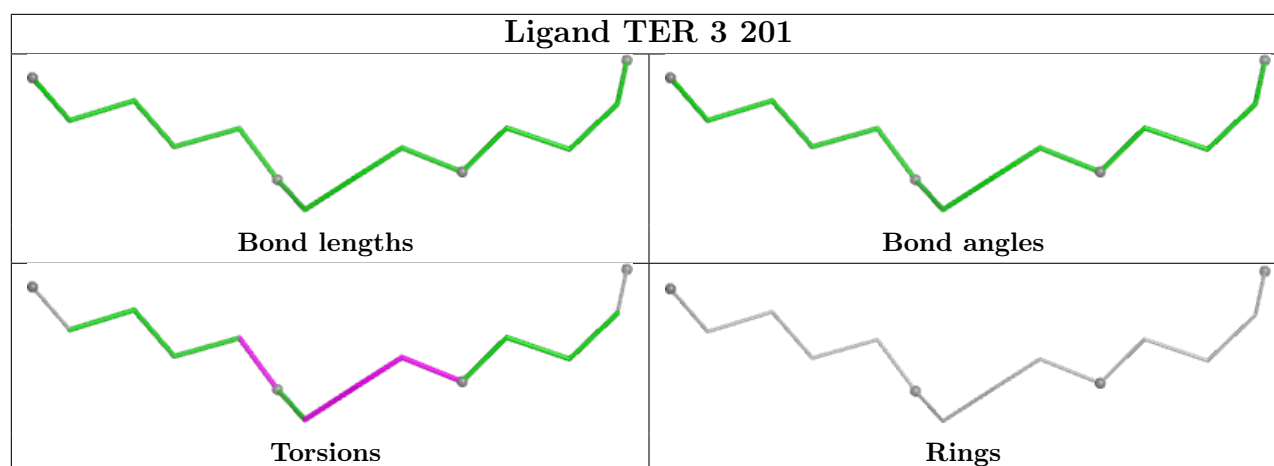












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
75	h1	3
74	Ca	1
73	AY	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h1	1784:G	O3'	1785:MA6	P	3.45
1	Ca	53:ILE	C	54:LYS	N	2.57
1	AY	76:THR	C	77:CYS	N	2.52
1	h1	1191:C	O3'	1192:C4J	P	1.88
1	h1	601:A	O3'	602:UY1	P	1.75

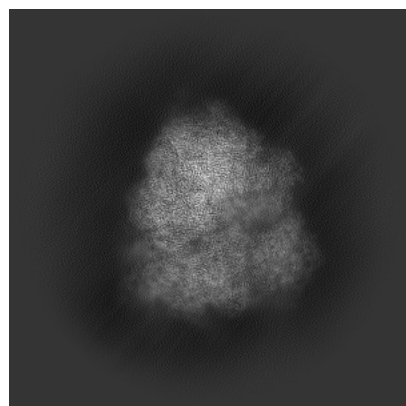
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51899. These allow visual inspection of the internal detail of the map and identification of artifacts.

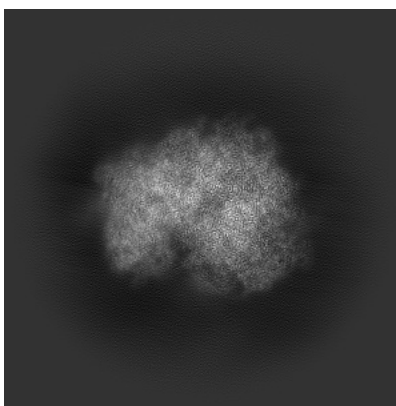
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

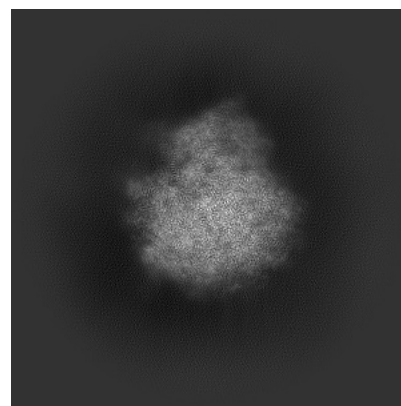
6.1.1 Primary map



X

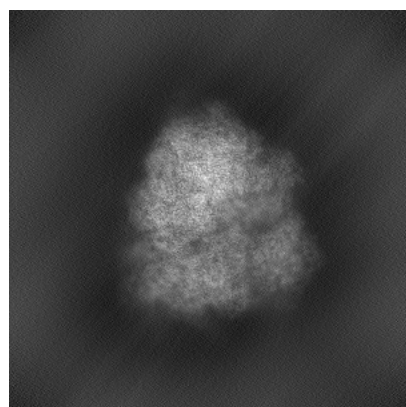


Y

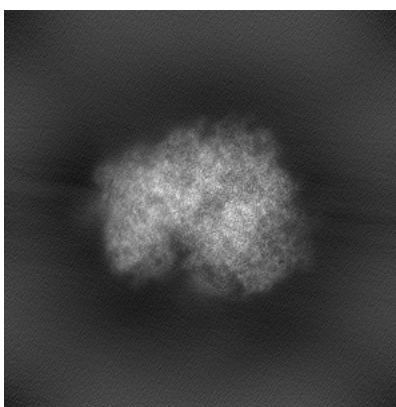


Z

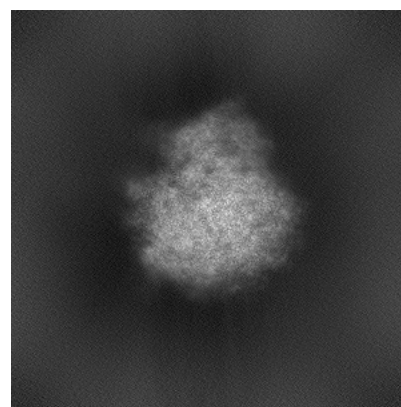
6.1.2 Raw map



X



Y

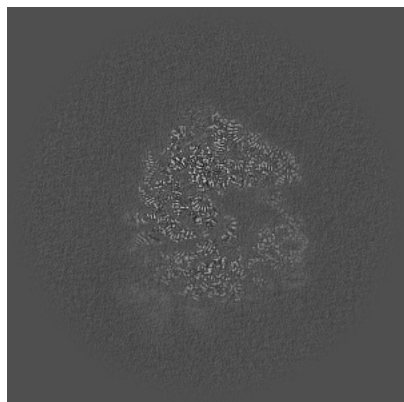


Z

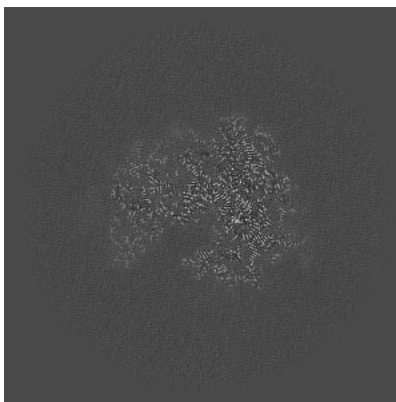
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

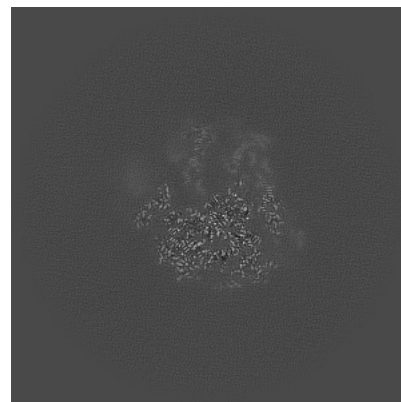
6.2.1 Primary map



X Index: 300

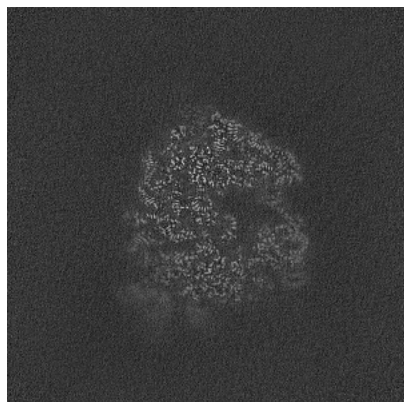


Y Index: 300

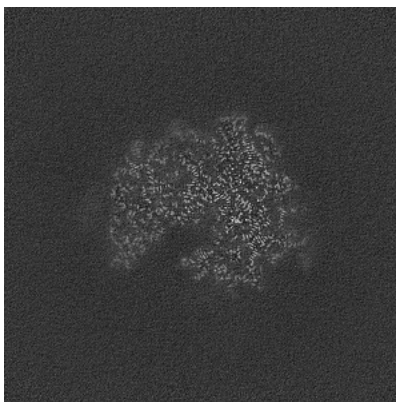


Z Index: 300

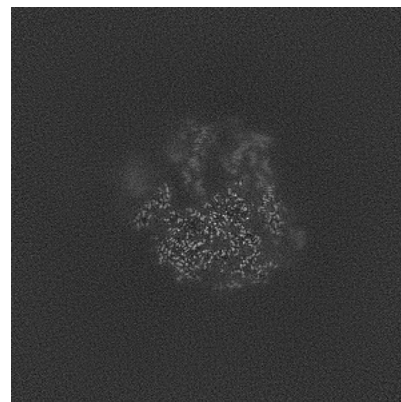
6.2.2 Raw map



X Index: 300



Y Index: 300

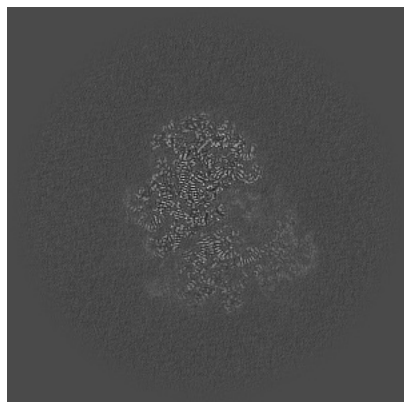


Z Index: 300

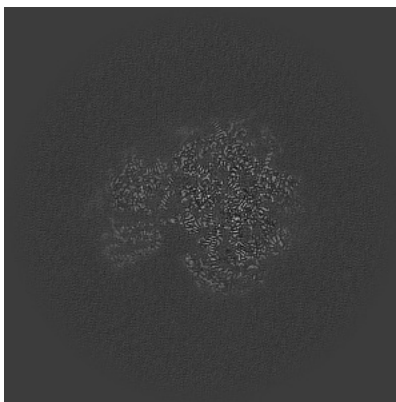
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

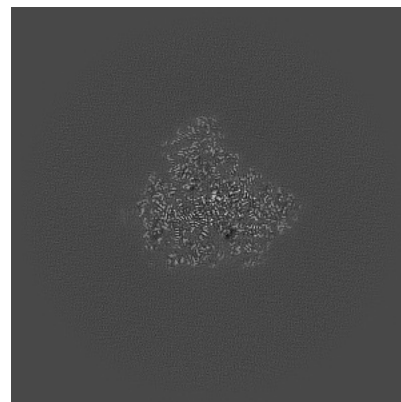
6.3.1 Primary map



X Index: 331

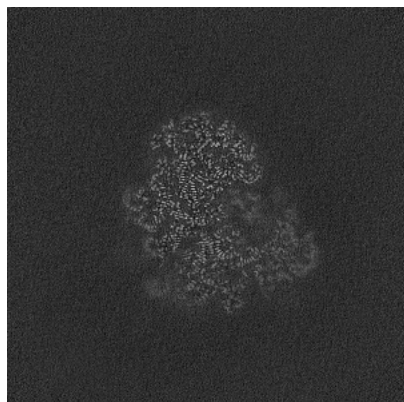


Y Index: 288

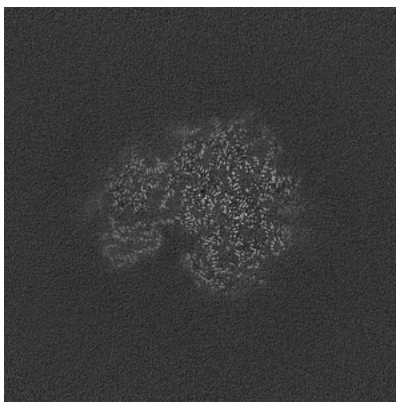


Z Index: 351

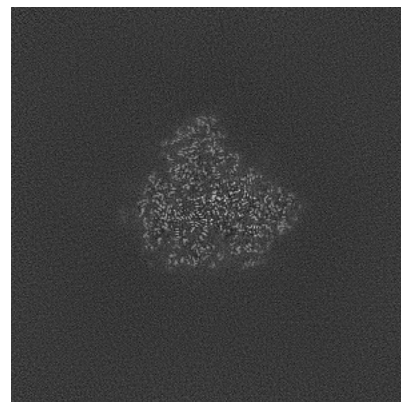
6.3.2 Raw map



X Index: 331



Y Index: 289

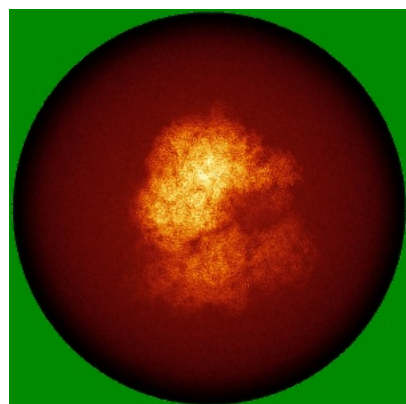


Z Index: 351

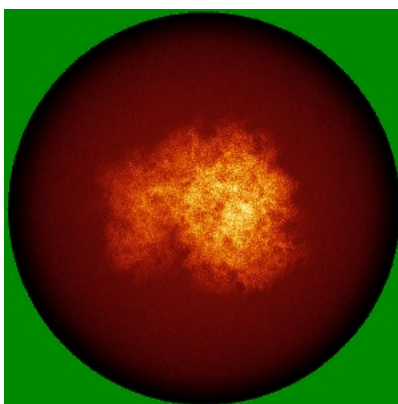
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

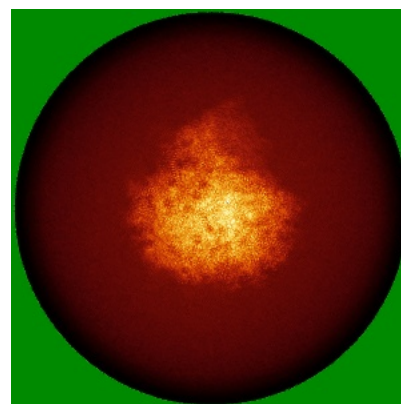
6.4.1 Primary map



X

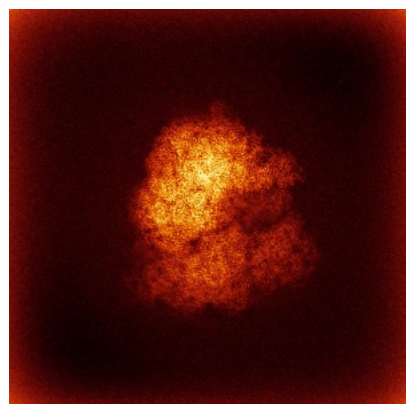


Y

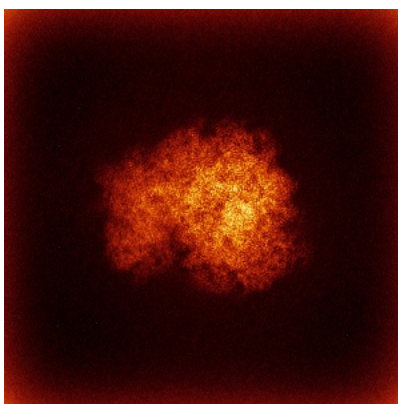


Z

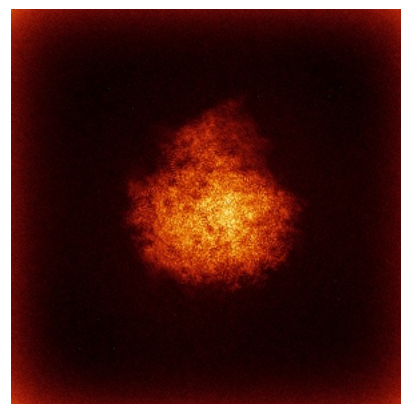
6.4.2 Raw map



X



Y

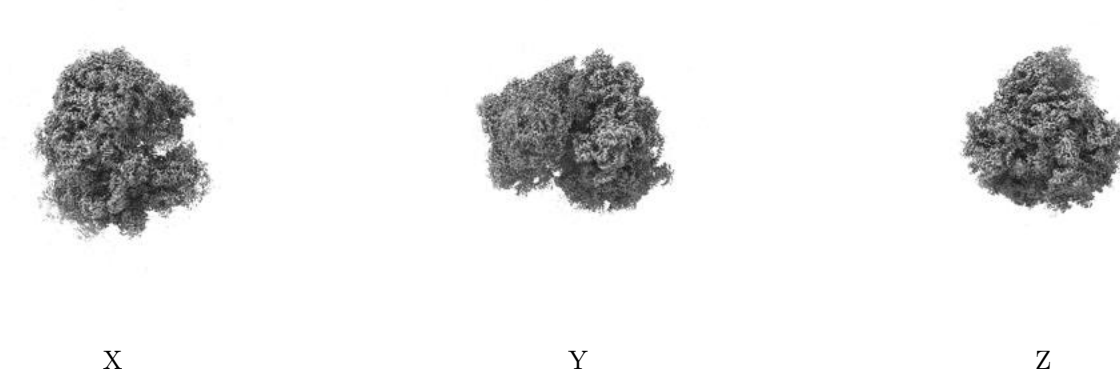


Z

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.

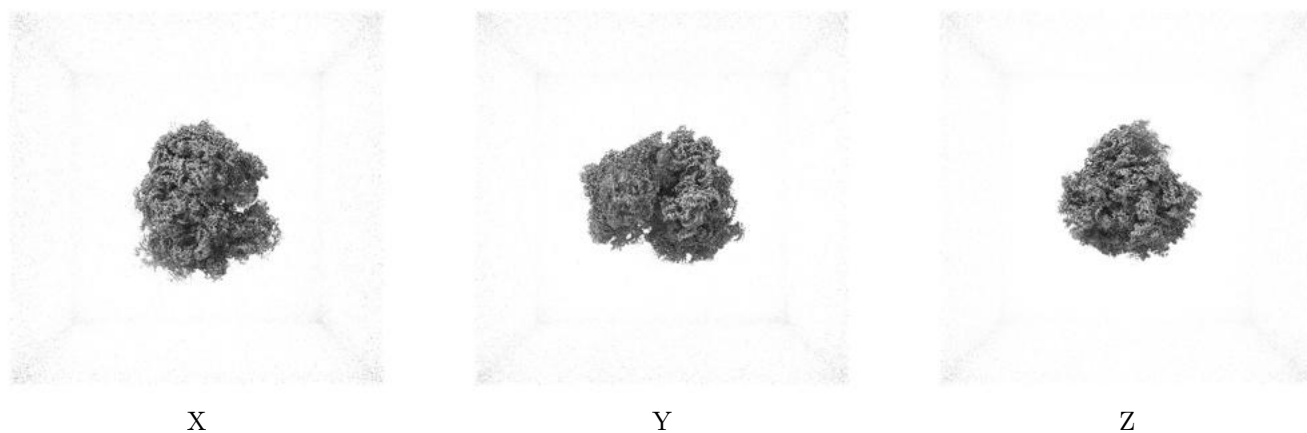
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

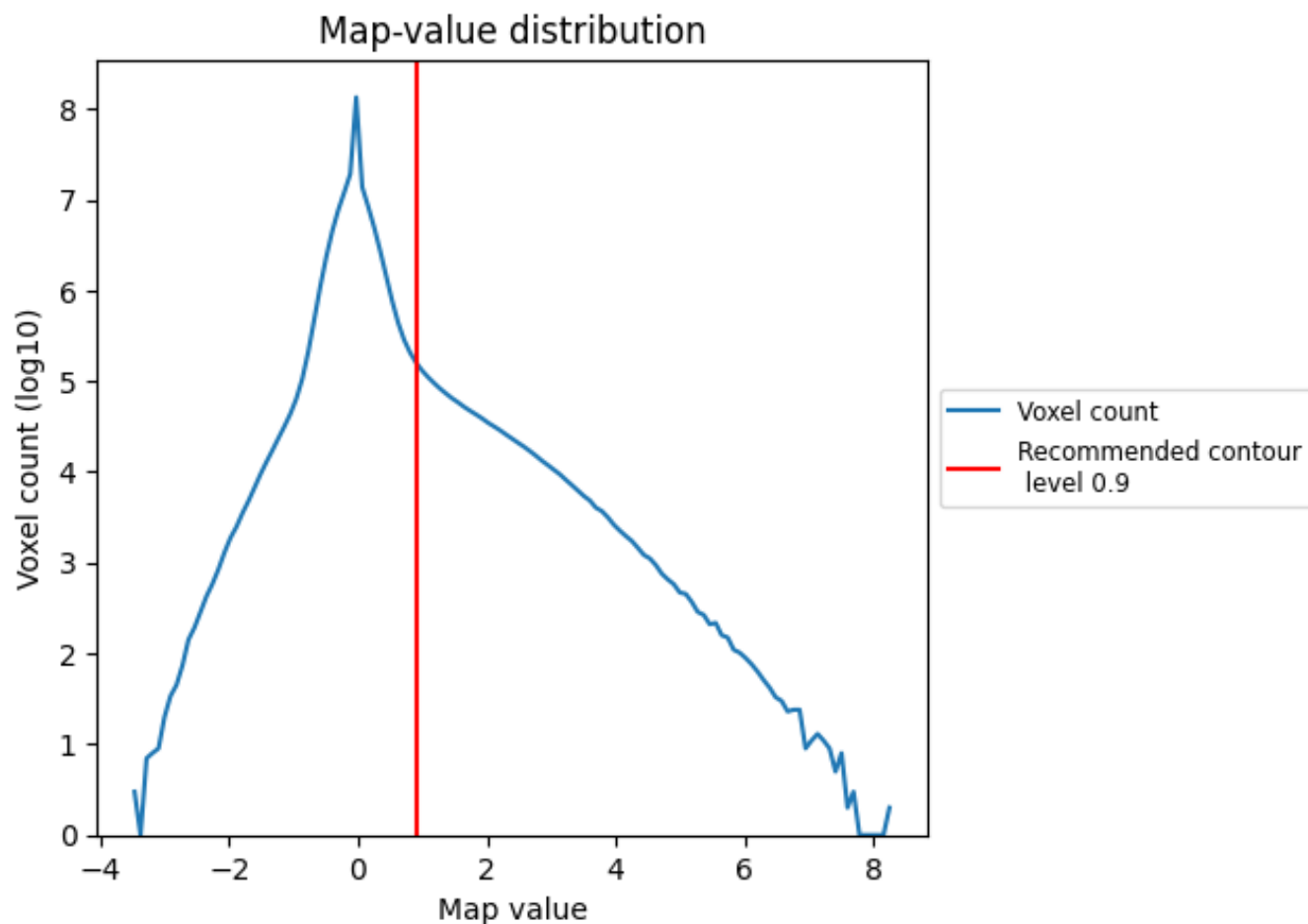
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

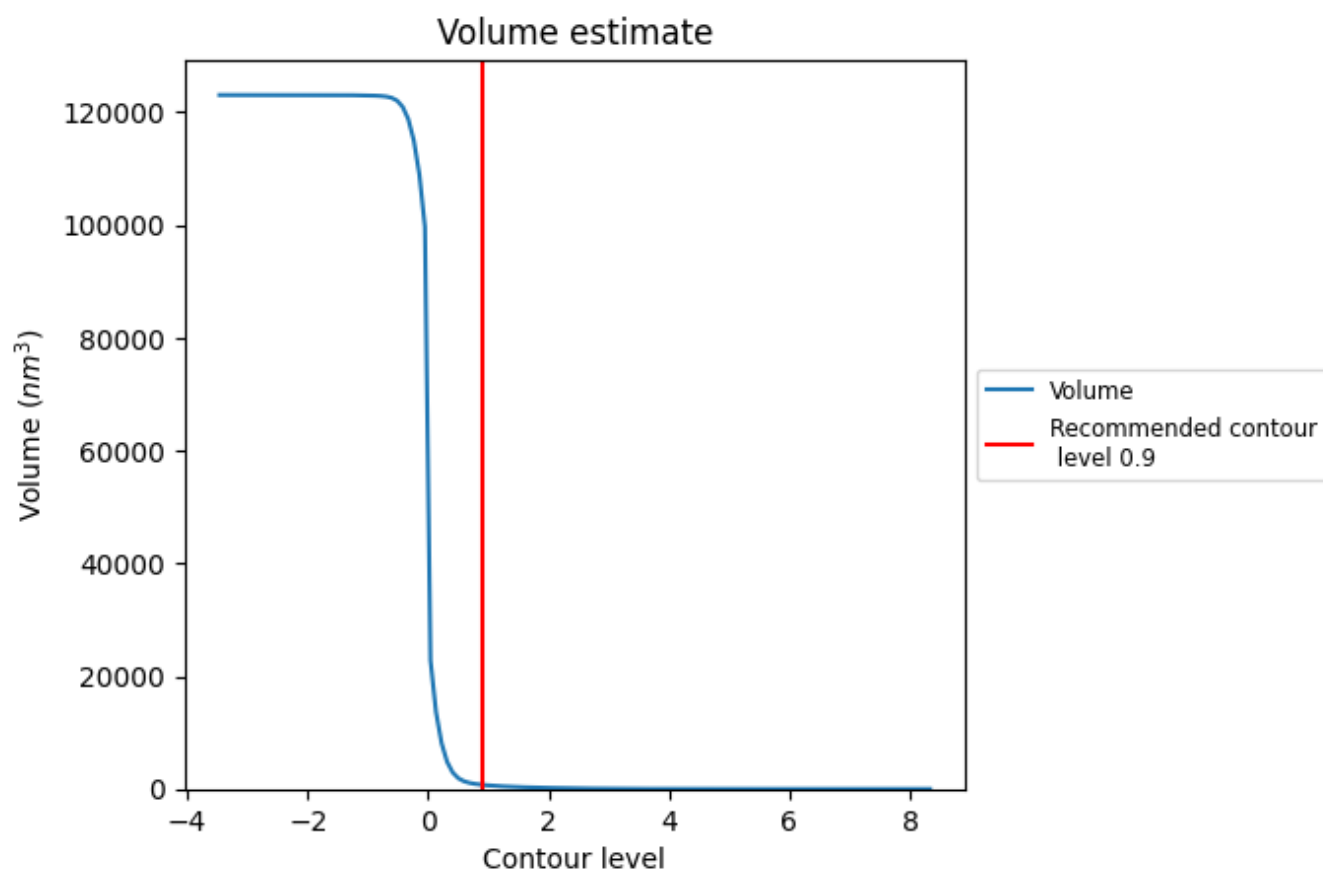
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

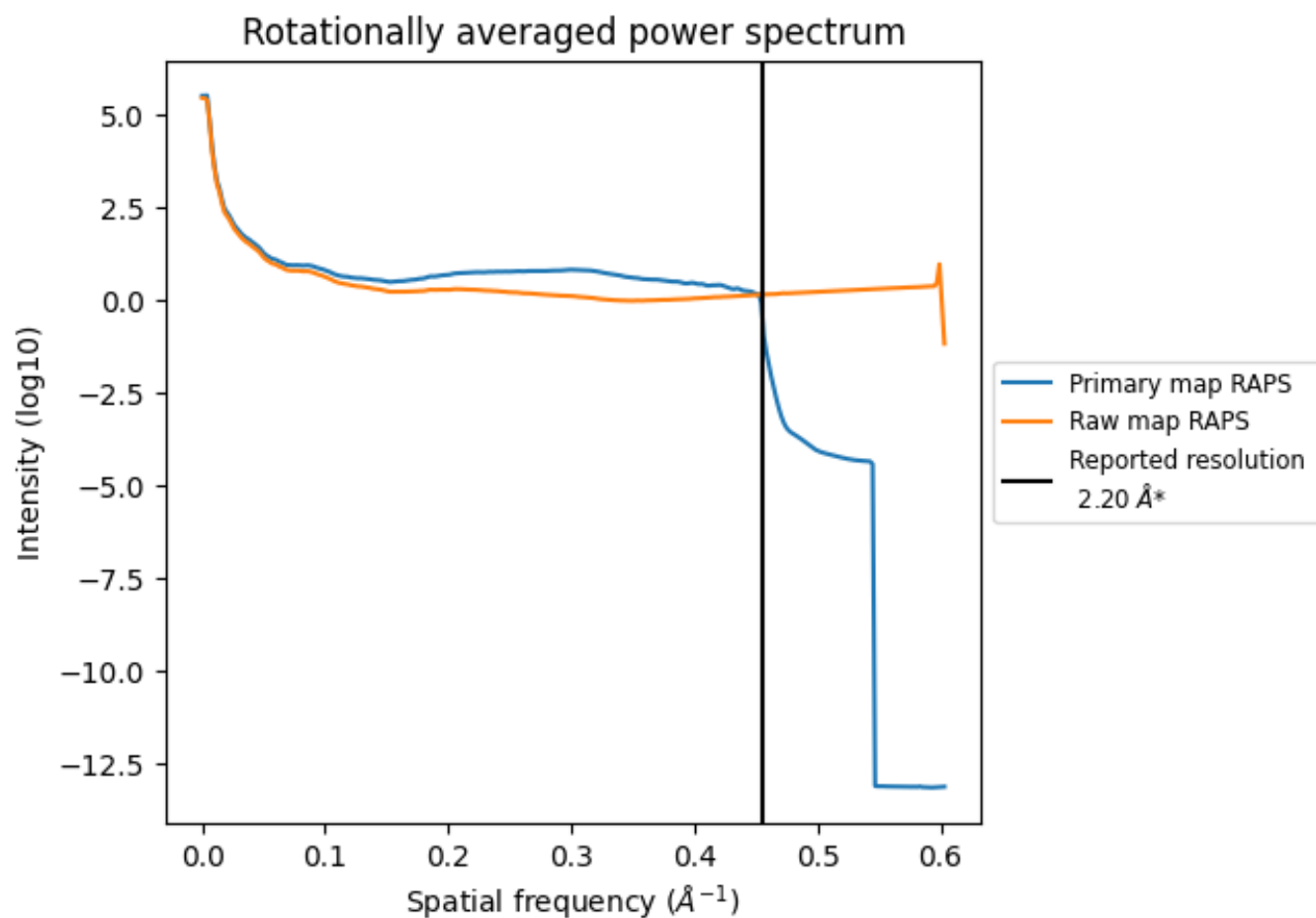
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 735 nm³; this corresponds to an approximate mass of 664 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 ⓘ

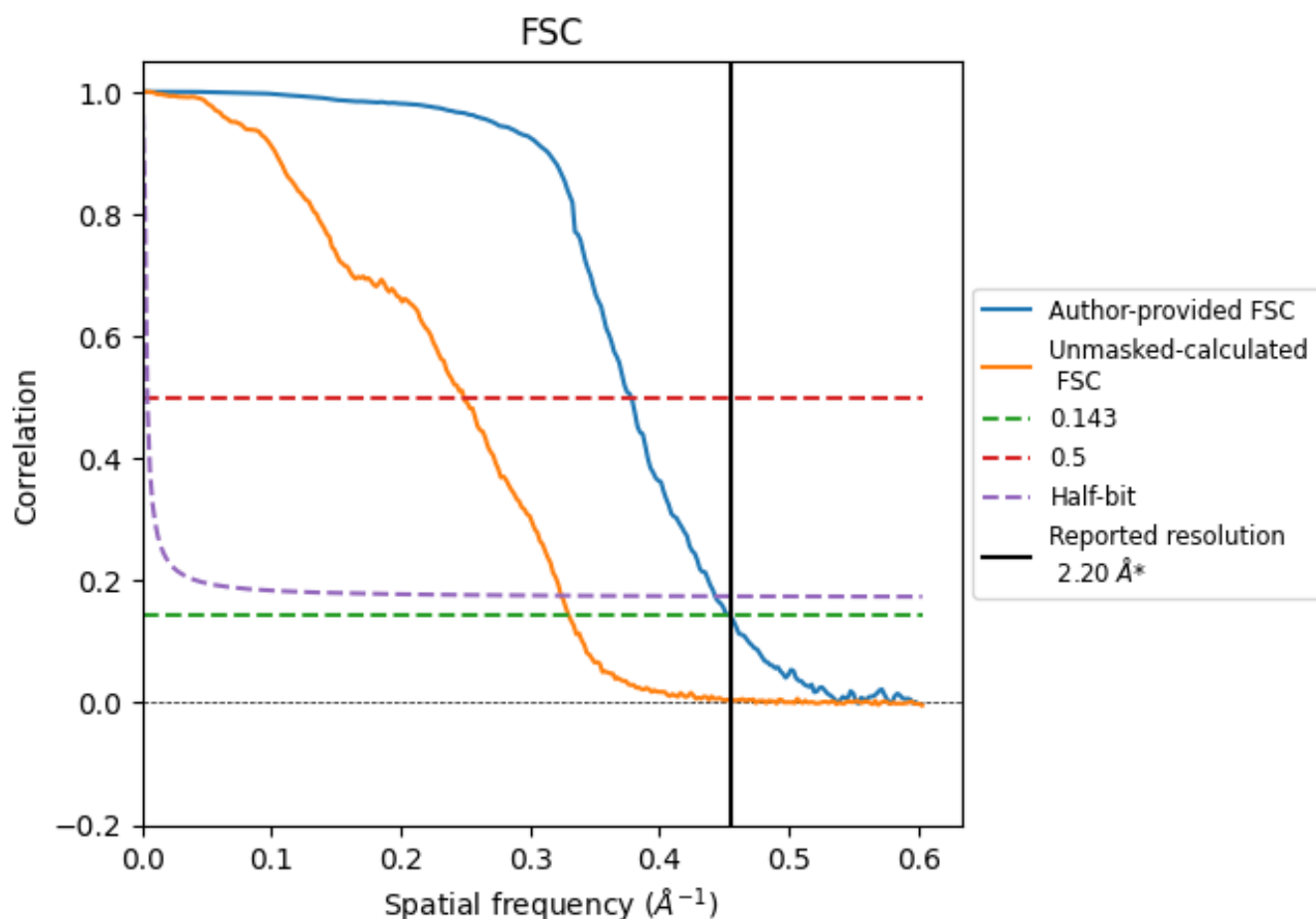


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

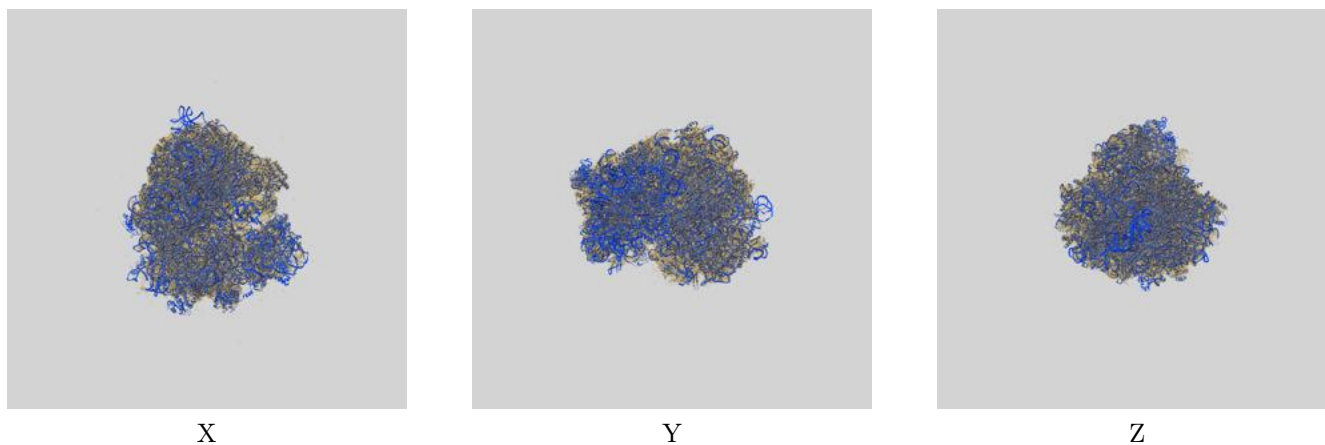
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.65	2.26
Unmasked-calculated*	3.03	4.02	3.09

*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 3.03 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

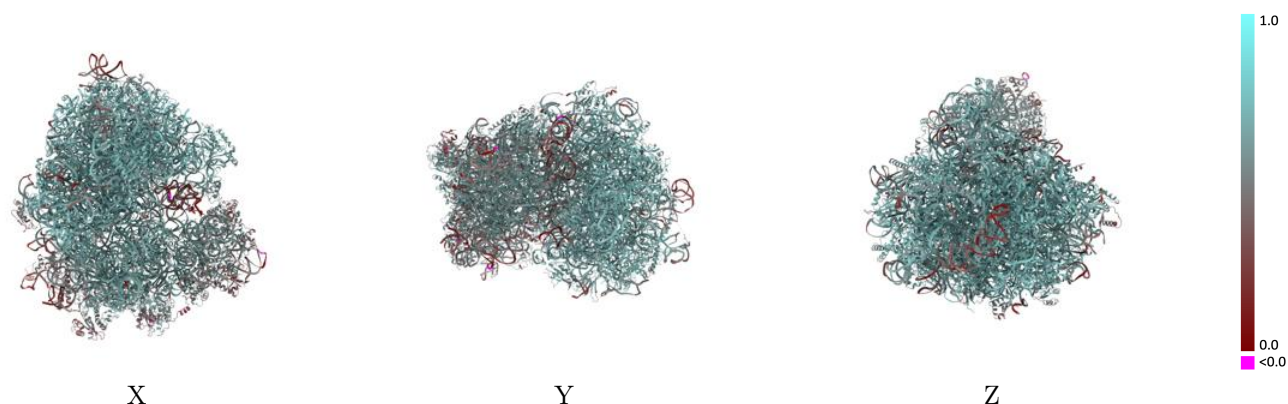
This section contains information regarding the fit between EMDB map EMD-51899 and PDB model 9H6I. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



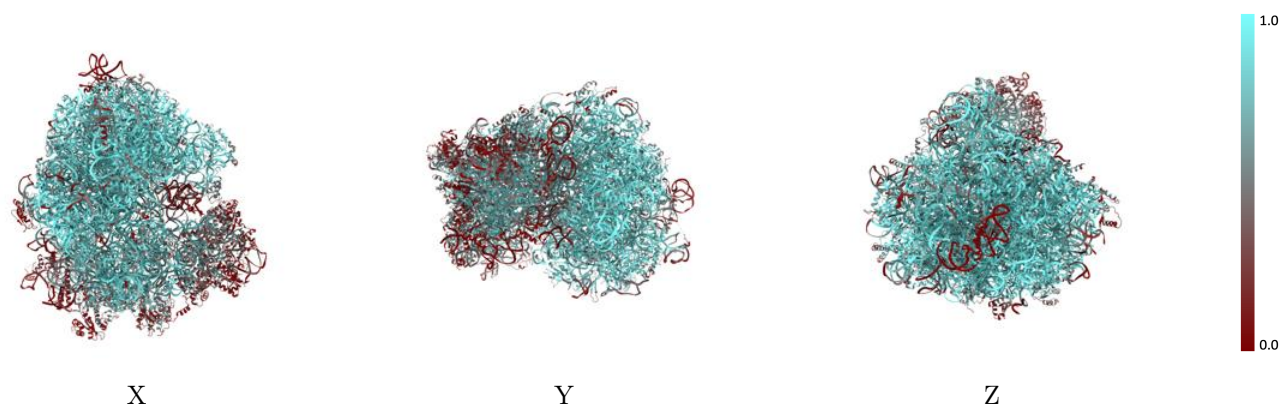
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



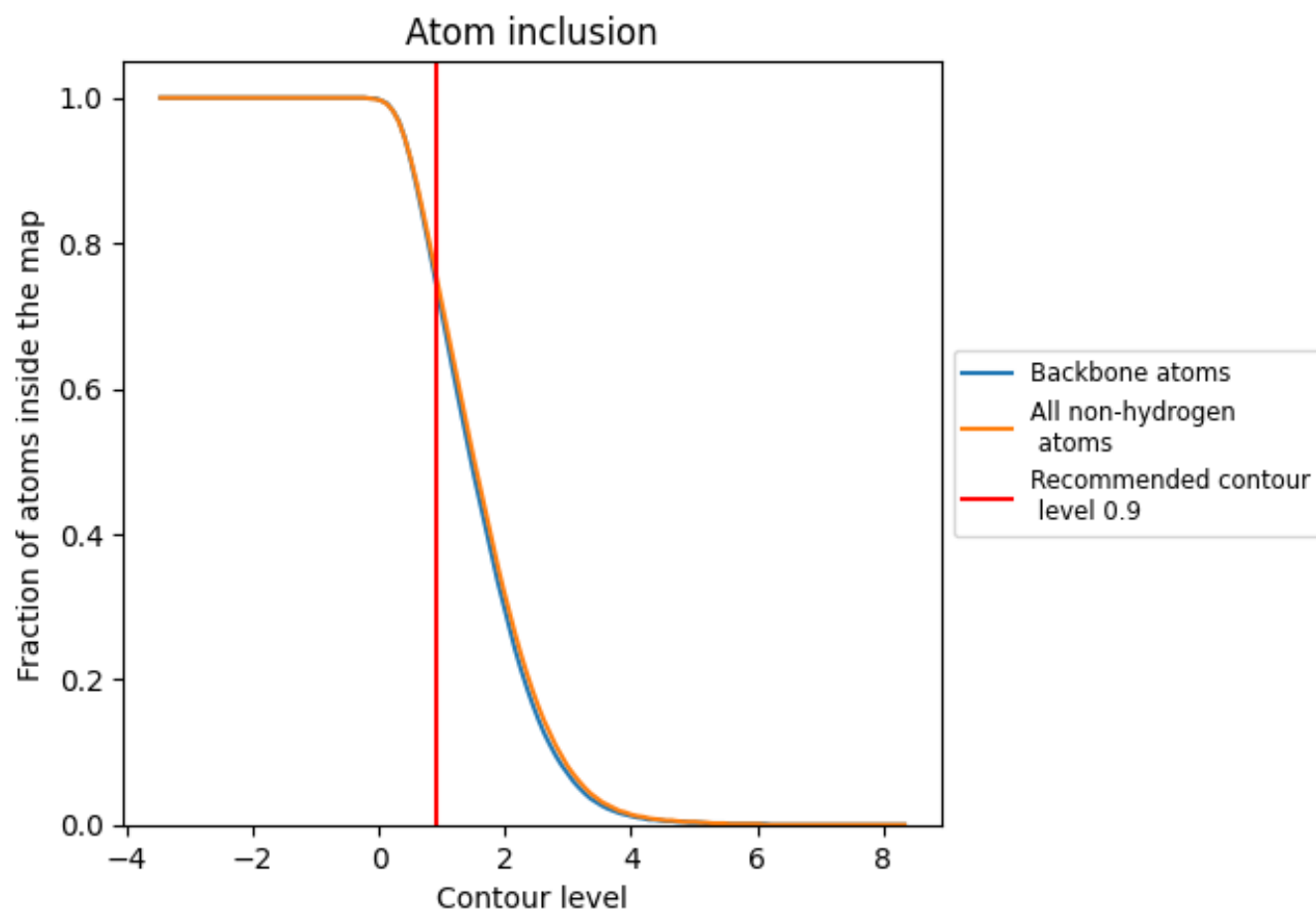
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.6260
2	 0.4470	 0.4720
3	 0.8600	 0.6390
A	 0.8800	 0.6580
AA	 0.2800	 0.4890
AB	 0.5430	 0.5760
AC	 0.7510	 0.6520
AD	 0.3430	 0.5410
AE	 0.8590	 0.6820
AF	 0.3010	 0.4990
AG	 0.8460	 0.6810
AH	 0.8130	 0.6650
AI	 0.1060	 0.3750
AJ	 0.9490	 0.7180
AK	 0.7700	 0.6340
AL	 0.9130	 0.6990
AM	 0.8510	 0.6730
AN	 0.0880	 0.4450
AO	 0.8940	 0.6960
AP	 0.7950	 0.6570
AQ	 0.3000	 0.5880
AR	 0.9220	 0.7050
AT	 0.8370	 0.6620
AU	 0.8000	 0.6610
AV	 0.9430	 0.7140
AW	 0.9480	 0.7170
AX	 0.8160	 0.6590
AY	 0.9570	 0.7170
AZ	 0.5680	 0.5970
Aa	 0.4070	 0.5280
B1	 0.7420	 0.6010
BA	 0.9340	 0.7030
BB	 0.1490	 0.3920
BC	 0.8170	 0.6910
BD	 0.9400	 0.7090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BE	 0.9070	 0.7050
BF	 0.6880	 0.6290
BG	 0.7060	 0.6210
BH	 0.8940	 0.7000
BI	 0.9120	 0.7070
BJ	 0.8160	 0.6690
BK	 0.7720	 0.6520
BL	 0.3090	 0.5050
BM	 0.9220	 0.7090
BN	 0.8180	 0.6680
BO	 0.8960	 0.6950
BP	 0.7940	 0.6640
BQ	 0.9670	 0.7240
BR	 0.8640	 0.6880
BS	 0.9270	 0.7110
BT	 0.8570	 0.6870
BU	 0.6400	 0.6040
BV	 0.6370	 0.6060
BW	 0.6120	 0.6210
Ba	 0.2080	 0.4320
C3	 0.9560	 0.6790
Ca	 0.4620	 0.5570
Da	 0.6710	 0.6180
Ea	 0.9880	 0.7290
Fa	 0.8800	 0.6860
Ga	 0.8710	 0.6870
Ha	 0.9250	 0.7120
Ia	 0.7720	 0.6580
Ja	 0.5830	 0.5900
Ka	 0.3840	 0.5330
L3	 0.1040	 0.3200
La	 0.1670	 0.4420
Ma	 0.6890	 0.6370
Na	 0.5200	 0.5560
Oa	 0.3600	 0.5250
Pa	 0.4400	 0.5630
Ra	 0.2300	 0.4420
Ta	 0.2680	 0.4610
Ua	 0.7220	 0.6350
Va	 0.7970	 0.6580
W2	 0.4430	 0.4360
Wa	 0.3440	 0.5290

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Xa	 0.6470	 0.6060
Ya	 0.2310	 0.4460
Za	 0.4740	 0.5660
h1	 0.7170	 0.5790