



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:24 AM UTC

PDB ID : 9HES / pdb\_00009hes  
EMDB ID : EMD-52095  
Title : Structure of the Arabidopsis thaliana 80S ribosome OVAC mutant in complex with P- and E-site tRNAs, mRNA, and thermospermine  
Authors : Faille, A.; Warren, A.J.  
Deposited on : 2024-11-14  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

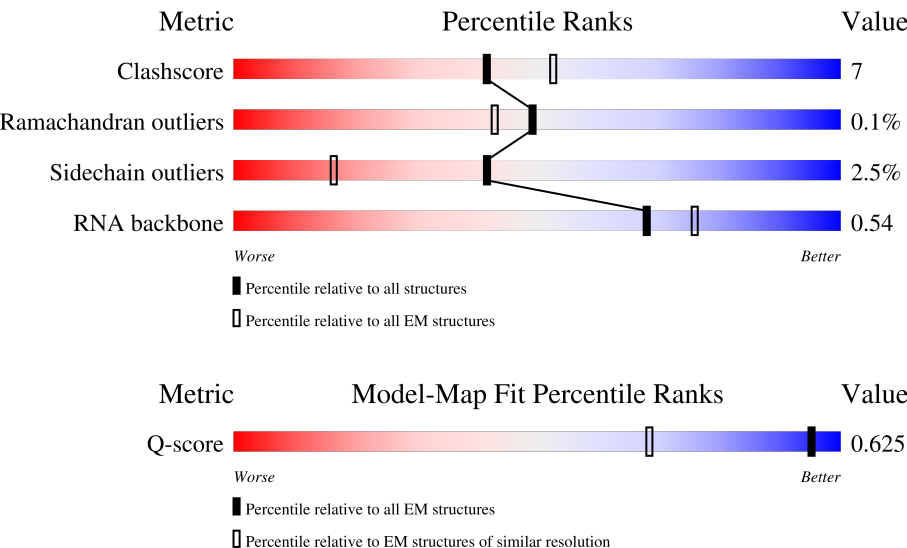


# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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	3458 ( 1.75 - 2.75 )

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  $\geq 3$ , 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	3	164	
2	A	3385	
3	2	76	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
3	W2	76	
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	<div><div><div></div><div></div><div></div></div><div>49%35%15%•48%</div></div>
79	L3	23	<div><div><div></div><div></div></div><div>100%100%</div></div>



## 2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 207912 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 Ribosomal RNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	162	Total	C	N	O	P	0	0
			3453	1544	617	1130	162		

- Molecule 2 is a RNA chain called Ribosomal RNA 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3149	Total	C	N	O	P	0	0
			67504	30152	12264	21939	3149		

- Molecule 3 is a RNA chain called Transfer RNA Phe GAA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	76	Total	C	N	O	P	0	0
			1630	726	298	530	76		
3	W2	76	Total	C	N	O	P	0	0
			1629	726	298	529	76		

- 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.



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		

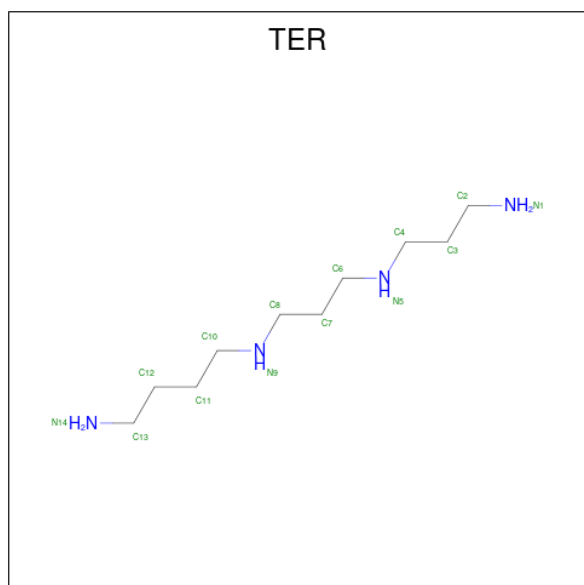
- Molecule 78 is a protein called Small ribosomal subunit protein eS10z.

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-DIAMINOBTANE (CCD ID: TER) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>) (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	BS	2	Total	Mg	0
			2	2	
81	AC	1	Total	Mg	0
			1	1	
81	BI	1	Total	Mg	0
			1	1	
81	BR	1	Total	Mg	0
			1	1	
81	BV	1	Total	Mg	0
			1	1	
81	Wa	1	Total	Mg	0
			1	1	
81	Ta	1	Total	Mg	0
			1	1	
81	AY	2	Total	Mg	0
			2	2	
81	h1	77	Total	Mg	0
			77	77	

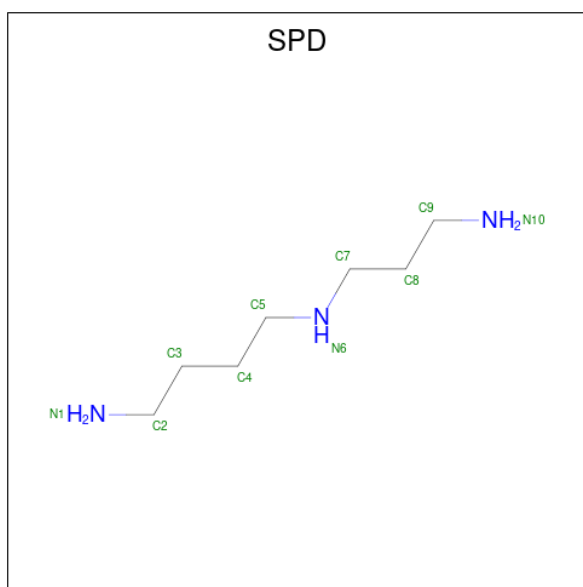
- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).



Mol	Chain	Residues	Atoms	AltConf
82	3	3	Total K 3 3	0
82	A	122	Total K 122 122	0
82	C3	1	Total K 1 1	0
82	BM	2	Total K 2 2	0
82	AR	1	Total K 1 1	0
82	Ea	1	Total K 1 1	0
82	Va	1	Total K 1 1	0
82	BD	1	Total K 1 1	0
82	BS	2	Total K 2 2	0
82	AV	1	Total K 1 1	0
82	AD	1	Total K 1 1	0
82	AJ	1	Total K 1 1	0
82	BQ	2	Total K 2 2	0
82	Fa	1	Total K 1 1	0
82	BJ	1	Total K 1 1	0
82	AG	2	Total K 2 2	0
82	Wa	1	Total K 1 1	0
82	Ua	1	Total K 1 1	0
82	Ca	1	Total K 1 1	0
82	h1	40	Total K 40 40	0

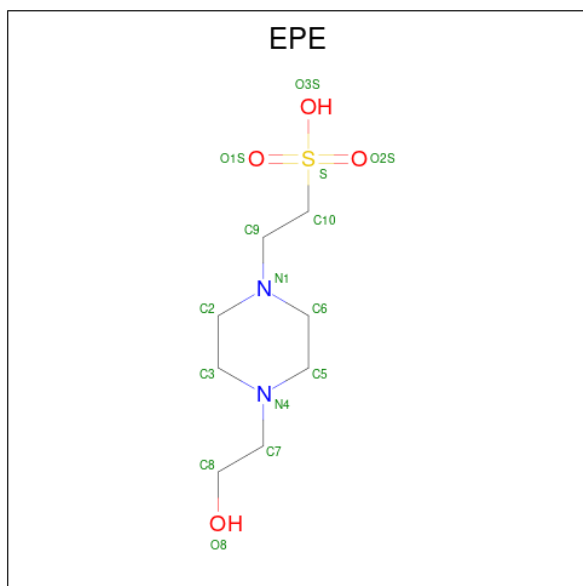
- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).





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	3	298	Total 298	O 298	0
86	A	6794	Total 6794	O 6794	0
86	2	2	Total 2	O 2	0
86	C3	154	Total 154	O 154	0
86	BC	9	Total 9	O 9	0
86	BM	59	Total 59	O 59	0
86	BO	31	Total 31	O 31	0
86	AR	41	Total 41	O 41	0
86	AU	26	Total 26	O 26	0
86	Ma	17	Total 17	O 17	0
86	Ia	20	Total 20	O 20	0
86	AE	14	Total 14	O 14	0
86	AX	21	Total 21	O 21	0
86	AP	11	Total 11	O 11	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
86	Ja	13	Total 13	O 13	0
86	Ea	123	Total 123	O 123	0
86	AL	58	Total 58	O 58	0
86	Va	19	Total 19	O 19	0
86	Ka	1	Total 1	O 1	0
86	AW	53	Total 53	O 53	0
86	BD	53	Total 53	O 53	0
86	BS	151	Total 151	O 151	0
86	AM	78	Total 78	O 78	0
86	AC	11	Total 11	O 11	0
86	BI	36	Total 36	O 36	0
86	AH	19	Total 19	O 19	0
86	BT	127	Total 127	O 127	0
86	AV	61	Total 61	O 61	0
86	AD	5	Total 5	O 5	0
86	AJ	108	Total 108	O 108	0
86	BQ	129	Total 129	O 129	0
86	BH	86	Total 86	O 86	0
86	Da	19	Total 19	O 19	0
86	BK	58	Total 58	O 58	0
86	AT	7	Total 7	O 7	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
86	Pa	2	Total 2	O 2	0
86	BP	21	Total 21	O 21	0
86	BN	30	Total 30	O 30	0
86	BG	31	Total 31	O 31	0
86	Fa	56	Total 56	O 56	0
86	Ha	88	Total 88	O 88	0
86	BU	5	Total 5	O 5	0
86	BR	69	Total 69	O 69	0
86	Xa	13	Total 13	O 13	0
86	BV	12	Total 12	O 12	0
86	BJ	30	Total 30	O 30	0
86	AO	17	Total 17	O 17	0
86	AK	42	Total 42	O 42	0
86	Na	2	Total 2	O 2	0
86	AB	5	Total 5	O 5	0
86	BF	14	Total 14	O 14	0
86	AA	1	Total 1	O 1	0
86	AG	82	Total 82	O 82	0
86	Ga	11	Total 11	O 11	0
86	BA	23	Total 23	O 23	0
86	AF	5	Total 5	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
86	Ta	4	Total 4	O 4	0
86	AZ	2	Total 2	O 2	0
86	BE	32	Total 32	O 32	0
86	AQ	4	Total 4	O 4	0
86	Oa	1	Total 1	O 1	0
86	Ua	22	Total 22	O 22	0
86	BL	1	Total 1	O 1	0
86	Aa	6	Total 6	O 6	0
86	AY	70	Total 70	O 70	0
86	Ca	2	Total 2	O 2	0
86	h1	1197	Total 1197	O 1197	0
86	B1	19	Total 19	O 19	0
86	W2	22	Total 22	O 22	0
86	Ba	2	Total 2	O 2	0
86	L3	1	Total 1	O 1	0

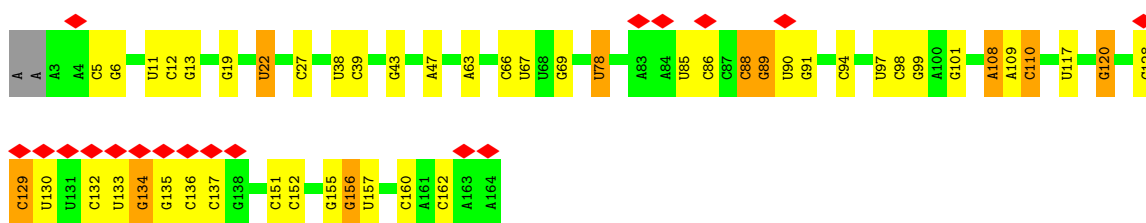


### 3 Residue-property plots

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.

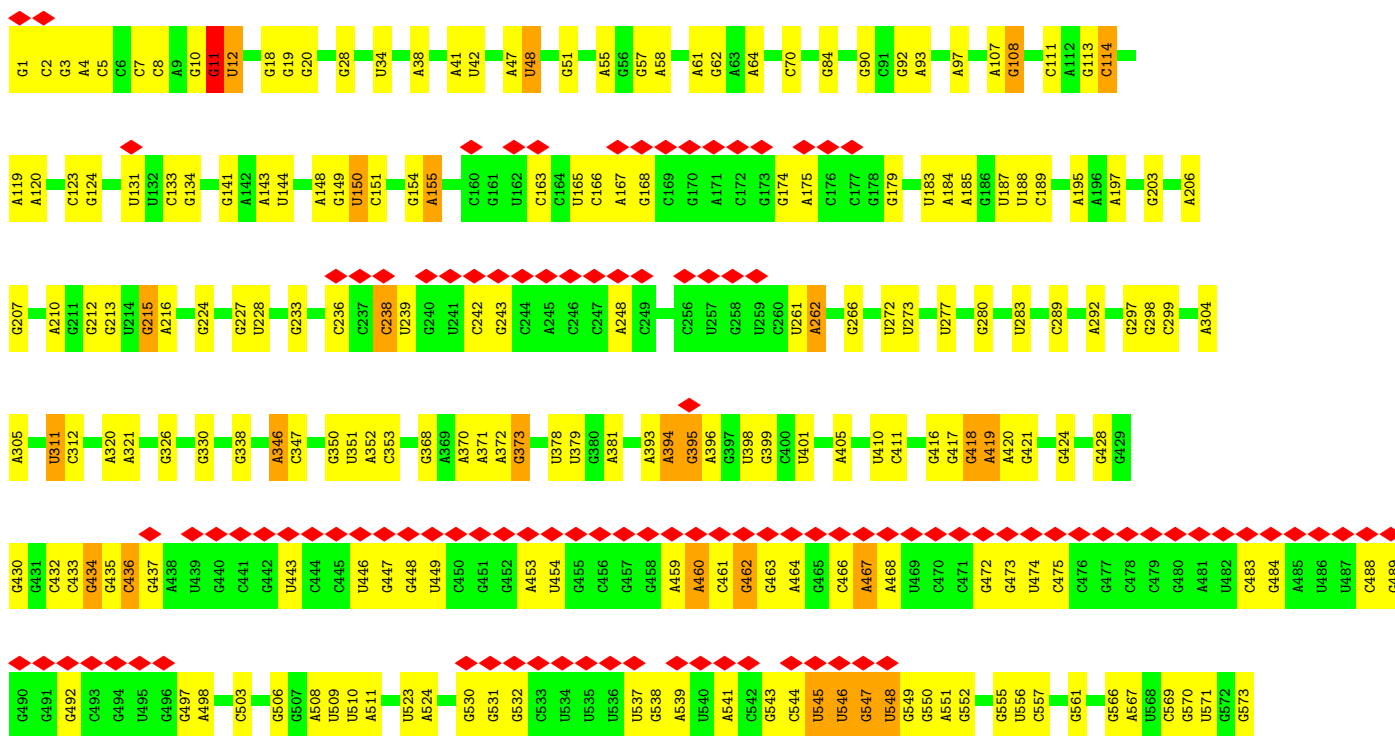
#### • Molecule 1: Ribosomal RNA 5.8S

Chain 3: 



#### • Molecule 2: Ribosomal RNA 25S

Chain A: 





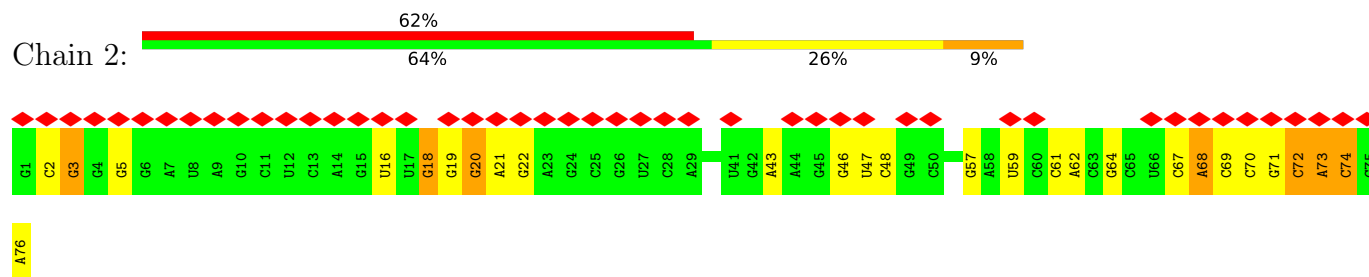




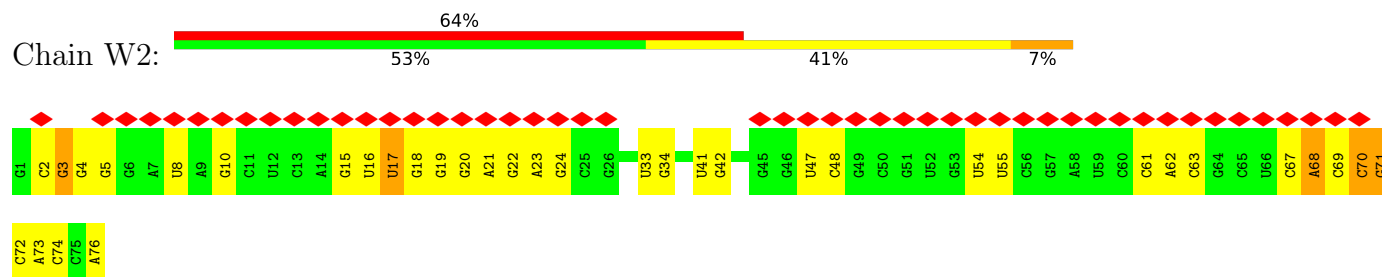




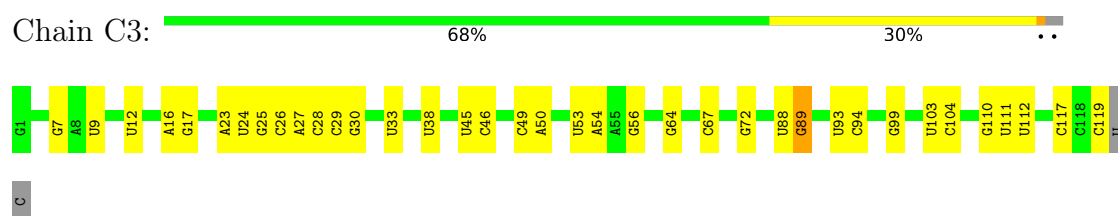
- Molecule 3: Transfer RNA Phe GAA



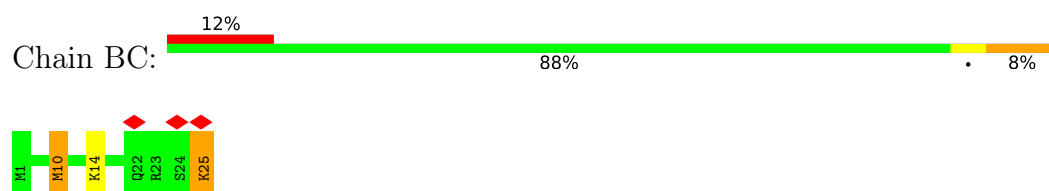
- Molecule 3: Transfer RNA Phe GAA



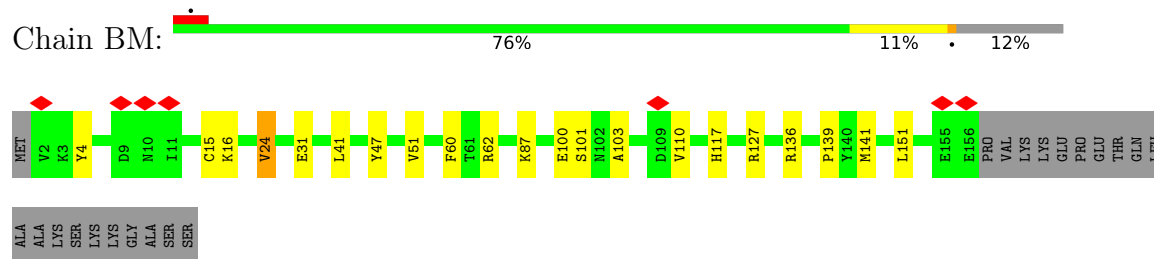
- Molecule 4: Ribosomal RNA 5S



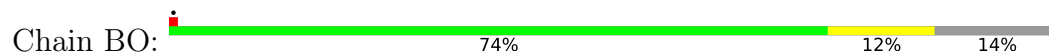
- Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v



- Molecule 6: Large ribosomal subunit protein uL22z



- Molecule 7: Large ribosomal subunit protein uL24z

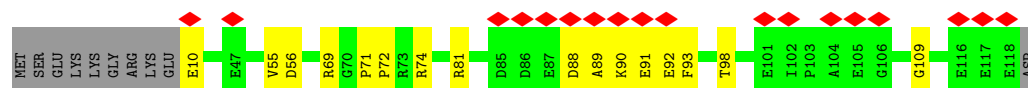
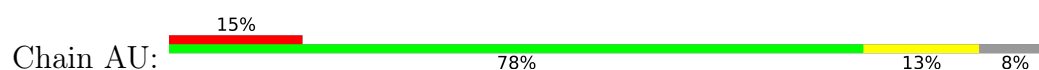




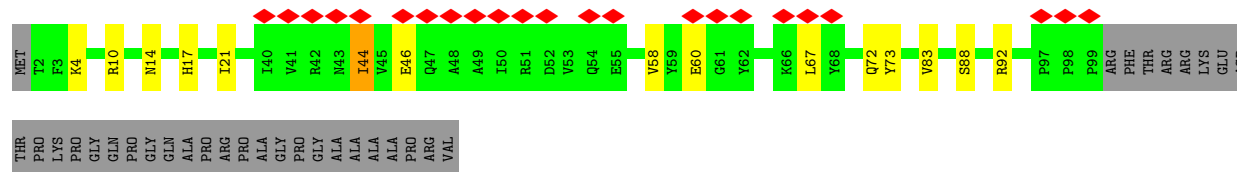
- Molecule 8: 60S ribosomal protein L29



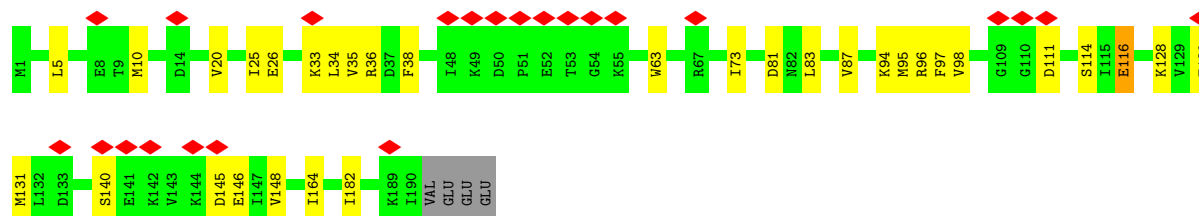
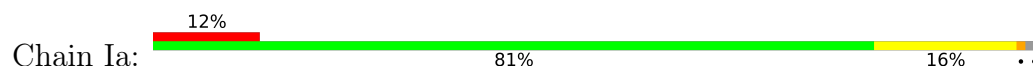
- Molecule 9: Large ribosomal subunit protein eL31y



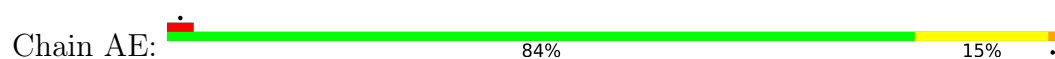
- Molecule 10: Small ribosomal subunit protein eS26y



- Molecule 11: Large ribosomal subunit protein uL6z/uL6y

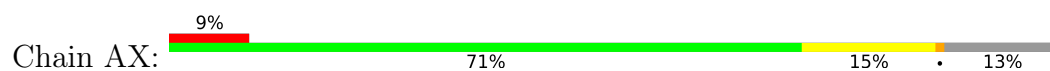


- Molecule 12: Small ribosomal subunit protein uS8z/uS8w

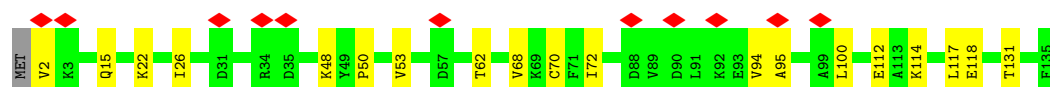
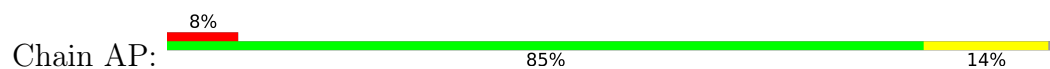




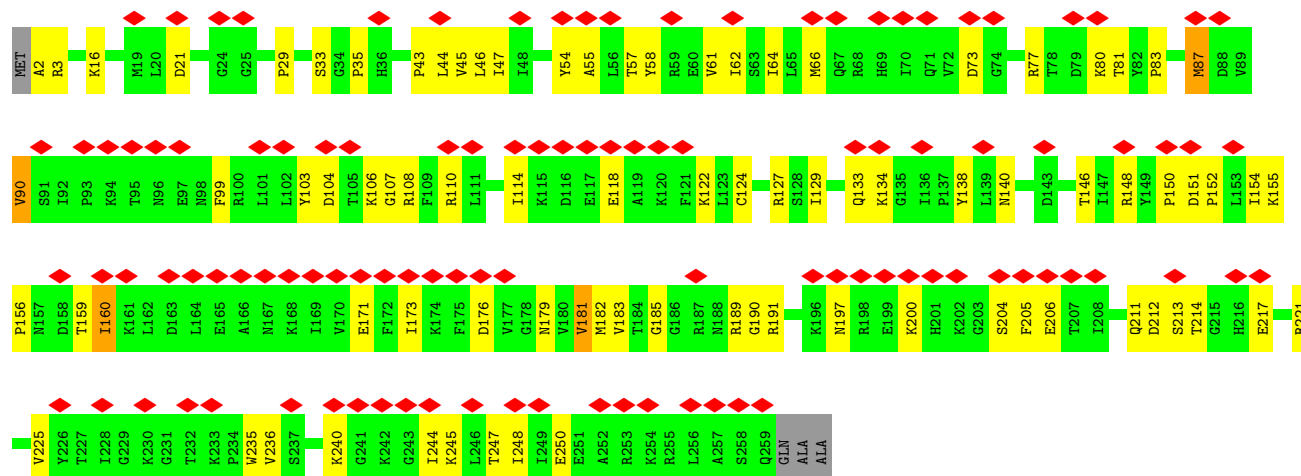
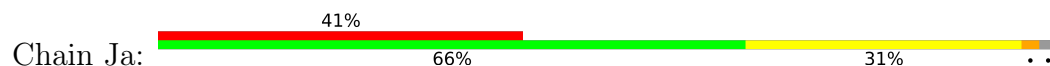
- Molecule 13: Large ribosomal subunit protein eL36y



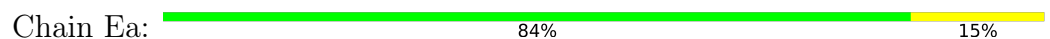
- Molecule 14: Large ribosomal subunit protein eL27x



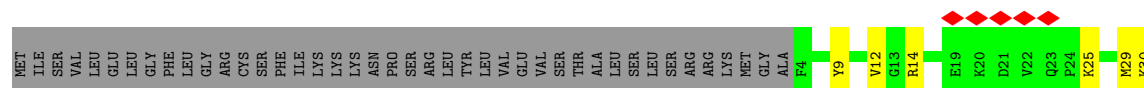
- Molecule 15: Small ribosomal subunit protein eS4x



- Molecule 16: Large ribosomal subunit protein eL15z



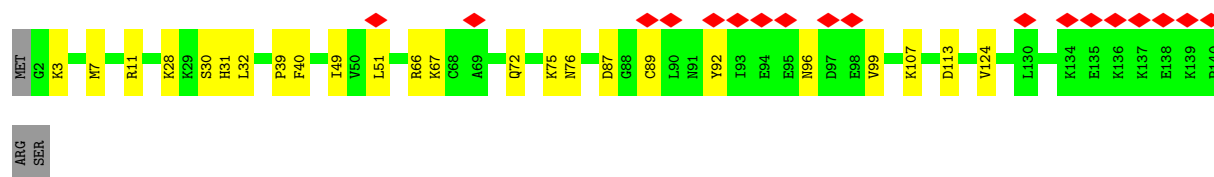
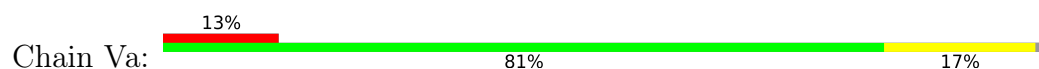
- Molecule 17: Ribosomal protein L18ae/LX family protein



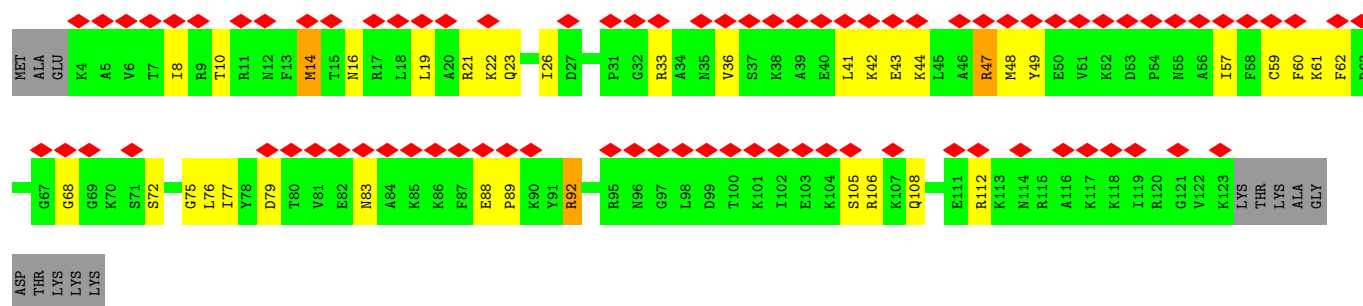




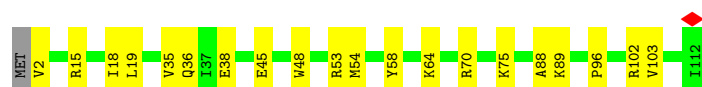
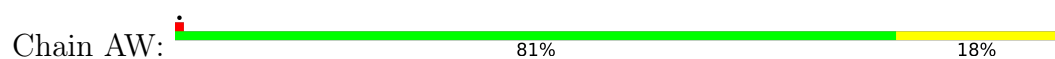
- Molecule 18: Small ribosomal subunit protein uS12y



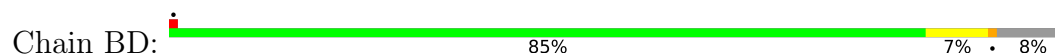
- Molecule 19: Small ribosomal subunit protein eS24y



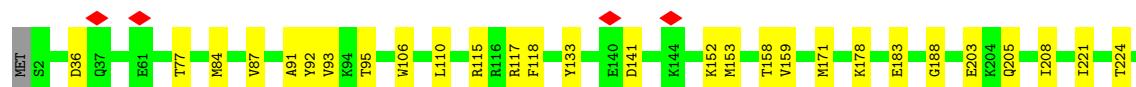
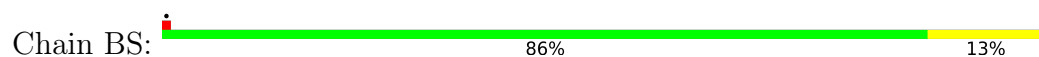
- Molecule 20: Large ribosomal subunit protein eL33y



- Molecule 21: Large ribosomal subunit protein eL42z/eL42y



- Molecule 22: Large ribosomal subunit protein uL3z

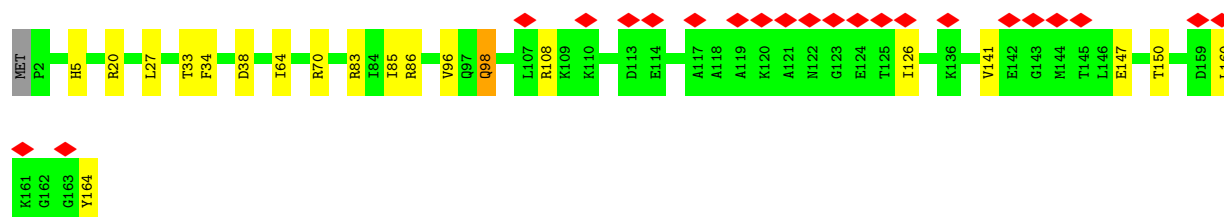






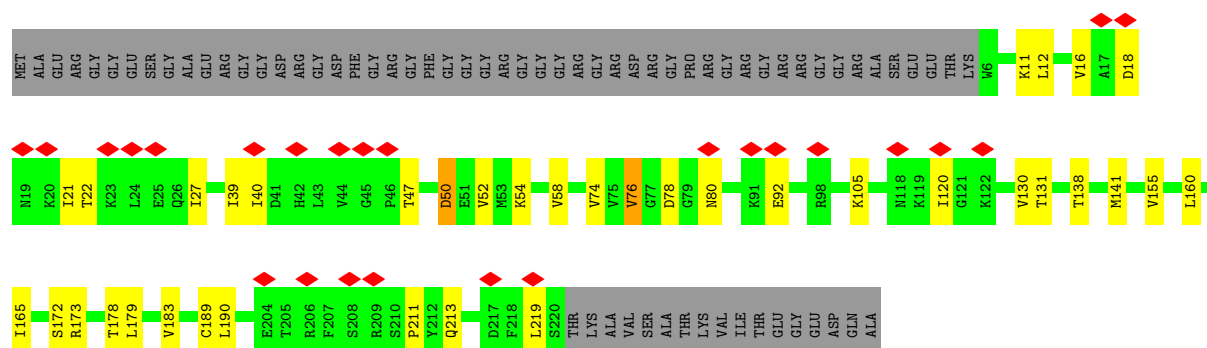
- Molecule 23: Large ribosomal subunit protein eL21z/eL21y

Chain AM: 13% 87% 12% ..



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

Chain AC: 9% 62% 13% 24%



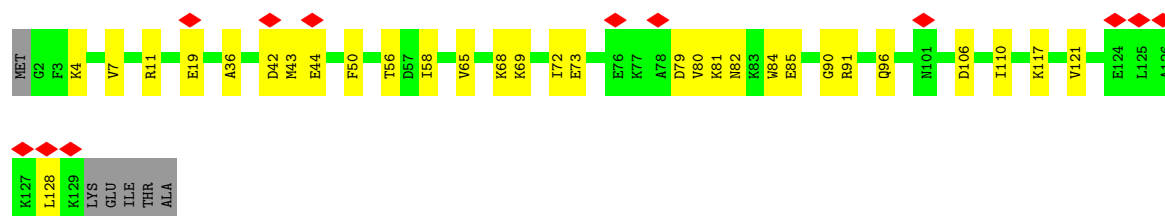
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI: 81% 12% 6%



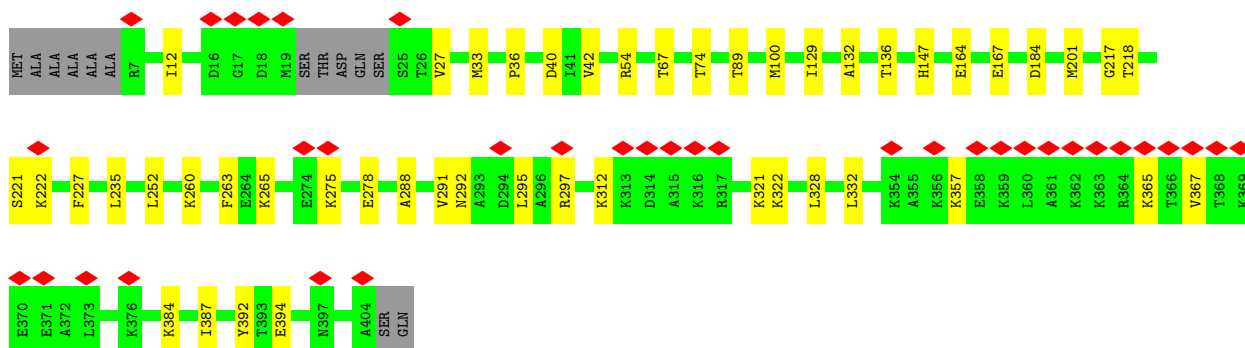
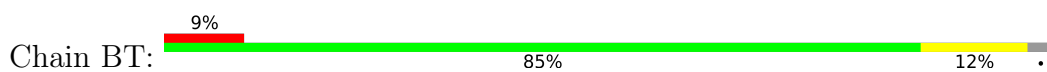
- Molecule 26: Large ribosomal subunit protein eL14y

Chain AH: 9% 73% 22%

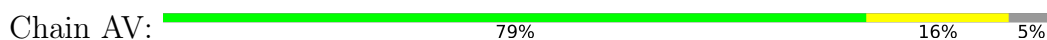


- Molecule 27: Large ribosomal subunit protein uL4z

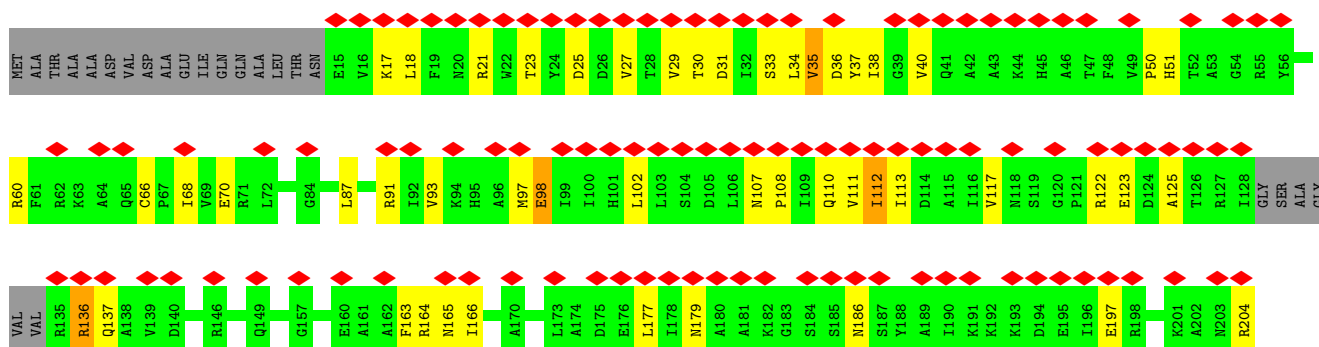




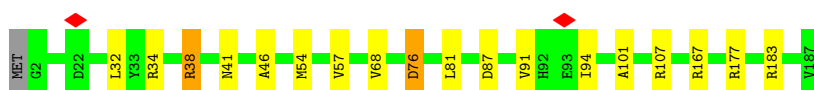
- Molecule 28: Large ribosomal subunit protein eL32z



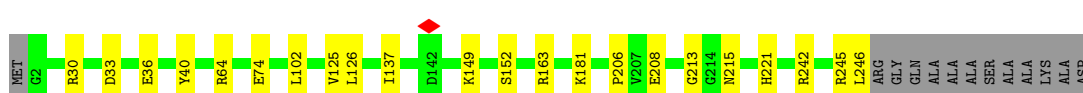
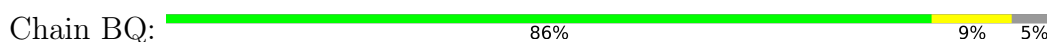
- Molecule 29: Small ribosomal subunit protein uS7y



- Molecule 30: Large ribosomal subunit protein eL18x

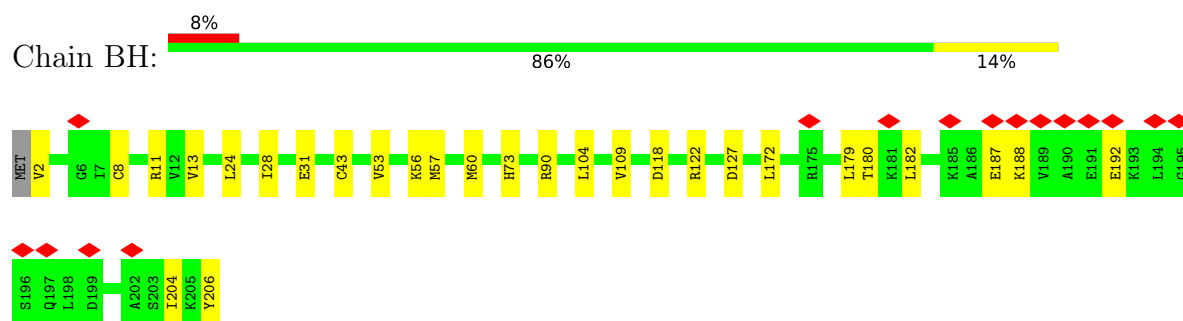


- Molecule 31: Large ribosomal subunit protein uL2z

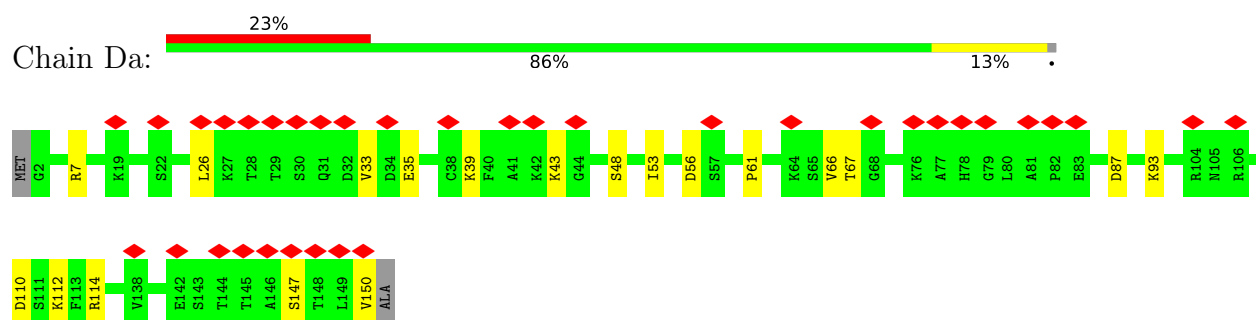




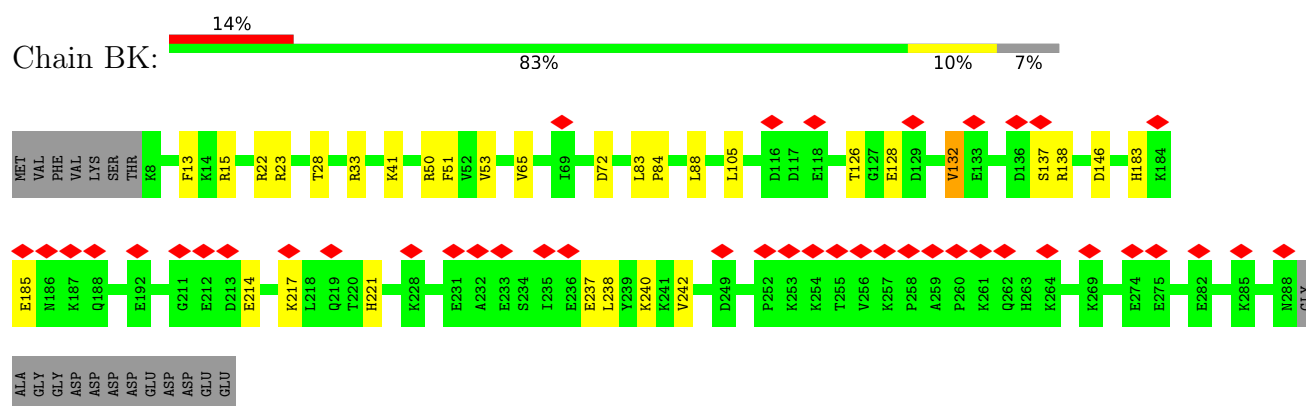
- Molecule 32: Large ribosomal subunit protein uL13y



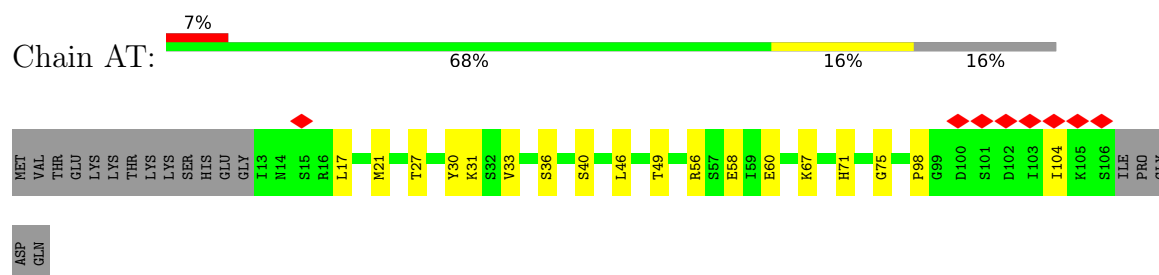
- Molecule 33: Small ribosomal subunit protein uS15y



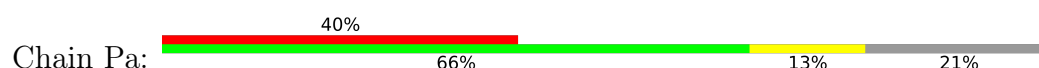
- Molecule 34: Large ribosomal subunit protein uL18z



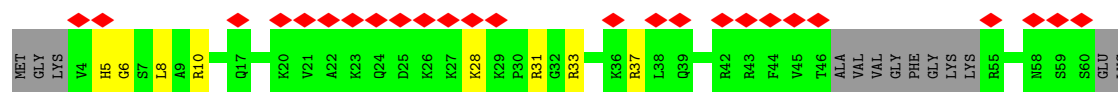
- Molecule 35: Large ribosomal subunit protein eL30y



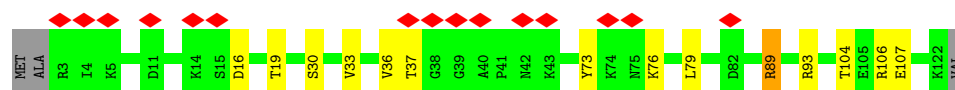
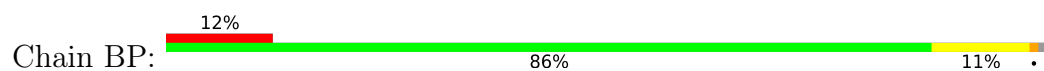
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x



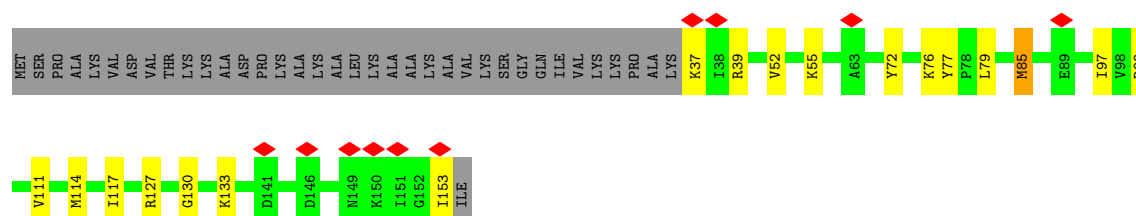




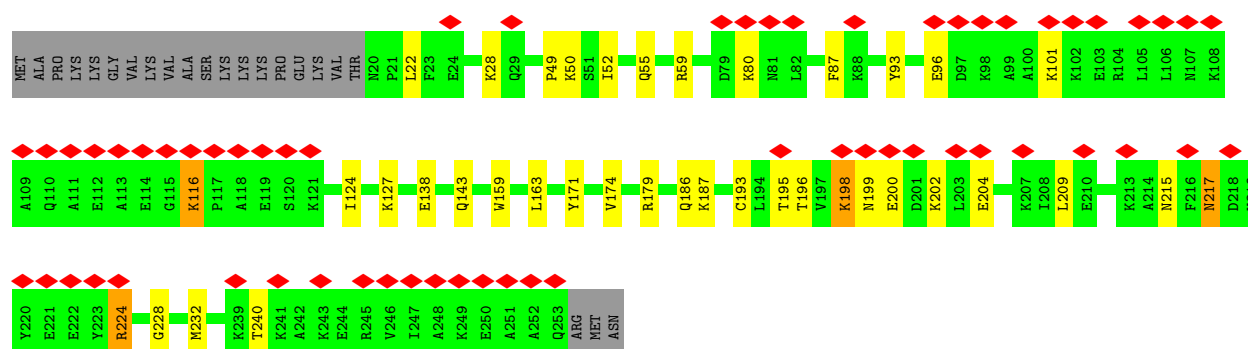
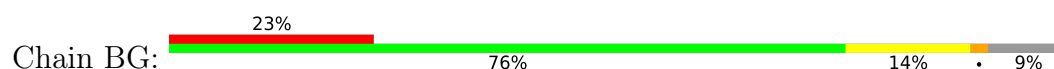
- Molecule 37: Large ribosomal subunit protein uL29x



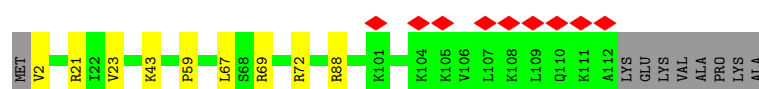
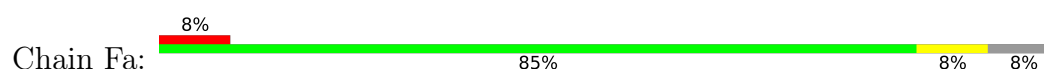
- Molecule 38: Large ribosomal subunit protein uL23y



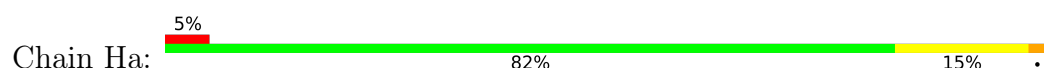
- Molecule 39: Large ribosomal subunit protein eL8y



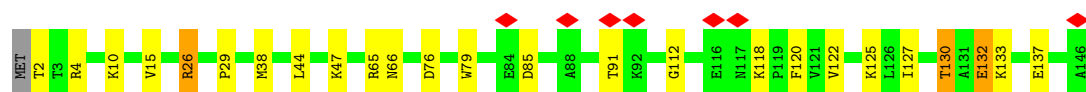
- Molecule 40: Large ribosomal subunit protein eL34z



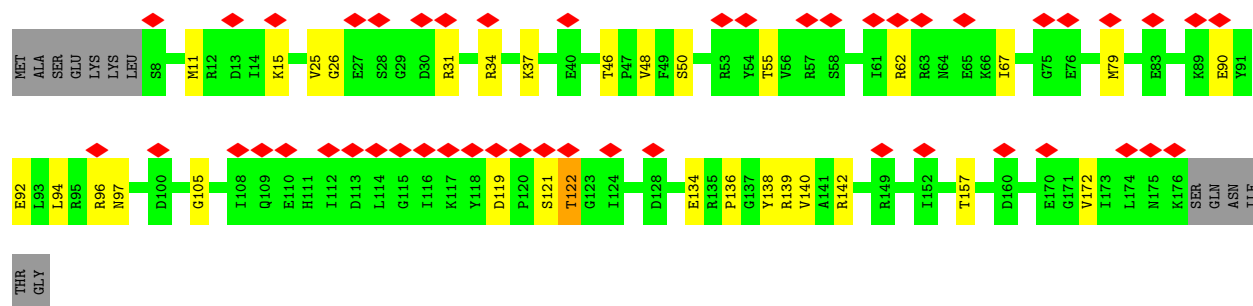
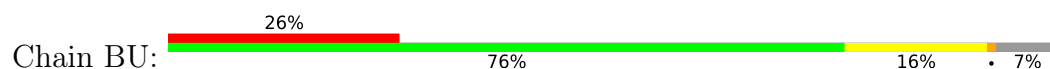
- Molecule 41: Large ribosomal subunit protein uL15x



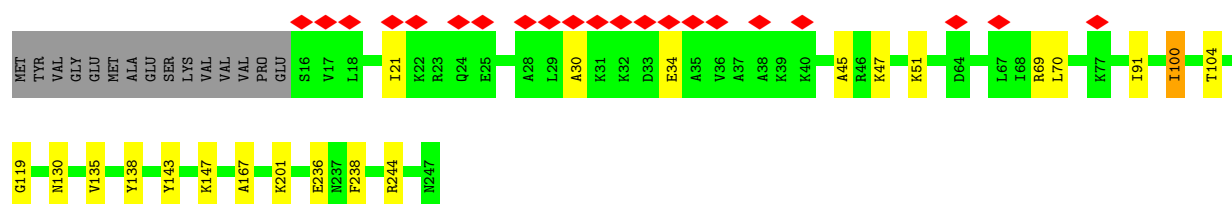
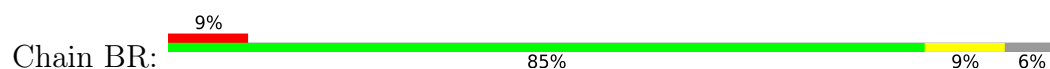




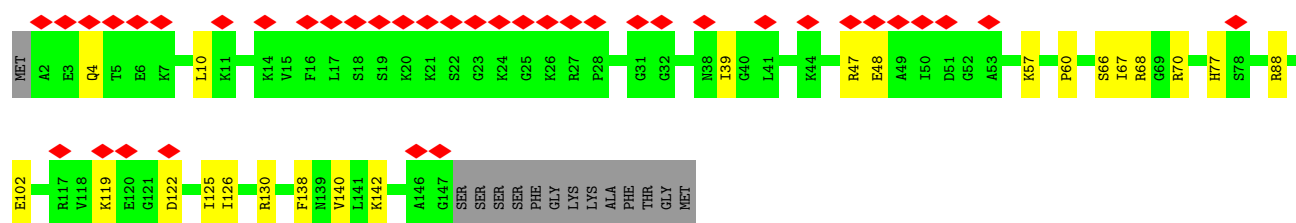
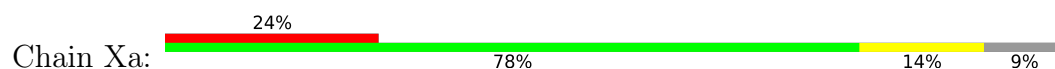
- Molecule 42: Large ribosomal subunit protein uL5z



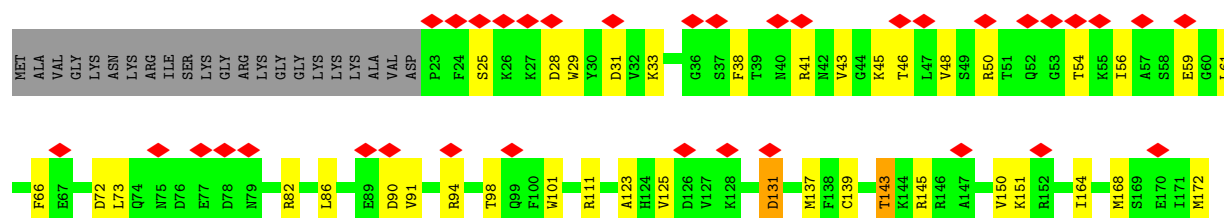
- Molecule 43: Ribosomal protein L30/L7 family protein



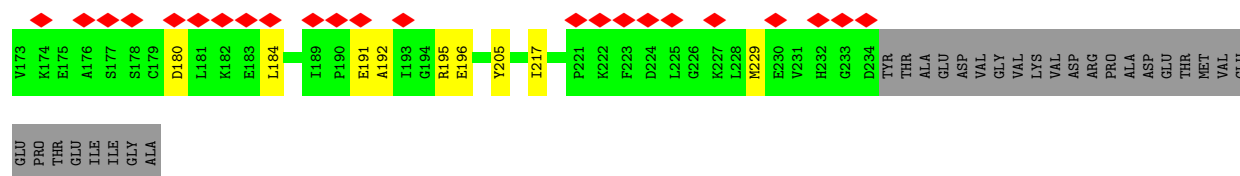
- Molecule 44: Small ribosomal subunit protein uS17z



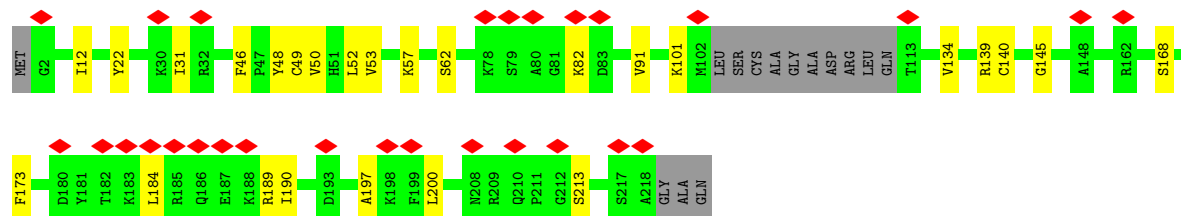
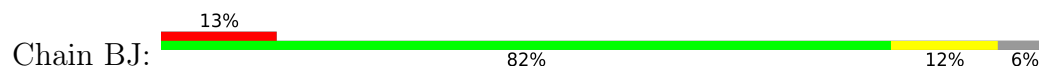
- Molecule 45: Small ribosomal subunit protein eS1y



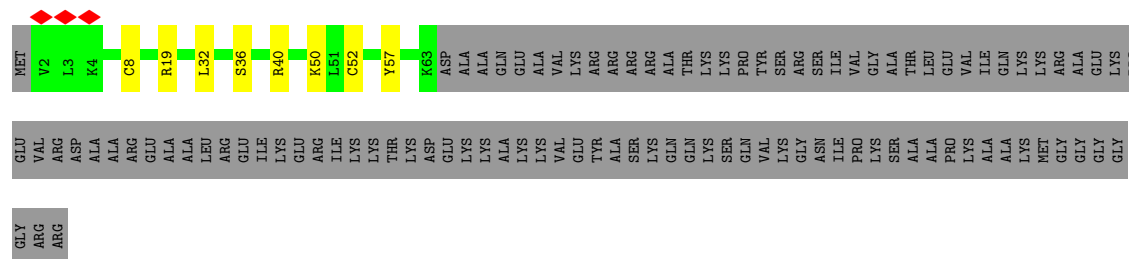
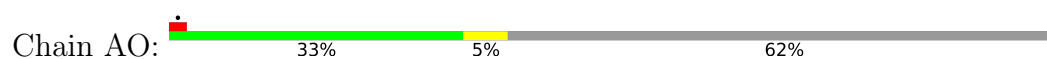




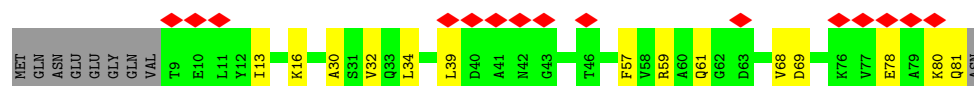
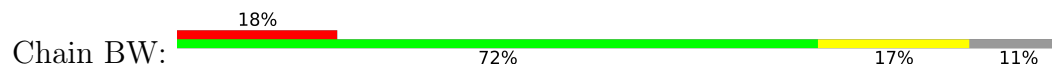
- Molecule 46: Large ribosomal subunit protein uL16y



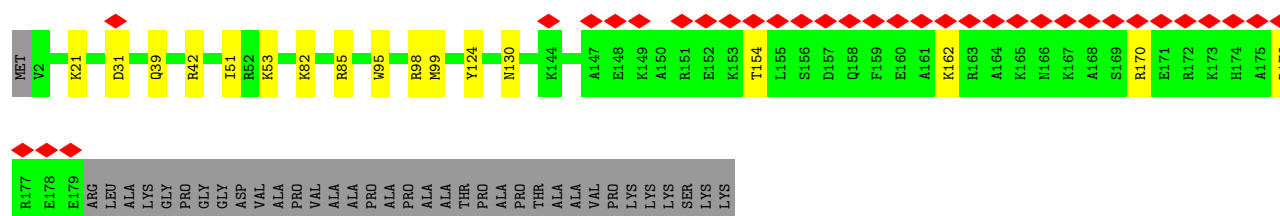
- Molecule 47: Large ribosomal subunit protein eL24z



- Molecule 48: Small ribosomal subunit protein eS21y

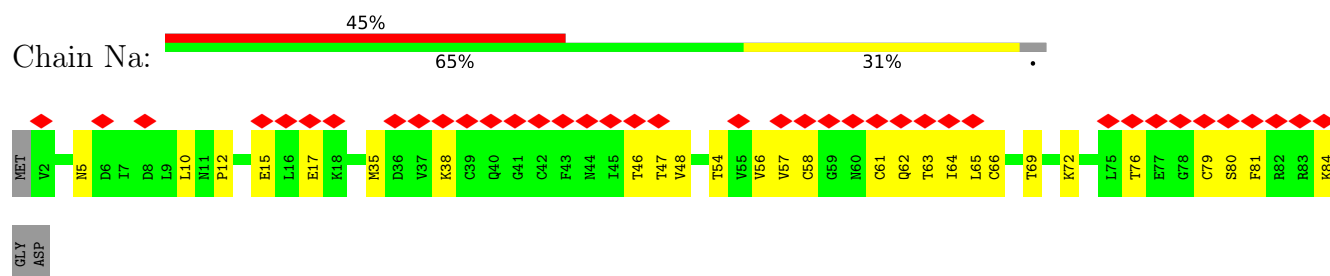


- Molecule 49: Large ribosomal subunit protein eL19x

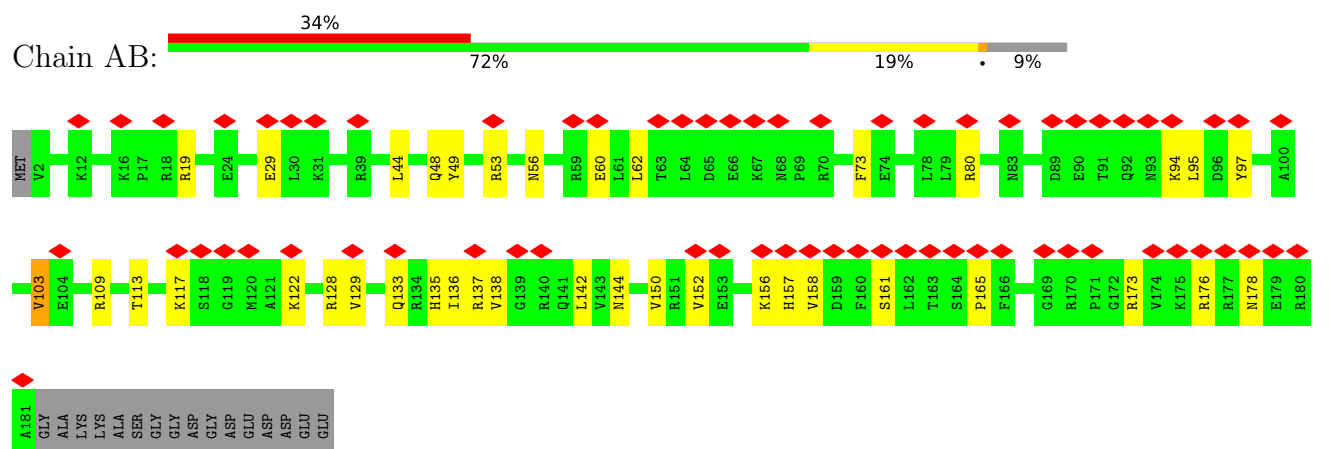


- Molecule 50: Small ribosomal subunit protein eS27y

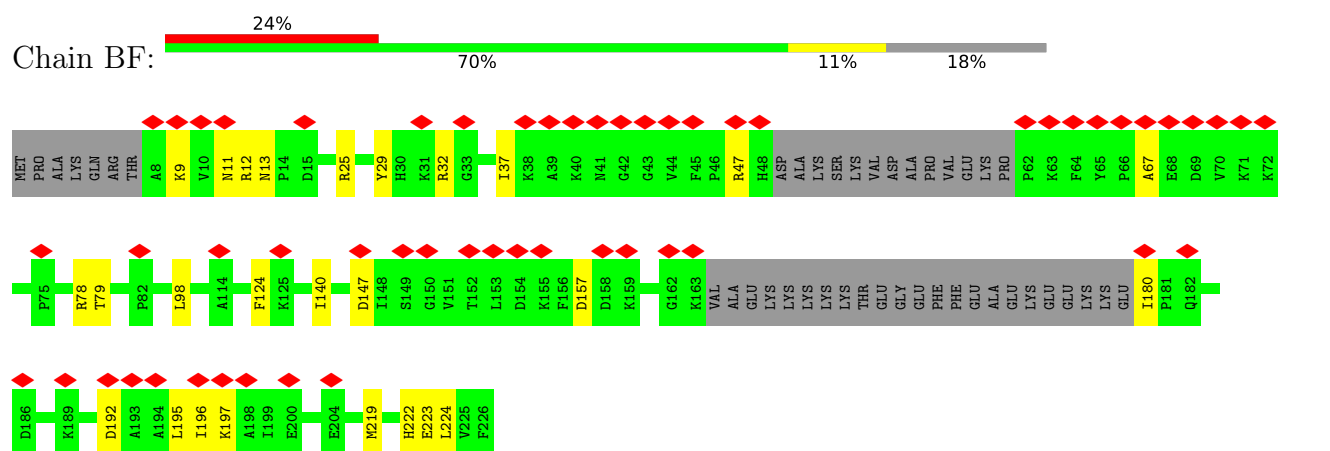




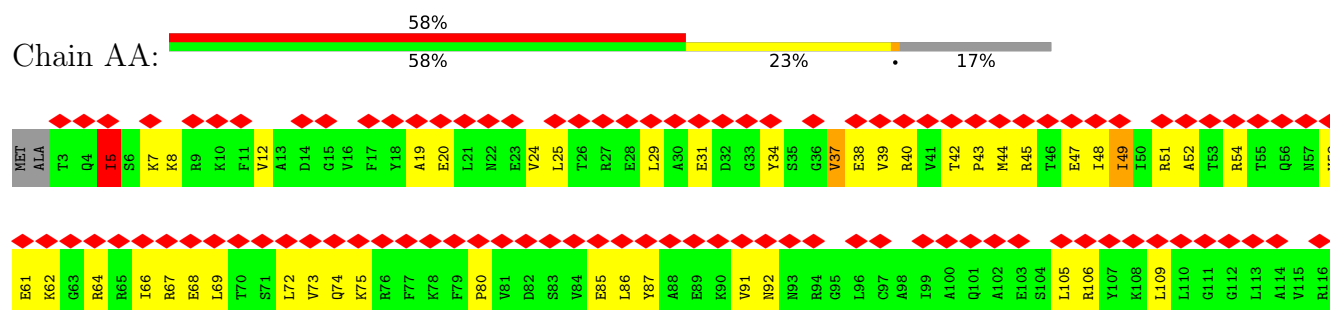
- Molecule 51: Small ribosomal subunit protein uS4y



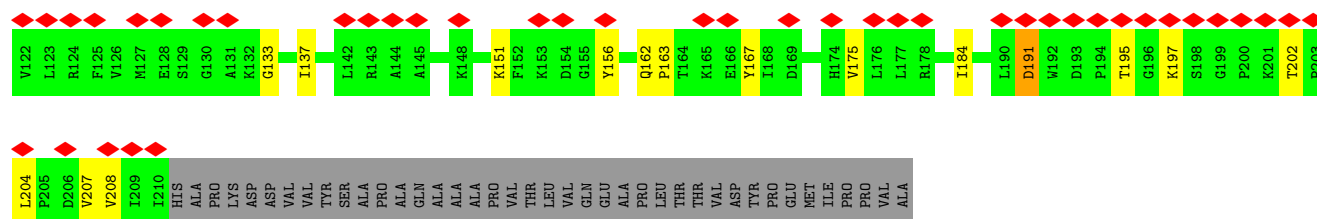
- Molecule 52: Large ribosomal subunit protein eL6y



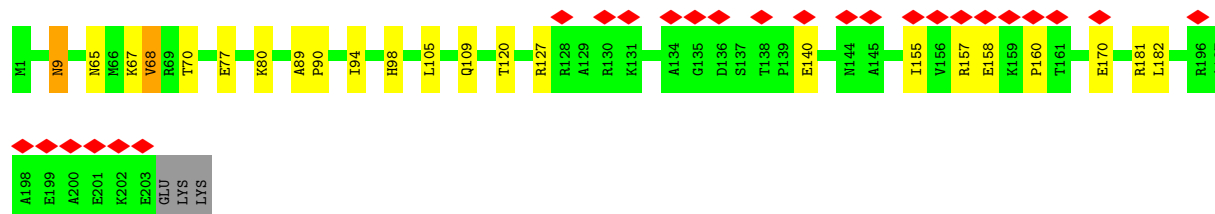
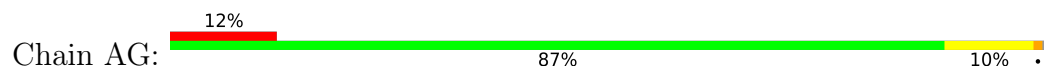
- Molecule 53: Small ribosomal subunit protein uS3z



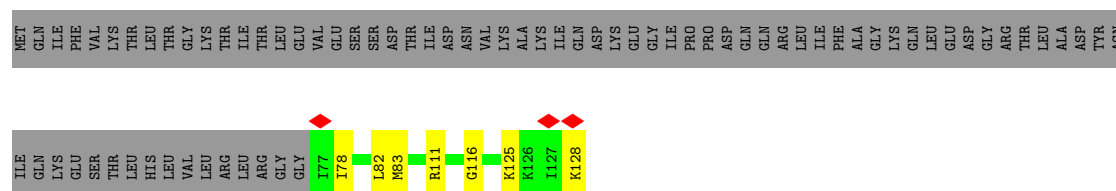
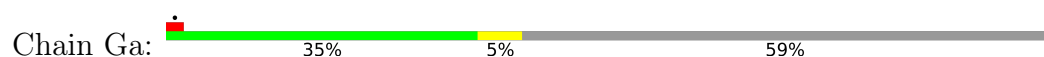




- Molecule 54: Large ribosomal subunit protein eL13z



- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein



- Molecule 56: Large ribosomal subunit protein eL39z/eL39x

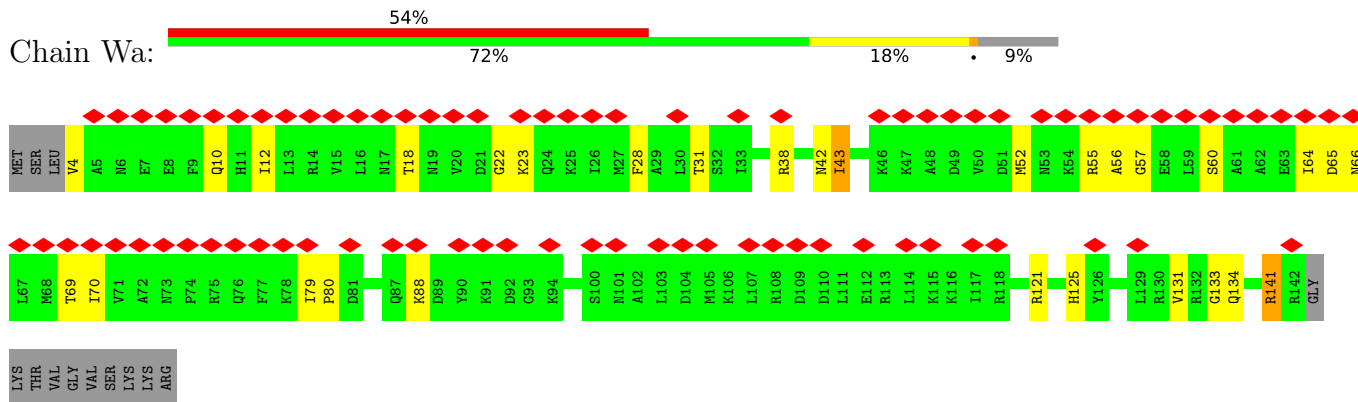


- Molecule 57: Small ribosomal subunit protein uS9z





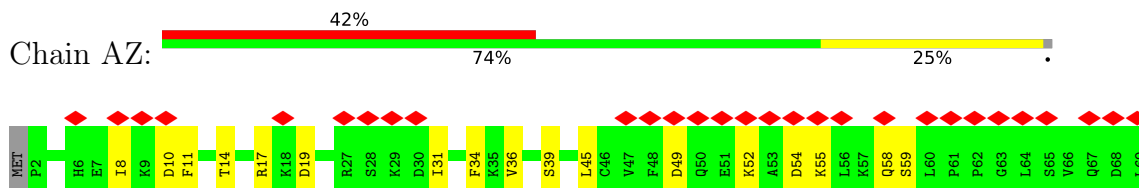
- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x



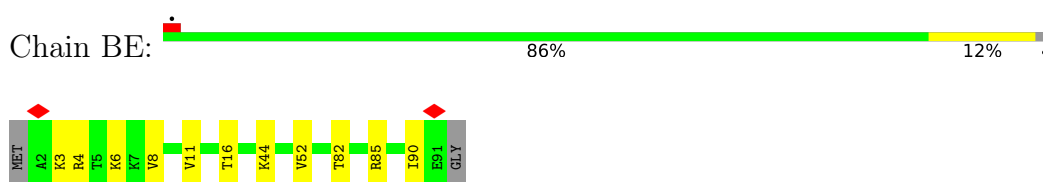
- Molecule 59: Small ribosomal subunit protein eS6y



- Molecule 60: Large ribosomal subunit protein eL38z/eL38y



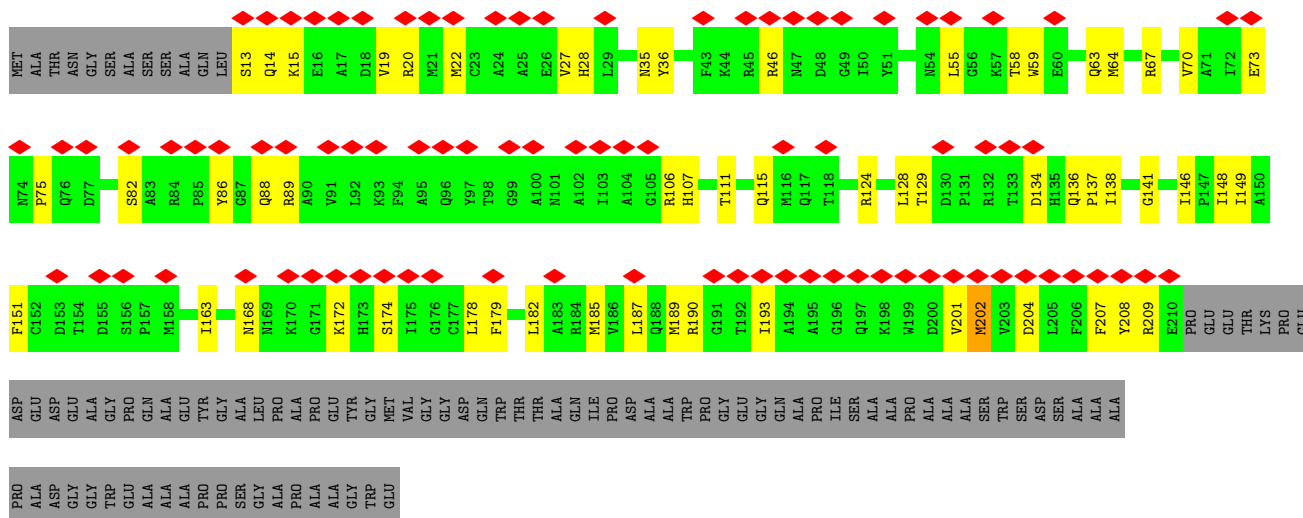
- Molecule 61: Large ribosomal subunit protein eL43y



- Molecule 62: Small ribosomal subunit protein uS2z



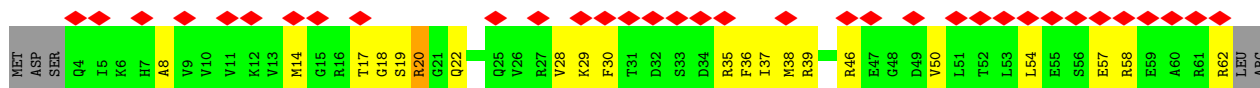




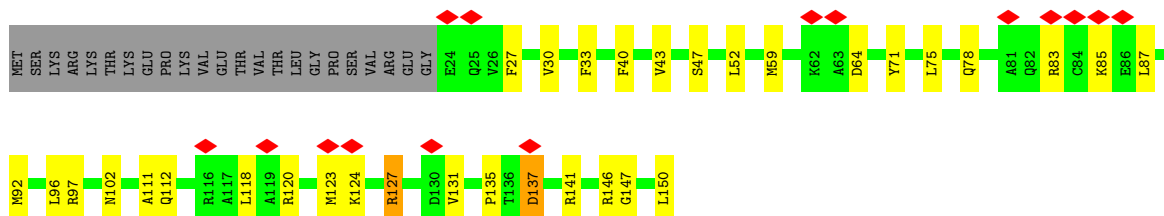
• Molecule 63: Large ribosomal subunit protein eL28z



• Molecule 64: Small ribosomal subunit protein eS28x

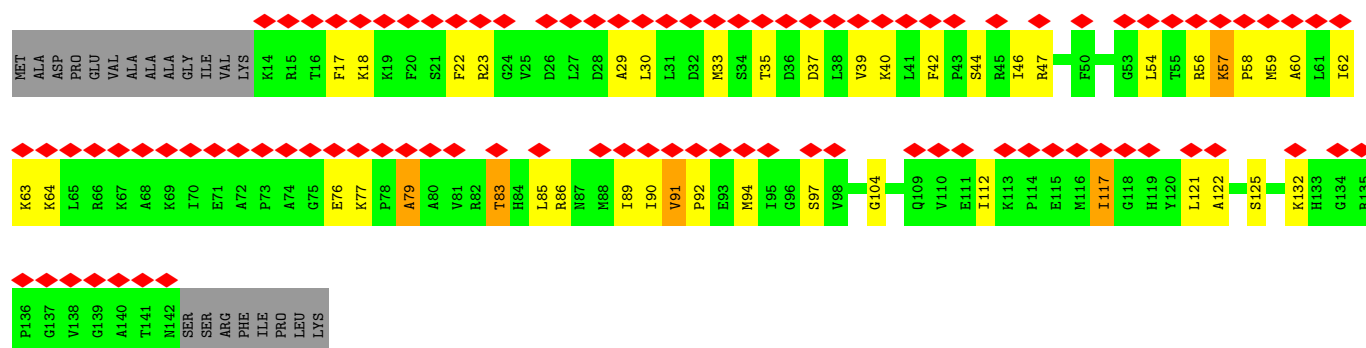


• Molecule 65: Small ribosomal subunit protein uS11y

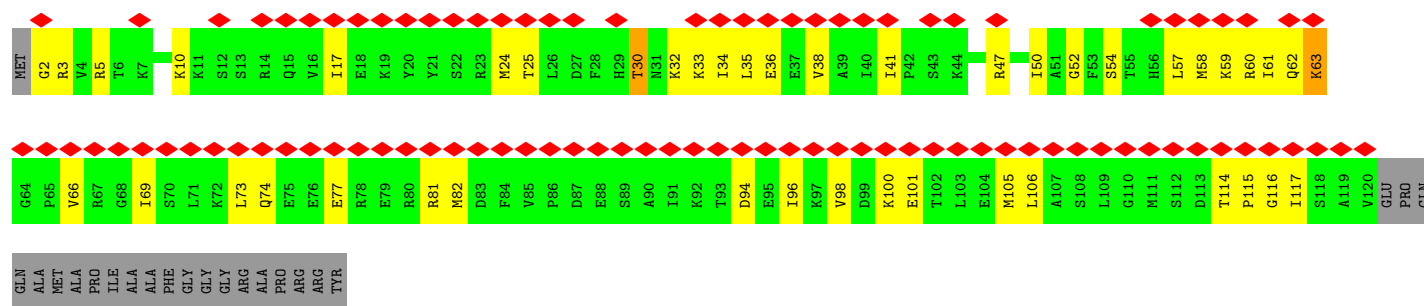


• Molecule 66: Small ribosomal subunit protein uS19y

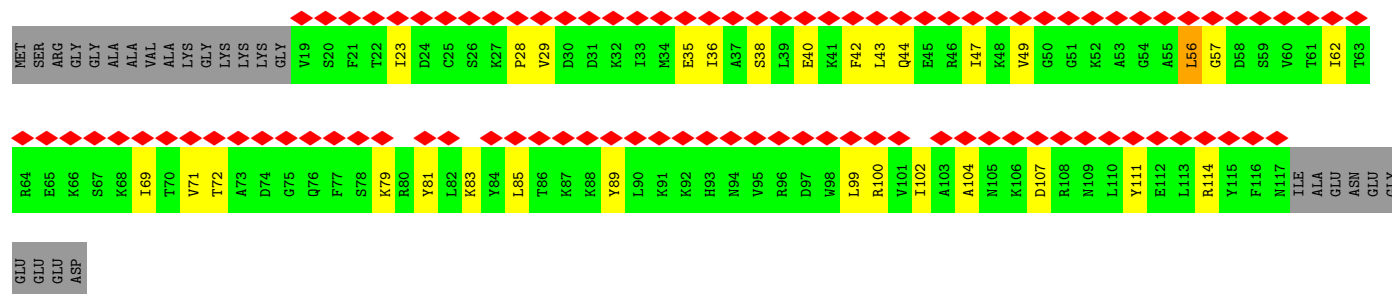
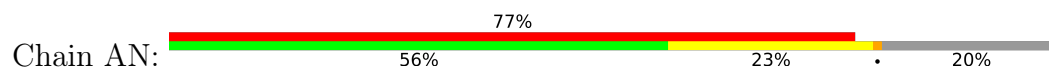




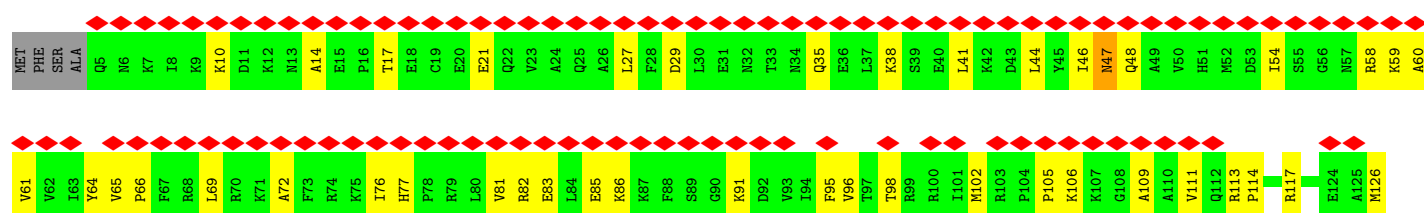
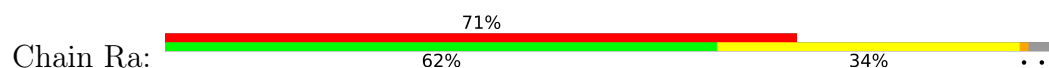
- Molecule 67: Small ribosomal subunit protein eS17w



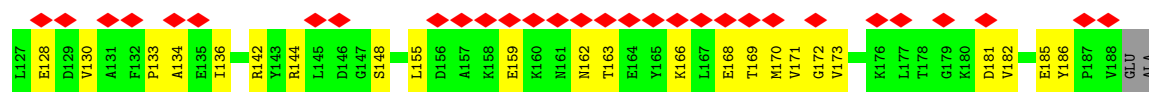
- Molecule 68: Large ribosomal subunit protein eL22z



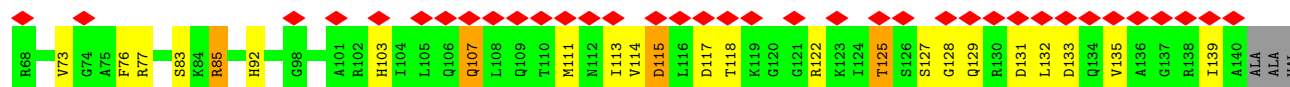
- Molecule 69: Small ribosomal subunit protein eS7x



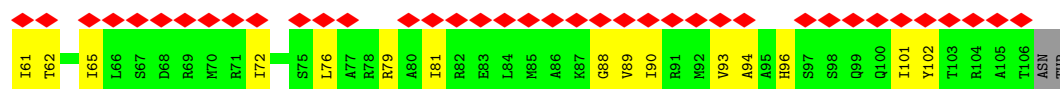
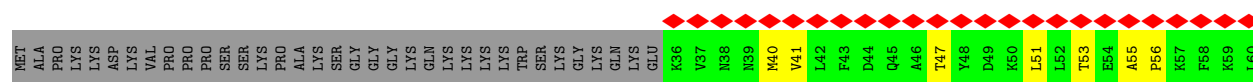




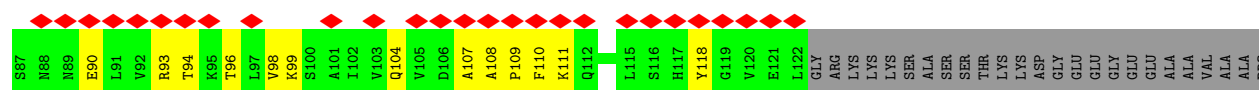
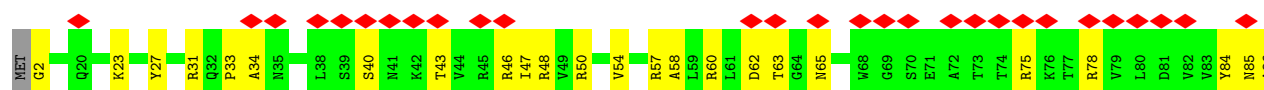
- Molecule 70: Small ribosomal subunit protein eS19x



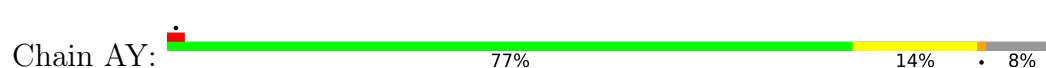
- Molecule 71: Small ribosomal subunit protein eS25w



- Molecule 72: Small ribosomal subunit protein eS8z



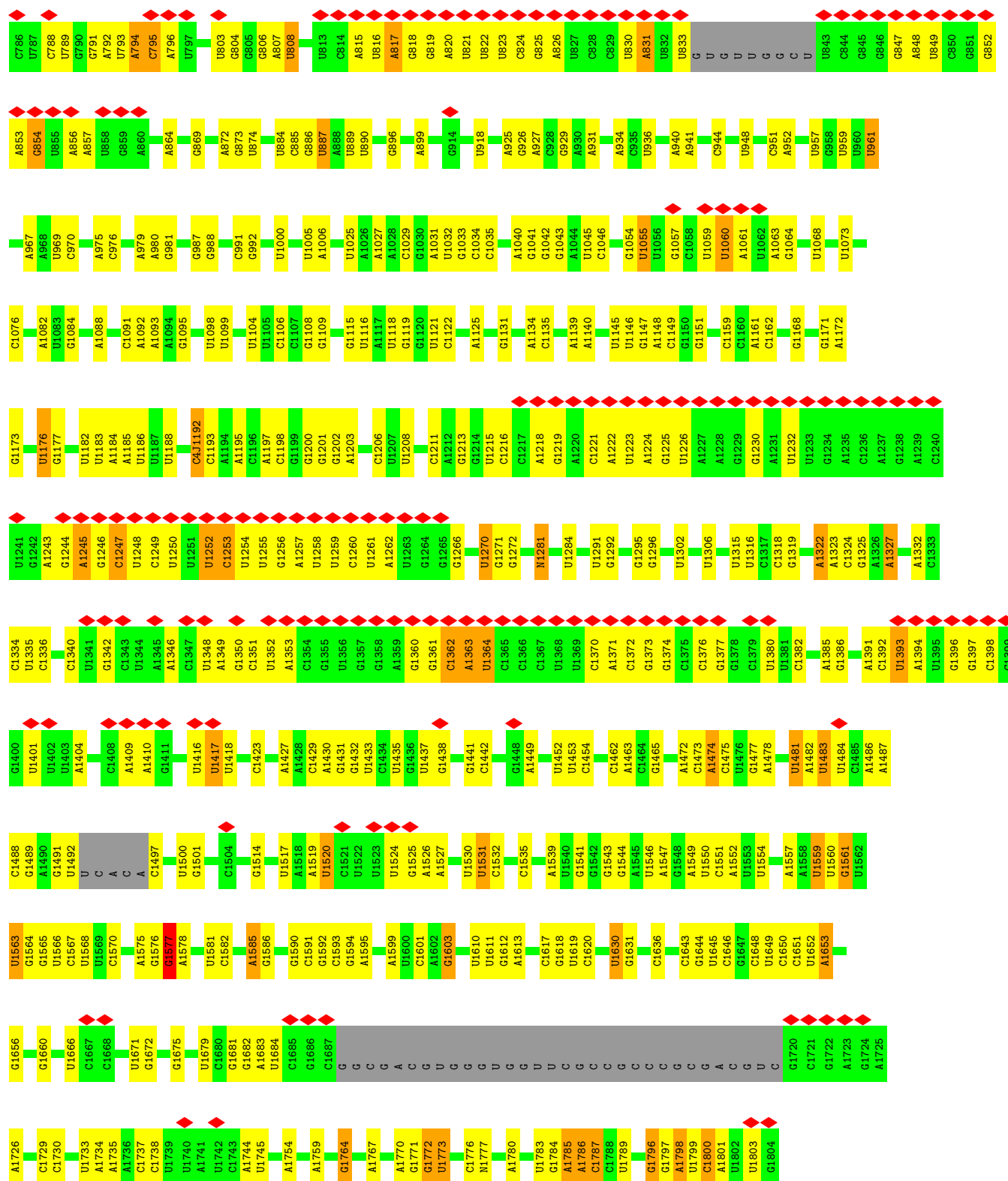
- Molecule 73: Large ribosomal subunit protein eL37z



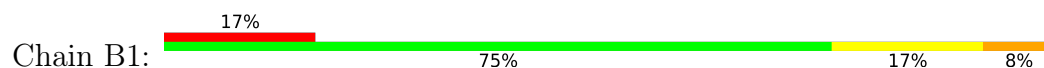




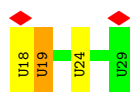




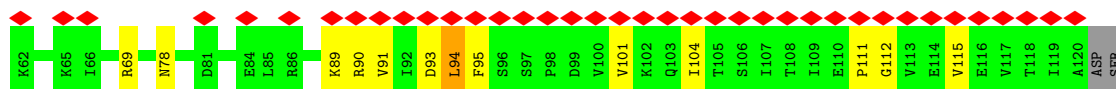
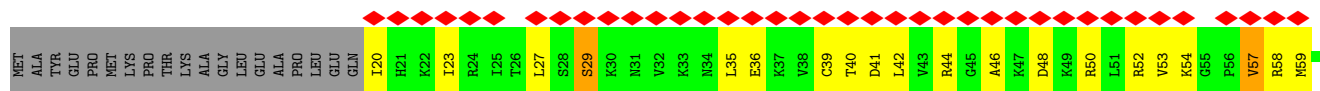
• Molecule 76: Messenger RNA



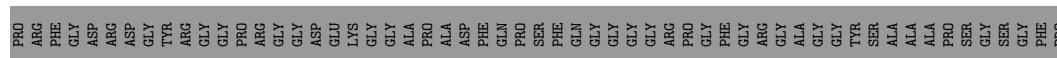
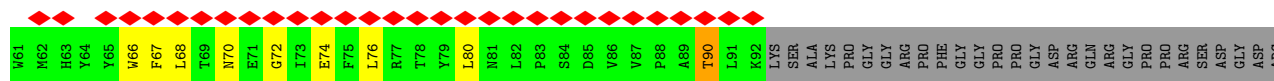
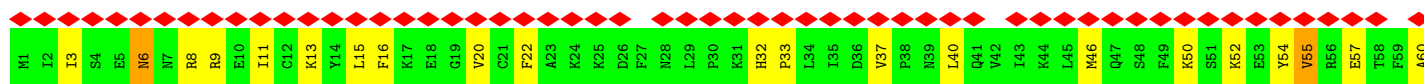
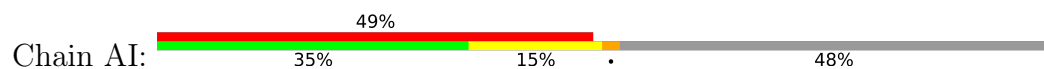




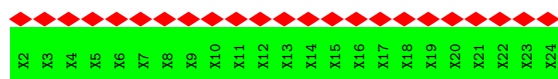
- Molecule 77: Small ribosomal subunit protein uS10y



- Molecule 78: Small ribosomal subunit protein eS10z



- Molecule 79: Nascent polypeptide





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31655	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 ( $e^-/\text{\AA}^2$ )	53.85	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.925	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	500.094, 500.094, 500.094	wwPDB
Map dimensions	686, 686, 686	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	3	0.59	1/3713 (0.0%)	0.80	1/5784 (0.0%)
2	A	0.59	8/72590 (0.0%)	0.82	14/113222 (0.0%)
3	2	0.54	0/1823	0.68	0/2840
3	W2	0.54	0/1822	0.68	0/2840
4	C3	0.57	0/2834	0.77	0/4415
5	BC	0.68	0/238	0.94	0/302
6	BM	0.65	0/1269	0.85	0/1705
7	BO	0.59	0/1042	0.81	0/1390
8	AR	0.64	0/435	0.90	0/577
9	AU	0.60	0/900	0.78	0/1202
10	Ma	0.56	0/804	0.73	0/1081
11	Ia	0.53	0/1533	0.71	0/2050
12	AE	0.54	0/1051	0.78	0/1406
13	AX	0.53	0/793	0.81	0/1047
14	AP	0.54	0/1110	0.77	0/1477
15	Ja	0.48	0/2116	0.71	0/2841
16	Ea	0.69	0/1743	0.87	0/2335
17	AL	0.59	0/1523	0.80	0/2042
18	Va	0.53	0/1100	0.72	0/1465
19	Ka	0.46	0/1001	0.68	0/1329
20	AW	0.63	0/921	0.78	0/1234
21	BD	0.59	0/806	0.79	0/1065
22	BS	0.61	0/3165	0.80	0/4238
23	AM	0.59	0/1335	0.80	0/1789
24	AC	0.52	0/1709	0.72	0/2310
25	BI	0.65	0/1002	0.84	1/1347 (0.1%)
26	AH	0.51	0/1054	0.78	0/1408
27	BT	0.63	0/3112	0.80	0/4187
28	AV	0.66	0/1045	0.88	1/1399 (0.1%)
29	AD	0.47	0/1473	0.69	0/1985
30	AJ	0.63	0/1492	0.84	0/1995



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	BQ	0.70	0/1921	0.86	0/2584
32	BH	0.64	0/1664	0.81	0/2224
33	Da	0.54	0/1214	0.76	0/1630
34	BK	0.55	0/2321	0.74	0/3119
35	AT	0.56	0/731	0.74	0/982
36	Pa	0.52	0/394	0.82	0/519
37	BP	0.56	0/984	0.78	0/1306
38	BN	0.57	0/972	0.77	0/1309
39	BG	0.54	0/1908	0.80	0/2561
40	Fa	0.63	0/909	0.88	0/1214
41	Ha	0.73	0/1187	0.96	2/1584 (0.1%)
42	BU	0.48	0/1388	0.70	0/1858
43	BR	0.59	0/1931	0.79	0/2584
44	Xa	0.50	0/1189	0.70	0/1590
45	BV	0.48	0/1746	0.72	0/2341
46	BJ	0.56	0/1691	0.71	0/2263
47	AO	0.58	0/541	0.76	0/718
48	BW	0.50	0/577	0.69	0/777
49	AK	0.60	0/1499	0.81	0/1975
50	Na	0.48	0/657	0.73	0/883
51	AB	0.46	0/1540	0.71	0/2061
52	BF	0.54	0/1521	0.73	0/2040
53	AA	0.47	0/1647	0.73	0/2212
54	AG	0.57	0/1680	0.83	0/2251
55	Ga	0.55	0/428	0.78	0/564
56	BA	0.67	0/456	0.88	0/603
57	AF	0.47	0/1133	0.71	0/1513
58	Wa	0.46	0/1152	0.70	0/1541
59	Ta	0.47	0/1819	0.73	0/2422
60	AZ	0.54	0/570	0.71	0/758
61	BE	0.65	0/711	0.83	0/942
62	Za	0.46	0/1609	0.71	0/2173
63	AQ	0.47	0/1070	0.71	0/1436
64	Oa	0.45	0/474	0.71	0/632
65	Ua	0.55	0/974	0.80	0/1305
66	Ya	0.48	0/1044	0.74	1/1398 (0.1%)
67	BB	0.46	0/965	0.75	0/1287
68	AN	0.44	0/820	0.68	0/1097
69	Ra	0.45	0/1530	0.73	0/2052
70	BL	0.48	0/1086	0.75	1/1459 (0.1%)
71	La	0.46	0/568	0.66	0/762
72	Aa	0.48	0/1517	0.71	0/2027
73	AY	0.74	0/717	1.01	1/951 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	Ca	0.51	0/450	0.76	0/598
75	h1	0.56	7/36567 (0.0%)	0.74	2/56975 (0.0%)
76	B1	0.62	0/263	0.76	0/404
77	Ba	0.46	0/809	0.71	0/1090
78	AI	0.44	0/801	0.70	0/1082
All	All	0.57	16/205899 (0.0%)	0.78	24/301963 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
8	AR	0	1
16	Ea	0	1
23	AM	0	1
30	AJ	0	1
34	BK	0	1
37	BP	0	1
39	BG	0	1
40	Fa	0	1
54	AG	0	1
55	Ga	0	1
57	AF	0	1
65	Ua	0	1
70	BL	0	1
72	Aa	0	1
All	All	0	16

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	621	A2M	O3'-P	6.56	1.62	1.56
2	A	2279	A2M	O3'-P	6.54	1.62	1.56
2	A	48	OMU	O3'-P	5.96	1.62	1.56
75	h1	1754	A2M	O3'-P	5.74	1.61	1.56
75	h1	422	A2M	O3'-P	5.51	1.61	1.56
2	A	676	OMU	O3'-P	5.38	1.61	1.56
75	h1	778	A2M	O3'-P	5.36	1.61	1.56
2	A	1142	A2M	O3'-P	5.26	1.61	1.56
75	h1	123	OMU	O3'-P	5.23	1.61	1.56

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1376	A2M	O3'-P	5.19	1.61	1.56
2	A	2324	A2M	O3'-P	5.15	1.61	1.56
2	A	2639	A2M	O3'-P	5.08	1.61	1.56
75	h1	543	A2M	O3'-P	5.08	1.61	1.56
2	A	2716	OMU	O3'-P	5.07	1.61	1.56
1	3	47	A2M	O3'-P	5.04	1.61	1.56
75	h1	1327	A2M	O3'-P	5.01	1.61	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	Ha	26	ARG	CD-NE-CZ	10.25	138.75	124.40
2	A	10	G	O3'-P-O5'	-7.72	92.42	104.00
2	A	11	G	P-O5'-C5'	-7.64	109.44	120.90
2	A	346	A	O3'-P-O5'	-6.85	93.72	104.00
2	A	1902	A	O3'-P-O5'	-6.30	94.55	104.00
41	Ha	26	ARG	CG-CD-NE	-5.94	98.93	112.00
73	AY	3	LYS	N-CA-CB	-5.90	101.44	110.12
25	BI	48	ARG	N-CA-CB	-5.86	101.87	111.66
1	3	156	G	O3'-P-O5'	-5.81	95.29	104.00
2	A	2870	G	C4'-C3'-O3'	-5.81	104.29	113.00
70	BL	113	ILE	N-CA-C	-5.60	108.04	113.53
2	A	206	A	O3'-P-O5'	-5.58	95.63	104.00
2	A	280	G	C4'-C3'-O3'	-5.51	104.73	113.00
2	A	888	U	C4'-C3'-O3'	-5.43	104.85	113.00
75	h1	386	G	O3'-P-O5'	-5.43	95.86	104.00
2	A	2162	C	C4'-C3'-C2'	-5.41	97.19	102.60
2	A	826	A2M	OP1-P-O3'	5.24	116.72	105.20
75	h1	1115	G	C3'-C2'-C1'	-5.23	96.27	101.50
28	AV	42	ARG	CB-CA-C	-5.19	102.50	110.81
2	A	2398	G	C2'-C3'-O3'	-5.15	105.97	113.70
2	A	1820	C	O3'-P-O5'	-5.11	96.34	104.00
2	A	1222	G	O3'-P-O5'	-5.05	96.42	104.00
2	A	1936	G	O3'-P-O5'	-5.05	96.43	104.00
66	Ya	104	GLY	N-CA-C	-5.04	108.70	114.69

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	113	G	Sidechain
2	A	2374	G	Sidechain

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Group
57	AF	145	ARG	Sidechain
54	AG	181	ARG	Sidechain
30	AJ	38	ARG	Sidechain
23	AM	70	ARG	Sidechain
8	AR	20	GLY	Peptide
72	Aa	50	ARG	Sidechain
39	BG	59	ARG	Sidechain
34	BK	23	ARG	Sidechain
70	BL	85	ARG	Sidechain
37	BP	89	ARG	Sidechain
16	Ea	108	ARG	Sidechain
40	Fa	69	ARG	Sidechain
55	Ga	111	ARG	Sidechain
65	Ua	137	ASP	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	3	3453	0	1754	28	0
2	A	67504	0	34099	646	0
3	2	1630	0	822	16	0
3	W2	1629	0	823	18	0
4	C3	2536	0	1284	20	0
5	BC	237	0	289	3	0
6	BM	1246	0	1264	14	0
7	BO	1030	0	1110	14	0
8	AR	425	0	440	7	0
9	AU	888	0	933	10	0
10	Ma	789	0	810	14	0
11	Ia	1512	0	1598	17	0
12	AE	1033	0	1070	12	0
13	AX	786	0	888	14	0
14	AP	1092	0	1182	12	0
15	Ja	2074	0	2180	65	0
16	Ea	1705	0	1764	27	0
17	AL	1485	0	1547	23	0
18	Va	1082	0	1153	16	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Ka	986	0	1053	29	0
20	AW	901	0	926	16	0
21	BD	792	0	843	6	0
22	BS	3111	0	3221	41	0
23	AM	1307	0	1359	15	0
24	AC	1672	0	1748	25	0
25	BI	986	0	1048	8	0
26	AH	1042	0	1119	20	0
27	BT	3056	0	3214	33	0
28	AV	1028	0	1105	16	0
29	AD	1454	0	1512	36	0
30	AJ	1468	0	1577	13	0
31	BQ	1877	0	1922	19	0
32	BH	1636	0	1752	20	0
33	Da	1190	0	1273	10	0
34	BK	2277	0	2311	25	0
35	AT	720	0	754	9	0
36	Pa	389	0	419	6	0
37	BP	975	0	1100	8	0
38	BN	955	0	1037	11	0
39	BG	1874	0	2015	34	0
40	Fa	896	0	975	9	0
41	Ha	1156	0	1207	18	0
42	BU	1366	0	1407	16	0
43	BR	1898	0	2005	18	0
44	Xa	1163	0	1222	18	0
45	BV	1718	0	1774	39	0
46	BJ	1653	0	1707	15	0
47	AO	528	0	557	6	0
48	BW	568	0	566	9	0
49	AK	1480	0	1610	13	0
50	Na	647	0	663	14	0
51	AB	1514	0	1576	26	0
52	BF	1491	0	1596	20	0
53	AA	1625	0	1718	46	0
54	AG	1648	0	1755	16	0
55	Ga	433	0	475	4	0
56	BA	444	0	477	4	0
57	AF	1113	0	1169	37	0
58	Wa	1136	0	1177	22	0
59	Ta	1795	0	1920	50	0
60	AZ	562	0	606	12	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BE	702	0	741	6	0
62	Za	1575	0	1578	44	0
63	AQ	1056	0	1128	26	0
64	Oa	471	0	497	15	0
65	Ua	962	0	994	29	0
66	Ya	1024	0	1090	32	0
67	BB	955	0	1012	33	0
68	AN	808	0	845	18	0
69	Ra	1506	0	1571	43	0
70	BL	1064	0	1097	25	0
71	La	562	0	599	18	0
72	Aa	1494	0	1538	46	0
73	AY	705	0	724	20	0
74	Ca	440	0	431	12	0
75	h1	34449	0	17387	421	0
76	B1	240	0	121	2	0
77	Ba	799	0	868	25	0
78	AI	779	0	790	30	0
79	L3	115	0	33	0	0
80	3	28	0	52	0	0
80	A	266	0	494	19	0
80	h1	84	0	156	3	0
81	3	4	0	0	0	0
81	A	193	0	0	0	0
81	AC	1	0	0	0	0
81	AY	2	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	2	0	0	0	0
81	BV	1	0	0	0	0
81	C3	4	0	0	0	0
81	Ta	1	0	0	0	0
81	Wa	1	0	0	0	0
81	h1	77	0	0	1	0
82	3	3	0	0	0	0
82	A	122	0	0	0	0
82	AD	1	0	0	0	0
82	AG	2	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	40	0	0	0	0
83	A	10	0	19	0	0
84	A	15	0	18	0	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
86	2	2	0	0	0	0
86	3	298	0	0	9	0
86	A	6794	0	0	181	0
86	AA	1	0	0	0	0
86	AB	5	0	0	0	0
86	AC	11	0	0	0	0
86	AD	5	0	0	0	0
86	AE	14	0	0	0	0
86	AF	5	0	0	0	0
86	AG	82	0	0	2	0
86	AH	19	0	0	1	0
86	AJ	108	0	0	3	0
86	AK	42	0	0	3	0
86	AL	58	0	0	5	0
86	AM	78	0	0	7	0
86	AO	17	0	0	1	0
86	AP	11	0	0	0	0
86	AQ	4	0	0	1	0
86	AR	41	0	0	2	0
86	AT	7	0	0	0	0
86	AU	26	0	0	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	AV	61	0	0	3	0
86	AW	53	0	0	3	0
86	AX	21	0	0	4	0
86	AY	70	0	0	7	0
86	AZ	2	0	0	0	0
86	Aa	6	0	0	4	0
86	B1	19	0	0	0	0
86	BA	23	0	0	1	0
86	BC	9	0	0	0	0
86	BD	53	0	0	1	0
86	BE	32	0	0	1	0
86	BF	14	0	0	1	0
86	BG	31	0	0	4	0
86	BH	86	0	0	3	0
86	BI	36	0	0	1	0
86	BJ	30	0	0	0	0
86	BK	58	0	0	2	0
86	BL	1	0	0	0	0
86	BM	59	0	0	3	0
86	BN	30	0	0	2	0
86	BO	31	0	0	4	0
86	BP	21	0	0	0	0
86	BQ	129	0	0	6	0
86	BR	69	0	0	7	0
86	BS	151	0	0	6	0
86	BT	127	0	0	2	0
86	BU	5	0	0	0	0
86	BV	12	0	0	1	0
86	Ba	2	0	0	0	0
86	C3	154	0	0	8	0
86	Ca	2	0	0	0	0
86	Da	19	0	0	1	0
86	Ea	123	0	0	8	0
86	Fa	56	0	0	3	0
86	Ga	11	0	0	0	0
86	Ha	88	0	0	5	0
86	Ia	20	0	0	0	0
86	Ja	13	0	0	1	0
86	Ka	1	0	0	0	0
86	L3	1	0	0	0	0
86	Ma	17	0	0	2	0
86	Na	2	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Oa	1	0	0	0	0
86	Pa	2	0	0	0	0
86	Ta	4	0	0	2	0
86	Ua	22	0	0	1	0
86	Va	19	0	0	1	0
86	W2	22	0	0	0	0
86	Xa	13	0	0	1	0
86	h1	1197	0	0	52	0
All	All	207912	0	146263	2320	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 7.

All (2320) 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)
31:BQ:102:LEU:HD13	86:BQ:412:HOH:O	1.32	1.29
6:BM:141:MET:SD	86:BM:358:HOH:O	1.92	1.22
73:AY:76:THR:O	73:AY:77:CYS:N	1.75	1.18
22:BS:93:VAL:HB	86:BS:633:HOH:O	1.43	1.17
73:AY:76:THR:C	73:AY:77:CYS:N	2.06	1.13
22:BS:251:LYS:N	86:BS:501:HOH:O	1.82	1.12
23:AM:5:HIS:ND1	86:AM:201:HOH:O	1.85	1.07
2:A:1491:A:N7	86:A:3802:HOH:O	1.87	1.07
2:A:1354:G:N7	86:A:3803:HOH:O	1.88	1.05
75:h1:1284:U:OP2	86:h1:2101:HOH:O	1.74	1.05
4:C3:119:C:O3'	86:C3:301:HOH:O	1.76	1.03
16:Ea:104:GLU:OE1	86:Ea:401:HOH:O	1.81	0.98
2:A:3167:G:O2'	86:A:3801:HOH:O	1.82	0.97
2:A:1605:A:N7	86:A:3808:HOH:O	1.98	0.96
17:AL:29:MET:SD	86:AM:267:HOH:O	2.24	0.96
2:A:28:G:H5''	16:Ea:172:ARG:HD3	1.47	0.96
44:Xa:70:ARG:NH1	75:h1:306:U:O2	2.01	0.93
75:h1:1681:G:H21	75:h1:1726:A:H62	1.00	0.92
5:BC:14:LYS:HD3	86:h1:2410:HOH:O	1.68	0.92
75:h1:1681:G:N2	75:h1:1726:A:H62	1.67	0.91
2:A:203:G:N7	86:A:3812:HOH:O	2.03	0.90
72:Aa:27:TYR:N	86:Aa:301:HOH:O	2.04	0.90
2:A:2450:G:H1	2:A:2492:A:H61	1.20	0.89
43:BR:167:ALA:O	86:BR:401:HOH:O	1.88	0.89
2:A:3139:A:N1	86:A:3814:HOH:O	2.05	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:554:G:OP2	86:h1:2102:HOH:O	1.91	0.88
22:BS:91:ALA:HB2	22:BS:153:MET:HG2	1.55	0.88
66:Ya:60:ALA:HA	66:Ya:63:LYS:HD3	1.53	0.88
15:Ja:114:ILE:HD11	15:Ja:118:GLU:HG2	1.56	0.87
2:A:330:G:N7	86:A:3818:HOH:O	2.07	0.87
2:A:2495:U:H2'	86:A:5948:HOH:O	1.74	0.87
69:Ra:41:LEU:HD12	69:Ra:44:LEU:HD11	1.55	0.87
2:A:320:A:OP1	86:A:3804:HOH:O	1.93	0.86
2:A:3184:G:H1	2:A:3190:U:H3	1.18	0.86
59:Ta:90:ARG:HD3	86:Ta:401:HOH:O	1.75	0.85
57:AF:145:ARG:NH2	3:W2:33:U:OP2	2.09	0.85
2:A:2119:A:N1	86:A:3819:HOH:O	2.08	0.85
2:A:847:G:O6	61:BE:4:ARG:NH2	2.10	0.85
2:A:1017:A:N7	86:A:3827:HOH:O	2.10	0.85
2:A:2362:G:N7	86:A:3820:HOH:O	2.08	0.84
24:AC:178:THR:HB	86:h1:2425:HOH:O	1.74	0.84
59:Ta:168:ASN:HD21	59:Ta:172:LYS:HB2	1.42	0.83
22:BS:250:ARG:C	86:BS:501:HOH:O	2.16	0.83
12:AE:51:GLU:OE1	69:Ra:142:ARG:HB2	1.78	0.82
2:A:2113:C:OP2	86:A:3805:HOH:O	1.97	0.82
2:A:874:C:N3	86:A:3832:HOH:O	2.11	0.82
2:A:373:G:N7	86:A:3833:HOH:O	2.11	0.82
2:A:3223:U:H3	2:A:3240:U:H3	1.28	0.81
72:Aa:181:ARG:HD3	86:Aa:303:HOH:O	1.80	0.81
4:C3:72:G:N2	4:C3:103:U:O4	2.12	0.81
59:Ta:10:THR:OG1	59:Ta:12:CYS:SG	2.37	0.81
69:Ra:54:ILE:HG23	69:Ra:172:GLY:HA3	1.63	0.81
75:h1:869:G:H1	75:h1:961:U:H3	1.26	0.81
59:Ta:164:ARG:NH1	75:h1:66:U:O2	2.14	0.80
2:A:1823:U:O2	40:Fa:72:ARG:NH2	2.13	0.80
2:A:621:G:N7	86:A:3836:HOH:O	2.12	0.80
75:h1:248:A:N3	86:h1:2119:HOH:O	2.15	0.80
75:h1:563:G:N7	86:h1:2112:HOH:O	2.12	0.80
2:A:424:G:H22	2:A:644:U:H3	1.28	0.80
67:BB:24:MET:HB2	67:BB:58:MET:HE2	1.64	0.80
2:A:155:A:N7	86:A:3837:HOH:O	2.13	0.79
2:A:736:G:N7	86:A:3848:HOH:O	2.15	0.79
41:Ha:132:GLU:OE1	86:Ha:201:HOH:O	2.01	0.79
75:h1:1591:C:OP1	86:h1:2104:HOH:O	2.01	0.78
69:Ra:35:GLN:HA	69:Ra:38:LYS:HD2	1.64	0.78
75:h1:1385:A:HO2'	75:h1:1386:G:H8	1.32	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3182:G:H1	2:A:3192:U:H3	1.30	0.78
2:A:785:PSU:O4'	86:A:3810:HOH:O	2.01	0.78
2:A:1714:G:O6	35:AT:31:LYS:HE3	1.82	0.78
2:A:1039:C:H2'	2:A:1040:G:C8	2.19	0.78
8:AR:16:ALA:O	8:AR:20:GLY:HA2	1.83	0.78
75:h1:112:U:O2	86:h1:2105:HOH:O	2.02	0.78
54:AG:65:ASN:O	86:AG:401:HOH:O	2.02	0.78
75:h1:1492:U:O3'	86:h1:2103:HOH:O	2.00	0.78
72:Aa:31:ARG:NH1	75:h1:334:U:OP1	2.14	0.77
75:h1:1681:G:H21	75:h1:1726:A:N6	1.81	0.77
2:A:353:C:O2'	86:A:3811:HOH:O	2.02	0.77
2:A:2230:A:O2'	86:A:3809:HOH:O	2.01	0.77
2:A:381:A:N3	86:A:3856:HOH:O	2.17	0.77
35:AT:30:TYR:OH	35:AT:58:GLU:OE2	2.03	0.77
76:B1:24:U:H3	3:W2:34:G:H1	1.28	0.77
73:AY:11:ARG:NH2	86:AY:301:HOH:O	2.16	0.77
29:AD:97:MET:HE2	29:AD:108:PRO:HB2	1.66	0.76
1:3:120:G:N7	86:3:301:HOH:O	2.18	0.76
4:C3:56:G:O6	86:C3:302:HOH:O	2.04	0.76
45:BV:54:THR:HA	86:BV:406:HOH:O	1.85	0.76
72:Aa:90:GLU:HA	72:Aa:93:ARG:HD2	1.68	0.76
86:AX:215:HOH:O	54:AG:98:HIS:HD2	1.69	0.75
75:h1:406:G:N3	86:h1:2127:HOH:O	2.18	0.75
53:AA:72:LEU:HD21	78:AI:20:VAL:HB	1.69	0.75
75:h1:381:U:OP2	86:h1:2106:HOH:O	2.05	0.75
62:Za:55:LEU:HA	62:Za:58:THR:HG22	1.69	0.75
29:AD:23:THR:OG1	29:AD:25:ASP:OD1	2.05	0.74
2:A:1486:G:OP2	86:A:3815:HOH:O	2.05	0.74
2:A:3070:A:OP2	86:A:3813:HOH:O	2.03	0.74
49:AK:98:ARG:NH2	49:AK:130:ASN:OD1	2.19	0.74
2:A:609:A:N6	52:BF:25:ARG:O	2.19	0.74
69:Ra:54:ILE:HD11	69:Ra:60:ALA:HB2	1.69	0.74
53:AA:48:ILE:HB	53:AA:86:LEU:HD22	1.70	0.74
36:Pa:6:GLY:HA2	36:Pa:10:ARG:HD2	1.70	0.73
59:Ta:2:LYS:HB2	59:Ta:110:VAL:HG22	1.68	0.73
2:A:62:G:OP1	16:Ea:185:ARG:NH1	2.21	0.73
53:AA:39:VAL:HG22	53:AA:48:ILE:HD12	1.70	0.73
59:Ta:96:ARG:NH2	75:h1:1675:G:OP1	2.20	0.73
64:Oa:57:GLU:OE1	65:Ua:78:GLN:NE2	2.21	0.73
2:A:3226:G:H1	2:A:3237:U:H3	1.33	0.73
2:A:1486:G:O6	86:A:3816:HOH:O	2.05	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BU:37:LYS:O	42:BU:37:LYS:NZ	2.20	0.73
54:AG:68:VAL:O	54:AG:157:ARG:NH1	2.21	0.73
2:A:3246:C:N3	86:A:3878:HOH:O	2.21	0.73
38:BN:130:GLY:HA2	86:BN:222:HOH:O	1.86	0.73
33:Da:33:VAL:HG21	33:Da:66:VAL:HG11	1.71	0.73
68:AN:56:LEU:HD12	68:AN:57:GLY:H	1.53	0.73
3:2:5:G:H22	3:2:68:A:H2	1.36	0.72
73:AY:8:PHE:CD1	86:AY:358:HOH:O	2.42	0.72
2:A:584:G:OP2	52:BF:12:ARG:NH2	2.21	0.72
31:BQ:181:LYS:NZ	86:BQ:402:HOH:O	2.22	0.72
67:BB:96:ILE:HB	67:BB:117:ILE:HG12	1.70	0.72
22:BS:93:VAL:CG1	86:BS:633:HOH:O	2.35	0.72
67:BB:114:THR:HB	67:BB:117:ILE:HB	1.70	0.72
6:BM:117:HIS:ND1	86:BM:301:HOH:O	2.23	0.72
75:h1:428:G:OP2	86:h1:2107:HOH:O	2.08	0.72
2:A:416:G:N7	86:A:3887:HOH:O	2.22	0.71
2:A:1631:G:N7	14:AP:48:LYS:NZ	2.39	0.71
57:AF:137:ARG:NH1	75:h1:1585:A:OP1	2.23	0.71
66:Ya:86:ARG:NH2	66:Ya:125:SER:O	2.22	0.71
2:A:1587:G:H2'	86:A:8334:HOH:O	1.91	0.71
15:Ja:127:ARG:HB2	15:Ja:140:ASN:HB2	1.70	0.71
2:A:945:A2M:HM'3	86:A:5503:HOH:O	1.91	0.71
2:A:1778:G:N7	86:A:3898:HOH:O	2.23	0.71
2:A:1136:G:O6	86:A:3817:HOH:O	2.05	0.71
2:A:3310:A:N7	86:A:3894:HOH:O	2.22	0.71
80:A:3405:TER:H81	86:A:9559:HOH:O	1.90	0.71
2:A:2399:A:N3	86:A:3896:HOH:O	2.23	0.71
75:h1:99:U:OP1	86:h1:2110:HOH:O	2.09	0.71
2:A:2803:A:N3	86:A:3905:HOH:O	2.24	0.70
10:Ma:58:VAL:HG21	65:Ua:27:PHE:HZ	1.56	0.70
2:A:2175:A:N7	86:A:3908:HOH:O	2.24	0.70
2:A:1138:A:OP2	86:A:3825:HOH:O	2.10	0.70
34:BK:50:ARG:NH1	34:BK:146:ASP:OD2	2.23	0.70
61:BE:85:ARG:HB2	86:BE:228:HOH:O	1.91	0.70
60:AZ:17:ARG:NH2	60:AZ:19:ASP:OD2	2.24	0.70
2:A:742:U:H3	2:A:747:G:H1	1.40	0.70
2:A:1222:G:OP2	86:A:3823:HOH:O	2.09	0.70
62:Za:82:SER:O	62:Za:88:GLN:NE2	2.24	0.70
75:h1:795:C:O2'	75:h1:796:A:O4'	2.10	0.70
8:AR:17:HIS:HA	8:AR:20:GLY:HA3	1.72	0.70
15:Ja:212:ASP:OD1	15:Ja:213:SER:N	2.24	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AQ:106:VAL:HG21	63:AQ:115:LYS:HG3	1.74	0.70
20:AW:89:LYS:NZ	86:AW:201:HOH:O	2.22	0.70
2:A:2995:C:O4'	86:A:3824:HOH:O	2.10	0.69
2:A:3124:C:O2'	86:A:3822:HOH:O	2.09	0.69
2:A:297:G:N7	86:A:3911:HOH:O	2.24	0.69
77:Ba:48:ASP:O	77:Ba:50:ARG:NH1	2.25	0.69
17:AL:134:LYS:NZ	86:AL:201:HOH:O	1.99	0.69
2:A:2496:U:C6	86:A:5948:HOH:O	2.44	0.69
2:A:3174:C:N4	32:BH:172:LEU:HD13	2.08	0.69
42:BU:55:THR:HG23	42:BU:62:ARG:HA	1.74	0.69
42:BU:79:MET:HE2	42:BU:79:MET:HA	1.74	0.69
51:AB:144:ASN:OD1	75:h1:770:U:N3	2.24	0.69
52:BF:11:ASN:ND2	52:BF:13:ASN:O	2.26	0.69
2:A:976:A:OP1	41:Ha:47:LYS:NZ	2.26	0.69
17:AL:82:ARG:NE	86:AL:203:HOH:O	2.26	0.69
49:AK:170:ARG:HH12	75:h1:817:A:H2'	1.58	0.69
53:AA:68:GLU:HG3	78:AI:90:THR:HG21	1.75	0.69
2:A:393:A:O2'	2:A:396:A:OP1	2.09	0.69
2:A:1212:A:N1	86:A:3919:HOH:O	2.25	0.69
2:A:3071:A:N7	86:A:3927:HOH:O	2.26	0.69
2:A:299:C:OP2	86:A:3826:HOH:O	2.10	0.68
25:BI:90:ARG:CZ	25:BI:96:MET:HE1	2.23	0.68
19:Ka:79:ASP:OD1	19:Ka:83:ASN:ND2	2.26	0.68
54:AG:140:GLU:OE1	54:AG:140:GLU:N	2.27	0.68
75:h1:826:A:H61	75:h1:849:U:H3	1.39	0.68
24:AC:16:VAL:HG21	24:AC:39:ILE:HG23	1.74	0.68
74:Ca:53:ILE:C	74:Ca:54:LYS:N	2.51	0.68
66:Ya:23:ARG:NH2	75:h1:1550:U:OP1	2.27	0.68
13:AX:6:VAL:O	13:AX:15:ASN:ND2	2.25	0.68
65:Ua:30:VAL:HB	65:Ua:92:MET:HE2	1.76	0.68
16:Ea:30:TYR:OH	86:Ea:402:HOH:O	2.09	0.68
65:Ua:135:PRO:O	86:Ua:301:HOH:O	2.12	0.68
2:A:1552:G:OP2	86:A:3828:HOH:O	2.10	0.68
49:AK:170:ARG:NH2	75:h1:819:G:N7	2.41	0.68
59:Ta:13:GLN:NE2	75:h1:150:U:O4'	2.26	0.68
75:h1:927:A:N1	86:h1:2139:HOH:O	2.26	0.68
16:Ea:7:VAL:HA	86:BG:302:HOH:O	1.94	0.68
3:W2:70:C:H2'	3:W2:71:G:C8	2.28	0.68
2:A:3046:A:O4'	86:A:3829:HOH:O	2.11	0.67
51:AB:129:VAL:O	51:AB:133:GLN:HG3	1.94	0.67
2:A:401:U:OP2	86:A:3835:HOH:O	2.12	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2275:C:OP2	86:A:3838:HOH:O	2.13	0.67
2:A:2110:G:H5'	47:AO:50:LYS:HG2	1.76	0.67
29:AD:51:HIS:ND1	29:AD:51:HIS:O	2.26	0.67
2:A:1013:A:O5'	86:A:3831:HOH:O	2.11	0.67
54:AG:170:GLU:N	54:AG:170:GLU:OE1	2.26	0.67
75:h1:382:U:OP1	86:h1:2111:HOH:O	2.11	0.67
2:A:817:A:N7	86:A:3954:HOH:O	2.28	0.67
2:A:446:U:H2'	2:A:447:G:H8	1.60	0.67
75:h1:1084:G:N7	86:h1:2141:HOH:O	2.26	0.67
2:A:1350:G:N7	86:A:3935:HOH:O	2.26	0.67
2:A:1526:A:OP1	56:BA:41:ARG:NH2	2.28	0.67
15:Ja:66:MET:HE2	15:Ja:66:MET:HA	1.77	0.67
75:h1:17:C:OP2	86:h1:2114:HOH:O	2.13	0.67
1:3:156:G:OP1	38:BN:39:ARG:NH2	2.27	0.67
10:Ma:10:ARG:NH1	86:Ma:301:HOH:O	2.28	0.67
22:BS:93:VAL:CB	86:BS:633:HOH:O	2.16	0.67
73:AY:8:PHE:CG	86:AY:358:HOH:O	2.47	0.67
75:h1:1202:G:OP1	86:h1:2113:HOH:O	2.13	0.67
1:3:69:G:N3	86:3:308:HOH:O	2.27	0.66
2:A:1493:A:N7	86:A:3962:HOH:O	2.28	0.66
2:A:1807:G:N7	86:A:3952:HOH:O	2.28	0.66
4:C3:93:U:H2'	4:C3:94:C:C6	2.30	0.66
15:Ja:103:TYR:HB2	15:Ja:182:MET:HE2	1.77	0.66
75:h1:1261:OMU:HM22	75:h1:1262:A:H5'	1.78	0.66
62:Za:89:ARG:NH1	62:Za:207:PHE:O	2.28	0.66
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HD2	1.77	0.66
75:h1:872:A:H2'	75:h1:873:G:C8	2.29	0.66
75:h1:1092:A:N3	86:h1:2145:HOH:O	2.27	0.66
2:A:992:C:OP2	2:A:1111:G:N2	2.22	0.66
6:BM:136:ARG:NH2	86:BM:302:HOH:O	2.27	0.66
70:BL:57:ARG:NH2	75:h1:1482:A:OP2	2.29	0.66
75:h1:385:G:O6	86:h1:2109:HOH:O	2.09	0.66
20:AW:54:MET:HE1	20:AW:88:ALA:HB1	1.76	0.66
59:Ta:51:LYS:HB3	59:Ta:114:VAL:HG12	1.78	0.66
2:A:1620:A:N7	86:A:3936:HOH:O	2.26	0.66
58:Wa:43:ILE:HD11	70:BL:37:ILE:HG22	1.76	0.66
2:A:2649:UY1:OP2	86:A:3839:HOH:O	2.13	0.66
2:A:19:G:N7	86:A:3948:HOH:O	2.27	0.66
8:AR:24:PRO:HG2	23:AM:86:ARG:CZ	2.25	0.66
2:A:2115:G:OP2	86:A:3834:HOH:O	2.12	0.66
24:AC:131:THR:OG1	75:h1:1099:U:OP1	2.14	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1403:A:OP1	86:A:3843:HOH:O	2.14	0.66
12:AE:2:VAL:N	75:h1:1035:C:HO2'	1.94	0.66
27:BT:42:VAL:HG21	27:BT:252:LEU:HD21	1.77	0.66
45:BV:72:ASP:OD1	65:Ua:127:ARG:NH1	2.29	0.66
2:A:3317:A:N7	86:A:3974:HOH:O	2.29	0.66
4:C3:17:G:N7	86:C3:304:HOH:O	2.28	0.66
15:Ja:35:PRO:HD2	15:Ja:83:PRO:HG2	1.78	0.66
25:BI:15:ARG:HD2	86:BI:301:HOH:O	1.96	0.66
72:Aa:142:LEU:O	72:Aa:146:ILE:HG12	1.96	0.66
2:A:3195:A:O4'	86:A:3842:HOH:O	2.14	0.65
12:AE:11:LEU:HD12	12:AE:74:VAL:HG23	1.77	0.65
24:AC:178:THR:HG21	75:h1:14:C:OP2	1.97	0.65
2:A:710:G:N7	86:A:3983:HOH:O	2.30	0.65
29:AD:60:ARG:HD3	75:h1:1617:C:H2'	1.79	0.65
75:h1:1780:A:N3	86:h1:2159:HOH:O	2.29	0.65
2:A:835:G:N7	86:A:3985:HOH:O	2.30	0.65
49:AK:85:ARG:HD3	86:AK:311:HOH:O	1.97	0.65
54:AG:68:VAL:HG13	54:AG:155:ILE:HD11	1.78	0.65
75:h1:350:U:OP2	86:h1:2117:HOH:O	2.14	0.65
75:h1:1172:A:H2'	75:h1:1173:G:C8	2.31	0.65
2:A:1033:G:N2	2:A:1040:G:H1	1.95	0.65
75:h1:951:C:O2'	86:h1:2120:HOH:O	2.15	0.65
32:BH:127:ASP:OD2	86:BH:301:HOH:O	2.14	0.65
71:La:40:MET:HE1	71:La:47:THR:HG21	1.78	0.65
81:h1:1969:MG:MG	86:h1:2106:HOH:O	1.40	0.65
2:A:3183:A:H61	2:A:3191:C:H42	1.45	0.65
15:Ja:90:VAL:HG13	15:Ja:99:PHE:HB2	1.79	0.65
20:AW:19:LEU:HD11	20:AW:36:GLN:HB2	1.79	0.65
27:BT:40:ASP:OD1	86:BT:501:HOH:O	2.14	0.65
38:BN:85:MET:HE1	38:BN:153:ILE:HG23	1.79	0.65
2:A:352:A:N1	27:BT:89:THR:HG22	2.11	0.65
2:A:701:A:N7	2:A:703:U:O2'	2.25	0.65
11:Ia:97:PHE:HB2	11:Ia:145:ASP:HB3	1.79	0.65
72:Aa:99:LYS:HB3	75:h1:331:G:H5'	1.77	0.65
75:h1:1296:G:O6	86:h1:2116:HOH:O	2.14	0.65
78:AI:46:MET:HE1	78:AI:55:VAL:HG21	1.77	0.65
2:A:2883:C:C6	86:A:6307:HOH:O	2.49	0.64
75:h1:141:G:H2'	75:h1:142:G:C8	2.32	0.64
55:Ga:78:ILE:HB	55:Ga:83:MET:HE3	1.80	0.64
2:A:111:C:OP2	37:BP:106:ARG:NH2	2.30	0.64
2:A:1104:C:O2'	23:AM:126:ILE:O	2.14	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1922:U:O2'	86:A:3847:HOH:O	2.15	0.64
75:h1:337:PSU:OP1	86:h1:2118:HOH:O	2.15	0.64
54:AG:127:ARG:N	86:AG:403:HOH:O	2.30	0.64
68:AN:40:GLU:O	68:AN:44:GLN:HG3	1.98	0.64
75:h1:1332:A:N7	86:h1:2162:HOH:O	2.30	0.64
10:Ma:4:LYS:NZ	75:h1:1798:A:OP2	2.31	0.64
2:A:1033:G:H22	2:A:1040:G:H1	1.46	0.64
2:A:1043:U:H2'	2:A:1044:C:C6	2.33	0.64
2:A:1808:A:N3	86:A:3997:HOH:O	2.30	0.64
69:Ra:59:LYS:HB2	69:Ra:91:LYS:HB3	1.79	0.64
2:A:61:A:OP1	16:Ea:172:ARG:NH2	2.28	0.64
2:A:2450:G:H1	2:A:2492:A:N6	1.93	0.64
27:BT:167:GLU:HG2	27:BT:222:LYS:HE3	1.79	0.64
75:h1:395:C:O2	86:h1:2115:HOH:O	2.13	0.64
2:A:1446:OMC:HM22	2:A:1447:U:H5'	1.78	0.64
2:A:2886:A:N1	86:A:3992:HOH:O	2.30	0.64
2:A:472:G:H2'	2:A:473:G:C8	2.32	0.63
75:h1:466:A2M:HM'2	75:h1:467:G:H5'	1.80	0.63
1:3:98:C:O3'	73:AY:76:THR:HG21	1.99	0.63
2:A:1406:C:OP1	86:A:3850:HOH:O	2.15	0.63
2:A:2894:G:O2'	86:A:3846:HOH:O	2.15	0.63
44:Xa:125:ILE:HD12	44:Xa:142:LYS:HD3	1.79	0.63
62:Za:63:GLN:NE2	62:Za:185:MET:SD	2.71	0.63
69:Ra:64:TYR:HA	69:Ra:96:VAL:O	1.97	0.63
2:A:1223:G:H4'	17:AL:92:MET:HG2	1.80	0.63
15:Ja:33:SER:OG	75:h1:299:U:O2	2.16	0.63
75:h1:515:U:H2'	75:h1:516:G:C8	2.33	0.63
2:A:1146:C:N3	86:A:3994:HOH:O	2.30	0.63
2:A:1941:G:OP1	86:A:3845:HOH:O	2.15	0.63
41:Ha:127:ILE:O	86:Ha:202:HOH:O	2.15	0.63
69:Ra:17:THR:O	69:Ra:21:GLU:HG3	1.99	0.63
2:A:1754:G:O6	86:A:3841:HOH:O	2.14	0.63
69:Ra:66:PRO:HG2	69:Ra:69:LEU:HB2	1.80	0.63
70:BL:85:ARG:NH2	75:h1:1543:G:OP1	2.31	0.63
19:Ka:60:PHE:HB2	19:Ka:61:LYS:HG2	1.81	0.63
42:BU:119:ASP:HB3	42:BU:122:THR:HB	1.80	0.63
75:h1:96:G:HO2'	75:h1:462:A:HO2'	1.43	0.63
10:Ma:44:ILE:O	65:Ua:112:GLN:NE2	2.32	0.62
75:h1:1784:G:H3'	75:h1:1785:MA6:P	2.39	0.62
2:A:990:C:H3'	2:A:991:G:H5''	1.81	0.62
2:A:2548:U:H5	31:BQ:40:TYR:O	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AD:91:ARG:NH2	75:h1:1530:U:OP1	2.32	0.62
2:A:188:U:O4	86:A:3852:HOH:O	2.16	0.62
47:AO:40:ARG:NH1	86:AO:201:HOH:O	2.29	0.62
2:A:611:C:O2'	52:BF:47:ARG:O	2.17	0.62
18:Va:107:LYS:HD2	75:h1:603:A:OP2	1.99	0.62
43:BR:104:THR:HG23	43:BR:135:VAL:HG12	1.81	0.62
53:AA:40:ARG:HH12	53:AA:49:ILE:HD11	1.64	0.62
75:h1:749:A:H62	75:h1:806:G:H21	1.47	0.62
75:h1:1042:G:H2'	75:h1:1043:G:C8	2.35	0.62
75:h1:1776:C:OP1	86:h1:2124:HOH:O	2.16	0.62
2:A:2211:A:H2'	2:A:2212:A2M:C8	2.30	0.62
2:A:3241:U:H2'	2:A:3242:G:C8	2.34	0.62
75:h1:1787:C:OP1	86:h1:2123:HOH:O	2.16	0.62
2:A:1954:G:H2'	2:A:2091:A:H61	1.65	0.62
66:Ya:94:MET:O	66:Ya:97:SER:OG	2.18	0.62
35:AT:17:LEU:O	35:AT:21:MET:HG2	2.00	0.61
70:BL:115:ASP:OD1	70:BL:125:THR:OG1	2.18	0.61
75:h1:342:U:H2'	75:h1:343:A:C8	2.35	0.61
19:Ka:19:LEU:HD13	19:Ka:21:ARG:HH21	1.63	0.61
39:BG:143:GLN:NE2	39:BG:195:THR:O	2.33	0.61
51:AB:133:GLN:HB3	75:h1:515:U:H4'	1.81	0.61
77:Ba:35:LEU:HD22	77:Ba:90:ARG:HD3	1.82	0.61
14:AP:114:LYS:NZ	14:AP:118:GLU:OE2	2.33	0.61
32:BH:43:CYS:SG	32:BH:109:VAL:CG1	2.88	0.61
65:Ua:150:LEU:HD12	75:h1:1789:U:OP1	2.00	0.61
71:La:88:GLY:O	71:La:90:ILE:N	2.30	0.61
2:A:3341:C:H4'	2:A:3342:U:H3'	1.82	0.61
75:h1:979:A:OP2	86:h1:2122:HOH:O	2.16	0.61
2:A:880:U:P	86:A:4003:HOH:O	2.58	0.61
75:h1:896:G:H1	75:h1:918:U:H3	1.48	0.61
2:A:1039:C:H2'	2:A:1040:G:H8	1.62	0.61
2:A:2211:A:H2'	2:A:2212:A2M:H8	1.82	0.61
15:Ja:151:ASP:HB3	15:Ja:154:ILE:HG12	1.83	0.61
52:BF:196:ILE:HD12	52:BF:197:LYS:N	2.15	0.61
2:A:2935:A:N3	86:A:4001:HOH:O	2.30	0.61
3:2:61:C:H2'	3:2:62:A:H8	1.65	0.61
75:h1:1652:U:H2'	75:h1:1653:A:C8	2.36	0.61
2:A:588:C:H2'	2:A:589:U:H2'	1.81	0.61
2:A:1575:A:H2'	2:A:1576:A:O4'	2.00	0.61
27:BT:295:LEU:HD11	30:AJ:32:LEU:HB2	1.83	0.61
72:Aa:84:TYR:CE2	72:Aa:198:LYS:HB3	2.35	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Ua:96:LEU:HD11	65:Ua:111:ALA:HB1	1.82	0.61
75:h1:1489:G:O6	75:h1:1525:G:N2	2.33	0.61
2:A:410:U:H2'	2:A:411:C:C6	2.36	0.60
2:A:692:C:OP2	86:A:3851:HOH:O	2.16	0.60
2:A:2728:U:OP2	86:A:3849:HOH:O	2.15	0.60
51:AB:56:ASN:O	51:AB:60:GLU:HG3	2.01	0.60
75:h1:886:G:H2'	75:h1:887:U:C6	2.36	0.60
15:Ja:248:ILE:HD11	75:h1:793:U:H4'	1.83	0.60
27:BT:12:ILE:HD13	27:BT:260:LYS:HD2	1.81	0.60
50:Na:56:VAL:HG12	50:Na:66:CYS:SG	2.41	0.60
72:Aa:84:TYR:HE2	72:Aa:198:LYS:HB3	1.66	0.60
75:h1:1566:U:H2'	75:h1:1567:C:C6	2.36	0.60
2:A:1442:A:OP2	86:A:3853:HOH:O	2.16	0.60
58:Wa:134:GLN:NE2	75:h1:1546:U:OP1	2.34	0.60
2:A:1953:U:H2'	2:A:1954:G:C8	2.35	0.60
26:AH:96:GLN:NE2	86:AH:201:HOH:O	2.32	0.60
69:Ra:10:LYS:HE2	69:Ra:14:ALA:HB3	1.84	0.60
75:h1:194:A:HO2'	75:h1:195:A:H8	1.48	0.60
75:h1:371:U:O2'	75:h1:372:A:OP1	2.17	0.60
2:A:3127:A:H1'	86:A:4295:HOH:O	1.99	0.60
75:h1:321:U:H4'	75:h1:325:A:C8	2.37	0.60
2:A:3141:G:N7	86:A:4019:HOH:O	2.31	0.60
51:AB:138:VAL:HG22	51:AB:158:VAL:HG22	1.82	0.60
2:A:530:G:H1	2:A:546:U:H3	1.48	0.60
86:A:6145:HOH:O	34:BK:15:ARG:HD3	2.01	0.60
59:Ta:7:ASN:HB3	59:Ta:12:CYS:SG	2.42	0.60
63:AQ:74:LYS:HB2	63:AQ:77:LYS:HB2	1.83	0.60
2:A:1597:C:H2'	2:A:1598:C:C6	2.36	0.60
59:Ta:140:ALA:O	59:Ta:143:ILE:HG22	2.01	0.60
44:Xa:126:ILE:CG2	44:Xa:138:PHE:HB3	2.32	0.59
14:AP:15:GLN:HE21	40:Fa:88:ARG:HH11	1.51	0.59
28:AV:66:HIS:CE1	63:AQ:29:SER:HB3	2.36	0.59
51:AB:48:GLN:HG2	51:AB:103:VAL:HG21	1.83	0.59
66:Ya:29:ALA:O	66:Ya:33:MET:HG2	2.02	0.59
75:h1:1059:U:H3'	75:h1:1060:U:C5'	2.31	0.59
15:Ja:3:ARG:HB3	75:h1:94:A:H1'	1.84	0.59
23:AM:98:GLN:NE2	86:AM:202:HOH:O	1.94	0.59
31:BQ:30:ARG:HG2	31:BQ:74:GLU:HG3	1.84	0.59
2:A:2503:U:H2'	2:A:2504:A:H8	1.67	0.59
45:BV:139:CYS:HB2	45:BV:172:MET:CE	2.33	0.59
2:A:2971:G:O6	86:A:3854:HOH:O	2.16	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3158:C:H2'	2:A:3159:G:H8	1.64	0.59
20:AW:53:ARG:HD3	86:AW:249:HOH:O	2.03	0.59
59:Ta:32:LEU:HB2	59:Ta:102:CYS:HB2	1.84	0.59
27:BT:218:THR:HG23	27:BT:221:SER:HB2	1.83	0.59
75:h1:1477:G:H2'	75:h1:1478:A:H8	1.68	0.59
2:A:1169:A:O2'	2:A:1376:A2M:H5'	2.03	0.59
32:BH:43:CYS:SG	32:BH:109:VAL:HG13	2.43	0.59
32:BH:90:ARG:HG3	32:BH:104:LEU:HD11	1.84	0.59
2:A:119:A:C2	39:BG:96:GLU:OE1	2.55	0.59
2:A:1953:U:H2'	2:A:1954:G:H8	1.66	0.59
66:Ya:56:ARG:O	66:Ya:57:LYS:HG3	2.02	0.59
67:BB:105:MET:HE3	67:BB:106:LEU:HG	1.84	0.59
71:La:56:PRO:HB3	71:La:89:VAL:HG13	1.85	0.59
73:AY:55:ARG:CB	73:AY:55:ARG:HH11	2.16	0.59
75:h1:1225:G:H2'	75:h1:1226:U:C6	2.38	0.59
10:Ma:10:ARG:CZ	86:Ma:301:HOH:O	2.50	0.59
45:BV:131:ASP:OD1	45:BV:131:ASP:N	2.28	0.59
75:h1:76:C:O2'	75:h1:77:A:O4'	2.20	0.59
2:A:2785:A:OP1	86:A:3857:HOH:O	2.17	0.58
86:A:3870:HOH:O	40:Fa:2:VAL:HG23	2.03	0.58
6:BM:139:PRO:HB3	6:BM:141:MET:HE3	1.85	0.58
15:Ja:2:ALA:O	75:h1:95:PSU:OP1	2.20	0.58
72:Aa:43:THR:OG1	72:Aa:60:ARG:NH2	2.36	0.58
75:h1:1491:G:O2'	75:h1:1497:C:O2	2.19	0.58
78:AI:13:LYS:HA	78:AI:80:LEU:HD11	1.85	0.58
25:BI:13:LYS:HD3	25:BI:128:LEU:HD11	1.86	0.58
33:Da:7:ARG:HB2	86:Da:219:HOH:O	2.03	0.58
77:Ba:69:ARG:NH2	77:Ba:78:ASN:OD1	2.36	0.58
2:A:2508:U:H2'	2:A:2509:A:H8	1.68	0.58
12:AE:14:MET:HE2	12:AE:27:ILE:HD11	1.85	0.58
73:AY:10:LYS:O	86:AY:302:HOH:O	2.17	0.58
15:Ja:124:CYS:HB2	15:Ja:160:ILE:HG22	1.86	0.58
60:AZ:10:ASP:O	60:AZ:14:THR:HG23	2.03	0.58
63:AQ:3:THR:O	63:AQ:4:VAL:HG22	2.03	0.58
2:A:3133:G:N3	86:A:4042:HOH:O	2.32	0.58
3:2:70:C:H2'	3:2:71:G:C8	2.38	0.58
45:BV:25:SER:O	45:BV:50:ARG:NH2	2.36	0.58
46:BJ:12:ILE:HD12	46:BJ:57:LYS:HG2	1.86	0.58
60:AZ:49:ASP:HB3	60:AZ:52:LYS:HG3	1.84	0.58
2:A:262:A:H1'	86:AX:211:HOH:O	2.01	0.58
2:A:3337:C:O2'	2:A:3339:U:OP2	2.22	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AZ:19:ASP:OD1	60:AZ:19:ASP:N	2.36	0.58
2:A:1354:G:O6	86:A:3840:HOH:O	2.13	0.58
16:Ea:147:ARG:CZ	86:Ea:409:HOH:O	2.52	0.58
37:BP:73:TYR:HB3	37:BP:79:LEU:HD22	1.85	0.58
48:BW:81:GLN:OE1	62:Za:67:ARG:NH2	2.37	0.58
62:Za:89:ARG:HH22	62:Za:209:ARG:HG3	1.68	0.58
75:h1:1590:G:H1	75:h1:1610:U:H3	1.51	0.58
2:A:320:A:P	86:A:3804:HOH:O	2.59	0.58
2:A:461:C:H2'	2:A:462:G:H8	1.68	0.58
2:A:954:C:H2'	2:A:955:C:C6	2.39	0.58
26:AH:106:ASP:O	26:AH:110:ILE:HG12	2.04	0.58
45:BV:29:TRP:O	45:BV:94:ARG:NH1	2.37	0.58
58:Wa:60:SER:O	58:Wa:64:ILE:HD12	2.03	0.58
75:h1:618:G:O2'	86:h1:2125:HOH:O	2.17	0.58
75:h1:940:A:H2'	75:h1:941:A:C8	2.39	0.58
2:A:148:A:N7	86:A:4040:HOH:O	2.32	0.57
2:A:462:G:H5'	63:AQ:74:LYS:HD3	1.85	0.57
29:AD:87:LEU:HD21	57:AF:46:LEU:HD13	1.86	0.57
36:Pa:33:ARG:HD3	51:AB:128:ARG:HD3	1.84	0.57
57:AF:61:ARG:HD2	57:AF:107:ILE:HD11	1.85	0.57
77:Ba:53:VAL:HG22	77:Ba:94:LEU:HD11	1.86	0.57
78:AI:16:PHE:CD1	78:AI:76:LEU:HD22	2.38	0.57
2:A:674:U:H2'	2:A:675:OMC:C6	2.39	0.57
15:Ja:204:SER:OG	15:Ja:205:PHE:N	2.37	0.57
24:AC:50:ASP:HB3	24:AC:76:VAL:HG22	1.87	0.57
75:h1:1396:G:H2'	75:h1:1397:G:C8	2.39	0.57
15:Ja:200:LYS:HA	15:Ja:206:GLU:OE2	2.04	0.57
2:A:2719:G:N7	86:A:4043:HOH:O	2.32	0.57
2:A:2959:C:H2'	2:A:2960:G:C8	2.40	0.57
24:AC:173:ARG:NE	75:h1:609:G:O2'	2.38	0.57
75:h1:139:U:H4'	75:h1:140:C:O5'	2.03	0.57
86:3:514:HOH:O	7:BO:75:ARG:HD3	2.03	0.57
14:AP:22:LYS:NZ	14:AP:131:THR:O	2.24	0.57
43:BR:45:ALA:HB2	86:BR:469:HOH:O	2.04	0.57
45:BV:145:ARG:NH2	45:BV:151:LYS:O	2.37	0.57
75:h1:1386:G:H4'	77:Ba:36:GLU:OE2	2.04	0.57
78:AI:16:PHE:HB2	78:AI:76:LEU:CD2	2.35	0.57
15:Ja:159:THR:HG22	15:Ja:173:ILE:HB	1.87	0.57
75:h1:395:C:H1'	86:h1:2115:HOH:O	2.05	0.57
3:2:20:G:C6	3:2:59:U:O4	2.57	0.57
13:AX:7:LYS:HE3	13:AX:17:GLY:HA3	1.87	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AD:40:VAL:HG21	29:AD:113:ILE:HD11	1.85	0.57
34:BK:132:VAL:HG22	86:BK:435:HOH:O	2.05	0.57
46:BJ:53:VAL:HG22	46:BJ:134:VAL:HG22	1.87	0.57
59:Ta:115:ILE:HD11	59:Ta:126:LEU:HD23	1.87	0.57
62:Za:149:ILE:HG12	62:Za:163:ILE:HB	1.87	0.57
75:h1:1171:G:C2	75:h1:1172:A:C8	2.92	0.57
2:A:114:C:OP2	86:A:3860:HOH:O	2.18	0.57
15:Ja:191:ARG:HG2	15:Ja:245:LYS:HG3	1.87	0.57
2:A:242:C:H2'	2:A:243:G:H8	1.70	0.57
2:A:1167:G:N3	86:A:4053:HOH:O	2.33	0.57
2:A:2810:A:O2'	86:A:3859:HOH:O	2.18	0.57
3:2:72:C:H2'	3:2:73:A:C5	2.40	0.57
56:BA:30:ARG:NE	86:BA:101:HOH:O	2.25	0.57
63:AQ:16:ASN:HB3	86:AQ:203:HOH:O	2.03	0.57
72:Aa:104:GLN:HG2	72:Aa:167:ARG:HB2	1.86	0.57
78:AI:76:LEU:HD21	78:AI:80:LEU:HD12	1.86	0.57
2:A:867:A:N1	86:A:4052:HOH:O	2.33	0.56
75:h1:395:C:H2'	75:h1:396:C:C6	2.40	0.56
78:AI:3:ILE:O	78:AI:8:ARG:NH2	2.37	0.56
2:A:28:G:C5'	16:Ea:172:ARG:HD3	2.27	0.56
2:A:2782:U:OP2	86:A:3855:HOH:O	2.17	0.56
40:Fa:21:ARG:NH1	86:Fa:301:HOH:O	2.08	0.56
45:BV:48:VAL:HG21	45:BV:61:LEU:HG	1.87	0.56
53:AA:106:ARG:HG3	53:AA:175:VAL:HG22	1.86	0.56
62:Za:168:ASN:O	62:Za:174:SER:OG	2.17	0.56
75:h1:342:U:H2'	75:h1:343:A:H8	1.71	0.56
19:Ka:19:LEU:CD1	19:Ka:21:ARG:HH21	2.18	0.56
67:BB:94:ASP:O	67:BB:116:GLY:HA3	2.05	0.56
75:h1:427:A:OP1	86:h1:2126:HOH:O	2.18	0.56
75:h1:1230:G:N2	75:h1:1256:G:O2'	2.38	0.56
15:Ja:181:VAL:HG11	15:Ja:225:VAL:HG13	1.86	0.56
15:Ja:211:GLN:HG3	15:Ja:217:GLU:HG2	1.87	0.56
45:BV:31:ASP:OD1	45:BV:33:LYS:NZ	2.39	0.56
51:AB:173:ARG:HA	51:AB:176:ARG:HH12	1.68	0.56
57:AF:44:GLU:OE2	57:AF:47:ARG:NH1	2.38	0.56
75:h1:925:A:H2'	75:h1:926:G:C8	2.41	0.56
75:h1:1477:G:H2'	75:h1:1478:A:C8	2.40	0.56
65:Ua:147:GLY:O	65:Ua:150:LEU:HD23	2.05	0.56
71:La:89:VAL:HG12	71:La:90:ILE:HG23	1.86	0.56
75:h1:465:U:H2'	75:h1:466:A2M:H8	1.87	0.56
77:Ba:29:SER:OG	77:Ba:112:GLY:O	2.16	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2503:U:H2'	2:A:2504:A:C8	2.40	0.56
39:BG:199:ASN:HA	39:BG:202:LYS:HB2	1.88	0.56
57:AF:13:GLY:HA2	57:AF:85:GLN:HE21	1.69	0.56
69:Ra:159:GLU:OE2	69:Ra:162:ASN:ND2	2.39	0.56
77:Ba:57:VAL:HG23	77:Ba:91:VAL:HB	1.87	0.56
17:AL:70:ASN:O	17:AL:75:LYS:NZ	2.32	0.56
53:AA:167:TYR:OH	53:AA:202:THR:O	2.18	0.56
64:Oa:14:MET:HG3	64:Oa:38:MET:HE1	1.88	0.56
66:Ya:54:LEU:HB3	66:Ya:58:PRO:HG2	1.88	0.56
69:Ra:47:ASN:O	69:Ra:64:TYR:HB2	2.05	0.56
72:Aa:60:ARG:NH1	75:h1:1679:U:OP1	2.37	0.56
74:Ca:10:HIS:O	74:Ca:12:LYS:HD2	2.06	0.56
75:h1:1258:U:O2'	78:AI:8:ARG:NH2	2.35	0.56
2:A:584:G:N7	52:BF:32:ARG:NH2	2.54	0.56
2:A:2995:C:C4'	86:A:3824:HOH:O	2.53	0.56
45:BV:82:ARG:NH2	45:BV:191:GLU:OE2	2.39	0.56
52:BF:67:ALA:HA	63:AQ:120:ALA:HB1	1.87	0.56
75:h1:1452:U:H2'	75:h1:1453:U:C6	2.40	0.56
2:A:443:U:H3	2:A:492:G:H1	1.54	0.56
2:A:2205:A:H2'	2:A:2206:A:O4'	2.06	0.56
28:AV:10:VAL:HG22	28:AV:64:THR:HB	1.87	0.56
2:A:1917:A:OP2	80:A:3411:TER:H111	2.05	0.56
3:2:67:C:H2'	3:2:68:A:C8	2.40	0.56
39:BG:124:ILE:HD12	39:BG:198:LYS:HG3	1.88	0.56
67:BB:17:ILE:HD12	67:BB:58:MET:SD	2.46	0.56
72:Aa:147:ALA:HA	72:Aa:150:GLN:NE2	2.21	0.56
75:h1:593:A:H2'	75:h1:594:A:C8	2.41	0.56
2:A:1364:C:N3	63:AQ:30:LYS:NZ	2.55	0.55
7:BO:48:PRO:HD2	86:BO:205:HOH:O	2.06	0.55
15:Ja:248:ILE:HG22	51:AB:73:PHE:CE1	2.41	0.55
2:A:3149:U:N3	86:A:3933:HOH:O	2.26	0.55
45:BV:125:VAL:HG11	45:BV:172:MET:HB3	1.88	0.55
51:AB:113:THR:O	51:AB:117:LYS:HG2	2.06	0.55
68:AN:79:LYS:HG2	68:AN:111:TYR:CE2	2.41	0.55
2:A:789:A:N3	86:A:4037:HOH:O	2.32	0.55
2:A:3014:A:H2'	2:A:3015:A:H8	1.71	0.55
24:AC:172:SER:OG	75:h1:4:C:OP1	2.19	0.55
2:A:224:G:OP1	86:A:3862:HOH:O	2.18	0.55
2:A:939:U:H5''	80:A:3407:TER:H42	1.88	0.55
2:A:1576:A:H2'	2:A:1577:C:C6	2.42	0.55
2:A:3275:C:H2'	2:A:3276:G:H8	1.71	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BO:6:ARG:NH1	86:BO:202:HOH:O	2.38	0.55
31:BQ:137:ILE:HD11	31:BQ:149:LYS:HB2	1.89	0.55
53:AA:191:ASP:OD1	53:AA:191:ASP:N	2.32	0.55
73:AY:55:ARG:HH11	73:AY:55:ARG:HB3	1.72	0.55
2:A:822:G:N3	86:A:4039:HOH:O	2.32	0.55
2:A:1446:OMC:HM23	27:BT:100:MET:HG3	1.88	0.55
24:AC:11:LYS:HE3	24:AC:219:LEU:HD13	1.89	0.55
69:Ra:102:MET:HE3	69:Ra:117:ARG:HG3	1.88	0.55
74:Ca:26:ASN:ND2	75:h1:1270:OMU:O4	2.35	0.55
75:h1:154:A:H2'	75:h1:155:A:O4'	2.05	0.55
75:h1:397:U:H2'	75:h1:398:G:O4'	2.07	0.55
75:h1:484:U:H2'	75:h1:485:A:H8	1.71	0.55
2:A:311:PSU:H2'	2:A:312:C:C6	2.41	0.55
2:A:1339:U:O4	86:A:3863:HOH:O	2.18	0.55
2:A:2696:A:H2'	2:A:2697:G:C8	2.42	0.55
2:A:3014:A:H2'	2:A:3015:A:C8	2.42	0.55
48:BW:57:PHE:O	48:BW:61:GLN:HG2	2.07	0.55
3:2:61:C:H2'	3:2:62:A:C8	2.41	0.55
16:Ea:108:ARG:NH1	86:Ea:407:HOH:O	2.40	0.55
29:AD:165:ASN:OD1	29:AD:166:ILE:N	2.40	0.55
60:AZ:14:THR:HA	60:AZ:17:ARG:HG3	1.89	0.55
67:BB:96:ILE:O	67:BB:117:ILE:HA	2.06	0.55
70:BL:10:VAL:HG11	70:BL:139:ILE:HG13	1.89	0.55
75:h1:1594:G:H2'	75:h1:1595:A:C8	2.42	0.55
2:A:2362:G:H22	2:A:2394:G:H1'	1.72	0.55
27:BT:12:ILE:HD11	27:BT:27:VAL:CG2	2.37	0.55
62:Za:70:VAL:HG23	62:Za:190:ARG:HG3	1.89	0.55
68:AN:44:GLN:HG2	68:AN:62:ILE:HD11	1.89	0.55
2:A:304:A:H2'	2:A:305:A:C8	2.42	0.55
2:A:488:C:H2'	2:A:489:G:C8	2.42	0.55
12:AE:24:GLN:NE2	12:AE:64:GLU:OE1	2.36	0.55
10:Ma:58:VAL:HG13	65:Ua:124:LYS:HB3	1.89	0.55
70:BL:29:ILE:HG23	70:BL:107:GLN:HG2	1.89	0.55
86:C3:404:HOH:O	34:BK:221:HIS:HE1	1.88	0.54
24:AC:141:MET:HG3	24:AC:189:CYS:SG	2.47	0.54
25:BI:107:ASN:OD1	25:BI:111:GLU:N	2.38	0.54
39:BG:228:GLY:O	86:BG:301:HOH:O	2.18	0.54
58:Wa:121:ARG:NH2	75:h1:1549:A:OP2	2.41	0.54
62:Za:141:GLY:HA2	62:Za:146:ILE:HD12	1.88	0.54
75:h1:1252:U:HO2'	75:h1:1253:C:H6	1.53	0.54
75:h1:1260:C:H2'	75:h1:1261:OMU:H6	1.89	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3011:U:H2'	2:A:3012:U:C6	2.42	0.54
24:AC:78:ASP:OD1	24:AC:80:ASN:N	2.39	0.54
53:AA:24:VAL:HG22	78:AI:60:ALA:HB3	1.88	0.54
59:Ta:139:ARG:HD2	59:Ta:142:LYS:HG3	1.89	0.54
77:Ba:41:ASP:OD1	77:Ba:44:ARG:NH2	2.41	0.54
2:A:143:A:OP2	39:BG:187:LYS:NZ	2.30	0.54
2:A:582:A:H4'	52:BF:11:ASN:OD1	2.06	0.54
2:A:1129:A:H2'	2:A:1130:U:H6	1.73	0.54
2:A:1522:G:OP2	86:A:3861:HOH:O	2.18	0.54
78:AI:9:ARG:HH21	78:AI:80:LEU:HA	1.70	0.54
2:A:418:G:O6	32:BH:73:HIS:HE1	1.91	0.54
2:A:582:A:H2'	2:A:583:C:C6	2.42	0.54
2:A:3158:C:H2'	2:A:3159:G:C8	2.43	0.54
17:AL:75:LYS:NZ	17:AL:99:THR:O	2.38	0.54
19:Ka:108:GLN:HG2	19:Ka:112:ARG:HH21	1.72	0.54
29:AD:108:PRO:O	29:AD:112:ILE:HG13	2.07	0.54
35:AT:56:ARG:O	35:AT:60:GLU:HG3	2.07	0.54
75:h1:1161:A:H2'	75:h1:1162:C:H6	1.71	0.54
75:h1:1396:G:H2'	75:h1:1397:G:H8	1.73	0.54
2:A:1576:A:H2'	2:A:1577:C:H6	1.72	0.54
18:Va:40:PHE:O	18:Va:75:LYS:NZ	2.41	0.54
61:BE:82:THR:HG23	61:BE:85:ARG:HH12	1.70	0.54
67:BB:81:ARG:HA	67:BB:81:ARG:CZ	2.37	0.54
75:h1:1385:A:O2'	75:h1:1386:G:H5''	2.08	0.54
2:A:556:U:H2'	2:A:557:C:C6	2.42	0.54
2:A:661:A2M:OP2	2:A:2867:U:O2'	2.25	0.54
2:A:760:A:N7	86:A:4049:HOH:O	2.33	0.54
2:A:945:A2M:HM'2	2:A:947:C:C6	2.42	0.54
2:A:1818:G:H2'	2:A:1819:C:C6	2.42	0.54
18:Va:28:LYS:O	18:Va:32:LEU:HB2	2.08	0.54
50:Na:64:ILE:HG13	50:Na:76:THR:HG21	1.89	0.54
2:A:991:G:N1	2:A:1111:G:H2'	2.22	0.54
8:AR:16:ALA:O	8:AR:20:GLY:CA	2.54	0.54
16:Ea:135:VAL:HG21	16:Ea:151:ILE:HG21	1.88	0.54
69:Ra:58:ARG:HD3	69:Ra:169:THR:HG22	1.88	0.54
74:Ca:16:PRO:HD2	75:h1:1206:C:N3	2.22	0.54
75:h1:123:OMU:HM22	75:h1:124:G:H5'	1.89	0.54
75:h1:409:A:H2'	75:h1:410:C:C6	2.42	0.54
2:A:800:G:N7	86:A:4056:HOH:O	2.33	0.54
2:A:1564:U:O2	39:BG:50:LYS:NZ	2.37	0.54
2:A:1622:G:H2'	2:A:1623:U:C6	2.43	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2968:A:N7	31:BQ:215:ASN:ND2	2.55	0.54
4:C3:29:C:O2'	4:C3:50:A:N1	2.39	0.54
65:Ua:85:LYS:HG3	65:Ua:123:MET:HE1	1.89	0.54
75:h1:298:U:O2'	86:h1:2128:HOH:O	2.19	0.54
2:A:883:U:OP2	2:A:1909:C:O2'	2.21	0.54
2:A:1129:A:H2'	2:A:1130:U:C6	2.43	0.54
16:Ea:176:GLY:O	16:Ea:185:ARG:NH2	2.41	0.54
18:Va:3:LYS:HA	86:Va:315:HOH:O	2.08	0.54
22:BS:91:ALA:CB	22:BS:153:MET:HG2	2.31	0.54
27:BT:365:LYS:HB2	27:BT:367:VAL:HG23	1.89	0.54
53:AA:19:ALA:HB2	74:Ca:49:GLU:OE2	2.08	0.54
59:Ta:57:ASP:HB3	59:Ta:100:ARG:HD2	1.89	0.54
65:Ua:59:MET:HE3	75:h1:899:A:H5'	1.90	0.54
78:AI:50:LYS:HE2	78:AI:57:GLU:HB2	1.90	0.54
27:BT:132:ALA:O	27:BT:136:THR:HG23	2.08	0.53
62:Za:15:LYS:HD3	62:Za:59:TRP:CE3	2.43	0.53
67:BB:33:LYS:HA	67:BB:36:GLU:HG3	1.90	0.53
2:A:1655:G:OP2	86:A:3864:HOH:O	2.18	0.53
2:A:3002:C:H2'	2:A:3003:G:O4'	2.09	0.53
86:A:8310:HOH:O	49:AK:82:LYS:HE3	2.08	0.53
53:AA:64:ARG:HH11	53:AA:64:ARG:HG3	1.72	0.53
69:Ra:83:GLU:HA	69:Ra:86:LYS:HE2	1.91	0.53
71:La:94:ALA:HB3	71:La:101:ILE:HD12	1.89	0.53
75:h1:1543:G:O6	86:h1:2121:HOH:O	2.15	0.53
1:3:130:U:H6	1:3:134:G:H1	1.55	0.53
2:A:989:A:N3	2:A:991:G:H1'	2.23	0.53
2:A:2841:U:O2	2:A:2841:U:H2'	2.09	0.53
15:Ja:43:PRO:HG2	15:Ja:46:LEU:HG	1.89	0.53
17:AL:172:ASN:ND2	86:AL:202:HOH:O	2.17	0.53
33:Da:93:LYS:HG2	33:Da:150:VAL:HG11	1.91	0.53
42:BU:34:ARG:HD3	42:BU:122:THR:HA	1.88	0.53
72:Aa:150:GLN:HG2	72:Aa:150:GLN:O	2.07	0.53
2:A:1722:U:OP2	49:AK:124:TYR:OH	2.20	0.53
2:A:3275:C:H2'	2:A:3276:G:C8	2.43	0.53
19:Ka:68:GLY:HA3	75:h1:534:U:H4'	1.90	0.53
29:AD:17:LYS:HD3	29:AD:23:THR:HB	1.91	0.53
50:Na:76:THR:OG1	50:Na:79:CYS:SG	2.66	0.53
66:Ya:58:PRO:O	66:Ya:62:ILE:HG23	2.09	0.53
2:A:896:G:H2'	2:A:897:U:C6	2.43	0.53
2:A:1003:G:N7	86:A:4072:HOH:O	2.34	0.53
2:A:1445:U:O4	27:BT:74:THR:HG22	2.08	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1456:G:OP1	80:A:3415:TER:N14	2.33	0.53
15:Ja:104:ASP:OD1	15:Ja:110:ARG:HG3	2.09	0.53
29:AD:123:GLU:HG3	64:Oa:54:LEU:HD12	1.90	0.53
35:AT:98:PRO:HB3	35:AT:104:ILE:HG13	1.91	0.53
43:BR:201:LYS:CE	86:BR:404:HOH:O	2.56	0.53
50:Na:63:THR:HG23	50:Na:63:THR:O	2.08	0.53
65:Ua:150:LEU:HB2	75:h1:1773:U:O2	2.09	0.53
66:Ya:37:ASP:OD1	66:Ya:40:LYS:NZ	2.41	0.53
75:h1:196:G:H2'	75:h1:197:G:H8	1.72	0.53
75:h1:1409:A:H2'	75:h1:1410:A:H8	1.74	0.53
75:h1:1619:U:H2'	75:h1:1620:C:C6	2.44	0.53
6:BM:41:LEU:HD21	6:BM:100:GLU:HG3	1.90	0.53
67:BB:57:LEU:HD22	67:BB:69:ILE:HD11	1.91	0.53
72:Aa:2:GLY:N	75:h1:395:C:OP1	2.42	0.53
2:A:394:A:H4'	2:A:395:G:H3'	1.90	0.53
2:A:2595:U:H5	86:A:9669:HOH:O	1.92	0.53
9:AU:72:PRO:HD3	86:AU:219:HOH:O	2.08	0.53
18:Va:28:LYS:HG3	18:Va:32:LEU:HD13	1.89	0.53
59:Ta:43:GLU:HB3	59:Ta:45:PHE:CD2	2.44	0.53
59:Ta:160:ASN:HA	59:Ta:163:ARG:HG3	1.90	0.53
62:Za:187:LEU:HB3	62:Za:193:ILE:HD12	1.89	0.53
72:Aa:146:ILE:HG22	72:Aa:150:GLN:OE1	2.08	0.53
73:AY:39:TYR:CD1	73:AY:40:PRO:HA	2.44	0.53
2:A:1204:G:H2'	2:A:1205:A:C8	2.44	0.53
2:A:2713:G:H5''	2:A:2715:U:C6	2.44	0.53
15:Ja:108:ARG:HH22	75:h1:791:G:P	2.32	0.53
73:AY:25:ARG:HD3	86:AY:306:HOH:O	2.08	0.53
75:h1:522:A:H2'	75:h1:523:A:C8	2.44	0.53
75:h1:1535:C:H4'	75:h1:1541:G:O6	2.09	0.53
3:W2:61:C:H2'	3:W2:62:A:H8	1.74	0.53
7:BO:99:GLN:HB3	86:BO:203:HOH:O	2.09	0.53
15:Ja:148:ARG:NH1	75:h1:126:U:H5'	2.24	0.53
17:AL:95:GLU:HB3	17:AL:141:THR:HG21	1.90	0.53
26:AH:68:LYS:O	26:AH:72:ILE:HG13	2.09	0.53
38:BN:37:LYS:HD2	38:BN:39:ARG:NE	2.24	0.53
53:AA:69:LEU:O	53:AA:73:VAL:HG23	2.09	0.53
75:h1:1594:G:H2'	75:h1:1595:A:H8	1.74	0.53
2:A:261:U:H4'	2:A:262:A:C2	2.44	0.53
3:2:69:C:H2'	3:2:70:C:C6	2.44	0.53
15:Ja:80:LYS:HG3	15:Ja:81:THR:HG23	1.91	0.53
15:Ja:87:MET:HE1	15:Ja:236:VAL:HG11	1.91	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:394:GLU:H	27:BT:394:GLU:CD	2.17	0.53
29:AD:37:TYR:OH	64:Oa:46:ARG:NH2	2.42	0.53
75:h1:31:C:O2'	75:h1:549:U:OP1	2.25	0.53
80:A:3414:TER:H32	80:A:3414:TER:H72	1.91	0.52
14:AP:26:ILE:HD12	14:AP:95:ALA:HB3	1.89	0.52
16:Ea:6:TYR:OH	39:BG:138:GLU:OE2	2.24	0.52
20:AW:102:ARG:NH1	32:BH:8:CYS:HB3	2.23	0.52
44:Xa:126:ILE:HG21	44:Xa:138:PHE:HB3	1.91	0.52
59:Ta:7:ASN:H	59:Ta:12:CYS:HB2	1.74	0.52
62:Za:89:ARG:HH22	62:Za:209:ARG:CG	2.22	0.52
74:Ca:12:LYS:NZ	75:h1:1454:C:OP1	2.40	0.52
2:A:2923:U:O4	86:A:3844:HOH:O	2.14	0.52
72:Aa:118:TYR:CD2	72:Aa:153:ARG:HG3	2.44	0.52
2:A:969:PSU:N1	86:A:4071:HOH:O	2.34	0.52
2:A:990:C:C3'	2:A:991:G:H5''	2.39	0.52
2:A:2704:A:O2'	86:A:3866:HOH:O	2.19	0.52
3:2:70:C:H2'	3:2:71:G:H8	1.73	0.52
24:AC:179:LEU:O	24:AC:183:VAL:HG23	2.09	0.52
59:Ta:104:VAL:HG13	59:Ta:108:LEU:HD12	1.90	0.52
72:Aa:107:ALA:O	72:Aa:111:LYS:HB2	2.10	0.52
72:Aa:118:TYR:CE2	72:Aa:153:ARG:HG3	2.44	0.52
2:A:609:A:H4'	2:A:610:G:O5'	2.09	0.52
2:A:1072:G:O2'	23:AM:108:ARG:NH2	2.42	0.52
75:h1:1223:U:H2'	75:h1:1224:A:H8	1.73	0.52
77:Ba:50:ARG:HH11	77:Ba:50:ARG:HG3	1.74	0.52
2:A:3168:C:H4'	2:A:3171:A:C6	2.45	0.52
4:C3:45:U:H2'	4:C3:46:C:C6	2.44	0.52
25:BI:117:ILE:O	25:BI:137:ASN:ND2	2.32	0.52
31:BQ:36:GLU:OE1	31:BQ:163:ARG:NH1	2.42	0.52
58:Wa:65:ASP:O	58:Wa:69:THR:HG23	2.10	0.52
66:Ya:86:ARG:HB3	66:Ya:122:ALA:HB2	1.90	0.52
68:AN:62:ILE:HG22	68:AN:71:VAL:HG13	1.91	0.52
75:h1:109:A:H2'	75:h1:110:G:C8	2.44	0.52
75:h1:633:G:O2'	86:h1:2129:HOH:O	2.19	0.52
2:A:488:C:H2'	2:A:489:G:H8	1.75	0.52
45:BV:164:ILE:O	45:BV:168:MET:HG3	2.09	0.52
59:Ta:148:ASN:OD1	59:Ta:150:GLY:N	2.36	0.52
67:BB:54:SER:O	67:BB:58:MET:HG2	2.10	0.52
75:h1:67:G:O2'	75:h1:69:A:OP1	2.22	0.52
2:A:401:U:P	86:A:3835:HOH:O	2.68	0.52
2:A:875:A:OP2	86:A:3865:HOH:O	2.19	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:77:ARG:NH2	75:h1:124:G:OP1	2.41	0.52
19:Ka:59:CYS:HB3	19:Ka:62:PHE:HE2	1.75	0.52
39:BG:204:GLU:H	39:BG:204:GLU:CD	2.17	0.52
65:Ua:33:PHE:HB3	65:Ua:40:PHE:HB2	1.91	0.52
65:Ua:83:ARG:O	65:Ua:87:LEU:HD22	2.10	0.52
2:A:1372:G:N7	86:A:4080:HOH:O	2.34	0.52
2:A:1758:C:O3'	68:AN:114:ARG:NH2	2.42	0.52
2:A:3181:G:O6	26:AH:4:LYS:NZ	2.40	0.52
53:AA:162:GLN:NE2	75:h1:1334:C:H4'	2.24	0.52
57:AF:70:ARG:NH1	75:h1:1351:C:H4'	2.24	0.52
66:Ya:46:ILE:HD12	66:Ya:89:ILE:HD12	1.90	0.52
75:h1:79:A:H2'	75:h1:80:C:C6	2.44	0.52
75:h1:117:U:H2'	75:h1:118:U:C6	2.44	0.52
75:h1:484:U:H2'	75:h1:485:A:C8	2.45	0.52
75:h1:803:U:H2'	75:h1:804:G:C8	2.44	0.52
77:Ba:27:LEU:HD12	77:Ba:39:CYS:SG	2.49	0.52
2:A:2268:A:H2'	2:A:2269:A:C8	2.44	0.52
2:A:3384:G:N2	2:A:3385:A:H62	2.07	0.52
14:AP:50:PRO:HD3	14:AP:68:VAL:HG12	1.92	0.52
45:BV:139:CYS:SG	45:BV:168:MET:HE3	2.50	0.52
66:Ya:91:VAL:HG22	66:Ya:92:PRO:HD2	1.90	0.52
75:h1:1059:U:H3'	75:h1:1060:U:H5''	1.90	0.52
2:A:1032:G:C6	2:A:1033:G:C6	2.97	0.52
9:AU:10:GLU:O	9:AU:81:ARG:NH1	2.39	0.52
75:h1:1161:A:H2'	75:h1:1162:C:C6	2.45	0.52
18:Va:51:LEU:HD11	18:Va:72:GLN:HB2	1.92	0.51
29:AD:27:VAL:HG12	29:AD:110:GLN:HG2	1.91	0.51
34:BK:53:VAL:O	86:BK:401:HOH:O	2.19	0.51
75:h1:1764:G:N7	86:h1:2175:HOH:O	2.34	0.51
2:A:2266:U:H2'	2:A:2267:U:H2'	1.91	0.51
2:A:3247:G:H1'	86:A:8902:HOH:O	2.10	0.51
51:AB:122:LYS:HD2	75:h1:481:C:H4'	1.90	0.51
75:h1:409:A:H2'	75:h1:410:C:H6	1.75	0.51
75:h1:1346:A:H1'	77:Ba:57:VAL:HG12	1.92	0.51
75:h1:1374:G:O2'	75:h1:1377:G:OP2	2.16	0.51
28:AV:74:LYS:HE2	28:AV:96:GLU:OE2	2.10	0.51
32:BH:2:VAL:N	86:BH:308:HOH:O	2.43	0.51
75:h1:1221:C:H2'	75:h1:1222:A:H8	1.76	0.51
77:Ba:23:ILE:HG21	77:Ba:101:VAL:HG11	1.92	0.51
2:A:671:G:OP2	86:A:3869:HOH:O	2.19	0.51
2:A:1152:A:H1'	86:A:5142:HOH:O	2.10	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2304:C:O2'	2:A:2305:G:OP2	2.23	0.51
17:AL:14:ARG:HG2	17:AL:61:LEU:HD11	1.92	0.51
28:AV:97:ILE:HG21	28:AV:106:ARG:HG2	1.92	0.51
29:AD:93:VAL:O	29:AD:97:MET:HG3	2.10	0.51
72:Aa:65:ASN:ND2	75:h1:258:A:N3	2.58	0.51
6:BM:127:ARG:HE	6:BM:141:MET:HE1	1.76	0.51
26:AH:81:LYS:O	26:AH:85:GLU:HG3	2.10	0.51
38:BN:79:LEU:HD13	38:BN:97:ILE:HD11	1.93	0.51
53:AA:109:LEU:HD12	53:AA:184:ILE:HD11	1.92	0.51
67:BB:61:ILE:HD11	67:BB:69:ILE:HD13	1.92	0.51
70:BL:6:THR:HG23	70:BL:133:ASP:OD2	2.11	0.51
75:h1:1225:G:H2'	75:h1:1226:U:H6	1.73	0.51
11:Ia:83:LEU:O	11:Ia:87:VAL:HG23	2.09	0.51
17:AL:34:THR:OG1	17:AL:38:ARG:HD2	2.10	0.51
18:Va:67:LYS:HD2	36:Pa:8:LEU:HD23	1.92	0.51
40:Fa:43:LYS:HB2	86:Fa:354:HOH:O	2.11	0.51
53:AA:67:ARG:NH1	78:AI:90:THR:O	2.43	0.51
75:h1:1486:A:H2'	75:h1:1487:A:C8	2.45	0.51
2:A:446:U:H2'	2:A:447:G:C8	2.44	0.51
2:A:642:A:H2'	2:A:643:U:C6	2.45	0.51
86:A:9215:HOH:O	16:Ea:193:LYS:HD3	2.10	0.51
12:AE:77:PRO:HB2	18:Va:7:MET:HE2	1.93	0.51
15:Ja:29:PRO:HD3	75:h1:450:C:OP1	2.11	0.51
22:BS:158:THR:HG23	86:BS:544:HOH:O	2.10	0.51
31:BQ:221:HIS:HB2	86:BQ:403:HOH:O	2.11	0.51
66:Ya:22:PHE:HB3	66:Ya:30:LEU:HD11	1.93	0.51
2:A:1515:G:N7	86:A:4086:HOH:O	2.34	0.51
45:BV:137:MET:HE3	45:BV:172:MET:HG2	1.91	0.51
62:Za:106:ARG:NH1	75:h1:1322:A:OP2	2.44	0.51
63:AQ:19:PHE:HB3	63:AQ:35:LYS:H	1.76	0.51
75:h1:793:U:H2'	75:h1:794:A2M:H8	1.92	0.51
75:h1:1140:A:N1	86:h1:2181:HOH:O	2.34	0.51
1:3:110:C:OP2	86:3:302:HOH:O	2.19	0.51
34:BK:237:GLU:HA	34:BK:240:LYS:HE2	1.92	0.51
65:Ua:83:ARG:HE	65:Ua:87:LEU:HD21	1.76	0.51
2:A:474:U:H2'	2:A:475:C:C6	2.46	0.51
12:AE:23:ARG:NH2	50:Na:5:ASN:O	2.44	0.51
15:Ja:21:ASP:HB2	75:h1:776:C:H5''	1.93	0.51
42:BU:25:VAL:HG11	42:BU:31:ARG:HG2	1.92	0.51
50:Na:58:CYS:HB2	50:Na:65:LEU:HD21	1.92	0.51
59:Ta:111:LEU:HD23	59:Ta:113:LEU:HD21	1.93	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Oa:30:PHE:HE2	64:Oa:37:ILE:HD13	1.75	0.51
70:BL:40:THR:OG1	75:h1:1481:U:OP1	2.27	0.51
72:Aa:84:TYR:HE1	72:Aa:86:ALA:HA	1.76	0.51
75:h1:1577:G7M:H2'	75:h1:1578:A:C8	2.46	0.51
1:3:11:U:H2'	1:3:12:C:C6	2.47	0.50
2:A:1510:U:H2'	86:A:7959:HOH:O	2.11	0.50
2:A:2404:C:H2'	2:A:2405:C:C6	2.46	0.50
2:A:2557:C:OP1	39:BG:28:LYS:NZ	2.43	0.50
72:Aa:138:LYS:HG3	72:Aa:142:LEU:HD12	1.94	0.50
75:h1:30:G:H2'	75:h1:31:C:C6	2.47	0.50
77:Ba:59:MET:HG3	77:Ba:89:LYS:HE3	1.93	0.50
2:A:1056:A:H2'	2:A:1059:C:C5	2.45	0.50
2:A:2452:G:O6	2:A:2459:A:O2'	2.28	0.50
2:A:2841:U:OP1	2:A:2843:C:N4	2.41	0.50
2:A:2881:U:H2'	2:A:2882:OMU:H6	1.94	0.50
2:A:2888:C:N4	2:A:2910:A2M:H2	2.25	0.50
75:h1:1348:U:C2	77:Ba:59:MET:HE1	2.46	0.50
2:A:144:OMU:HM23	39:BG:186:GLN:HG3	1.93	0.50
2:A:608:C:H5'	2:A:609:A:H5''	1.93	0.50
2:A:2713:G:OP2	21:BD:10:THR:HG22	2.12	0.50
2:A:2878:OMC:HM21	22:BS:242:PRO:HD3	1.93	0.50
86:A:7448:HOH:O	21:BD:71:ARG:HD2	2.11	0.50
41:Ha:79:TRP:CZ2	41:Ha:118:LYS:HB3	2.46	0.50
45:BV:180:ASP:OD1	45:BV:180:ASP:N	2.45	0.50
46:BJ:190:ILE:CG2	46:BJ:197:ALA:HB1	2.42	0.50
51:AB:94:LYS:HB2	51:AB:97:TYR:CD1	2.47	0.50
51:AB:136:ILE:O	51:AB:142:LEU:HD12	2.12	0.50
59:Ta:8:PRO:HD3	59:Ta:114:VAL:HG22	1.93	0.50
75:h1:87:A:H2'	75:h1:88:C:H6	1.76	0.50
2:A:227:G:OP1	2:A:702:G:N1	2.33	0.50
2:A:378:U:H2'	2:A:379:U:C6	2.46	0.50
2:A:1086:C:OP2	86:A:3858:HOH:O	2.17	0.50
2:A:1089:U:O2	34:BK:138:ARG:NH2	2.43	0.50
2:A:2630:U:OP1	2:A:2756:U:O2'	2.28	0.50
42:BU:11:MET:HE3	42:BU:136:PRO:HB2	1.92	0.50
45:BV:139:CYS:HB2	45:BV:172:MET:HE3	1.92	0.50
59:Ta:1:MET:HE3	59:Ta:3:PHE:HE1	1.76	0.50
67:BB:2:GLY:N	75:h1:1417:U:OP1	2.45	0.50
69:Ra:105:PRO:HD3	69:Ra:113:ARG:HD3	1.92	0.50
69:Ra:166:LYS:HE3	69:Ra:170:MET:HE3	1.93	0.50
2:A:693:A:N6	2:A:709:C:H2'	2.26	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1670:C:OP1	86:A:3870:HOH:O	2.19	0.50
2:A:3053:C:O2	2:A:3055:U:H5'	2.11	0.50
2:A:3312:G:O2'	9:AU:109:GLY:HA2	2.11	0.50
2:A:3349:A:H2'	2:A:3350:U:O4'	2.12	0.50
43:BR:143:TYR:CE2	43:BR:236:GLU:HG2	2.46	0.50
49:AK:21:LYS:HA	49:AK:53:LYS:HE2	1.94	0.50
59:Ta:139:ARG:HG2	59:Ta:140:ALA:H	1.77	0.50
65:Ua:146:ARG:HB2	65:Ua:150:LEU:HD22	1.93	0.50
72:Aa:33:PRO:HA	75:h1:333:A:H5'	1.94	0.50
74:Ca:24:CYS:HB2	75:h1:1437:U:H4'	1.93	0.50
75:h1:758:A:H2'	75:h1:759:A:O4'	2.11	0.50
2:A:569:C:O2'	2:A:570:G:H5'	2.12	0.50
2:A:1058:A:H2'	46:BJ:22:TYR:CZ	2.46	0.50
2:A:1581:A:H2'	2:A:1581:A:N3	2.26	0.50
11:Ia:94:LYS:HG2	11:Ia:148:VAL:HG22	1.93	0.50
13:AX:39:ARG:NH2	16:Ea:2:GLY:O	2.44	0.50
15:Ja:151:ASP:OD1	15:Ja:152:PRO:HD2	2.11	0.50
16:Ea:147:ARG:NE	86:Ea:409:HOH:O	2.44	0.50
28:AV:85:LEU:HD21	63:AQ:35:LYS:HG2	1.94	0.50
29:AD:102:LEU:HD11	71:La:93:VAL:HG21	1.94	0.50
32:BH:31:GLU:HA	32:BH:31:GLU:OE2	2.11	0.50
51:AB:137:ARG:HD3	51:AB:161:SER:HA	1.92	0.50
52:BF:98:LEU:HD11	52:BF:140:ILE:HG13	1.92	0.50
57:AF:97:LYS:HG2	57:AF:98:TYR:CE1	2.46	0.50
62:Za:138:ILE:HD13	62:Za:148:ILE:HD13	1.93	0.50
68:AN:49:VAL:HG21	68:AN:56:LEU:HA	1.94	0.50
2:A:2565:G:H2'	2:A:2566:C:C6	2.46	0.50
8:AR:43:GLN:OE1	86:AR:201:HOH:O	2.17	0.50
33:Da:35:GLU:O	33:Da:39:LYS:HG3	2.11	0.50
45:BV:111:ARG:NH2	75:h1:931:A:N3	2.59	0.50
66:Ya:83:THR:HG22	66:Ya:85:LEU:H	1.76	0.50
69:Ra:185:GLU:HG3	69:Ra:186:TYR:N	2.26	0.50
2:A:298:G:N7	86:A:4092:HOH:O	2.35	0.50
13:AX:54:ALA:HB3	13:AX:57:GLU:HG3	1.92	0.50
46:BJ:49:CYS:HB3	46:BJ:168:SER:HB3	1.94	0.50
75:h1:129:U:H3'	75:h1:130:A:H5'	1.93	0.50
19:Ka:21:ARG:HH11	19:Ka:76:LEU:HD21	1.77	0.50
22:BS:117:ARG:HA	22:BS:178:LYS:HD2	1.93	0.50
62:Za:86:TYR:CD2	62:Za:172:LYS:HB2	2.47	0.50
75:h1:12:U:H2'	75:h1:13:C:C6	2.46	0.50
75:h1:1566:U:H2'	75:h1:1567:C:H6	1.75	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1057:A:O3'	80:A:3404:TER:N1	2.45	0.49
22:BS:92:TYR:HB2	22:BS:159:VAL:HB	1.93	0.49
45:BV:139:CYS:HB3	45:BV:168:MET:HE3	1.94	0.49
62:Za:89:ARG:NE	67:BB:82:MET:SD	2.82	0.49
67:BB:58:MET:O	67:BB:62:GLN:HG2	2.12	0.49
75:h1:568:C:H2'	75:h1:569:A:O4'	2.12	0.49
2:A:1048:C:H2'	2:A:1049:U:H6	1.77	0.49
2:A:2232:G:N7	86:A:4081:HOH:O	2.34	0.49
32:BH:73:HIS:ND1	32:BH:73:HIS:O	2.43	0.49
32:BH:118:ASP:OD1	32:BH:118:ASP:N	2.45	0.49
45:BV:192:ALA:O	45:BV:196:GLU:HG2	2.11	0.49
62:Za:202:MET:HE3	62:Za:204:ASP:HB2	1.94	0.49
75:h1:452:U:H2'	75:h1:453:G:C8	2.47	0.49
2:A:1397:C:OP1	28:AV:105:LYS:NZ	2.38	0.49
2:A:3190:U:H2'	2:A:3191:C:C6	2.47	0.49
6:BM:24:VAL:HG13	6:BM:87:LYS:HG2	1.94	0.49
19:Ka:16:ASN:HB2	19:Ka:23:GLN:HE21	1.77	0.49
66:Ya:92:PRO:HA	66:Ya:117:ILE:HD11	1.94	0.49
69:Ra:77:HIS:CE1	69:Ra:81:VAL:HG11	2.47	0.49
2:A:421:G:O2'	28:AV:24:ASP:OD2	2.22	0.49
2:A:2391:G:H4'	22:BS:255:ILE:HD13	1.94	0.49
2:A:3169:C:OP1	20:AW:15:ARG:HD2	2.12	0.49
2:A:3240:U:H2'	2:A:3241:U:C6	2.48	0.49
2:A:3323:A:N1	86:A:4089:HOH:O	2.35	0.49
62:Za:46:ARG:HG2	67:BB:101:GLU:HG3	1.94	0.49
64:Oa:39:ARG:NH1	64:Oa:58:ARG:O	2.35	0.49
68:AN:29:VAL:HG21	68:AN:36:ILE:HG23	1.92	0.49
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HG3	1.94	0.49
78:AI:9:ARG:HE	78:AI:80:LEU:HD23	1.77	0.49
78:AI:70:ASN:O	78:AI:74:GLU:HG2	2.12	0.49
16:Ea:50:ARG:HD3	86:Ea:418:HOH:O	2.12	0.49
67:BB:81:ARG:HA	67:BB:81:ARG:NH1	2.28	0.49
69:Ra:109:ALA:O	69:Ra:111:VAL:HG12	2.13	0.49
75:h1:16:G:H2'	75:h1:17:C:C6	2.48	0.49
75:h1:1295:G:O2'	75:h1:1322:A:N1	2.45	0.49
75:h1:1322:A:H4'	75:h1:1323:A:O5'	2.12	0.49
2:A:419:A:C2	2:A:2361:A:H4'	2.47	0.49
2:A:483:C:H2'	2:A:484:G:H8	1.78	0.49
2:A:602:C:H4'	2:A:603:G:O5'	2.13	0.49
86:A:8369:HOH:O	27:BT:67:THR:HG22	2.12	0.49
12:AE:18:GLU:OE1	12:AE:67:GLY:HA2	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AX:7:LYS:HD3	13:AX:18:HIS:O	2.13	0.49
75:h1:65:A:N6	75:h1:85:A:OP2	2.43	0.49
75:h1:585:C:P	86:h1:2195:HOH:O	2.70	0.49
75:h1:615:G:H4'	75:h1:616:C:OP1	2.13	0.49
75:h1:889:U:H2'	75:h1:890:U:C6	2.48	0.49
2:A:1827:G:OP1	60:AZ:39:SER:OG	2.30	0.49
2:A:2661:A:H2'	2:A:2662:G:C8	2.48	0.49
2:A:2688:G:N3	2:A:2688:G:H2'	2.27	0.49
86:AX:207:HOH:O	16:Ea:18:VAL:HG23	2.12	0.49
18:Va:49:ILE:HG22	18:Va:96:ASN:HA	1.94	0.49
33:Da:26:LEU:HD22	33:Da:61:PRO:HD2	1.93	0.49
42:BU:26:GLY:HA2	42:BU:67:ILE:HB	1.94	0.49
53:AA:19:ALA:CB	74:Ca:49:GLU:OE2	2.61	0.49
59:Ta:193:ARG:O	59:Ta:196:ILE:HG22	2.13	0.49
65:Ua:59:MET:HE3	75:h1:899:A:C5'	2.43	0.49
72:Aa:107:ALA:HB2	72:Aa:168:LEU:HG	1.93	0.49
75:h1:1372:C:H2'	75:h1:1373:G:H8	1.77	0.49
86:3:566:HOH:O	2:A:2994:C:H5''	2.13	0.49
2:A:174:G:C4	2:A:175:A:C8	3.01	0.49
2:A:466:C:O2'	2:A:467:A:O4'	2.31	0.49
2:A:712:A:H3'	2:A:712:A:OP2	2.12	0.49
2:A:754:C:H2'	2:A:755:C:C6	2.48	0.49
2:A:1183:G:P	86:A:3928:HOH:O	2.70	0.49
2:A:1401:A:OP1	28:AV:126:ARG:NH1	2.44	0.49
2:A:1787:C:OP1	86:A:3871:HOH:O	2.19	0.49
2:A:2208:G:H4'	3:W2:4:G:O2'	2.13	0.49
19:Ka:26:ILE:HD11	19:Ka:75:GLY:HA3	1.94	0.49
23:AM:27:LEU:HB2	86:AM:223:HOH:O	2.13	0.49
29:AD:125:ALA:HB1	29:AD:136:ARG:HG2	1.94	0.49
36:Pa:28:LYS:HZ2	36:Pa:31:ARG:HE	1.60	0.49
43:BR:30:ALA:O	43:BR:34:GLU:HG2	2.13	0.49
65:Ua:97:ARG:HB3	65:Ua:131:VAL:HG23	1.95	0.49
71:La:96:HIS:HE2	75:h1:1531:PSU:P	2.35	0.49
75:h1:757:G:C6	75:h1:796:A:N6	2.81	0.49
75:h1:1084:G:O2'	75:h1:1095:G:O2'	2.30	0.49
2:A:11:G:H5''	2:A:11:G:H8	1.77	0.49
2:A:1952:C:H2'	2:A:1953:U:H6	1.78	0.49
4:C3:24:U:H2'	4:C3:25:G:O4'	2.13	0.49
11:Ia:20:VAL:HG22	11:Ia:25:ILE:HG12	1.95	0.49
11:Ia:95:MET:HE2	11:Ia:182:ILE:HG22	1.95	0.49
13:AX:46:LEU:HD11	39:BG:163:LEU:HA	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:107:GLY:HA2	15:Ja:189:ARG:HG2	1.95	0.49
46:BJ:46:PHE:HB3	46:BJ:139:ARG:HG2	1.94	0.49
70:BL:125:THR:O	70:BL:129:GLN:HG3	2.13	0.49
75:h1:187:C:H2'	75:h1:188:U:C6	2.48	0.49
2:A:462:G:C5'	63:AQ:74:LYS:HD3	2.42	0.49
2:A:550:G:H2'	2:A:551:A:C8	2.48	0.49
2:A:634:G:OP2	20:AW:64:LYS:HE2	2.13	0.49
2:A:2496:U:O2'	2:A:2497:U:OP1	2.29	0.49
2:A:2555:C:C4	31:BQ:64:ARG:HD2	2.48	0.49
19:Ka:33:ARG:HH11	19:Ka:36:VAL:HG22	1.78	0.49
20:AW:48:TRP:CD1	86:AW:224:HOH:O	2.65	0.49
31:BQ:102:LEU:CD1	86:BQ:412:HOH:O	2.16	0.49
34:BK:214:GLU:HG2	34:BK:217:LYS:HB2	1.93	0.49
48:BW:78:GLU:HA	48:BW:78:GLU:OE2	2.13	0.49
57:AF:17:THR:HG21	75:h1:1487:A:H5'	1.95	0.49
59:Ta:7:ASN:HB2	59:Ta:115:ILE:HD12	1.93	0.49
72:Aa:34:ALA:HB2	72:Aa:57:ARG:CD	2.43	0.49
75:h1:957:U:OP1	75:h1:1073:U:O2'	2.29	0.49
22:BS:208:ILE:HG12	22:BS:326:LEU:HD21	1.94	0.48
22:BS:221:ILE:HG12	22:BS:279:THR:HG23	1.95	0.48
26:AH:36:ALA:HB2	26:AH:50:PHE:CZ	2.48	0.48
32:BH:53:VAL:O	32:BH:57:MET:HG3	2.12	0.48
33:Da:56:ASP:OD2	50:Na:54:THR:HG23	2.13	0.48
52:BF:219:MET:HA	86:BF:314:HOH:O	2.12	0.48
53:AA:42:THR:HB	53:AA:43:PRO:HD2	1.93	0.48
62:Za:201:VAL:O	62:Za:202:MET:HB3	2.13	0.48
75:h1:969:U:OP1	75:h1:1034:C:O2'	2.28	0.48
2:A:801:C:H2'	2:A:802:C:C6	2.48	0.48
2:A:1518:A:N3	86:A:4098:HOH:O	2.35	0.48
2:A:2501:G:H2'	2:A:2502:U:H6	1.78	0.48
2:A:2672:A:OP1	42:BU:96:ARG:NH1	2.46	0.48
15:Ja:73:ASP:OD1	15:Ja:122:LYS:HD3	2.13	0.48
16:Ea:64:VAL:HG21	16:Ea:106:ALA:HB2	1.94	0.48
17:AL:169:TYR:OH	32:BH:31:GLU:HG3	2.13	0.48
26:AH:79:ASP:OD1	26:AH:82:ASN:HB2	2.13	0.48
29:AD:34:LEU:HD12	29:AD:117:VAL:HG22	1.94	0.48
29:AD:164:ARG:NH1	75:h1:1474:A:OP2	2.38	0.48
42:BU:119:ASP:OD1	42:BU:121:SER:OG	2.17	0.48
52:BF:157:ASP:OD1	52:BF:157:ASP:N	2.43	0.48
54:AG:158:GLU:HG2	54:AG:160:PRO:HD3	1.95	0.48
69:Ra:106:LYS:HA	69:Ra:106:LYS:HE3	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:BL:28:LYS:HB2	70:BL:111:MET:SD	2.54	0.48
70:BL:114:VAL:CG1	70:BL:122:ARG:HB3	2.43	0.48
75:h1:141:G:H2'	75:h1:142:G:H8	1.75	0.48
75:h1:1380:U:O2	75:h1:1382:C:N4	2.37	0.48
75:h1:1409:A:H2'	75:h1:1410:A:C8	2.48	0.48
2:A:1838:C:O2'	2:A:1844:A:N1	2.36	0.48
4:C3:26:C:H2'	4:C3:27:A:O4'	2.12	0.48
11:Ia:116:GLU:HG3	11:Ia:128:LYS:HG3	1.95	0.48
26:AH:58:ILE:HG21	26:AH:80:VAL:HG22	1.95	0.48
28:AV:75:PHE:CD2	28:AV:86:LEU:HD21	2.48	0.48
64:Oa:35:ARG:NH1	64:Oa:37:ILE:HD11	2.28	0.48
75:h1:1176:PSU:H2'	75:h1:1177:G:C8	2.48	0.48
2:A:710:G:H5''	2:A:711:U:C5	2.48	0.48
2:A:1625:G:O2'	2:A:1643:A:N1	2.46	0.48
2:A:1870:G:N7	86:A:4088:HOH:O	2.34	0.48
15:Ja:133:GLN:OE1	15:Ja:134:LYS:HG3	2.14	0.48
21:BD:90:HIS:HA	86:BD:348:HOH:O	2.12	0.48
29:AD:29:VAL:HB	29:AD:35:VAL:HG22	1.96	0.48
54:AG:105:LEU:O	54:AG:109:GLN:HG3	2.13	0.48
59:Ta:168:ASN:OD1	59:Ta:172:LYS:N	2.46	0.48
62:Za:22:MET:HB3	62:Za:27:VAL:HB	1.95	0.48
72:Aa:47:ILE:CD1	72:Aa:57:ARG:HB2	2.44	0.48
75:h1:1350:G:H2'	75:h1:1351:C:C6	2.48	0.48
75:h1:1630:PSU:H2'	75:h1:1631:G:C8	2.49	0.48
2:A:151:C:OP2	37:BP:106:ARG:NH1	2.46	0.48
2:A:1117:U:H2'	2:A:1118:C:C6	2.48	0.48
2:A:2676:G:N3	2:A:2676:G:H2'	2.29	0.48
29:AD:38:ILE:HG23	29:AD:68:ILE:HD13	1.95	0.48
37:BP:36:VAL:HG11	38:BN:77:TYR:CD1	2.48	0.48
64:Oa:20:ARG:H	64:Oa:22:GLN:HE21	1.62	0.48
72:Aa:63:THR:HG22	72:Aa:78:ARG:HG2	1.94	0.48
2:A:18:G:N7	86:A:4109:HOH:O	2.35	0.48
2:A:2452:G:H2'	2:A:2455:G:O6	2.14	0.48
2:A:2969:C:H4'	2:A:2970:A:C6	2.48	0.48
2:A:3163:G:H2'	2:A:3164:A:H8	1.78	0.48
11:Ia:34:LEU:HB3	11:Ia:83:LEU:HD22	1.94	0.48
19:Ka:43:GLU:OE1	19:Ka:47:ARG:NH2	2.42	0.48
24:AC:12:LEU:HD11	24:AC:27:ILE:HD12	1.96	0.48
29:AD:51:HIS:NE2	75:h1:1612:G:OP1	2.47	0.48
31:BQ:125:VAL:HG23	31:BQ:126:LEU:HG	1.95	0.48
63:AQ:96:ARG:HA	63:AQ:99:LYS:HE2	1.96	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ra:72:ALA:O	69:Ra:76:ILE:HD12	2.13	0.48
72:Aa:90:GLU:HB2	86:Aa:304:HOH:O	2.13	0.48
75:h1:1172:A:H2'	75:h1:1173:G:H8	1.76	0.48
75:h1:1427:A:H3'	86:h1:2333:HOH:O	2.12	0.48
78:Al:16:PHE:HB2	78:Al:76:LEU:HD21	1.95	0.48
2:A:1117:U:H2'	2:A:1118:C:H6	1.79	0.48
2:A:1292:G:H2'	2:A:1293:C:C6	2.49	0.48
2:A:2929:A:N7	86:A:4111:HOH:O	2.35	0.48
2:A:2946:G:N3	22:BS:253:ALA:HB1	2.28	0.48
68:AN:100:ARG:CZ	68:AN:102:ILE:HD11	2.43	0.48
72:Aa:111:LYS:HE3	72:Aa:163:PHE:HD1	1.77	0.48
72:Aa:140:ASN:HB2	75:h1:190:A:C2	2.49	0.48
2:A:769:G:N2	2:A:779:G:O2'	2.40	0.48
2:A:1929:G:C8	61:BE:16:THR:HG22	2.49	0.48
2:A:2446:A:H2'	2:A:2447:G:C8	2.48	0.48
19:Ka:22:LYS:HG3	19:Ka:77:ILE:HB	1.96	0.48
58:Wa:88:LYS:HG2	66:Ya:23:ARG:HD3	1.96	0.48
59:Ta:160:ASN:HA	59:Ta:163:ARG:CG	2.43	0.48
75:h1:176:A:H2'	75:h1:177:C:C6	2.48	0.48
75:h1:302:A:H2'	75:h1:303:A:C8	2.49	0.48
75:h1:1327:A2M:HM'3	75:h1:1327:A2M:H1'	1.62	0.48
2:A:4:A:H2'	2:A:5:C:O4'	2.13	0.48
2:A:472:G:H2'	2:A:473:G:H8	1.78	0.48
2:A:1079:U:H2'	2:A:1080:C:C6	2.48	0.48
2:A:1195:G:N3	17:AL:114:SER:OG	2.37	0.48
2:A:1469:A:H5'	9:AU:55:VAL:O	2.14	0.48
2:A:3186:U:O2'	2:A:3188:A:N6	2.47	0.48
8:AR:33:ARG:HD3	86:AR:235:HOH:O	2.11	0.48
13:AX:58:LYS:O	13:AX:61:THR:HG22	2.13	0.48
15:Ja:55:ALA:HB2	15:Ja:64:ILE:HD12	1.96	0.48
35:AT:46:LEU:HD22	35:AT:71:HIS:HB3	1.94	0.48
50:Na:47:THR:HG23	50:Na:84:LYS:HD2	1.96	0.48
59:Ta:157:LYS:HA	59:Ta:160:ASN:ND2	2.29	0.48
63:AQ:111:ARG:NH2	63:AQ:113:ASP:OD2	2.46	0.48
69:Ra:114:PRO:HB2	69:Ra:117:ARG:HG2	1.95	0.48
73:AY:76:THR:O	73:AY:77:CYS:CA	2.59	0.48
75:h1:406:G:H2'	75:h1:407:C:H6	1.78	0.48
75:h1:1593:C:H2'	75:h1:1594:G:H8	1.78	0.48
69:Ra:81:VAL:HG12	69:Ra:95:PHE:HE2	1.79	0.48
2:A:428:G:OP1	86:A:3872:HOH:O	2.20	0.47
2:A:1032:G:H2'	2:A:1033:G:C8	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2682:U:H2'	2:A:2683:C:C6	2.49	0.47
15:Ja:247:THR:OG1	15:Ja:250:GLU:HG3	2.14	0.47
32:BH:24:LEU:O	32:BH:28:ILE:HG12	2.14	0.47
62:Za:129:THR:HG22	62:Za:179:PHE:CE2	2.49	0.47
63:AQ:38:ASN:HB2	63:AQ:50:GLY:HA3	1.95	0.47
63:AQ:70:LEU:HD13	63:AQ:101:VAL:HG22	1.96	0.47
75:h1:1318:C:H2'	75:h1:1319:G:O4'	2.14	0.47
77:Ba:36:GLU:O	77:Ba:40:THR:HG22	2.13	0.47
78:AI:11:ILE:HD11	78:AI:37:VAL:HG21	1.96	0.47
1:3:78:PSU:OP1	7:BO:75:ARG:NH1	2.47	0.47
19:Ka:8:ILE:HG23	19:Ka:26:ILE:HG23	1.96	0.47
20:AW:15:ARG:NH2	20:AW:38:GLU:OE2	2.43	0.47
22:BS:87:VAL:HB	22:BS:110:LEU:HD22	1.96	0.47
28:AV:89:HIS:NE2	63:AQ:41:THR:O	2.46	0.47
31:BQ:242:ARG:NH2	31:BQ:245:ARG:O	2.47	0.47
37:BP:89:ARG:O	37:BP:93:ARG:HG2	2.13	0.47
45:BV:28:ASP:HB3	45:BV:94:ARG:NH1	2.29	0.47
53:AA:195:THR:HG22	53:AA:197:LYS:HE2	1.96	0.47
57:AF:99:VAL:HG12	57:AF:100:ASP:OD1	2.14	0.47
1:3:133:U:H2'	1:3:134:G:C8	2.49	0.47
2:A:123:C:H2'	2:A:124:G:H8	1.79	0.47
2:A:827:C:H2'	2:A:828:PSU:O4'	2.14	0.47
2:A:2506:U:H2'	2:A:2507:U:C6	2.49	0.47
20:AW:15:ARG:NH2	32:BH:8:CYS:HB2	2.29	0.47
27:BT:147:HIS:ND1	27:BT:184:ASP:OD2	2.45	0.47
39:BG:217:ASN:HB2	86:BG:316:HOH:O	2.14	0.47
48:BW:32:VAL:HG22	48:BW:59:ARG:HD2	1.96	0.47
70:BL:117:ASP:OD1	70:BL:118:THR:N	2.48	0.47
75:h1:1729:C:H2'	75:h1:1730:C:C6	2.49	0.47
77:Ba:27:LEU:HD22	77:Ba:115:VAL:HG22	1.95	0.47
77:Ba:46:ALA:HB2	77:Ba:94:LEU:HD21	1.96	0.47
2:A:710:G:N2	86:A:3873:HOH:O	2.20	0.47
2:A:2451:U:N3	2:A:2453:U:OP1	2.43	0.47
22:BS:77:THR:HB	22:BS:328:ILE:HG22	1.96	0.47
26:AH:84:TRP:O	26:AH:90:GLY:HA3	2.14	0.47
50:Na:38:LYS:HE2	50:Na:80:SER:OG	2.15	0.47
53:AA:25:LEU:CD1	53:AA:37:VAL:HG21	2.44	0.47
57:AF:134:ARG:HG3	57:AF:140:TYR:HE1	1.78	0.47
75:h1:450:C:H2'	75:h1:451:C:C6	2.48	0.47
75:h1:1223:U:H2'	75:h1:1224:A:C8	2.50	0.47
10:Ma:46:GLU:HG3	65:Ua:112:GLN:CD	2.39	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AP:68:VAL:HG22	14:AP:118:GLU:HG3	1.96	0.47
24:AC:213:GLN:HG3	62:Za:124:ARG:NH2	2.30	0.47
38:BN:130:GLY:CA	86:BN:222:HOH:O	2.55	0.47
52:BF:219:MET:HE3	52:BF:224:LEU:HD21	1.95	0.47
57:AF:12:PHE:HA	57:AF:20:ALA:O	2.14	0.47
57:AF:75:GLY:H	57:AF:78:SER:HG	1.62	0.47
62:Za:28:HIS:HB3	62:Za:55:LEU:HD13	1.95	0.47
75:h1:175:A:H4'	75:h1:176:A:H5''	1.95	0.47
75:h1:1184:A:N3	75:h1:1211:C:O2'	2.44	0.47
75:h1:1581:U:H2'	75:h1:1582:C:C6	2.49	0.47
2:A:693:A:N3	86:A:4112:HOH:O	2.36	0.47
2:A:2881:U:H2'	2:A:2882:OMU:C6	2.45	0.47
14:AP:53:VAL:HG13	14:AP:62:THR:HG23	1.96	0.47
19:Ka:21:ARG:NH1	19:Ka:76:LEU:HD11	2.30	0.47
24:AC:120:ILE:HD12	24:AC:120:ILE:O	2.15	0.47
27:BT:164:GLU:OE1	27:BT:218:THR:HG22	2.14	0.47
45:BV:90:ASP:OD1	45:BV:91:VAL:N	2.47	0.47
45:BV:150:VAL:HG23	75:h1:1068:U:H5''	1.97	0.47
69:Ra:128:GLU:HG2	69:Ra:136:ILE:HD12	1.97	0.47
75:h1:438:A2M:H8	75:h1:438:A2M:O5'	2.13	0.47
75:h1:1671:U:H2'	75:h1:1672:G:O4'	2.14	0.47
2:A:826:A2M:HM'3	2:A:929:A:C4	2.50	0.47
2:A:2196:A:N1	86:A:4115:HOH:O	2.36	0.47
2:A:2501:G:H2'	2:A:2502:U:C6	2.50	0.47
2:A:3193:C:OP2	2:A:3194:C:N4	2.35	0.47
4:C3:16:A:H2'	4:C3:17:G:C8	2.50	0.47
6:BM:15:CYS:SG	6:BM:103:ALA:HB2	2.55	0.47
10:Ma:60:GLU:N	10:Ma:60:GLU:OE1	2.47	0.47
15:Ja:148:ARG:NH1	75:h1:125:A:O3'	2.48	0.47
24:AC:78:ASP:OD1	24:AC:78:ASP:C	2.56	0.47
26:AH:121:VAL:HG21	32:BH:187:GLU:HG3	1.97	0.47
29:AD:66:CYS:SG	29:AD:70:GLU:HG2	2.54	0.47
32:BH:56:LYS:O	32:BH:60:MET:HG2	2.15	0.47
41:Ha:85:ASP:OD1	41:Ha:85:ASP:N	2.45	0.47
42:BU:134:GLU:HG2	42:BU:138:TYR:CD2	2.49	0.47
49:AK:162:LYS:NZ	75:h1:818:G:O4'	2.45	0.47
60:AZ:11:PHE:CZ	60:AZ:34:PHE:HB3	2.50	0.47
63:AQ:17:ASN:HD22	63:AQ:19:PHE:H	1.63	0.47
63:AQ:94:PHE:N	63:AQ:95:PRO:HD2	2.30	0.47
66:Ya:63:LYS:HG2	66:Ya:64:LYS:N	2.29	0.47
66:Ya:91:VAL:O	66:Ya:94:MET:HB2	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BB:74:GLN:O	67:BB:77:GLU:HG3	2.15	0.47
71:La:62:THR:H	71:La:65:ILE:HG22	1.80	0.47
75:h1:192:G:C2'	75:h1:193:G:H5'	2.44	0.47
75:h1:502:C:H2'	75:h1:503:U:O4'	2.15	0.47
75:h1:823:U:H2'	75:h1:824:C:C6	2.50	0.47
75:h1:1376:C:OP2	77:Ba:52:ARG:NH1	2.47	0.47
75:h1:1385:A:O2'	75:h1:1386:G:H8	1.95	0.47
75:h1:1432:G:H2'	75:h1:1433:U:C6	2.50	0.47
2:A:931:U:O4'	86:A:3874:HOH:O	2.20	0.47
2:A:2446:A:H2'	2:A:2447:G:H8	1.80	0.47
2:A:2767:U:H2'	2:A:2768:A:H8	1.80	0.47
2:A:3163:G:H2'	2:A:3164:A:C8	2.49	0.47
15:Ja:205:PHE:HB3	15:Ja:221:ARG:HD3	1.97	0.47
29:AD:137:GLN:OE1	29:AD:204:ARG:NE	2.48	0.47
75:h1:1221:C:H2'	75:h1:1222:A:C8	2.50	0.47
1:3:12:C:OP2	86:3:304:HOH:O	2.21	0.47
2:A:2498:A:H1'	2:A:2499:A:C8	2.49	0.47
2:A:2767:U:H2'	2:A:2768:A:C8	2.50	0.47
80:A:3414:TER:H71	22:BS:247:ARG:HD3	1.96	0.47
29:AD:21:ARG:NH2	29:AD:98:GLU:OE1	2.44	0.47
30:AJ:68:VAL:HG21	30:AJ:94:ILE:HD12	1.97	0.47
53:AA:208:VAL:HG13	67:BB:41:ILE:HG12	1.96	0.47
58:Wa:10:GLN:HB2	58:Wa:57:GLY:HA2	1.96	0.47
70:BL:66:TYR:CD2	70:BL:132:LEU:HD12	2.49	0.47
75:h1:137:A:N6	75:h1:173:G:O2'	2.48	0.47
2:A:497:G:H2'	2:A:498:A:C8	2.50	0.47
2:A:1897:A:O2'	2:A:3051:G:H4'	2.15	0.47
29:AD:51:HIS:O	57:AF:81:TYR:OH	2.32	0.47
44:Xa:88:ARG:NH1	86:Xa:201:HOH:O	2.34	0.47
57:AF:18:ALA:HB2	57:AF:74:GLY:HA3	1.97	0.47
66:Ya:59:MET:HA	66:Ya:62:ILE:HG12	1.96	0.47
71:La:72:ILE:HD12	71:La:76:LEU:HD23	1.97	0.47
75:h1:521:C:C4	75:h1:536:A:N7	2.83	0.47
75:h1:1352:U:H2'	75:h1:1353:A:C8	2.50	0.47
2:A:497:G:H2'	2:A:498:A:H8	1.79	0.46
2:A:712:A:O2'	54:AG:67:LYS:CD	2.62	0.46
2:A:1341:U:H5''	86:A:5896:HOH:O	2.14	0.46
2:A:2926:C:H2'	2:A:2927:C:C6	2.49	0.46
14:AP:94:VAL:HG13	14:AP:112:GLU:HB3	1.96	0.46
15:Ja:148:ARG:HH12	75:h1:126:U:P	2.37	0.46
23:AM:20:ARG:NH2	86:AM:203:HOH:O	2.35	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AA:204:LEU:HB2	53:AA:207:VAL:HG23	1.96	0.46
69:Ra:168:GLU:H	69:Ra:168:GLU:CD	2.23	0.46
2:A:1143:G:O2'	2:A:2641:A:N3	2.44	0.46
2:A:2696:A:H2'	2:A:2697:G:H8	1.80	0.46
2:A:3155:C:H2'	2:A:3156:G:H8	1.80	0.46
4:C3:23:A:H2'	4:C3:24:U:C6	2.50	0.46
9:AU:92:GLU:HG2	9:AU:93:PHE:CD2	2.49	0.46
15:Ja:106:LYS:HD2	15:Ja:108:ARG:HH21	1.81	0.46
43:BR:147:LYS:HD3	43:BR:244:ARG:HE	1.80	0.46
70:BL:23:LEU:HB3	70:BL:29:ILE:HD11	1.97	0.46
2:A:2176:A:N1	86:A:4096:HOH:O	2.35	0.46
2:A:3031:A:H2'	2:A:3032:C:H6	1.80	0.46
39:BG:116:LYS:HE2	39:BG:116:LYS:O	2.15	0.46
41:Ha:66:ASN:OD1	86:Ha:203:HOH:O	2.21	0.46
44:Xa:125:ILE:HB	44:Xa:142:LYS:HB3	1.97	0.46
62:Za:15:LYS:O	62:Za:19:VAL:HG13	2.15	0.46
70:BL:83:SER:OG	75:h1:1527:A:O3'	2.32	0.46
75:h1:1648:C:H2'	75:h1:1649:U:C6	2.50	0.46
77:Ba:54:LYS:HB3	77:Ba:93:ASP:HB2	1.98	0.46
1:3:13:G:OP1	86:3:303:HOH:O	2.20	0.46
2:A:973:G:H5'	41:Ha:29:PRO:HB2	1.97	0.46
2:A:1598:C:H2'	2:A:1599:G:C8	2.50	0.46
2:A:2216:G:H2'	2:A:2217:A:H8	1.80	0.46
2:A:3045:C:O2'	2:A:3046:A:H5'	2.14	0.46
2:A:3090:C:O2'	2:A:3092:G:OP2	2.22	0.46
80:A:3415:TER:H62	6:BM:62:ARG:HD3	1.96	0.46
4:C3:7:G:OP1	34:BK:33:ARG:NH1	2.48	0.46
11:Ia:26:GLU:HG2	11:Ia:35:VAL:HG13	1.96	0.46
24:AC:18:ASP:O	24:AC:18:ASP:OD1	2.33	0.46
52:BF:222:HIS:CD2	52:BF:223:GLU:HG2	2.50	0.46
58:Wa:66:ASN:O	58:Wa:70:ILE:HG13	2.16	0.46
59:Ta:166:PHE:CE1	59:Ta:174:VAL:HB	2.50	0.46
67:BB:106:LEU:HD13	67:BB:117:ILE:HG21	1.97	0.46
75:h1:130:A:N6	75:h1:175:A:O2'	2.48	0.46
75:h1:1472:A:H2'	75:h1:1473:C:C6	2.50	0.46
1:3:117:U:C4	56:BA:7:PHE:CZ	3.04	0.46
2:A:643:U:H2'	2:A:644:U:C6	2.50	0.46
2:A:729:A:OP1	41:Ha:130:THR:HB	2.16	0.46
16:Ea:68:ARG:HD2	16:Ea:128:LYS:HG3	1.97	0.46
23:AM:83:ARG:HE	23:AM:85:ILE:HD11	1.79	0.46
25:BI:18:LEU:HD23	25:BI:56:CYS:HB3	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BP:104:THR:OG1	37:BP:107:GLU:HG3	2.15	0.46
51:AB:94:LYS:HB2	51:AB:97:TYR:HD1	1.81	0.46
57:AF:52:GLU:OE2	57:AF:114:TYR:OH	2.34	0.46
61:BE:8:VAL:O	61:BE:11:VAL:HG22	2.15	0.46
75:h1:1134:A:H2'	75:h1:1135:C:O4'	2.16	0.46
2:A:754:C:H2'	2:A:755:C:H6	1.81	0.46
2:A:1557:A:H5''	86:A:3902:HOH:O	2.14	0.46
2:A:1592:G:P	86:A:5086:HOH:O	2.72	0.46
2:A:2618:OMG:HM23	2:A:2618:OMG:H1'	1.66	0.46
4:C3:28:C:H5''	42:BU:139:ARG:HD3	1.97	0.46
24:AC:178:THR:CB	86:h1:2425:HOH:O	2.44	0.46
66:Ya:83:THR:CG2	66:Ya:85:LEU:H	2.28	0.46
68:AN:38:SER:OG	68:AN:89:TYR:OH	2.22	0.46
69:Ra:61:VAL:HG23	69:Ra:91:LYS:HD3	1.98	0.46
74:Ca:53:ILE:O	74:Ca:54:LYS:HA	2.16	0.46
75:h1:757:G:H4'	75:h1:758:A:OP1	2.16	0.46
1:3:155:OMG:HM22	39:BG:52:ILE:HD11	1.96	0.46
2:A:985:U:H2'	2:A:986:C:O4'	2.16	0.46
2:A:2326:U:O4	86:A:3867:HOH:O	2.19	0.46
2:A:2367:G:H2'	2:A:2368:G:C8	2.51	0.46
2:A:3189:G:H2'	2:A:3190:U:H6	1.80	0.46
2:A:3290:OMG:H5''	86:A:5542:HOH:O	2.16	0.46
17:AL:150:LYS:HA	26:AH:7:VAL:O	2.16	0.46
18:Va:30:SER:OG	18:Va:31:HIS:ND1	2.49	0.46
31:BQ:206:PRO:HG3	31:BQ:213:GLY:HA3	1.98	0.46
37:BP:33:VAL:O	37:BP:37:THR:HG23	2.16	0.46
39:BG:127:LYS:HB2	39:BG:193:CYS:SG	2.56	0.46
41:Ha:76:ASP:HB3	41:Ha:112:GLY:HA3	1.96	0.46
46:BJ:139:ARG:HB2	46:BJ:173:PHE:CE1	2.50	0.46
53:AA:19:ALA:HA	74:Ca:49:GLU:OE2	2.16	0.46
68:AN:104:ALA:HB3	68:AN:107:ASP:O	2.16	0.46
73:AY:11:ARG:HD3	86:AY:303:HOH:O	2.16	0.46
75:h1:1340:C:O2'	75:h1:1342:G:N7	2.46	0.46
2:A:988:G:H4'	2:A:989:A:C4	2.51	0.46
2:A:2723:U:H5	86:A:9602:HOH:O	1.99	0.46
11:Ia:114:SER:HB3	11:Ia:130:GLU:OE1	2.16	0.46
13:AX:8:THR:HG23	13:AX:15:ASN:HB3	1.97	0.46
15:Ja:44:LEU:HD23	15:Ja:47:ILE:HD12	1.98	0.46
48:BW:30:ALA:O	48:BW:59:ARG:NH1	2.44	0.46
51:AB:156:LYS:HG3	51:AB:157:HIS:ND1	2.31	0.46
67:BB:52:GLY:HA3	75:h1:1392:C:O2'	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ra:81:VAL:O	69:Ra:85:GLU:HB2	2.15	0.46
75:h1:1176:PSU:H2'	75:h1:1177:G:H8	1.80	0.46
77:Ba:42:LEU:HG	77:Ba:104:ILE:HG22	1.96	0.46
1:3:22:PSU:O2'	86:3:305:HOH:O	2.21	0.46
2:A:467:A:H2'	2:A:468:A:C8	2.50	0.46
2:A:1026:A:H2'	2:A:1028:U:C5	2.51	0.46
2:A:2243:C:H4'	31:BQ:221:HIS:O	2.16	0.46
15:Ja:151:ASP:OD1	59:Ta:220:ARG:NH1	2.49	0.46
28:AV:33:TRP:CZ2	28:AV:54:PRO:HD2	2.50	0.46
62:Za:209:ARG:HG3	62:Za:209:ARG:HH11	1.80	0.46
75:h1:402:A:H4'	75:h1:403:A:H5''	1.98	0.46
2:A:462:G:H2'	2:A:463:G:C8	2.51	0.46
2:A:1026:A:O2'	2:A:1027:U:OP1	2.29	0.46
2:A:2970:A:N3	3:2:74:C:H4'	2.31	0.46
10:Ma:88:SER:O	10:Ma:92:ARG:HG3	2.16	0.46
29:AD:33:SER:HA	64:Oa:50:VAL:HB	1.98	0.46
45:BV:31:ASP:OD2	45:BV:45:LYS:NZ	2.49	0.46
53:AA:5:ILE:O	53:AA:5:ILE:HG13	2.16	0.46
58:Wa:131:VAL:HG22	75:h1:1547:A:OP1	2.15	0.46
65:Ua:43:VAL:HG12	65:Ua:52:LEU:HD12	1.97	0.46
67:BB:32:LYS:HG3	67:BB:47:ARG:HD3	1.97	0.46
70:BL:73:VAL:O	70:BL:77:ARG:HG3	2.16	0.46
75:h1:823:U:H2'	75:h1:824:C:H6	1.80	0.46
2:A:804:G:H2'	2:A:805:U:C6	2.51	0.45
2:A:1037:A:OP2	2:A:1037:A:H8	1.99	0.45
2:A:3239:U:H2'	2:A:3240:U:C6	2.51	0.45
22:BS:298:ALA:HB3	22:BS:307:LYS:HG3	1.98	0.45
53:AA:133:GLY:HA3	53:AA:156:TYR:O	2.16	0.45
75:h1:206:U:H2'	75:h1:207:A:H8	1.81	0.45
75:h1:1487:A:H2'	75:h1:1488:C:C6	2.51	0.45
2:A:2216:G:H2'	2:A:2217:A:C8	2.51	0.45
2:A:2345:OMU:H5	86:A:7685:HOH:O	2.16	0.45
2:A:3039:U:H2'	2:A:3040:U:C6	2.52	0.45
2:A:3168:C:H5'	86:A:3801:HOH:O	2.16	0.45
11:Ia:10:MET:HE1	11:Ia:81:ASP:HB2	1.98	0.45
26:AH:36:ALA:HB2	26:AH:50:PHE:CE1	2.51	0.45
43:BR:201:LYS:NZ	86:BR:404:HOH:O	2.41	0.45
53:AA:68:GLU:CG	78:AI:90:THR:HG21	2.43	0.45
59:Ta:65:GLN:HE21	75:h1:1684:U:H4'	1.82	0.45
72:Aa:175:ARG:HB2	72:Aa:178:GLN:HB2	1.98	0.45
2:A:2389:OMG:HM23	2:A:2389:OMG:H1'	1.78	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:181:VAL:CG1	15:Ja:225:VAL:HG13	2.46	0.45
28:AV:65:ARG:HD3	63:AQ:28:ASN:ND2	2.31	0.45
1:3:108:A:N3	2:A:20:G:H1'	2.30	0.45
2:A:119:A:O2'	39:BG:101:LYS:NZ	2.48	0.45
2:A:610:G:H2'	2:A:611:C:C6	2.51	0.45
2:A:668:A:H2'	2:A:669:A:C8	2.51	0.45
2:A:1786:C:O2'	86:A:3877:HOH:O	2.21	0.45
2:A:2631:G:N7	86:A:4123:HOH:O	2.36	0.45
40:Fa:67:LEU:HD23	40:Fa:72:ARG:HG3	1.98	0.45
69:Ra:81:VAL:HG12	69:Ra:95:PHE:CE2	2.51	0.45
72:Aa:23:LYS:HE3	75:h1:389:A:OP1	2.16	0.45
2:A:433:C:H2'	2:A:436:C:C6	2.52	0.45
2:A:2403:C:O2	2:A:2818:A:N1	2.50	0.45
80:A:3404:TER:C11	86:AM:248:HOH:O	2.65	0.45
15:Ja:103:TYR:CE1	15:Ja:189:ARG:HD2	2.51	0.45
28:AV:47:PHE:CZ	86:AV:361:HOH:O	2.69	0.45
43:BR:45:ALA:CB	86:BR:469:HOH:O	2.63	0.45
57:AF:61:ARG:CD	57:AF:107:ILE:HD11	2.46	0.45
66:Ya:17:PHE:CD2	66:Ya:18:LYS:HG2	2.51	0.45
68:AN:35:GLU:HG3	68:AN:38:SER:H	1.81	0.45
70:BL:61:MET:O	70:BL:65:VAL:HG23	2.16	0.45
71:La:72:ILE:HG23	71:La:76:LEU:HD23	1.98	0.45
75:h1:1649:U:H2'	75:h1:1650:C:C6	2.52	0.45
2:A:114:C:H5''	13:AX:39:ARG:NH1	2.31	0.45
2:A:338:G:C6	27:BT:201:MET:CE	3.00	0.45
2:A:582:A:H2'	2:A:583:C:H6	1.81	0.45
2:A:1031:G:C2	2:A:1032:G:C5	3.05	0.45
22:BS:259:HIS:HA	22:BS:260:PRO:C	2.42	0.45
26:AH:117:LYS:O	26:AH:121:VAL:HG23	2.16	0.45
45:BV:28:ASP:HB3	45:BV:94:ARG:HH12	1.81	0.45
45:BV:33:LYS:HA	45:BV:41:ARG:O	2.17	0.45
51:AB:178:ASN:ND2	75:h1:513:A:OP2	2.48	0.45
53:AA:47:GLU:C	53:AA:48:ILE:HD13	2.41	0.45
57:AF:50:ILE:HD11	57:AF:80:VAL:HG22	1.98	0.45
62:Za:89:ARG:HG2	62:Za:207:PHE:O	2.17	0.45
75:h1:795:C:H2'	75:h1:796:A:C4	2.52	0.45
75:h1:884:U:H2'	75:h1:885:C:C6	2.52	0.45
75:h1:1221:C:H5''	78:AI:52:LYS:HE3	1.97	0.45
75:h1:1441:G:H2'	75:h1:1442:C:C6	2.52	0.45
75:h1:1500:U:C2	75:h1:1501:G:C8	3.05	0.45
2:A:547:G:O3'	2:A:548:U:H4'	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1572:C:H2'	2:A:1573:U:O4'	2.16	0.45
2:A:1800:A:H2'	2:A:1801:A:C8	2.51	0.45
2:A:2695:A:H2'	2:A:2696:A:C8	2.52	0.45
2:A:2807:A:C6	80:A:3421:TER:H111	2.52	0.45
4:C3:88:U:H2'	4:C3:89:G:O4'	2.17	0.45
13:AX:49:GLU:O	39:BG:224:ARG:NH2	2.49	0.45
13:AX:66:VAL:HG23	13:AX:68:LYS:HG3	1.99	0.45
14:AP:2:VAL:HG21	35:AT:67:LYS:HD2	1.99	0.45
22:BS:171:MET:HE3	22:BS:171:MET:HB2	1.79	0.45
27:BT:12:ILE:CD1	27:BT:260:LYS:HG3	2.47	0.45
27:BT:321:LYS:HD2	43:BR:167:ALA:HB1	1.99	0.45
33:Da:87:ASP:N	33:Da:87:ASP:OD1	2.49	0.45
44:Xa:68:ARG:HH12	44:Xa:130:ARG:N	2.15	0.45
45:BV:143:THR:HG23	45:BV:205:TYR:CE1	2.51	0.45
45:BV:195:ARG:HH11	45:BV:195:ARG:HG3	1.82	0.45
59:Ta:30:LYS:HD2	59:Ta:36:VAL:HG22	1.97	0.45
69:Ra:126:MET:HE3	69:Ra:126:MET:HB2	1.78	0.45
70:BL:24:LYS:HA	70:BL:55:TYR:CE2	2.52	0.45
2:A:2453:U:C5	2:A:2454:A:H1'	2.52	0.45
2:A:2896:A:OP2	2:A:2898:C:N4	2.47	0.45
2:A:3212:G:H2'	2:A:3213:C:C6	2.51	0.45
3:2:18:G:H2'	3:2:57:G:H1	1.82	0.45
24:AC:155:VAL:HG13	24:AC:183:VAL:HG22	1.98	0.45
28:AV:47:PHE:CD1	86:AV:361:HOH:O	2.65	0.45
30:AJ:167:ARG:HA	86:AJ:404:HOH:O	2.17	0.45
31:BQ:30:ARG:NH2	31:BQ:33:ASP:OD2	2.48	0.45
44:Xa:47:ARG:NH1	75:h1:848:A:H5'	2.32	0.45
53:AA:75:LYS:HB3	78:AI:22:PHE:HE2	1.81	0.45
58:Wa:125:HIS:CD2	58:Wa:131:VAL:HG11	2.51	0.45
62:Za:134:ASP:O	62:Za:137:PRO:HD2	2.17	0.45
64:Oa:8:ALA:HB1	64:Oa:28:VAL:HB	1.99	0.45
69:Ra:77:HIS:O	69:Ra:81:VAL:HG13	2.17	0.45
72:Aa:58:ALA:HB2	72:Aa:180:GLY:HA2	1.98	0.45
75:h1:1361:G:C2	75:h1:1362:C:H5	2.34	0.45
2:A:763:G:H2'	2:A:764:A:H8	1.82	0.45
2:A:784:G:O2'	2:A:786:U:OP2	2.32	0.45
2:A:2280:U:O2	2:A:2308:U:H4'	2.16	0.45
2:A:2496:U:HO2'	2:A:2497:U:P	2.40	0.45
2:A:2883:C:H3'	86:A:6307:HOH:O	2.17	0.45
2:A:2888:C:H41	2:A:2910:A2M:H2	1.82	0.45
2:A:3119:U:H1'	2:A:3120:A:H5''	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:C3:426:HOH:O	34:BK:13:PHE:HD1	2.00	0.45
19:Ka:106:ARG:HB2	75:h1:445:C:OP2	2.17	0.45
41:Ha:120:PHE:HE1	41:Ha:122:VAL:HG23	1.82	0.45
46:BJ:184:LEU:HB3	46:BJ:190:ILE:HG12	1.99	0.45
49:AK:42:ARG:NH1	86:AK:301:HOH:O	2.10	0.45
58:Wa:141:ARG:NH2	75:h1:1465:G:N7	2.63	0.45
72:Aa:108:ALA:HB3	72:Aa:109:PRO:HD3	1.98	0.45
75:h1:821:U:H2'	75:h1:822:U:C6	2.52	0.45
75:h1:1370:C:H2'	75:h1:1371:A:H8	1.82	0.45
2:A:188:U:H2'	2:A:189:C:C6	2.52	0.45
2:A:1029:G:C6	2:A:1045:G:C4	3.05	0.45
2:A:1630:U:H2'	2:A:1631:G:C4	2.52	0.45
2:A:1917:A:H2'	2:A:1918:U:C6	2.52	0.45
2:A:2304:C:H5''	86:A:5048:HOH:O	2.15	0.45
2:A:2896:A:H5''	55:Ga:125:LYS:HG3	1.99	0.45
2:A:3230:G:N7	22:BS:152:LYS:HE2	2.32	0.45
16:Ea:145:ASP:HB3	16:Ea:148:ILE:HG22	1.98	0.45
23:AM:34:PHE:HB3	23:AM:64:ILE:HD13	1.99	0.45
39:BG:171:TYR:CE1	39:BG:217:ASN:HB3	2.53	0.45
41:Ha:10:LYS:NZ	86:Ha:208:HOH:O	2.44	0.45
43:BR:91:ILE:O	43:BR:119:GLY:HA2	2.17	0.45
49:AK:170:ARG:NH1	75:h1:817:A:H2'	2.30	0.45
50:Na:69:THR:OG1	50:Na:72:LYS:O	2.34	0.45
51:AB:49:TYR:HE2	51:AB:53:ARG:HH21	1.64	0.45
54:AG:89:ALA:N	54:AG:90:PRO:HD2	2.32	0.45
75:h1:15:U:H2'	75:h1:16:G:O4'	2.16	0.45
75:h1:465:U:H2'	75:h1:466:A2M:C8	2.47	0.45
75:h1:1610:U:H5''	86:h1:2203:HOH:O	2.15	0.45
2:A:107:A:H4'	2:A:108:G:OP1	2.17	0.44
2:A:592:C:H2'	2:A:593:G:O4'	2.16	0.44
2:A:774:U:N3	54:AG:182:LEU:HD21	2.32	0.44
2:A:1952:C:H2'	2:A:1953:U:C6	2.51	0.44
2:A:2548:U:C5	31:BQ:40:TYR:O	2.68	0.44
9:AU:71:PRO:HD2	86:AU:206:HOH:O	2.16	0.44
15:Ja:104:ASP:O	15:Ja:190:GLY:HA3	2.17	0.44
43:BR:238:PHE:HA	86:BR:407:HOH:O	2.17	0.44
44:Xa:60:PRO:HB3	44:Xa:67:ILE:HD11	1.99	0.44
75:h1:821:U:H2'	75:h1:822:U:H6	1.81	0.44
75:h1:1131:G:N7	80:h1:1903:TER:N5	2.65	0.44
3:W2:62:A:H2'	3:W2:63:C:H6	1.82	0.44
1:3:134:G:H2'	1:3:135:G:H8	1.83	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:580:G:H2'	2:A:581:C:O4'	2.17	0.44
2:A:583:C:H2'	2:A:584:G:H8	1.82	0.44
86:A:3988:HOH:O	21:BD:61:LYS:NZ	2.45	0.44
3:2:16:U:H3	3:2:59:U:H3	1.65	0.44
16:Ea:147:ARG:HD2	86:Ea:409:HOH:O	2.17	0.44
22:BS:36:ASP:O	22:BS:188:GLY:HA2	2.17	0.44
22:BS:141:ASP:C	22:BS:141:ASP:OD1	2.60	0.44
35:AT:49:THR:HG23	35:AT:75:GLY:H	1.82	0.44
46:BJ:213:SER:O	46:BJ:213:SER:OG	2.35	0.44
54:AG:89:ALA:HB1	54:AG:94:ILE:HB	1.99	0.44
57:AF:95:TYR:HA	57:AF:99:VAL:HG23	2.00	0.44
68:AN:28:PRO:HB3	68:AN:99:LEU:HD21	1.99	0.44
72:Aa:40:SER:HA	72:Aa:62:ASP:OD2	2.17	0.44
72:Aa:90:GLU:O	72:Aa:94:THR:HG23	2.17	0.44
75:h1:1091:C:H2'	75:h1:1092:A:H5''	1.98	0.44
3:W2:67:C:H2'	3:W2:68:A:C8	2.52	0.44
1:3:110:C:H5''	86:3:346:HOH:O	2.16	0.44
2:A:2660:G:H2'	2:A:2661:A:C8	2.52	0.44
2:A:3317:A:H3'	86:A:3951:HOH:O	2.16	0.44
30:AJ:41:ASN:C	86:AJ:327:HOH:O	2.60	0.44
53:AA:137:ILE:HD13	53:AA:151:LYS:HE2	2.00	0.44
57:AF:99:VAL:HG12	57:AF:100:ASP:H	1.82	0.44
62:Za:128:LEU:HD12	62:Za:138:ILE:HD11	2.00	0.44
66:Ya:54:LEU:HD12	66:Ya:58:PRO:HG2	2.00	0.44
3:W2:54:U:H2'	3:W2:55:U:O4'	2.17	0.44
2:A:510:U:H2'	2:A:511:A:C8	2.53	0.44
2:A:555:G:H2'	2:A:556:U:C6	2.53	0.44
2:A:964:U:H2'	2:A:965:PSU:C6	2.53	0.44
2:A:1030:G:C6	2:A:1031:G:C5	3.05	0.44
2:A:1119:C:H2'	2:A:1120:A:O4'	2.18	0.44
7:BO:54:GLU:HB2	7:BO:107:LYS:HB3	2.00	0.44
11:Ia:96:ARG:CD	11:Ia:146:GLU:HG3	2.48	0.44
15:Ja:57:THR:O	15:Ja:61:VAL:HG23	2.17	0.44
15:Ja:110:ARG:NH1	86:Ja:301:HOH:O	2.50	0.44
44:Xa:66:SER:HG	75:h1:115:A:HO2'	1.61	0.44
46:BJ:189:ARG:NH2	46:BJ:200:LEU:O	2.42	0.44
51:AB:173:ARG:HA	51:AB:176:ARG:NH1	2.32	0.44
53:AA:20:GLU:O	53:AA:24:VAL:HG23	2.16	0.44
62:Za:55:LEU:HA	62:Za:58:THR:CG2	2.43	0.44
74:Ca:7:TRP:CZ3	75:h1:1453:U:H1'	2.53	0.44
75:h1:406:G:H2'	75:h1:407:C:C6	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:817:A:H2'	75:h1:817:A:N3	2.33	0.44
75:h1:944:C:OP2	86:h1:2131:HOH:O	2.21	0.44
2:A:321:A:OP2	86:A:3880:HOH:O	2.21	0.44
2:A:395:G:N2	2:A:1424:C:H4'	2.32	0.44
2:A:432:C:H2'	2:A:433:C:C6	2.52	0.44
2:A:790:G:H4'	86:A:4057:HOH:O	2.17	0.44
2:A:985:U:OP1	30:AJ:54:MET:HE1	2.18	0.44
80:A:3414:TER:HN11	80:A:3414:TER:H41	1.49	0.44
3:2:2:C:H2'	3:2:3:G:C8	2.52	0.44
6:BM:4:TYR:CE1	6:BM:16:LYS:HE3	2.53	0.44
15:Ja:155:LYS:HA	15:Ja:155:LYS:HD3	1.75	0.44
17:AL:134:LYS:N	86:AL:201:HOH:O	2.45	0.44
19:Ka:105:SER:HB3	19:Ka:108:GLN:HB3	1.99	0.44
26:AH:91:ARG:NE	32:BH:206:TYR:OXT	2.48	0.44
45:BV:66:PHE:CE2	65:Ua:47:SER:HB3	2.53	0.44
46:BJ:48:TYR:HB3	46:BJ:140:CYS:O	2.18	0.44
54:AG:9:ASN:HD22	54:AG:9:ASN:N	2.15	0.44
62:Za:136:GLN:HB3	62:Za:137:PRO:HD3	2.00	0.44
64:Oa:17:THR:OG1	64:Oa:18:GLY:N	2.51	0.44
67:BB:60:ARG:NH1	75:h1:1404:A:OP1	2.50	0.44
75:h1:609:G:H5'	75:h1:615:G:N2	2.33	0.44
75:h1:1272:OMG:HM23	75:h1:1272:OMG:HI'	1.71	0.44
75:h1:1324:C:H2'	75:h1:1325:G:O4'	2.18	0.44
75:h1:1441:G:H2'	75:h1:1442:C:H6	1.83	0.44
75:h1:1610:U:C5'	86:h1:2203:HOH:O	2.65	0.44
3:W2:69:C:H2'	3:W2:70:C:O4'	2.18	0.44
77:Ba:20:ILE:HD12	77:Ba:95:PHE:HB3	1.99	0.44
2:A:1222:G:H5''	86:A:3823:HOH:O	2.16	0.44
2:A:2359:A2M:H2'	2:A:2360:C:C6	2.52	0.44
2:A:2672:A:H4'	42:BU:105:GLY:C	2.43	0.44
2:A:3000:C:O2'	22:BS:183:GLU:OE2	2.23	0.44
80:A:3413:TER:H21	86:A:8677:HOH:O	2.18	0.44
23:AM:38:ASP:HB2	23:AM:64:ILE:HD12	2.00	0.44
23:AM:160:LEU:HD12	23:AM:160:LEU:HA	1.86	0.44
28:AV:47:PHE:CG	86:AV:361:HOH:O	2.70	0.44
39:BG:96:GLU:H	39:BG:96:GLU:HG2	1.64	0.44
45:BV:137:MET:CE	45:BV:172:MET:HG2	2.47	0.44
52:BF:219:MET:HE2	52:BF:224:LEU:HD11	2.00	0.44
60:AZ:8:ILE:HG12	60:AZ:45:LEU:HD21	2.00	0.44
75:h1:193:G:HI'	75:h1:194:A:H5'	1.99	0.44
2:A:1029:G:H2'	2:A:1030:G:H8	1.82	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2391:G:O2'	2:A:2392:G:OP2	2.34	0.44
2:A:2454:A:N3	2:A:2454:A:H2'	2.33	0.44
5:BC:10:MET:HE1	75:h1:1116:U:H4'	1.99	0.44
11:Ia:5:LEU:HB2	11:Ia:63:TRP:CZ3	2.53	0.44
15:Ja:197:ASN:N	15:Ja:197:ASN:OD1	2.50	0.44
27:BT:295:LEU:HD12	27:BT:295:LEU:HA	1.81	0.44
34:BK:126:THR:HG22	34:BK:128:GLU:H	1.83	0.44
51:AB:129:VAL:HG13	51:AB:133:GLN:NE2	2.33	0.44
69:Ra:82:ARG:O	69:Ra:86:LYS:HG3	2.18	0.44
75:h1:306:U:H2'	75:h1:307:C:C6	2.53	0.44
75:h1:830:U:O4	86:h1:2130:HOH:O	2.20	0.44
75:h1:1198:C:H5''	86:h1:2718:HOH:O	2.17	0.44
75:h1:1559:U:O2'	75:h1:1560:U:H2'	2.17	0.44
75:h1:1567:C:H2'	75:h1:1568:U:O4'	2.18	0.44
1:3:151:C:H2'	1:3:152:C:C6	2.53	0.44
2:A:434:G:O4'	2:A:436:C:H2'	2.18	0.44
2:A:945:A2M:HM'2	2:A:947:C:C5	2.53	0.44
2:A:2117:C:H2'	2:A:2118:A:O4'	2.18	0.44
2:A:3241:U:H2'	2:A:3242:G:H8	1.79	0.44
16:Ea:147:ARG:CD	86:Ea:409:HOH:O	2.65	0.44
20:AW:18:ILE:HD11	20:AW:103:VAL:HG11	2.00	0.44
24:AC:52:VAL:HG22	24:AC:74:VAL:HG22	2.00	0.44
27:BT:227:PHE:HB2	27:BT:235:LEU:HD11	2.00	0.44
29:AD:18:LEU:HD11	29:AD:50:PRO:HD3	2.00	0.44
29:AD:179:ASN:ND2	29:AD:186:ASN:HB2	2.33	0.44
30:AJ:81:LEU:O	30:AJ:101:ALA:HA	2.18	0.44
53:AA:45:ARG:NH2	53:AA:87:TYR:OH	2.50	0.44
69:Ra:44:LEU:O	69:Ra:44:LEU:HD12	2.17	0.44
75:h1:28:A2M:H1'	75:h1:28:A2M:HM'3	1.63	0.44
75:h1:98:C:H2'	75:h1:99:U:C6	2.53	0.44
75:h1:548:U:H2'	75:h1:549:U:C6	2.53	0.44
75:h1:1796:G:OP1	80:h1:1906:TER:N1	2.51	0.44
2:A:503:C:OP1	20:AW:53:ARG:NH2	2.51	0.44
2:A:1030:G:C4	2:A:1031:G:C8	3.06	0.44
2:A:3129:U:H2'	2:A:3130:C:C6	2.53	0.44
6:BM:15:CYS:SG	6:BM:151:LEU:HB2	2.58	0.44
17:AL:153:LEU:HD23	17:AL:153:LEU:HA	1.87	0.44
24:AC:54:LYS:HD2	24:AC:179:LEU:HD13	2.00	0.44
34:BK:183:HIS:CE1	34:BK:185:GLU:HB2	2.53	0.44
40:Fa:67:LEU:O	40:Fa:72:ARG:NH1	2.43	0.44
46:BJ:52:LEU:HD12	46:BJ:52:LEU:HA	1.85	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:203:ILE:HD13	75:h1:128:G:C2	2.53	0.44
62:Za:172:LYS:HG3	62:Za:208:TYR:HB3	2.00	0.44
72:Aa:187:LEU:C	72:Aa:192:LEU:HD13	2.42	0.44
2:A:210:A:N3	7:BO:9:SER:HB3	2.33	0.43
2:A:1396:G:N7	86:A:4142:HOH:O	2.37	0.43
2:A:2910:A2M:H8	2:A:2910:A2M:H2'	1.55	0.43
2:A:3215:A:H2'	2:A:3216:A:C8	2.53	0.43
45:BV:123:ALA:HB3	45:BV:168:MET:HE2	2.00	0.43
59:Ta:3:PHE:O	59:Ta:15:LYS:HA	2.17	0.43
63:AQ:71:ALA:HA	63:AQ:86:ASN:O	2.18	0.43
65:Ua:102:ASN:HB2	65:Ua:141:ARG:HB3	1.99	0.43
70:BL:92:HIS:NE2	75:h1:1603:G:OP2	2.41	0.43
75:h1:1249:C:C2	75:h1:1250:U:C5	3.06	0.43
75:h1:1281:4AC:O7	75:h1:1281:4AC:H5	2.18	0.43
75:h1:1349:A:H2'	75:h1:1350:G:O4'	2.18	0.43
75:h1:1544:G:N2	75:h1:1570:C:H1'	2.33	0.43
2:A:351:U:H2'	2:A:352:A:H8	1.83	0.43
2:A:1373:A:H2'	2:A:1374:U:O4'	2.18	0.43
2:A:1556:A:H2'	2:A:1557:A:C8	2.52	0.43
2:A:1598:C:H2'	2:A:1599:G:H8	1.83	0.43
2:A:1827:G:H5''	60:AZ:19:ASP:OD2	2.17	0.43
9:AU:56:ASP:HB2	9:AU:98:THR:HG22	2.00	0.43
38:BN:76:LYS:HE2	38:BN:99:ASP:HA	2.00	0.43
39:BG:93:TYR:HE1	39:BG:198:LYS:HD3	1.83	0.43
39:BG:159:TRP:CD1	39:BG:159:TRP:H	2.36	0.43
45:BV:184:LEU:HD12	45:BV:184:LEU:HA	1.80	0.43
58:Wa:42:ASN:HA	58:Wa:52:MET:HE1	2.00	0.43
66:Ya:35:THR:O	66:Ya:39:VAL:HG13	2.18	0.43
66:Ya:60:ALA:O	66:Ya:64:LYS:HG3	2.18	0.43
68:AN:42:PHE:HD2	68:AN:89:TYR:HB2	1.83	0.43
73:AY:38:ALA:HB2	73:AY:45:ARG:HB2	2.00	0.43
73:AY:65:ARG:HD3	86:AY:326:HOH:O	2.18	0.43
75:h1:1121:U:H2'	75:h1:1122:C:C6	2.53	0.43
2:A:212:G:H5''	7:BO:11:ARG:HG3	2.00	0.43
2:A:1510:U:O2'	2:A:1511:G:H5'	2.18	0.43
2:A:1808:A:N7	86:A:4143:HOH:O	2.37	0.43
2:A:2405:C:H2'	2:A:2406:U:C6	2.54	0.43
2:A:3056:C:N4	9:AU:69:ARG:HH11	2.16	0.43
2:A:3189:G:H2'	2:A:3190:U:C6	2.53	0.43
9:AU:88:ASP:OD1	9:AU:89:ALA:N	2.50	0.43
29:AD:17:LYS:HG2	29:AD:23:THR:HA	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BK:22:ARG:CB	34:BK:28:THR:HG22	2.48	0.43
41:Ha:65:ARG:HD2	86:Ha:279:HOH:O	2.19	0.43
45:BV:139:CYS:HB2	45:BV:172:MET:HE1	1.99	0.43
50:Na:12:PRO:HG2	50:Na:17:GLU:HG3	2.00	0.43
57:AF:102:GLN:O	57:AF:106:GLU:HG3	2.18	0.43
65:Ua:71:TYR:O	65:Ua:75:LEU:HD13	2.18	0.43
69:Ra:54:ILE:HG21	69:Ra:169:THR:HA	2.00	0.43
75:h1:987:G:H2'	75:h1:988:G:O4'	2.17	0.43
78:AI:16:PHE:HB2	78:AI:76:LEU:HD22	1.98	0.43
2:A:1016:G:N7	86:A:4136:HOH:O	2.37	0.43
2:A:3215:A:H2'	2:A:3216:A:H8	1.82	0.43
4:C3:12:U:OP2	4:C3:67:C:O2'	2.34	0.43
15:Ja:87:MET:CE	15:Ja:236:VAL:HG11	2.48	0.43
35:AT:40:SER:O	35:AT:40:SER:OG	2.30	0.43
49:AK:95:TRP:CH2	49:AK:99:MET:HE3	2.53	0.43
59:Ta:45:PHE:HB2	59:Ta:48:TYR:CD1	2.52	0.43
59:Ta:66:GLY:HA2	75:h1:1683:A:H1'	2.00	0.43
64:Oa:36:PHE:C	64:Oa:37:ILE:HD12	2.44	0.43
67:BB:30:THR:O	67:BB:34:ILE:HG13	2.18	0.43
75:h1:991:C:H2'	75:h1:992:G:O4'	2.18	0.43
75:h1:1397:G:H2'	75:h1:1398:C:C6	2.54	0.43
1:3:130:U:O2'	1:3:134:G:N2	2.52	0.43
2:A:998:C:OP1	43:BR:130:ASN:ND2	2.41	0.43
2:A:1695:U:O2'	2:A:1750:A:N1	2.40	0.43
2:A:2130:A:H5'	86:A:6201:HOH:O	2.19	0.43
2:A:2398:G:H5''	2:A:2399:A:OP2	2.19	0.43
2:A:2399:A:H1'	86:A:3896:HOH:O	2.19	0.43
86:A:6669:HOH:O	16:Ea:169:LYS:HD3	2.18	0.43
15:Ja:64:ILE:HG13	19:Ka:19:LEU:HD21	2.01	0.43
17:AL:12:VAL:HG12	17:AL:61:LEU:HB2	1.99	0.43
23:AM:150:THR:HG21	27:BT:392:TYR:HE1	1.83	0.43
24:AC:190:LEU:HD23	24:AC:190:LEU:HA	1.90	0.43
29:AD:163:PHE:O	75:h1:1475:C:OP2	2.37	0.43
30:AJ:76:ASP:OD1	30:AJ:76:ASP:N	2.40	0.43
39:BG:217:ASN:CB	86:BG:316:HOH:O	2.66	0.43
58:Wa:133:GLY:HA3	75:h1:1561:G:H5''	2.00	0.43
59:Ta:135:ARG:HH22	75:h1:147:C:H1'	1.84	0.43
68:AN:81:TYR:CZ	68:AN:85:LEU:HD11	2.53	0.43
75:h1:1733:U:H2'	75:h1:1734:A:O4'	2.18	0.43
75:h1:1800:C:H5'	75:h1:1801:A:N7	2.33	0.43
2:A:1033:G:N2	2:A:1040:G:H22	2.17	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1696:A:H2'	2:A:1697:A:C8	2.54	0.43
2:A:2212:A2M:H2	2:A:2428:A:O4'	2.18	0.43
2:A:2814:OMG:H2'	2:A:2869:5MC:HM51	2.01	0.43
86:A:6783:HOH:O	56:BA:45:ARG:HD2	2.19	0.43
29:AD:179:ASN:HD22	29:AD:186:ASN:HB2	1.84	0.43
34:BK:83:LEU:HD13	34:BK:88:LEU:HD23	2.00	0.43
53:AA:52:ALA:O	53:AA:91:VAL:HG23	2.19	0.43
53:AA:105:LEU:HG	53:AA:184:ILE:HD13	2.00	0.43
57:AF:52:GLU:OE1	57:AF:84:ARG:NH1	2.51	0.43
62:Za:172:LYS:HE3	62:Za:172:LYS:HB3	1.63	0.43
75:h1:1119:G:N7	86:h1:2196:HOH:O	2.36	0.43
75:h1:1360:G:OP2	75:h1:1363:A:N6	2.51	0.43
75:h1:1643:C:H2'	75:h1:1644:G:C8	2.54	0.43
2:A:1719:G:N3	86:A:4135:HOH:O	2.37	0.43
2:A:2959:C:H2'	2:A:2960:G:H8	1.81	0.43
3:2:69:C:C2	3:2:70:C:C5	3.06	0.43
20:AW:18:ILE:HD13	20:AW:35:VAL:HG22	2.00	0.43
27:BT:12:ILE:HD11	27:BT:27:VAL:HG23	2.00	0.43
29:AD:31:ASP:O	29:AD:35:VAL:HG23	2.19	0.43
43:BR:100:ILE:HD13	43:BR:138:TYR:CE2	2.54	0.43
67:BB:59:LYS:HE2	67:BB:59:LYS:HB3	1.94	0.43
75:h1:1586:G:O2'	75:h1:1612:G:O6	2.28	0.43
2:A:48:OMU:OP2	86:A:3884:HOH:O	2.21	0.43
2:A:680:A:H2'	2:A:681:U:C6	2.53	0.43
2:A:1335:G:H2'	2:A:1336:A:O4'	2.19	0.43
2:A:2610:U:H2'	2:A:2611:U:C6	2.54	0.43
17:AL:92:MET:HE1	17:AL:116:HIS:CE1	2.54	0.43
19:Ka:88:GLU:CD	19:Ka:89:PRO:HD2	2.44	0.43
26:AH:65:VAL:HG13	26:AH:65:VAL:O	2.18	0.43
27:BT:33:MET:HE3	27:BT:263:PHE:HE1	1.84	0.43
30:AJ:91:VAL:HG13	30:AJ:94:ILE:HD11	2.01	0.43
46:BJ:31:ILE:HG22	46:BJ:62:SER:HB2	2.00	0.43
48:BW:69:ASP:C	48:BW:69:ASP:OD1	2.61	0.43
59:Ta:1:MET:HE3	59:Ta:3:PHE:CE1	2.54	0.43
59:Ta:166:PHE:CE2	75:h1:68:A:H5'	2.53	0.43
74:Ca:14:TYR:OH	75:h1:1557:A:N6	2.51	0.43
75:h1:332:G:H2'	75:h1:333:A:C8	2.53	0.43
75:h1:521:C:C5	75:h1:522:A:C8	3.07	0.43
75:h1:778:A2M:H1'	75:h1:778:A2M:HM'3	1.57	0.43
75:h1:1106:C:O3'	80:h1:1902:TER:H112	2.18	0.43
75:h1:1531:PSU:H2'	75:h1:1532:C:C6	2.54	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2946:G:C2	22:BS:253:ALA:HB1	2.54	0.43
2:A:2952:U:H2'	2:A:2953:U:H2'	2.00	0.43
7:BO:18:HIS:ND1	86:BO:201:HOH:O	2.36	0.43
12:AE:55:ASP:OD1	12:AE:57:ARG:HB2	2.19	0.43
18:Va:66:ARG:NH2	18:Va:113:ASP:OD2	2.35	0.43
34:BK:50:ARG:NH2	34:BK:72:ASP:OD2	2.52	0.43
75:h1:450:C:H2'	75:h1:451:C:H6	1.83	0.43
75:h1:453:G:H2'	75:h1:455:C:O2	2.18	0.43
75:h1:1247:C:H2'	75:h1:1248:U:O4'	2.18	0.43
75:h1:1363:A:O2'	75:h1:1364:U:H5'	2.18	0.43
75:h1:1576:G:H5''	75:h1:1577:G7M:OP1	2.18	0.43
75:h1:1672:G:O2'	75:h1:1735:A:N6	2.47	0.43
2:A:459:A:H2'	2:A:460:A:C8	2.54	0.43
2:A:710:G:H5''	2:A:711:U:H5	1.84	0.43
2:A:2417:A:H2'	2:A:2418:C:C6	2.53	0.43
2:A:3219:C:H2'	2:A:3220:C:C6	2.54	0.43
80:A:3403:TER:H132	80:A:3403:TER:H102	1.86	0.43
27:BT:292:ASN:OD1	27:BT:297:ARG:HD2	2.19	0.43
45:BV:56:ILE:HB	45:BV:59:GLU:HG2	2.01	0.43
60:AZ:55:LYS:O	60:AZ:59:SER:OG	2.31	0.43
62:Za:73:GLU:O	62:Za:75:PRO:HD3	2.19	0.43
66:Ya:90:ILE:HA	66:Ya:94:MET:SD	2.59	0.43
73:AY:55:ARG:CB	73:AY:55:ARG:NH1	2.82	0.43
75:h1:184:C:H2'	75:h1:185:G:O4'	2.19	0.43
75:h1:193:G:O2'	75:h1:194:A:H8	2.01	0.43
3:W2:2:C:H2'	3:W2:3:G:C8	2.54	0.43
2:A:446:U:C2	2:A:447:G:C8	3.07	0.42
2:A:681:U:O2'	2:A:1118:C:O2'	2.37	0.42
2:A:990:C:O2'	2:A:992:C:N4	2.52	0.42
6:BM:127:ARG:HG3	6:BM:141:MET:HE1	2.00	0.42
11:Ia:131:MET:HE1	11:Ia:164:ILE:HD11	2.01	0.42
21:BD:4:ILE:HG13	21:BD:91:PHE:HE1	1.84	0.42
26:AH:11:ARG:NH1	26:AH:56:THR:O	2.46	0.42
26:AH:69:LYS:O	26:AH:73:GLU:HG3	2.19	0.42
34:BK:22:ARG:HB3	34:BK:28:THR:HG22	2.01	0.42
39:BG:204:GLU:OE2	39:BG:204:GLU:N	2.32	0.42
43:BR:47:LYS:O	43:BR:51:LYS:HG2	2.18	0.42
53:AA:44:MET:SD	53:AA:80:PRO:HG2	2.59	0.42
59:Ta:149:LEU:HD23	59:Ta:149:LEU:HA	1.89	0.42
63:AQ:103:ASN:HA	63:AQ:107:ASP:HB2	2.01	0.42
73:AY:72:ARG:O	73:AY:76:THR:HG23	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:251:C:H2'	75:h1:252:A:H8	1.84	0.42
75:h1:1145:U:H2'	75:h1:1146:U:C6	2.54	0.42
2:A:1568:A:H5'	2:A:1569:G:OP2	2.18	0.42
2:A:2879:PSU:H1'	22:BS:253:ALA:HB3	2.00	0.42
2:A:2886:A:H2'	2:A:2886:A:N3	2.33	0.42
10:Ma:14:ASN:HB2	75:h1:1076:C:O2'	2.18	0.42
26:AH:43:MET:HG3	26:AH:44:GLU:O	2.19	0.42
27:BT:275:LYS:HZ1	27:BT:278:GLU:HG2	1.84	0.42
44:XA:68:ARG:NE	75:h1:113:A:O2'	2.51	0.42
47:AO:36:SER:O	47:AO:40:ARG:HG3	2.19	0.42
51:AB:109:ARG:NH2	51:AB:150:VAL:O	2.52	0.42
63:AQ:97:MET:HE2	63:AQ:122:LEU:HD11	2.01	0.42
68:AN:23:ILE:HG22	68:AN:69:ILE:HB	2.01	0.42
78:AI:54:TYR:HB3	78:AI:72:GLY:HA2	2.01	0.42
2:A:11:G:H5'	2:A:12:U:OP2	2.19	0.42
2:A:506:G:O2'	52:BF:78:ARG:HD3	2.19	0.42
2:A:2405:C:H2'	2:A:2406:U:H6	1.83	0.42
17:AL:25:LYS:NZ	23:AM:147:GLU:OE1	2.35	0.42
22:BS:224:THR:HG22	22:BS:333:VAL:HG23	2.01	0.42
34:BK:51:PHE:CE1	34:BK:105:LEU:HD23	2.54	0.42
57:AF:33:LEU:HD23	57:AF:69:ILE:HB	2.01	0.42
66:Ya:44:SER:OG	75:h1:1551:C:H3'	2.18	0.42
69:Ra:27:LEU:HD11	69:Ra:46:ILE:HD11	2.02	0.42
71:La:61:ILE:HB	71:La:102:TYR:HB2	2.00	0.42
75:h1:536:A:C5	75:h1:537:A:C8	3.07	0.42
1:3:19:G:H1'	2:A:405:A:N6	2.34	0.42
1:3:162:C:OP2	39:BG:80:LYS:NZ	2.45	0.42
2:A:462:G:C2	2:A:463:G:C5	3.07	0.42
2:A:795:A:H4'	2:A:796:G:H5'	2.01	0.42
2:A:1816:G:N3	2:A:1817:U:N3	2.67	0.42
2:A:3087:C:H2'	2:A:3088:U:O4'	2.20	0.42
10:Ma:44:ILE:HG13	10:Ma:67:LEU:HG	2.01	0.42
22:BS:84:MET:O	22:BS:205:GLN:HA	2.18	0.42
37:BP:73:TYR:CD1	37:BP:76:LYS:HD2	2.54	0.42
45:BV:101:TRP:CE3	45:BV:217:ILE:HD12	2.55	0.42
48:BW:39:LEU:HD11	62:Za:189:MET:HE2	2.00	0.42
49:AK:176:ARG:NH2	75:h1:854:G:OP2	2.45	0.42
53:AA:42:THR:O	53:AA:43:PRO:C	2.63	0.42
57:AF:13:GLY:N	57:AF:86:SER:OG	2.53	0.42
72:Aa:194:PHE:CE1	72:Aa:198:LYS:HE2	2.54	0.42
75:h1:17:C:H2'	75:h1:18:C:C6	2.55	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:819:G:H2'	75:h1:820:A:H8	1.85	0.42
1:3:155:OMG:HM23	1:3:155:OMG:H1'	1.64	0.42
2:A:544:C:O2'	2:A:545:U:H5'	2.20	0.42
2:A:796:G:H2'	2:A:797:C:C6	2.54	0.42
2:A:1357:C:H3'	30:AJ:38:ARG:HH12	1.84	0.42
2:A:1916:G:H5''	80:A:3411:TER:H132	2.01	0.42
2:A:2156:G:N7	31:BQ:152:SER:OG	2.47	0.42
2:A:2374:G:H2'	2:A:2375:G:C8	2.55	0.42
2:A:2427:G:H2'	2:A:2428:A:C8	2.55	0.42
2:A:2685:U:H2'	2:A:2686:G:O4'	2.20	0.42
10:Ma:17:HIS:ND1	86:h1:2131:HOH:O	2.37	0.42
15:Ja:133:GLN:O	15:Ja:134:LYS:HB2	2.19	0.42
15:Ja:176:ASP:OD1	15:Ja:179:ASN:ND2	2.53	0.42
27:BT:328:LEU:O	27:BT:332:LEU:HG	2.20	0.42
28:AV:80:THR:HG23	28:AV:112:ARG:HG2	2.01	0.42
43:BR:201:LYS:HE3	86:BR:404:HOH:O	2.18	0.42
44:Xa:77:HIS:HB2	44:Xa:88:ARG:HB2	2.01	0.42
51:AB:80:ARG:HH22	75:h1:767:U:P	2.43	0.42
53:AA:29:LEU:HB3	53:AA:34:TYR:HB2	2.01	0.42
53:AA:38:GLU:HB2	53:AA:51:ARG:HH22	1.85	0.42
57:AF:52:GLU:O	57:AF:56:LEU:HD13	2.18	0.42
59:Ta:133:ARG:O	59:Ta:134:MET:HB3	2.19	0.42
65:Ua:118:LEU:HD12	65:Ua:118:LEU:HA	1.85	0.42
75:h1:1737:C:H2'	75:h1:1738:C:H6	1.84	0.42
3:W2:71:G:H2'	3:W2:72:C:O4'	2.19	0.42
78:Al:32:HIS:CG	78:Al:33:PRO:HD2	2.54	0.42
2:A:165:U:H2'	2:A:166:C:C6	2.54	0.42
2:A:556:U:H2'	2:A:557:C:H6	1.83	0.42
2:A:591:A:H4'	2:A:592:C:O5'	2.20	0.42
2:A:916:G:H2'	2:A:935:A:H62	1.83	0.42
2:A:2660:G:H2'	2:A:2661:A:H8	1.84	0.42
2:A:2969:C:H4'	2:A:2970:A:C5	2.54	0.42
2:A:3190:U:H2'	2:A:3191:C:H6	1.83	0.42
16:Ea:65:ARG:HD2	16:Ea:127:TYR:CD1	2.54	0.42
19:Ka:8:ILE:HD12	19:Ka:44:LYS:HB3	2.02	0.42
19:Ka:62:PHE:HA	19:Ka:72:SER:O	2.19	0.42
34:BK:41:LYS:HA	34:BK:41:LYS:HD3	1.93	0.42
45:BV:229:MET:HA	45:BV:229:MET:HE3	2.02	0.42
47:AO:8:CYS:HA	47:AO:32:LEU:O	2.19	0.42
50:Na:35:MET:HB2	50:Na:81:PHE:HB2	2.01	0.42
51:AB:62:LEU:HD21	51:AB:95:LEU:HB2	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:96:GLN:HG2	57:AF:104:LYS:CD	2.50	0.42
66:Ya:94:MET:HB3	66:Ya:112:ILE:HD12	2.02	0.42
75:h1:437:C:H2'	75:h1:438:A2M:O4'	2.19	0.42
75:h1:847:G:O6	75:h1:848:A:N6	2.52	0.42
75:h1:1800:C:H5'	75:h1:1801:A:C8	2.55	0.42
2:A:7:C:H2'	2:A:8:C:O4'	2.19	0.42
2:A:183:U:OP1	7:BO:121:LYS:NZ	2.42	0.42
2:A:668:A:N3	86:A:4146:HOH:O	2.37	0.42
2:A:925:G:H5'	2:A:926:A:OP1	2.19	0.42
2:A:1030:G:H2'	2:A:1031:G:O4'	2.20	0.42
2:A:2766:U:H2'	2:A:2767:U:C6	2.55	0.42
80:A:3409:TER:H102	86:A:9179:HOH:O	2.18	0.42
11:Ia:96:ARG:HD2	11:Ia:146:GLU:HG3	2.01	0.42
24:AC:50:ASP:N	24:AC:50:ASP:OD1	2.52	0.42
41:Ha:2:THR:HG22	41:Ha:4:ARG:HG2	2.01	0.42
48:BW:68:VAL:HG12	62:Za:64:MET:HE1	2.00	0.42
53:AA:162:GLN:N	53:AA:163:PRO:CD	2.82	0.42
59:Ta:123:LEU:HA	59:Ta:124:PRO:HD3	1.96	0.42
69:Ra:65:VAL:O	69:Ra:98:THR:HG22	2.19	0.42
70:BL:32:PRO:HD3	70:BL:103:HIS:CE1	2.55	0.42
75:h1:824:C:H3'	75:h1:825:G:H21	1.85	0.42
75:h1:1032:U:H4'	75:h1:1033:G:OP2	2.20	0.42
75:h1:1255:U:H2'	75:h1:1256:G:C8	2.55	0.42
75:h1:1644:G:H2'	75:h1:1645:U:H6	1.83	0.42
2:A:474:U:H2'	2:A:475:C:H6	1.85	0.42
2:A:1175:G:H5'	86:A:8079:HOH:O	2.20	0.42
2:A:1189:C:C2	2:A:1191:G:C8	3.08	0.42
2:A:2511:U:H4'	39:BG:232:MET:SD	2.60	0.42
2:A:3085:A:H4'	22:BS:369:PHE:CE1	2.55	0.42
2:A:3216:A:H2'	2:A:3217:G:O4'	2.19	0.42
2:A:3248:C:H2'	2:A:3249:C:C6	2.54	0.42
2:A:3365:C:O2'	22:BS:316:PRO:HA	2.20	0.42
15:Ja:138:TYR:CD2	15:Ja:146:THR:HG23	2.55	0.42
19:Ka:42:LYS:HG3	19:Ka:57:ILE:HB	2.02	0.42
36:Pa:5:HIS:O	75:h1:568:C:H4'	2.20	0.42
44:Xa:68:ARG:NH2	75:h1:113:A:O2'	2.46	0.42
53:AA:40:ARG:HD3	77:Ba:111:PRO:HB3	2.02	0.42
53:AA:85:GLU:OE2	53:AA:85:GLU:HA	2.20	0.42
58:Wa:28:PHE:CE2	58:Wa:38:ARG:HD2	2.55	0.42
59:Ta:196:ILE:O	59:Ta:200:LYS:HG3	2.20	0.42
64:Oa:57:GLU:HG2	65:Ua:120:ARG:NH2	2.35	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:BL:128:GLY:O	70:BL:132:LEU:HG	2.19	0.42
71:La:51:LEU:HD12	71:La:55:ALA:HB2	2.02	0.42
71:La:55:ALA:N	71:La:56:PRO:HD2	2.34	0.42
75:h1:277:C:H1'	75:h1:283:G:N2	2.35	0.42
75:h1:422:A2M:HM'3	75:h1:422:A2M:H1'	1.87	0.42
2:A:174:G:H2'	2:A:175:A:H8	1.85	0.42
2:A:2282:C:N4	2:A:2306:C:OP2	2.52	0.42
15:Ja:171:GLU:HG2	15:Ja:235:TRP:HH2	1.85	0.42
18:Va:87:ASP:HA	75:h1:570:G:O5'	2.19	0.42
42:BU:94:LEU:O	42:BU:97:ASN:HB2	2.19	0.42
57:AF:85:GLN:HE22	57:AF:121:ALA:HB2	1.85	0.42
58:Wa:22:GLY:HA2	58:Wa:56:ALA:HB3	2.01	0.42
58:Wa:64:ILE:HD12	58:Wa:64:ILE:H	1.84	0.42
60:AZ:54:ASP:O	60:AZ:58:GLN:HG2	2.20	0.42
62:Za:70:VAL:HG21	62:Za:189:MET:HB3	2.02	0.42
66:Ya:77:LYS:O	66:Ya:79:ALA:N	2.49	0.42
67:BB:100:LYS:HD3	67:BB:100:LYS:N	2.35	0.42
69:Ra:144:ARG:HH21	69:Ra:148:SER:HB3	1.85	0.42
75:h1:192:G:O2'	75:h1:193:G:H5'	2.20	0.42
75:h1:830:U:H2'	75:h1:831:A:C8	2.55	0.42
75:h1:1554:U:O2'	75:h1:1599:A:N3	2.37	0.42
2:A:148:A:H3'	2:A:149:G:H8	1.85	0.42
2:A:930:A:C6	73:AY:8:PHE:HE2	2.37	0.42
2:A:1029:G:C6	2:A:1045:G:C5	3.07	0.42
2:A:1356:G:H5''	27:BT:312:LYS:HD2	2.02	0.42
2:A:1543:A:H2'	2:A:1544:A:C8	2.54	0.42
2:A:2265:C:H2'	2:A:2266:U:C6	2.55	0.42
2:A:3035:U:H5''	22:BS:352:ARG:CZ	2.50	0.42
11:Ia:111:ASP:OD1	11:Ia:111:ASP:N	2.43	0.42
13:AX:11:PHE:CD1	41:Ha:125:LYS:HD3	2.55	0.42
15:Ja:127:ARG:N	15:Ja:140:ASN:O	2.33	0.42
22:BS:285:ILE:HA	22:BS:328:ILE:HD12	2.02	0.42
30:AJ:87:ASP:OD2	30:AJ:107:ARG:HD2	2.20	0.42
47:AO:52:CYS:HA	47:AO:57:TYR:CD1	2.54	0.42
59:Ta:112:ASN:OD1	75:h1:161:G:H1'	2.20	0.42
72:Aa:75:ARG:HB2	72:Aa:110:PHE:CE1	2.55	0.42
75:h1:78:G:O2'	75:h1:80:C:OP2	2.26	0.42
75:h1:438:A2M:H1'	75:h1:438:A2M:HM'3	1.64	0.42
75:h1:1054:G:C4	75:h1:1055:U:C5	3.08	0.42
75:h1:1243:A:N6	75:h1:1245:A:C6	2.88	0.42
75:h1:1483:PSU:O2'	75:h1:1484:U:H5'	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:51:G:H4'	2:A:821:G:H4'	2.02	0.41
2:A:948:U:OP2	41:Ha:26:ARG:NH2	2.36	0.41
2:A:1669:C:H4'	40:Fa:2:VAL:HG21	2.01	0.41
2:A:1675:G:H2'	2:A:1676:A:H8	1.85	0.41
2:A:2980:U:OP1	86:A:3883:HOH:O	2.21	0.41
13:AX:31:SER:HB3	86:AX:218:HOH:O	2.19	0.41
17:AL:164:LYS:HG2	20:AW:45:GLU:OE1	2.20	0.41
18:Va:39:PRO:O	18:Va:76:ASN:ND2	2.46	0.41
38:BN:127:ARG:HD3	38:BN:133:LYS:HE3	2.01	0.41
57:AF:101:GLU:HA	57:AF:104:LYS:HB3	2.01	0.41
66:Ya:47:ARG:HH21	75:h1:1552:A:P	2.43	0.41
70:BL:61:MET:HE3	70:BL:76:PHE:CG	2.55	0.41
75:h1:172:U:H2'	75:h1:173:G:O4'	2.19	0.41
75:h1:783:A:N7	75:h1:785:G:C2	2.88	0.41
75:h1:1335:U:H2'	75:h1:1336:C:H6	1.85	0.41
75:h1:1651:C:H2'	75:h1:1652:U:C6	2.55	0.41
75:h1:1771:G:H4'	75:h1:1772:G:C4	2.55	0.41
3:W2:41:U:H2'	3:W2:42:G:C8	2.55	0.41
3:W2:62:A:H2'	3:W2:63:C:C6	2.53	0.41
1:3:128:C:H2'	1:3:129:C:C1'	2.50	0.41
2:A:463:G:H2'	2:A:464:A:C8	2.55	0.41
2:A:931:U:P	73:AY:3:LYS:HD3	2.60	0.41
2:A:958:C:O2'	2:A:980:G:OP1	2.37	0.41
2:A:1675:G:H2'	2:A:1676:A:C8	2.55	0.41
2:A:2247:G:C8	2:A:2270:G:C8	3.08	0.41
2:A:2500:C:H2'	2:A:2501:G:C8	2.55	0.41
2:A:3205:G:N3	2:A:3208:G:H2'	2.35	0.41
12:AE:14:MET:HE3	12:AE:14:MET:HB2	1.87	0.41
31:BQ:102:LEU:N	86:BQ:412:HOH:O	2.52	0.41
31:BQ:246:LEU:HA	86:BQ:526:HOH:O	2.19	0.41
32:BH:13:VAL:HG12	32:BH:122:ARG:HG3	2.02	0.41
33:Da:112:LYS:NZ	75:h1:976:C:OP1	2.53	0.41
44:Xa:4:GLN:HE21	44:Xa:10:LEU:H	1.67	0.41
57:AF:31:ILE:HG22	57:AF:38:ILE:HD12	2.01	0.41
57:AF:72:ASN:O	75:h1:1486:A:OP1	2.38	0.41
59:Ta:59:GLN:HG3	86:Ta:404:HOH:O	2.19	0.41
66:Ya:121:LEU:HD23	66:Ya:121:LEU:HA	1.92	0.41
69:Ra:133:PRO:HG2	69:Ra:163:THR:CG2	2.50	0.41
75:h1:206:U:H2'	75:h1:207:A:C8	2.53	0.41
75:h1:823:U:H3	75:h1:852:G:H1	1.69	0.41
75:h1:856:A:O2'	75:h1:857:A:H3'	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:981:G:H4'	75:h1:1780:A:H4'	2.03	0.41
75:h1:1183:U:O2'	75:h1:1185:A:N7	2.45	0.41
75:h1:1564:G:C2	75:h1:1565:G:C8	3.07	0.41
3:W2:16:U:H5''	3:W2:17:U:OP1	2.20	0.41
3:W2:61:C:H2'	3:W2:62:A:C8	2.53	0.41
2:A:446:U:H3	2:A:489:G:H1	1.68	0.41
2:A:461:C:H2'	2:A:462:G:C8	2.53	0.41
2:A:794:G:H2'	2:A:794:G:N3	2.35	0.41
2:A:1095:G:H2'	2:A:1096:C:O4'	2.20	0.41
2:A:1173:G:OP1	86:A:3876:HOH:O	2.21	0.41
2:A:1507:A:H2'	2:A:1508:U:C6	2.55	0.41
2:A:1768:G:H2'	2:A:1769:U:O4'	2.20	0.41
2:A:3053:C:O2'	2:A:3055:U:OP2	2.35	0.41
6:BM:31:GLU:OE1	6:BM:60:PHE:HA	2.21	0.41
20:AW:54:MET:HE2	20:AW:75:LYS:N	2.36	0.41
20:AW:58:TYR:CZ	20:AW:70:ARG:HB2	2.56	0.41
22:BS:285:ILE:HG12	22:BS:328:ILE:CD1	2.50	0.41
25:BI:16:MET:HE1	25:BI:57:VAL:HB	2.01	0.41
39:BG:22:LEU:HA	39:BG:22:LEU:HD23	1.80	0.41
51:AB:94:LYS:HD3	51:AB:94:LYS:HA	1.82	0.41
53:AA:68:GLU:HG3	78:AI:90:THR:CG2	2.48	0.41
58:Wa:55:ARG:HE	71:La:41:VAL:HG21	1.85	0.41
63:AQ:129:LEU:HD12	63:AQ:129:LEU:HA	1.86	0.41
72:Aa:85:ASN:HD21	72:Aa:98:VAL:HG21	1.85	0.41
75:h1:76:C:HO2'	75:h1:77:A:C1'	2.32	0.41
75:h1:778:A2M:H2'	75:h1:779:G:H8	1.85	0.41
75:h1:969:U:H2'	75:h1:970:C:O4'	2.20	0.41
2:A:149:G:H2'	2:A:150:PSU:H6	1.84	0.41
2:A:195:A:N3	2:A:215:G:O2'	2.51	0.41
2:A:801:C:H2'	2:A:802:C:H6	1.85	0.41
2:A:932:C:O4'	86:A:3885:HOH:O	2.22	0.41
2:A:1304:A:H3'	86:AL:210:HOH:O	2.20	0.41
2:A:1338:C:H2'	2:A:1339:U:O4'	2.20	0.41
2:A:1869:A:H2'	2:A:1870:G:C8	2.55	0.41
2:A:2253:A:N1	75:h1:1646:C:O2'	2.53	0.41
2:A:2286:OMG:HM23	2:A:2286:OMG:H1'	1.81	0.41
2:A:3253:A:H2'	52:BF:124:PHE:CZ	2.55	0.41
3:2:18:G:O2'	3:2:57:G:N2	2.53	0.41
8:AR:44:ARG:HH11	8:AR:44:ARG:HD3	1.72	0.41
11:Ia:36:ARG:HG2	11:Ia:38:PHE:CZ	2.55	0.41
15:Ja:138:TYR:HD2	15:Ja:146:THR:HG23	1.84	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ja:185:GLY:HA2	15:Ja:189:ARG:HH11	1.84	0.41
16:Ea:201:ARG:O	16:Ea:204:ARG:HD3	2.20	0.41
21:BD:28:TYR:HB3	21:BD:69:VAL:HB	2.01	0.41
30:Aj:177:ARG:HA	30:Aj:183:ARG:O	2.19	0.41
32:BH:11:ARG:NH1	86:BH:306:HOH:O	2.40	0.41
34:BK:51:PHE:HE1	34:BK:105:LEU:HD23	1.86	0.41
39:BG:87:PHE:CE1	39:BG:179:ARG:HG2	2.55	0.41
39:BG:209:LEU:HD23	39:BG:209:LEU:HA	1.91	0.41
41:Ha:44:LEU:HD23	41:Ha:44:LEU:C	2.45	0.41
48:BW:34:LEU:HD21	62:Za:163:ILE:HD11	2.01	0.41
54:AG:80:LYS:HE2	54:AG:80:LYS:HB2	1.69	0.41
59:Ta:3:PHE:HB2	59:Ta:16:LEU:HB2	2.02	0.41
69:Ra:48:GLN:HB3	69:Ra:64:TYR:HD2	1.85	0.41
72:Aa:46:ARG:NH1	72:Aa:54:VAL:HG22	2.35	0.41
75:h1:794:A2M:H1'	75:h1:794:A2M:HM'3	1.65	0.41
75:h1:1148:A:H2'	75:h1:1149:C:C6	2.56	0.41
75:h1:1563:PSU:H4'	75:h1:1601:C:H4'	2.01	0.41
2:A:312:C:H3'	13:AX:30:ARG:NH1	2.35	0.41
2:A:434:G:H4'	2:A:435:G:H5''	2.01	0.41
2:A:566:G:H2'	2:A:567:A:H8	1.86	0.41
2:A:909:G:H1'	2:A:1590:A:N6	2.34	0.41
2:A:1566:A:C8	39:BG:49:PRO:HB3	2.55	0.41
2:A:2123:G:N7	86:A:4149:HOH:O	2.37	0.41
2:A:3265:C:H2'	2:A:3266:A:O4'	2.19	0.41
4:C3:7:G:OP2	34:BK:28:THR:HB	2.20	0.41
4:C3:111:U:H2'	4:C3:112:U:O4'	2.21	0.41
9:Au:90:LYS:HD3	9:Au:91:GLU:HG3	2.01	0.41
12:AE:111:MET:HE2	12:AE:111:MET:HB3	1.89	0.41
15:Ja:54:TYR:CD1	19:Ka:14:MET:HE1	2.56	0.41
24:AC:21:ILE:HD11	24:AC:211:PRO:HB3	2.02	0.41
46:BJ:48:TYR:CE2	46:BJ:145:GLY:HA2	2.56	0.41
49:AK:42:ARG:HD3	86:AK:301:HOH:O	2.20	0.41
58:Wa:4:VAL:HG23	71:La:79:ARG:HH21	1.85	0.41
58:Wa:10:GLN:O	58:Wa:12:ILE:N	2.53	0.41
59:Ta:69:THR:O	59:Ta:101:GLY:HA3	2.21	0.41
59:Ta:77:LEU:HD12	59:Ta:97:LYS:HB2	2.02	0.41
59:Ta:162:TYR:O	59:Ta:163:ARG:C	2.63	0.41
62:Za:36:TYR:CD1	75:h1:1041:G:H4'	2.56	0.41
66:Ya:76:GLU:O	66:Ya:77:LYS:C	2.63	0.41
75:h1:853:A:H2'	75:h1:854:G:O4'	2.21	0.41
2:A:586:G:C8	52:BF:37:ILE:CD1	3.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1348:C:H5'	86:A:6995:HOH:O	2.20	0.41
2:A:1575:A:C8	2:A:1575:A:H3'	2.56	0.41
2:A:2456:G:P	2:A:2456:G:H21	2.44	0.41
2:A:2701:A:OP2	86:A:3889:HOH:O	2.22	0.41
2:A:3001:G:HO2'	22:BS:92:TYR:HH	1.65	0.41
12:AE:4:ILE:HG23	75:h1:636:G:H5'	2.03	0.41
19:Ka:48:MET:HG2	19:Ka:49:TYR:CD1	2.56	0.41
19:Ka:89:PRO:HG2	19:Ka:92:ARG:HB2	2.02	0.41
24:AC:40:ILE:HG13	24:AC:105:LYS:O	2.20	0.41
51:AB:29:GLU:HB2	51:AB:44:LEU:CD2	2.51	0.41
59:Ta:193:ARG:NH2	75:h1:286:G:O6	2.54	0.41
63:AQ:59:ILE:HB	63:AQ:121:ARG:HG2	2.01	0.41
66:Ya:42:PHE:HB3	66:Ya:46:ILE:HB	2.03	0.41
69:Ra:134:ALA:HB1	69:Ra:155:LEU:HB3	2.03	0.41
75:h1:379:G:O2'	75:h1:380:A:OP2	2.32	0.41
75:h1:471:OMC:HM23	75:h1:471:OMC:H1'	1.92	0.41
75:h1:594:A:O2'	75:h1:598:C:OP1	2.37	0.41
75:h1:1108:G:O2'	75:h1:1109:G:H5'	2.20	0.41
75:h1:1477:G:C2	75:h1:1478:A:C5	3.09	0.41
3:W2:23:A:H2'	3:W2:24:G:H8	1.86	0.41
2:A:213:G:OP1	7:BO:15:ARG:NH1	2.49	0.41
2:A:2234:OMG:H4'	3:W2:71:G:OP1	2.21	0.41
2:A:2397:A:H2'	2:A:2398:G:O4'	2.20	0.41
2:A:2453:U:C4	2:A:2454:A:H1'	2.56	0.41
2:A:3161:C:H2'	2:A:3162:C:H6	1.86	0.41
2:A:3247:G:O2'	2:A:3248:C:OP1	2.39	0.41
10:Ma:21:ILE:HD13	10:Ma:72:GLN:HB3	2.02	0.41
17:AL:9:TYR:O	17:AL:30:LYS:HA	2.21	0.41
18:Va:89:CYS:HA	18:Va:92:TYR:CD2	2.56	0.41
23:AM:160:LEU:HD22	23:AM:164:TYR:CD1	2.55	0.41
39:BG:198:LYS:HB3	39:BG:200:GLU:HG2	2.02	0.41
45:BV:86:LEU:HB3	45:BV:98:THR:HB	2.03	0.41
62:Za:20:ARG:HD3	67:BB:117:ILE:HD11	2.01	0.41
62:Za:20:ARG:NH1	67:BB:115:PRO:HD2	2.35	0.41
62:Za:151:PHE:CE1	62:Za:178:LEU:HB3	2.56	0.41
75:h1:1253:C:H2'	75:h1:1254:U:H6	1.86	0.41
2:A:1:G:H2'	2:A:2:C:C6	2.56	0.41
2:A:238:C:H2'	2:A:239:U:O4'	2.21	0.41
2:A:371:A:N3	2:A:373:G:H5''	2.35	0.41
2:A:410:U:H2'	2:A:411:C:H6	1.80	0.41
2:A:420:A:H2'	2:A:421:G:O4'	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:C:H2'	2:A:484:G:C8	2.56	0.41
2:A:1691:U:H2'	2:A:1692:G:C8	2.54	0.41
2:A:3160:C:H2'	2:A:3161:C:C6	2.56	0.41
2:A:3225:C:O2'	2:A:3226:G:OP1	2.32	0.41
10:Ma:73:TYR:CE2	10:Ma:83:VAL:HG21	2.56	0.41
22:BS:320:ILE:HG22	22:BS:322:LYS:HD2	2.03	0.41
26:AH:79:ASP:O	26:AH:79:ASP:CG	2.64	0.41
34:BK:238:LEU:O	34:BK:242:VAL:HG23	2.21	0.41
39:BG:198:LYS:HB2	39:BG:198:LYS:HE2	1.89	0.41
51:AB:135:HIS:CE1	51:AB:165:PRO:HD2	2.56	0.41
53:AA:7:LYS:NZ	77:Ba:89:LYS:HD2	2.36	0.41
58:Wa:23:LYS:HE2	71:La:41:VAL:HB	2.02	0.41
60:AZ:11:PHE:CE2	60:AZ:36:VAL:HG23	2.56	0.41
70:BL:57:ARG:O	70:BL:61:MET:HG3	2.20	0.41
73:AY:55:ARG:NH1	73:AY:55:ARG:HB2	2.36	0.41
75:h1:597:OMG:HM23	75:h1:597:OMG:H1'	1.83	0.41
2:A:92:G:H2'	2:A:93:A:C8	2.56	0.41
2:A:371:A:H4'	2:A:372:A:OP1	2.20	0.41
2:A:531:G:H1	2:A:545:U:H3	1.68	0.41
2:A:667:C:H2'	2:A:668:A:C8	2.56	0.41
2:A:712:A:O2'	54:AG:67:LYS:HD3	2.21	0.41
2:A:1112:A:H2'	2:A:1112:A:N3	2.36	0.41
2:A:2455:G:N1	2:A:2457:A:H3'	2.36	0.41
2:A:2590:G:N7	86:A:4166:HOH:O	2.37	0.41
2:A:2884:C:O2'	2:A:2885:U:H5'	2.21	0.41
2:A:3104:A:H2'	2:A:3105:U:O4'	2.21	0.41
2:A:3219:C:H2'	2:A:3220:C:H6	1.85	0.41
2:A:3340:G:H1'	2:A:3343:G:C8	2.55	0.41
3:2:20:G:H3'	3:2:20:G:N3	2.36	0.41
6:BM:47:TYR:O	6:BM:51:VAL:HG23	2.21	0.41
11:Ia:98:VAL:HG22	55:Ga:82:LEU:HB3	2.03	0.41
14:AP:70:CYS:SG	14:AP:117:LEU:HD12	2.61	0.41
14:AP:72:ILE:HG22	14:AP:100:LEU:HD21	2.03	0.41
19:Ka:16:ASN:HB2	19:Ka:23:GLN:NE2	2.36	0.41
22:BS:110:LEU:O	22:BS:115:ARG:NH1	2.53	0.41
24:AC:160:LEU:HD23	24:AC:165:ILE:HD13	2.02	0.41
29:AD:107:ASN:O	29:AD:111:VAL:HG23	2.21	0.41
29:AD:112:ILE:HG12	29:AD:177:LEU:HD13	2.01	0.41
33:Da:53:ILE:HD13	33:Da:53:ILE:HA	1.93	0.41
34:BK:65:VAL:CG1	34:BK:72:ASP:HB3	2.50	0.41
39:BG:52:ILE:O	39:BG:55:GLN:HB2	2.21	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ha:133:LYS:O	41:Ha:137:GLU:HG3	2.21	0.41
43:BR:70:LEU:HD23	43:BR:70:LEU:HA	1.91	0.41
57:AF:26:ARG:H	57:AF:26:ARG:HG3	1.71	0.41
57:AF:52:GLU:N	57:AF:53:PRO:HD2	2.36	0.41
57:AF:100:ASP:OD1	57:AF:100:ASP:N	2.40	0.41
58:Wa:79:ILE:HA	58:Wa:80:PRO:HD3	1.93	0.41
62:Za:13:SER:OG	62:Za:14:GLN:N	2.50	0.41
62:Za:107:HIS:CE1	62:Za:111:THR:HB	2.55	0.41
65:Ua:83:ARG:HA	65:Ua:83:ARG:HD2	1.86	0.41
67:BB:60:ARG:O	67:BB:63:LYS:HG2	2.21	0.41
67:BB:66:VAL:HB	67:BB:69:ILE:HD12	2.03	0.41
69:Ra:58:ARG:CZ	69:Ra:58:ARG:HA	2.50	0.41
69:Ra:171:VAL:HG22	69:Ra:182:VAL:HG23	2.02	0.41
70:BL:127:SER:O	70:BL:131:ASP:OD1	2.39	0.41
70:BL:131:ASP:O	70:BL:135:VAL:HG22	2.20	0.41
75:h1:162:A2M:HM'3	75:h1:162:A2M:H1'	1.67	0.41
75:h1:979:A:H2'	75:h1:980:A:O4'	2.21	0.41
75:h1:1249:C:H2'	75:h1:1250:U:C6	2.56	0.41
75:h1:1453:U:H2'	75:h1:1454:C:C6	2.56	0.41
78:AI:46:MET:HE2	78:AI:66:TRP:CG	2.56	0.41
2:A:272:U:H2'	2:A:273:U:C6	2.55	0.41
2:A:370:A:O2'	86:A:3890:HOH:O	2.22	0.41
2:A:583:C:H2'	2:A:584:G:C8	2.55	0.41
2:A:784:G:H3'	86:A:9443:HOH:O	2.19	0.41
2:A:1004:G:N3	2:A:2636:A:H2'	2.36	0.41
2:A:2746:A:H1'	86:A:6056:HOH:O	2.21	0.41
44:Xa:126:ILE:HD13	44:Xa:140:VAL:HA	2.03	0.41
50:Na:57:VAL:HG13	50:Na:62:GLN:O	2.21	0.41
53:AA:8:LYS:O	53:AA:12:VAL:HG23	2.20	0.41
53:AA:31:GLU:C	53:AA:54:ARG:HH21	2.29	0.41
53:AA:92:ASN:N	53:AA:92:ASN:OD1	2.53	0.41
64:Oa:57:GLU:HA	65:Ua:120:ARG:HH22	1.86	0.41
72:Aa:48:ARG:NH2	75:h1:400:G:OP2	2.50	0.41
75:h1:87:A:H2'	75:h1:88:C:C6	2.55	0.41
75:h1:1063:A:H3'	75:h1:1064:G:H8	1.86	0.41
75:h1:1125:A:OP2	86:h1:2132:HOH:O	2.22	0.41
75:h1:1270:OMU:H4'	75:h1:1271:G:C5'	2.51	0.41
76:B1:18:U:O2'	76:B1:19:U:OP1	2.37	0.41
78:AI:54:TYR:HB3	78:AI:72:GLY:CA	2.50	0.41
2:A:368:G:H4'	2:A:393:A:N1	2.36	0.40
2:A:1048:C:H2'	2:A:1049:U:C6	2.55	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2944:G:O2'	2:A:2947:OMC:OP2	2.28	0.40
80:A:3418:TER:H112	86:A:8901:HOH:O	2.20	0.40
4:C3:93:U:H2'	4:C3:94:C:H6	1.80	0.40
15:Ja:66:MET:HG3	75:h1:456:A:O4'	2.21	0.40
17:AL:61:LEU:HD22	23:AM:141:VAL:HG21	2.02	0.40
18:Va:11:ARG:NH2	44:Xa:102:GLU:OE1	2.54	0.40
26:AH:42:ASP:OD1	26:AH:42:ASP:N	2.53	0.40
27:BT:54:ARG:NH2	86:BT:508:HOH:O	2.39	0.40
30:AJ:46:ALA:HB3	86:AJ:330:HOH:O	2.22	0.40
34:BK:83:LEU:N	34:BK:84:PRO:CD	2.84	0.40
36:Pa:37:ARG:NH1	75:h1:480:A:OP1	2.48	0.40
38:BN:85:MET:CE	38:BN:153:ILE:HG23	2.50	0.40
43:BR:69:ARG:HH12	43:BR:70:LEU:HD23	1.86	0.40
46:BJ:46:PHE:CB	46:BJ:139:ARG:HG2	2.51	0.40
52:BF:147:ASP:OD1	52:BF:147:ASP:C	2.63	0.40
52:BF:192:ASP:O	52:BF:196:ILE:HG13	2.21	0.40
57:AF:46:LEU:HB3	57:AF:80:VAL:HG21	2.01	0.40
61:BE:44:LYS:HE2	61:BE:44:LYS:HB3	1.73	0.40
65:Ua:137:ASP:OD1	75:h1:929:G:H4'	2.21	0.40
69:Ra:61:VAL:CG2	69:Ra:91:LYS:HD3	2.51	0.40
3:W2:73:A:O2'	3:W2:74:C:H5'	2.21	0.40
78:Al:52:LYS:CD	78:Al:54:TYR:HE2	2.35	0.40
1:3:156:G:N2	39:BG:55:GLN:OE1	2.44	0.40
2:A:185:A:OP2	7:BO:45:ARG:NH1	2.54	0.40
2:A:447:G:C2	2:A:448:G:C8	3.10	0.40
2:A:609:A:OP1	52:BF:29:TYR:OH	2.36	0.40
2:A:885:A2M:HM'3	2:A:885:A2M:H1'	1.93	0.40
2:A:3282:A:H2'	2:A:3283:A:H8	1.86	0.40
4:C3:99:G:N7	17:AL:54:LYS:NZ	2.64	0.40
5:BC:25:LYS:NZ	75:h1:1656:G:OP1	2.47	0.40
15:Ja:64:ILE:HD11	19:Ka:19:LEU:HD11	2.02	0.40
25:BI:69:LYS:HA	25:BI:70:PRO:HD3	1.94	0.40
27:BT:36:PRO:HB3	27:BT:288:ALA:HB2	2.03	0.40
27:BT:384:LYS:NZ	27:BT:387:ILE:HD11	2.37	0.40
29:AD:122:ARG:HD2	64:Oa:54:LEU:HD21	2.02	0.40
33:Da:110:ASP:O	33:Da:114:ARG:HG2	2.20	0.40
40:Fa:21:ARG:HD2	86:Fa:301:HOH:O	2.21	0.40
44:Xa:122:ASP:OD1	44:Xa:122:ASP:N	2.53	0.40
45:BV:28:ASP:OD2	45:BV:50:ARG:HG2	2.21	0.40
57:AF:33:LEU:HD11	57:AF:83:ILE:HD13	2.04	0.40
63:AQ:47:LYS:HE3	63:AQ:48:HIS:CE1	2.56	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AQ:63:ASP:O	63:AQ:65:ASP:N	2.54	0.40
67:BB:5:ARG:O	67:BB:10:LYS:NZ	2.55	0.40
67:BB:41:ILE:HD13	67:BB:50:ILE:HD12	2.02	0.40
72:Aa:109:PRO:C	72:Aa:111:LYS:H	2.29	0.40
75:h1:43:A:O2'	75:h1:100:C:OP1	2.34	0.40
75:h1:627:C:H2'	75:h1:628:U:C6	2.56	0.40
75:h1:1031:A:N1	86:h1:2207:HOH:O	2.37	0.40
75:h1:1045:U:H2'	75:h1:1046:C:C6	2.56	0.40
77:Ba:50:ARG:NH1	77:Ba:50:ARG:HG3	2.35	0.40
1:3:136:C:H2'	1:3:137:C:C6	2.57	0.40
2:A:289:C:OP2	16:Ea:68:ARG:NH2	2.51	0.40
2:A:1162:A:OP1	86:A:3891:HOH:O	2.22	0.40
2:A:2614:G:H2'	2:A:2615:C:C6	2.56	0.40
2:A:3110:G:O6	80:A:3416:TER:N14	2.54	0.40
80:A:3404:TER:H112	86:AM:248:HOH:O	2.21	0.40
86:A:6943:HOH:O	55:Ga:116:GLY:HA2	2.20	0.40
86:C3:442:HOH:O	42:BU:142:ARG:HG3	2.19	0.40
15:Ja:129:ILE:HG22	75:h1:244:OMG:HM21	2.02	0.40
15:Ja:214:THR:OG1	15:Ja:244:ILE:HD13	2.22	0.40
15:Ja:240:LYS:HB2	75:h1:788:C:C2	2.56	0.40
17:AL:83:TYR:CD2	17:AL:118:VAL:HG21	2.57	0.40
22:BS:364:ASP:OD1	47:AO:19:ARG:NH2	2.55	0.40
27:BT:217:GLY:O	27:BT:265:LYS:NZ	2.31	0.40
34:BK:240:LYS:HE2	34:BK:240:LYS:HB2	1.92	0.40
44:Xa:48:GLU:H	44:Xa:48:GLU:CD	2.29	0.40
45:BV:139:CYS:N	45:BV:172:MET:HE1	2.36	0.40
53:AA:61:GLU:OE1	53:AA:62:LYS:HE3	2.20	0.40
67:BB:3:ARG:HD3	75:h1:1393:U:H5''	2.03	0.40
68:AN:43:LEU:HD22	68:AN:47:ILE:HD11	2.04	0.40
72:Aa:181:ARG:CD	86:Aa:303:HOH:O	2.53	0.40
75:h1:781:C:C4	75:h1:782:U:C4	3.09	0.40
75:h1:1385:A:N3	77:Ba:58:ARG:HD2	2.37	0.40
75:h1:1744:A:H2'	75:h1:1745:U:C6	2.57	0.40
78:AI:6:ASN:OD1	78:AI:6:ASN:N	2.54	0.40
78:AI:15:LEU:HG	78:AI:68:LEU:HD12	2.03	0.40
78:AI:55:VAL:HA	78:AI:67:PHE:O	2.21	0.40
1:3:88:C:H5''	1:3:89:G:C4	2.56	0.40
2:A:2217:A:H2'	2:A:2218:A2M:H8	2.04	0.40
2:A:2614:G:H2'	2:A:2615:C:H6	1.87	0.40
2:A:3116:C:H2'	2:A:3117:U:O4'	2.21	0.40
4:C3:9:U:H5''	86:C3:359:HOH:O	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:C3:404:HOH:O	34:BK:221:HIS:CE1	2.68	0.40
15:Ja:58:TYR:O	15:Ja:62:ILE:HG12	2.22	0.40
15:Ja:183:VAL:HG12	15:Ja:189:ARG:HA	2.03	0.40
22:BS:106:TRP:HB2	22:BS:133:TYR:CE1	2.56	0.40
29:AD:87:LEU:HD23	29:AD:87:LEU:HA	1.93	0.40
38:BN:72:TYR:CD1	38:BN:114:MET:HE1	2.57	0.40
50:Na:61:CYS:SG	50:Na:62:GLN:N	2.95	0.40
53:AA:5:ILE:N	75:h1:1517:U:O2	2.54	0.40
57:AF:29:GLY:HA2	57:AF:65:VAL:O	2.22	0.40
71:La:81:ILE:HG21	71:La:102:TYR:CZ	2.56	0.40
75:h1:20:G:N7	86:h1:2206:HOH:O	2.37	0.40
75:h1:361:G:OP2	75:h1:362:A:H5''	2.22	0.40
75:h1:807:A:H2'	75:h1:808:PSU:H6	1.87	0.40
75:h1:1593:C:H2'	75:h1:1594:G:C8	2.56	0.40
1:3:5:C:H2'	1:3:6:G:O4'	2.22	0.40
1:3:135:G:H2'	1:3:136:C:C6	2.57	0.40
2:A:373:G:O5'	7:BO:88:LYS:NZ	2.53	0.40
2:A:508:A:H5''	27:BT:322:LYS:HG2	2.03	0.40
2:A:1868:C:C2	80:A:3408:TER:H101	2.56	0.40
2:A:3155:C:H2'	2:A:3156:G:C8	2.56	0.40
2:A:3303:A:H61	2:A:3308:C:H1'	1.87	0.40
7:BO:47:MET:HE1	7:BO:117:LEU:HD23	2.04	0.40
16:Ea:42:PRO:HG3	16:Ea:61:VAL:HG21	2.04	0.40
18:Va:99:VAL:HG12	18:Va:124:VAL:HG23	2.03	0.40
19:Ka:36:VAL:HG12	19:Ka:41:LEU:HG	2.03	0.40
19:Ka:57:ILE:HG12	19:Ka:77:ILE:HG12	2.04	0.40
41:Ha:120:PHE:CE1	41:Ha:122:VAL:HG23	2.56	0.40
42:BU:90:GLU:HB3	42:BU:92:GLU:CD	2.47	0.40
45:BV:38:PHE:CG	45:BV:73:LEU:HD12	2.57	0.40
57:AF:57:LEU:HB2	57:AF:62:PHE:HE1	1.87	0.40
58:Wa:55:ARG:HH21	71:La:41:VAL:HG23	1.87	0.40
68:AN:83:LYS:HB2	68:AN:111:TYR:CE2	2.56	0.40
72:Aa:194:PHE:HE2	72:Aa:195:TYR:CE1	2.40	0.40
75:h1:244:OMG:HM23	75:h1:244:OMG:H1'	1.92	0.40
75:h1:1216:OMC:HM23	75:h1:1216:OMC:H1'	1.88	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BC	23/25 (92%)	23 (100%)	0	0	100	100
6	BM	153/176 (87%)	151 (99%)	2 (1%)	0	100	100
7	BO	123/146 (84%)	119 (97%)	4 (3%)	0	100	100
8	AR	49/83 (59%)	43 (88%)	6 (12%)	0	100	100
9	AU	107/119 (90%)	105 (98%)	2 (2%)	0	100	100
10	Ma	96/131 (73%)	93 (97%)	3 (3%)	0	100	100
11	Ia	188/194 (97%)	183 (97%)	5 (3%)	0	100	100
12	AE	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
13	AX	95/112 (85%)	93 (98%)	2 (2%)	0	100	100
14	AP	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
15	Ja	256/262 (98%)	240 (94%)	15 (6%)	1 (0%)	30	31
16	Ea	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	AL	173/217 (80%)	169 (98%)	4 (2%)	0	100	100
18	Va	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
19	Ka	118/133 (89%)	113 (96%)	5 (4%)	0	100	100
20	AW	109/112 (97%)	109 (100%)	0	0	100	100
21	BD	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
22	BS	383/389 (98%)	377 (98%)	6 (2%)	0	100	100
23	AM	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
24	AC	213/284 (75%)	209 (98%)	4 (2%)	0	100	100
25	BI	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
26	AH	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
27	BT	389/406 (96%)	380 (98%)	9 (2%)	0	100	100
28	AV	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
29	AD	180/207 (87%)	173 (96%)	7 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	AJ	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
31	BQ	243/258 (94%)	230 (95%)	13 (5%)	0	100	100
32	BH	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
33	Da	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
34	BK	279/301 (93%)	274 (98%)	5 (2%)	0	100	100
35	AT	92/112 (82%)	91 (99%)	1 (1%)	0	100	100
36	Pa	45/62 (73%)	41 (91%)	4 (9%)	0	100	100
37	BP	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
38	BN	115/154 (75%)	115 (100%)	0	0	100	100
39	BG	232/256 (91%)	226 (97%)	6 (3%)	0	100	100
40	Fa	109/120 (91%)	106 (97%)	3 (3%)	0	100	100
41	Ha	143/146 (98%)	138 (96%)	4 (3%)	1 (1%)	18	17
42	BU	167/182 (92%)	164 (98%)	3 (2%)	0	100	100
43	BR	230/247 (93%)	223 (97%)	7 (3%)	0	100	100
44	Xa	144/160 (90%)	138 (96%)	6 (4%)	0	100	100
45	BV	210/262 (80%)	208 (99%)	2 (1%)	0	100	100
46	BJ	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
47	AO	60/164 (37%)	59 (98%)	1 (2%)	0	100	100
48	BW	71/82 (87%)	70 (99%)	0	1 (1%)	9	5
49	AK	176/214 (82%)	173 (98%)	3 (2%)	0	100	100
50	Na	81/86 (94%)	71 (88%)	10 (12%)	0	100	100
51	AB	178/197 (90%)	174 (98%)	4 (2%)	0	100	100
52	BF	184/233 (79%)	176 (96%)	8 (4%)	0	100	100
53	AA	206/250 (82%)	192 (93%)	13 (6%)	1 (0%)	24	24
54	AG	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
55	Ga	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
56	BA	48/51 (94%)	48 (100%)	0	0	100	100
57	AF	136/146 (93%)	124 (91%)	12 (9%)	0	100	100
58	Wa	137/152 (90%)	131 (96%)	6 (4%)	0	100	100
59	Ta	223/249 (90%)	204 (92%)	17 (8%)	2 (1%)	14	12
60	AZ	66/69 (96%)	63 (96%)	3 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	BE	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	11	8
62	Za	196/298 (66%)	187 (95%)	8 (4%)	1 (0%)	24	24
63	AQ	134/143 (94%)	122 (91%)	11 (8%)	1 (1%)	18	17
64	Oa	57/64 (89%)	57 (100%)	0	0	100	100
65	Ua	125/150 (83%)	120 (96%)	5 (4%)	0	100	100
66	Ya	127/150 (85%)	112 (88%)	13 (10%)	2 (2%)	7	4
67	BB	117/141 (83%)	109 (93%)	8 (7%)	0	100	100
68	AN	97/124 (78%)	88 (91%)	9 (9%)	0	100	100
69	Ra	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
70	BL	134/143 (94%)	130 (97%)	4 (3%)	0	100	100
71	La	69/108 (64%)	68 (99%)	1 (1%)	0	100	100
72	Aa	181/222 (82%)	176 (97%)	5 (3%)	0	100	100
73	AY	83/95 (87%)	82 (99%)	1 (1%)	0	100	100
74	Ca	51/56 (91%)	51 (100%)	0	0	100	100
77	Ba	99/122 (81%)	97 (98%)	2 (2%)	0	100	100
78	AI	90/177 (51%)	89 (99%)	1 (1%)	0	100	100
All	All	10397/11933 (87%)	10050 (97%)	336 (3%)	11 (0%)	49	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	Ta	29	ASP
66	Ya	57	LYS
59	Ta	14	LYS
48	BW	80	LYS
53	AA	5	ILE
61	BE	3	LYS
63	AQ	21	VAL
66	Ya	79	ALA
15	Ja	150	PRO
62	Za	202	MET
41	Ha	15	VAL



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BC	24/24 (100%)	22 (92%)	2 (8%)	10	8
6	BM	131/148 (88%)	128 (98%)	3 (2%)	44	55
7	BO	116/133 (87%)	114 (98%)	2 (2%)	53	65
8	AR	44/71 (62%)	44 (100%)	0	100	100
9	AU	96/105 (91%)	95 (99%)	1 (1%)	68	77
10	Ma	87/110 (79%)	86 (99%)	1 (1%)	65	75
11	Ia	171/175 (98%)	167 (98%)	4 (2%)	44	55
12	AE	111/112 (99%)	106 (96%)	5 (4%)	24	29
13	AX	84/94 (89%)	83 (99%)	1 (1%)	63	74
14	AP	116/117 (99%)	116 (100%)	0	100	100
15	Ja	225/227 (99%)	218 (97%)	7 (3%)	35	44
16	Ea	179/180 (99%)	176 (98%)	3 (2%)	53	65
17	AL	161/198 (81%)	157 (98%)	4 (2%)	42	52
18	Va	111/114 (97%)	111 (100%)	0	100	100
19	Ka	104/114 (91%)	100 (96%)	4 (4%)	29	36
20	AW	97/98 (99%)	95 (98%)	2 (2%)	47	58
21	BD	87/93 (94%)	86 (99%)	1 (1%)	65	75
22	BS	326/329 (99%)	324 (99%)	2 (1%)	78	84
23	AM	137/138 (99%)	134 (98%)	3 (2%)	45	56
24	AC	183/225 (81%)	175 (96%)	8 (4%)	25	29
25	BI	104/110 (94%)	103 (99%)	1 (1%)	68	77
26	AH	112/117 (96%)	110 (98%)	2 (2%)	51	63
27	BT	323/331 (98%)	320 (99%)	3 (1%)	70	79
28	AV	114/121 (94%)	114 (100%)	0	100	100
29	AD	156/171 (91%)	149 (96%)	7 (4%)	24	29
30	AJ	157/158 (99%)	155 (99%)	2 (1%)	61	72

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	BQ	191/197 (97%)	190 (100%)	1 (0%)	81	87
32	BH	176/177 (99%)	170 (97%)	6 (3%)	32	40
33	Da	132/133 (99%)	128 (97%)	4 (3%)	36	45
34	BK	238/254 (94%)	236 (99%)	2 (1%)	73	80
35	AT	81/97 (84%)	78 (96%)	3 (4%)	30	37
36	Pa	40/49 (82%)	40 (100%)	0	100	100
37	BP	108/110 (98%)	105 (97%)	3 (3%)	38	48
38	BN	108/136 (79%)	103 (95%)	5 (5%)	24	28
39	BG	200/219 (91%)	192 (96%)	8 (4%)	28	34
40	Fa	97/104 (93%)	95 (98%)	2 (2%)	47	58
41	Ha	120/121 (99%)	116 (97%)	4 (3%)	33	42
42	BU	147/158 (93%)	139 (95%)	8 (5%)	20	21
43	BR	199/212 (94%)	197 (99%)	2 (1%)	68	77
44	Xa	124/135 (92%)	121 (98%)	3 (2%)	43	54
45	BV	187/226 (83%)	183 (98%)	4 (2%)	47	58
46	BJ	170/179 (95%)	166 (98%)	4 (2%)	43	54
47	AO	58/137 (42%)	58 (100%)	0	100	100
48	BW	60/68 (88%)	58 (97%)	2 (3%)	33	42
49	AK	158/181 (87%)	154 (98%)	4 (2%)	42	52
50	Na	76/78 (97%)	72 (95%)	4 (5%)	20	22
51	AB	161/172 (94%)	158 (98%)	3 (2%)	50	61
52	BF	157/194 (81%)	153 (98%)	4 (2%)	42	52
53	AA	174/207 (84%)	167 (96%)	7 (4%)	28	34
54	AG	174/177 (98%)	169 (97%)	5 (3%)	37	47
55	Ga	47/114 (41%)	46 (98%)	1 (2%)	47	58
56	BA	47/48 (98%)	45 (96%)	2 (4%)	26	31
57	AF	117/123 (95%)	111 (95%)	6 (5%)	21	23
58	Wa	121/132 (92%)	117 (97%)	4 (3%)	33	42
59	Ta	193/213 (91%)	187 (97%)	6 (3%)	35	44
60	AZ	64/65 (98%)	63 (98%)	1 (2%)	55	66
61	BE	72/73 (99%)	69 (96%)	3 (4%)	26	31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	Za	166/228 (73%)	163 (98%)	3 (2%)	51	63
63	AQ	116/122 (95%)	112 (97%)	4 (3%)	32	40
64	Oa	52/57 (91%)	48 (92%)	4 (8%)	12	10
65	Ua	100/121 (83%)	98 (98%)	2 (2%)	48	59
66	Ya	110/126 (87%)	106 (96%)	4 (4%)	31	39
67	BB	108/122 (88%)	101 (94%)	7 (6%)	15	14
68	AN	88/104 (85%)	86 (98%)	2 (2%)	44	55
69	Ra	165/169 (98%)	160 (97%)	5 (3%)	36	45
70	BL	110/113 (97%)	104 (94%)	6 (6%)	19	20
71	La	61/92 (66%)	60 (98%)	1 (2%)	55	66
72	Aa	158/183 (86%)	157 (99%)	1 (1%)	78	84
73	AY	73/78 (94%)	73 (100%)	0	100	100
74	Ca	47/48 (98%)	46 (98%)	1 (2%)	47	58
77	Ba	93/110 (84%)	90 (97%)	3 (3%)	34	43
78	AI	87/139 (63%)	83 (95%)	4 (5%)	24	28
All	All	9087/10114 (90%)	8861 (98%)	226 (2%)	42	52

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BC	10	MET
5	BC	25	LYS
6	BM	24	VAL
6	BM	101	SER
6	BM	110	VAL
7	BO	61	THR
7	BO	66	GLU
9	AU	74	ARG
10	Ma	44	ILE
11	Ia	33	LYS
11	Ia	73	ILE
11	Ia	116	GLU
11	Ia	140	SER
12	AE	26	MET
12	AE	51	GLU
12	AE	96	SER
12	AE	117	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
12	AE	121	VAL
13	AX	15	ASN
15	Ja	16	LYS
15	Ja	45	VAL
15	Ja	87	MET
15	Ja	90	VAL
15	Ja	156	PRO
15	Ja	160	ILE
15	Ja	181	VAL
16	Ea	27	CYS
16	Ea	131	GLU
16	Ea	155	VAL
17	AL	87	THR
17	AL	149	ILE
17	AL	156	ARG
17	AL	162	SER
19	Ka	10	THR
19	Ka	14	MET
19	Ka	47	ARG
19	Ka	92	ARG
20	AW	2	VAL
20	AW	96	PRO
21	BD	10	THR
22	BS	95	THR
22	BS	203	GLU
23	AM	33	THR
23	AM	96	VAL
23	AM	98	GLN
24	AC	22	THR
24	AC	47	THR
24	AC	50	ASP
24	AC	58	VAL
24	AC	76	VAL
24	AC	92	GLU
24	AC	130	VAL
24	AC	138	THR
25	BI	71	ASP
26	AH	19	GLU
26	AH	128	LEU
27	BT	129	ILE
27	BT	291	VAL
27	BT	357	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
29	AD	30	THR
29	AD	35	VAL
29	AD	36	ASP
29	AD	98	GLU
29	AD	112	ILE
29	AD	136	ARG
29	AD	197	GLU
30	AJ	57	VAL
30	AJ	76	ASP
31	BQ	208	GLU
32	BH	179	LEU
32	BH	180	THR
32	BH	182	LEU
32	BH	188	LYS
32	BH	192	GLU
32	BH	204	ILE
33	Da	43	LYS
33	Da	48	SER
33	Da	67	THR
33	Da	147	SER
34	BK	132	VAL
34	BK	137	SER
35	AT	27	THR
35	AT	33	VAL
35	AT	36	SER
37	BP	16	ASP
37	BP	19	THR
37	BP	30	SER
38	BN	52	VAL
38	BN	55	LYS
38	BN	85	MET
38	BN	111	VAL
38	BN	117	ILE
39	BG	116	LYS
39	BG	174	VAL
39	BG	196	THR
39	BG	198	LYS
39	BG	215	ASN
39	BG	217	ASN
39	BG	224	ARG
39	BG	240	THR
40	Fa	23	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
40	Fa	59	PRO
41	Ha	38	MET
41	Ha	91	THR
41	Ha	130	THR
41	Ha	132	GLU
42	BU	15	LYS
42	BU	46	THR
42	BU	48	VAL
42	BU	50	SER
42	BU	122	THR
42	BU	140	VAL
42	BU	157	THR
42	BU	172	VAL
43	BR	21	ILE
43	BR	100	ILE
44	Xa	39	ILE
44	Xa	57	LYS
44	Xa	119	LYS
45	BV	43	VAL
45	BV	46	THR
45	BV	131	ASP
45	BV	143	THR
46	BJ	50	VAL
46	BJ	82	LYS
46	BJ	91	VAL
46	BJ	101	LYS
48	BW	13	ILE
48	BW	16	LYS
49	AK	31	ASP
49	AK	39	GLN
49	AK	51	ILE
49	AK	154	THR
50	Na	10	LEU
50	Na	15	GLU
50	Na	46	THR
50	Na	48	VAL
51	AB	19	ARG
51	AB	103	VAL
51	AB	152	VAL
52	BF	9	LYS
52	BF	79	THR
52	BF	180	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
52	BF	195	LEU
53	AA	5	ILE
53	AA	37	VAL
53	AA	49	ILE
53	AA	58	VAL
53	AA	66	ILE
53	AA	74	GLN
53	AA	191	ASP
54	AG	9	ASN
54	AG	68	VAL
54	AG	70	THR
54	AG	77	GLU
54	AG	120	THR
55	Ga	128	LYS
56	BA	17	MET
56	BA	47	THR
57	AF	19	VAL
57	AF	51	PHE
57	AF	60	HIS
57	AF	71	VAL
57	AF	99	VAL
57	AF	119	LEU
58	Wa	18	THR
58	Wa	31	THR
58	Wa	43	ILE
58	Wa	141	ARG
59	Ta	45	PHE
59	Ta	114	VAL
59	Ta	129	THR
59	Ta	143	ILE
59	Ta	185	THR
59	Ta	188	THR
60	AZ	31	ILE
61	BE	6	LYS
61	BE	52	VAL
61	BE	90	ILE
62	Za	35	ASN
62	Za	115	GLN
62	Za	182	LEU
63	AQ	4	VAL
63	AQ	20	LEU
63	AQ	36	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
63	AQ	85	VAL
64	Oa	19	SER
64	Oa	20	ARG
64	Oa	29	LYS
64	Oa	62	ARG
65	Ua	64	ASP
65	Ua	127	ARG
66	Ya	83	THR
66	Ya	91	VAL
66	Ya	117	ILE
66	Ya	132	LYS
67	BB	25	THR
67	BB	30	THR
67	BB	35	LEU
67	BB	38	VAL
67	BB	63	LYS
67	BB	73	LEU
67	BB	98	VAL
68	AN	56	LEU
68	AN	72	THR
69	Ra	29	ASP
69	Ra	47	ASN
69	Ra	130	VAL
69	Ra	173	VAL
69	Ra	181	ASP
70	BL	16	VAL
70	BL	31	LEU
70	BL	40	THR
70	BL	107	GLN
70	BL	115	ASP
70	BL	125	THR
71	La	53	THR
72	Aa	96	THR
74	Ca	54	LYS
77	Ba	29	SER
77	Ba	57	VAL
77	Ba	94	LEU
78	AI	6	ASN
78	AI	40	LEU
78	AI	55	VAL
78	AI	90	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78)



such sidechains are listed below:

Mol	Chain	Res	Type
6	BM	98	ASN
7	BO	71	GLN
8	AR	19	ASN
8	AR	27	HIS
11	Ia	105	ASN
14	AP	15	GLN
15	Ja	50	ASN
15	Ja	67	GLN
15	Ja	188	ASN
15	Ja	201	HIS
16	Ea	171	ASN
16	Ea	181	ASN
18	Va	60	GLN
18	Va	91	ASN
19	Ka	16	ASN
19	Ka	23	GLN
19	Ka	83	ASN
20	AW	27	ASN
20	AW	28	GLN
20	AW	36	GLN
20	AW	68	HIS
22	BS	109	HIS
22	BS	136	GLN
22	BS	344	GLN
22	BS	349	GLN
27	BT	48	GLN
27	BT	123	ASN
29	AD	83	ASN
29	AD	101	HIS
29	AD	179	ASN
30	AJ	134	ASN
30	AJ	161	ASN
31	BQ	38	ASN
31	BQ	118	HIS
32	BH	18	HIS
32	BH	68	ASN
34	BK	85	GLN
34	BK	183	HIS
36	Pa	17	GLN
36	Pa	24	GLN
38	BN	118	GLN
40	Fa	19	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
41	Ha	19	HIS
42	BU	153	GLN
43	BR	55	GLN
43	BR	98	ASN
43	BR	118	ASN
43	BR	164	GLN
44	Xa	38	ASN
44	Xa	99	GLN
44	Xa	111	HIS
44	Xa	139	ASN
45	BV	95	ASN
45	BV	163	GLN
46	BJ	177	ASN
49	AK	39	GLN
50	Na	4	GLN
51	AB	93	ASN
51	AB	105	ASN
51	AB	125	HIS
52	BF	222	HIS
53	AA	57	ASN
54	AG	58	HIS
55	Ga	104	HIS
57	AF	85	GLN
59	Ta	13	GLN
59	Ta	22	GLN
62	Za	76	GLN
62	Za	117	GLN
62	Za	136	GLN
62	Za	188	GLN
63	AQ	42	ASN
64	Oa	40	ASN
69	Ra	22	GLN
69	Ra	47	ASN
69	Ra	77	HIS
73	AY	69	ASN
78	AI	39	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	161/164 (98%)	25 (15%)	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3143/3385 (92%)	435 (13%)	20 (0%)
3	2	75/76 (98%)	16 (21%)	0
3	W2	75/76 (98%)	17 (22%)	1 (1%)
4	C3	118/121 (97%)	11 (9%)	0
75	h1	1603/1805 (88%)	225 (14%)	0
76	B1	11/12 (91%)	1 (9%)	0
All	All	5186/5639 (91%)	730 (14%)	21 (0%)

All (730) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	27	C
1	3	38	U
1	3	39	C
1	3	43	G
1	3	63	A
1	3	66	C
1	3	67	U
1	3	85	U
1	3	86	C
1	3	88	C
1	3	89	G
1	3	90	U
1	3	91	G
1	3	94	C
1	3	99	G
1	3	101	G
1	3	108	A
1	3	109	A
1	3	110	C
1	3	120	G
1	3	129	C
1	3	132	C
1	3	134	G
1	3	157	U
1	3	160	C
2	A	3	G
2	A	11	G
2	A	12	U
2	A	38	A
2	A	41	A
2	A	47	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	55	A
2	A	57	G
2	A	58	A
2	A	64	A
2	A	70	C
2	A	84	G
2	A	90	G
2	A	97	A
2	A	108	G
2	A	114	C
2	A	120	A
2	A	131	U
2	A	133	C
2	A	134	G
2	A	141	G
2	A	154	G
2	A	155	A
2	A	163	C
2	A	167	A
2	A	168	G
2	A	179	G
2	A	184	A
2	A	187	U
2	A	197	A
2	A	207	G
2	A	215	G
2	A	216	A
2	A	233	G
2	A	236	C
2	A	238	C
2	A	248	A
2	A	262	A
2	A	266	G
2	A	283	U
2	A	292	A
2	A	326	G
2	A	346	A
2	A	347	C
2	A	350	G
2	A	373	G
2	A	394	A
2	A	395	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	398	U
2	A	399	G
2	A	417	G
2	A	418	G
2	A	419	A
2	A	430	G
2	A	434	G
2	A	436	C
2	A	437	G
2	A	449	U
2	A	453	A
2	A	454	U
2	A	460	A
2	A	462	G
2	A	467	A
2	A	523	U
2	A	524	A
2	A	532	G
2	A	537	U
2	A	538	G
2	A	539	A
2	A	541	A
2	A	543	G
2	A	545	U
2	A	546	U
2	A	547	G
2	A	548	U
2	A	549	G
2	A	552	G
2	A	561	G
2	A	571	U
2	A	573	G
2	A	574	U
2	A	581	C
2	A	589	U
2	A	591	A
2	A	592	C
2	A	602	C
2	A	603	G
2	A	607	U
2	A	608	C
2	A	610	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	621	G
2	A	632	U
2	A	637	U
2	A	648	C
2	A	661	A2M
2	A	672	A
2	A	673	G
2	A	689	A
2	A	694	A
2	A	702	G
2	A	711	U
2	A	712	A
2	A	713	A
2	A	719	A
2	A	726	C
2	A	729	A
2	A	730	U
2	A	732	G
2	A	745	G
2	A	746	C
2	A	774	U
2	A	776	U
2	A	786	U
2	A	789	A
2	A	790	G
2	A	794	G
2	A	824	G
2	A	826	A2M
2	A	839	G
2	A	846	A
2	A	858	C
2	A	870	C
2	A	883	U
2	A	888	U
2	A	905	A
2	A	906	C
2	A	916	G
2	A	917	OMG
2	A	923	A
2	A	925	G
2	A	926	A
2	A	930	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	932	C
2	A	934	A
2	A	946	G
2	A	953	C
2	A	968	C
2	A	969	PSU
2	A	986	C
2	A	989	A
2	A	990	C
2	A	991	G
2	A	992	C
2	A	993	G
2	A	1005	G
2	A	1011	C
2	A	1012	C
2	A	1027	U
2	A	1031	G
2	A	1032	G
2	A	1035	G
2	A	1036	C
2	A	1039	C
2	A	1045	G
2	A	1046	A
2	A	1055	C
2	A	1057	A
2	A	1073	G
2	A	1074	A
2	A	1085	G
2	A	1091	U
2	A	1092	U
2	A	1104	C
2	A	1105	G
2	A	1106	G
2	A	1107	A
2	A	1112	A
2	A	1113	G
2	A	1126	G
2	A	1140	G
2	A	1153	U
2	A	1162	A
2	A	1168	A
2	A	1183	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	1189	C
2	A	1190	U
2	A	1200	C
2	A	1203	A
2	A	1211	C
2	A	1219	G
2	A	1226	G
2	A	1293	C
2	A	1295	G
2	A	1297	A
2	A	1315	U
2	A	1317	G
2	A	1319	U
2	A	1326	U
2	A	1327	A
2	A	1333	G
2	A	1358	A
2	A	1359	A
2	A	1360	G
2	A	1361	A
2	A	1362	G
2	A	1363	C
2	A	1364	C
2	A	1408	A
2	A	1411	G
2	A	1428	G
2	A	1440	G
2	A	1443	G
2	A	1446	OMC
2	A	1455	A
2	A	1460	C
2	A	1464	U
2	A	1484	A
2	A	1490	A
2	A	1492	G
2	A	1511	G
2	A	1536	C
2	A	1545	G
2	A	1564	U
2	A	1567	U
2	A	1569	G
2	A	1573	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	1575	A
2	A	1576	A
2	A	1581	A
2	A	1588	A
2	A	1589	A
2	A	1590	A
2	A	1594	G
2	A	1606	A
2	A	1621	C
2	A	1629	U
2	A	1645	G
2	A	1657	C
2	A	1662	G
2	A	1676	A
2	A	1683	A
2	A	1692	G
2	A	1714	G
2	A	1725	G
2	A	1744	G
2	A	1751	A
2	A	1752	G
2	A	1759	G
2	A	1763	G
2	A	1765	C
2	A	1766	G
2	A	1767	C
2	A	1768	G
2	A	1799	A
2	A	1815	A
2	A	1816	G
2	A	1817	U
2	A	1818	G
2	A	1823	U
2	A	1844	A
2	A	1868	C
2	A	1880	G
2	A	1881	A
2	A	1882	U
2	A	1908	G
2	A	2091	A
2	A	2092	A
2	A	2100	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	2101	U
2	A	2110	G
2	A	2111	OMU
2	A	2113	C
2	A	2121	G
2	A	2130	A
2	A	2139	U
2	A	2143	A
2	A	2157	A
2	A	2190	C
2	A	2203	U
2	A	2208	G
2	A	2226	A
2	A	2247	G
2	A	2256	PSU
2	A	2271	G
2	A	2278	A
2	A	2305	G
2	A	2306	C
2	A	2308	U
2	A	2311	A
2	A	2313	G
2	A	2332	U
2	A	2333	G
2	A	2334	U
2	A	2370	A
2	A	2371	A
2	A	2372	C
2	A	2373	G
2	A	2383	G
2	A	2391	G
2	A	2392	G
2	A	2395	A
2	A	2400	A
2	A	2401	G
2	A	2402	A
2	A	2409	U
2	A	2410	G
2	A	2433	G
2	A	2438	A
2	A	2443	U
2	A	2446	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	2450	G
2	A	2451	U
2	A	2452	G
2	A	2453	U
2	A	2454	A
2	A	2455	G
2	A	2456	G
2	A	2457	A
2	A	2458	U
2	A	2459	A
2	A	2460	A
2	A	2461	G
2	A	2496	U
2	A	2497	U
2	A	2498	A
2	A	2499	A
2	A	2506	U
2	A	2512	U
2	A	2520	G
2	A	2522	A
2	A	2550	U
2	A	2552	G
2	A	2573	G
2	A	2586	C
2	A	2592	A
2	A	2605	G
2	A	2606	G
2	A	2613	G
2	A	2625	A
2	A	2651	U
2	A	2655	A
2	A	2673	A
2	A	2676	G
2	A	2679	A
2	A	2688	G
2	A	2689	G
2	A	2690	A
2	A	2693	A
2	A	2703	A
2	A	2713	G
2	A	2718	U
2	A	2727	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	2728	U
2	A	2752	G
2	A	2754	C
2	A	2761	A
2	A	2776	G
2	A	2777	G
2	A	2795	G
2	A	2798	A
2	A	2799	G
2	A	2800	A
2	A	2802	A
2	A	2809	C
2	A	2816	A
2	A	2841	U
2	A	2844	A
2	A	2870	G
2	A	2886	A
2	A	2898	C
2	A	2910	A2M
2	A	2934	U
2	A	2935	A
2	A	2941	C
2	A	2946	G
2	A	2970	A
2	A	2982	C
2	A	2989	G
2	A	2996	G
2	A	3010	A
2	A	3028	G
2	A	3056	C
2	A	3057	G
2	A	3076	G
2	A	3077	U
2	A	3090	C
2	A	3099	G
2	A	3111	A
2	A	3114	G
2	A	3120	A
2	A	3129	U
2	A	3139	A
2	A	3140	A
2	A	3142	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	3150	G
2	A	3152	G
2	A	3166	U
2	A	3167	G
2	A	3168	C
2	A	3170	G
2	A	3171	A
2	A	3172	C
2	A	3175	U
2	A	3181	G
2	A	3188	A
2	A	3189	G
2	A	3195	A
2	A	3202	C
2	A	3203	G
2	A	3205	G
2	A	3206	U
2	A	3215	A
2	A	3217	G
2	A	3218	U
2	A	3222	G
2	A	3223	U
2	A	3224	U
2	A	3225	C
2	A	3226	G
2	A	3231	A
2	A	3235	G
2	A	3244	G
2	A	3248	C
2	A	3252	G
2	A	3273	G
2	A	3281	G
2	A	3290	OMG
2	A	3291	C
2	A	3303	A
2	A	3304	U
2	A	3306	C
2	A	3307	G
2	A	3328	C
2	A	3338	U
2	A	3339	U
2	A	3341	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	3343	G
2	A	3344	C
2	A	3347	C
2	A	3356	G
2	A	3365	C
2	A	3369	U
2	A	3377	A
2	A	3379	G
2	A	3385	A
3	2	3	G
3	2	18	G
3	2	19	G
3	2	20	G
3	2	21	A
3	2	22	G
3	2	43	A
3	2	46	G
3	2	47	U
3	2	48	C
3	2	64	G
3	2	68	A
3	2	72	C
3	2	73	A
3	2	74	C
3	2	76	A
4	C3	30	G
4	C3	33	U
4	C3	38	U
4	C3	49	C
4	C3	53	U
4	C3	54	A
4	C3	64	G
4	C3	89	G
4	C3	104	C
4	C3	110	G
4	C3	117	C
75	h1	17	C
75	h1	25	C
75	h1	26	A
75	h1	34	G
75	h1	42	G
75	h1	45	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	47	A
75	h1	56	U
75	h1	63	G
75	h1	67	G
75	h1	68	A
75	h1	82	G
75	h1	84	G
75	h1	105	A
75	h1	115	A
75	h1	126	U
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	151	A
75	h1	158	C
75	h1	164	C
75	h1	174	C
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	213	U
75	h1	214	A
75	h1	250	U
75	h1	251	C
75	h1	258	A
75	h1	262	G
75	h1	264	C
75	h1	266	G
75	h1	272	A
75	h1	273	U
75	h1	301	A
75	h1	316	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	318	A
75	h1	322	U
75	h1	324	G
75	h1	335	A
75	h1	339	G
75	h1	340	C
75	h1	361	G
75	h1	363	C
75	h1	372	A
75	h1	380	A
75	h1	382	U
75	h1	383	C
75	h1	387	A
75	h1	402	A
75	h1	403	A
75	h1	404	C
75	h1	418	A
75	h1	425	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	461	G
75	h1	470	A
75	h1	479	A
75	h1	503	U
75	h1	504	G
75	h1	509	U
75	h1	512	G
75	h1	516	G
75	h1	517	A
75	h1	536	A
75	h1	540	A
75	h1	544	U
75	h1	545	C
75	h1	553	G
75	h1	559	G
75	h1	567	C
75	h1	570	G
75	h1	580	OMU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	581	A
75	h1	583	PSU
75	h1	584	U
75	h1	585	C
75	h1	596	A
75	h1	597	OMG
75	h1	608	A
75	h1	612	G
75	h1	613	OMU
75	h1	621	A2M
75	h1	622	A
75	h1	624	A
75	h1	625	A
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	784	C
75	h1	785	G
75	h1	789	U
75	h1	792	A
75	h1	795	C
75	h1	815	A
75	h1	816	U
75	h1	817	A
75	h1	831	A
75	h1	833	U
75	h1	854	G
75	h1	864	A
75	h1	874	U
75	h1	887	U
75	h1	934	A
75	h1	936	U
75	h1	952	A
75	h1	961	U
75	h1	967	A
75	h1	1005	U
75	h1	1006	A
75	h1	1027	A
75	h1	1029	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	1040	A
75	h1	1055	U
75	h1	1057	G
75	h1	1060	U
75	h1	1061	A
75	h1	1082	A
75	h1	1088	A
75	h1	1093	A
75	h1	1098	U
75	h1	1139	A
75	h1	1147	G
75	h1	1151	G
75	h1	1159	C
75	h1	1168	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	1213	G
75	h1	1218	A
75	h1	1219	G
75	h1	1232	OMU
75	h1	1244	G
75	h1	1245	A
75	h1	1246	G
75	h1	1247	C
75	h1	1252	U
75	h1	1253	C
75	h1	1257	A
75	h1	1259	U
75	h1	1266	G
75	h1	1270	OMU
75	h1	1292	G
75	h1	1315	U
75	h1	1316	U
75	h1	1322	A
75	h1	1362	C
75	h1	1363	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	1364	U
75	h1	1391	A
75	h1	1393	U
75	h1	1394	A
75	h1	1401	U
75	h1	1416	U
75	h1	1417	U
75	h1	1418	U
75	h1	1423	C
75	h1	1429	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	1481	U
75	h1	1514	G
75	h1	1519	A
75	h1	1520	PSU
75	h1	1524	U
75	h1	1526	A
75	h1	1539	A
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	1613	A
75	h1	1618	G
75	h1	1636	C
75	h1	1653	A
75	h1	1660	G
75	h1	1666	U
75	h1	1682	G
75	h1	1759	A
75	h1	1764	G
75	h1	1770	A
75	h1	1772	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	h1	1773	U
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
76	B1	19	U
3	W2	3	G
3	W2	5	G
3	W2	8	U
3	W2	10	G
3	W2	15	G
3	W2	17	U
3	W2	18	G
3	W2	19	G
3	W2	20	G
3	W2	21	A
3	W2	22	G
3	W2	47	U
3	W2	48	C
3	W2	68	A
3	W2	70	C
3	W2	71	G
3	W2	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	547	G
2	A	591	A
2	A	602	C
2	A	609	A
2	A	882	C
2	A	905	A
2	A	925	G
2	A	990	C
2	A	1004	G
2	A	1026	A
2	A	1606	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	2304	C
2	A	2370	A
2	A	2496	U
2	A	2585	G
2	A	2727	G
2	A	3119	U
2	A	3225	C
2	A	3247	G
2	A	3303	A
3	W2	70	C

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

215 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
75	PSU	h1	604	75	18,21,22	0.72	1 (5%)	21,30,33	1.08	2 (9%)
1	A2M	3	47	1	22,25,26	0.58	0	30,36,39	1.62	5 (16%)
2	OMU	A	2111	2	19,22,23	0.30	0	25,31,34	0.60	0
75	PSU	h1	1104	75	18,21,22	0.94	1 (5%)	21,30,33	1.08	2 (9%)
75	PSU	h1	1118	75	18,21,22	0.92	1 (5%)	21,30,33	0.89	1 (4%)
2	OMU	A	2408	2,82	19,22,23	0.42	0	25,31,34	0.64	0
2	PSU	A	2893	2	18,21,22	0.77	1 (5%)	21,30,33	0.96	3 (14%)
75	MA6	h1	1786	75	23,26,27	0.43	0	33,38,41	1.58	3 (9%)
75	6MZ	h1	1767	82,75,81	22,25,26	0.48	0	29,36,39	0.90	1 (3%)
75	PSU	h1	634	75	18,21,22	1.05	2 (11%)	21,30,33	1.06	2 (9%)
75	PSU	h1	1563	75	18,21,22	0.92	1 (5%)	21,30,33	1.11	2 (9%)
2	PSU	A	2189	2,82	18,21,22	0.84	2 (11%)	21,30,33	1.04	2 (9%)
2	PSU	A	975	2,82	18,21,22	1.27	3 (16%)	21,30,33	0.94	2 (9%)
75	PSU	h1	468	75	18,21,22	0.92	1 (5%)	21,30,33	0.96	2 (9%)
2	PSU	A	1054	2	18,21,22	0.95	2 (11%)	21,30,33	1.11	3 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	A	2864	2	18,21,22	0.84	1 (5%)	21,30,33	0.91	0
75	PSU	h1	752	75	18,21,22	1.04	2 (11%)	21,30,33	0.96	1 (4%)
1	OMG	3	155	2,1	23,26,27	0.41	0	32,38,41	0.43	0
2	PSU	A	2974	2	18,21,22	1.03	1 (5%)	21,30,33	1.21	4 (19%)
2	OMC	A	2878	2	19,22,23	0.61	0	25,31,34	0.61	0
75	PSU	h1	95	75	18,21,22	1.01	1 (5%)	21,30,33	1.06	3 (14%)
2	A2M	A	2254	2	22,25,26	0.58	0	30,36,39	1.87	9 (30%)
75	OMC	h1	471	75	19,22,23	0.42	0	25,31,34	0.47	0
75	PSU	h1	1208	75	18,21,22	0.96	2 (11%)	21,30,33	0.89	1 (4%)
2	A2M	A	826	2,82,81	22,25,26	0.57	0	30,36,39	1.61	6 (20%)
2	OMU	A	144	2,82	19,22,23	0.24	0	25,31,34	0.58	0
75	OMU	h1	1232	75	19,22,23	0.51	0	25,31,34	0.53	0
2	A2M	A	2945	2,81	22,25,26	0.62	0	30,36,39	1.62	5 (16%)
75	PSU	h1	762	75	18,21,22	0.86	1 (5%)	21,30,33	1.07	3 (14%)
75	PSU	h1	808	75	18,21,22	0.98	2 (11%)	21,30,33	0.97	2 (9%)
2	PSU	A	1015	2,82	18,21,22	0.87	2 (11%)	21,30,33	1.09	3 (14%)
2	OMC	A	1858	2	19,22,23	0.37	0	25,31,34	0.52	0
2	OMG	A	2650	2	23,26,27	0.38	0	32,38,41	0.56	1 (3%)
75	PSU	h1	360	75	18,21,22	0.95	1 (5%)	21,30,33	1.22	3 (14%)
2	1MA	A	657	2,81	21,25,26	0.71	1 (4%)	30,37,40	0.92	0
75	PSU	h1	256	75	18,21,22	0.95	1 (5%)	21,30,33	0.98	1 (4%)
75	OMG	h1	390	82,75	23,26,27	0.36	0	32,38,41	0.51	1 (3%)
22	HIC	BS	246	22	10,11,12	0.44	0	9,14,16	1.78	2 (22%)
75	OMC	h1	1641	75,81	19,22,23	0.47	0	25,31,34	0.57	0
2	OMC	A	2363	2	19,22,23	0.47	0	25,31,34	0.41	0
75	PSU	h1	304	75	18,21,22	0.87	1 (5%)	21,30,33	1.26	3 (14%)
2	OMU	A	2716	2	19,22,23	0.43	0	25,31,34	0.57	0
2	OMC	A	2835	2	19,22,23	0.49	0	25,31,34	0.52	0
75	OMU	h1	1270	75,81	19,22,23	0.31	0	25,31,34	0.65	0
2	OMU	A	2345	2	19,22,23	0.55	0	25,31,34	0.60	0
75	A2M	h1	422	75	22,25,26	0.60	0	30,36,39	1.83	6 (20%)
2	UY1	A	2649	2	19,22,23	0.86	1 (5%)	21,31,34	0.74	0
2	A2M	A	1376	2,81	22,25,26	0.53	0	30,36,39	1.48	3 (10%)
2	OMG	A	2122	2	23,26,27	0.39	0	32,38,41	0.55	0
75	OMG	h1	1272	82,75	23,26,27	0.32	0	32,38,41	0.32	0
2	OMG	A	1459	2,81	23,26,27	0.47	0	32,38,41	0.53	0
75	PSU	h1	1483	75	18,21,22	1.02	2 (11%)	21,30,33	0.74	0
75	PSU	h1	1176	75	18,21,22	0.90	1 (5%)	21,30,33	1.01	3 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
75	PSU	h1	121	75,81	18,21,22	0.83	1 (5%)	21,30,33	0.77	0
75	PSU	h1	761	75	18,21,22	0.85	1 (5%)	21,30,33	0.76	0
75	PSU	h1	337	82,75	18,21,22	1.01	2 (11%)	21,30,33	0.76	0
2	PSU	A	894	2	18,21,22	1.08	2 (11%)	21,30,33	1.10	1 (4%)
75	PSU	h1	1531	75	18,21,22	0.96	1 (5%)	21,30,33	0.95	2 (9%)
75	PSU	h1	1215	75	18,21,22	0.92	1 (5%)	21,30,33	0.94	0
75	PSU	h1	1306	75	18,21,22	0.91	2 (11%)	21,30,33	0.87	2 (9%)
2	A2M	A	2124	2	22,25,26	0.52	0	30,36,39	1.44	3 (10%)
2	OMG	A	2814	2	23,26,27	0.48	0	32,38,41	0.37	0
75	PSU	h1	959	82,75	18,21,22	1.15	2 (11%)	21,30,33	1.06	1 (4%)
2	PSU	A	34	2	18,21,22	0.96	1 (5%)	21,30,33	1.06	2 (9%)
2	PSU	A	2743	2	18,21,22	0.85	2 (11%)	21,30,33	1.01	2 (9%)
1	OMG	3	79	1	23,26,27	0.38	0	32,38,41	0.44	0
2	OMG	A	2921	2	23,26,27	0.32	0	32,38,41	0.44	0
2	OMC	A	1517	2,81	19,22,23	0.58	0	25,31,34	0.61	0
75	PSU	h1	449	82,75	18,21,22	1.03	2 (11%)	21,30,33	0.94	1 (4%)
2	PSU	A	2134	2	18,21,22	1.20	2 (11%)	21,30,33	1.10	2 (9%)
2	PSU	A	2209	2	18,21,22	0.97	2 (11%)	21,30,33	1.03	3 (14%)
1	PSU	3	97	82,1	18,21,22	0.92	2 (11%)	21,30,33	1.10	2 (9%)
2	PSU	A	965	2	18,21,22	0.93	1 (5%)	21,30,33	1.16	3 (14%)
75	A2M	h1	543	75	22,25,26	0.68	0	30,36,39	2.10	8 (26%)
2	OMU	A	803	2	19,22,23	0.42	0	25,31,34	0.59	0
75	OMG	h1	244	75	23,26,27	0.33	0	32,38,41	0.38	0
2	OMU	A	3299	2	19,22,23	0.31	0	25,31,34	0.54	0
75	PSU	h1	415	75	18,21,22	0.91	1 (5%)	21,30,33	0.85	0
75	PSU	h1	1611	75	18,21,22	0.90	1 (5%)	21,30,33	1.08	2 (9%)
2	OMG	A	2916	2	23,26,27	0.41	0	32,38,41	0.48	0
75	PSU	h1	1302	75	18,21,22	0.98	2 (11%)	21,30,33	0.83	0
1	PSU	3	22	2,1	18,21,22	1.02	1 (5%)	21,30,33	1.44	5 (23%)
2	A2M	A	1142	2	22,25,26	0.61	0	30,36,39	1.60	7 (23%)
2	OMC	A	1446	2	19,22,23	0.35	0	25,31,34	0.60	0
75	A2M	h1	28	75,81	22,25,26	0.51	0	30,36,39	1.67	7 (23%)
2	OMU	A	2734	2,81	19,22,23	0.29	0	25,31,34	0.68	0
2	OMC	A	1848	2,81	19,22,23	0.41	0	25,31,34	0.58	0
75	A2M	h1	466	75	22,25,26	0.55	0	30,36,39	1.88	6 (20%)
2	PSU	A	969	2	18,21,22	0.70	0	21,30,33	1.50	6 (28%)
2	A2M	A	2279	2	22,25,26	0.66	0	30,36,39	1.93	10 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A2M	A	2910	2	22,25,26	0.68	0	30,36,39	1.54	5 (16%)
2	PSU	A	685	2	18,21,22	1.09	2 (11%)	21,30,33	1.43	3 (14%)
2	OMU	A	676	2	19,22,23	0.51	0	25,31,34	0.76	0
2	A2M	A	945	2	22,25,26	0.55	0	30,36,39	1.54	4 (13%)
2	OMC	A	1478	2	19,22,23	0.41	0	25,31,34	0.64	0
75	OMC	h1	1216	75	19,22,23	0.33	0	25,31,34	0.60	0
75	OMU	h1	1381	75,81	19,22,23	0.39	0	25,31,34	0.54	0
2	OMU	A	2419	2	19,22,23	0.48	0	25,31,34	0.64	0
75	PSU	h1	103	75	18,21,22	0.98	2 (11%)	21,30,33	0.73	0
2	PSU	A	150	2,82	18,21,22	1.07	2 (11%)	21,30,33	0.85	0
2	5MC	A	2869	2,82	19,22,23	1.12	1 (5%)	26,32,35	0.86	0
75	OMU	h1	613	75	19,22,23	0.37	0	25,31,34	0.57	0
2	OMU	A	2920	2,82	19,22,23	0.30	0	25,31,34	0.62	0
75	OMU	h1	1010	75	19,22,23	0.41	0	25,31,34	0.61	0
2	OMC	A	2681	2	19,22,23	0.38	0	25,31,34	0.51	0
2	1MG	A	1646	2	23,26,27	0.94	0	33,39,42	0.83	1 (3%)
75	PSU	h1	948	75	18,21,22	0.85	1 (5%)	21,30,33	0.96	3 (14%)
2	PSU	A	2922	2,82	18,21,22	1.12	2 (11%)	21,30,33	1.10	1 (4%)
2	PSU	A	228	2	18,21,22	1.05	2 (11%)	21,30,33	0.90	1 (4%)
75	A2M	h1	1754	75	22,25,26	0.54	0	30,36,39	1.66	5 (16%)
2	OMG	A	2792	2	23,26,27	0.43	0	32,38,41	0.42	0
2	PSU	A	2132	2,82	18,21,22	0.96	0	21,30,33	1.47	3 (14%)
75	OMU	h1	1263	75	19,22,23	0.46	0	25,31,34	0.50	0
75	A2M	h1	162	75	22,25,26	0.54	0	30,36,39	1.79	8 (26%)
2	PSU	A	1681	2	18,21,22	1.09	2 (11%)	21,30,33	0.88	1 (4%)
2	A2M	A	661	2	22,25,26	0.64	0	30,36,39	1.32	3 (10%)
2	5MC	A	2276	2,81	19,22,23	1.03	1 (5%)	26,32,35	0.70	0
2	OMG	A	3290	2,81	23,26,27	0.45	0	32,38,41	0.72	1 (3%)
2	PSU	A	3109	2	18,21,22	0.96	1 (5%)	21,30,33	1.07	2 (9%)
75	OMU	h1	1261	75	19,22,23	0.53	0	25,31,34	0.61	0
2	A2M	A	2212	2,81	22,25,26	0.63	0	30,36,39	1.66	6 (20%)
2	PSU	A	2430	2	18,21,22	1.06	1 (5%)	21,30,33	1.00	3 (14%)
2	OMC	A	1845	2	19,22,23	0.47	0	25,31,34	0.53	0
2	OMC	A	2958	2,81	19,22,23	0.55	0	25,31,34	0.51	0
2	PSU	A	2853	2	18,21,22	0.92	2 (11%)	21,30,33	1.11	3 (14%)
2	PSU	A	2262	2	18,21,22	0.95	2 (11%)	21,30,33	1.17	3 (14%)
2	A2M	A	2359	2	22,25,26	0.57	0	30,36,39	1.60	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A2M	A	2218	2	22,25,26	0.54	0	30,36,39	1.81	6 (20%)
2	PSU	A	2252	2	18,21,22	0.85	1 (5%)	21,30,33	1.03	2 (9%)
2	PSU	A	2943	2,82,81	18,21,22	1.01	1 (5%)	21,30,33	1.02	0
75	OMC	h1	416	75	19,22,23	0.30	0	25,31,34	0.51	0
2	OMG	A	2393	2,81	23,26,27	0.47	0	32,38,41	0.62	0
2	PSU	A	311	2,82	18,21,22	1.11	2 (11%)	21,30,33	1.03	2 (9%)
2	PSU	A	1133	2	18,21,22	0.86	2 (11%)	21,30,33	1.06	2 (9%)
75	OMG	h1	597	75	23,26,27	0.36	0	32,38,41	0.54	0
2	OMG	A	814	2	23,26,27	0.35	0	32,38,41	0.58	0
2	PSU	A	509	2	18,21,22	1.04	2 (11%)	21,30,33	1.05	2 (9%)
2	OMU	A	1890	2	19,22,23	0.44	0	25,31,34	0.83	0
2	OMC	A	2291	2	19,22,23	0.34	0	25,31,34	0.70	0
2	OMC	A	2947	2	19,22,23	0.59	0	25,31,34	0.54	0
75	A2M	h1	621	75,81	22,25,26	0.65	0	30,36,39	1.52	5 (16%)
2	PSU	A	2312	2,82	18,21,22	1.03	2 (11%)	21,30,33	1.12	3 (14%)
2	PSU	A	1472	2	18,21,22	0.77	1 (5%)	21,30,33	1.15	3 (14%)
75	OMC	h1	38	75	19,22,23	0.35	0	25,31,34	0.49	0
75	UY1	h1	602	75	19,22,23	1.07	1 (5%)	21,31,34	1.07	2 (9%)
75	4AC	h1	1281	75	21,24,25	0.84	1 (4%)	28,34,37	1.12	3 (10%)
75	PSU	h1	583	75	18,21,22	1.07	2 (11%)	21,30,33	0.86	1 (4%)
2	A2M	A	1458	2,81	22,25,26	0.62	0	30,36,39	1.41	4 (13%)
2	OMG	A	917	2,82	23,26,27	0.47	0	32,38,41	0.48	0
75	A2M	h1	1327	75	22,25,26	0.44	0	30,36,39	1.79	6 (20%)
75	OMU	h1	1445	75	19,22,23	0.46	0	25,31,34	0.44	0
2	OMU	A	2882	2	19,22,23	0.38	0	25,31,34	0.76	0
75	PSU	h1	605	75	18,21,22	0.88	1 (5%)	21,30,33	1.20	3 (14%)
2	OMG	A	2389	2	23,26,27	0.35	0	32,38,41	0.42	0
2	PSU	A	42	2,82	18,21,22	1.03	2 (11%)	21,30,33	1.29	4 (19%)
2	PSU	A	785	2	18,21,22	1.03	1 (5%)	21,30,33	0.84	0
2	PSU	A	901	2,82	18,21,22	1.13	2 (11%)	21,30,33	1.12	2 (9%)
2	OMC	A	2195	2,82	19,22,23	0.57	0	25,31,34	0.83	1 (4%)
2	OMU	A	1066	2	19,22,23	0.31	0	25,31,34	0.75	0
2	A2M	A	2319	2	22,25,26	0.53	0	30,36,39	1.63	6 (20%)
2	A2M	A	2324	2	22,25,26	0.57	0	30,36,39	1.45	3 (10%)
75	PSU	h1	1000	75	18,21,22	0.89	1 (5%)	21,30,33	1.13	3 (14%)
75	A2M	h1	1575	75	22,25,26	0.61	0	30,36,39	2.01	9 (30%)
2	PSU	A	1480	2	18,21,22	0.91	1 (5%)	21,30,33	1.10	3 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
75	PSU	h1	606	75	18,21,22	1.16	2 (11%)	21,30,33	0.97	0
2	OMG	A	2618	2,3	23,26,27	0.45	0	32,38,41	0.42	0
2	PSU	A	2825	2,82	18,21,22	1.05	1 (5%)	21,30,33	1.13	2 (9%)
75	OMG	h1	1431	75,81	23,26,27	0.37	0	32,38,41	0.32	0
2	PSU	A	277	2	18,21,22	1.23	3 (16%)	21,30,33	1.14	3 (14%)
1	PSU	3	78	1	18,21,22	0.93	1 (5%)	21,30,33	0.99	2 (9%)
2	OMU	A	44	2,82	19,22,23	0.37	0	25,31,34	0.57	0
75	A2M	h1	975	75	22,25,26	0.58	0	30,36,39	1.62	6 (20%)
75	PSU	h1	1630	75	18,21,22	1.07	2 (11%)	21,30,33	1.13	3 (14%)
75	A2M	h1	778	75	22,25,26	0.46	0	30,36,39	1.70	7 (23%)
2	OMU	A	48	2	19,22,23	0.39	0	25,31,34	0.66	0
2	OMG	A	2234	2	23,26,27	0.40	0	32,38,41	0.58	0
75	4AC	h1	1777	75	21,24,25	0.70	1 (4%)	28,34,37	1.00	3 (10%)
2	OMC	A	675	2	19,22,23	0.45	0	25,31,34	0.54	0
2	OMG	A	1853	2	23,26,27	0.37	0	32,38,41	0.53	0
75	A2M	h1	438	75	22,25,26	0.56	0	30,36,39	1.75	6 (20%)
2	PSU	A	2954	2	18,21,22	0.89	2 (11%)	21,30,33	0.80	0
2	OMG	A	2790	2	23,26,27	0.45	0	32,38,41	0.52	0
75	PSU	h1	1520	75	18,21,22	0.92	1 (5%)	21,30,33	0.91	1 (4%)
2	PSU	A	2316	2,81	18,21,22	1.06	2 (11%)	21,30,33	0.84	0
2	PSU	A	1062	2,82	18,21,22	1.01	1 (5%)	21,30,33	1.19	3 (14%)
2	PSU	A	1131	2	18,21,22	0.98	1 (5%)	21,30,33	1.09	4 (19%)
75	PSU	h1	1188	75	18,21,22	0.95	1 (5%)	21,30,33	1.04	2 (9%)
2	PSU	A	2414	2,81	18,21,22	1.06	2 (11%)	21,30,33	1.07	2 (9%)
2	A2M	A	2639	2	22,25,26	0.56	0	30,36,39	1.56	3 (10%)
75	PSU	h1	308	75	18,21,22	1.01	2 (11%)	21,30,33	1.31	3 (14%)
2	PSU	A	2258	2	18,21,22	0.90	1 (5%)	21,30,33	0.82	0
75	PSU	h1	1182	75	18,21,22	0.82	1 (5%)	21,30,33	1.00	2 (9%)
75	OMU	h1	580	75	19,22,23	0.33	0	25,31,34	0.62	0
75	MA6	h1	1785	75	23,26,27	0.34	0	33,38,41	1.39	3 (9%)
2	OMG	A	2286	2	23,26,27	0.46	0	32,38,41	0.37	0
75	A2M	h1	799	75	22,25,26	0.31	0	30,36,39	0.53	0
75	A2M	h1	794	75	22,25,26	0.54	0	30,36,39	1.69	5 (16%)
2	OMG	A	2407	2,82	23,26,27	0.36	0	32,38,41	0.51	0
2	PSU	A	1132	2	18,21,22	0.72	1 (5%)	21,30,33	1.37	4 (19%)
75	OMU	h1	123	75	19,22,23	0.51	0	25,31,34	0.66	0
2	PSU	A	2256	2	18,21,22	1.02	2 (11%)	21,30,33	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A2M	A	2933	2	22,25,26	0.65	0	30,36,39	1.70	6 (20%)
2	OMC	A	2335	2	19,22,23	0.40	0	25,31,34	0.62	0
75	PSU	h1	1291	75	18,21,22	1.00	2 (11%)	21,30,33	0.96	1 (4%)
75	C4J	h1	1192	75	25,29,30	1.24	3 (12%)	28,42,45	0.97	2 (7%)
75	PSU	h1	1783	75	18,21,22	0.91	1 (5%)	21,30,33	0.77	0
2	PSU	A	1001	2	18,21,22	1.02	2 (11%)	21,30,33	0.84	0
2	A2M	A	885	2	22,25,26	0.57	0	30,36,39	1.59	4 (13%)
55	MLY	Ga	113	55	9,10,11	0.43	0	6,11,13	0.16	0
2	PSU	A	828	2	18,21,22	1.20	3 (16%)	21,30,33	1.28	3 (14%)
75	G7M	h1	1577	3,75	23,26,27	0.98	1 (4%)	34,39,42	0.85	1 (2%)
2	A2M	A	816	2	22,25,26	0.73	0	30,36,39	1.99	8 (26%)
2	PSU	A	2879	2	18,21,22	0.99	1 (5%)	21,30,33	1.02	1 (4%)
2	PSU	A	2264	2	18,21,22	1.12	2 (11%)	21,30,33	1.01	1 (4%)
75	PSU	h1	1025	75	18,21,22	0.91	1 (5%)	21,30,33	1.35	2 (9%)

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
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
1	A2M	3	47	1	-	0/9/27/28	0/3/3/3
2	OMU	A	2111	2	-	2/9/27/28	0/2/2/2
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2408	2,82	-	0/9/27/28	0/2/2/2
2	PSU	A	2893	2	-	0/7/25/26	0/2/2/2
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
75	6MZ	h1	1767	82,75,81	-	2/9/27/28	0/3/3/3
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2189	2,82	-	0/7/25/26	0/2/2/2
2	PSU	A	975	2,82	-	0/7/25/26	0/2/2/2
75	PSU	h1	468	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1054	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2864	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	752	75	-	0/7/25/26	0/2/2/2
1	OMG	3	155	2,1	-	1/9/27/28	0/3/3/3

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2974	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2878	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	95	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2254	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	471	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	1208	75	-	2/7/25/26	0/2/2/2
2	A2M	A	826	2,82,81	-	0/9/27/28	0/3/3/3
2	OMU	A	144	2,82	-	0/9/27/28	0/2/2/2
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
2	A2M	A	2945	2,81	-	1/9/27/28	0/3/3/3
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	808	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1015	2,82	-	0/7/25/26	0/2/2/2
2	OMC	A	1858	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2650	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
2	1MA	A	657	2,81	-	2/7/25/26	0/3/3/3
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
75	OMG	h1	390	82,75	-	0/9/27/28	0/3/3/3
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
75	OMC	h1	1641	75,81	-	1/9/27/28	0/2/2/2
2	OMC	A	2363	2	-	1/9/27/28	0/2/2/2
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2716	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2835	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	1270	75,81	-	3/9/27/28	0/2/2/2
2	OMU	A	2345	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	422	75	-	0/9/27/28	0/3/3/3
2	UY1	A	2649	2	-	0/9/27/28	0/2/2/2
2	A2M	A	1376	2,81	-	1/9/27/28	0/3/3/3
2	OMG	A	2122	2	-	0/9/27/28	0/3/3/3
75	OMG	h1	1272	82,75	-	1/9/27/28	0/3/3/3
2	OMG	A	1459	2,81	-	0/9/27/28	0/3/3/3
75	PSU	h1	1483	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	121	75,81	-	0/7/25/26	0/2/2/2
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	337	82,75	-	0/7/25/26	0/2/2/2
2	PSU	A	894	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PSU	h1	1306	75	-	2/7/25/26	0/2/2/2
2	A2M	A	2124	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2814	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	959	82,75	-	0/7/25/26	0/2/2/2
2	PSU	A	34	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2743	2	-	0/7/25/26	0/2/2/2
1	OMG	3	79	1	-	0/9/27/28	0/3/3/3
2	OMG	A	2921	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1517	2,81	-	2/9/27/28	0/2/2/2
75	PSU	h1	449	82,75	-	0/7/25/26	0/2/2/2
2	PSU	A	2134	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2209	2	-	0/7/25/26	0/2/2/2
1	PSU	3	97	82,1	-	0/7/25/26	0/2/2/2
2	PSU	A	965	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	543	75	-	2/9/27/28	0/3/3/3
2	OMU	A	803	2	-	0/9/27/28	0/2/2/2
75	OMG	h1	244	75	-	0/9/27/28	0/3/3/3
2	OMU	A	3299	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	415	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1611	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2916	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
1	PSU	3	22	2,1	-	0/7/25/26	0/2/2/2
2	A2M	A	1142	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1446	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	28	75,81	-	1/9/27/28	0/3/3/3
2	OMU	A	2734	2,81	-	0/9/27/28	0/2/2/2
2	OMC	A	1848	2,81	-	0/9/27/28	0/2/2/2
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
2	PSU	A	969	2	-	1/7/25/26	0/2/2/2
2	A2M	A	2279	2	-	2/9/27/28	0/3/3/3
2	A2M	A	2910	2	-	4/9/27/28	0/3/3/3
2	PSU	A	685	2	-	0/7/25/26	0/2/2/2
2	OMU	A	676	2	-	0/9/27/28	0/2/2/2
2	A2M	A	945	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1478	2	-	0/9/27/28	0/2/2/2
75	OMC	h1	1216	75	-	0/9/27/28	0/2/2/2
75	OMU	h1	1381	75,81	-	0/9/27/28	0/2/2/2
2	OMU	A	2419	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	103	75	-	0/7/25/26	0/2/2/2
2	PSU	A	150	2,82	-	0/7/25/26	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	A	2869	2,82	-	4/7/25/26	0/2/2/2
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
2	OMU	A	2920	2,82	-	0/9/27/28	0/2/2/2
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
2	OMC	A	2681	2	-	0/9/27/28	0/2/2/2
2	1MG	A	1646	2	-	0/7/25/26	0/3/3/3
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2922	2,82	-	2/7/25/26	0/2/2/2
2	PSU	A	228	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1754	75	-	1/9/27/28	0/3/3/3
2	OMG	A	2792	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2132	2,82	-	0/7/25/26	0/2/2/2
75	OMU	h1	1263	75	-	0/9/27/28	0/2/2/2
75	A2M	h1	162	75	-	1/9/27/28	0/3/3/3
2	PSU	A	1681	2	-	0/7/25/26	0/2/2/2
2	A2M	A	661	2	-	1/9/27/28	0/3/3/3
2	5MC	A	2276	2,81	-	0/7/25/26	0/2/2/2
2	OMG	A	3290	2,81	-	0/9/27/28	0/3/3/3
2	PSU	A	3109	2	-	0/7/25/26	0/2/2/2
75	OMU	h1	1261	75	-	1/9/27/28	0/2/2/2
2	A2M	A	2212	2,81	-	1/9/27/28	0/3/3/3
2	PSU	A	2430	2	-	0/7/25/26	0/2/2/2
2	OMC	A	1845	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2958	2,81	-	0/9/27/28	0/2/2/2
2	PSU	A	2853	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2262	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2359	2	-	1/9/27/28	0/3/3/3
2	A2M	A	2218	2	-	1/9/27/28	0/3/3/3
2	PSU	A	2252	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2943	2,82,81	-	0/7/25/26	0/2/2/2
75	OMC	h1	416	75	-	1/9/27/28	0/2/2/2
2	OMG	A	2393	2,81	-	0/9/27/28	0/3/3/3
2	PSU	A	311	2,82	-	0/7/25/26	0/2/2/2
2	PSU	A	1133	2	-	0/7/25/26	0/2/2/2
75	OMG	h1	597	75	-	4/9/27/28	0/3/3/3
2	OMG	A	814	2	-	0/9/27/28	0/3/3/3
2	PSU	A	509	2	-	0/7/25/26	0/2/2/2
2	OMU	A	1890	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2291	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2947	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	621	75,81	-	3/9/27/28	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2312	2,82	-	1/7/25/26	0/2/2/2
2	PSU	A	1472	2	-	0/7/25/26	0/2/2/2
75	OMC	h1	38	75	-	0/9/27/28	0/2/2/2
75	UY1	h1	602	75	-	1/9/27/28	0/2/2/2
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
75	PSU	h1	583	75	-	4/7/25/26	0/2/2/2
2	A2M	A	1458	2,81	-	0/9/27/28	0/3/3/3
2	OMG	A	917	2,82	-	0/9/27/28	0/3/3/3
75	A2M	h1	1327	75	-	1/9/27/28	0/3/3/3
75	OMU	h1	1445	75	-	0/9/27/28	0/2/2/2
2	OMU	A	2882	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2389	2	-	1/9/27/28	0/3/3/3
2	PSU	A	42	2,82	-	0/7/25/26	0/2/2/2
2	PSU	A	785	2	-	2/7/25/26	0/2/2/2
2	PSU	A	901	2,82	-	0/7/25/26	0/2/2/2
2	OMC	A	2195	2,82	-	4/9/27/28	0/2/2/2
2	OMU	A	1066	2	-	0/9/27/28	0/2/2/2
2	A2M	A	2319	2	-	0/9/27/28	0/3/3/3
2	A2M	A	2324	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
2	PSU	A	1480	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	606	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2618	2,3	-	1/9/27/28	0/3/3/3
2	PSU	A	2825	2,82	-	0/7/25/26	0/2/2/2
75	OMG	h1	1431	75,81	-	1/9/27/28	0/3/3/3
2	PSU	A	277	2	-	0/7/25/26	0/2/2/2
1	PSU	3	78	1	-	0/7/25/26	0/2/2/2
2	OMU	A	44	2,82	-	0/9/27/28	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	778	75	-	3/9/27/28	0/3/3/3
2	OMU	A	48	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2234	2	-	1/9/27/28	0/3/3/3
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
2	OMC	A	675	2	-	0/9/27/28	0/2/2/2
2	OMG	A	1853	2	-	1/9/27/28	0/3/3/3
75	A2M	h1	438	75	-	1/9/27/28	0/3/3/3
2	PSU	A	2954	2	-	0/7/25/26	0/2/2/2
2	OMG	A	2790	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	PSU	h1	1520	75	-	3/7/25/26	0/2/2/2
2	PSU	A	2316	2,81	-	0/7/25/26	0/2/2/2
2	PSU	A	1062	2,82	-	1/7/25/26	0/2/2/2
2	PSU	A	1131	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1188	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2414	2,81	-	0/7/25/26	0/2/2/2
2	A2M	A	2639	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	308	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2258	2	-	1/7/25/26	0/2/2/2
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
75	OMU	h1	580	75	-	5/9/27/28	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
2	OMG	A	2286	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	799	75	-	0/9/27/28	0/3/3/3
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3
2	OMG	A	2407	2,82	-	0/9/27/28	0/3/3/3
2	PSU	A	1132	2	-	0/7/25/26	0/2/2/2
75	OMU	h1	123	75	-	3/9/27/28	0/2/2/2
2	PSU	A	2256	2	-	2/7/25/26	0/2/2/2
2	A2M	A	2933	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2335	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
75	C4J	h1	1192	75	-	5/16/34/35	0/2/2/2
75	PSU	h1	1783	75	-	1/7/25/26	0/2/2/2
2	PSU	A	1001	2	-	0/7/25/26	0/2/2/2
2	A2M	A	885	2	-	0/9/27/28	0/3/3/3
55	MLY	Ga	113	55	-	0/8/9/11	-
2	PSU	A	828	2	-	0/7/25/26	0/2/2/2
75	G7M	h1	1577	3,75	-	0/7/25/26	0/3/3/3
2	A2M	A	816	2	-	2/9/27/28	0/3/3/3
2	PSU	A	2879	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2869	5MC	C5-C4	-4.43	1.40	1.44
75	h1	606	PSU	C6-C5	4.13	1.39	1.35
2	A	2922	PSU	C6-C5	3.95	1.39	1.35
75	h1	602	UY1	C6-C5	3.94	1.39	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2276	5MC	C5-C4	-3.92	1.41	1.44
75	h1	583	PSU	C6-C5	3.79	1.39	1.35
75	h1	959	PSU	C6-C5	3.76	1.39	1.35
2	A	2264	PSU	C6-C5	3.74	1.39	1.35
2	A	785	PSU	C6-C5	3.68	1.39	1.35
2	A	901	PSU	C6-C5	3.64	1.39	1.35
2	A	311	PSU	C6-C5	3.52	1.39	1.35
75	h1	752	PSU	C6-C5	3.51	1.39	1.35
75	h1	256	PSU	C6-C5	3.49	1.39	1.35
2	A	509	PSU	C6-C5	3.49	1.39	1.35
2	A	2825	PSU	C6-C5	3.49	1.39	1.35
75	h1	337	PSU	C6-C5	3.49	1.39	1.35
75	h1	1483	PSU	C6-C5	3.47	1.39	1.35
2	A	2134	PSU	C6-C5	3.46	1.39	1.35
75	h1	360	PSU	C6-C5	3.45	1.39	1.35
75	h1	1577	G7M	C8-N7	3.44	1.38	1.33
75	h1	1192	C4J	C6-C5	3.42	1.40	1.35
2	A	1062	PSU	C6-C5	3.42	1.39	1.35
75	h1	95	PSU	C6-C5	3.41	1.39	1.35
75	h1	1531	PSU	C6-C5	3.40	1.39	1.35
75	h1	1215	PSU	C6-C5	3.39	1.39	1.35
75	h1	1630	PSU	C6-C5	3.38	1.39	1.35
2	A	2430	PSU	C6-C5	3.37	1.39	1.35
2	A	228	PSU	C6-C5	3.37	1.39	1.35
75	h1	415	PSU	C6-C5	3.31	1.39	1.35
75	h1	1291	PSU	C6-C5	3.29	1.38	1.35
75	h1	449	PSU	C6-C5	3.28	1.38	1.35
2	A	2879	PSU	C6-C5	3.27	1.38	1.35
2	A	1681	PSU	C6-C5	3.26	1.38	1.35
2	A	2209	PSU	C6-C5	3.21	1.38	1.35
2	A	1480	PSU	C6-C5	3.21	1.38	1.35
1	3	78	PSU	C6-C5	3.20	1.38	1.35
75	h1	468	PSU	C6-C5	3.20	1.38	1.35
2	A	2316	PSU	C6-C5	3.19	1.38	1.35
2	A	685	PSU	C6-C5	3.18	1.38	1.35
75	h1	308	PSU	C6-C5	3.15	1.38	1.35
75	h1	1176	PSU	C6-C5	3.15	1.38	1.35
75	h1	1520	PSU	C6-C5	3.15	1.38	1.35
2	A	1001	PSU	C6-C5	3.14	1.38	1.35
75	h1	1563	PSU	C6-C5	3.13	1.38	1.35
75	h1	1188	PSU	C6-C5	3.13	1.38	1.35
2	A	1054	PSU	C6-C5	3.12	1.38	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	277	PSU	C4-C5	-3.11	1.35	1.44
75	h1	1783	PSU	C6-C5	3.11	1.38	1.35
2	A	2943	PSU	C6-C5	3.09	1.38	1.35
75	h1	1104	PSU	C6-C5	3.09	1.38	1.35
2	A	3109	PSU	C6-C5	3.08	1.38	1.35
2	A	2256	PSU	C6-C5	3.08	1.38	1.35
75	h1	1611	PSU	C6-C5	3.06	1.38	1.35
75	h1	1208	PSU	C6-C5	3.05	1.38	1.35
1	3	22	PSU	C6-C5	3.04	1.38	1.35
2	A	2649	UY1	C6-C5	3.02	1.38	1.35
75	h1	948	PSU	C6-C5	3.01	1.38	1.35
2	A	2312	PSU	C6-C5	3.00	1.38	1.35
75	h1	103	PSU	C6-C5	2.95	1.38	1.35
2	A	1131	PSU	C6-C5	2.95	1.38	1.35
2	A	975	PSU	C6-C5	2.94	1.38	1.35
75	h1	605	PSU	C6-C5	2.93	1.38	1.35
75	h1	1118	PSU	C6-C5	2.91	1.38	1.35
2	A	34	PSU	C6-C5	2.88	1.38	1.35
2	A	150	PSU	C6-C5	2.88	1.38	1.35
2	A	150	PSU	C4-C5	-2.88	1.36	1.44
2	A	2252	PSU	C6-C5	2.88	1.38	1.35
75	h1	1192	C4J	C4-C5	-2.88	1.41	1.47
75	h1	1182	PSU	C6-C5	2.86	1.38	1.35
75	h1	1000	PSU	C6-C5	2.85	1.38	1.35
75	h1	1306	PSU	C6-C5	2.84	1.38	1.35
2	A	2262	PSU	C6-C5	2.84	1.38	1.35
75	h1	121	PSU	C6-C5	2.82	1.38	1.35
2	A	965	PSU	C6-C5	2.81	1.38	1.35
75	h1	634	PSU	C6-C5	2.81	1.38	1.35
75	h1	304	PSU	C6-C5	2.81	1.38	1.35
75	h1	762	PSU	C6-C5	2.78	1.38	1.35
2	A	1472	PSU	C6-C5	2.77	1.38	1.35
75	h1	761	PSU	C6-C5	2.75	1.38	1.35
75	h1	808	PSU	C6-C5	2.72	1.38	1.35
2	A	657	1MA	C5-C6	-2.71	1.36	1.43
75	h1	1281	4AC	C4-N4	2.70	1.43	1.39
2	A	685	PSU	C4-C5	-2.70	1.36	1.44
2	A	277	PSU	C6-C5	2.70	1.38	1.35
75	h1	1025	PSU	C6-C5	2.70	1.38	1.35
2	A	2864	PSU	C6-C5	2.70	1.38	1.35
75	h1	1302	PSU	C6-C5	2.70	1.38	1.35
2	A	2853	PSU	C6-C5	2.69	1.38	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	42	PSU	C6-C5	2.65	1.38	1.35
2	A	1681	PSU	C4-C5	-2.65	1.37	1.44
2	A	828	PSU	C6-N1	-2.63	1.32	1.36
2	A	1001	PSU	C4-C5	-2.61	1.37	1.44
75	h1	959	PSU	C4-C5	-2.61	1.37	1.44
2	A	2414	PSU	C6-C5	2.59	1.38	1.35
75	h1	308	PSU	C4-C5	-2.59	1.37	1.44
2	A	2258	PSU	C6-C5	2.59	1.38	1.35
2	A	828	PSU	C4-C5	-2.58	1.37	1.44
2	A	901	PSU	C4-C5	-2.57	1.37	1.44
2	A	894	PSU	C6-C5	2.56	1.38	1.35
75	h1	1192	C4J	C4-N3	2.55	1.44	1.40
75	h1	1777	4AC	C4-N4	2.54	1.43	1.39
1	3	97	PSU	C6-C5	2.54	1.38	1.35
75	h1	1630	PSU	C4-C5	-2.52	1.37	1.44
2	A	975	PSU	C4-C5	-2.51	1.37	1.44
2	A	2134	PSU	C4-C5	-2.48	1.37	1.44
75	h1	1291	PSU	C4-C5	-2.45	1.37	1.44
2	A	2264	PSU	C4-C5	-2.43	1.37	1.44
2	A	228	PSU	C4-C5	-2.41	1.37	1.44
2	A	2954	PSU	C6-C5	2.41	1.38	1.35
75	h1	1302	PSU	C4-C5	-2.39	1.37	1.44
2	A	2189	PSU	C6-C5	2.39	1.37	1.35
75	h1	634	PSU	C4-C5	-2.38	1.37	1.44
75	h1	808	PSU	C4-C5	-2.35	1.37	1.44
75	h1	103	PSU	C4-C5	-2.34	1.37	1.44
2	A	2312	PSU	C4-C5	-2.34	1.37	1.44
2	A	2262	PSU	C4-C5	-2.32	1.37	1.44
75	h1	752	PSU	C4-C5	-2.32	1.37	1.44
2	A	1132	PSU	C6-C5	2.31	1.37	1.35
2	A	2743	PSU	C4-C5	-2.31	1.37	1.44
2	A	311	PSU	C4-C5	-2.30	1.38	1.44
2	A	2954	PSU	C4-C5	-2.29	1.38	1.44
2	A	2256	PSU	C4-C5	-2.27	1.38	1.44
75	h1	606	PSU	C4-C5	-2.26	1.38	1.44
2	A	2974	PSU	C6-C5	2.23	1.37	1.35
2	A	277	PSU	C4-N3	-2.22	1.34	1.38
2	A	894	PSU	C4-N3	-2.21	1.34	1.38
2	A	975	PSU	C4-N3	-2.19	1.34	1.38
2	A	2316	PSU	C4-C5	-2.18	1.38	1.44
2	A	2743	PSU	C6-C5	2.17	1.37	1.35
2	A	2893	PSU	C6-C5	2.17	1.37	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	1483	PSU	C4-C5	-2.17	1.38	1.44
2	A	2189	PSU	C4-C5	-2.15	1.38	1.44
75	h1	337	PSU	C4-C5	-2.15	1.38	1.44
2	A	2414	PSU	C4-C5	-2.14	1.38	1.44
75	h1	449	PSU	C4-C5	-2.13	1.38	1.44
2	A	1133	PSU	C4-C5	-2.13	1.38	1.44
2	A	1015	PSU	C6-C5	2.13	1.37	1.35
75	h1	1208	PSU	C4-C5	-2.13	1.38	1.44
2	A	1054	PSU	C4-C5	-2.12	1.38	1.44
2	A	1015	PSU	C4-C5	-2.12	1.38	1.44
75	h1	583	PSU	C4-C5	-2.11	1.38	1.44
2	A	828	PSU	C4-N3	-2.09	1.34	1.38
2	A	1133	PSU	C6-C5	2.08	1.37	1.35
75	h1	604	PSU	C6-C5	2.07	1.37	1.35
2	A	2853	PSU	C4-C5	-2.07	1.38	1.44
2	A	509	PSU	C4-C5	-2.06	1.38	1.44
1	3	97	PSU	C4-C5	-2.05	1.38	1.44
2	A	42	PSU	C4-C5	-2.05	1.38	1.44
2	A	2922	PSU	C4-C5	-2.05	1.38	1.44
75	h1	1306	PSU	C4-C5	-2.03	1.38	1.44
2	A	2209	PSU	C4-C5	-2.01	1.38	1.44

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	543	A2M	C1'-N9-C8	-6.41	112.86	127.09
2	A	816	A2M	C1'-N9-C8	-6.22	113.28	127.09
75	h1	1575	A2M	C1'-N9-C8	-5.73	114.39	127.09
75	h1	466	A2M	C1'-N9-C8	-5.58	114.70	127.09
75	h1	1327	A2M	C1'-N9-C8	-5.41	115.09	127.09
75	h1	438	A2M	C1'-N9-C8	-5.39	115.12	127.09
75	h1	1786	MA6	C5-C6-N6	5.32	133.75	125.33
2	A	2279	A2M	C1'-N9-C8	-5.29	115.36	127.09
75	h1	422	A2M	C1'-N9-C8	-5.27	115.40	127.09
75	h1	1786	MA6	N1-C6-N6	-5.25	110.46	116.86
2	A	2933	A2M	C1'-N9-C8	-5.16	115.64	127.09
75	h1	778	A2M	C1'-N9-C8	-5.15	115.66	127.09
75	h1	162	A2M	C1'-N9-C8	-5.15	115.66	127.09
2	A	2218	A2M	C1'-N9-C8	-5.12	115.73	127.09
75	h1	543	A2M	C4-N9-C1'	5.12	138.60	126.63
2	A	1376	A2M	C1'-N9-C8	-5.10	115.78	127.09
2	A	2212	A2M	C1'-N9-C8	-5.05	115.89	127.09

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2639	A2M	C1'-N9-C8	-5.04	115.90	127.09
2	A	2254	A2M	C1'-N9-C8	-5.03	115.93	127.09
2	A	2359	A2M	C1'-N9-C8	-4.99	116.02	127.09
75	h1	1785	MA6	N1-C6-N6	-4.98	110.79	116.86
75	h1	794	A2M	C1'-N9-C8	-4.97	116.08	127.09
75	h1	1754	A2M	C1'-N9-C8	-4.94	116.14	127.09
2	A	885	A2M	C1'-N9-C8	-4.93	116.15	127.09
75	h1	28	A2M	C1'-N9-C8	-4.85	116.33	127.09
2	A	826	A2M	C1'-N9-C8	-4.67	116.72	127.09
75	h1	1327	A2M	C4-N9-C1'	4.61	137.41	126.63
2	A	816	A2M	C4-N9-C1'	4.59	137.37	126.63
2	A	2910	A2M	C1'-N9-C8	-4.57	116.95	127.09
75	h1	975	A2M	C1'-N9-C8	-4.56	116.97	127.09
2	A	945	A2M	C1'-N9-C8	-4.55	117.00	127.09
1	3	47	A2M	C1'-N9-C8	-4.54	117.01	127.09
75	h1	438	A2M	C4-N9-C1'	4.52	137.21	126.63
2	A	1458	A2M	C1'-N9-C8	-4.52	117.07	127.09
2	A	2324	A2M	C1'-N9-C8	-4.45	117.23	127.09
75	h1	1785	MA6	C5-C6-N6	4.43	132.34	125.33
2	A	2639	A2M	C4-N9-C1'	4.41	136.94	126.63
2	A	1376	A2M	C4-N9-C1'	4.41	136.94	126.63
75	h1	1575	A2M	C4-N9-C1'	4.37	136.84	126.63
75	h1	466	A2M	C4-N9-C1'	4.36	136.83	126.63
2	A	2319	A2M	C1'-N9-C8	-4.36	117.43	127.09
2	A	2945	A2M	C1'-N9-C8	-4.35	117.45	127.09
75	h1	422	A2M	C4-N9-C1'	4.32	136.74	126.63
2	A	885	A2M	C4-N9-C1'	4.31	136.70	126.63
2	A	1142	A2M	C1'-N9-C8	-4.25	117.66	127.09
75	h1	621	A2M	C1'-N9-C8	-4.23	117.70	127.09
2	A	2218	A2M	C4-N9-C1'	4.21	136.47	126.63
75	h1	778	A2M	C4-N9-C1'	4.17	136.39	126.63
2	A	2359	A2M	C4-N9-C1'	4.14	136.31	126.63
2	A	2124	A2M	C1'-N9-C8	-4.10	117.99	127.09
1	3	47	A2M	C2'-C1'-N9	-4.08	107.04	113.75
75	h1	794	A2M	C4-N9-C1'	4.03	136.05	126.63
2	A	2933	A2M	C4-N9-C1'	4.01	136.01	126.63
2	A	661	A2M	C1'-N9-C8	-3.95	118.33	127.09
75	h1	162	A2M	C4-N9-C1'	3.94	135.85	126.63
2	A	2212	A2M	C4-N9-C1'	3.93	135.83	126.63
2	A	2945	A2M	C2'-C1'-N9	-3.92	107.30	113.75
75	h1	1754	A2M	C4-N9-C1'	3.85	135.64	126.63
75	h1	28	A2M	C4-N9-C1'	3.79	135.49	126.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2279	A2M	C4-N9-C1'	3.78	135.47	126.63
2	A	2319	A2M	C2'-C1'-N9	-3.69	107.67	113.75
75	h1	1786	MA6	C2-N1-C6	3.69	120.83	111.83
22	BS	246	HIC	NE2-CE1-ND1	-3.67	111.26	112.66
2	A	2324	A2M	C4-N9-C1'	3.66	135.18	126.63
2	A	685	PSU	C6-C5-C4	3.65	120.64	118.17
2	A	826	A2M	C3'-C2'-C1'	-3.62	95.87	102.81
1	3	47	A2M	C4-N9-C1'	3.62	135.10	126.63
75	h1	1575	A2M	C2'-C1'-N9	-3.61	107.81	113.75
2	A	2124	A2M	C4-N9-C1'	3.61	135.07	126.63
2	A	945	A2M	C4-N9-C1'	3.58	135.00	126.63
75	h1	975	A2M	C4-N9-C1'	3.53	134.90	126.63
2	A	1458	A2M	C4-N9-C1'	3.53	134.88	126.63
2	A	2218	A2M	O2'-C2'-C1'	3.52	115.68	108.99
75	h1	621	A2M	O2'-C2'-C1'	3.52	115.67	108.99
2	A	2254	A2M	C4-N9-C1'	3.51	134.84	126.63
2	A	661	A2M	C4-N9-C1'	3.51	134.84	126.63
2	A	2254	A2M	C2'-C1'-N9	-3.49	108.01	113.75
2	A	2132	PSU	C5-C6-N1	-3.46	117.33	122.14
2	A	816	A2M	C5-C4-N9	-3.42	102.08	105.81
2	A	2910	A2M	C4-N9-C1'	3.42	134.62	126.63
1	3	22	PSU	C6-C5-C4	3.41	120.48	118.17
2	A	2132	PSU	C4-N3-C2	-3.36	121.74	126.37
2	A	826	A2M	C4-N9-C1'	3.34	134.45	126.63
2	A	2319	A2M	C4-N9-C1'	3.33	134.43	126.63
2	A	2922	PSU	C6-C5-C4	3.33	120.42	118.17
2	A	2254	A2M	C4-N9-C8	3.30	109.21	105.74
75	h1	621	A2M	C4-N9-C1'	3.30	134.35	126.63
75	h1	1327	A2M	O2'-C2'-C1'	3.28	115.22	108.99
2	A	1142	A2M	C2'-C1'-N9	-3.28	108.35	113.75
2	A	2945	A2M	C4-N9-C1'	3.28	134.30	126.63
75	h1	543	A2M	O4'-C1'-C2'	3.26	112.20	106.59
2	A	2279	A2M	O2'-C2'-C1'	3.25	115.15	108.99
75	h1	959	PSU	C6-C5-C4	3.24	120.36	118.17
2	A	1142	A2M	C4-N9-C1'	3.24	134.20	126.63
75	h1	1785	MA6	C2-N1-C6	3.23	119.73	111.83
75	h1	1575	A2M	O2'-C2'-C1'	3.19	115.05	108.99
75	h1	1281	4AC	N4-C4-N3	3.19	119.05	113.87
2	A	685	PSU	C5-C6-N1	-3.11	117.83	122.14
75	h1	794	A2M	O2'-C2'-C1'	3.09	114.85	108.99
75	h1	308	PSU	C6-C5-C4	3.09	120.26	118.17
22	BS	246	HIC	CZ-NE2-CD2	-3.05	122.03	126.03

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2134	PSU	C6-C5-C4	3.05	120.23	118.17
2	A	969	PSU	C5-C6-N1	-3.04	117.92	122.14
2	A	816	A2M	O4'-C1'-C2'	3.02	111.79	106.59
2	A	2279	A2M	C2'-C1'-N9	-3.02	108.78	113.75
2	A	2933	A2M	C2'-C1'-N9	-3.02	108.78	113.75
75	h1	1025	PSU	C5-C6-N1	-3.01	117.96	122.14
75	h1	360	PSU	C5-C6-N1	-3.00	117.98	122.14
75	h1	308	PSU	C5-C6-N1	-2.98	118.01	122.14
75	h1	304	PSU	C6-C5-C4	2.97	120.18	118.17
75	h1	543	A2M	N3-C4-N9	2.97	132.22	127.17
75	h1	162	A2M	C2'-C1'-N9	-2.96	108.89	113.75
2	A	1132	PSU	C5-C6-N1	-2.94	118.06	122.14
75	h1	466	A2M	C5-C4-N9	-2.94	102.61	105.81
2	A	2218	A2M	C2'-C1'-N9	-2.91	108.96	113.75
2	A	885	A2M	C2'-C1'-N9	-2.90	108.98	113.75
75	h1	621	A2M	O4'-C1'-N9	-2.89	102.53	108.09
75	h1	975	A2M	C2'-C1'-N9	-2.89	108.99	113.75
75	h1	28	A2M	C2'-C1'-N9	-2.89	109.00	113.75
75	h1	1575	A2M	O4'-C1'-N9	-2.87	102.57	108.09
75	h1	1575	A2M	C4-N9-C8	2.87	108.75	105.74
2	A	42	PSU	C4-N3-C2	-2.85	122.45	126.37
2	A	816	A2M	C2'-C1'-N9	-2.83	109.10	113.75
2	A	2262	PSU	C6-C5-C4	2.80	120.06	118.17
2	A	2974	PSU	C5-C6-N1	-2.78	118.28	122.14
2	A	828	PSU	C4-N3-C2	-2.78	122.55	126.37
2	A	2910	A2M	C2'-C1'-N9	-2.77	109.19	113.75
75	h1	543	A2M	C4'-O4'-C1'	-2.76	103.36	109.47
75	h1	422	A2M	N3-C4-N9	2.75	131.85	127.17
75	h1	605	PSU	C5-C6-N1	-2.75	118.32	122.14
75	h1	422	A2M	C2'-C1'-N9	-2.75	109.23	113.75
75	h1	360	PSU	C6-C5-C4	2.75	120.03	118.17
75	h1	1754	A2M	O2'-C2'-C1'	2.75	114.20	108.99
75	h1	466	A2M	N3-C4-N9	2.74	131.84	127.17
2	A	2324	A2M	C2'-C1'-N9	-2.74	109.24	113.75
2	A	1132	PSU	C6-C5-C4	2.73	120.01	118.17
1	3	22	PSU	C4-N3-C2	-2.72	122.62	126.37
2	A	1472	PSU	C5-C6-N1	-2.72	118.36	122.14
1	3	22	PSU	C5-C6-N1	-2.71	118.38	122.14
2	A	42	PSU	C5-C6-N1	-2.71	118.38	122.14
2	A	1132	PSU	C4-N3-C2	-2.70	122.66	126.37
2	A	685	PSU	C4-N3-C2	-2.69	122.66	126.37
2	A	2945	A2M	O2'-C2'-C1'	2.69	114.09	108.99

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1376	A2M	O4'-C1'-N9	-2.68	102.95	108.09
75	h1	438	A2M	O2'-C2'-C1'	2.66	114.05	108.99
2	A	2264	PSU	C6-C5-C4	2.65	119.96	118.17
75	h1	1192	C4J	C4-N3-C2	-2.65	122.36	125.62
75	h1	304	PSU	C5-C6-N1	-2.64	118.47	122.14
2	A	816	A2M	N3-C4-N9	2.64	131.66	127.17
2	A	2254	A2M	O3'-C3'-C2'	-2.64	103.80	111.19
75	h1	543	A2M	C5-C4-N9	-2.64	102.93	105.81
2	A	2279	A2M	C4-N9-C8	2.63	108.50	105.74
75	h1	1611	PSU	C6-C5-C4	2.62	119.94	118.17
2	A	901	PSU	C4-N3-C2	-2.62	122.76	126.37
75	h1	438	A2M	N3-C4-N9	2.62	131.62	127.17
75	h1	1777	4AC	N4-C4-N3	2.61	118.11	113.87
75	h1	1563	PSU	C6-C5-C4	2.60	119.93	118.17
2	A	2124	A2M	C2'-C1'-N9	-2.60	109.47	113.75
75	h1	28	A2M	C5-C4-N9	-2.59	102.99	105.81
2	A	2189	PSU	C4-N3-C2	-2.59	122.81	126.37
2	A	34	PSU	C6-C5-C4	2.59	119.92	118.17
2	A	969	PSU	C4-N3-C2	-2.59	122.81	126.37
75	h1	95	PSU	C5-C6-N1	-2.58	118.56	122.14
2	A	2359	A2M	C2'-C1'-N9	-2.58	109.51	113.75
75	h1	1577	G7M	N9-C8-N7	-2.58	106.22	112.48
75	h1	162	A2M	N3-C4-N9	2.58	131.55	127.17
2	A	2212	A2M	O2'-C2'-C1'	2.58	113.88	108.99
75	h1	778	A2M	C2'-C1'-N9	-2.57	109.52	113.75
2	A	1054	PSU	C4-N3-C2	-2.56	122.84	126.37
2	A	826	A2M	O3'-C3'-C2'	-2.56	104.02	111.19
2	A	828	PSU	C5-C6-N1	-2.56	118.59	122.14
2	A	826	A2M	O4'-C1'-N9	-2.56	103.18	108.09
75	h1	162	A2M	O2'-C2'-C1'	2.56	113.84	108.99
75	h1	1520	PSU	C6-C5-C4	2.55	119.89	118.17
2	A	661	A2M	C2'-C1'-N9	-2.55	109.56	113.75
75	h1	605	PSU	C4-N3-C2	-2.54	122.87	126.37
2	A	969	PSU	C6-C5-C4	2.54	119.89	118.17
75	h1	1630	PSU	C6-C5-C4	2.53	119.88	118.17
2	A	816	A2M	C4-N9-C8	2.53	108.40	105.74
2	A	3109	PSU	C6-C5-C4	2.53	119.88	118.17
2	A	945	A2M	N3-C4-N9	2.52	131.46	127.17
75	h1	466	A2M	C4-N9-C8	2.52	108.39	105.74
2	A	2252	PSU	C6-C5-C4	2.52	119.88	118.17
2	A	2853	PSU	C5-C6-N1	-2.51	118.66	122.14
2	A	2134	PSU	C4-N3-C2	-2.51	122.92	126.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1015	PSU	C4-N3-C2	-2.51	122.92	126.37
75	h1	422	A2M	C5-C4-N9	-2.50	103.08	105.81
2	A	2312	PSU	C6-C5-C4	2.50	119.86	118.17
75	h1	1327	A2M	N3-C4-N9	2.49	131.40	127.17
2	A	965	PSU	C5-C6-N1	-2.49	118.69	122.14
2	A	1646	1MG	C2-N3-C4	2.48	117.56	111.98
2	A	2279	A2M	C3'-C2'-C1'	-2.48	98.06	102.81
75	h1	308	PSU	C4-N3-C2	-2.47	122.97	126.37
2	A	2254	A2M	O2'-C2'-C1'	2.47	113.68	108.99
75	h1	543	A2M	C4-N9-C8	2.47	108.33	105.74
2	A	1142	A2M	N3-C4-N9	2.46	131.35	127.17
2	A	277	PSU	C6-C5-C4	2.46	119.83	118.17
75	h1	1767	6MZ	C1'-N9-C8	2.46	132.55	127.09
75	h1	1000	PSU	C6-C5-C4	2.45	119.83	118.17
2	A	1062	PSU	C4-N3-C2	-2.45	123.00	126.37
75	h1	1563	PSU	C5-C6-N1	-2.44	118.75	122.14
2	A	3290	OMG	C3'-C2'-C1'	-2.44	98.13	102.81
2	A	2212	A2M	C5-C4-N9	-2.44	103.15	105.81
2	A	228	PSU	C6-C5-C4	2.44	119.82	118.17
2	A	1133	PSU	C6-C5-C4	2.44	119.82	118.17
75	h1	1104	PSU	C4-N3-C2	-2.43	123.02	126.37
75	h1	634	PSU	C6-C5-C4	2.43	119.82	118.17
75	h1	1575	A2M	C5-C4-N9	-2.43	103.16	105.81
2	A	42	PSU	C6-C5-C4	2.43	119.81	118.17
75	h1	1291	PSU	C6-C5-C4	2.43	119.81	118.17
2	A	2974	PSU	C4-N3-C2	-2.43	123.03	126.37
2	A	2974	PSU	C6-C5-C4	2.42	119.81	118.17
2	A	2254	A2M	C3'-C2'-C1'	-2.42	98.17	102.81
75	h1	438	A2M	C2'-C1'-N9	-2.42	109.77	113.75
2	A	2933	A2M	C4-N9-C8	2.41	108.27	105.74
2	A	894	PSU	C6-C5-C4	2.41	119.80	118.17
75	h1	1025	PSU	C4-N3-C2	-2.41	123.05	126.37
2	A	1054	PSU	C5-C6-N1	-2.41	118.79	122.14
2	A	2254	A2M	C5-C4-N9	-2.41	103.19	105.81
2	A	2279	A2M	N3-C4-N9	2.41	131.26	127.17
2	A	1015	PSU	C5-C6-N1	-2.41	118.80	122.14
1	3	22	PSU	N1-C2-N3	2.41	117.70	115.17
2	A	2209	PSU	C5-C6-N1	-2.40	118.80	122.14
2	A	2359	A2M	N3-C4-N9	2.40	131.25	127.17
75	h1	1777	4AC	C6-C5-C4	2.40	119.89	117.00
75	h1	162	A2M	C5-C4-N9	-2.39	103.20	105.81
2	A	816	A2M	C4'-O4'-C1'	-2.39	104.19	109.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	602	UY1	C5-C6-N1	-2.39	118.82	122.14
2	A	2212	A2M	C4-N9-C8	2.38	108.24	105.74
2	A	1480	PSU	C6-C5-C4	2.38	119.78	118.17
2	A	2312	PSU	C5-C6-N1	-2.38	118.84	122.14
2	A	2189	PSU	C5-C6-N1	-2.38	118.84	122.14
2	A	1472	PSU	C4-N3-C2	-2.37	123.10	126.37
2	A	2319	A2M	C5-C4-N9	-2.37	103.23	105.81
75	h1	95	PSU	C6-C5-C4	2.37	119.77	118.17
1	3	97	PSU	C5-C6-N1	-2.36	118.86	122.14
1	3	78	PSU	C5-C6-N1	-2.36	118.86	122.14
2	A	2279	A2M	C4'-O4'-C1'	-2.36	104.26	109.47
75	h1	604	PSU	C5-C6-N1	-2.36	118.87	122.14
75	h1	778	A2M	N3-C4-N9	2.36	131.18	127.17
2	A	1062	PSU	N1-C2-N3	2.35	117.65	115.17
1	3	97	PSU	C6-C5-C4	2.35	119.76	118.17
2	A	1142	A2M	C5-C4-N9	-2.35	103.25	105.81
75	h1	28	A2M	O2'-C2'-C1'	2.34	113.44	108.99
2	A	1458	A2M	C5-C4-N9	-2.34	103.26	105.81
75	h1	256	PSU	C6-C5-C4	2.34	119.75	118.17
2	A	969	PSU	O2'-C2'-C1'	-2.34	105.66	111.21
2	A	2319	A2M	N3-C4-N9	2.34	131.15	127.17
2	A	2639	A2M	N3-C4-N9	2.34	131.14	127.17
75	h1	360	PSU	C4-N3-C2	-2.33	123.16	126.37
75	h1	621	A2M	C4'-O4'-C1'	-2.33	104.31	109.47
2	A	2414	PSU	C4-N3-C2	-2.33	123.16	126.37
2	A	2218	A2M	C5-C4-N9	-2.33	103.27	105.81
2	A	2430	PSU	C4-N3-C2	-2.33	123.17	126.37
75	h1	778	A2M	C5-C4-N9	-2.33	103.28	105.81
2	A	2359	A2M	O3'-C3'-C2'	-2.31	104.71	111.19
2	A	965	PSU	C4-N3-C2	-2.31	123.18	126.37
75	h1	162	A2M	C4-N9-C8	2.31	108.17	105.74
2	A	2825	PSU	C4-N3-C2	-2.31	123.19	126.37
2	A	277	PSU	C5-C6-N1	-2.31	118.94	122.14
75	h1	794	A2M	N3-C4-N9	2.31	131.09	127.17
75	h1	28	A2M	C4-N9-C8	2.30	108.16	105.74
2	A	1480	PSU	C5-C6-N1	-2.30	118.95	122.14
75	h1	28	A2M	N3-C4-N9	2.29	131.07	127.17
75	h1	1754	A2M	C4-N9-C8	2.29	108.14	105.74
2	A	2910	A2M	C4-N9-C8	2.28	108.14	105.74
2	A	2262	PSU	C5-C6-N1	-2.28	118.97	122.14
2	A	901	PSU	C5-C6-N1	-2.28	118.98	122.14
75	h1	1754	A2M	C2'-C1'-N9	-2.27	110.01	113.75

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2254	A2M	O4'-C1'-N9	-2.27	103.73	108.09
2	A	969	PSU	C3'-C2'-C1'	2.26	104.36	101.69
2	A	1142	A2M	C4-N9-C8	2.26	108.11	105.74
75	h1	1182	PSU	C6-C5-C4	2.26	119.70	118.17
75	h1	449	PSU	C3'-C2'-C1'	2.26	104.35	101.69
2	A	1131	PSU	C6-C5-C4	2.26	119.70	118.17
2	A	2879	PSU	C4-N3-C2	-2.26	123.26	126.37
75	h1	762	PSU	C6-C5-C4	2.25	119.69	118.17
75	h1	1188	PSU	C4-N3-C2	-2.25	123.27	126.37
2	A	2132	PSU	C6-C5-C4	2.25	119.69	118.17
2	A	2933	A2M	C5-C4-N9	-2.25	103.36	105.81
1	3	22	PSU	O2-C2-N1	-2.25	120.47	122.79
2	A	311	PSU	C4-N3-C2	-2.25	123.28	126.37
2	A	1062	PSU	C5-C6-N1	-2.24	119.03	122.14
75	h1	605	PSU	C6-C5-C4	2.24	119.68	118.17
2	A	277	PSU	C4-N3-C2	-2.23	123.29	126.37
2	A	2743	PSU	C4-N3-C2	-2.23	123.30	126.37
2	A	2414	PSU	C5-C6-N1	-2.22	119.05	122.14
2	A	2853	PSU	C4-N3-C2	-2.22	123.31	126.37
75	h1	1306	PSU	C6-C5-C4	2.22	119.67	118.17
75	h1	1192	C4J	C3'-C2'-C1'	2.21	104.30	101.69
75	h1	975	A2M	C4-N9-C8	2.21	108.06	105.74
2	A	2195	OMC	C3'-C2'-C1'	-2.21	98.57	102.81
2	A	2218	A2M	N3-C4-N9	2.21	130.92	127.17
2	A	1142	A2M	O4'-C4'-C3'	-2.21	100.77	105.15
2	A	2743	PSU	C5-C6-N1	-2.21	119.08	122.14
75	h1	1327	A2M	C2'-C1'-N9	-2.21	110.12	113.75
75	h1	304	PSU	C4-N3-C2	-2.21	123.33	126.37
2	A	2910	A2M	O2'-C2'-C1'	2.21	113.18	108.99
75	h1	468	PSU	C5-C6-N1	-2.21	119.08	122.14
2	A	885	A2M	O2'-C2'-C1'	2.20	113.17	108.99
2	A	2209	PSU	C6-C5-C4	2.20	119.66	118.17
2	A	826	A2M	C4-N9-C8	2.20	108.04	105.74
2	A	34	PSU	C5-C6-N1	-2.20	119.09	122.14
2	A	2262	PSU	C4-N3-C2	-2.19	123.35	126.37
2	A	969	PSU	C6-N1-C2	2.19	124.72	122.69
2	A	311	PSU	C5-C6-N1	-2.19	119.11	122.14
2	A	1458	A2M	C4-N9-C8	2.18	108.03	105.74
75	h1	1176	PSU	C6-C5-C4	2.18	119.65	118.17
75	h1	1000	PSU	C5-C6-N1	-2.18	119.11	122.14
75	h1	466	A2M	C2'-C1'-N9	-2.18	110.17	113.75
75	h1	604	PSU	C4-N3-C2	-2.18	123.37	126.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2893	PSU	C4-N3-C2	-2.17	123.37	126.37
75	h1	762	PSU	C4-N3-C2	-2.17	123.38	126.37
2	A	1681	PSU	C5-C6-N1	-2.17	119.13	122.14
75	h1	975	A2M	C5-C4-N9	-2.17	103.45	105.81
2	A	2853	PSU	C6-C5-C4	2.17	119.64	118.17
75	h1	808	PSU	C6-C5-C4	2.17	119.64	118.17
75	h1	1176	PSU	C4-N3-C2	-2.17	123.39	126.37
2	A	1015	PSU	C6-C5-C4	2.16	119.63	118.17
75	h1	1575	A2M	C3'-C2'-C1'	-2.16	98.67	102.81
75	h1	762	PSU	C5-C6-N1	-2.16	119.14	122.14
2	A	945	A2M	C4'-O4'-C1'	-2.16	104.70	109.47
75	h1	438	A2M	C5-C4-N9	-2.15	103.47	105.81
75	h1	543	A2M	O2'-C2'-C1'	2.15	113.07	108.99
75	h1	1000	PSU	C2'-C3'-C4'	-2.15	98.46	102.61
2	A	1131	PSU	C4-N3-C2	-2.14	123.42	126.37
2	A	2945	A2M	C4-N9-C8	2.14	107.99	105.74
2	A	2279	A2M	O3'-C3'-C4'	2.14	117.22	111.08
75	h1	1777	4AC	C5-C4-N3	-2.14	119.26	122.60
1	3	78	PSU	C6-C5-C4	2.13	119.61	118.17
2	A	2893	PSU	C5-C6-N1	-2.13	119.18	122.14
2	A	975	PSU	C5-C6-N1	-2.13	119.18	122.14
75	h1	162	A2M	C4'-O4'-C1'	-2.13	104.76	109.47
75	h1	1531	PSU	C5-C6-N1	-2.12	119.19	122.14
2	A	2825	PSU	C5-C6-N1	-2.12	119.20	122.14
2	A	42	PSU	C2'-C3'-C4'	-2.12	98.51	102.61
75	h1	948	PSU	C6-C5-C4	2.12	119.60	118.17
75	h1	602	UY1	C6-N1-C2	2.12	124.66	122.69
2	A	2933	A2M	N3-C4-N9	2.12	130.77	127.17
75	h1	975	A2M	N3-C4-N9	2.12	130.77	127.17
75	h1	1630	PSU	C4-N3-C2	-2.12	123.45	126.37
75	h1	752	PSU	C6-C5-C4	2.11	119.60	118.17
2	A	2319	A2M	C4-N9-C8	2.11	107.96	105.74
2	A	1131	PSU	C2'-C3'-C4'	-2.11	98.53	102.61
2	A	1132	PSU	C6-N1-C2	2.11	124.65	122.69
1	3	47	A2M	N3-C4-N9	2.11	130.76	127.17
2	A	2209	PSU	C4-N3-C2	-2.11	123.47	126.37
2	A	1131	PSU	C5-C6-N1	-2.11	119.22	122.14
75	h1	1188	PSU	C6-C5-C4	2.11	119.59	118.17
75	h1	1118	PSU	C4-N3-C2	-2.10	123.47	126.37
2	A	1480	PSU	C4-N3-C2	-2.09	123.50	126.37
2	A	2650	OMG	C3'-C2'-C1'	-2.08	98.82	102.81
75	h1	1630	PSU	C5-C6-N1	-2.08	119.25	122.14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	778	A2M	O2'-C2'-C1'	2.08	112.93	108.99
75	h1	1104	PSU	C5-C6-N1	-2.07	119.26	122.14
2	A	3109	PSU	C4-N3-C2	-2.07	123.51	126.37
2	A	2430	PSU	C6-C5-C4	2.07	119.57	118.17
75	h1	778	A2M	C4-N9-C8	2.07	107.91	105.74
75	h1	634	PSU	C4-N3-C2	-2.07	123.52	126.37
2	A	1133	PSU	C4-N3-C2	-2.07	123.52	126.37
2	A	1472	PSU	C6-C5-C4	2.07	119.57	118.17
2	A	2359	A2M	C5-C4-N9	-2.06	103.56	105.81
75	h1	390	OMG	C2'-C1'-N9	-2.06	110.34	114.24
2	A	2279	A2M	C5-C4-N9	-2.06	103.57	105.81
75	h1	583	PSU	C6-C5-C4	2.05	119.56	118.17
75	h1	1611	PSU	C5-C6-N1	-2.05	119.29	122.14
75	h1	95	PSU	C4-N3-C2	-2.05	123.54	126.37
75	h1	1327	A2M	C5-C4-N9	-2.05	103.58	105.81
1	3	47	A2M	C5-C4-N9	-2.05	103.58	105.81
2	A	965	PSU	C2'-C3'-C4'	-2.04	98.66	102.61
75	h1	1575	A2M	O3'-C3'-C2'	-2.04	105.47	111.19
2	A	509	PSU	C6-C5-C4	2.04	119.55	118.17
75	h1	794	A2M	C4'-O4'-C1'	-2.04	104.97	109.47
75	h1	1306	PSU	C5-C6-N1	-2.04	119.31	122.14
2	A	2212	A2M	N3-C4-N9	2.03	130.63	127.17
2	A	2974	PSU	C2'-C3'-C4'	-2.03	98.68	102.61
75	h1	1208	PSU	C6-C5-C4	2.03	119.55	118.17
75	h1	468	PSU	C4-N3-C2	-2.03	123.57	126.37
75	h1	1281	4AC	C6-C5-C4	2.03	119.44	117.00
2	A	2312	PSU	C4-N3-C2	-2.03	123.58	126.37
2	A	2252	PSU	C5-C6-N1	-2.03	119.33	122.14
75	h1	948	PSU	C4-N3-C2	-2.03	123.58	126.37
75	h1	1281	4AC	C5-C4-N3	-2.03	119.43	122.60
2	A	509	PSU	C4-N3-C2	-2.02	123.58	126.37
2	A	975	PSU	C4-N3-C2	-2.02	123.58	126.37
75	h1	1531	PSU	C6-C5-C4	2.02	119.54	118.17
75	h1	1176	PSU	C5-C6-N1	-2.02	119.34	122.14
75	h1	1182	PSU	C5-C6-N1	-2.02	119.34	122.14
2	A	828	PSU	C6-N1-C2	2.02	124.56	122.69
2	A	2893	PSU	C6-C5-C4	2.02	119.53	118.17
2	A	2430	PSU	C5-C6-N1	-2.02	119.34	122.14
75	h1	422	A2M	O3'-C3'-C4'	2.01	116.86	111.08
2	A	1054	PSU	C6-C5-C4	2.01	119.53	118.17
75	h1	948	PSU	C5-C6-N1	-2.01	119.35	122.14
75	h1	808	PSU	C4-N3-C2	-2.00	123.61	126.37



There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	3	155	OMG	C1'-C2'-O2'-CM2
2	A	785	PSU	C2'-C1'-C5-C4
2	A	2111	OMU	O4'-C4'-C5'-O5'
2	A	2195	OMC	C2'-C1'-N1-C2
2	A	2195	OMC	C2'-C1'-N1-C6
2	A	2212	A2M	C1'-C2'-O2'-CM'
2	A	2218	A2M	C1'-C2'-O2'-CM'
2	A	2234	OMG	C1'-C2'-O2'-CM2
2	A	2256	PSU	O4'-C4'-C5'-O5'
2	A	2359	A2M	C1'-C2'-O2'-CM'
2	A	2389	OMG	C1'-C2'-O2'-CM2
2	A	2618	OMG	C1'-C2'-O2'-CM2
2	A	2945	A2M	C1'-C2'-O2'-CM'
75	h1	28	A2M	C1'-C2'-O2'-CM'
75	h1	162	A2M	C1'-C2'-O2'-CM'
75	h1	416	OMC	C1'-C2'-O2'-CM2
75	h1	438	A2M	C1'-C2'-O2'-CM'
75	h1	597	OMG	O4'-C4'-C5'-O5'
75	h1	602	UY1	C1'-C2'-O2'-CM2
75	h1	621	A2M	C1'-C2'-O2'-CM'
75	h1	778	A2M	O4'-C4'-C5'-O5'
75	h1	778	A2M	C1'-C2'-O2'-CM'
75	h1	794	A2M	C1'-C2'-O2'-CM'
75	h1	1192	C4J	C4'-C5'-O5'-P
75	h1	1232	OMU	O4'-C4'-C5'-O5'
75	h1	1272	OMG	C1'-C2'-O2'-CM2
75	h1	1327	A2M	C1'-C2'-O2'-CM'
75	h1	1520	PSU	C2'-C1'-C5-C4
75	h1	1520	PSU	C2'-C1'-C5-C6
75	h1	1754	A2M	C1'-C2'-O2'-CM'
2	A	2111	OMU	C3'-C4'-C5'-O5'
75	h1	778	A2M	C3'-C4'-C5'-O5'
2	A	2910	A2M	O4'-C4'-C5'-O5'
2	A	2910	A2M	C3'-C4'-C5'-O5'
75	h1	466	A2M	O4'-C4'-C5'-O5'
75	h1	580	OMU	O4'-C4'-C5'-O5'
75	h1	583	PSU	C3'-C4'-C5'-O5'
75	h1	583	PSU	O4'-C4'-C5'-O5'
75	h1	1192	C4J	O4'-C4'-C5'-O5'
75	h1	1232	OMU	C3'-C4'-C5'-O5'

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
75	h1	1270	OMU	C3'-C4'-C5'-O5'
75	h1	1270	OMU	O4'-C4'-C5'-O5'
2	A	2256	PSU	C3'-C4'-C5'-O5'
75	h1	597	OMG	C3'-C4'-C5'-O5'
75	h1	621	A2M	C3'-C4'-C5'-O5'
75	h1	1192	C4J	C3'-C4'-C5'-O5'
2	A	2279	A2M	O4'-C4'-C5'-O5'
75	h1	123	OMU	C3'-C4'-C5'-O5'
75	h1	621	A2M	O4'-C4'-C5'-O5'
2	A	2279	A2M	C3'-C4'-C5'-O5'
2	A	1517	OMC	O4'-C4'-C5'-O5'
75	h1	580	OMU	C3'-C4'-C5'-O5'
2	A	1517	OMC	C3'-C4'-C5'-O5'
75	h1	123	OMU	O4'-C4'-C5'-O5'
75	h1	466	A2M	C3'-C4'-C5'-O5'
75	h1	597	OMG	C1'-C2'-O2'-CM2
2	A	2910	A2M	C2'-C1'-N9-C8
75	h1	1767	6MZ	N1-C6-N6-C9
2	A	2869	5MC	C2'-C1'-N1-C6
75	h1	1767	6MZ	C5-C6-N6-C9
75	h1	1641	OMC	O4'-C4'-C5'-O5'
2	A	2312	PSU	C4'-C5'-O5'-P
2	A	2869	5MC	O4'-C1'-N1-C6
2	A	816	A2M	C3'-C2'-O2'-CM'
2	A	2922	PSU	C4'-C5'-O5'-P
75	h1	1431	OMG	C4'-C5'-O5'-P
2	A	969	PSU	O4'-C1'-C5-C4
2	A	2922	PSU	O4'-C1'-C5-C4
75	h1	1208	PSU	O4'-C1'-C5-C4
75	h1	1306	PSU	O4'-C1'-C5-C4
75	h1	1786	MA6	C4'-C5'-O5'-P
2	A	2910	A2M	C2'-C1'-N9-C4
2	A	2195	OMC	O4'-C1'-N1-C6
75	h1	1261	OMU	C3'-C2'-O2'-CM2
2	A	657	1MA	C2'-C1'-N9-C4
2	A	1376	A2M	O4'-C4'-C5'-O5'
2	A	2258	PSU	O4'-C4'-C5'-O5'
2	A	661	A2M	C4'-C5'-O5'-P
75	h1	1270	OMU	C4'-C5'-O5'-P
75	h1	1783	PSU	O4'-C4'-C5'-O5'
2	A	2195	OMC	O4'-C1'-N1-C2
2	A	2869	5MC	O4'-C1'-N1-C2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1853	OMG	C1'-C2'-O2'-CM2
75	h1	580	OMU	O4'-C1'-N1-C6
75	h1	583	PSU	O4'-C1'-C5-C6
75	h1	1208	PSU	O4'-C1'-C5-C6
75	h1	1306	PSU	O4'-C1'-C5-C6
75	h1	543	A2M	O4'-C1'-N9-C8
75	h1	580	OMU	C2'-C1'-N1-C6
2	A	2363	OMC	C3'-C2'-O2'-CM2
75	h1	1192	C4J	N33-C32-C34-O35
2	A	785	PSU	C2'-C1'-C5-C6
75	h1	583	PSU	C2'-C1'-C5-C6
75	h1	597	OMG	C4'-C5'-O5'-P
75	h1	543	A2M	C2'-C1'-N9-C4
75	h1	1520	PSU	O4'-C4'-C5'-O5'
75	h1	580	OMU	O4'-C1'-N1-C2
2	A	816	A2M	O4'-C1'-N9-C8
75	h1	1192	C4J	N3-C3-C31-C32
2	A	657	1MA	C2'-C1'-N9-C8
2	A	2869	5MC	C2'-C1'-N1-C2
75	h1	123	OMU	C2'-C1'-N1-C2
2	A	1062	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

62 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	h1	1563	PSU	1	0
1	3	155	OMG	2	0
2	A	2878	OMC	1	0
75	h1	95	PSU	1	0
75	h1	471	OMC	1	0
2	A	826	A2M	1	0
2	A	144	OMU	1	0
75	h1	808	PSU	1	0
75	h1	1270	OMU	2	0
2	A	2345	OMU	1	0
75	h1	422	A2M	1	0
2	A	2649	UY1	1	0
2	A	1376	A2M	1	0
75	h1	1272	OMG	1	0
75	h1	1483	PSU	1	0
75	h1	1176	PSU	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	h1	337	PSU	1	0
75	h1	1531	PSU	2	0
2	A	2814	OMG	1	0
2	A	965	PSU	1	0
75	h1	244	OMG	2	0
1	3	22	PSU	1	0
2	A	1446	OMC	2	0
75	h1	28	A2M	1	0
75	h1	466	A2M	3	0
2	A	969	PSU	1	0
2	A	2910	A2M	3	0
2	A	945	A2M	3	0
75	h1	1216	OMC	1	0
2	A	150	PSU	1	0
2	A	2869	5MC	1	0
75	h1	162	A2M	1	0
2	A	661	A2M	1	0
2	A	3290	OMG	1	0
75	h1	1261	OMU	2	0
2	A	2212	A2M	3	0
2	A	2359	A2M	1	0
2	A	2218	A2M	1	0
2	A	311	PSU	1	0
75	h1	597	OMG	1	0
2	A	2947	OMC	1	0
75	h1	1281	4AC	1	0
75	h1	1327	A2M	1	0
2	A	2882	OMU	2	0
2	A	2389	OMG	1	0
2	A	785	PSU	1	0
2	A	2618	OMG	1	0
1	3	78	PSU	1	0
75	h1	1630	PSU	1	0
75	h1	778	A2M	2	0
2	A	48	OMU	1	0
2	A	2234	OMG	1	0
2	A	675	OMC	1	0
75	h1	438	A2M	3	0
75	h1	1785	MA6	1	0
2	A	2286	OMG	1	0
75	h1	794	A2M	2	0
75	h1	123	OMU	1	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	885	A2M	1	0
2	A	828	PSU	1	0
75	h1	1577	G7M	2	0
2	A	2879	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 481 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	$\# Z  > 2$
83	SPD	A	3401	-	9,9,9	0.18	0	8,8,8	0.79	0
80	TER	h1	1902	-	13,13,13	0.23	0	12,12,12	0.28	0
84	EPE	A	3402	-	15,15,15	0.74	1 (6%)	19,20,20	0.84	0
80	TER	A	3418	-	13,13,13	0.17	0	12,12,12	0.33	0
80	TER	A	3419	-	13,13,13	0.18	0	12,12,12	0.23	0
80	TER	A	3412	-	13,13,13	0.13	0	12,12,12	0.25	0
80	TER	h1	1903	-	13,13,13	0.15	0	12,12,12	0.49	0
80	TER	A	3404	-	13,13,13	0.34	0	12,12,12	0.52	0
80	TER	A	3407	-	13,13,13	0.25	0	12,12,12	0.67	0
80	TER	3	201	-	13,13,13	0.27	0	12,12,12	0.31	0
80	TER	A	3409	-	13,13,13	0.29	0	12,12,12	0.44	0
80	TER	A	3415	-	13,13,13	0.19	0	12,12,12	0.45	0
80	TER	h1	1905	-	13,13,13	0.16	0	12,12,12	0.29	0
80	TER	A	3421	-	13,13,13	0.16	0	12,12,12	0.28	0
80	TER	3	202	-	13,13,13	0.16	0	12,12,12	0.27	0
80	TER	A	3414	-	13,13,13	0.36	0	12,12,12	0.37	0
80	TER	A	3417	-	13,13,13	0.17	0	12,12,12	0.20	0
80	TER	h1	1904	-	13,13,13	0.17	0	12,12,12	0.25	0
80	TER	h1	1906	-	13,13,13	0.17	0	12,12,12	0.30	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
80	TER	A	3420	-	13,13,13	0.24	0	12,12,12	0.57	0
80	TER	A	3411	-	13,13,13	0.15	0	12,12,12	0.45	0
80	TER	A	3410	-	13,13,13	0.15	0	12,12,12	0.31	0
80	TER	A	3403	-	13,13,13	0.19	0	12,12,12	0.36	0
80	TER	A	3408	-	13,13,13	0.15	0	12,12,12	0.28	0
80	TER	A	3416	-	13,13,13	0.20	0	12,12,12	0.28	0
80	TER	A	3406	-	13,13,13	0.17	0	12,12,12	0.34	0
80	TER	h1	1901	-	13,13,13	0.18	0	12,12,12	0.41	0
80	TER	A	3405	-	13,13,13	0.26	0	12,12,12	0.34	0
80	TER	A	3413	-	13,13,13	0.29	0	12,12,12	0.47	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
83	SPD	A	3401	-	-	4/7/7/7	-
80	TER	h1	1902	-	-	7/11/11/11	-
84	EPE	A	3402	-	-	4/9/19/19	0/1/1/1
80	TER	A	3418	-	-	5/11/11/11	-
80	TER	A	3419	-	-	4/11/11/11	-
80	TER	A	3412	-	-	5/11/11/11	-
80	TER	h1	1903	-	-	11/11/11/11	-
80	TER	A	3404	-	-	5/11/11/11	-
80	TER	A	3407	-	-	5/11/11/11	-
80	TER	3	201	-	-	4/11/11/11	-
80	TER	A	3409	-	-	8/11/11/11	-
80	TER	A	3415	-	-	4/11/11/11	-
80	TER	h1	1905	-	-	6/11/11/11	-
80	TER	A	3421	-	-	5/11/11/11	-
80	TER	3	202	-	-	4/11/11/11	-
80	TER	A	3414	-	-	6/11/11/11	-
80	TER	A	3417	-	-	1/11/11/11	-
80	TER	h1	1904	-	-	6/11/11/11	-
80	TER	h1	1906	-	-	10/11/11/11	-
80	TER	A	3420	-	-	6/11/11/11	-
80	TER	A	3411	-	-	6/11/11/11	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	TER	A	3410	-	-	4/11/11/11	-
80	TER	A	3403	-	-	2/11/11/11	-
80	TER	A	3408	-	-	6/11/11/11	-
80	TER	A	3416	-	-	5/11/11/11	-
80	TER	A	3406	-	-	5/11/11/11	-
80	TER	h1	1901	-	-	7/11/11/11	-
80	TER	A	3405	-	-	8/11/11/11	-
80	TER	A	3413	-	-	3/11/11/11	-

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

There are no bond angle outliers.

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	h1	1903	TER	C7-C6-N5-C4
80	h1	1906	TER	C2-C3-C4-N5
84	A	3402	EPE	C8-C7-N4-C5
80	A	3405	TER	C2-C3-C4-N5
80	A	3407	TER	N5-C6-C7-C8
80	A	3415	TER	N5-C6-C7-C8
80	h1	1903	TER	N9-C10-C11-C12
80	A	3409	TER	C2-C3-C4-N5
80	A	3417	TER	C2-C3-C4-N5
80	A	3421	TER	C2-C3-C4-N5
80	h1	1902	TER	N9-C10-C11-C12
80	A	3404	TER	N9-C10-C11-C12
80	A	3412	TER	N9-C10-C11-C12
80	A	3413	TER	N9-C10-C11-C12
80	h1	1906	TER	N9-C10-C11-C12
80	A	3414	TER	C2-C3-C4-N5
80	A	3421	TER	N5-C6-C7-C8
80	h1	1903	TER	C6-C7-C8-N9
80	h1	1904	TER	C2-C3-C4-N5
80	h1	1906	TER	N5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
80	A	3407	TER	C6-C7-C8-N9
80	A	3413	TER	C6-C7-C8-N9
80	A	3418	TER	N5-C6-C7-C8
80	A	3418	TER	C6-C7-C8-N9
80	A	3406	TER	N9-C10-C11-C12
80	A	3418	TER	N9-C10-C11-C12
80	A	3405	TER	N5-C6-C7-C8
80	A	3420	TER	C2-C3-C4-N5
80	A	3421	TER	C6-C7-C8-N9
80	h1	1902	TER	C2-C3-C4-N5
83	A	3401	SPD	N6-C7-C8-C9
80	A	3415	TER	C2-C3-C4-N5
80	A	3405	TER	C7-C6-N5-C4
80	A	3406	TER	C11-C10-N9-C8
80	A	3418	TER	C11-C10-N9-C8
80	h1	1901	TER	C7-C8-N9-C10
83	A	3401	SPD	C8-C7-N6-C5
80	h1	1905	TER	C10-C11-C12-C13
80	3	201	TER	C7-C6-N5-C4
80	A	3406	TER	C7-C6-N5-C4
80	A	3412	TER	C7-C8-N9-C10
80	A	3420	TER	C7-C6-N5-C4
80	A	3408	TER	N9-C10-C11-C12
80	A	3408	TER	C2-C3-C4-N5
80	h1	1905	TER	N5-C6-C7-C8
80	A	3410	TER	C3-C4-N5-C6
80	A	3410	TER	C7-C6-N5-C4
80	A	3411	TER	C7-C6-N5-C4
80	A	3412	TER	C7-C6-N5-C4
80	h1	1901	TER	C11-C10-N9-C8
80	h1	1903	TER	C3-C4-N5-C6
80	h1	1903	TER	C7-C8-N9-C10
80	h1	1904	TER	N1-C2-C3-C4
80	h1	1906	TER	C11-C10-N9-C8
80	A	3408	TER	C10-C11-C12-C13
80	A	3406	TER	N5-C6-C7-C8
80	h1	1902	TER	N5-C6-C7-C8
80	h1	1906	TER	C6-C7-C8-N9
80	h1	1901	TER	N9-C10-C11-C12
80	h1	1906	TER	C11-C12-C13-N14
80	A	3421	TER	C10-C11-C12-C13
80	A	3407	TER	C7-C6-N5-C4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
80	A	3419	TER	C7-C6-N5-C4
80	h1	1906	TER	C7-C8-N9-C10
80	3	202	TER	C10-C11-C12-C13
80	h1	1901	TER	C10-C11-C12-C13
80	A	3404	TER	C10-C11-C12-C13
80	A	3416	TER	C10-C11-C12-C13
80	A	3403	TER	C10-C11-C12-C13
80	A	3412	TER	C6-C7-C8-N9
80	A	3410	TER	C10-C11-C12-C13
80	A	3415	TER	C10-C11-C12-C13
80	h1	1904	TER	C10-C11-C12-C13
80	h1	1903	TER	C10-C11-C12-C13
80	A	3409	TER	N5-C6-C7-C8
80	A	3409	TER	C7-C8-N9-C10
80	h1	1904	TER	N5-C6-C7-C8
80	3	202	TER	C3-C4-N5-C6
80	A	3405	TER	N1-C2-C3-C4
80	A	3409	TER	N1-C2-C3-C4
80	A	3414	TER	N1-C2-C3-C4
84	A	3402	EPE	C9-C10-S-O1S
80	3	201	TER	C6-C7-C8-N9
80	A	3409	TER	C6-C7-C8-N9
80	A	3411	TER	N5-C6-C7-C8
80	h1	1901	TER	C7-C6-N5-C4
80	h1	1903	TER	C11-C10-N9-C8
80	h1	1904	TER	C7-C6-N5-C4
83	A	3401	SPD	C4-C5-N6-C7
80	A	3405	TER	C10-C11-C12-C13
80	A	3406	TER	C11-C12-C13-N14
80	h1	1906	TER	C10-C11-C12-C13
80	A	3411	TER	C7-C8-N9-C10
80	A	3419	TER	C7-C8-N9-C10
80	h1	1902	TER	C7-C6-N5-C4
80	h1	1905	TER	C7-C8-N9-C10
80	A	3412	TER	N5-C6-C7-C8
80	h1	1901	TER	C2-C3-C4-N5
80	A	3407	TER	C11-C10-N9-C8
80	A	3414	TER	C11-C10-N9-C8
80	3	202	TER	C6-C7-C8-N9
80	h1	1905	TER	C2-C3-C4-N5
80	A	3404	TER	N1-C2-C3-C4
80	A	3413	TER	N1-C2-C3-C4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
80	A	3420	TER	N1-C2-C3-C4
80	h1	1902	TER	N1-C2-C3-C4
80	h1	1904	TER	C11-C10-N9-C8
83	A	3401	SPD	C7-C8-C9-N10
80	A	3420	TER	C11-C12-C13-N14
80	A	3421	TER	C11-C12-C13-N14
80	h1	1901	TER	C11-C12-C13-N14
80	h1	1903	TER	C11-C12-C13-N14
80	A	3414	TER	N9-C10-C11-C12
80	A	3409	TER	C7-C6-N5-C4
80	h1	1906	TER	C7-C6-N5-C4
80	3	201	TER	N9-C10-C11-C12
80	A	3419	TER	N9-C10-C11-C12
80	A	3411	TER	C3-C4-N5-C6
80	A	3415	TER	C7-C8-N9-C10
80	A	3416	TER	C7-C8-N9-C10
80	A	3420	TER	C7-C8-N9-C10
80	h1	1906	TER	C3-C4-N5-C6
84	A	3402	EPE	C9-C10-S-O3S
84	A	3402	EPE	C8-C7-N4-C3
80	A	3418	TER	C7-C8-N9-C10
80	h1	1902	TER	C7-C8-N9-C10
80	h1	1903	TER	C2-C3-C4-N5
80	A	3405	TER	C7-C8-N9-C10
80	A	3409	TER	C11-C10-N9-C8
80	3	201	TER	N5-C6-C7-C8
80	A	3405	TER	C3-C4-N5-C6
80	A	3407	TER	N1-C2-C3-C4
80	A	3420	TER	C11-C10-N9-C8
80	A	3403	TER	N9-C10-C11-C12
80	A	3411	TER	C11-C10-N9-C8
80	A	3416	TER	C7-C6-N5-C4
80	h1	1902	TER	C11-C10-N9-C8
80	A	3408	TER	C6-C7-C8-N9
80	A	3414	TER	N5-C6-C7-C8
80	h1	1903	TER	N5-C6-C7-C8
80	A	3419	TER	C11-C12-C13-N14
80	h1	1905	TER	C11-C12-C13-N14
80	A	3414	TER	C7-C6-N5-C4
80	3	202	TER	N9-C10-C11-C12
80	A	3404	TER	N5-C6-C7-C8
80	A	3404	TER	C7-C8-N9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
80	A	3410	TER	C7-C8-N9-C10
80	A	3405	TER	C11-C12-C13-N14
80	A	3408	TER	C7-C8-N9-C10
80	A	3409	TER	C10-C11-C12-C13
80	A	3408	TER	N1-C2-C3-C4
80	A	3416	TER	N1-C2-C3-C4
80	h1	1903	TER	N1-C2-C3-C4
80	h1	1905	TER	C7-C6-N5-C4
80	A	3416	TER	C11-C10-N9-C8
80	A	3411	TER	C10-C11-C12-C13

There are no ring outliers.

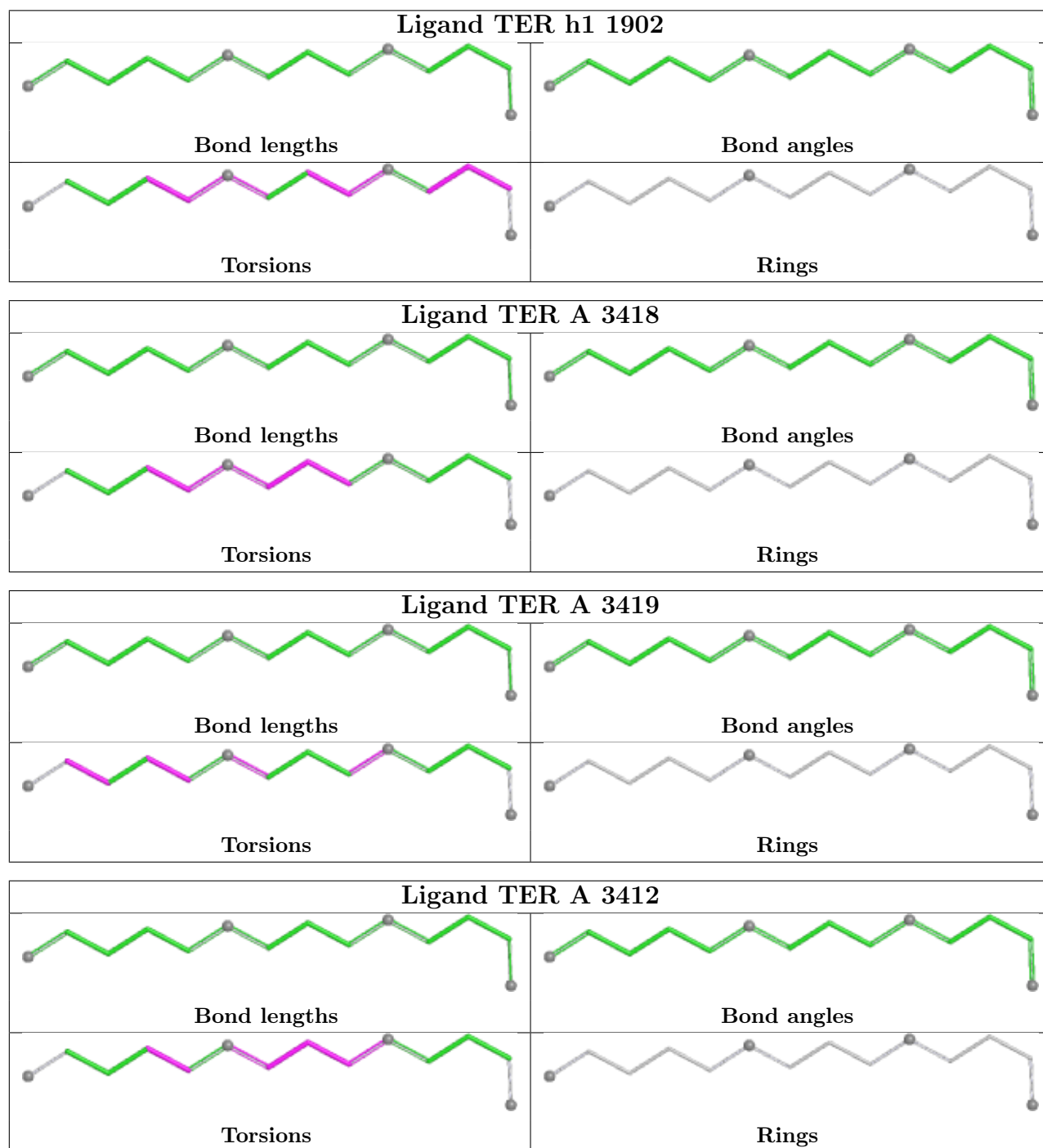
16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	h1	1902	TER	1	0
80	A	3418	TER	1	0
80	h1	1903	TER	1	0
80	A	3404	TER	3	0
80	A	3407	TER	1	0
80	A	3409	TER	1	0
80	A	3415	TER	2	0
80	A	3421	TER	1	0
80	A	3414	TER	3	0
80	h1	1906	TER	1	0
80	A	3411	TER	2	0
80	A	3403	TER	1	0
80	A	3408	TER	1	0
80	A	3416	TER	1	0
80	A	3405	TER	1	0
80	A	3413	TER	1	0

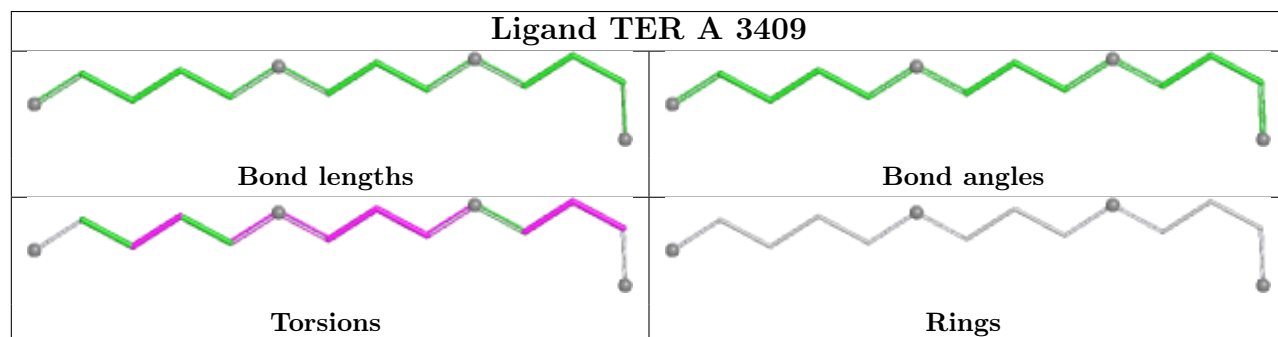
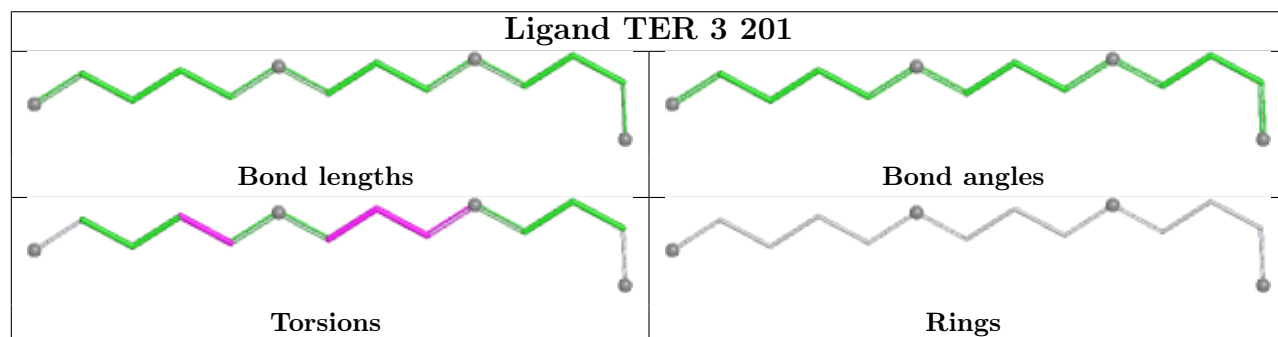
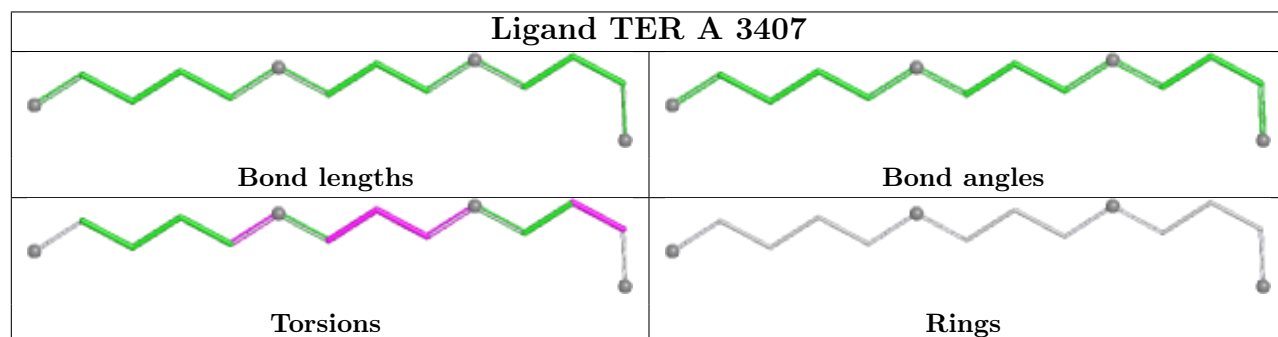
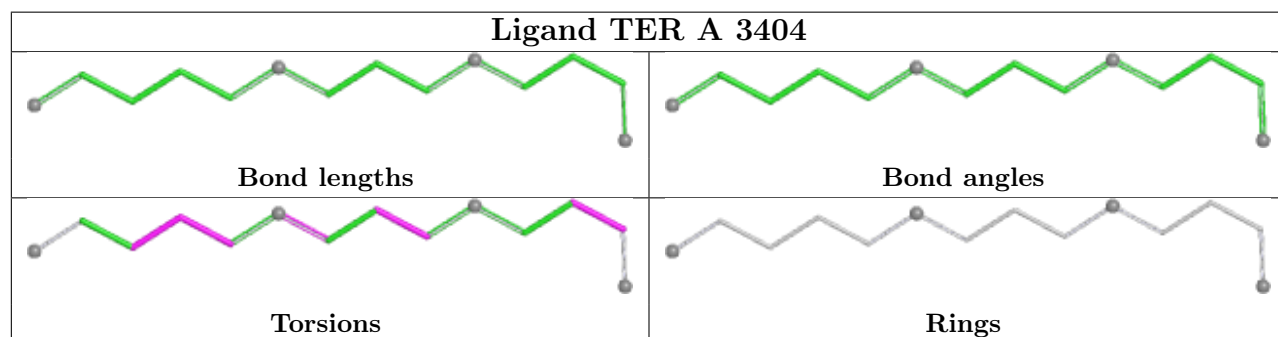
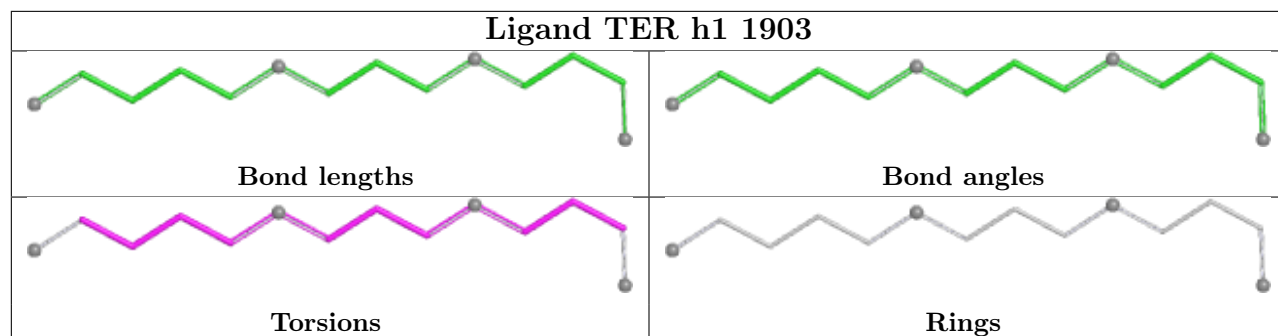
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



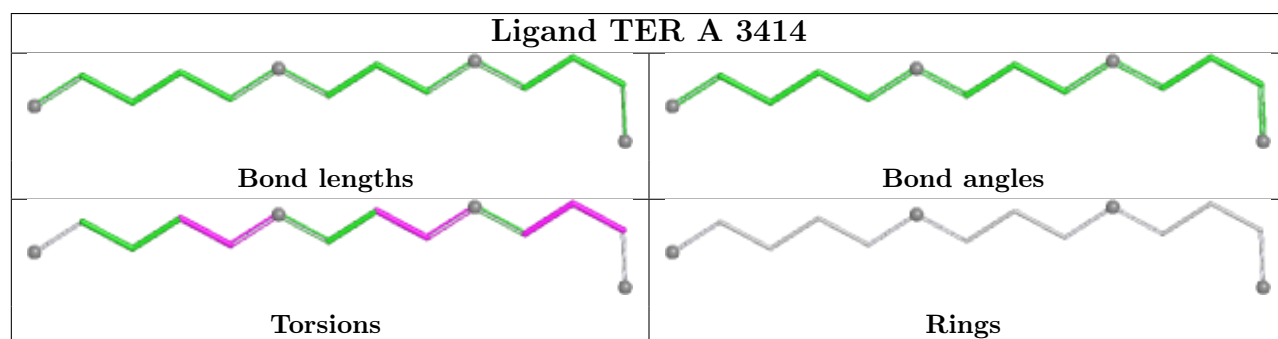
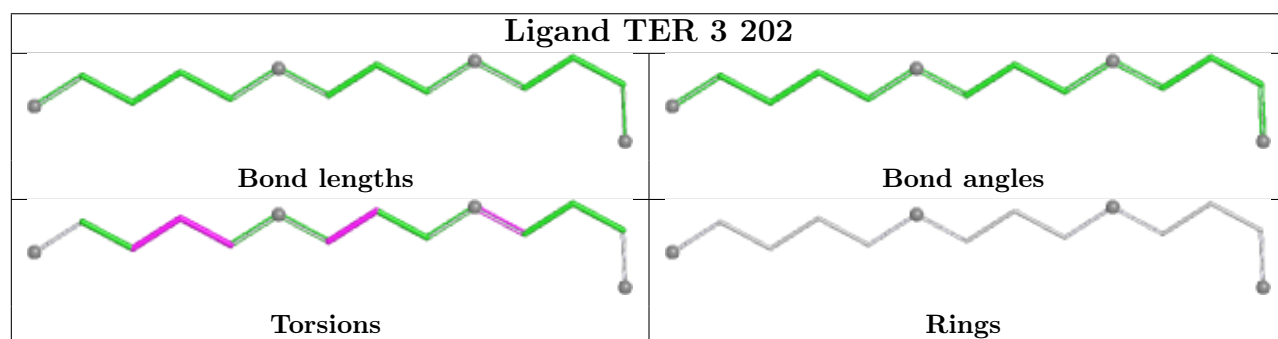
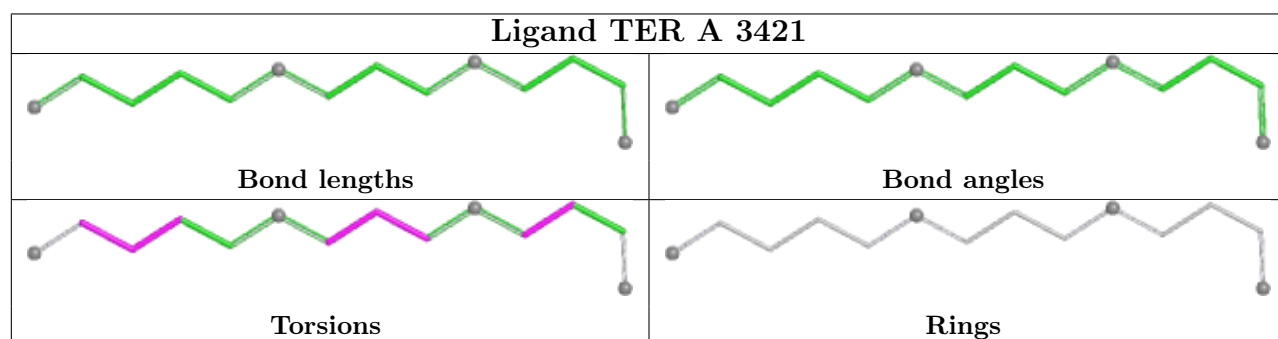
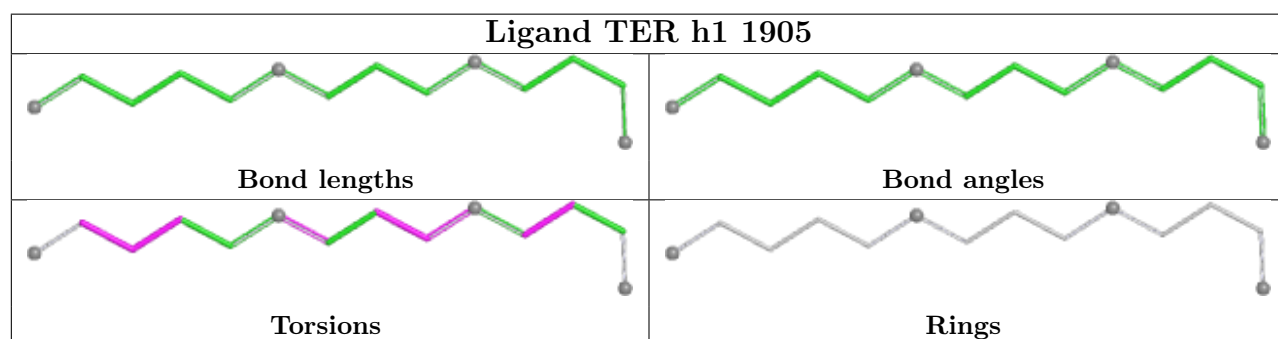
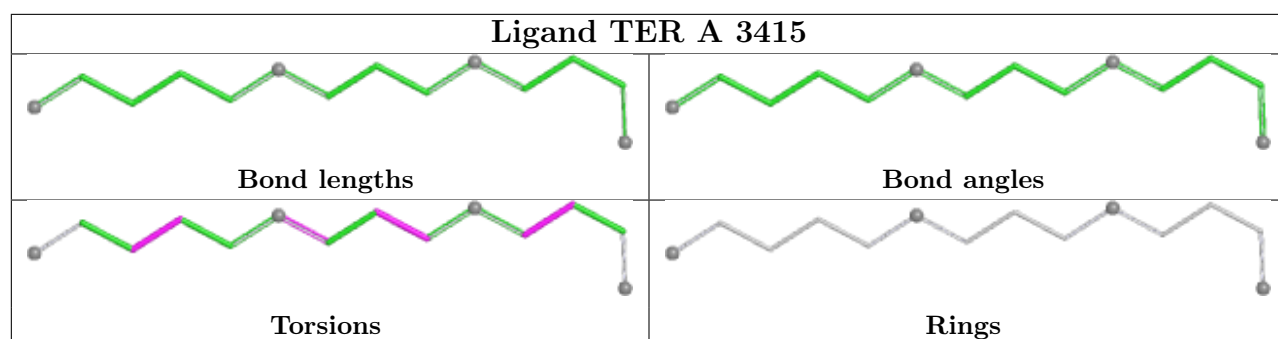
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



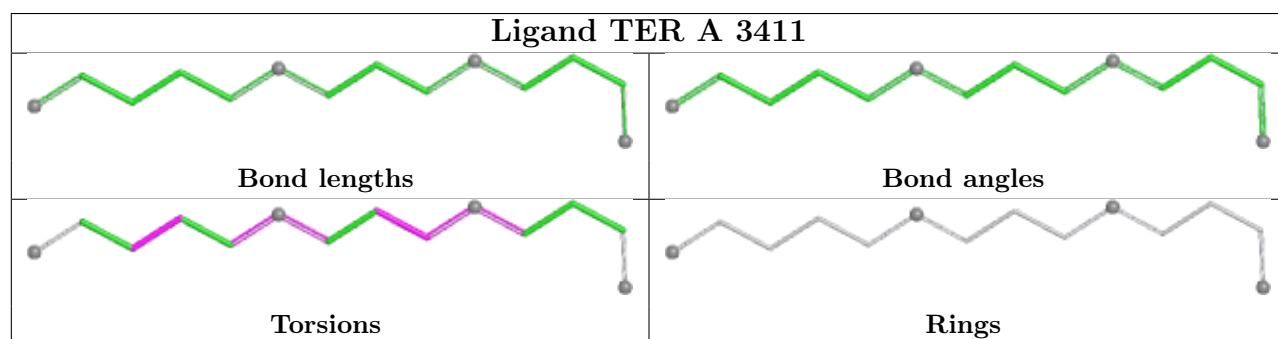
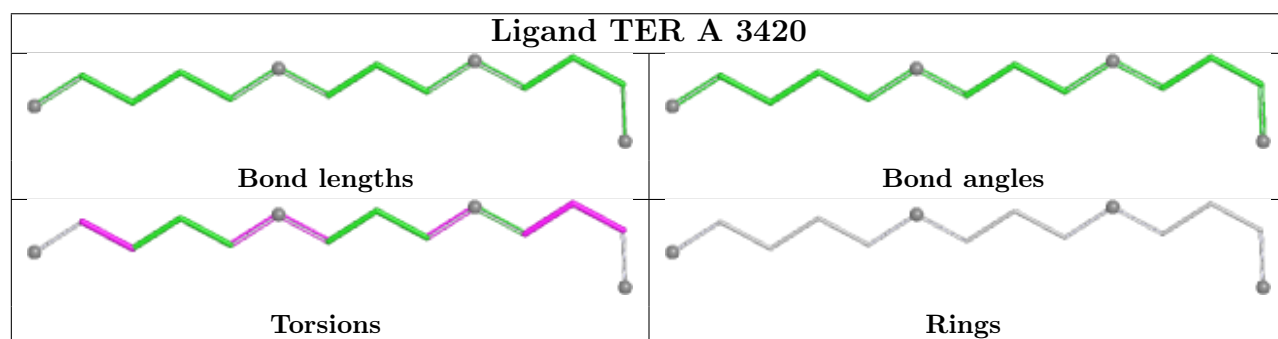
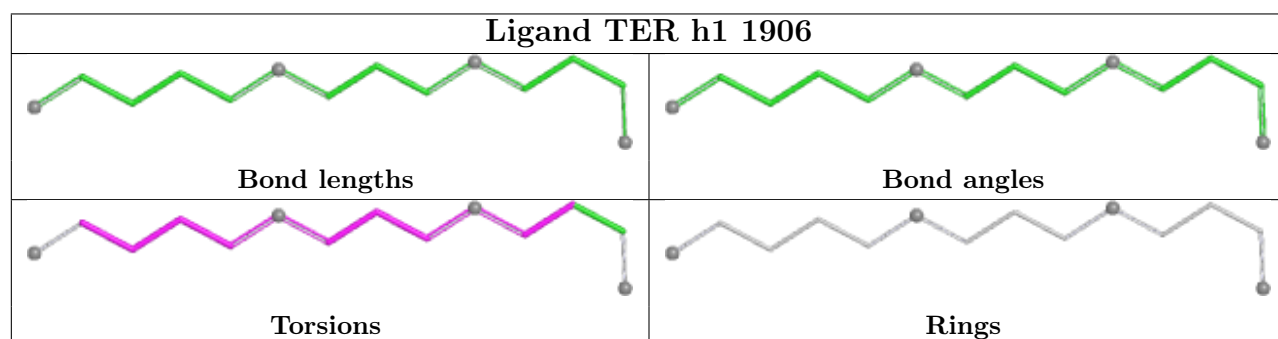
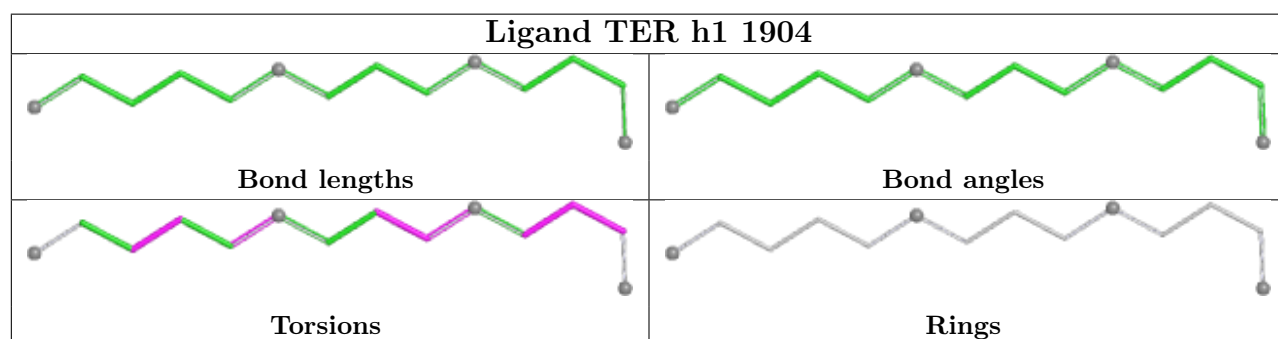
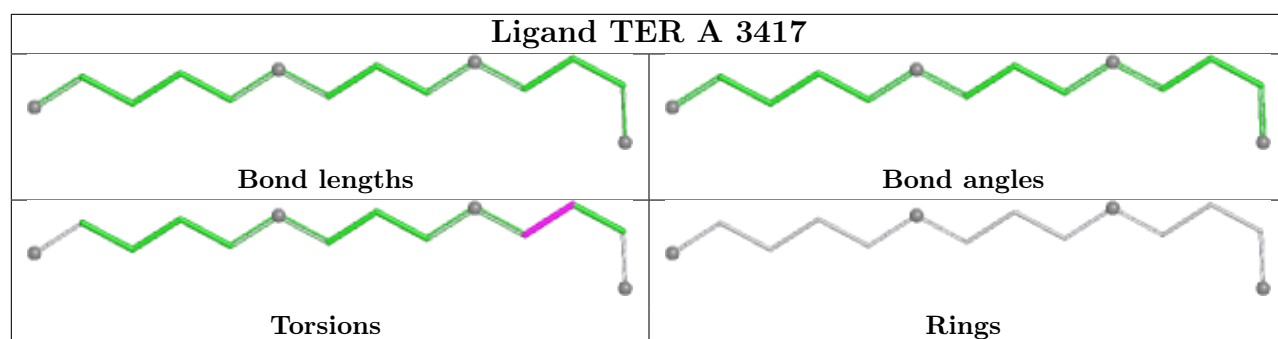




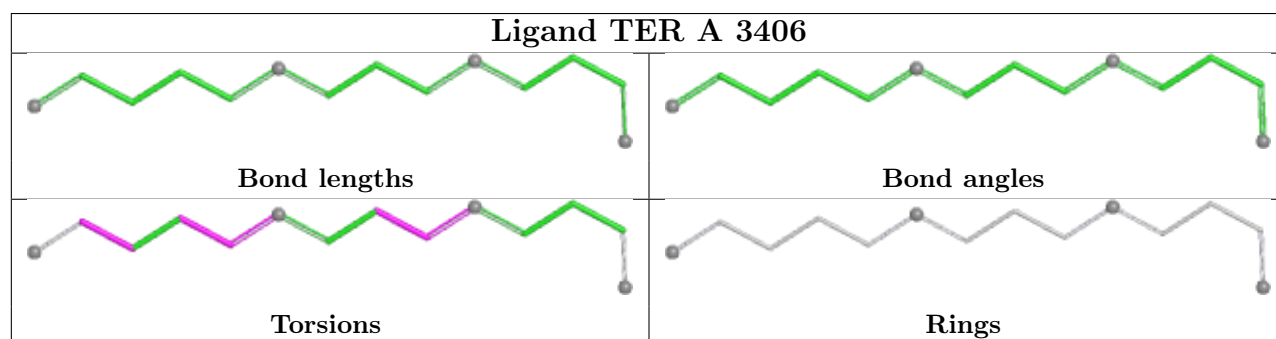
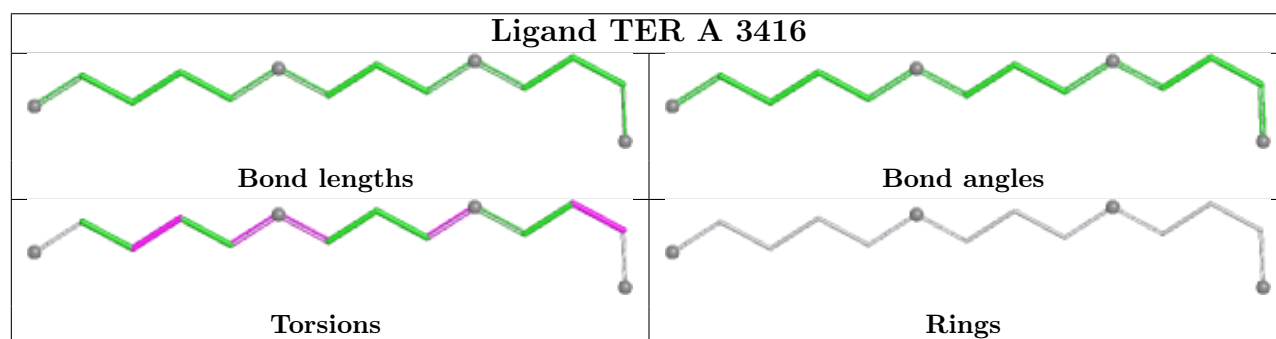
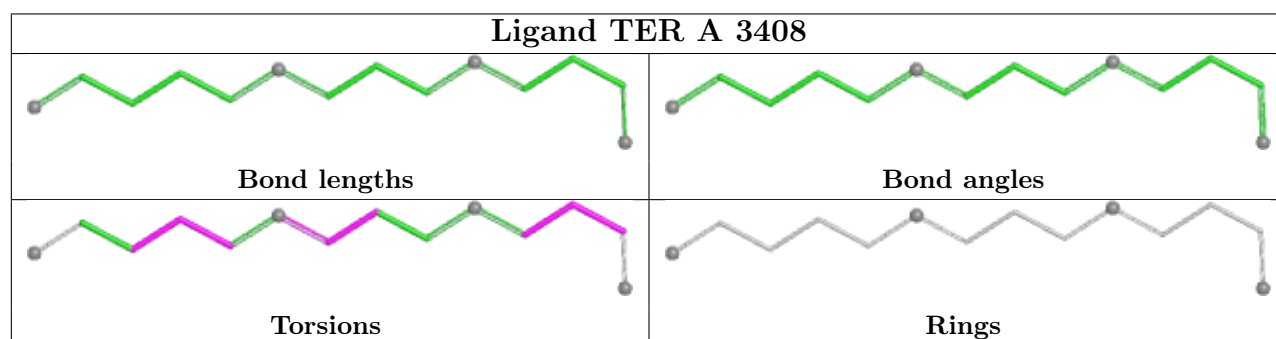
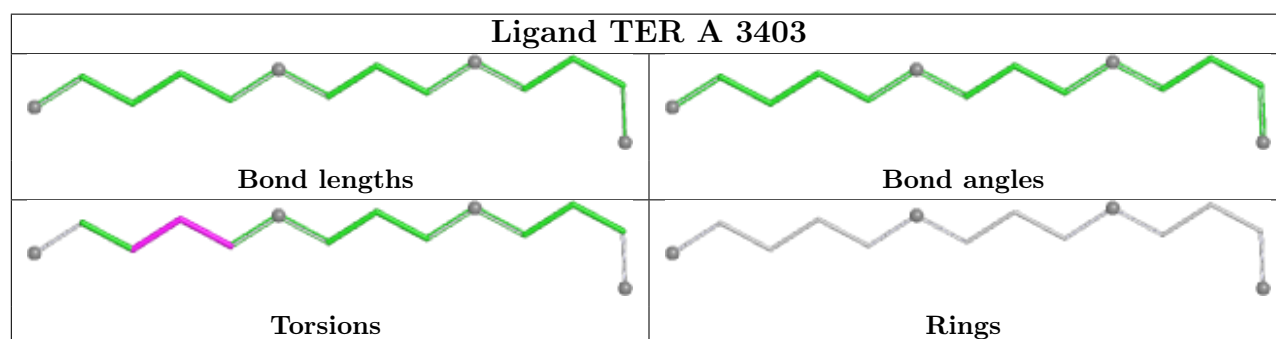
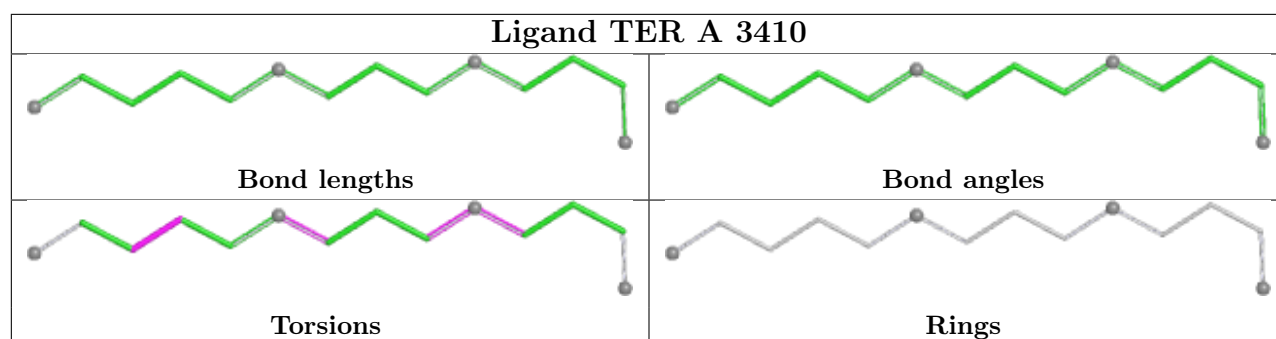




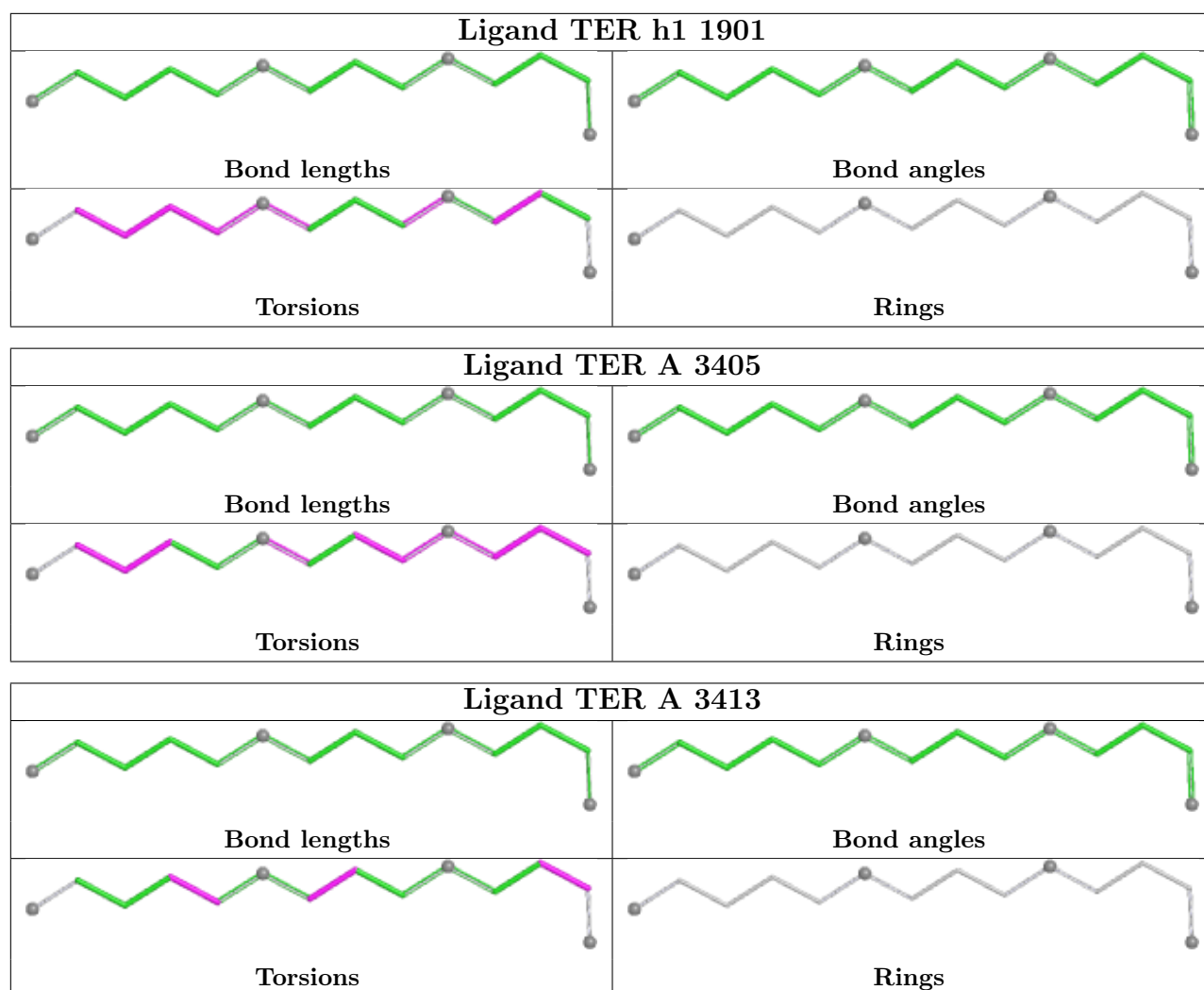












## 5.7 Other polymers [i](#)

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	1
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	4.15
1	Ca	53:ILE	C	54:LYS	N	2.51
1	AY	76:THR	C	77:CYS	N	2.06



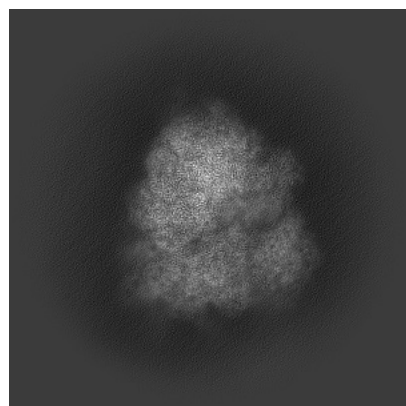
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52095. These allow visual inspection of the internal detail of the map and identification of artifacts.

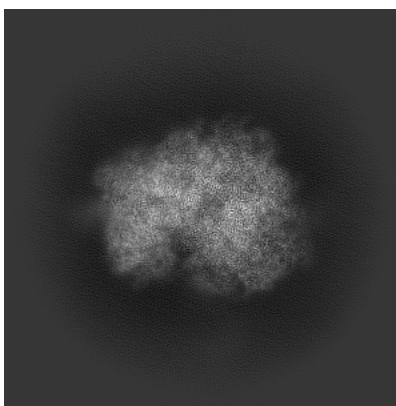
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

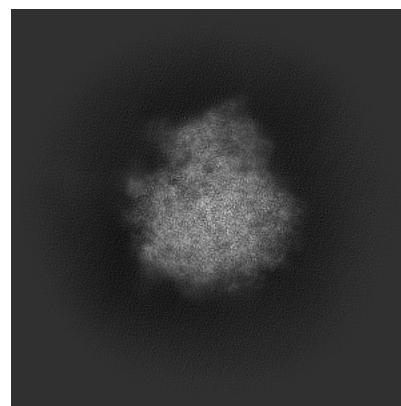
#### 6.1.1 Primary map



X

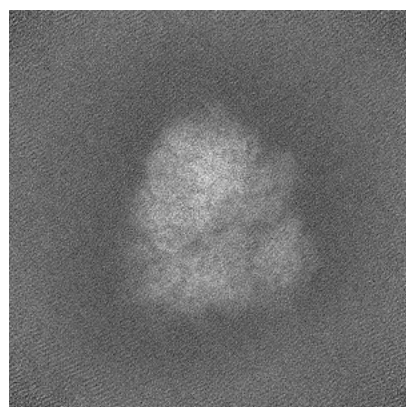


Y

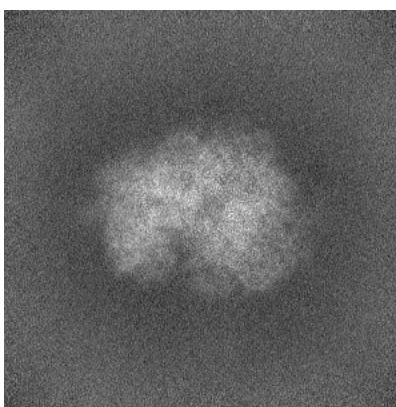


Z

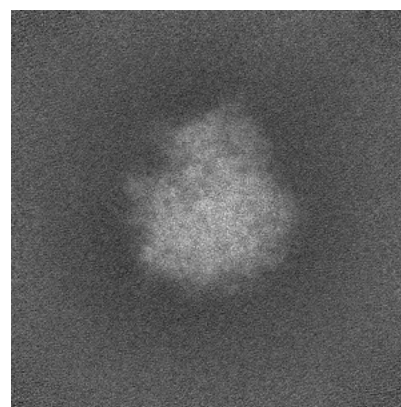
#### 6.1.2 Raw map



X



Y



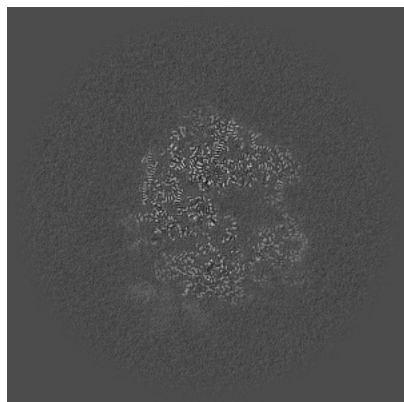
Z

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

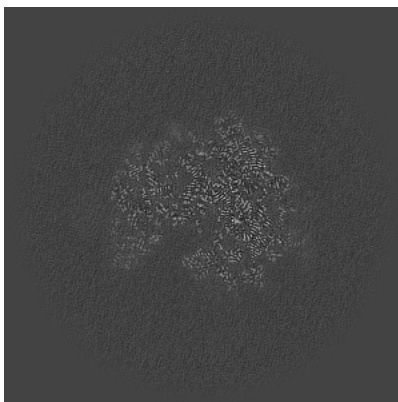


## 6.2 Central slices [i](#)

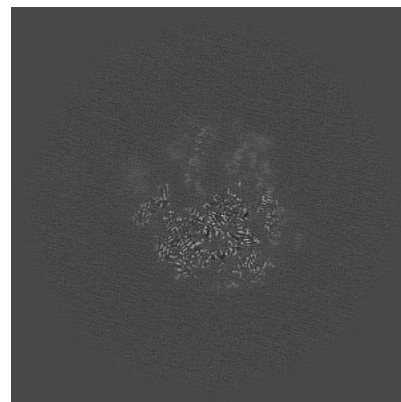
### 6.2.1 Primary map



X Index: 343

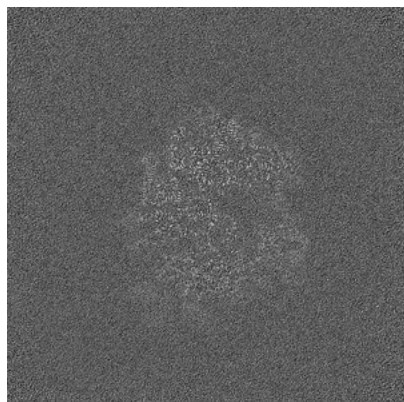


Y Index: 343

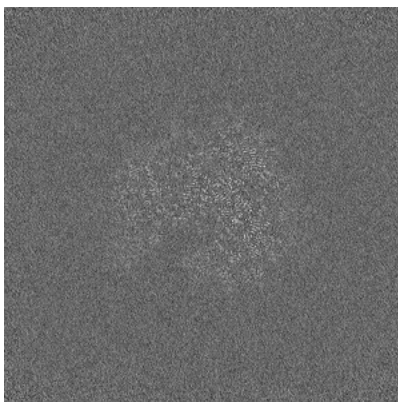


Z Index: 343

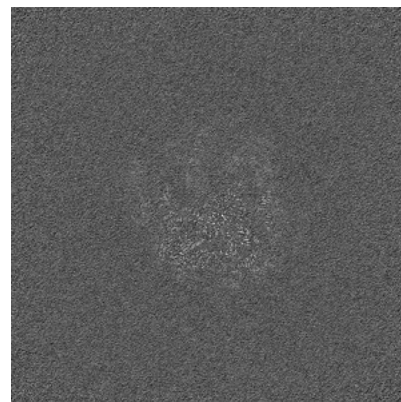
### 6.2.2 Raw map



X Index: 343



Y Index: 343



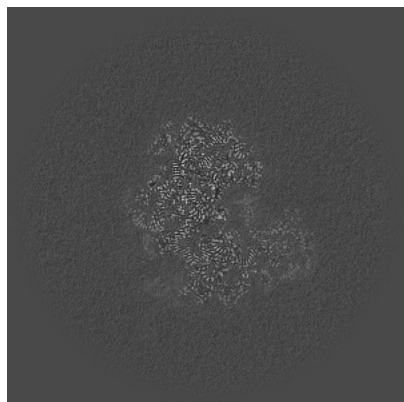
Z Index: 343

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

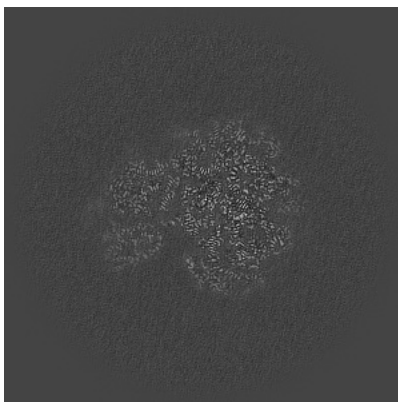


## 6.3 Largest variance slices [i](#)

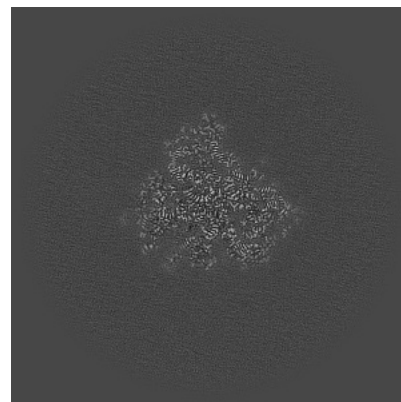
### 6.3.1 Primary map



X Index: 371

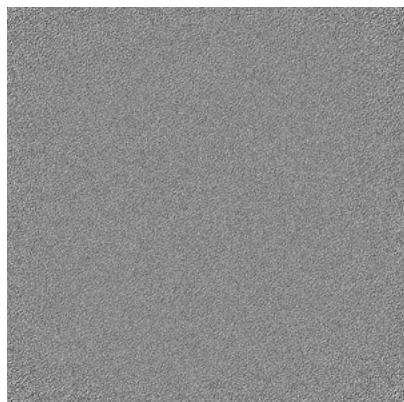


Y Index: 331

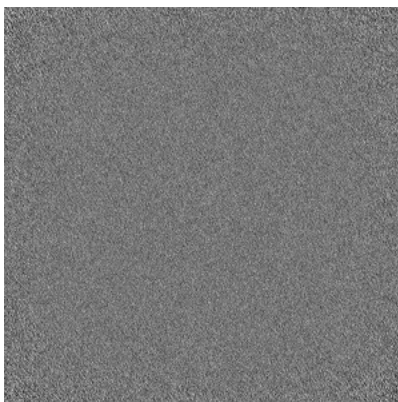


Z Index: 409

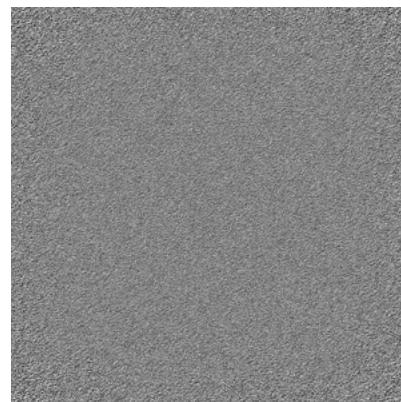
### 6.3.2 Raw map



X Index: 0



Y Index: 0



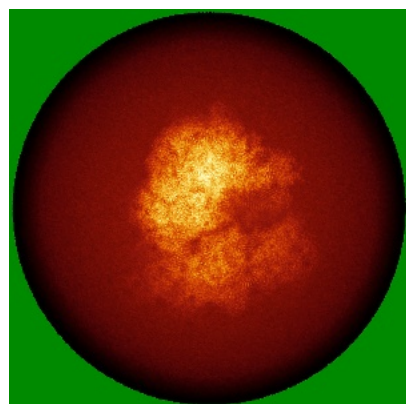
Z Index: 0

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

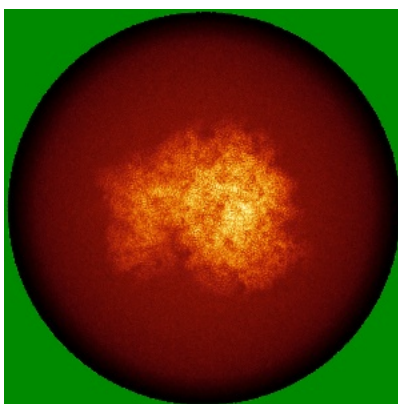


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

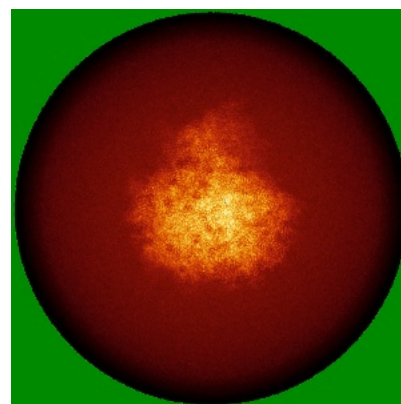
### 6.4.1 Primary map



X

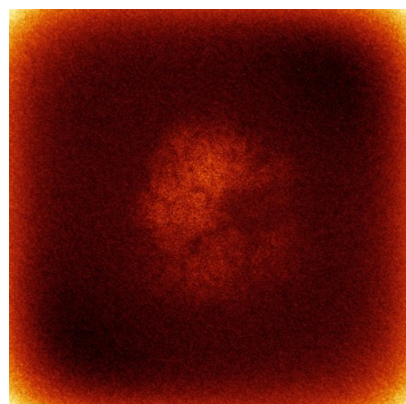


Y

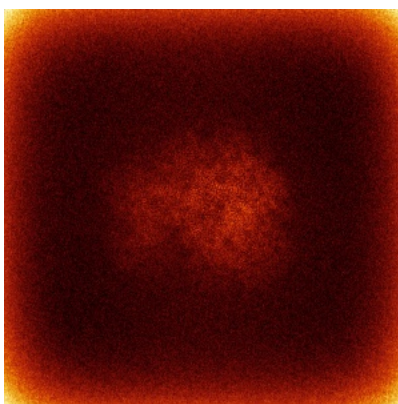


Z

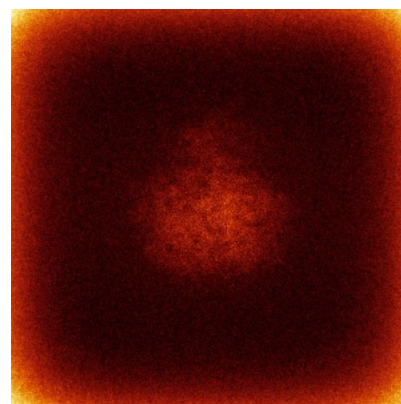
### 6.4.2 Raw map



X



Y



Z

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



## 6.5 Orthogonal surface views [i](#)

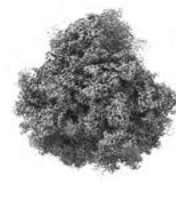
### 6.5.1 Primary map



X



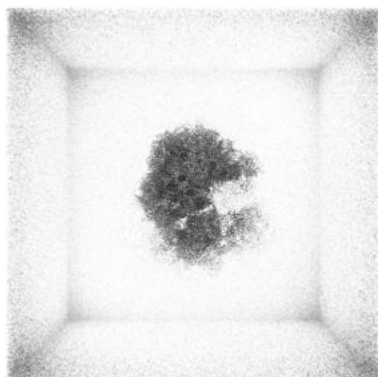
Y



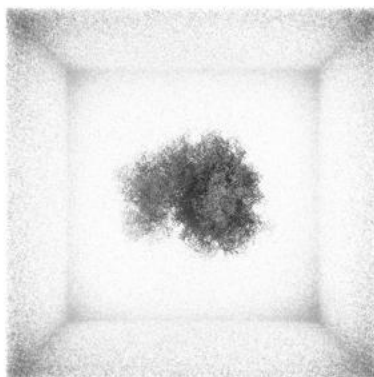
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

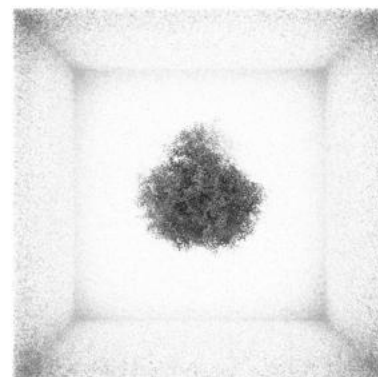
### 6.5.2 Raw map



X



Y



Z

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



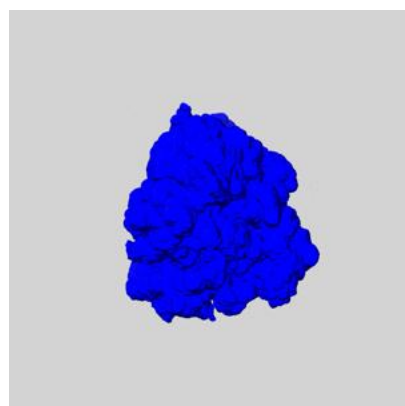
## 6.6 Mask visualisation [i](#)

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

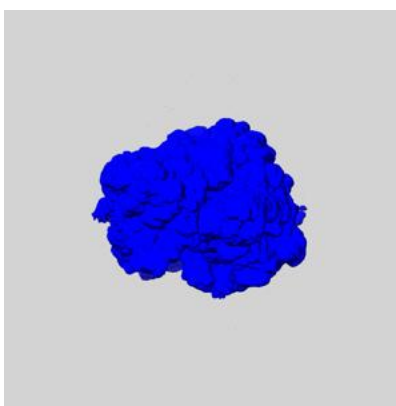
A mask typically either:

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

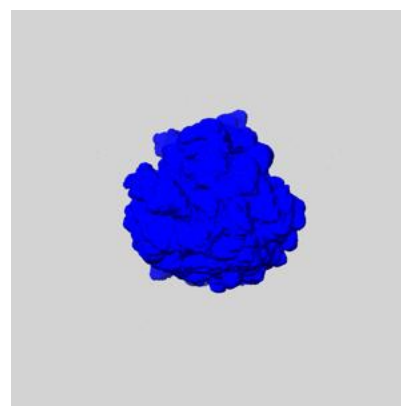
### 6.6.1 emd\_52095\_msk\_1.map [i](#)



X



Y



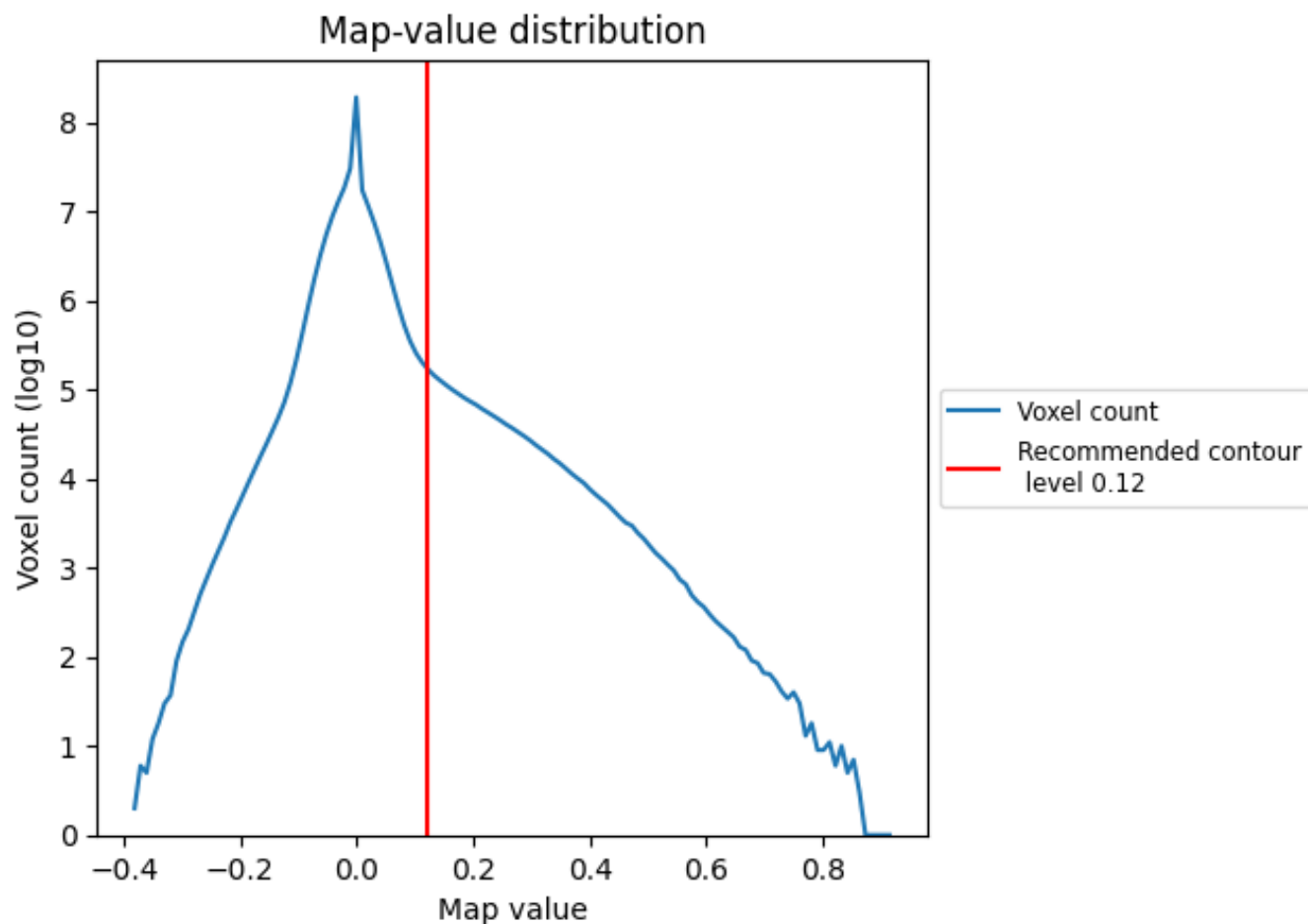
Z



## 7 Map analysis [i](#)

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

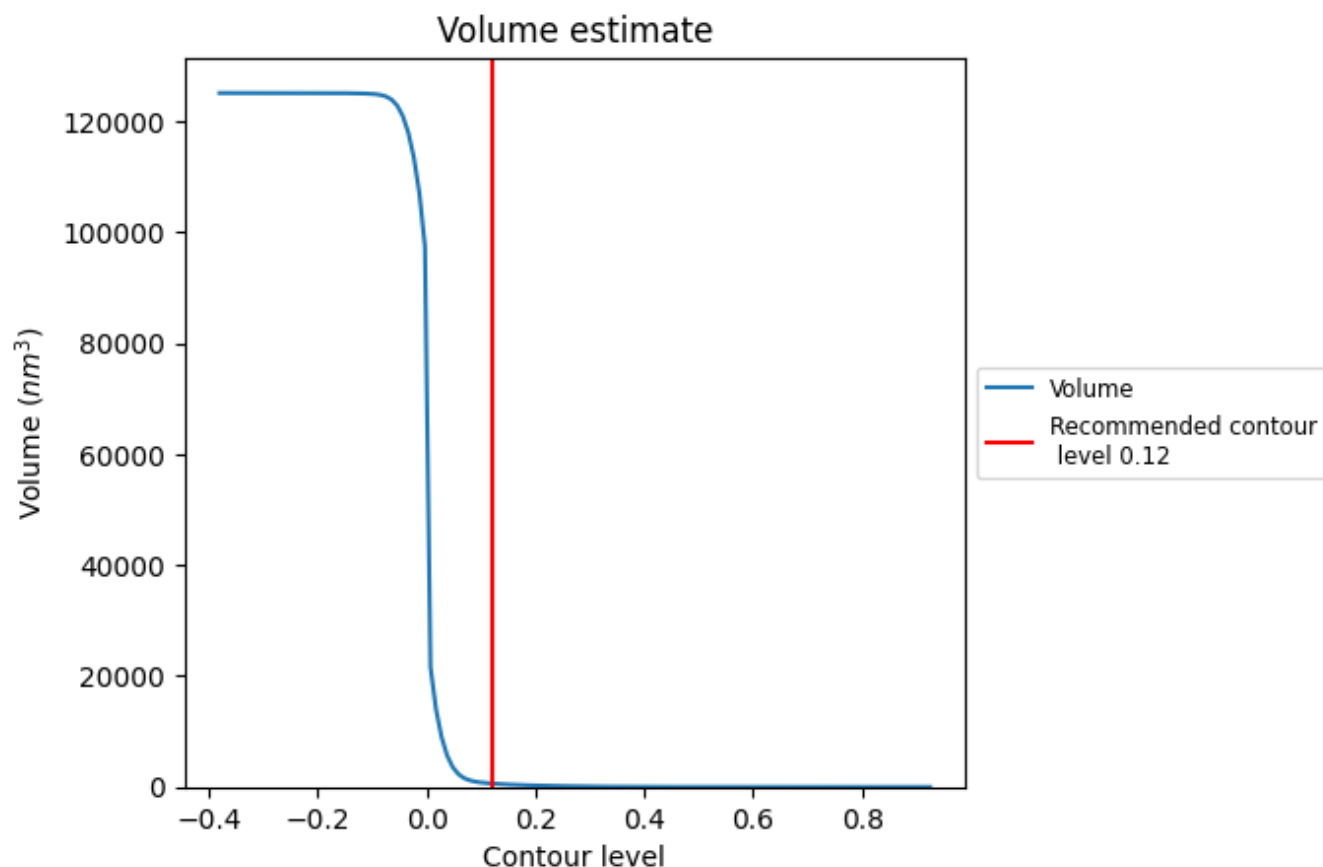
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

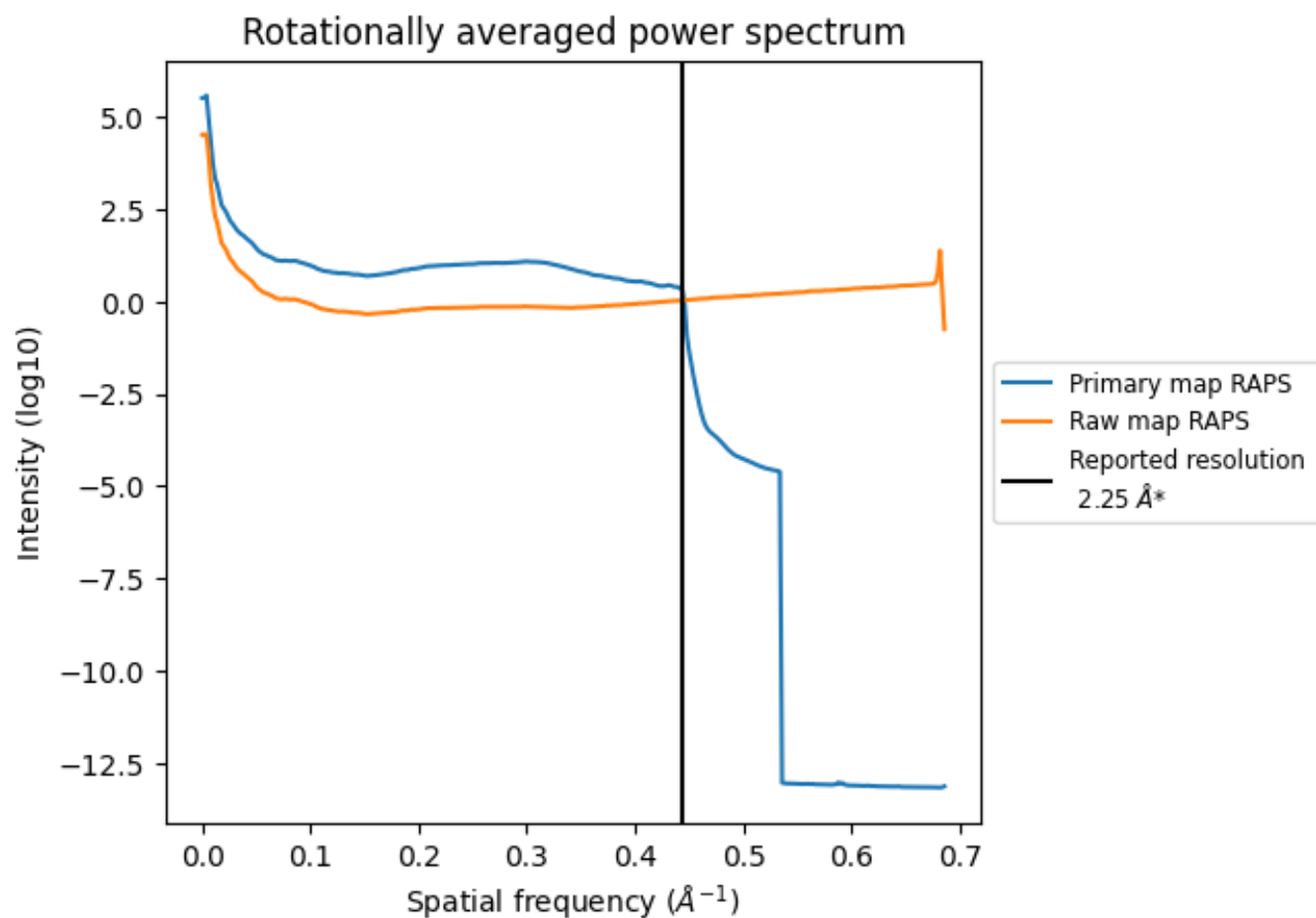


The volume at the recommended contour level is 618  $\text{nm}^3$ ; this corresponds to an approximate mass of 558 kDa.

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 ⓘ



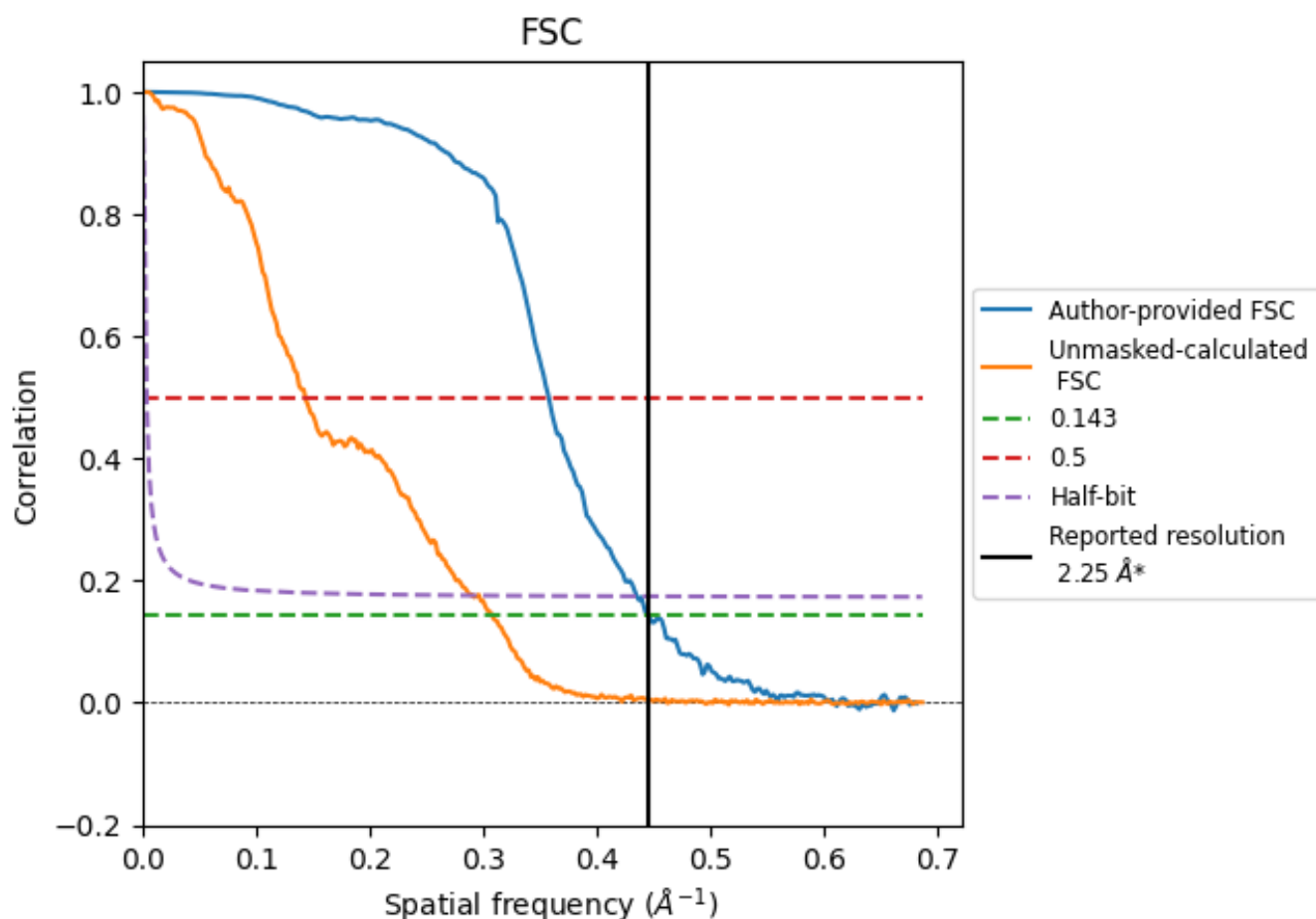
\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>



## 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 0.444  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.80	2.30
Unmasked-calculated*	3.25	6.97	3.44

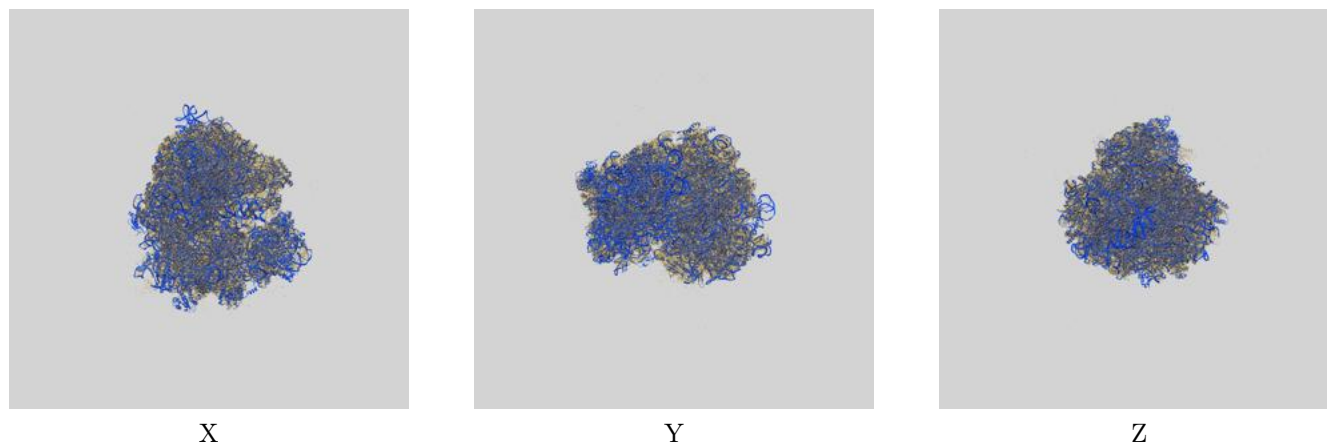
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.25 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52095 and PDB model 9HES. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

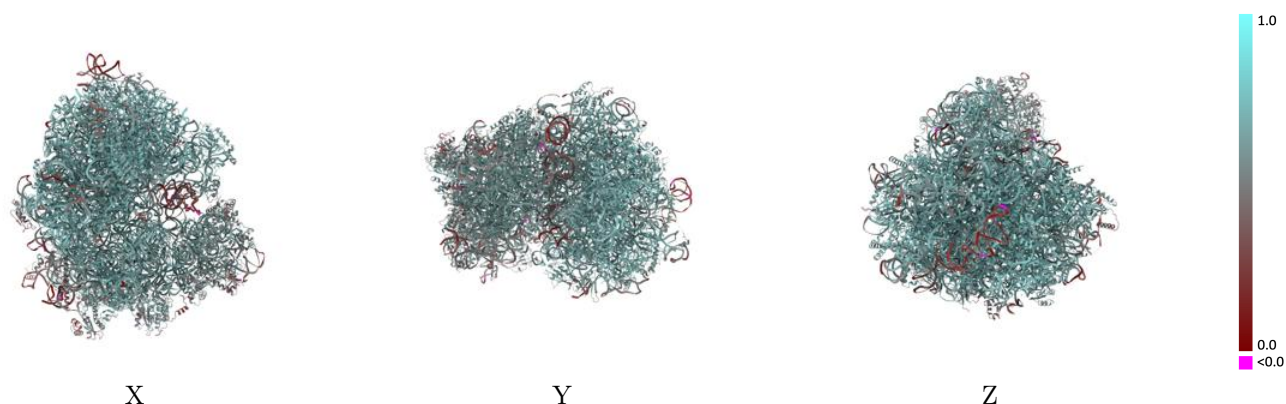
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

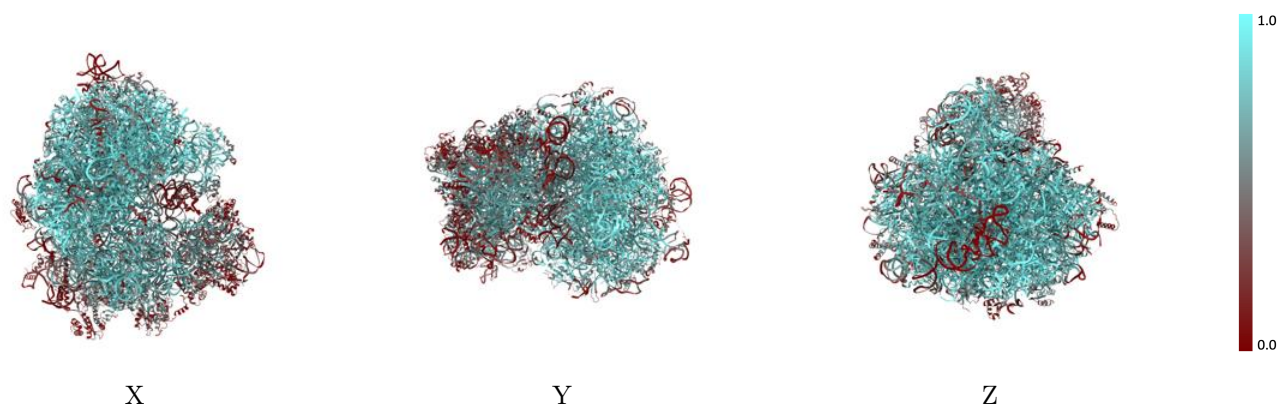


## 9.2 Q-score mapped to coordinate model [i](#)



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.

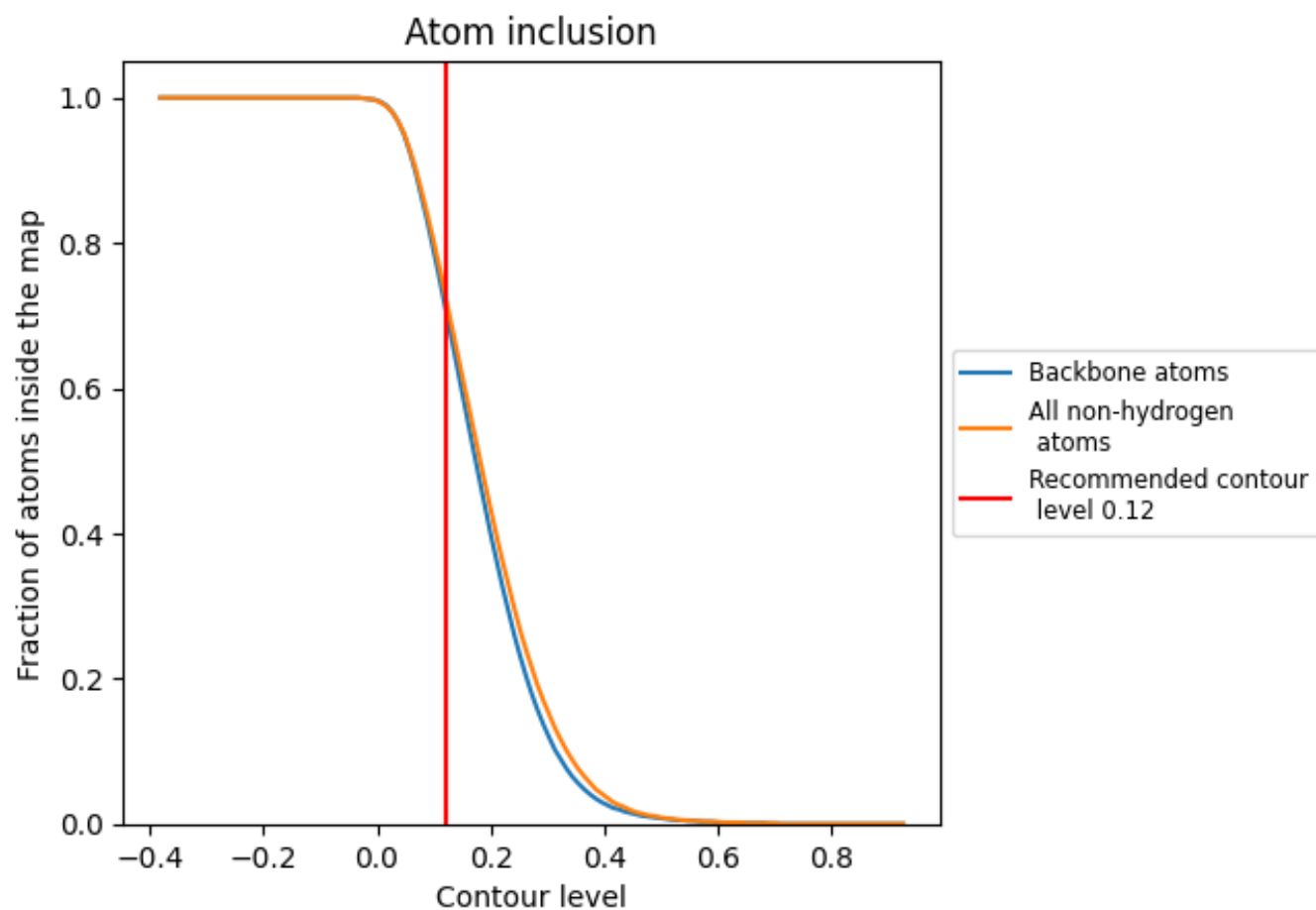
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.12).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 71% of all backbone atoms, 73% 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 (0.12) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.7290	 0.6250
2	 0.3340	 0.4510
3	 0.8350	 0.6330
A	 0.8500	 0.6480
AA	 0.2930	 0.5160
AB	 0.4950	 0.5760
AC	 0.6940	 0.6380
AD	 0.3600	 0.5630
AE	 0.8170	 0.6780
AF	 0.3540	 0.5380
AG	 0.7850	 0.6660
AH	 0.7280	 0.6510
AI	 0.1750	 0.4560
AJ	 0.9190	 0.7040
AK	 0.7250	 0.6250
AL	 0.8790	 0.6910
AM	 0.7980	 0.6770
AN	 0.0650	 0.4300
AO	 0.8380	 0.6890
AP	 0.7580	 0.6520
AQ	 0.2470	 0.5760
AR	 0.8830	 0.6900
AT	 0.7800	 0.6650
AU	 0.7370	 0.6440
AV	 0.8840	 0.7000
AW	 0.9090	 0.7070
AX	 0.7210	 0.6510
AY	 0.9240	 0.7050
AZ	 0.5460	 0.6180
Aa	 0.4180	 0.5580
B1	 0.6880	 0.5910
BA	 0.9220	 0.7020
BB	 0.1920	 0.4210
BC	 0.7610	 0.6650
BD	 0.8920	 0.7030



*Continued on next page...*











*Continued from previous page...*

Chain	Atom inclusion	Q-score
BE	 0.8470	 0.6930
BF	 0.5910	 0.6150
BG	 0.6300	 0.6160
BH	 0.8450	 0.6870
BI	 0.8680	 0.6980
BJ	 0.7440	 0.6620
BK	 0.7080	 0.6420
BL	 0.3920	 0.5580
BM	 0.8790	 0.6970
BN	 0.7580	 0.6660
BO	 0.8510	 0.6860
BP	 0.7320	 0.6600
BQ	 0.9460	 0.7160
BR	 0.8280	 0.6830
BS	 0.8850	 0.7020
BT	 0.7990	 0.6750
BU	 0.5850	 0.6110
BV	 0.5780	 0.6130
BW	 0.5930	 0.6270
Ba	 0.2410	 0.4910
C3	 0.9260	 0.6710
Ca	 0.5230	 0.5910
Da	 0.6300	 0.6170
Ea	 0.9660	 0.7200
Fa	 0.8550	 0.6810
Ga	 0.8230	 0.6710
Ha	 0.8980	 0.6980
Ia	 0.6960	 0.6430
Ja	 0.4870	 0.5860
Ka	 0.3310	 0.5510
L3	 0.0260	 0.1860
La	 0.1850	 0.4990
Ma	 0.6900	 0.6460
Na	 0.4520	 0.5550
Oa	 0.3580	 0.5730
Pa	 0.4070	 0.5480
Ra	 0.2280	 0.4790
Ta	 0.2630	 0.4860
Ua	 0.6840	 0.6440
Va	 0.7290	 0.6630
W2	 0.3920	 0.4590
Wa	 0.3940	 0.5550

*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
Xa	 0.6100	 0.6150
Ya	 0.2720	 0.5090
Za	 0.4640	 0.5880
h1	 0.7070	 0.5920