



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 10:00 PM EDT

PDB ID : 9PN5 / pdb_00009pn5
EMDB ID : EMD-71745
Title : Composite map of hypomethylated 80S ribosome treated with hygromycin B
Authors : Zhao, Y.; Li, H.
Deposited on : 2025-07-19
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

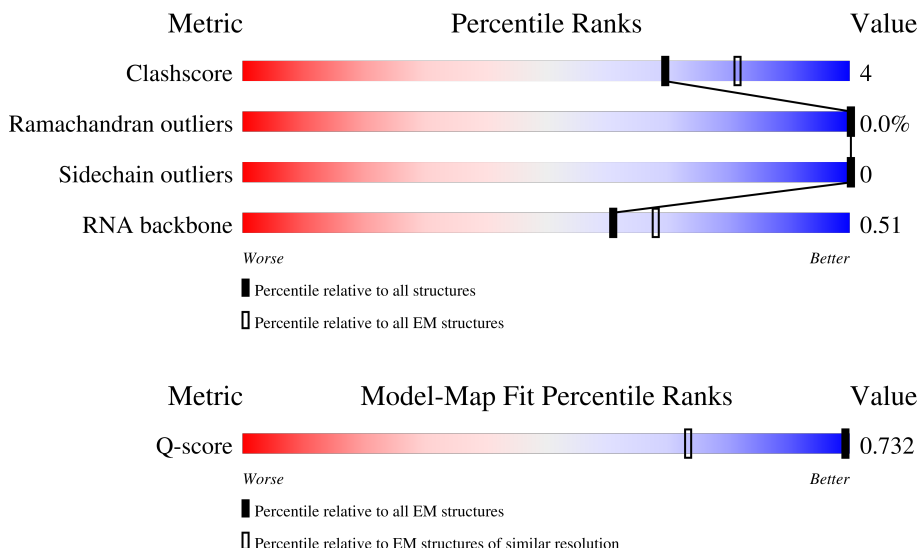
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.75 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	657 (1.25 - 2.25)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	252	
2	BB	255	
3	BC	254	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	

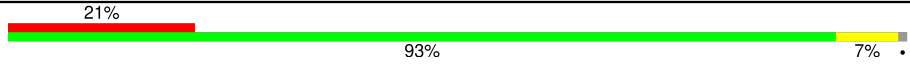







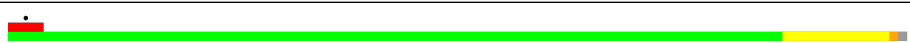

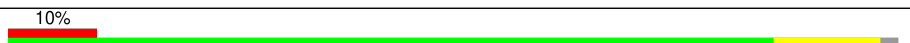


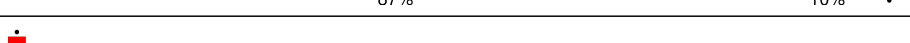
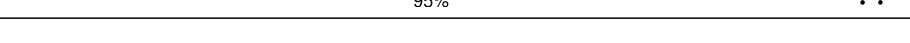
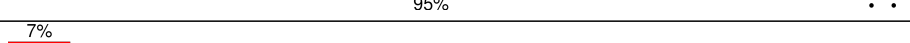
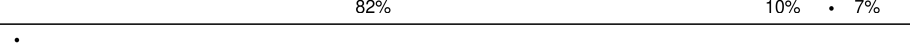
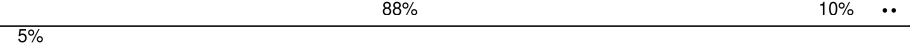
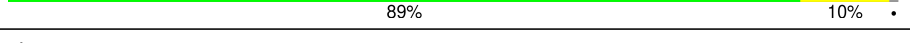
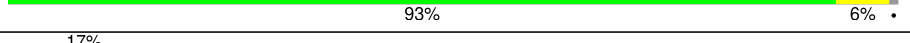




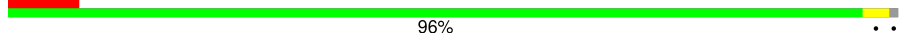
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3184	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	G7M	B5	1575	X	-	-	-

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 200291 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called Small ribosomal subunit protein eS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 5 is a protein called Small ribosomal subunit protein eS6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 6 is a protein called Small ribosomal subunit protein eS7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BH	184	Total	C	N	O		0	0
			1481	951	265	265			

- Molecule 7 is a protein called Small ribosomal subunit protein eS8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS12A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called Small ribosomal subunit protein eS24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called Small ribosomal subunit protein eS27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 18 is a protein called Small ribosomal subunit protein eS30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called Small ribosomal subunit protein uS9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 24 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	123	Total	C	N	O	S	0	0
			982	616	186	178	2		

- Molecule 25 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called Small ribosomal subunit protein eS19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	71	Total	C	N	O	0	0
			574	366	108	100		

- Molecule 29 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1757	Total	C	N	O	P	1	0
			37463	16754	6635	12317	1757		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 37 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3161	Total	C	N	O	P	0	0
			67606	30202	12171	22072	3161		

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called Large ribosomal subunit protein eL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	167	Total	C	N	O	S	0	0
			1303	840	234	228	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	120	LYS	ASN	conflict	UNP Q02326

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	217	Total	C	N	O	S	0	0
			1759	1114	333	305	7		

- Molecule 47 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 50 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 51 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 55 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	-5	MET	-	initiating methionine	UNP P0CX23
AS	-4	PRO	-	expression tag	UNP P0CX23
AS	-3	GLN	-	expression tag	UNP P0CX23
AS	-2	LYS	-	expression tag	UNP P0CX23
AS	-1	TRP	-	expression tag	UNP P0CX23
AS	0	LYS	-	expression tag	UNP P0CX23

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AU	100	Total	C	N	O		0	0
			796	516	131	149			

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 60 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AY	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 64 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ak	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-ribosomal protein eL40A fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called Small ribosomal subunit protein eS32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called Large ribosomal subunit protein eL42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	B5	35	Total	Mg	0
			35	35	
79	A1	134	Total	Mg	0
			134	134	
79	A3	1	Total	Mg	0
			1	1	
79	A4	1	Total	Mg	0
			1	1	
79	AP	1	Total	Mg	0
			1	1	
79	AV	1	Total	Mg	0
			1	1	
79	Aj	1	Total	Mg	0
			1	1	

- Molecule 80 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
80	B5	8	Total 8	K 8	0
80	A1	17	Total 17	K 17	0
80	Ab	1	Total 1	K 1	0
80	Ae	1	Total 1	K 1	0

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Ao	1	Total 1	Zn 1	0

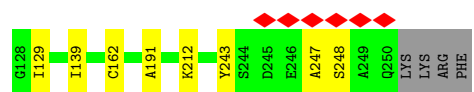
- Molecule 82 is water.

Mol	Chain	Residues	Atoms		AltConf
82	BB	1	Total 1	O 1	0
82	BE	1	Total 1	O 1	0
82	BL	1	Total 1	O 1	0
82	BO	1	Total 1	O 1	0
82	BX	2	Total 2	O 2	0
82	Ba	3	Total 3	O 3	0
82	BD	1	Total 1	O 1	0
82	BT	2	Total 2	O 2	0
82	Bd	1	Total 1	O 1	0
82	B5	224	Total 224	O 224	0
82	AA	19	Total 19	O 19	0
82	AB	3	Total 3	O 3	0
82	AC	8	Total 8	O 8	0

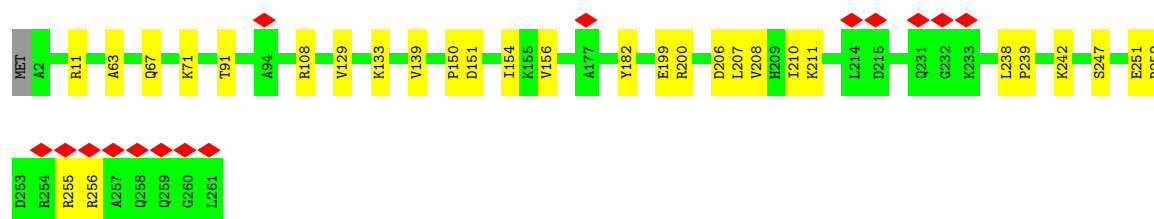
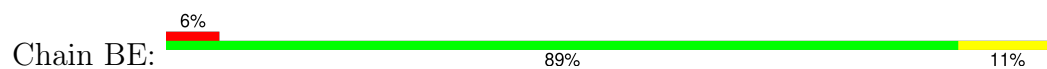
Continued on next page...

Continued from previous page...

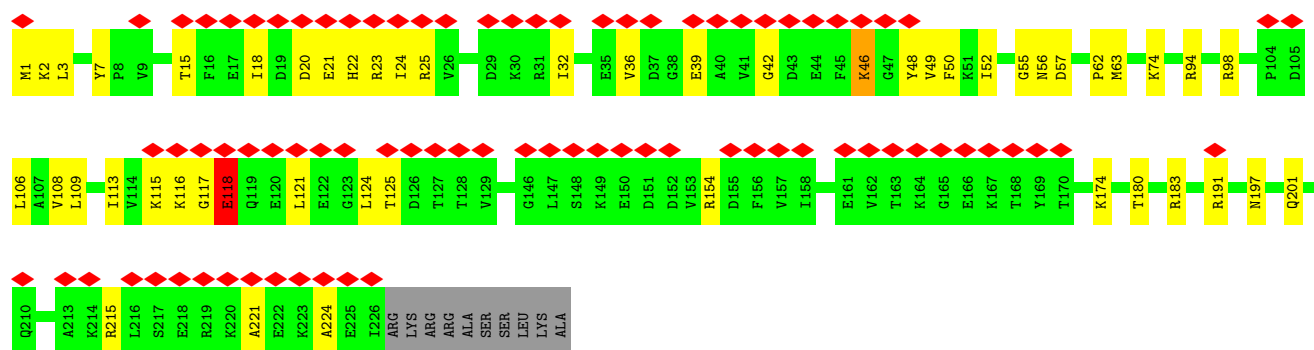
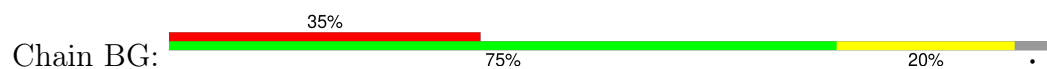
Mol	Chain	Residues	Atoms		AltConf
82	A1	941	Total 941	O 941	0
82	A3	5	Total 5	O 5	0
82	A4	9	Total 9	O 9	0
82	AF	1	Total 1	O 1	0
82	AN	7	Total 7	O 7	0
82	AO	3	Total 3	O 3	0
82	AP	3	Total 3	O 3	0
82	AR	2	Total 2	O 2	0
82	AT	1	Total 1	O 1	0
82	AV	2	Total 2	O 2	0
82	AX	2	Total 2	O 2	0
82	Aa	10	Total 10	O 10	0
82	Ab	1	Total 1	O 1	0
82	Ae	6	Total 6	O 6	0
82	Aj	6	Total 6	O 6	0
82	Ao	2	Total 2	O 2	0



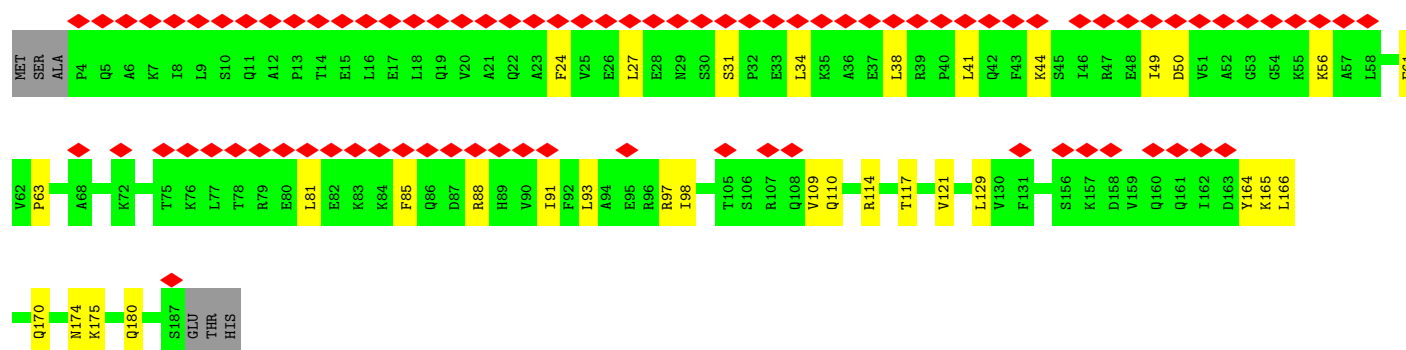
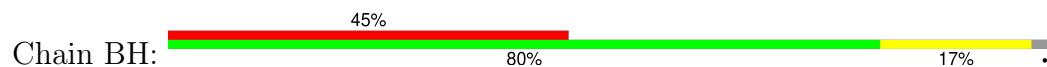
- Molecule 4: Small ribosomal subunit protein eS4A



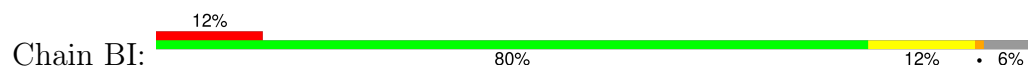
- Molecule 5: Small ribosomal subunit protein eS6A

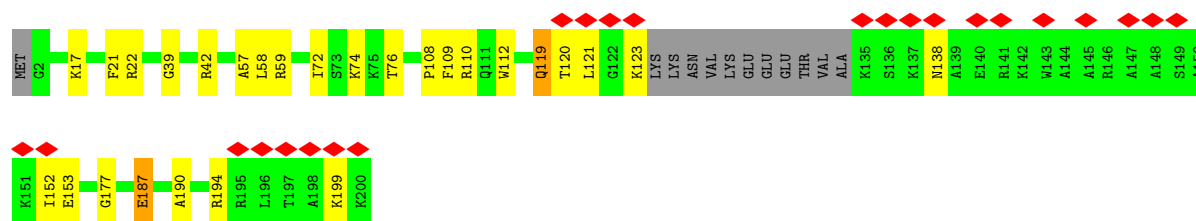


- Molecule 6: Small ribosomal subunit protein eS7A

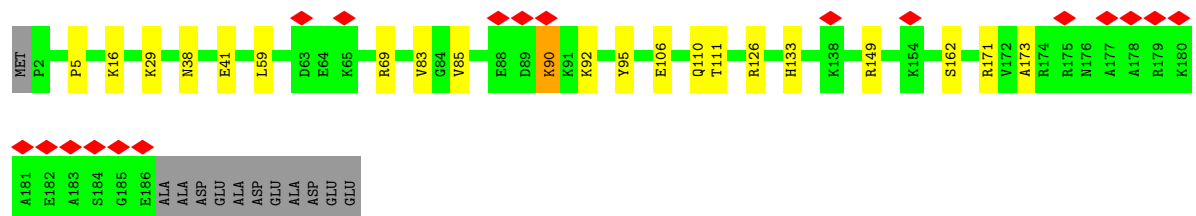
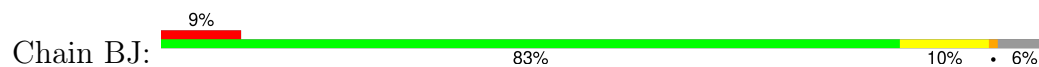


- Molecule 7: Small ribosomal subunit protein eS8A

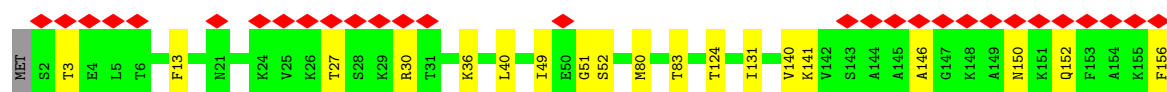
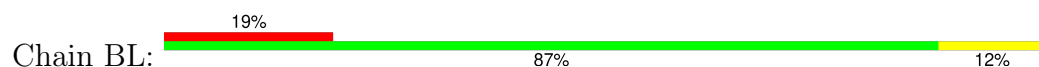




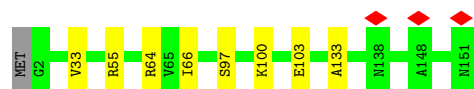
- Molecule 8: Small ribosomal subunit protein uS4A



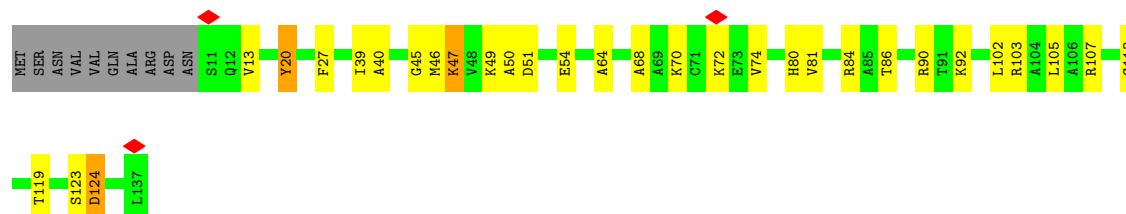
- Molecule 9: Small ribosomal subunit protein uS17A



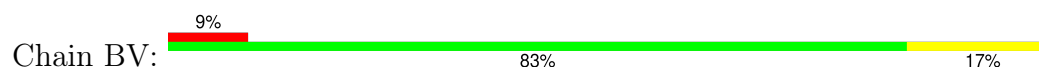
- Molecule 10: Small ribosomal subunit protein uS15

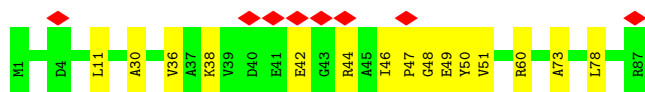


- Molecule 11: Small ribosomal subunit protein uS11A



- Molecule 12: Small ribosomal subunit protein eS21A





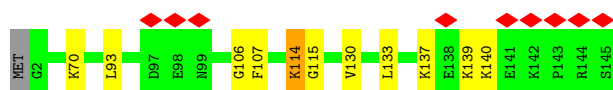
- Molecule 13: Small ribosomal subunit protein uS8A

Chain BW: 93% 6%



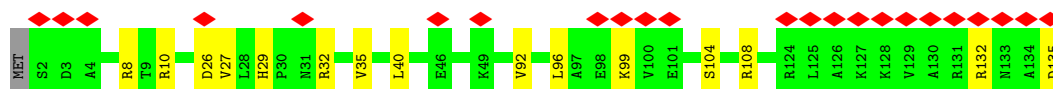
- Molecule 14: Small ribosomal subunit protein uS12A

Chain BX: 92% 7% ..



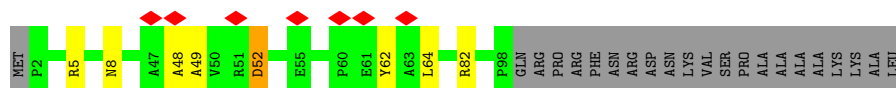
- Molecule 15: Small ribosomal subunit protein eS24A

Chain BY: 88% 11% ..



- Molecule 16: Small ribosomal subunit protein eS26B

Chain Ba: 75% 6% 18%



- Molecule 17: Small ribosomal subunit protein eS27A

Chain Bb: 78% 16% 5%

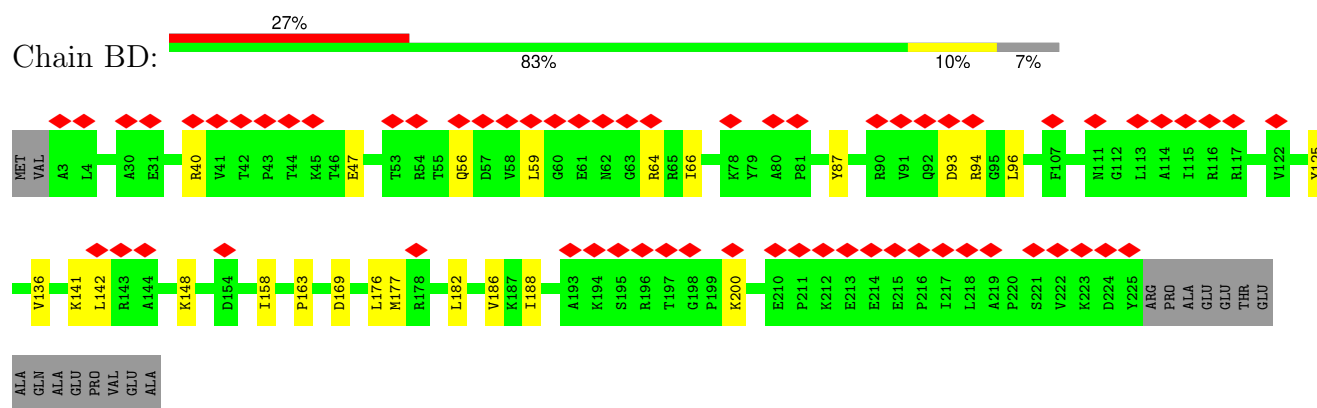


- Molecule 18: Small ribosomal subunit protein eS30A

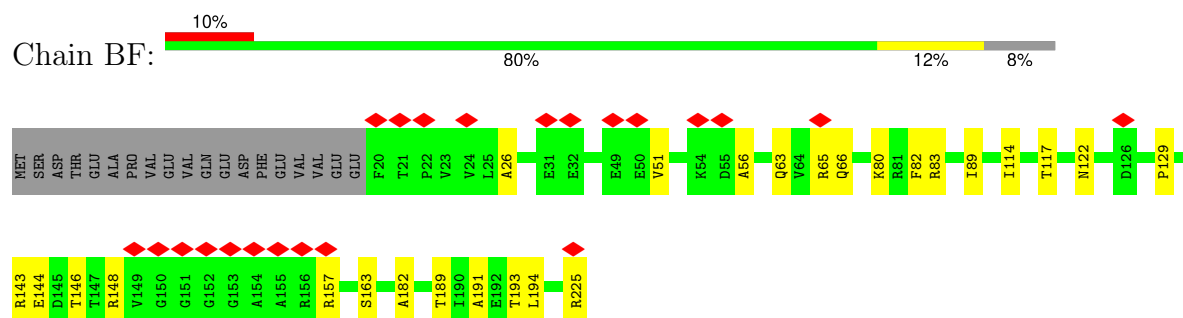
Chain Be: 79% 16% 5%



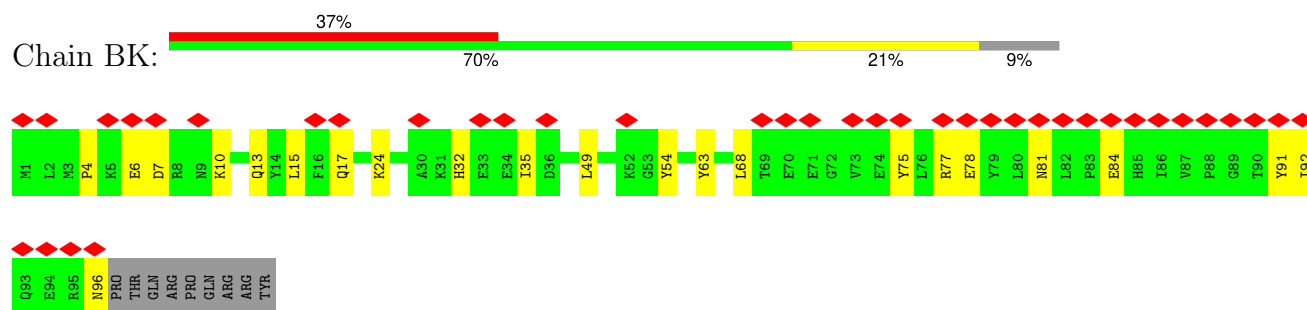
- Molecule 19: Small ribosomal subunit protein uS3



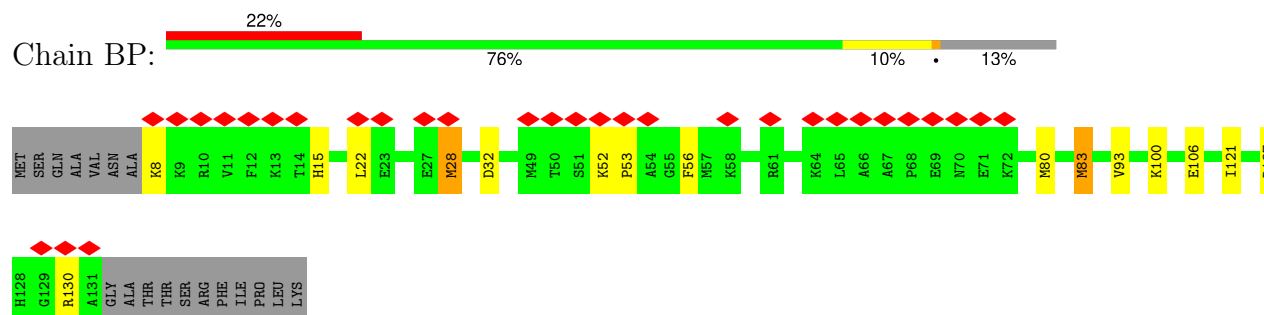
- Molecule 20: Small ribosomal subunit protein uS7



- Molecule 21: Small ribosomal subunit protein eS10A

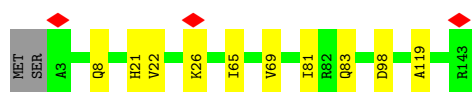


- Molecule 22: Small ribosomal subunit protein uS19

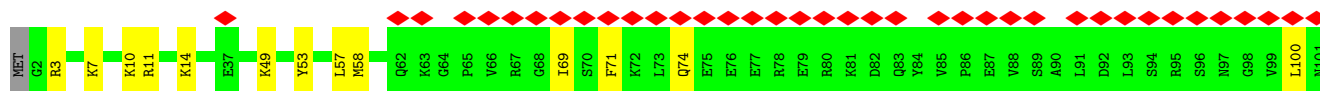
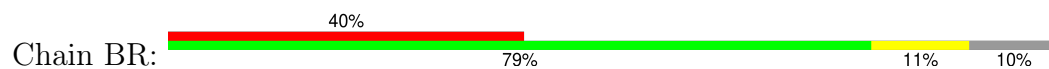


- Molecule 23: Small ribosomal subunit protein uS9A

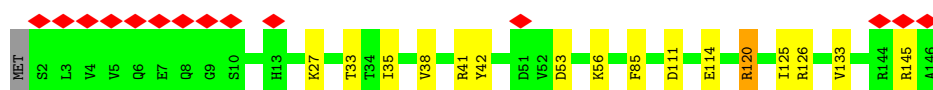
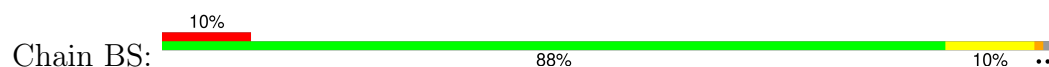




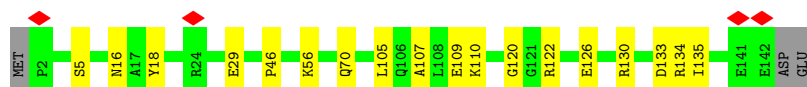
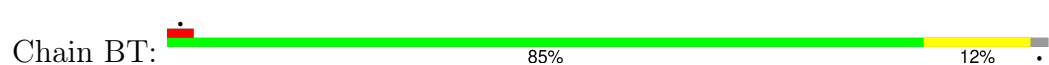
- Molecule 24: Small ribosomal subunit protein eS17A



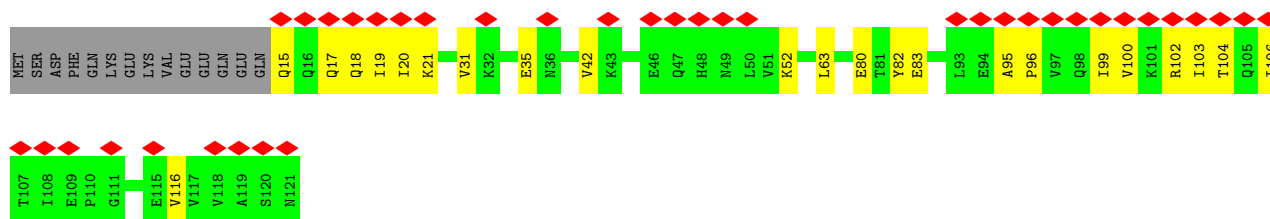
- Molecule 25: Small ribosomal subunit protein uS13A



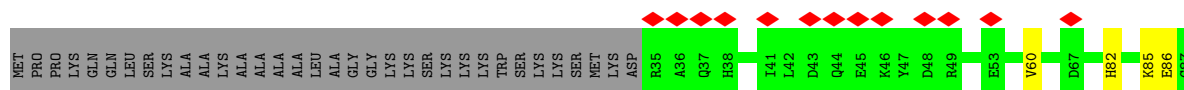
- Molecule 26: Small ribosomal subunit protein eS19A

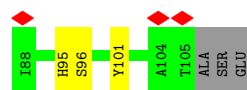


- Molecule 27: Small ribosomal subunit protein uS10

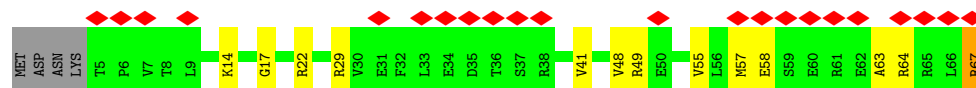
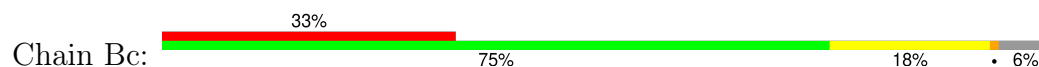


- Molecule 28: Small ribosomal subunit protein eS25A

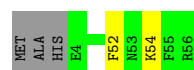




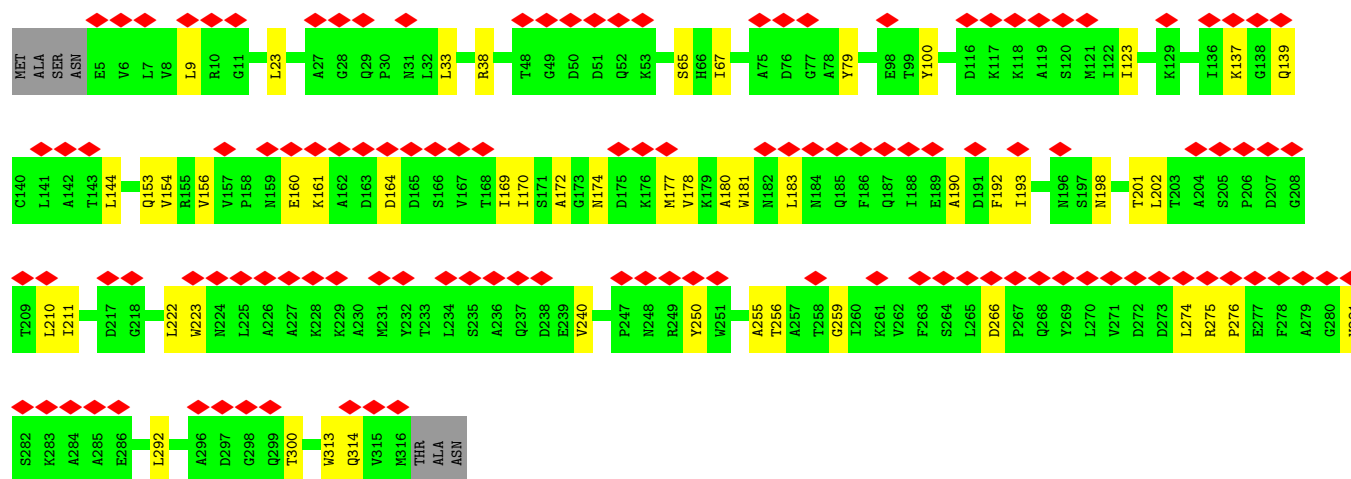
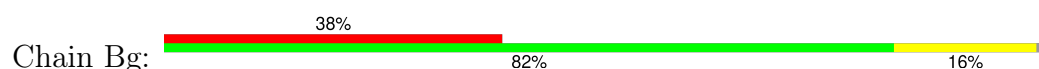
- Molecule 29: Small ribosomal subunit protein eS28A



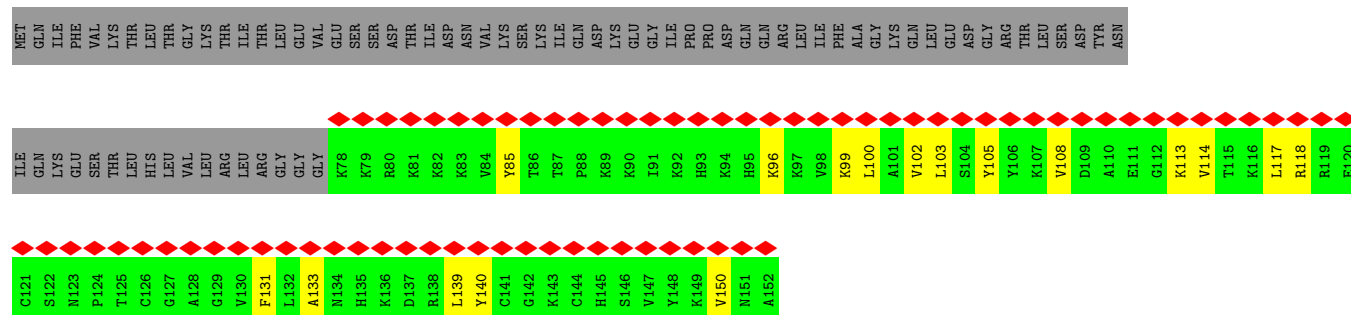
- Molecule 30: Small ribosomal subunit protein uS14A



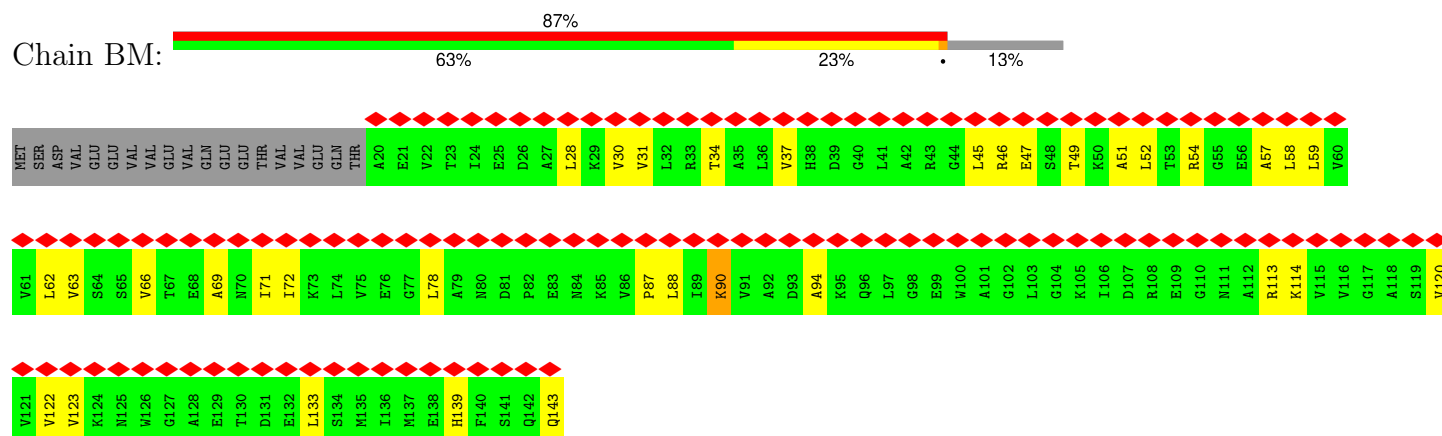
- Molecule 31: Small ribosomal subunit protein RACK1



- Molecule 32: Ubiquitin-ribosomal protein eS31 fusion protein

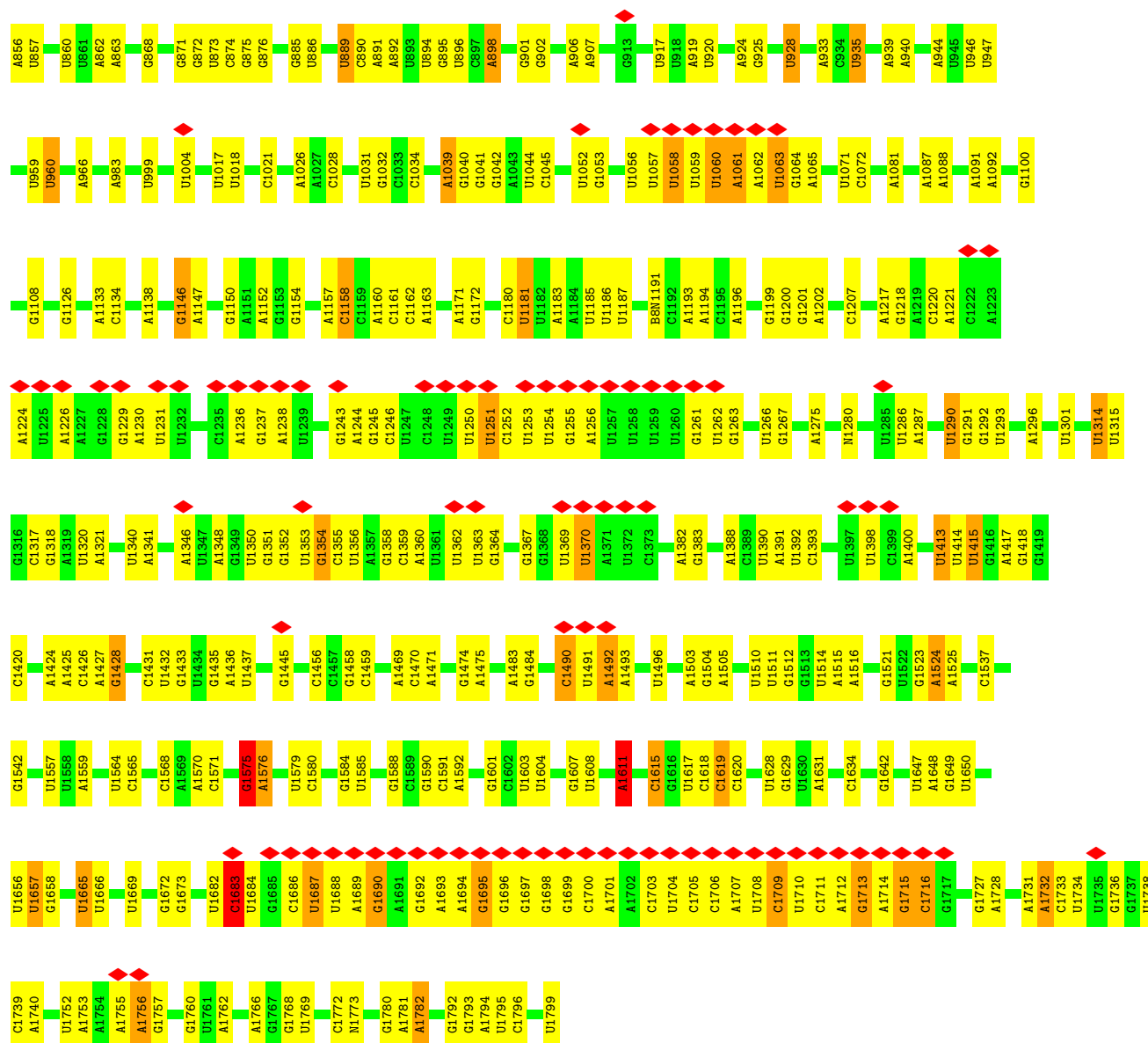


Chain BM:



Chain B5:





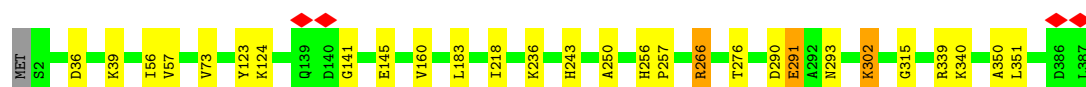
• Molecule 35: 60S ribosomal protein L2-A

Chain AA: 90% 6% ..



• Molecule 36: Large ribosomal subunit protein uL3

Chain AB: 93% 6% .



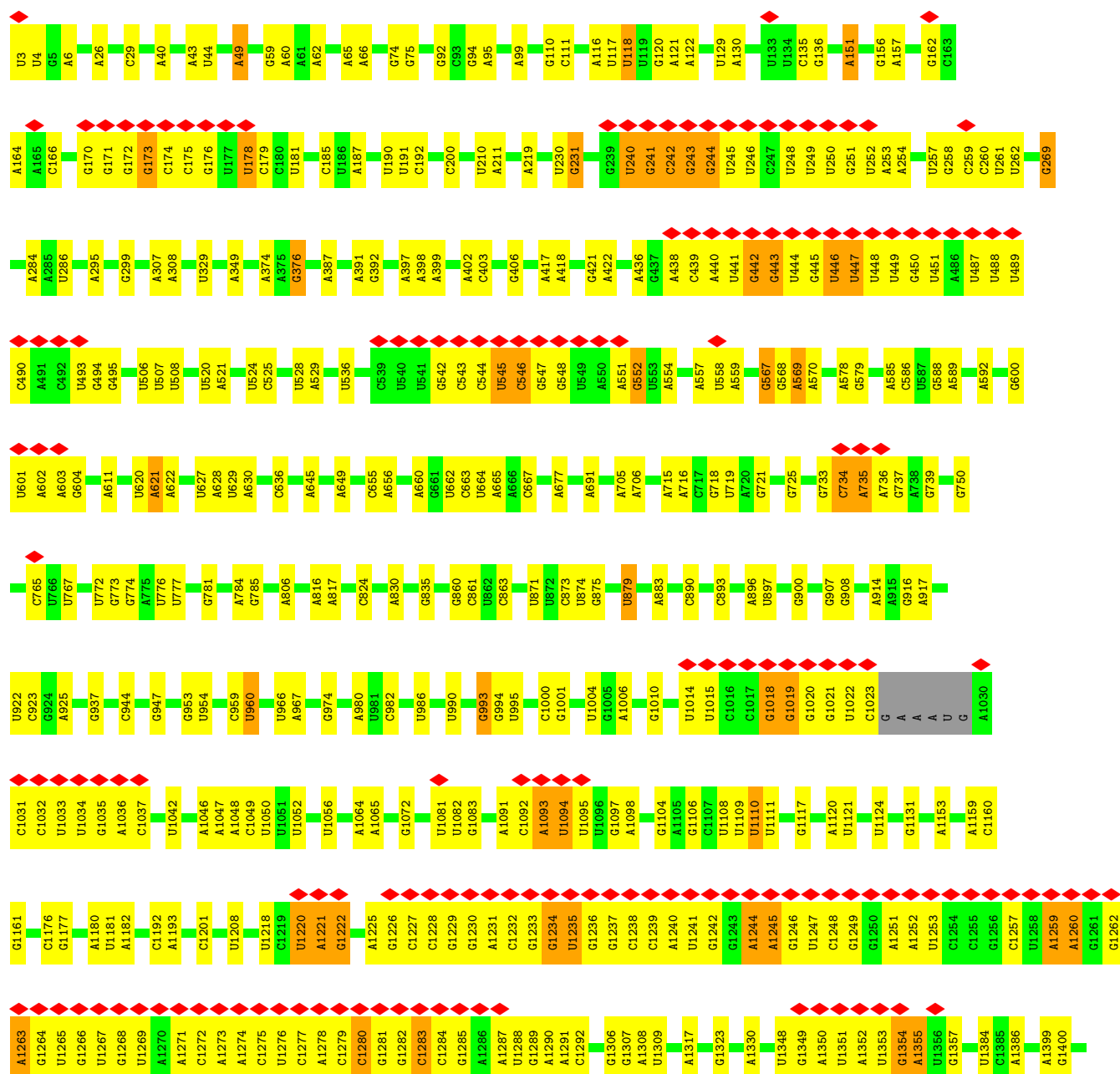
- Molecule 37: 60S ribosomal protein L4-A

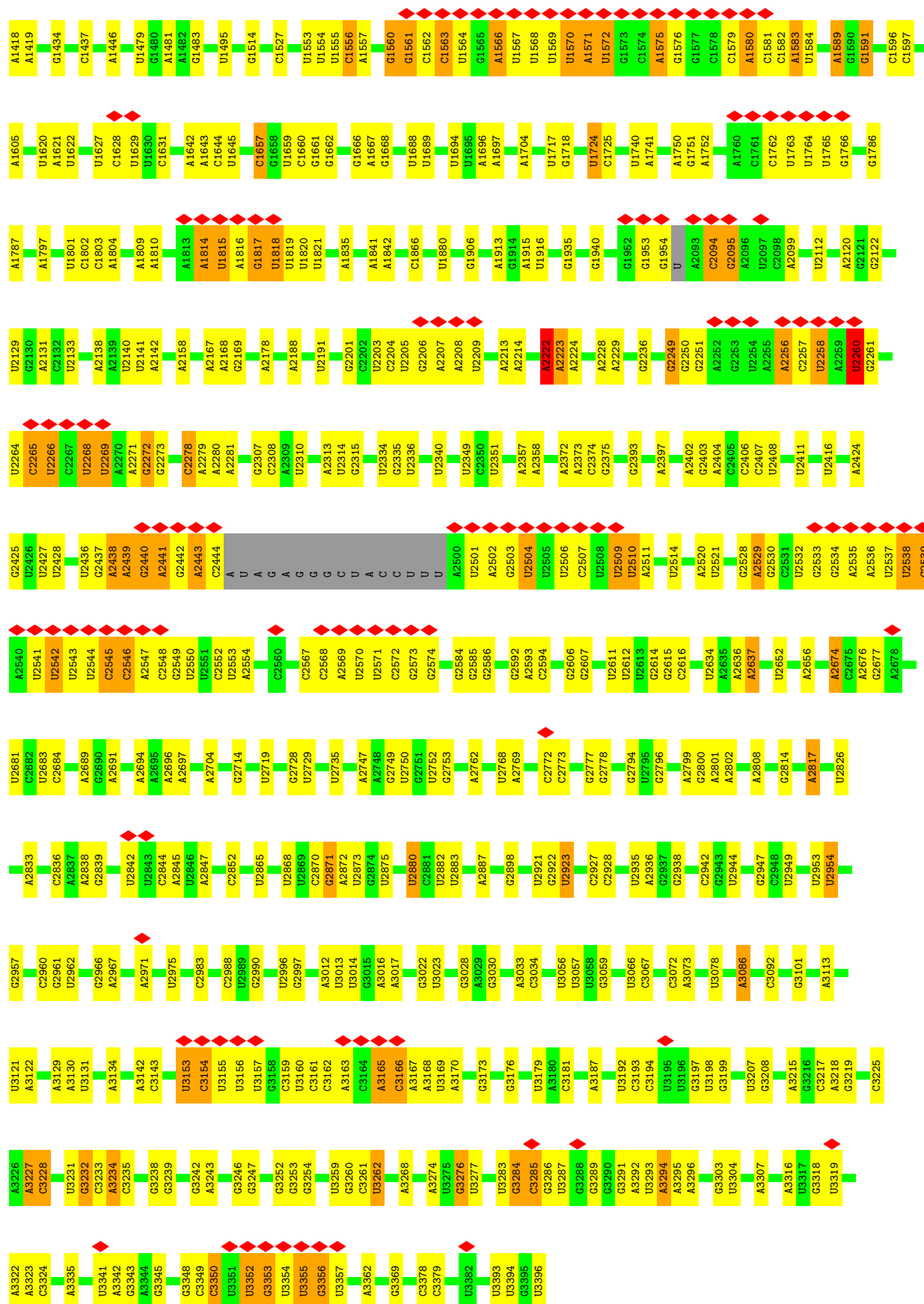
Chain AC:  93% 6%




- Molecule 38: 25S rRNA

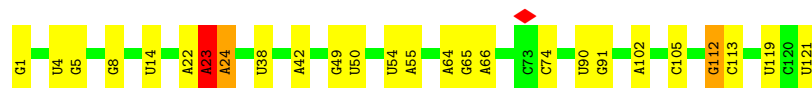
Chain A1:  9% 71% 24%






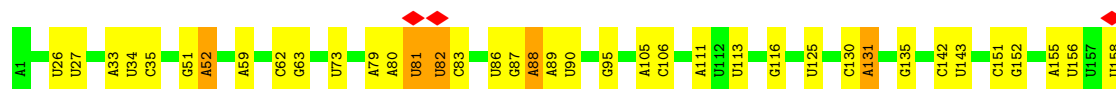
- Molecule 39: 5S rRNA

Chain A3:  79% 19%




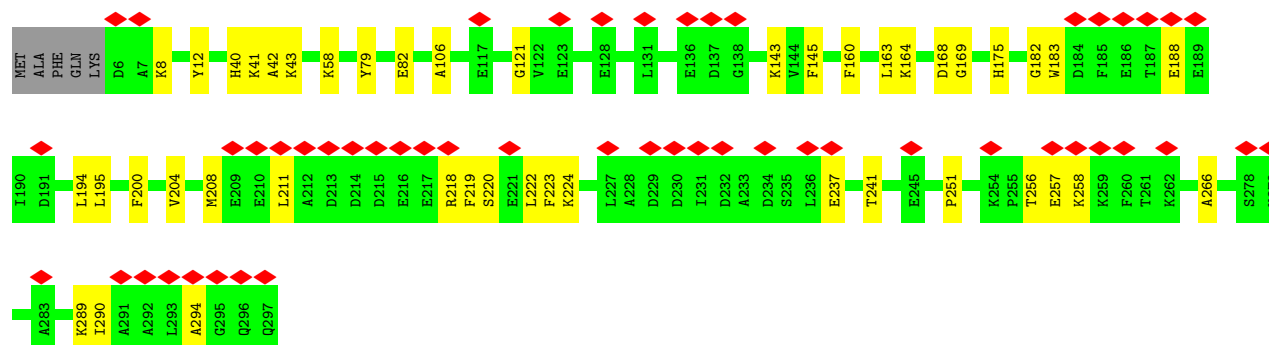
- Molecule 40: 5.8S rRNA

Chain A4:  76% 21%




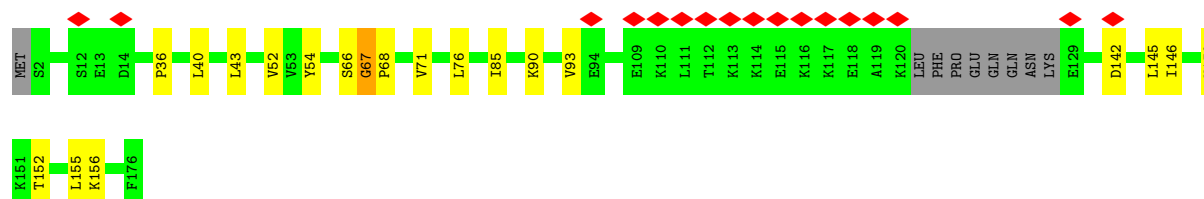
- Molecule 41: 60S ribosomal protein L5

Chain AD:  18% 84% 15%



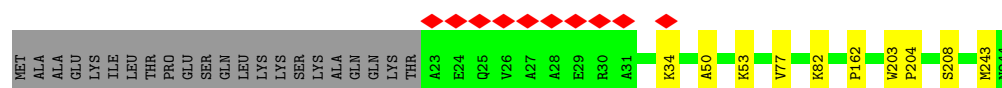
- Molecule 42: Large ribosomal subunit protein eL6A

Chain AE:  10% 84% 11% 5%

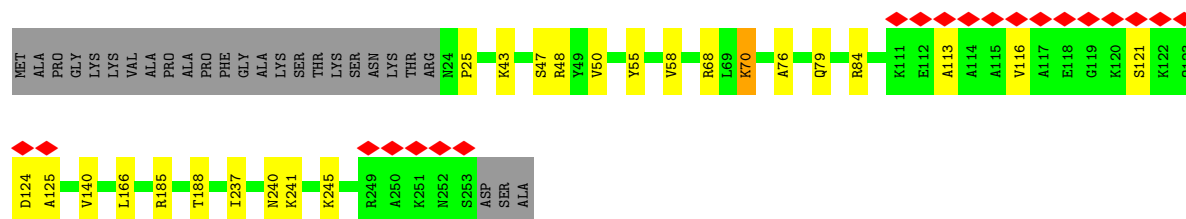
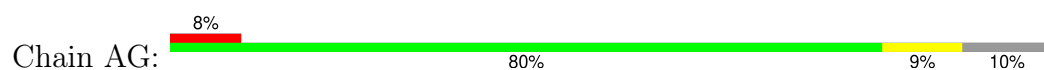


- Molecule 43: 60S ribosomal protein L7-A

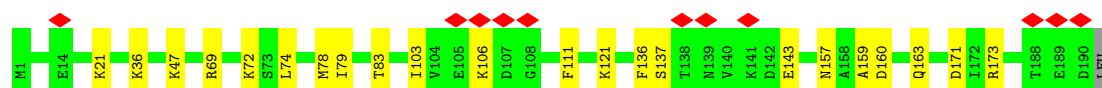
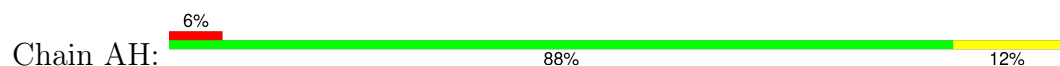
Chain AF:  87% 9%



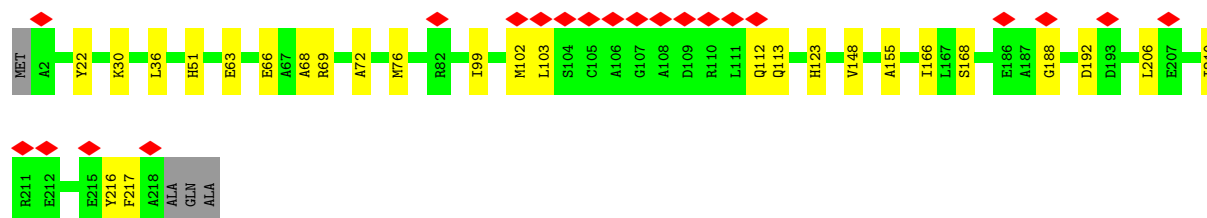
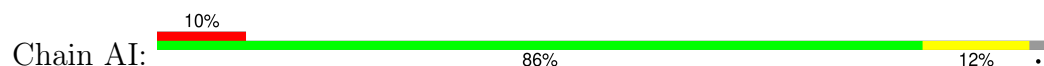
- Molecule 44: Large ribosomal subunit protein eL8A



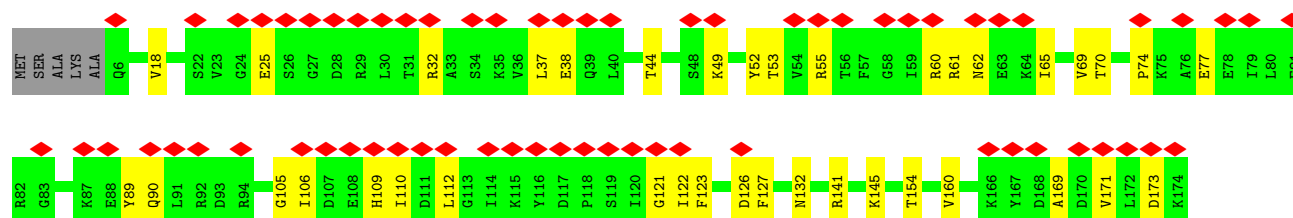
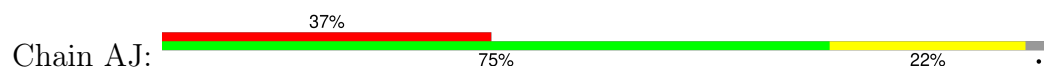
- Molecule 45: Large ribosomal subunit protein uL6A



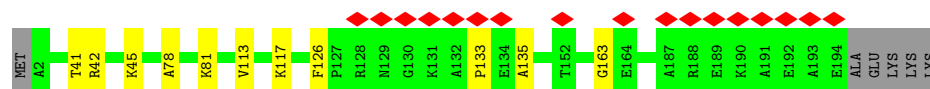
- Molecule 46: Large ribosomal subunit protein uL16



- Molecule 47: 60S ribosomal protein L11-A



- Molecule 48: 60S ribosomal protein L13-A



- Molecule 49: 60S ribosomal protein L14-A





- Molecule 50: Large ribosomal subunit protein eL15A

Chain AN: 96%



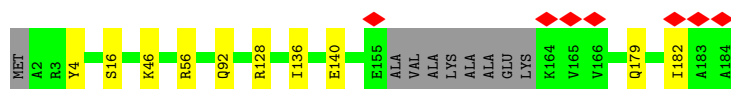
- Molecule 51: Large ribosomal subunit protein uL13A

Chain AO: 89% 10% ..



- Molecule 52: 60S ribosomal protein L17-A

Chain AP: 90% 5% 5%



- Molecule 53: 60S ribosomal protein L18-A

Chain AQ: 96% ..



- Molecule 54: 60S ribosomal protein L19-A

Chain AR: 21% 93% 7%

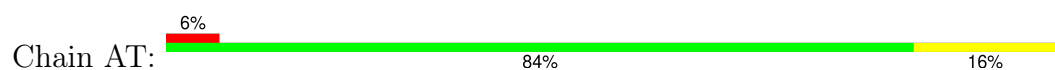


- Molecule 55: Large ribosomal subunit protein eL20A

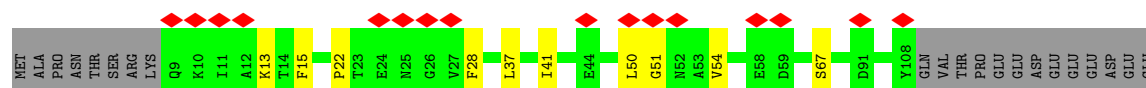
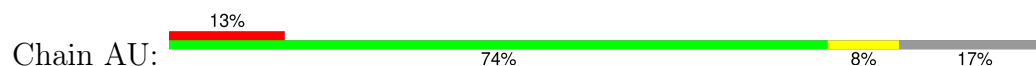
Chain AS: 85% 11%



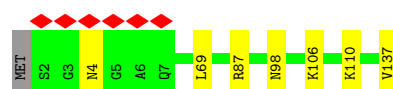
- Molecule 56: 60S ribosomal protein L21-A



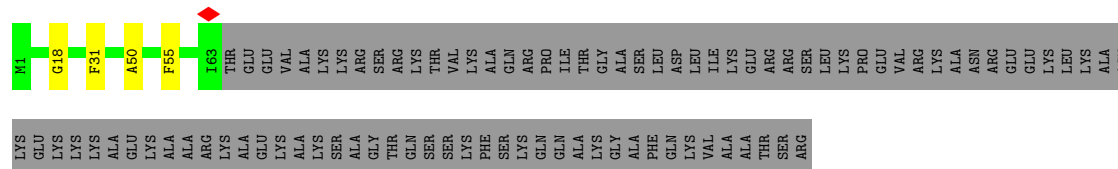
- Molecule 57: 60S ribosomal protein L22-A



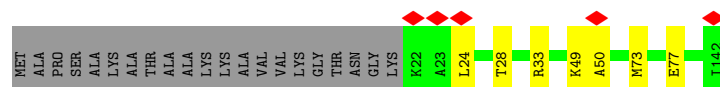
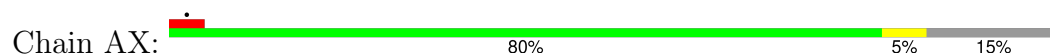
- Molecule 58: 60S ribosomal protein L23-A



- Molecule 59: Large ribosomal subunit protein eL24A



- Molecule 60: 60S ribosomal protein L25



- Molecule 61: 60S ribosomal protein L26-A

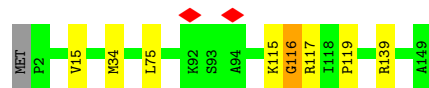


- Molecule 62: 60S ribosomal protein L27-A





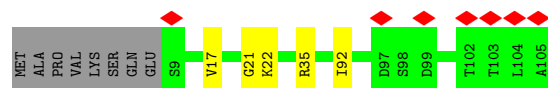
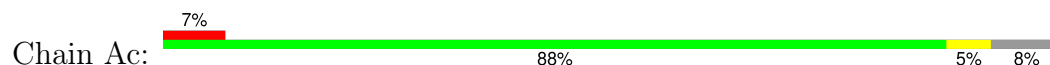
- Molecule 63: 60S ribosomal protein L28



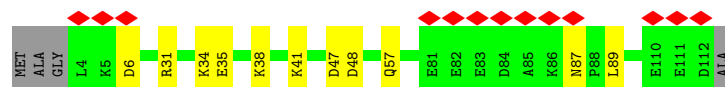
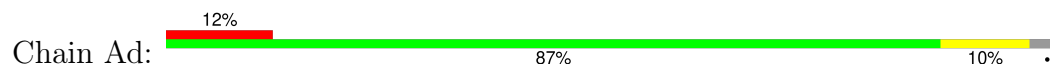
- Molecule 64: Large ribosomal subunit protein eL29



- Molecule 65: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L31-A



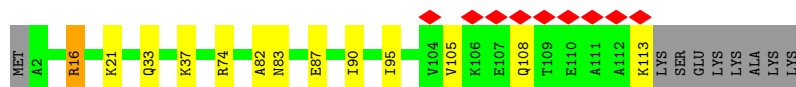
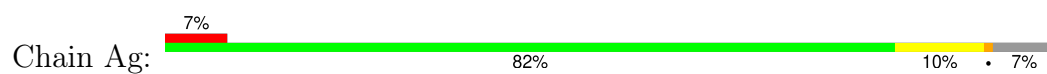
- Molecule 67: 60S ribosomal protein L32



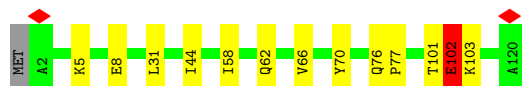
- Molecule 68: 60S ribosomal protein L33-A



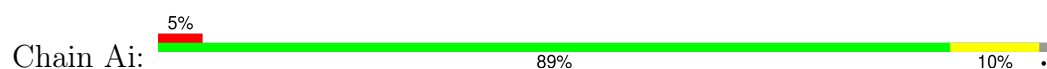
- Molecule 69: 60S ribosomal protein L34-A



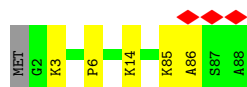
- Molecule 70: 60S ribosomal protein L35-A



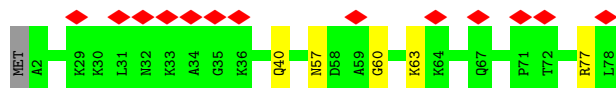
- Molecule 71: 60S ribosomal protein L36-A



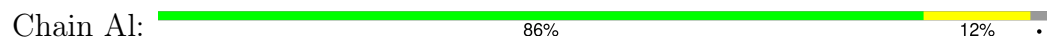
- Molecule 72: 60S ribosomal protein L37-A



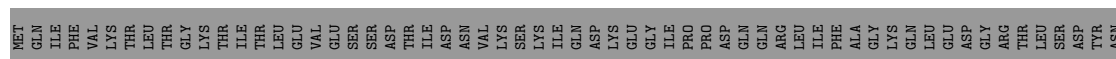
- Molecule 73: 60S ribosomal protein L38

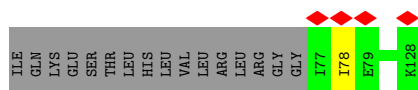


- Molecule 74: 60S ribosomal protein L39



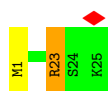
- Molecule 75: Ubiquitin-ribosomal protein eL40A fusion protein





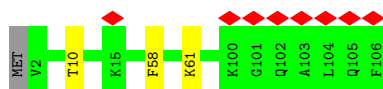
- Molecule 76: Small ribosomal subunit protein eS32A

Chain An: 92%



- Molecule 77: Large ribosomal subunit protein eL42A

Chain Ao: 8% 96%



- Molecule 78: 60S ribosomal protein L43-A

Chain Ap: 93% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	160722	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.595	Depositor
Minimum map value	-0.294	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	438.0, 438.0, 438.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.73, 0.73, 0.73	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, G7M, ZN, MG, 1MA, OMU, MA6, UR3, 5MC, OMG, 4AC, K, B8N, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	BA	0.56	2/1653 (0.1%)	0.66	2/2261 (0.1%)
2	BB	0.60	0/1735	0.78	1/2335 (0.0%)
3	BC	0.47	1/1665 (0.1%)	0.57	0/2263
4	BE	0.54	1/2109 (0.0%)	0.70	4/2839 (0.1%)
5	BG	0.56	0/1844	0.72	4/2464 (0.2%)
6	BH	0.53	0/1506	0.71	0/2028
7	BI	0.61	3/1514 (0.2%)	0.72	2/2021 (0.1%)
8	BJ	0.40	0/1519	0.58	1/2035 (0.0%)
9	BL	0.52	1/1272 (0.1%)	0.68	2/1712 (0.1%)
10	BN	0.42	0/1215	0.57	0/1638
11	BO	0.70	2/952 (0.2%)	0.92	2/1279 (0.2%)
12	BV	0.61	1/693 (0.1%)	0.75	3/935 (0.3%)
13	BW	0.48	0/1038	0.64	0/1395
14	BX	0.52	0/1139	0.71	3/1518 (0.2%)
15	BY	0.56	2/1087 (0.2%)	0.65	0/1449
16	Ba	0.53	1/782 (0.1%)	0.70	0/1047
17	Bb	0.78	3/620 (0.5%)	1.41	5/838 (0.6%)
18	Be	0.45	0/483	0.69	0/643
19	BD	0.52	1/1759 (0.1%)	0.65	0/2368
20	BF	0.47	0/1629	0.64	2/2202 (0.1%)
21	BK	0.60	1/837 (0.1%)	0.74	0/1131
22	BP	0.59	3/1012 (0.3%)	0.73	2/1356 (0.1%)
23	BQ	0.58	1/1125 (0.1%)	0.61	0/1510
24	BR	0.58	1/992 (0.1%)	0.67	1/1331 (0.1%)
25	BS	0.60	0/1211	0.77	0/1628
26	BT	0.48	0/1113	0.67	0/1494
27	BU	0.57	0/865	0.73	0/1169
28	BZ	0.50	0/582	0.62	0/782
29	Bc	0.56	0/499	0.71	0/670
30	Bd	0.42	0/452	0.55	0/600
31	Bg	0.48	0/2454	0.65	0/3340
32	Bf	0.48	0/616	0.70	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.52	1/943 (0.1%)	0.75	0/1274
34	B5	0.45	5/41450 (0.0%)	0.57	8/64582 (0.0%)
35	AA	0.50	2/1912 (0.1%)	0.73	0/2569
36	AB	0.51	3/3139 (0.1%)	0.72	4/4219 (0.1%)
37	AC	0.50	2/2800 (0.1%)	0.75	1/3790 (0.0%)
38	A1	0.47	23/74838 (0.0%)	0.62	7/116683 (0.0%)
39	A3	0.41	0/2861	0.55	1/4457 (0.0%)
40	A4	0.42	0/3724	0.61	1/5798 (0.0%)
41	AD	0.48	0/2390	0.72	0/3225
42	AE	0.44	0/1324	0.67	2/1782 (0.1%)
43	AF	0.40	0/1821	0.62	0/2451
44	AG	0.48	1/1830 (0.1%)	0.69	0/2469
45	AH	0.47	1/1531 (0.1%)	0.65	0/2062
46	AI	0.51	0/1796	0.68	2/2409 (0.1%)
47	AJ	0.51	0/1374	0.74	0/1842
48	AL	0.40	0/1568	0.61	0/2106
49	AM	0.42	0/1068	0.56	0/1438
50	AN	0.46	0/1757	0.72	0/2354
51	AO	0.53	1/1585 (0.1%)	0.75	2/2128 (0.1%)
52	AP	0.50	2/1410 (0.1%)	0.65	0/1893
53	AQ	0.43	0/1465	0.67	2/1965 (0.1%)
54	AR	0.40	0/1538	0.60	0/2050
55	AS	0.58	1/1481 (0.1%)	0.70	1/1990 (0.1%)
56	AT	0.50	1/1300 (0.1%)	0.65	0/1743
57	AU	0.52	0/812	0.82	2/1099 (0.2%)
58	AV	0.54	1/1018 (0.1%)	0.73	0/1369
59	AW	0.44	0/533	0.65	0/707
60	AX	0.42	0/983	0.67	0/1325
61	AY	0.76	5/1004 (0.5%)	0.77	3/1341 (0.2%)
62	AZ	0.51	1/1118 (0.1%)	0.61	0/1497
63	Aa	0.42	0/1204	0.69	0/1612
64	Ab	0.49	0/473	0.73	0/629
65	Ac	0.37	0/751	0.57	0/1008
66	Ad	0.47	0/904	0.64	0/1213
67	Ae	0.44	0/1041	0.61	0/1394
68	Af	0.39	0/868	0.60	0/1168
69	Ag	0.44	1/890 (0.1%)	0.70	0/1189
70	Ah	0.46	0/978	0.69	3/1301 (0.2%)
71	Ai	0.49	0/778	0.65	0/1034
72	Aj	0.64	2/696 (0.3%)	0.78	1/923 (0.1%)
73	Ak	0.53	0/618	0.78	2/826 (0.2%)
74	Al	0.41	0/443	0.68	0/588
75	Am	0.66	1/423 (0.2%)	0.74	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	1.12	3/234 (1.3%)	0.94	1/300 (0.3%)
77	Ao	0.45	1/860 (0.1%)	0.61	0/1136
78	Ap	0.45	0/701	0.65	0/934
All	All	0.48	82/212207 (0.0%)	0.64	77/311532 (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
1	BA	0	1
3	BC	0	1
5	BG	0	1
8	BJ	0	1
9	BL	0	1
11	BO	0	2
13	BW	0	1
25	BS	0	1
29	Bc	0	1
34	B5	2	0
35	AA	0	1
37	AC	0	3
41	AD	0	1
44	AG	0	3
50	AN	0	1
51	AO	0	3
54	AR	0	1
55	AS	0	2
56	AT	0	1
61	AY	0	1
62	AZ	0	1
63	Aa	0	2
70	Ah	0	1
71	Ai	0	1
All	All	2	32

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	An	23	ARG	NE-CZ	-12.72	1.19	1.33
23	BQ	98	ASP	CG-OD1	-12.38	1.01	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Bb	15	GLU	CD-OE2	-11.17	1.04	1.25
61	AY	74	TYR	CE2-CZ	-10.61	1.12	1.38
55	AS	21	GLU	C-O	10.37	1.28	1.23
12	BV	47	PRO	N-CD	-10.33	1.33	1.47
22	BP	28	MET	SD-CE	-9.69	1.55	1.79
24	BR	49	LYS	CD-CE	-9.39	1.24	1.52
72	Aj	6	PRO	N-CA	8.51	1.58	1.47
52	AP	140	GLU	CD-OE2	-8.03	1.10	1.25
34	B5	935	U	C2-O2	-7.84	1.06	1.22
35	AA	137	ILE	CG1-CD1	-7.43	1.22	1.51
75	Am	78	ILE	CG1-CD1	-7.36	1.23	1.51
38	A1	2141	U	P-OP2	-7.29	1.34	1.49
72	Aj	6	PRO	N-CD	-7.21	1.37	1.47
17	Bb	23	THR	CB-CG2	7.19	1.76	1.52
38	A1	2141	U	P-OP1	-7.19	1.34	1.49
38	A1	893	C	P-OP1	-7.17	1.34	1.49
36	AB	302	LYS	CD-CE	-6.98	1.31	1.52
38	A1	2138	A	P-OP1	-6.84	1.35	1.49
62	AZ	103	GLN	CD-NE2	-6.83	1.18	1.33
34	B5	1428	G	P-OP2	-6.82	1.35	1.49
16	Ba	52	ASP	CG-OD2	-6.79	1.12	1.25
1	BA	30	GLN	CD-NE2	-6.65	1.19	1.33
7	BI	119	GLN	CG-CD	-6.56	1.35	1.52
38	A1	875	G	P-OP1	-6.50	1.35	1.49
61	AY	77	LYS	CD-CE	-6.45	1.33	1.52
11	BO	47	LYS	CD-CE	-6.38	1.33	1.52
76	An	23	ARG	CZ-NH2	-6.35	1.25	1.33
38	A1	2817	A	P-OP1	-6.27	1.36	1.49
38	A1	863	C	P-OP2	-6.25	1.36	1.49
3	BC	115	ILE	CG1-CD1	-6.23	1.27	1.51
76	An	23	ARG	CZ-NH1	6.12	1.41	1.32
1	BA	33	GLN	CG-CD	-6.08	1.36	1.52
38	A1	2268	U	C2-O2	-6.04	1.10	1.22
37	AC	110	ASN	C-O	-6.01	1.15	1.23
38	A1	2873	U	P-OP2	-6.00	1.36	1.49
56	AT	110	LYS	CE-NZ	-5.98	1.31	1.49
15	BY	40	LEU	CG-CD1	-5.97	1.32	1.52
37	AC	319	LYS	CE-NZ	-5.93	1.31	1.49
61	AY	77	LYS	CG-CD	5.92	1.70	1.52
34	B5	403	G	P-OP2	-5.86	1.37	1.49
7	BI	119	GLN	CD-OE1	-5.84	1.12	1.23
61	AY	105	VAL	CB-CG1	-5.83	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	AB	56	ILE	CG1-CD1	-5.81	1.29	1.51
51	AO	84[A]	LEU	CG-CD2	-5.77	1.33	1.52
7	BI	187	GLU	CD-OE1	-5.76	1.14	1.25
15	BY	40	LEU	CG-CD2	-5.63	1.33	1.52
38	A1	1591	G	P-OP1	-5.61	1.37	1.49
58	AV	98	ASN	CG-OD1	-5.52	1.13	1.23
38	A1	2949	U	P-OP1	-5.48	1.38	1.49
34	B5	1611	A	C2-N3	-5.46	1.22	1.33
33	BM	90	LYS	CE-NZ	-5.44	1.33	1.49
22	BP	80	MET	SD-CE	-5.43	1.66	1.79
45	AH	160	ASP	CG-OD2	-5.43	1.15	1.25
38	A1	871	U	P-OP2	-5.42	1.38	1.49
22	BP	83	MET	SD-CE	-5.41	1.66	1.79
38	A1	2269	U	C2-O2	-5.39	1.11	1.22
36	AB	291	GLU	CB-CG	-5.36	1.36	1.52
38	A1	49	A	P-OP2	-5.34	1.38	1.49
44	AG	70	LYS	CD-CE	-5.33	1.36	1.52
52	AP	92	GLN	CD-NE2	-5.32	1.22	1.33
38	A1	2871	G	P-OP2	-5.31	1.38	1.49
34	B5	1575	G7M	O3'-P	5.24	1.61	1.56
4	BE	182	TYR	CZ-OH	-5.22	1.27	1.38
11	BO	20	TYR	CG-CD1	-5.22	1.28	1.39
17	Bb	51	GLN	CG-CD	-5.21	1.39	1.52
38	A1	1514	G	P-OP1	-5.20	1.38	1.49
69	Ag	16	ARG	CZ-NH2	-5.20	1.26	1.33
77	Ao	10	THR	CB-CG2	-5.18	1.35	1.52
38	A1	1605	A	P-OP1	-5.17	1.38	1.49
38	A1	2868	U	P-OP1	-5.16	1.38	1.49
35	AA	109	GLU	CD-OE1	-5.16	1.15	1.25
38	A1	883	A	P-OP1	-5.13	1.38	1.49
61	AY	74	TYR	CD1-CE1	5.11	1.53	1.38
19	BD	200	LYS	CE-NZ	-5.10	1.34	1.49
38	A1	893	C	P-OP2	-5.09	1.38	1.49
38	A1	1479	U	P-OP2	-5.09	1.38	1.49
9	BL	49	ILE	CG1-CD1	-5.08	1.31	1.51
21	BK	81	ASN	CG-ND2	-5.06	1.22	1.33
38	A1	2957	G	P-OP1	-5.04	1.38	1.49
38	A1	2898	G	P-OP2	-5.01	1.39	1.49

All (77) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Bb	15	GLU	OE1-CD-OE2	-26.47	59.38	122.90
17	Bb	15	GLU	CG-CD-OE2	-20.25	71.82	118.40
24	BR	49	LYS	CD-CE-NZ	11.58	148.95	111.90
76	An	23	ARG	NE-CZ-NH2	-10.12	110.09	119.20
22	BP	28	MET	CA-CB-CG	9.79	133.69	114.10
5	BG	118	GLU	OE1-CD-OE2	-9.47	100.18	122.90
12	BV	47	PRO	N-CD-CG	9.36	117.24	103.20
36	AB	266	ARG	CB-CG-CD	8.96	131.91	111.30
22	BP	28	MET	CG-SD-CE	8.66	119.95	100.90
51	AO	166[A]	GLU	CG-CD-OE1	-8.60	98.62	118.40
5	BG	46	LYS	CG-CD-CE	7.95	129.57	111.30
37	AC	319	LYS	CD-CE-NZ	7.69	136.52	111.90
38	A1	406	G	O4'-C1'-N9	6.96	118.64	108.20
34	B5	1426	C	C1'-C2'-O2'	-6.82	101.56	111.80
53	AQ	31	LYS	CA-CB-CG	-6.75	100.60	114.10
1	BA	33	GLN	N-CA-CB	6.61	120.28	110.49
51	AO	162[A]	VAL	CA-C-O	-6.52	114.25	121.17
17	Bb	23	THR	OG1-CB-CG2	-6.50	96.31	109.30
57	AU	51	GLY	CA-C-N	6.46	133.88	121.54
57	AU	51	GLY	C-N-CA	6.46	133.88	121.54
14	BX	114	LYS	CB-CG-CD	6.39	126.01	111.30
14	BX	106	GLY	CA-C-N	-6.25	110.01	121.52
14	BX	106	GLY	C-N-CA	-6.25	110.01	121.52
38	A1	151	A	O5'-P-OP1	6.20	126.60	108.00
34	B5	889	U	C2'-C3'-O3'	6.10	122.85	113.70
36	AB	291	GLU	CB-CG-CD	6.01	122.81	112.60
12	BV	46	ILE	CA-C-N	5.99	126.93	119.98
12	BV	46	ILE	C-N-CA	5.99	126.93	119.98
55	AS	50	LYS	O-C-N	-5.95	114.52	122.38
72	Aj	6	PRO	N-CD-CG	5.90	112.05	103.20
34	B5	928	U	N1-C1'-C2'	5.87	122.81	114.00
34	B5	1146	G	C1'-C2'-O2'	-5.86	99.61	108.40
38	A1	506	U	O5'-P-OP2	-5.81	90.57	108.00
42	AE	67	GLY	N-CA-C	-5.80	100.50	112.34
38	A1	3086	A	C5'-C4'-C3'	-5.80	107.31	116.00
73	Ak	77	ARG	CA-C-N	5.80	132.13	121.70
73	Ak	77	ARG	C-N-CA	5.80	132.13	121.70
70	Ah	102	GLU	CB-CG-CD	5.79	122.45	112.60
34	B5	1146	G	P-O3'-C3'	5.75	128.83	120.20
61	AY	74	TYR	CD1-CG-CD2	-5.70	109.56	118.10
42	AE	93	VAL	CA-CB-CG1	5.69	120.07	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	33	GLN	CG-CD-NE2	-5.68	107.88	116.40
9	BL	146	ALA	CA-C-N	-5.67	112.95	122.25
9	BL	146	ALA	C-N-CA	-5.67	112.95	122.25
38	A1	835	G	O4'-C1'-N9	5.66	116.69	108.20
61	AY	52	ARG	CA-C-N	-5.66	113.67	122.67
61	AY	52	ARG	C-N-CA	-5.66	113.67	122.67
4	BE	11	ARG	CA-C-N	5.58	132.19	121.54
4	BE	11	ARG	C-N-CA	5.58	132.19	121.54
38	A1	1657	C	C3'-C2'-O2'	-5.57	106.24	114.60
11	BO	50	ALA	CA-C-N	5.55	132.15	121.54
11	BO	50	ALA	C-N-CA	5.55	132.15	121.54
7	BI	119	GLN	CA-C-N	5.51	131.42	121.06
7	BI	119	GLN	C-N-CA	5.51	131.42	121.06
53	AQ	180	ARG	CG-CD-NE	5.50	124.11	112.00
2	BB	117	TRP	CA-CB-CG	-5.49	103.17	113.60
46	AI	192	ASP	OD1-CG-OD2	-5.45	109.83	122.90
36	AB	266	ARG	CG-CD-NE	5.42	123.92	112.00
34	B5	1683	C	P-O3'-C3'	5.34	128.21	120.20
70	Ah	101	THR	CA-C-N	5.34	128.83	120.82
70	Ah	101	THR	C-N-CA	5.34	128.83	120.82
5	BG	118	GLU	CG-CD-OE1	5.32	130.63	118.40
4	BE	156	VAL	CA-C-N	5.27	130.05	122.40
4	BE	156	VAL	C-N-CA	5.27	130.05	122.40
46	AI	102	MET	CA-CB-CG	5.25	124.59	114.10
40	A4	88	A	C1'-C2'-O2'	-5.22	100.56	108.40
5	BG	46	LYS	CD-CE-NZ	5.20	128.53	111.90
36	AB	302	LYS	CA-CB-CG	5.18	124.47	114.10
39	A3	23	A	C2'-C3'-O3'	5.13	121.40	113.70
20	BF	56	ALA	CA-C-N	5.11	131.31	121.54
20	BF	56	ALA	C-N-CA	5.11	131.31	121.54
34	B5	556	A	OP1-P-OP2	-5.08	104.35	119.60
38	A1	2222	A	C2'-C3'-O3'	5.08	121.32	113.70
8	BJ	90	LYS	CA-CB-CG	5.07	124.24	114.10
17	Bb	50	ALA	CA-C-N	5.02	134.94	125.66
17	Bb	50	ALA	C-N-CA	5.02	134.94	125.66
34	B5	196	G	OP1-P-O3'	5.02	123.05	108.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1575	G7M	C4',C3'

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	AA	190	ARG	Sidechain
37	AC	182	LEU	Peptide
37	AC	24	ALA	Peptide
37	AC	83	GLY	Peptide
41	AD	251	PRO	Peptide
44	AG	48	ARG	Sidechain
44	AG	76	ALA	Peptide
44	AG	79	GLN	Peptide
50	AN	187	ARG	Sidechain
51	AO	162[A]	VAL	Mainchain
51	AO	49[A]	ARG	Sidechain
51	AO	86[A]	GLY	Peptide
54	AR	131	ALA	Peptide
55	AS	19	VAL	Peptide
55	AS	2	ALA	Peptide
56	AT	83	ARG	Sidechain
61	AY	74	TYR	Sidechain
62	AZ	91	ALA	Peptide
63	Aa	115	LYS	Peptide
63	Aa	116	GLY	Peptide
70	Ah	102	GLU	Sidechain
71	Ai	78	GLY	Peptide
1	BA	187	ALA	Peptide
3	BC	95	ARG	Sidechain
5	BG	118	GLU	Sidechain
8	BJ	171	ARG	Sidechain
9	BL	150	ASN	Sidechain
11	BO	123	SER	Mainchain
11	BO	124	ASP	Sidechain
25	BS	120	ARG	Sidechain
13	BW	54	ASP	Peptide
29	Bc	67	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1612	0	1623	25	0
2	BB	1709	0	1784	22	0
3	BC	1635	0	1723	19	0
4	BE	2068	0	2154	17	0
5	BG	1820	0	1918	38	0
6	BH	1481	0	1572	23	0
7	BI	1489	0	1525	22	0
8	BJ	1494	0	1573	19	0
9	BL	1244	0	1314	14	0
10	BN	1192	0	1255	7	0
11	BO	941	0	979	25	0
12	BV	684	0	672	7	0
13	BW	1021	0	1060	6	0
14	BX	1121	0	1196	7	0
15	BY	1073	0	1132	9	0
16	Ba	769	0	818	9	0
17	Bb	610	0	633	15	0
18	Be	475	0	525	7	0
19	BD	1734	0	1817	17	0
20	BF	1609	0	1675	18	0
21	BK	817	0	804	14	0
22	BP	991	0	1035	10	0
23	BQ	1105	0	1166	6	0
24	BR	982	0	1047	10	0
25	BS	1192	0	1222	16	0
26	BT	1095	0	1114	12	0
27	BU	855	0	917	15	0
28	BZ	574	0	616	4	0
29	Bc	497	0	535	13	0
30	Bd	442	0	432	3	0
31	Bg	2401	0	2356	31	0
32	Bf	605	0	654	15	0
33	BM	935	0	975	21	0
34	B5	37463	0	18812	261	0
35	AA	1878	0	1946	13	0
36	AB	3081	0	3162	15	0
37	AC	2748	0	2859	14	0
38	A1	67606	0	33960	254	0
39	A3	2579	0	1303	12	0
40	A4	3353	0	1695	12	0
41	AD	2341	0	2290	30	0
42	AE	1303	0	1376	11	0
43	AF	1784	0	1862	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	AG	1798	0	1894	16	0
45	AH	1510	0	1576	15	0
46	AI	1759	0	1799	26	0
47	AJ	1353	0	1383	23	0
48	AL	1543	0	1608	8	0
49	AM	1053	0	1149	8	0
50	AN	1720	0	1779	5	0
51	AO	1555	0	1659	9	0
52	AP	1388	0	1423	5	0
53	AQ	1441	0	1543	6	0
54	AR	1521	0	1617	11	0
55	AS	1445	0	1487	13	0
56	AT	1276	0	1323	18	0
57	AU	796	0	812	5	0
58	AV	1003	0	1048	3	0
59	AW	521	0	551	2	0
60	AX	968	0	1036	9	0
61	AY	993	0	1081	5	0
62	AZ	1092	0	1155	11	0
63	Aa	1173	0	1215	6	0
64	Ab	462	0	491	5	0
65	Ac	743	0	797	3	0
66	Ad	890	0	938	7	0
67	Ae	1020	0	1090	2	0
68	Af	850	0	880	2	0
69	Ag	880	0	945	9	0
70	Ah	969	0	1078	12	0
71	Ai	771	0	849	6	0
72	Aj	681	0	687	3	0
73	Ak	612	0	682	2	0
74	Al	436	0	475	4	0
75	Am	417	0	459	0	0
76	An	233	0	284	2	0
77	Ao	847	0	914	2	0
78	Ap	694	0	738	3	0
79	A1	134	0	0	0	0
79	A3	1	0	0	0	0
79	A4	1	0	0	0	0
79	AP	1	0	0	0	0
79	AV	1	0	0	0	0
79	Aj	1	0	0	0	0
79	B5	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	A1	17	0	0	0	0
80	Ab	1	0	0	0	0
80	Ae	1	0	0	0	0
80	B5	8	0	0	0	0
81	Ao	1	0	0	0	0
82	A1	941	0	0	0	0
82	A3	5	0	0	0	0
82	A4	9	0	0	0	0
82	AA	19	0	0	0	0
82	AB	3	0	0	0	0
82	AC	8	0	0	0	0
82	AF	1	0	0	0	0
82	AN	7	0	0	0	0
82	AO	3	0	0	0	0
82	AP	3	0	0	0	0
82	AR	2	0	0	0	0
82	AT	1	0	0	0	0
82	AV	2	0	0	0	0
82	AX	2	0	0	0	0
82	Aa	10	0	0	0	0
82	Ab	1	0	0	0	0
82	Ae	6	0	0	0	0
82	Aj	6	0	0	0	0
82	Ao	2	0	0	0	0
82	B5	224	0	0	0	0
82	BB	1	0	0	0	0
82	BD	1	0	0	0	0
82	BE	1	0	0	0	0
82	BL	1	0	0	0	0
82	BO	1	0	0	0	0
82	BT	2	0	0	0	0
82	BX	2	0	0	0	0
82	Ba	3	0	0	0	0
82	Bd	1	0	0	0	0
All	All	200291	0	147531	1228	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 4.

All (1228) 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)
17:Bb:23:THR:CB	17:Bb:23:THR:CG2	1.76	1.57
34:B5:649:U:H3	34:B5:684:A:N6	1.49	1.10
5:BG:32:ILE:HD11	5:BG:63:MET:HE2	1.43	0.98
46:AI:30:LYS:HD3	46:AI:63:GLU:HA	1.44	0.98
11:BO:20:TYR:HD1	11:BO:84:ARG:HD3	1.33	0.94
7:BI:119:GLN:HG2	7:BI:120:THR:H	1.32	0.92
46:AI:103:LEU:H	46:AI:112:GLN:HE22	1.18	0.92
34:B5:1665:U:H3	34:B5:1736:G:H1	0.91	0.90
60:AX:50:ALA:HB1	70:Ah:66:VAL:HG11	1.54	0.89
5:BG:21:GLU:HA	5:BG:24:ILE:HG12	1.56	0.86
51:AO:22[A]:VAL:HG22	51:AO:122[A]:GLN:HE21	1.40	0.86
7:BI:110:ARG:HE	7:BI:121:LEU:HD12	1.39	0.86
78:Ap:36:ARG:HG2	78:Ap:48:LYS:HD3	1.59	0.84
5:BG:22:HIS:HA	5:BG:25:ARG:HE	1.41	0.83
34:B5:895:G:H1	34:B5:917:U:H3	1.27	0.82
1:BA:30:GLN:HE21	1:BA:33:GLN:HG2	1.45	0.81
69:Ag:16:ARG:HG2	69:Ag:37:LYS:HD3	1.62	0.81
46:AI:36:LEU:HD21	46:AI:69:ARG:HH11	1.45	0.80
2:BB:115:ARG:HE	2:BB:116:LYS:H	1.28	0.80
5:BG:2:LYS:HB3	5:BG:108:VAL:HG22	1.62	0.79
34:B5:868:G:H1	34:B5:960:U:H3	1.31	0.79
11:BO:20:TYR:CD1	11:BO:84:ARG:HD3	2.18	0.79
5:BG:18:ILE:HG12	5:BG:24:ILE:HG22	1.66	0.77
34:B5:487:G:H2'	34:B5:488:G:H4'	1.65	0.76
1:BA:197:ILE:HD12	1:BA:201:LEU:HD21	1.68	0.76
31:Bg:23:LEU:HD12	31:Bg:33:LEU:HD11	1.68	0.76
12:BV:42:GLU:HG3	12:BV:44:ARG:HD3	1.68	0.75
40:A4:81:U:H4'	40:A4:82:U:H4'	1.65	0.75
31:Bg:144:LEU:HD21	31:Bg:183:LEU:HD11	1.67	0.75
38:A1:436:A:H2	38:A1:621:A:H62	1.34	0.74
38:A1:1940:G:H21	38:A1:3362:A:H8	1.36	0.74
25:BS:145:ARG:HH12	34:B5:1172:G:H5''	1.49	0.74
1:BA:30:GLN:HE22	1:BA:32:HIS:HB2	1.52	0.74
31:Bg:156:VAL:HA	31:Bg:169:ILE:HG22	1.69	0.73
33:BM:52:LEU:HD22	33:BM:78:LEU:HB3	1.71	0.73
31:Bg:300:THR:HG22	31:Bg:314:GLN:HG2	1.70	0.73
47:AJ:90:GLN:NE2	47:AJ:173:ASP:HB3	2.04	0.73
2:BB:134:VAL:HG22	2:BB:219:LYS:HG2	1.69	0.72
13:BW:23:ARG:HG3	17:Bb:4:VAL:HG22	1.71	0.72
74:Al:43:ASN:HB3	74:Al:46:ARG:HE	1.53	0.72
7:BI:76:THR:HG22	7:BI:108:PRO:HG2	1.70	0.72
17:Bb:51:GLN:HA	17:Bb:66:PRO:HB3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:849:C:H5'	34:B5:850:A:H5'	1.70	0.72
57:AU:50:LEU:HD22	57:AU:54:VAL:HB	1.72	0.72
11:BO:51:ASP:HA	11:BO:54:GLU:HG3	1.73	0.71
70:Ah:102:GLU:HG2	70:Ah:103:LYS:N	2.05	0.71
38:A1:2436:U:H4'	44:AG:70:LYS:HE3	1.73	0.71
38:A1:551:A:HO2'	38:A1:552:G:H8	1.39	0.71
34:B5:490:C:H41	34:B5:493:U:H5'	1.57	0.70
38:A1:1627:U:H2'	38:A1:1814:A:H61	1.56	0.70
38:A1:2209:U:H3	38:A1:2236:G:H22	1.39	0.70
31:Bg:177:MET:HE1	31:Bg:193:ILE:HG13	1.74	0.69
46:AI:30:LYS:HE2	46:AI:66:GLU:HB3	1.72	0.69
34:B5:1490:C:H4'	34:B5:1492:A:H5'	1.74	0.69
38:A1:3234:A:H2	38:A1:3253:G:H22	1.40	0.69
29:Bc:17:GLY:HA3	29:Bc:67:ARG:HE	1.58	0.69
3:BC:91:ARG:CZ	34:B5:1147:A:H5'	2.23	0.68
40:A4:52:A:H5'	74:Al:21:ARG:HD3	1.76	0.68
21:BK:4:PRO:HB2	21:BK:6:GLU:HG2	1.75	0.68
17:Bb:23:THR:CG2	17:Bb:23:THR:OG1	2.38	0.68
17:Bb:36:LYS:HZ3	17:Bb:43:ILE:HB	1.59	0.68
6:BH:174:ASN:HD21	6:BH:180:GLN:HE21	1.41	0.68
31:Bg:210:LEU:HD21	31:Bg:222:LEU:HD12	1.75	0.68
31:Bg:250:TYR:HE2	31:Bg:266:ASP:HB2	1.59	0.67
31:Bg:281:TYR:HE2	34:B5:1393:C:H4'	1.57	0.67
21:BK:15:LEU:HG	21:BK:68:LEU:HD21	1.76	0.67
5:BG:32:ILE:CD1	5:BG:63:MET:HE2	2.21	0.66
34:B5:1669:U:H3	34:B5:1732:A:H62	1.43	0.66
37:AC:138:ARG:HH21	37:AC:240:PRO:HG2	1.61	0.66
4:BE:129:VAL:HG22	4:BE:139:VAL:HG12	1.75	0.66
34:B5:1207:C:H42	34:B5:1456:C:H5	1.44	0.66
47:AJ:32:ARG:HH21	47:AJ:121:GLY:HA3	1.59	0.65
37:AC:20:LEU:HD11	37:AC:252:GLU:HG3	1.78	0.65
2:BB:132:ASP:HB2	2:BB:221:PRO:HB3	1.78	0.65
37:AC:316:ASN:H	37:AC:319:LYS:NZ	1.94	0.65
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.32	0.65
18:Be:49:LEU:HG	18:Be:58:PRO:HG3	1.78	0.65
20:BF:225:ARG:HD3	29:Bc:58:GLU:HG2	1.79	0.65
19:BD:142:LEU:HD12	19:BD:148:LYS:HG3	1.78	0.65
5:BG:154:ARG:HD3	34:B5:78:A:C8	2.32	0.65
34:B5:1665:U:O2	34:B5:1736:G:N2	2.26	0.65
5:BG:55:GLY:H	5:BG:63:MET:HG2	1.62	0.64
34:B5:649:U:C2	34:B5:684:A:N6	2.65	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.33	0.64
38:A1:1222:G:H2'	38:A1:1285:G:H22	1.62	0.64
47:AJ:49:LYS:HB3	47:AJ:62:ASN:HA	1.78	0.64
46:AI:103:LEU:H	46:AI:112:GLN:NE2	1.95	0.64
34:B5:131:C:H1'	34:B5:135:A:H8	1.62	0.64
55:AS:77:VAL:HG11	55:AS:106:LEU:HD22	1.79	0.64
11:BO:124:ASP:HB2	34:B5:885:G:N2	2.13	0.64
26:BT:107:ALA:HA	26:BT:110:LYS:HE3	1.80	0.64
15:BY:27:VAL:HG21	15:BY:35:VAL:HG21	1.81	0.63
11:BO:40:ALA:HB2	11:BO:70:LYS:HD3	1.80	0.63
33:BM:88:LEU:HD21	33:BM:90:LYS:HE3	1.79	0.63
34:B5:502:U:H2'	34:B5:503:G:C8	2.33	0.63
7:BI:39:GLY:O	7:BI:59:ARG:HB3	1.97	0.63
33:BM:34:THR:HA	33:BM:37:VAL:HG12	1.81	0.63
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.34	0.63
45:AH:47:LYS:HB2	49:AM:7:VAL:HG22	1.80	0.63
5:BG:74:LYS:HE2	5:BG:94:ARG:HG2	1.81	0.63
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.81	0.63
34:B5:181:A:H2'	34:B5:182:A:C8	2.34	0.63
46:AI:36:LEU:HD11	46:AI:69:ARG:HD2	1.79	0.63
63:Aa:75:LEU:HB2	63:Aa:116:GLY:HA2	1.79	0.62
6:BH:44:LYS:HG3	6:BH:63:PRO:HD3	1.81	0.62
6:BH:91:ILE:HG21	6:BH:129:LEU:HD12	1.80	0.62
38:A1:1247:U:H3	38:A1:1267:U:H5	1.47	0.62
69:Ag:83:ASN:O	69:Ag:87:GLU:HG3	1.99	0.62
8:BJ:29:LYS:HD2	18:Be:40:TYR:HE1	1.64	0.62
20:BF:189:THR:HG22	20:BF:191:ALA:H	1.65	0.62
26:BT:5:SER:HA	26:BT:133:ASP:OD1	1.99	0.62
69:Ag:105:VAL:HG13	69:Ag:108:GLN:HE21	1.65	0.62
22:BP:28:MET:HE3	22:BP:32:ASP:CG	2.24	0.61
22:BP:127:ARG:HH22	22:BP:130:ARG:HH12	1.46	0.61
17:Bb:23:THR:CG2	17:Bb:23:THR:CA	2.74	0.61
5:BG:1:MET:HE2	5:BG:109:LEU:HB2	1.82	0.61
37:AC:182:LEU:HD23	37:AC:223:PRO:HG2	1.82	0.61
12:BV:38:LYS:HE3	12:BV:49:GLU:HG3	1.83	0.61
48:AL:78:ALA:HA	48:AL:81:LYS:HE3	1.83	0.61
54:AR:173:ARG:HA	54:AR:176:ARG:HB2	1.83	0.61
6:BH:98:ILE:HG12	6:BH:121:VAL:HG21	1.83	0.61
17:Bb:34:ASP:HB3	17:Bb:43:ILE:HD11	1.83	0.61
42:AE:142:ASP:O	42:AE:146:ILE:HG13	2.01	0.61
27:BU:17:GLN:HG2	27:BU:96:PRO:HG3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:119:GLN:HG2	7:BI:120:THR:N	2.12	0.60
46:AI:188:GLY:HA3	46:AI:216:TYR:HB2	1.84	0.60
41:AD:211:LEU:HD23	41:AD:223:PHE:HE2	1.66	0.60
34:B5:822:U:H3	34:B5:849:C:H2'	1.66	0.60
34:B5:65:A:H2	34:B5:84:A:H62	1.50	0.60
54:AR:134:HIS:CE1	54:AR:136:ARG:HB3	2.35	0.60
39:A3:23:A:H2'	39:A3:24:A:C8	2.36	0.60
41:AD:218:ARG:HH21	41:AD:222:LEU:HG	1.65	0.60
47:AJ:74:PRO:HA	47:AJ:77:GLU:HG2	1.84	0.60
34:B5:647:G:H2'	34:B5:648:G:C8	2.37	0.60
38:A1:120:G:H22	44:AG:124:ASP:HA	1.67	0.60
10:BN:64:ARG:HH12	34:B5:862:A:H8	1.49	0.59
15:BY:8:ARG:HD2	34:B5:780:A:N3	2.17	0.59
38:A1:1277:C:H2'	38:A1:1278:A:C8	2.37	0.59
38:A1:2836:C:H5	38:A1:2852:C:H42	1.48	0.59
33:BM:113:ARG:HG3	33:BM:114:LYS:HG3	1.83	0.59
19:BD:93:ASP:HB2	19:BD:96:LEU:HD13	1.83	0.59
38:A1:2443:A:H2'	38:A1:2504:U:H5	1.67	0.59
7:BI:194:ARG:HA	7:BI:199:LYS:HB2	1.84	0.59
32:Bf:96:LYS:HE3	34:B5:1252:C:H41	1.67	0.59
13:BW:27:ILE:HG22	13:BW:30:SER:HB3	1.85	0.59
34:B5:850:A:H4'	54:AR:170:ARG:HE	1.67	0.59
38:A1:2249:G:H22	38:A1:2268:U:H1'	1.68	0.59
5:BG:57:ASP:HB3	5:BG:98:ARG:HD2	1.85	0.59
13:BW:2:THR:N	34:B5:1034:C:HO2'	2.00	0.59
64:Ab:35:VAL:HB	64:Ab:40:ARG:HE	1.68	0.59
19:BD:64:ARG:HD3	21:BK:91:TYR:CD2	2.38	0.59
43:AF:82:LYS:HD3	56:AT:135:PRO:HG2	1.84	0.59
17:Bb:50:ALA:O	17:Bb:51:GLN:HG2	2.03	0.58
38:A1:1694:U:H5	38:A1:1752:A:N1	2.01	0.58
34:B5:509:G:H2'	34:B5:510:G:C8	2.38	0.58
38:A1:1220:U:H5''	38:A1:1221:A:H3'	1.86	0.58
46:AI:76:MET:HE2	46:AI:148:VAL:HA	1.86	0.58
34:B5:851:U:H4'	34:B5:852:C:H5'	1.84	0.58
34:B5:1236:A:H2'	34:B5:1237:G:C8	2.38	0.58
38:A1:1280:C:H2'	38:A1:1281:G:C8	2.38	0.58
38:A1:2509:U:H2'	38:A1:2510:U:C6	2.37	0.58
6:BH:49:ILE:HD12	6:BH:175:LYS:HG2	1.85	0.58
38:A1:528:U:H2'	38:A1:529:A:C8	2.39	0.58
55:AS:81:TYR:CE1	55:AS:90:MET:HE3	2.38	0.58
4:BE:108:ARG:HH12	34:B5:788:A:H3'	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:138:ARG:HH12	38:A1:1384:U:H5'	1.69	0.58
38:A1:129:U:H2'	38:A1:130:A:C8	2.38	0.58
38:A1:2222:A:H2'	38:A1:2223:A:C8	2.38	0.58
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.39	0.58
25:BS:42:TYR:HA	25:BS:85:PHE:CZ	2.39	0.58
31:Bg:172:ALA:HB2	31:Bg:202:LEU:HD23	1.86	0.58
48:AL:126:PHE:HZ	48:AL:135:ALA:HB2	1.69	0.58
38:A1:601:U:H3'	38:A1:602:A:C8	2.39	0.57
46:AI:76:MET:HE2	46:AI:148:VAL:HG12	1.86	0.57
3:BC:95:ARG:HH11	3:BC:97:ARG:HG3	1.69	0.57
38:A1:2533:G:H4'	69:Ag:113:LYS:HE3	1.86	0.57
25:BS:53:ASP:HB3	25:BS:56:LYS:HE2	1.86	0.57
38:A1:734:C:H3'	38:A1:735:A:C8	2.39	0.57
34:B5:1588:G:H1	34:B5:1608:U:H3	1.53	0.57
34:B5:591:A:H2'	34:B5:592:A:C8	2.40	0.57
34:B5:842:C:H41	34:B5:844:A:N6	2.03	0.57
35:AA:178:PRO:HG2	78:Ap:26:VAL:HG23	1.87	0.57
27:BU:42:VAL:HA	27:BU:52:LYS:HE2	1.87	0.57
27:BU:104:THR:HG22	27:BU:116:VAL:HG21	1.85	0.57
34:B5:655:G:H4'	34:B5:656:G:C8	2.40	0.57
34:B5:894:U:H2'	34:B5:895:G:C8	2.40	0.57
35:AA:109:GLU:OE1	35:AA:138:GLY:HA2	2.04	0.57
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.40	0.57
9:BL:124:THR:HG22	9:BL:141:LYS:HB3	1.86	0.56
24:BR:14:LYS:HE3	24:BR:69:ILE:HD11	1.86	0.56
25:BS:42:TYR:HA	25:BS:85:PHE:HZ	1.70	0.56
38:A1:2440:G:C2	38:A1:2441:A:H2'	2.40	0.56
22:BP:15:HIS:HB3	22:BP:22:LEU:HD12	1.87	0.56
25:BS:33:THR:HA	25:BS:38:VAL:HG23	1.87	0.56
41:AD:256:THR:HG22	41:AD:257:GLU:H	1.71	0.56
38:A1:269:G:H5''	50:AN:14:LYS:HE2	1.87	0.56
38:A1:2265:C:H2'	38:A1:2266:PSU:C6	2.41	0.56
65:Ac:17:VAL:HG11	65:Ac:92:ILE:HD12	1.87	0.56
67:Ae:60:ASN:OD1	67:Ae:62:LYS:HE2	2.04	0.56
49:AM:19:ARG:HG2	49:AM:65:LEU:HD22	1.88	0.56
34:B5:1356:U:H3	34:B5:1367:G:H1	1.53	0.56
16:Ba:82:ARG:NH2	34:B5:1152:A:H5''	2.20	0.56
44:AG:241:LYS:O	44:AG:245:LYS:HG2	2.04	0.56
61:AY:39:LEU:HD22	61:AY:43:TYR:HE2	1.69	0.56
38:A1:627:U:H2'	38:A1:628:A:C8	2.41	0.56
41:AD:164:LYS:HE2	41:AD:195:LEU:HD21	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AD:183:TRP:CH2	41:AD:188:GLU:HA	2.41	0.56
44:AG:121:SER:OG	44:AG:125:ALA:HB2	2.05	0.56
55:AS:90:MET:HE1	55:AS:114:HIS:CE1	2.41	0.56
1:BA:101:ARG:HH22	34:B5:1320:U:H3'	1.69	0.56
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.71	0.56
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.41	0.56
42:AE:68:PRO:HG3	42:AE:145:LEU:HD23	1.88	0.56
22:BP:8:LYS:HG2	47:AJ:90:GLN:HG2	1.86	0.56
11:BO:92:LYS:HB2	11:BO:119:THR:HG21	1.88	0.55
37:AC:138:ARG:NH1	38:A1:1384:U:H5'	2.21	0.55
38:A1:1817:G:C8	38:A1:1818:U:H5	2.24	0.55
38:A1:2443:A:H5''	38:A1:2443:A:H8	1.71	0.55
6:BH:31:SER:HA	6:BH:34:LEU:HB3	1.88	0.55
34:B5:186:C:H2'	34:B5:187:G:O4'	2.06	0.55
34:B5:1158:C:H5	34:B5:1163:A:H61	1.54	0.55
34:B5:846:G:H2'	34:B5:847:A:C8	2.40	0.55
38:A1:1495:U:H5	38:A1:1835:A:N1	2.04	0.55
38:A1:2209:U:H3	38:A1:2236:G:N2	2.05	0.55
64:Ab:32:LEU:HB3	64:Ab:40:ARG:HD3	1.89	0.55
17:Bb:36:LYS:NZ	17:Bb:43:ILE:HB	2.22	0.55
71:Ai:26:ILE:HD12	71:Ai:29:LYS:HD2	1.89	0.55
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.89	0.55
34:B5:649:U:N3	34:B5:684:A:N6	2.23	0.55
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.42	0.55
1:BA:15:GLN:HG3	24:BR:100:LEU:HD21	1.89	0.55
2:BB:28:GLU:OE1	2:BB:50:LYS:HD3	2.05	0.54
11:BO:45:GLY:HA2	11:BO:54:GLU:HG2	1.89	0.54
15:BY:92:VAL:HG11	15:BY:99:LYS:HG3	1.89	0.54
38:A1:1580:A:H2	60:AX:33:ARG:HD2	1.70	0.54
51:AO:187[A]:GLU:HA	51:AO:192[A]:LYS:HE3	1.89	0.54
31:Bg:250:TYR:CE2	31:Bg:266:ASP:HB2	2.40	0.54
31:Bg:276:PRO:HG3	31:Bg:313:TRP:HZ2	1.72	0.54
1:BA:30:GLN:NE2	1:BA:32:HIS:HB2	2.23	0.54
4:BE:139:VAL:HG13	4:BE:150:PRO:HG3	1.89	0.54
4:BE:251:GLU:HB2	4:BE:255:ARG:NH2	2.23	0.54
34:B5:1060:U:H3'	34:B5:1061:A:H5''	1.90	0.54
3:BC:40:LYS:HG2	3:BC:247:ALA:HB1	1.89	0.54
5:BG:1:MET:HE3	5:BG:106:LEU:HB3	1.90	0.54
6:BH:114:ARG:HG3	34:B5:860:U:O4'	2.08	0.54
31:Bg:240:VAL:HG22	31:Bg:256:THR:HG22	1.90	0.54
38:A1:3153:U:H4'	38:A1:3154:C:N3	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:123:TYR:CZ	36:AB:124:LYS:HG3	2.43	0.54
37:AC:74:ILE:HD12	37:AC:75:PRO:HD2	1.88	0.54
2:BB:175:GLU:HG2	2:BB:193:ILE:HG12	1.89	0.54
38:A1:551:A:O2'	38:A1:552:G:H8	1.89	0.54
38:A1:2953:U:H2'	38:A1:2954:U:H2'	1.90	0.54
38:A1:3154:C:N4	38:A1:3293:U:H3	2.06	0.54
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.42	0.54
34:B5:1236:A:H2'	34:B5:1237:G:H8	1.73	0.53
42:AE:152:THR:HG23	42:AE:155:LEU:HB2	1.90	0.53
34:B5:983:A:N1	34:B5:1018:U:H5	2.05	0.53
38:A1:1627:U:H2'	38:A1:1814:A:N6	2.24	0.53
54:AR:43:LYS:HG3	54:AR:46:LYS:HE3	1.89	0.53
9:BL:27:THR:HG23	9:BL:30:ARG:H	1.72	0.53
47:AJ:109:HIS:CE1	47:AJ:112:LEU:HD23	2.43	0.53
6:BH:27:LEU:HD11	6:BH:38:LEU:HD13	1.90	0.53
8:BJ:90:LYS:HB2	8:BJ:95:TYR:CD2	2.44	0.53
34:B5:1346:A:C8	34:B5:1370:U:H2'	2.42	0.53
36:AB:36:ASP:OD2	36:AB:39:LYS:HE2	2.08	0.53
38:A1:900:G:H1'	38:A1:1589:A:N6	2.24	0.53
38:A1:2510:U:H2'	38:A1:2511:A:H8	1.73	0.53
34:B5:844:A:H5'	34:B5:845:G:H5''	1.90	0.53
41:AD:289:LYS:HD3	46:AI:206:LEU:HD23	1.90	0.53
55:AS:152:LEU:HB2	55:AS:172:TYR:CE2	2.44	0.53
55:AS:1:MET:HG2	55:AS:32:SER:HB3	1.91	0.53
3:BC:91:ARG:NH2	34:B5:1147:A:H5'	2.23	0.53
23:BQ:8:GLN:HG2	23:BQ:21:HIS:CE1	2.43	0.53
27:BU:80:GLU:HG2	30:Bd:54:LYS:NZ	2.23	0.53
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.43	0.53
3:BC:91:ARG:HH11	3:BC:91:ARG:HG2	1.74	0.53
5:BG:39:GLU:HA	5:BG:46:LYS:HE2	1.91	0.53
6:BH:50:ASP:HA	6:BH:56:LYS:HG2	1.89	0.53
7:BI:119:GLN:CG	7:BI:120:THR:H	2.13	0.53
34:B5:1017:U:H2'	34:B5:1018:U:O2	2.09	0.53
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.44	0.53
19:BD:64:ARG:HD3	21:BK:91:TYR:HD2	1.73	0.53
34:B5:416:A:H3'	34:B5:417:A:C8	2.43	0.53
34:B5:1511:U:H2'	34:B5:1512:G:C8	2.44	0.53
34:B5:1649:G:H2'	34:B5:1650:U:C6	2.44	0.53
38:A1:3033:A:H2'	38:A1:3034:C:O2	2.09	0.53
38:A1:3353:G:H1'	38:A1:3356:G:H5'	1.89	0.53
42:AE:66:SER:HB2	42:AE:76:LEU:HD23	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AI:30:LYS:HE2	46:AI:66:GLU:CG	2.39	0.53
47:AJ:18:VAL:HG13	47:AJ:70:THR:HG22	1.91	0.53
34:B5:124:A:N1	34:B5:293:U:H5	2.07	0.52
34:B5:1359:C:H2'	34:B5:1360:A:C8	2.45	0.52
48:AL:126:PHE:HE1	48:AL:133:PRO:HG2	1.73	0.52
2:BB:134:VAL:HG23	2:BB:218:LEU:HB2	1.90	0.52
17:Bb:67:THR:HG22	17:Bb:68:GLY:H	1.75	0.52
34:B5:1615:C:H5''	34:B5:1615:C:H6	1.73	0.52
8:BJ:83:VAL:HA	8:BJ:149:ARG:HA	1.90	0.52
34:B5:650:U:H2'	34:B5:651:G:C8	2.45	0.52
38:A1:3231:U:H2'	38:A1:3232:G:C8	2.44	0.52
46:AI:166:ILE:HG21	56:AT:158:THR:HG21	1.91	0.52
34:B5:1220:C:H2'	34:B5:1221:A:C8	2.44	0.52
34:B5:1296:A:N1	34:B5:1301:U:H5	2.07	0.52
34:B5:1564:U:H2'	34:B5:1565:C:C6	2.44	0.52
45:AH:171:ASP:OD1	45:AH:173:ARG:HG2	2.10	0.52
28:BZ:85:LYS:HE2	28:BZ:86:GLU:OE1	2.10	0.52
34:B5:1738:U:H2'	34:B5:1739:C:C6	2.44	0.52
38:A1:1724:U:H1'	38:A1:1725:C:C6	2.45	0.52
57:AU:22:PRO:HB2	57:AU:28:PHE:HB2	1.91	0.52
24:BR:71:PHE:CZ	24:BR:74:GLN:HB2	2.45	0.52
27:BU:100:VAL:O	27:BU:104:THR:HG23	2.10	0.52
2:BB:86:LEU:HB3	2:BB:98:THR:HB	1.92	0.52
7:BI:138:ASN:HD21	34:B5:187:G:H3'	1.75	0.52
34:B5:12:U:H2'	34:B5:13:C:C6	2.45	0.52
35:AA:144:ASN:O	35:AA:145:LYS:HE2	2.09	0.52
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.45	0.52
34:B5:520:A:H2'	34:B5:521:A:C8	2.45	0.52
34:B5:1709:C:H4'	34:B5:1710:U:H5'	1.91	0.52
38:A1:242:C:H2'	38:A1:243:G:C8	2.44	0.52
1:BA:98:ILE:HD11	1:BA:116:LYS:HD2	1.91	0.52
4:BE:251:GLU:HB2	4:BE:255:ARG:HH22	1.75	0.52
34:B5:416:A:H3'	34:B5:417:A:H8	1.74	0.52
61:AY:39:LEU:HD22	61:AY:43:TYR:CE2	2.44	0.52
28:BZ:60:VAL:HB	28:BZ:101:TYR:HB2	1.91	0.52
51:AO:35[A]:VAL:HG21	51:AO:80[A]:PHE:HE2	1.74	0.52
32:Bf:108:VAL:HG22	32:Bf:114:VAL:HG22	1.92	0.51
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.45	0.51
38:A1:2094:C:H2'	38:A1:2095:G:H8	1.75	0.51
38:A1:3160:U:H2'	38:A1:3161:C:C6	2.45	0.51
62:AZ:103:GLN:NE2	62:AZ:106:GLN:CD	2.67	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BF:144:GLU:HG3	29:Bc:57:MET:HG2	1.92	0.51
34:B5:233:C:H1'	34:B5:235:G:C6	2.45	0.51
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.45	0.51
45:AH:137:SER:OG	45:AH:143:GLU:HB3	2.10	0.51
60:AX:50:ALA:HB2	70:Ah:77:PRO:HG2	1.91	0.51
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.46	0.51
50:AN:183:THR:HG22	50:AN:187:ARG:HB2	1.92	0.51
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.92	0.51
54:AR:162:ARG:O	54:AR:166:ASN:HB3	2.11	0.51
5:BG:116:LYS:HG2	5:BG:117:GLY:H	1.74	0.51
34:B5:1619:C:H2'	34:B5:1620:C:H6	1.76	0.51
38:A1:3034:C:H5	45:AH:121:LYS:H	1.58	0.51
5:BG:56:ASN:HD22	5:BG:62:PRO:HA	1.74	0.51
34:B5:76:A:H4'	34:B5:77:U:H5'	1.92	0.51
38:A1:1277:C:H2'	38:A1:1278:A:H8	1.75	0.51
47:AJ:110:ILE:HD12	47:AJ:110:ILE:H	1.75	0.51
5:BG:180:THR:HG23	5:BG:183:ARG:H	1.76	0.51
7:BI:57:ALA:HB2	7:BI:177:GLY:HA2	1.92	0.51
34:B5:1252:C:H2'	34:B5:1253:U:H6	1.76	0.51
66:Ad:41:LYS:HE3	66:Ad:47:ASP:OD1	2.10	0.51
34:B5:1226:A:H4'	34:B5:1230:A:H5'	1.92	0.51
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.45	0.51
31:Bg:259:GLY:HA3	31:Bg:275:ARG:HG2	1.92	0.51
34:B5:198:A:H2'	34:B5:199:G:O4'	2.11	0.51
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.46	0.51
34:B5:1648:A:H2'	34:B5:1649:G:C8	2.45	0.51
38:A1:1566:A:N7	38:A1:1570:U:H1'	2.26	0.51
38:A1:3284:G:H2'	38:A1:3285:C:C6	2.45	0.51
51:AO:18[A]:ARG:O	51:AO:22[A]:VAL:HG23	2.11	0.51
31:Bg:137:LYS:HZ2	31:Bg:139:GLN:HB2	1.76	0.51
31:Bg:160:GLU:HG2	31:Bg:161:LYS:H	1.76	0.51
34:B5:814:A:H3'	54:AR:167:ARG:HG2	1.91	0.51
34:B5:1665:U:O4	34:B5:1736:G:O6	2.28	0.51
36:AB:290:ASP:O	36:AB:293:ASN:OD1	2.29	0.51
38:A1:954:U:H5	38:A1:967:A:N1	2.08	0.51
38:A1:2584:G:H1'	44:AG:240:ASN:ND2	2.26	0.51
42:AE:52:VAL:HA	42:AE:67:GLY:HA3	1.93	0.51
44:AG:25:PRO:HB2	62:AZ:125:GLY:H	1.76	0.51
5:BG:191:ARG:HH22	34:B5:177:U:H2'	1.76	0.50
50:AN:45:PRO:O	50:AN:49:ARG:HG3	2.11	0.50
34:B5:480:G:H1	34:B5:508:U:H3	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:830:U:H1'	34:B5:831:U:H5	1.75	0.50
3:BC:95:ARG:NH1	3:BC:97:ARG:HE	2.09	0.50
33:BM:59:LEU:H	33:BM:123:VAL:HG22	1.77	0.50
34:B5:924:A:H2'	34:B5:925:G:C8	2.45	0.50
40:A4:130:C:H2'	40:A4:131:A:H5''	1.93	0.50
4:BE:71:LYS:HG3	4:BE:91:THR:HB	1.94	0.50
14:BX:133:LEU:HG	14:BX:137:LYS:HE2	1.93	0.50
21:BK:32:HIS:ND1	21:BK:35:ILE:HB	2.27	0.50
34:B5:730:G:H21	34:B5:732:G:H21	1.58	0.50
38:A1:176:G:H1	38:A1:242:C:H42	1.58	0.50
14:BX:130:VAL:HG13	14:BX:140:LYS:HE2	1.94	0.50
22:BP:56:PHE:CD2	22:BP:83:MET:HE1	2.47	0.50
25:BS:41:ARG:HH11	26:BT:46:PRO:HG3	1.77	0.50
34:B5:1039:A:HO2'	34:B5:1040:G:H8	1.60	0.50
38:A1:307:A:H2'	38:A1:308:A:C8	2.46	0.50
16:Ba:48:ALA:H	29:Bc:64:ARG:NH2	2.10	0.50
39:A3:14:U:H5	39:A3:66:A:N1	2.09	0.50
48:AL:163:GLY:HA2	63:Aa:139:ARG:NH2	2.26	0.50
56:AT:119:ALA:HA	56:AT:122:GLN:O	2.12	0.50
77:Ao:58:PHE:HE2	77:Ao:61:LYS:HD2	1.76	0.50
26:BT:105:LEU:O	26:BT:109:GLU:HG3	2.12	0.50
34:B5:851:U:H1'	34:B5:853:G:OP2	2.11	0.50
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.47	0.50
44:AG:68:ARG:HD3	44:AG:237:ILE:O	2.12	0.50
3:BC:88:LYS:HD3	3:BC:95:ARG:NH2	2.27	0.50
7:BI:21:PHE:CD2	7:BI:22:ARG:HG3	2.47	0.50
18:Be:55:ARG:HH12	34:B5:557:G:P	2.35	0.50
34:B5:407:A:H2'	34:B5:408:C:C6	2.47	0.50
38:A1:446:U:H2'	38:A1:447:U:H4'	1.93	0.50
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.77	0.50
20:BF:143:ARG:HD2	29:Bc:55:VAL:HG11	1.92	0.50
33:BM:66:VAL:HG21	33:BM:71:ILE:HG21	1.93	0.50
38:A1:2438:A:C2	38:A1:2439:A:H2'	2.46	0.50
47:AJ:52:TYR:HA	47:AJ:61:ARG:HG3	1.92	0.50
5:BG:116:LYS:HE3	5:BG:125:THR:HG21	1.94	0.49
34:B5:368:U:H2'	34:B5:369:A:O4'	2.11	0.49
34:B5:625:C:H2'	34:B5:626:U:C6	2.46	0.49
38:A1:299:G:C4	71:Ai:31:GLY:HA3	2.47	0.49
38:A1:3154:C:H42	38:A1:3293:U:H3	1.59	0.49
41:AD:294:ALA:HB1	46:AI:217:PHE:HB3	1.93	0.49
8:BJ:5:PRO:HB3	34:B5:380:U:C4	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:110:GLN:NE2	8:BJ:126:ARG:HB2	2.26	0.49
14:BX:114:LYS:HG2	14:BX:115:GLY:N	2.27	0.49
19:BD:136:VAL:HG22	19:BD:186:VAL:HG22	1.92	0.49
23:BQ:69:VAL:HG11	23:BQ:81:ILE:HD11	1.93	0.49
31:Bg:180:ALA:HB3	31:Bg:190:ALA:HB3	1.93	0.49
44:AG:43:LYS:HD3	60:AX:28:THR:HG21	1.93	0.49
48:AL:163:GLY:HA2	63:Aa:139:ARG:HH22	1.77	0.49
29:Bc:57:MET:HE2	29:Bc:57:MET:HA	1.92	0.49
34:B5:1352:G:H2'	34:B5:1354:G:C8	2.47	0.49
34:B5:1715:G:H2'	34:B5:1716:C:O4'	2.13	0.49
46:AI:30:LYS:HE2	46:AI:66:GLU:CB	2.39	0.49
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.48	0.49
38:A1:3343:G:H21	38:A1:3362:A:H2	1.60	0.49
52:AP:46:LYS:HZ1	52:AP:56:ARG:HH12	1.58	0.49
56:AT:39:ILE:HG13	56:AT:102:ARG:HG3	1.95	0.49
68:Af:10:LYS:O	68:Af:33:GLU:HG2	2.12	0.49
2:BB:84:ILE:HD12	2:BB:100:PHE:HE1	1.77	0.49
9:BL:152:GLN:HA	10:BN:133:ALA:HB2	1.94	0.49
11:BO:39:ILE:HG21	11:BO:74:VAL:HG21	1.94	0.49
31:Bg:123:ILE:HD12	31:Bg:154:VAL:HB	1.94	0.49
38:A1:3:U:H3	40:A4:156:U:H3	1.59	0.49
38:A1:2278:5MC:OP1	76:An:23:ARG:NH2	2.33	0.49
71:Ai:34:SER:H	71:Ai:37:THR:HG22	1.77	0.49
3:BC:88:LYS:HD3	3:BC:95:ARG:HH21	1.76	0.49
9:BL:80:MET:HE3	9:BL:83:THR:HB	1.95	0.49
34:B5:821:U:O2	34:B5:852:C:H1'	2.12	0.49
38:A1:2265:C:H2'	38:A1:2266:PSU:H6	1.78	0.49
40:A4:151:C:C5	60:AX:24:LEU:HD11	2.48	0.49
47:AJ:37:LEU:HD12	47:AJ:69:VAL:HG12	1.94	0.49
1:BA:181:VAL:O	1:BA:185:ARG:HG2	2.12	0.49
6:BH:56:LYS:HB2	6:BH:88:ARG:HH21	1.77	0.49
34:B5:226:A:H1'	34:B5:837:G:H1	1.78	0.49
34:B5:778:G:N2	34:B5:780:A:H5'	2.27	0.49
38:A1:1580:A:C2	60:AX:33:ARG:HD2	2.48	0.49
45:AH:103:ILE:HG12	45:AH:136:PHE:CE2	2.48	0.49
7:BI:121:LEU:HG	7:BI:123:LYS:H	1.78	0.49
7:BI:190:ALA:HB1	7:BI:194:ARG:HH12	1.77	0.49
34:B5:502:U:H2'	34:B5:503:G:H8	1.77	0.49
38:A1:151:A:H5''	70:Ah:102:GLU:CD	2.37	0.49
70:Ah:5:LYS:HD2	70:Ah:8:GLU:OE2	2.13	0.49
8:BJ:149:ARG:HG2	34:B5:765:G:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:30:VAL:HG11	33:BM:133:LEU:HD22	1.94	0.49
34:B5:144:U:H1'	34:B5:145:A:H5'	1.95	0.49
34:B5:221:A:H61	34:B5:839:U:H3	1.61	0.49
34:B5:241:U:H2'	34:B5:242:U:H5''	1.95	0.49
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.47	0.49
38:A1:953:G:H4'	38:A1:954:U:O2	2.12	0.49
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.48	0.49
39:A3:4:U:H2'	39:A3:5:G:C8	2.48	0.49
8:BJ:106:GLU:HA	8:BJ:111:THR:HG21	1.94	0.49
27:BU:102:ARG:O	27:BU:106:ILE:HG12	2.13	0.49
31:Bg:178:VAL:HB	31:Bg:192:PHE:HB2	1.95	0.49
33:BM:28:LEU:HA	33:BM:31:VAL:HG12	1.95	0.49
34:B5:1220:C:H2'	34:B5:1221:A:H8	1.78	0.49
53:AQ:180:ARG:HD3	53:AQ:180:ARG:H	1.77	0.49
31:Bg:255:ALA:HB2	31:Bg:292:LEU:HD23	1.95	0.48
32:Bf:105:TYR:HE1	34:B5:1252:C:H5'	1.78	0.48
34:B5:537:G:H5''	34:B5:537:G:H8	1.76	0.48
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.48	0.48
39:A3:4:U:H2'	39:A3:5:G:H8	1.77	0.48
43:AF:50:ALA:O	43:AF:53:LYS:HG3	2.13	0.48
56:AT:75:ILE:HD13	56:AT:88:ARG:HG2	1.93	0.48
70:Ah:70:TYR:HB3	70:Ah:76:GLN:OE1	2.13	0.48
8:BJ:16:LYS:HD2	34:B5:3:U:C4	2.48	0.48
22:BP:100:LYS:HD2	34:B5:1183:A:C4	2.48	0.48
27:BU:19:ILE:HD11	27:BU:21:LYS:HE3	1.95	0.48
40:A4:79:A:H2'	40:A4:80:A:O4'	2.13	0.48
46:AI:112:GLN:O	46:AI:113:GLN:HG2	2.14	0.48
49:AM:48:GLY:HA3	49:AM:53:VAL:HB	1.95	0.48
2:BB:32:ILE:HD11	2:BB:46:THR:HB	1.95	0.48
38:A1:29:C:H4'	38:A1:62:A:H4'	1.95	0.48
45:AH:159:ALA:O	45:AH:163:GLN:HG2	2.13	0.48
3:BC:49:LYS:HD2	3:BC:243:TYR:CD2	2.48	0.48
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.48	0.48
38:A1:1225:A:H2'	38:A1:1226:G:C8	2.49	0.48
38:A1:1288:U:H2'	38:A1:1289:G:C8	2.48	0.48
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.49	0.48
38:A1:2094:C:H2'	38:A1:2095:G:C8	2.48	0.48
38:A1:2536:A:N6	38:A1:2539:C:H4'	2.27	0.48
38:A1:2927:C:H2'	38:A1:2928:C:C6	2.48	0.48
19:BD:56:GLN:CD	19:BD:56:GLN:H	2.22	0.48
36:AB:250:ALA:HB3	38:A1:2880:PSU:H1'	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AI:51:HIS:HD2	56:AT:160:ILE:HG23	1.79	0.48
46:AI:99:ILE:HG22	46:AI:123:HIS:HB2	1.95	0.48
47:AJ:160:VAL:HG13	47:AJ:171:VAL:HG21	1.96	0.48
62:AZ:50:PRO:HD3	62:AZ:68:ILE:HG12	1.95	0.48
78:Ap:13:LYS:HE3	78:Ap:14:TYR:CZ	2.49	0.48
8:BJ:126:ARG:HD3	18:Be:33:ARG:HD3	1.95	0.48
8:BJ:149:ARG:HG2	34:B5:765:G:O6	2.13	0.48
19:BD:47:GLU:HG3	19:BD:87:TYR:HE1	1.79	0.48
34:B5:734:A:C8	34:B5:735:C:H5	2.31	0.48
38:A1:2257:C:H2'	38:A1:2258:PSU:O4'	2.14	0.48
41:AD:211:LEU:HD23	41:AD:223:PHE:CE2	2.48	0.48
46:AI:30:LYS:HE2	46:AI:66:GLU:HG2	1.95	0.48
7:BI:42:ARG:HB3	7:BI:58:LEU:O	2.12	0.48
11:BO:124:ASP:HB2	34:B5:885:G:H21	1.78	0.48
20:BF:117:THR:HG21	20:BF:194:LEU:HD23	1.94	0.48
21:BK:24:LYS:HD3	21:BK:63:TYR:CE1	2.47	0.48
24:BR:10:LYS:HG2	24:BR:53:TYR:CE2	2.48	0.48
34:B5:689:G:H2'	34:B5:690:G:H8	1.79	0.48
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.49	0.48
38:A1:2534:G:H2'	38:A1:2535:A:C8	2.47	0.48
46:AI:206:LEU:O	46:AI:210:ILE:HG12	2.13	0.48
20:BF:122:ASN:HB2	20:BF:129:PRO:HG3	1.95	0.48
33:BM:62:LEU:HD13	33:BM:120:VAL:HB	1.95	0.48
34:B5:1252:C:H2'	34:B5:1253:U:C6	2.49	0.48
40:A4:26:U:H2'	40:A4:27:U:C6	2.48	0.48
7:BI:22:ARG:HG2	34:B5:385:A:H5''	1.94	0.48
55:AS:4:PHE:HD2	55:AS:104:GLU:HG2	1.79	0.48
34:B5:116:U:H2'	34:B5:117:U:C6	2.49	0.48
36:AB:57:VAL:HG22	36:AB:73:VAL:HG22	1.96	0.48
38:A1:1235:U:H5''	38:A1:1263:A:C8	2.48	0.48
3:BC:95:ARG:HH12	3:BC:97:ARG:HE	1.62	0.47
8:BJ:92:LYS:HB2	8:BJ:95:TYR:HD2	1.78	0.47
32:Bf:102:VAL:HG22	33:BM:46:ARG:HD2	1.96	0.47
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.49	0.47
38:A1:3231:U:H2'	38:A1:3232:G:H8	1.78	0.47
44:AG:47:SER:HA	44:AG:50:VAL:HG23	1.95	0.47
49:AM:49:PRO:HG3	49:AM:78:THR:HG23	1.96	0.47
53:AQ:153:PHE:O	53:AQ:161:LYS:HE2	2.14	0.47
59:AW:50:ALA:HA	59:AW:55:PHE:CG	2.49	0.47
10:BN:100:LYS:O	10:BN:103:GLU:HG3	2.14	0.47
34:B5:209:U:H2'	34:B5:210:A:H5''	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:636:A:N1	34:B5:860:U:H5	2.12	0.47
34:B5:1689:A:H3'	34:B5:1690:G:H5''	1.96	0.47
38:A1:3232:G:H2'	38:A1:3233:C:C6	2.49	0.47
51:AO:62[A]:THR:H	51:AO:69[A]:GLY:HA3	1.79	0.47
62:AZ:97:SER:O	62:AZ:100:THR:HG22	2.15	0.47
3:BC:56:ILE:HG23	3:BC:61:LEU:HB2	1.97	0.47
7:BI:187:GLU:OE1	9:BL:13:PHE:CZ	2.67	0.47
11:BO:64:ALA:HB1	11:BO:105:LEU:HD22	1.96	0.47
33:BM:59:LEU:O	33:BM:122:VAL:HA	2.14	0.47
33:BM:62:LEU:HD12	33:BM:63:VAL:H	1.80	0.47
34:B5:513:U:H2'	34:B5:514:G:C8	2.49	0.47
38:A1:185:C:H5'	61:AY:121:ARG:HG2	1.96	0.47
38:A1:2545:C:H2'	38:A1:2546:C:C6	2.49	0.47
59:AW:18:GLY:HA3	59:AW:31:PHE:O	2.14	0.47
1:BA:127:ARG:NH2	1:BA:152:PRO:HD3	2.29	0.47
4:BE:247:SER:O	4:BE:251:GLU:HG2	2.15	0.47
5:BG:20:ASP:HB2	5:BG:23:ARG:HG2	1.97	0.47
20:BF:146:THR:HB	20:BF:157:ARG:HB3	1.96	0.47
34:B5:1617:U:H2'	34:B5:1618:C:C6	2.50	0.47
48:AL:42:ARG:HA	48:AL:45:LYS:HE2	1.96	0.47
34:B5:393:C:H2'	34:B5:394:C:C6	2.50	0.47
38:A1:3227:A:H2'	38:A1:3228:C:C6	2.50	0.47
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.49	0.47
58:AV:69:LEU:HD21	58:AV:110:LYS:HE2	1.97	0.47
60:AX:73:MET:O	60:AX:77:GLU:HG3	2.14	0.47
5:BG:174:LYS:HG3	34:B5:79:C:H1'	1.97	0.47
6:BH:109:VAL:HG22	6:BH:110:GLN:H	1.80	0.47
22:BP:93:VAL:HG22	22:BP:106:GLU:OE1	2.15	0.47
34:B5:794:U:H3'	34:B5:795:U:O2	2.14	0.47
34:B5:1713:G:H2'	34:B5:1715:G:OP2	2.14	0.47
34:B5:1756[A]:A:H2'	38:A1:2256:A:N1	2.29	0.47
38:A1:567:G:H2'	38:A1:568:G:C8	2.50	0.47
38:A1:2592:G:H4'	38:A1:2594:C:C2	2.50	0.47
39:A3:119:U:H3'	41:AD:258:LYS:NZ	2.29	0.47
57:AU:54:VAL:HG22	57:AU:67:SER:HB2	1.97	0.47
25:BS:111:ASP:HA	25:BS:114:GLU:HG3	1.96	0.47
32:Bf:96:LYS:HE2	34:B5:1251:U:C5	2.50	0.47
34:B5:1656:U:H5''	34:B5:1657:U:OP2	2.15	0.47
38:A1:507:U:H2'	38:A1:508:U:C6	2.50	0.47
38:A1:1018:G:H8	38:A1:1019:G:H5'	1.79	0.47
38:A1:1688:U:H2'	38:A1:1689:U:C6	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AD:204:VAL:O	41:AD:208:MET:HG3	2.14	0.47
46:AI:168:SER:HA	56:AT:160:ILE:C	2.40	0.47
6:BH:56:LYS:HB2	6:BH:88:ARG:HE	1.79	0.47
15:BY:29:HIS:HB2	15:BY:32:ARG:HB2	1.97	0.47
16:Ba:82:ARG:HH22	34:B5:1152:A:H5'	1.80	0.47
34:B5:1647:U:H2'	34:B5:1648:A:C8	2.50	0.47
38:A1:2836:C:H5	38:A1:2852:C:N4	2.12	0.47
72:Aj:14:LYS:HD3	74:Al:51:ILE:HD11	1.97	0.47
19:BD:169:ASP:OD1	19:BD:188:ILE:HB	2.15	0.47
21:BK:77:ARG:HD3	21:BK:84:GLU:HA	1.96	0.47
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.50	0.47
38:A1:3013:U:H2'	38:A1:3014:U:C6	2.50	0.47
2:BB:156:ALA:HB3	2:BB:161:ILE:HD11	1.97	0.46
10:BN:55:ARG:HH22	17:Bb:51:GLN:HE21	1.62	0.46
16:Ba:48:ALA:HB2	29:Bc:64:ARG:HH21	1.80	0.46
27:BU:31:VAL:O	27:BU:35:GLU:HG2	2.14	0.46
36:AB:141:GLY:O	36:AB:145:GLU:HG2	2.15	0.46
36:AB:266:ARG:HD3	38:A1:2988:C:O2'	2.14	0.46
38:A1:1591:G:P	69:Ag:16:ARG:HH21	2.38	0.46
38:A1:3072:C:H2'	38:A1:3073:A:O4'	2.15	0.46
49:AM:8:LYS:HA	49:AM:8:LYS:HD3	1.76	0.46
34:B5:162:A:H3'	34:B5:163:G:H21	1.80	0.46
34:B5:507:U:H2'	34:B5:508:U:H5'	1.97	0.46
41:AD:160:PHE:HA	41:AD:163:LEU:HB3	1.95	0.46
41:AD:182:GLY:HA2	41:AD:194:LEU:HD23	1.95	0.46
48:AL:113:VAL:O	48:AL:117:LYS:HG2	2.15	0.46
69:Ag:21:LYS:HE2	69:Ag:33:GLN:OE1	2.16	0.46
1:BA:139:VAL:HG23	1:BA:141:ILE:HG12	1.97	0.46
5:BG:106:LEU:HD13	5:BG:109:LEU:HD13	1.96	0.46
17:Bb:11:THR:HG22	17:Bb:13:ALA:H	1.80	0.46
34:B5:220:A:C8	34:B5:832:U:H1'	2.50	0.46
34:B5:319:U:H4'	34:B5:323:A:C8	2.51	0.46
38:A1:129:U:H2'	38:A1:130:A:H8	1.80	0.46
39:A3:112:G:H2'	39:A3:113:C:C6	2.51	0.46
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.98	0.46
3:BC:162:CYS:SG	3:BC:212:LYS:HE2	2.55	0.46
8:BJ:133:HIS:ND1	8:BJ:162:SER:HB2	2.31	0.46
31:Bg:274:LEU:HD22	31:Bg:313:TRP:CD1	2.50	0.46
33:BM:139:HIS:O	33:BM:143:GLN:HG3	2.15	0.46
34:B5:825:U:H5'	34:B5:826:U:C4	2.50	0.46
38:A1:1555:U:H5'	38:A1:1556:C:OP2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AD:237:GLU:O	41:AD:241:THR:HG23	2.15	0.46
51:AO:97[A]:ALA:O	51:AO:100[A]:GLU:HG3	2.15	0.46
10:BN:97:SER:O	10:BN:100:LYS:HG3	2.16	0.46
25:BS:41:ARG:NH1	26:BT:46:PRO:HG3	2.31	0.46
34:B5:1352:G:H2'	34:B5:1354:G:H8	1.81	0.46
38:A1:568:G:H2'	38:A1:569:A:O4'	2.15	0.46
38:A1:1244:A:H4'	38:A1:1245:A:H5'	1.97	0.46
39:A3:8:G:OP1	56:AT:27:LEU:HD12	2.16	0.46
52:AP:128:ARG:HD2	52:AP:136:ILE:HG21	1.96	0.46
6:BH:174:ASN:ND2	6:BH:180:GLN:HE21	2.10	0.46
11:BO:80:HIS:HA	11:BO:113:GLY:O	2.16	0.46
34:B5:653:C:H4'	34:B5:655:G:N7	2.30	0.46
40:A4:135:G:H5''	60:AX:49:LYS:HD3	1.97	0.46
66:Ad:38:LYS:HD3	66:Ad:38:LYS:N	2.30	0.46
9:BL:124:THR:CG2	9:BL:141:LYS:HB3	2.46	0.46
19:BD:141:LYS:HE3	34:B5:1275:A:O2'	2.15	0.46
20:BF:114:ILE:HA	20:BF:117:THR:HG22	1.97	0.46
27:BU:63:LEU:O	27:BU:83:GLU:HA	2.16	0.46
47:AJ:141:ARG:O	47:AJ:145:LYS:HE2	2.16	0.46
2:BB:94:LYS:HD2	2:BB:94:LYS:HA	1.75	0.46
13:BW:31:SER:HB3	34:B5:636:A:H5''	1.96	0.46
34:B5:181:A:H2'	34:B5:182:A:H8	1.80	0.46
9:BL:124:THR:HG23	9:BL:140:VAL:HG23	1.97	0.46
26:BT:126:GLU:OE2	34:B5:1358:G:H4'	2.16	0.46
31:Bg:170:ILE:HG21	31:Bg:211:ILE:HD11	1.97	0.46
34:B5:108:A:H2'	34:B5:109:G:C8	2.51	0.46
37:AC:191:LYS:HG2	37:AC:194:TYR:OH	2.16	0.46
44:AG:140:VAL:HG22	44:AG:166:LEU:HD21	1.97	0.46
66:Ad:48:ASP:HB2	66:Ad:87:ASN:HD21	1.80	0.46
3:BC:102:VAL:HG11	3:BC:129:ILE:HG12	1.98	0.46
19:BD:64:ARG:HA	19:BD:64:ARG:HD2	1.52	0.46
25:BS:27:LYS:HE2	25:BS:27:LYS:HB3	1.74	0.46
34:B5:1727:G:H2'	34:B5:1728:A:C8	2.50	0.46
38:A1:120:G:N2	44:AG:124:ASP:HA	2.29	0.46
38:A1:735:A:H2'	38:A1:736:A:C4	2.51	0.46
38:A1:2966:G:H2'	38:A1:2967:A:C8	2.50	0.46
38:A1:3165:A:H3'	38:A1:3166:C:H5''	1.97	0.46
46:AI:188:GLY:H	46:AI:216:TYR:HD1	1.64	0.46
60:AX:50:ALA:O	70:Ah:66:VAL:HG21	2.16	0.46
23:BQ:22:VAL:HG22	23:BQ:65:ILE:HG12	1.98	0.45
34:B5:939:A:H2'	34:B5:940:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:655:C:H2'	38:A1:656:A:C8	2.51	0.45
41:AD:121:GLY:HA3	41:AD:168:ASP:O	2.16	0.45
44:AG:185:ARG:O	44:AG:188:THR:HG22	2.15	0.45
54:AR:134:HIS:ND1	54:AR:136:ARG:HB3	2.31	0.45
70:Ah:102:GLU:HG2	70:Ah:103:LYS:H	1.80	0.45
5:BG:180:THR:HG22	5:BG:183:ARG:HB2	1.98	0.45
14:BX:137:LYS:HB2	14:BX:137:LYS:HE3	1.67	0.45
17:Bb:55:THR:OG1	17:Bb:60:SER:HA	2.17	0.45
19:BD:158:ILE:HD12	19:BD:163:PRO:HB2	1.98	0.45
21:BK:24:LYS:HD3	21:BK:63:TYR:CZ	2.52	0.45
21:BK:49:LEU:HD12	21:BK:54:TYR:HD2	1.82	0.45
27:BU:15:GLN:N	27:BU:18:GLN:HB3	2.32	0.45
34:B5:1266:U:H2'	34:B5:1267:G:C8	2.51	0.45
45:AH:79:ILE:O	45:AH:83:THR:HG22	2.16	0.45
1:BA:50:VAL:HG22	24:BR:109:LEU:HD21	1.98	0.45
5:BG:49:VAL:HB	5:BG:115:LYS:HB3	1.97	0.45
7:BI:74:LYS:HA	7:BI:74:LYS:HD3	1.78	0.45
20:BF:63:GLN:NE2	20:BF:66:GLN:H	2.14	0.45
34:B5:195:G:H2'	34:B5:196:G:C5	2.51	0.45
35:AA:104:LEU:HD11	35:AA:158:ILE:HD11	1.97	0.45
35:AA:137:ILE:HD11	35:AA:149:ARG:HB2	1.97	0.45
35:AA:190:ARG:HG3	35:AA:191:LEU:HD22	1.98	0.45
38:A1:1560:G:H4'	38:A1:1561:G:OP1	2.16	0.45
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.17	0.45
42:AE:150:LYS:HE3	42:AE:156:LYS:HD2	1.98	0.45
47:AJ:110:ILE:HD13	47:AJ:122:ILE:HA	1.98	0.45
62:AZ:116:LYS:O	62:AZ:120:GLU:HG3	2.16	0.45
14:BX:70:LYS:HG3	14:BX:93:LEU:HD22	1.98	0.45
24:BR:58:MET:HE3	24:BR:58:MET:HB3	1.87	0.45
26:BT:16:ASN:OD1	26:BT:56:LYS:HE3	2.17	0.45
33:BM:51:ALA:HA	33:BM:54:ARG:HE	1.82	0.45
34:B5:220:A:N7	34:B5:832:U:H1'	2.31	0.45
38:A1:718:G:C2	38:A1:721:G:H1'	2.52	0.45
38:A1:995:U:H1'	38:A1:2637:A:H5'	1.97	0.45
38:A1:1553:U:H4'	38:A1:1554:U:H5'	1.97	0.45
47:AJ:53:THR:HG22	47:AJ:55:ARG:HG2	1.99	0.45
11:BO:46:MET:O	11:BO:47:LYS:HD3	2.17	0.45
19:BD:47:GLU:HG3	19:BD:87:TYR:CE1	2.52	0.45
33:BM:63:VAL:HG21	33:BM:94:ALA:N	2.30	0.45
34:B5:82:U:H2'	34:B5:83:G:O4'	2.17	0.45
34:B5:485:A:N1	34:B5:504:U:H1'	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:490:C:N4	34:B5:493:U:H5'	2.28	0.45
34:B5:1064:G:H2'	34:B5:1065:A:C8	2.51	0.45
34:B5:1469:A:H2'	34:B5:1470:C:C6	2.52	0.45
34:B5:1570:A:H2'	34:B5:1571:C:O4'	2.16	0.45
36:AB:350:ALA:O	36:AB:351:LEU:HG	2.16	0.45
38:A1:1571:A:H3'	38:A1:1572:U:C5'	2.46	0.45
38:A1:2882:U:H2'	38:A1:2883:U:C6	2.51	0.45
38:A1:3215:A:C8	49:AM:121:MET:HE3	2.51	0.45
73:Ak:40:GLN:HG3	73:Ak:57:ASN:OD1	2.16	0.45
3:BC:95:ARG:NH1	3:BC:97:ARG:HG3	2.30	0.45
5:BG:1:MET:CE	5:BG:109:LEU:HB2	2.45	0.45
13:BW:31:SER:H	13:BW:34:ILE:HD12	1.82	0.45
32:Bf:113:LYS:HD3	32:Bf:113:LYS:HA	1.54	0.45
32:Bf:133:ALA:HB3	32:Bf:140:TYR:HB3	1.99	0.45
33:BM:58:LEU:O	33:BM:87:PRO:HD2	2.17	0.45
34:B5:1382:A:HO2'	34:B5:1383:G:H8	1.65	0.45
34:B5:1504:G:H2'	34:B5:1505:A:C8	2.52	0.45
34:B5:1772:C:H2'	34:B5:1773:4AC:H6	1.98	0.45
38:A1:2272:G:H5''	38:A1:2272:G:N3	2.31	0.45
58:AV:87:ARG:HH22	58:AV:137:VAL:CG2	2.29	0.45
4:BE:199:GLU:CD	4:BE:207:LEU:HB2	2.42	0.45
8:BJ:59:LEU:HD22	8:BJ:69:ARG:HA	1.98	0.45
9:BL:40:LEU:HG	34:B5:246:G:N3	2.32	0.45
34:B5:876:G:H1'	34:B5:944:A:O4'	2.16	0.45
34:B5:1686:C:H2'	34:B5:1687:U:H5''	1.98	0.45
38:A1:662:U:H2'	38:A1:663:C:C6	2.52	0.45
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.52	0.45
38:A1:3193:C:H2'	38:A1:3194:C:C6	2.51	0.45
45:AH:74:LEU:O	45:AH:78:MET:HG3	2.17	0.45
47:AJ:53:THR:HA	47:AJ:60:ARG:HA	1.99	0.45
1:BA:136:ALA:HB1	1:BA:141:ILE:HB	1.98	0.45
8:BJ:173:ALA:HB2	34:B5:511:A:H5'	1.98	0.45
15:BY:10:ARG:HD2	15:BY:26:ASP:OD2	2.17	0.45
17:Bb:11:THR:O	17:Bb:15:GLU:HG2	2.16	0.45
34:B5:871:G:H2'	34:B5:872:G:C8	2.52	0.45
34:B5:1044:U:H2'	34:B5:1045:C:C6	2.52	0.45
38:A1:191:U:H2'	38:A1:192:C:H6	1.82	0.45
38:A1:1913:A:N3	38:A1:2120:A:H2'	2.32	0.45
38:A1:2538:U:C5	38:A1:2543:U:H2'	2.52	0.45
38:A1:3161:C:H2'	38:A1:3162:C:C6	2.52	0.45
7:BI:72:ILE:HD13	7:BI:112:TRP:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bc:22:ARG:HD3	34:B5:1162:C:H4'	1.99	0.45
33:BM:45:LEU:O	33:BM:49:THR:HG23	2.17	0.45
34:B5:486:G:H1	34:B5:501:U:H3	1.65	0.45
34:B5:1642:G:H5'	76:An:1:MET:HB2	1.98	0.45
38:A1:151:A:H5''	70:Ah:102:GLU:HG3	1.99	0.45
38:A1:922:U:OP2	72:Aj:3:LYS:HD2	2.16	0.45
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.52	0.45
70:Ah:58:ILE:O	70:Ah:62:GLN:HG3	2.17	0.45
4:BE:151:ASP:HB3	4:BE:154:ILE:HG13	1.99	0.45
34:B5:1261:G:H2'	34:B5:1262:U:C6	2.52	0.45
34:B5:1579:U:H2'	34:B5:1580:C:C6	2.52	0.45
3:BC:116:LYS:HG2	3:BC:127:ALA:HB3	1.98	0.44
8:BJ:83:VAL:HG13	8:BJ:85:VAL:HG13	1.99	0.44
26:BT:18:TYR:CD1	26:BT:135:ILE:HG13	2.51	0.44
28:BZ:95:HIS:ND1	28:BZ:96:SER:O	2.51	0.44
34:B5:1193:A:H8	34:B5:1193:A:OP1	2.00	0.44
38:A1:2260:PSU:H2'	38:A1:2261:G:C8	2.52	0.44
38:A1:3192:U:H2'	38:A1:3193:C:C6	2.52	0.44
41:AD:106:ALA:HB3	41:AD:169:GLY:HA3	1.99	0.44
62:AZ:73:LYS:HG3	62:AZ:74:VAL:N	2.32	0.44
64:Ab:41:ARG:O	64:Ab:44:LYS:HG2	2.17	0.44
7:BI:17:LYS:HE3	7:BI:17:LYS:HB3	1.75	0.44
11:BO:49:LYS:HD3	11:BO:49:LYS:HA	1.79	0.44
11:BO:68:ALA:HB1	11:BO:72:LYS:NZ	2.32	0.44
31:Bg:160:GLU:HB3	31:Bg:164:ASP:HB2	2.00	0.44
32:Bf:99:LYS:HG2	32:Bf:100:LEU:HD13	1.98	0.44
34:B5:1350:U:H2'	34:B5:1351:G:H8	1.81	0.44
38:A1:2542:U:H5'	38:A1:2543:U:OP1	2.17	0.44
38:A1:2615:G:H2'	38:A1:2616:C:C6	2.52	0.44
38:A1:3355:U:OP1	38:A1:3355:U:H2'	2.17	0.44
44:AG:55:TYR:HA	44:AG:58:VAL:HG12	1.98	0.44
57:AU:13:LYS:HE2	57:AU:15:PHE:CZ	2.52	0.44
2:BB:134:VAL:CG2	2:BB:219:LYS:HG2	2.42	0.44
5:BG:3:LEU:O	5:BG:15:THR:HA	2.17	0.44
5:BG:221:ALA:HA	5:BG:224:ALA:HB3	1.99	0.44
20:BF:163:SER:HB3	29:Bc:48:VAL:HG22	1.99	0.44
25:BS:120:ARG:O	25:BS:120:ARG:HD3	2.17	0.44
31:Bg:174:ASN:OD1	31:Bg:198:ASN:HB2	2.17	0.44
38:A1:3231:U:O2'	38:A1:3232:G:H5'	2.17	0.44
52:AP:46:LYS:NZ	52:AP:56:ARG:HH12	2.15	0.44
5:BG:118:GLU:H	5:BG:118:GLU:HG2	1.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BY:132:ARG:HA	15:BY:135:ASP:OD2	2.16	0.44
34:B5:602:U:H2'	34:B5:603:U:C6	2.52	0.44
38:A1:1803:C:H2'	38:A1:1804:A:C8	2.53	0.44
43:AF:203:TRP:CD1	43:AF:204:PRO:HD2	2.52	0.44
44:AG:70:LYS:HD3	44:AG:70:LYS:N	2.33	0.44
53:AQ:94:PHE:CE2	63:Aa:119:PRO:HD3	2.53	0.44
62:AZ:14:VAL:HG11	69:Ag:90:ILE:HD11	2.00	0.44
74:Al:5:LYS:HE2	74:Al:13:MET:HE1	2.00	0.44
1:BA:41:ARG:HD3	24:BR:103:ASP:OD1	2.18	0.44
31:Bg:153:GLN:HG3	31:Bg:201:THR:HA	1.98	0.44
32:Bf:105:TYR:CE1	34:B5:1252:C:H5'	2.53	0.44
35:AA:132:ASN:ND2	38:A1:2178:A:H5''	2.32	0.44
41:AD:143:LYS:HD3	41:AD:145:PHE:CZ	2.52	0.44
15:BY:8:ARG:HD2	34:B5:780:A:C4	2.53	0.44
21:BK:49:LEU:O	21:BK:54:TYR:HB2	2.18	0.44
31:Bg:38:ARG:HG2	31:Bg:67:ILE:HG23	1.98	0.44
31:Bg:161:LYS:HD2	31:Bg:161:LYS:HA	1.81	0.44
37:AC:183:LYS:HA	37:AC:183:LYS:HD2	1.71	0.44
38:A1:3159:C:H2'	38:A1:3160:U:C6	2.53	0.44
38:A1:3393:U:H2'	38:A1:3394:U:C6	2.53	0.44
45:AH:21:LYS:NZ	49:AM:8:LYS:HE3	2.33	0.44
45:AH:36:LYS:HE3	45:AH:74:LEU:HB3	1.99	0.44
5:BG:197:ASN:O	5:BG:201:GLN:HG2	2.18	0.44
19:BD:176:LEU:HD11	34:B5:1437:U:H5''	1.98	0.44
38:A1:118:U:O2	38:A1:121:A:H5''	2.17	0.44
38:A1:1815:U:H1'	38:A1:1817:G:N2	2.33	0.44
38:A1:2747:A:H5'	41:AD:175:HIS:HA	1.99	0.44
41:AD:290:ILE:O	41:AD:294:ALA:HB3	2.18	0.44
1:BA:206:ASP:HA	1:BA:207:PRO:HA	1.62	0.44
3:BC:101:VAL:HG22	3:BC:115:ILE:HD12	2.00	0.44
4:BE:133:LYS:HZ1	34:B5:294:C:H5'	1.83	0.44
11:BO:46:MET:HE3	34:B5:898:A:H5'	2.00	0.44
17:Bb:33:LEU:HD23	17:Bb:81:ARG:HA	1.99	0.44
34:B5:182:A:H2'	34:B5:183:U:C6	2.53	0.44
34:B5:542:A:H5''	34:B5:544:A:O4'	2.18	0.44
34:B5:822:U:N3	34:B5:849:C:H2'	2.31	0.44
36:AB:160:VAL:HG13	36:AB:183:LEU:HD11	1.99	0.44
37:AC:92:ASN:HA	37:AC:98:ARG:O	2.18	0.44
38:A1:151:A:H5''	70:Ah:102:GLU:CG	2.48	0.44
38:A1:442:G:OP2	38:A1:443:G:H8	2.01	0.44
38:A1:1306:G:C6	51:AO:62[A]:THR:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3121:U:H1'	38:A1:3122:A:H5''	1.99	0.44
38:A1:3232:G:H2'	38:A1:3233:C:H6	1.83	0.44
40:A4:81:U:H4'	40:A4:82:U:O5'	2.18	0.44
66:Ad:34:LYS:O	66:Ad:38:LYS:HG2	2.17	0.44
34:B5:1585:U:N3	34:B5:1611:A:H2	2.15	0.44
38:A1:716:A:N7	63:Aa:117:ARG:HG3	2.33	0.44
38:A1:1226:G:H2'	38:A1:1227:C:C6	2.53	0.44
38:A1:3153:U:H4'	38:A1:3154:C:C4	2.53	0.44
45:AH:106:LYS:HG3	45:AH:111:PHE:CD1	2.53	0.44
54:AR:173:ARG:O	54:AR:177:VAL:HG22	2.18	0.44
1:BA:79:ARG:O	1:BA:83:GLN:HG3	2.18	0.43
5:BG:1:MET:HG3	5:BG:106:LEU:O	2.18	0.43
12:BV:30:ALA:O	12:BV:60:ARG:HD3	2.18	0.43
20:BF:80:LYS:CG	20:BF:83:ARG:HE	2.30	0.43
34:B5:226:A:H62	34:B5:834:G:H2'	1.82	0.43
34:B5:1064:G:H2'	34:B5:1065:A:H8	1.83	0.43
38:A1:1093:A:H1'	38:A1:1094:U:H4'	2.00	0.43
38:A1:2223:A:H2'	38:A1:2224:A:C8	2.52	0.43
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.53	0.43
38:A1:3349:C:H2'	38:A1:3350:C:O4'	2.18	0.43
42:AE:36:PRO:O	42:AE:90:LYS:HE2	2.18	0.43
45:AH:157:ASN:C	45:AH:157:ASN:HD22	2.25	0.43
1:BA:76:ILE:HD13	1:BA:98:ILE:HB	2.00	0.43
12:BV:11:LEU:HD23	12:BV:11:LEU:HA	1.83	0.43
21:BK:7:ASP:HA	21:BK:10:LYS:HB2	2.00	0.43
34:B5:538:A:H5'	34:B5:543:C:H41	1.82	0.43
38:A1:524:U:H2'	38:A1:525:C:H5'	1.99	0.43
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.53	0.43
38:A1:2794:G:H5''	77:Ao:61:LYS:NZ	2.33	0.43
38:A1:3034:C:H5	45:AH:121:LYS:HB2	1.82	0.43
71:Ai:34:SER:H	71:Ai:37:THR:CG2	2.30	0.43
5:BG:52:ILE:HD12	5:BG:109:LEU:HD21	2.01	0.43
21:BK:13:GLN:O	21:BK:17:GLN:HG2	2.18	0.43
26:BT:130:ARG:HD3	26:BT:134:ARG:HH21	1.84	0.43
27:BU:100:VAL:O	27:BU:103:ILE:HG22	2.17	0.43
29:Bc:41:VAL:HG12	29:Bc:63:ALA:HB3	2.01	0.43
34:B5:874:C:H2'	34:B5:875:G:C8	2.53	0.43
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.34	0.43
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.53	0.43
54:AR:43:LYS:O	54:AR:46:LYS:HG3	2.18	0.43
56:AT:32:LYS:NZ	56:AT:98:HIS:H	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:26:ALA:HB2	1:BA:148:ASP:OD2	2.18	0.43
11:BO:81:VAL:HG11	11:BO:102:LEU:HD13	2.00	0.43
19:BD:94:ARG:HH11	19:BD:125:TYR:HE2	1.65	0.43
20:BF:63:GLN:HE22	20:BF:66:GLN:H	1.64	0.43
31:Bg:65:SER:OG	34:B5:1341:A:H1'	2.18	0.43
33:BM:69:ALA:O	33:BM:72:ILE:HG12	2.19	0.43
34:B5:30:G:H2'	34:B5:31:C:C6	2.54	0.43
34:B5:256:A:H2'	34:B5:257:A:O4'	2.18	0.43
34:B5:413:U:H2'	34:B5:414:C:C6	2.53	0.43
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.54	0.43
37:AC:317:PRO:O	37:AC:318:LEU:HG	2.18	0.43
38:A1:391:A:H2'	38:A1:392:G:O4'	2.17	0.43
38:A1:784:A:C6	53:AQ:93:ILE:HG22	2.53	0.43
55:AS:1:MET:HB3	55:AS:4:PHE:CZ	2.53	0.43
8:BJ:92:LYS:HB2	8:BJ:95:TYR:CD2	2.54	0.43
11:BO:86:THR:HG21	11:BO:90:ARG:HE	1.84	0.43
18:Be:20:LYS:HE3	18:Be:22:GLU:OE2	2.17	0.43
25:BS:120:ARG:HG2	25:BS:125:ILE:HD11	1.99	0.43
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	1.99	0.43
38:A1:94:G:H2'	38:A1:95:A:C8	2.53	0.43
38:A1:1563:C:OP1	38:A1:1563:C:H4'	2.18	0.43
39:A3:90:U:H2'	39:A3:91:G:O4'	2.19	0.43
42:AE:43:LEU:HD11	42:AE:85:ILE:HG13	2.01	0.43
43:AF:34:LYS:HD3	43:AF:34:LYS:HA	1.72	0.43
2:BB:97:LEU:HB3	2:BB:232:HIS:CD2	2.53	0.43
11:BO:103:ARG:HD2	16:Ba:49:ALA:HB2	1.99	0.43
34:B5:1503:A:H2'	34:B5:1504:G:O4'	2.19	0.43
38:A1:772:U:H2'	38:A1:773:G:O4'	2.19	0.43
42:AE:71:VAL:HG22	42:AE:156:LYS:HE2	2.00	0.43
47:AJ:89:TYR:HB3	47:AJ:169:ALA:HB2	1.99	0.43
25:BS:126:ARG:HB2	25:BS:133:VAL:HG12	2.00	0.43
31:Bg:192:PHE:HD2	31:Bg:223:TRP:CE3	2.36	0.43
34:B5:640:U:H2'	34:B5:641:G:O4'	2.19	0.43
34:B5:647:G:H2'	34:B5:648:G:H8	1.80	0.43
34:B5:852:C:H2'	34:B5:853:G:O4'	2.19	0.43
37:AC:159:ILE:HD13	37:AC:164:GLU:HG3	2.01	0.43
38:A1:1288:U:H2'	38:A1:1289:G:H8	1.84	0.43
38:A1:2203:U:H2'	38:A1:2204:C:C6	2.54	0.43
38:A1:3274:A:H5''	38:A1:3276:G:OP2	2.18	0.43
47:AJ:106:ILE:HG13	47:AJ:127:PHE:HE2	1.84	0.43
55:AS:80:ARG:HG2	55:AS:122:HIS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:211:LYS:HE2	4:BE:211:LYS:HB2	1.79	0.43
5:BG:7:TYR:CE2	5:BG:125:THR:HG23	2.53	0.43
5:BG:113:ILE:HD11	5:BG:124:LEU:HD13	2.01	0.43
34:B5:778:G:C2	34:B5:780:A:H5'	2.54	0.43
34:B5:906:A:H2'	34:B5:907:A:C8	2.54	0.43
36:AB:291:GLU:HG3	36:AB:302:LYS:HE2	2.01	0.43
38:A1:261:U:H2'	38:A1:262:U:C6	2.54	0.43
38:A1:1282:G:O2'	38:A1:1283:C:H5'	2.18	0.43
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.54	0.43
41:AD:211:LEU:HG	41:AD:219:PHE:HB2	2.00	0.43
53:AQ:31:LYS:HD2	53:AQ:31:LYS:HA	1.65	0.43
55:AS:124:LEU:HD23	56:AT:153:PRO:HB2	2.01	0.43
65:Ac:21:GLY:O	65:Ac:22:LYS:HD3	2.18	0.43
2:BB:29:TRP:CZ3	11:BO:13:VAL:HG11	2.54	0.43
2:BB:41:ARG:HA	2:BB:41:ARG:HD3	1.76	0.43
7:BI:74:LYS:HB2	7:BI:109:PHE:CZ	2.54	0.43
31:Bg:169:ILE:HG13	31:Bg:181:TRP:HB2	1.99	0.43
34:B5:1287:A:H3'	34:B5:1314:U:OP1	2.19	0.43
34:B5:1695:G:N3	34:B5:1695:G:H2'	2.34	0.43
34:B5:1733:C:H2'	34:B5:1734:U:H6	1.83	0.43
35:AA:181:LYS:HB2	38:A1:860:G:C5	2.53	0.43
38:A1:1307:G:H4'	38:A1:1308:A:H5'	2.01	0.43
38:A1:2204:C:H2'	38:A1:2205:U:C6	2.54	0.43
39:A3:1:G:C4	41:AD:266:ALA:HA	2.54	0.43
2:BB:144:ARG:HB2	2:BB:208:GLN:HB2	2.01	0.43
7:BI:190:ALA:O	7:BI:194:ARG:HG2	2.18	0.43
23:BQ:8:GLN:HG2	23:BQ:21:HIS:ND1	2.34	0.43
34:B5:1160:A:H2'	34:B5:1161:C:H6	1.84	0.43
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.53	0.43
34:B5:1682:U:O2'	34:B5:1683:C:H5'	2.19	0.43
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.53	0.43
38:A1:3291:G:H2'	38:A1:3292:A:H8	1.83	0.43
55:AS:100:VAL:O	55:AS:104:GLU:HG3	2.19	0.43
56:AT:104:GLU:O	56:AT:107:GLU:HG3	2.19	0.43
69:Ag:74:ARG:NH2	69:Ag:82:ALA:HB2	2.34	0.43
4:BE:238:LEU:HB2	4:BE:242:LYS:HD2	2.00	0.42
14:BX:137:LYS:NZ	14:BX:139:LYS:HE3	2.34	0.42
18:Be:30:PRO:O	18:Be:35:TYR:HB2	2.18	0.42
22:BP:52:LYS:HG2	22:BP:53:PRO:HD3	2.01	0.42
30:Bd:54:LYS:HZ3	34:B5:1420:C:P	2.42	0.42
37:AC:314:LYS:HD2	43:AF:162:PRO:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2696:A:H2'	38:A1:2697:A:C8	2.54	0.42
43:AF:77:VAL:HB	56:AT:139:ARG:HG2	2.01	0.42
44:AG:113:ALA:HA	44:AG:116:VAL:HB	2.00	0.42
20:BF:89:ILE:HD12	20:BF:89:ILE:HA	1.92	0.42
32:Bf:102:VAL:HA	32:Bf:105:TYR:CD2	2.54	0.42
34:B5:780:A:H3'	34:B5:781:U:H5'	2.01	0.42
34:B5:1266:U:H2'	34:B5:1267:G:H8	1.85	0.42
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.84	0.42
42:AE:52:VAL:HB	42:AE:67:GLY:H	1.84	0.42
58:AV:4:ASN:HD21	58:AV:106:LYS:HE3	1.84	0.42
4:BE:239:PRO:O	4:BE:242:LYS:HD3	2.19	0.42
31:Bg:9:LEU:HB2	31:Bg:313:TRP:NE1	2.34	0.42
34:B5:919:A:H2'	34:B5:920:U:C6	2.54	0.42
34:B5:1391:A:H2'	34:B5:1392:U:C6	2.54	0.42
38:A1:2167:A:H2'	38:A1:2168:A:C8	2.54	0.42
41:AD:294:ALA:CB	46:AI:217:PHE:HB3	2.49	0.42
43:AF:208:SER:O	43:AF:243:MET:HB3	2.19	0.42
46:AI:72:ALA:HB2	46:AI:155:ALA:HB2	2.00	0.42
9:BL:3:THR:OG1	9:BL:51:GLY:HA2	2.19	0.42
13:BW:30:SER:HB2	13:BW:61:ILE:HD12	2.01	0.42
19:BD:59:LEU:HD12	19:BD:66:ILE:HG21	2.01	0.42
34:B5:60:U:H5'	34:B5:455:C:N4	2.33	0.42
38:A1:2438:A:H3'	38:A1:2439:A:H3'	1.99	0.42
41:AD:40:HIS:CE1	41:AD:42:ALA:HB3	2.55	0.42
63:Aa:34:MET:HE3	63:Aa:34:MET:HB3	1.94	0.42
4:BE:208:VAL:HG12	4:BE:210:ILE:HG13	2.01	0.42
6:BH:61:PHE:HA	6:BH:93:LEU:O	2.19	0.42
18:Be:53:LYS:HA	18:Be:53:LYS:HD2	1.70	0.42
38:A1:2674:A:H8	47:AJ:126:ASP:OD1	2.03	0.42
56:AT:102:ARG:O	56:AT:106:LEU:HD23	2.18	0.42
6:BH:24:PHE:HE1	6:BH:81:LEU:HD11	1.84	0.42
6:BH:164:TYR:CE2	6:BH:165:LYS:HG3	2.54	0.42
15:BY:104:SER:O	15:BY:108:ARG:HG3	2.20	0.42
16:Ba:62:TYR:HD2	16:Ba:64:LEU:HD22	1.84	0.42
34:B5:1133:A:H2'	34:B5:1134:C:O4'	2.19	0.42
34:B5:1648:A:H2'	34:B5:1649:G:H8	1.83	0.42
38:A1:664:U:H2'	38:A1:665:A:C8	2.55	0.42
38:A1:993:G:N3	38:A1:2637:A:H2'	2.34	0.42
47:AJ:105:GLY:HA2	47:AJ:126:ASP:HA	2.01	0.42
47:AJ:132:ASN:HA	47:AJ:154:THR:HG21	2.02	0.42
2:BB:30:PHE:HA	2:BB:94:LYS:HE3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:97:ARG:HE	6:BH:97:ARG:HB2	1.69	0.42
33:BM:47:GLU:HG3	34:B5:1229:G:O6	2.20	0.42
33:BM:52:LEU:HA	33:BM:57:ALA:HB2	2.01	0.42
34:B5:413:U:H2'	34:B5:414:C:H6	1.85	0.42
34:B5:1231:U:H5	34:B5:1254:U:O2	2.02	0.42
34:B5:1739:C:H2'	34:B5:1740:A:C8	2.54	0.42
39:A3:49:G:O2'	41:AD:58:LYS:HE3	2.19	0.42
9:BL:156:PHE:HB3	54:AR:156:ASN:ND2	2.35	0.42
11:BO:47:LYS:HD3	11:BO:47:LYS:HA	1.75	0.42
20:BF:26:ALA:HB2	23:BQ:26:LYS:HG3	2.01	0.42
34:B5:156:A:H2'	34:B5:157:A:O4'	2.19	0.42
34:B5:304:U:H2'	34:B5:305:C:C6	2.55	0.42
34:B5:946:U:H2'	34:B5:947:U:C6	2.54	0.42
34:B5:1063:U:H2'	34:B5:1064:G:C8	2.54	0.42
34:B5:1576:A:O5'	34:B5:1576:A:H8	2.03	0.42
38:A1:1048:A:H2'	46:AI:22:TYR:CZ	2.55	0.42
38:A1:1049:C:H2'	38:A1:1050:U:C6	2.55	0.42
38:A1:2567:C:H2'	38:A1:2568:C:C6	2.55	0.42
38:A1:3028:G:H8	38:A1:3028:G:OP2	2.03	0.42
47:AJ:110:ILE:HD11	47:AJ:123:PHE:HB2	2.01	0.42
61:AY:51:ARG:HG2	61:AY:52:ARG:N	2.35	0.42
62:AZ:60:LYS:HB2	62:AZ:60:LYS:HE2	1.66	0.42
71:AI:88:GLU:O	71:AI:92:ASN:OD1	2.38	0.42
2:BB:26:ARG:O	2:BB:50:LYS:HG2	2.20	0.42
5:BG:215:ARG:HD3	5:BG:215:ARG:HA	1.90	0.42
8:BJ:38:ASN:OD1	8:BJ:41:GLU:HG3	2.20	0.42
9:BL:36:LYS:HD3	34:B5:248:U:H4'	2.02	0.42
27:BU:17:GLN:CG	27:BU:96:PRO:HG3	2.48	0.42
34:B5:358:U:H5''	34:B5:359:A:C2	2.55	0.42
34:B5:649:U:H3	34:B5:684:A:H62	0.63	0.42
34:B5:651:G:O5'	34:B5:651:G:H8	2.02	0.42
34:B5:800:U:H2'	34:B5:801:G:C8	2.55	0.42
34:B5:901:G:H2'	34:B5:902:G:C8	2.55	0.42
34:B5:1157:A:H2'	34:B5:1160:A:N7	2.35	0.42
34:B5:1417:A:H2'	34:B5:1418:G:O4'	2.20	0.42
34:B5:1542:G:N2	34:B5:1568:C:H1'	2.35	0.42
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.55	0.42
41:AD:40:HIS:HB3	41:AD:43:LYS:HD2	2.02	0.42
45:AH:69:ARG:NH1	45:AH:72:LYS:HD3	2.34	0.42
2:BB:67:GLU:HG2	2:BB:83:LYS:HD3	2.01	0.42
11:BO:68:ALA:HB1	11:BO:72:LYS:HZ3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:35:ILE:HB	25:BS:38:VAL:HG22	2.01	0.42
26:BT:29:GLU:HB3	26:BT:110:LYS:HZ1	1.84	0.42
26:BT:105:LEU:HD13	26:BT:122:ARG:HD3	2.02	0.42
34:B5:1603:U:H2'	34:B5:1604:U:C6	2.55	0.42
38:A1:1284:C:H6	38:A1:1285:G:C8	2.38	0.42
38:A1:2424:A:H2'	38:A1:2425:G:O4'	2.20	0.42
38:A1:2532:U:H2'	38:A1:2533:G:C8	2.55	0.42
38:A1:3253:G:H2'	38:A1:3254:G:O4'	2.20	0.42
1:BA:188:LEU:HD23	1:BA:188:LEU:HA	1.88	0.41
4:BE:63:ALA:O	4:BE:67:GLN:HG3	2.20	0.41
5:BG:48:TYR:CZ	5:BG:121:LEU:HD23	2.55	0.41
20:BF:148:ARG:HD3	20:BF:157:ARG:HD3	2.02	0.41
23:BQ:83:GLN:HE22	23:BQ:119:ALA:HA	1.85	0.41
24:BR:14:LYS:HZ2	24:BR:57:LEU:HD21	1.85	0.41
32:Bf:85:TYR:CZ	34:B5:1445:G:H1'	2.55	0.41
34:B5:1355:C:H2'	34:B5:1356:U:O4'	2.19	0.41
35:AA:2:GLY:HA2	35:AA:207:VAL:HG23	2.01	0.41
36:AB:339:ARG:HG2	36:AB:340:LYS:O	2.20	0.41
38:A1:545:U:H5'	38:A1:546:C:H5	1.85	0.41
38:A1:1046:A:H2'	38:A1:1049:C:C5	2.55	0.41
38:A1:1809:A:H2'	38:A1:1810:A:O4'	2.20	0.41
41:AD:218:ARG:NH2	41:AD:222:LEU:HG	2.35	0.41
62:AZ:9:LYS:HA	62:AZ:9:LYS:HD3	1.79	0.41
66:Ad:6:ASP:HB2	66:Ad:89:LEU:HD11	2.01	0.41
72:Aj:85:LYS:HD2	72:Aj:86:ALA:H	1.85	0.41
1:BA:74:VAL:HG23	1:BA:118:PRO:HB3	2.02	0.41
2:BB:124:ASN:HD21	2:BB:136:ARG:HD3	1.84	0.41
5:BG:23:ARG:HH21	5:BG:42:GLY:HA2	1.85	0.41
6:BH:117:THR:HB	34:B5:639:U:OP2	2.19	0.41
10:BN:55:ARG:HD3	34:B5:960:U:H5'	2.02	0.41
15:BY:96:LEU:HA	15:BY:96:LEU:HD23	1.86	0.41
21:BK:75:TYR:O	21:BK:78:GLU:HG3	2.20	0.41
34:B5:526:A:H2'	34:B5:527:A:O4'	2.20	0.41
38:A1:417:A:H2'	38:A1:418:A:C8	2.56	0.41
38:A1:585:A:H2'	38:A1:586:C:C6	2.55	0.41
38:A1:1234:G:H5''	38:A1:1263:A:H5''	2.03	0.41
38:A1:3356:G:H2'	38:A1:3357:U:H6	1.86	0.41
53:AQ:180:ARG:HD3	53:AQ:180:ARG:N	2.35	0.41
1:BA:40:ALA:HA	1:BA:46:HIS:HA	2.01	0.41
3:BC:91:ARG:NH1	34:B5:1146:G:O3'	2.53	0.41
12:BV:36:VAL:HB	12:BV:51:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:62:LEU:HD23	33:BM:90:LYS:NZ	2.34	0.41
34:B5:734:A:H2'	34:B5:735:C:C5	2.55	0.41
38:A1:173:G:H1	38:A1:244:G:H1	1.68	0.41
38:A1:1354:G:H5''	38:A1:1355:A:C8	2.55	0.41
38:A1:2407:C:H2'	38:A1:2408:U:C6	2.56	0.41
41:AD:8:LYS:HD3	41:AD:12:TYR:CE1	2.54	0.41
41:AD:200:PHE:CE1	41:AD:241:THR:HG22	2.55	0.41
44:AG:84:ARG:HG3	44:AG:84:ARG:HH11	1.83	0.41
51:AO:12[A]:LYS:HD2	51:AO:40[A]:GLU:OE1	2.20	0.41
24:BR:3:ARG:HH21	34:B5:1413:U:H5'	1.84	0.41
26:BT:70:GLN:HG3	26:BT:120:GLY:HA3	2.02	0.41
29:Bc:14:LYS:HB3	29:Bc:29:ARG:HB3	2.01	0.41
34:B5:1317:C:H2'	34:B5:1318:G:O4'	2.20	0.41
38:A1:879:U:O2	38:A1:2357:A:H1'	2.20	0.41
38:A1:1803:C:H2'	38:A1:1804:A:H8	1.85	0.41
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.54	0.41
38:A1:2528:G:H2'	38:A1:2529:A:O4'	2.20	0.41
38:A1:2553:U:C4	69:Ag:95:ILE:HG12	2.55	0.41
38:A1:3261:C:O2'	38:A1:3262:U:H5'	2.21	0.41
40:A4:155:A:H2'	40:A4:156:U:O4'	2.19	0.41
66:Ad:57:GLN:HE21	66:Ad:57:GLN:HB3	1.56	0.41
3:BC:40:LYS:HE3	3:BC:248:SER:HB3	2.01	0.41
5:BG:109:LEU:HD12	5:BG:109:LEU:HA	1.83	0.41
11:BO:92:LYS:HE3	11:BO:92:LYS:HB3	1.76	0.41
22:BP:121:ILE:H	25:BS:120:ARG:HH22	1.69	0.41
25:BS:42:TYR:CD1	25:BS:85:PHE:CE2	3.08	0.41
34:B5:121:U:H2'	34:B5:122:U:C6	2.55	0.41
38:A1:178:U:H2'	38:A1:179:C:C6	2.56	0.41
32:Bf:117:LEU:C	32:Bf:118:ARG:HD2	2.45	0.41
34:B5:800:U:H2'	34:B5:801:G:H8	1.85	0.41
34:B5:1058:U:H2'	34:B5:1061:A:C2	2.56	0.41
35:AA:22:LEU:HD23	35:AA:22:LEU:HA	1.89	0.41
36:AB:218:ILE:HG13	36:AB:276:THR:HG23	2.02	0.41
37:AC:35:VAL:HG21	37:AC:244:LEU:HD21	2.03	0.41
38:A1:230:U:H2'	38:A1:231:G:O4'	2.21	0.41
38:A1:601:U:H3'	38:A1:602:A:H8	1.85	0.41
38:A1:1094:U:C6	56:AT:125:ALA:HB2	2.56	0.41
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.21	0.41
45:AH:103:ILE:HG12	45:AH:136:PHE:CZ	2.55	0.41
56:AT:84:TYR:HB2	64:Ab:24:PRO:HD3	2.03	0.41
62:AZ:5:LEU:HD11	65:Ac:35:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Ak:60:GLY:HA2	73:Ak:63:LYS:CE	2.51	0.41
1:BA:30:GLN:NE2	1:BA:33:GLN:HG2	2.23	0.41
5:BG:22:HIS:O	5:BG:25:ARG:HG2	2.21	0.41
6:BH:166:LEU:O	6:BH:170:GLN:HG3	2.21	0.41
11:BO:124:ASP:OD2	34:B5:928:U:H1'	2.20	0.41
12:BV:48:GLY:HA2	12:BV:50:TYR:CZ	2.56	0.41
21:BK:92:ILE:HG21	21:BK:96:ASN:N	2.36	0.41
28:BZ:82:HIS:O	28:BZ:86:GLU:HG2	2.21	0.41
34:B5:1292:G:H2'	34:B5:1293:U:C6	2.56	0.41
38:A1:191:U:H2'	38:A1:192:C:C6	2.56	0.41
38:A1:374:A:N3	38:A1:376:G:H5''	2.35	0.41
38:A1:528:U:H2'	38:A1:529:A:H8	1.81	0.41
38:A1:1583:A:H2'	38:A1:1584:U:O4'	2.20	0.41
40:A4:142:C:H2'	40:A4:143:U:C6	2.56	0.41
41:AD:79:TYR:O	41:AD:82:GLU:HG2	2.21	0.41
57:AU:37:LEU:O	57:AU:41:ILE:HG13	2.21	0.41
9:BL:3:THR:HA	9:BL:52:SER:N	2.35	0.41
24:BR:7:LYS:HG3	24:BR:11:ARG:HH12	1.85	0.41
34:B5:187:G:H21	34:B5:198:A:H62	1.68	0.41
34:B5:847:A:H2'	34:B5:848:C:O4'	2.21	0.41
38:A1:629:U:H2'	38:A1:630:A:C8	2.56	0.41
38:A1:1120:A:H2'	38:A1:1121:U:C6	2.56	0.41
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.55	0.41
38:A1:2271:A:H2'	38:A1:2272:G:O4'	2.21	0.41
39:A3:64:A:H5''	46:AI:206:LEU:HB2	2.02	0.41
42:AE:40:LEU:HD11	42:AE:54:TYR:HB2	2.01	0.41
55:AS:135:VAL:O	55:AS:141:LYS:HE3	2.20	0.41
1:BA:119:ARG:HA	1:BA:119:ARG:HD2	1.94	0.41
1:BA:121:VAL:HG23	1:BA:141:ILE:HG21	2.02	0.41
2:BB:103:MET:HE3	2:BB:215:VAL:HG23	2.02	0.41
2:BB:146:GLN:NE2	34:B5:1065:A:N3	2.68	0.41
5:BG:36:VAL:HG12	5:BG:50:PHE:HB2	2.03	0.41
7:BI:58:LEU:O	7:BI:59:ARG:HB2	2.20	0.41
10:BN:33:VAL:HG21	10:BN:66:ILE:HG21	2.03	0.41
11:BO:20:TYR:HB3	11:BO:27:PHE:HB2	2.03	0.41
11:BO:107:ARG:NE	16:Ba:52:ASP:OD2	2.53	0.41
16:Ba:64:LEU:HD13	16:Ba:64:LEU:HA	1.94	0.41
22:BP:100:LYS:HD2	34:B5:1183:A:C5	2.56	0.41
31:Bg:79:TYR:HE1	31:Bg:100:TYR:CE2	2.39	0.41
32:Bf:100:LEU:HD23	32:Bf:103:LEU:HD12	2.02	0.41
34:B5:16:G:H2'	34:B5:17:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:119:A:H1'	34:B5:397:A:C8	2.56	0.41
36:AB:236:LYS:HE2	36:AB:236:LYS:HB2	1.72	0.41
38:A1:59:G:H2'	40:A4:33:A:O2'	2.21	0.41
38:A1:655:C:H2'	38:A1:656:A:H8	1.85	0.41
38:A1:1259:A:H3'	38:A1:1260:A:C8	2.56	0.41
38:A1:1915:A:H2'	38:A1:1916:U:C6	2.56	0.41
38:A1:3238:G:H2'	38:A1:3239:G:O4'	2.19	0.41
39:A3:74:C:O2	39:A3:105:C:H5	2.04	0.41
46:AI:68:ALA:HB1	46:AI:155:ALA:HB1	2.03	0.41
47:AJ:25:GLU:HA	47:AJ:65:ILE:HG22	2.03	0.41
50:AN:154:PRO:O	50:AN:157:LYS:HG3	2.21	0.41
70:Ah:31:LEU:HB3	70:Ah:44:ILE:CD1	2.51	0.41
6:BH:81:LEU:O	6:BH:85:PHE:HB2	2.20	0.41
27:BU:95:ALA:HB1	27:BU:99:ILE:HD11	2.03	0.41
34:B5:585:A:H2'	34:B5:586:G:C8	2.56	0.41
34:B5:849:C:H5'	34:B5:850:A:C5'	2.46	0.41
34:B5:1180:C:H2'	34:B5:1181:PSU:O4'	2.21	0.41
38:A1:176:G:N2	38:A1:242:C:N3	2.69	0.41
38:A1:257:U:H2'	38:A1:258:G:C8	2.56	0.41
38:A1:1629:U:O4	62:AZ:111:LYS:HD2	2.21	0.41
38:A1:2615:G:H2'	38:A1:2616:C:H6	1.86	0.41
41:AD:220:SER:O	41:AD:224:LYS:HB2	2.20	0.41
52:AP:4:TYR:CE2	52:AP:16:SER:HB2	2.56	0.41
55:AS:50:LYS:HB2	55:AS:50:LYS:HE3	1.90	0.41
61:AY:39:LEU:HD23	61:AY:39:LEU:HA	1.88	0.41
6:BH:38:LEU:HA	6:BH:41:LEU:HD22	2.02	0.40
12:BV:73:ALA:HB1	12:BV:78:LEU:HB2	2.03	0.40
20:BF:82:PHE:CZ	29:Bc:49:ARG:HG3	2.57	0.40
34:B5:195:G:H2'	34:B5:196:G:C4	2.56	0.40
35:AA:40:TYR:O	38:A1:2550:U:H5	2.04	0.40
38:A1:947:G:H5''	67:Ae:55:ILE:HB	2.03	0.40
38:A1:1740:U:H1'	38:A1:1741:A:H2	1.87	0.40
38:A1:1801:U:H2'	38:A1:1802:C:C6	2.56	0.40
52:AP:179:GLN:HA	52:AP:182:ILE:HG22	2.03	0.40
1:BA:17:LEU:HD23	1:BA:22:THR:HG21	2.03	0.40
4:BE:252:ARG:O	4:BE:256:ARG:HG2	2.22	0.40
8:BJ:90:LYS:HB2	8:BJ:95:TYR:CE2	2.56	0.40
9:BL:131:ILE:HD13	9:BL:131:ILE:HA	1.83	0.40
9:BL:156:PHE:HB3	54:AR:156:ASN:HD22	1.87	0.40
16:Ba:5:ARG:HB2	16:Ba:8:ASN:O	2.21	0.40
19:BD:177:MET:HG3	19:BD:182:LEU:HG	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AJ:38:GLU:OE2	47:AJ:44:THR:HA	2.20	0.40
48:AL:41:THR:O	48:AL:45:LYS:HG3	2.21	0.40
50:AN:180:PHE:HB3	50:AN:183:THR:O	2.21	0.40
56:AT:14:MET:HG3	56:AT:15:PHE:CD1	2.55	0.40
66:Ad:31:ARG:HD2	66:Ad:35:GLU:OE2	2.20	0.40
6:BH:24:PHE:CE1	6:BH:81:LEU:HD11	2.56	0.40
19:BD:40:ARG:HG3	19:BD:47:GLU:HB3	2.02	0.40
34:B5:895:G:H2'	34:B5:896:U:C6	2.57	0.40
34:B5:1756[A]:A:H2'	38:A1:2256:A:C2	2.57	0.40
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	2.02	0.40
36:AB:256:HIS:HA	36:AB:257:PRO:C	2.47	0.40
38:A1:240:U:H1'	38:A1:241:G:C8	2.56	0.40
38:A1:1323:G:O2'	55:AS:2:ALA:HB3	2.22	0.40
38:A1:3352:U:H6	38:A1:3352:U:P	2.44	0.40
6:BH:56:LYS:O	6:BH:88:ARG:HA	2.21	0.40
14:BX:107:PHE:CZ	14:BX:114:LYS:HD3	2.56	0.40
20:BF:182:ALA:HB3	20:BF:193:THR:HG21	2.02	0.40
29:Bc:17:GLY:HA3	29:Bc:67:ARG:NE	2.31	0.40
34:B5:891:A:H2'	34:B5:892:A:C8	2.57	0.40
34:B5:1752:U:H2'	34:B5:1753:A:C8	2.56	0.40
35:AA:21:ARG:HD3	38:A1:824:C:H5''	2.03	0.40
38:A1:1575:A:H3'	38:A1:1575:A:N3	2.36	0.40
38:A1:2204:C:H2'	38:A1:2205:U:H6	1.86	0.40
56:AT:39:ILE:HD13	56:AT:63:VAL:HG22	2.03	0.40
71:Ai:4:LYS:HD2	71:Ai:13:LYS:O	2.22	0.40
1:BA:112:THR:HG22	1:BA:114:SER:H	1.86	0.40
4:BE:200:ARG:HA	4:BE:206:ASP:OD1	2.21	0.40
8:BJ:16:LYS:HE2	8:BJ:16:LYS:HB3	1.68	0.40
20:BF:51:VAL:O	20:BF:65:ARG:NH2	2.55	0.40
25:BS:145:ARG:H	25:BS:145:ARG:HD3	1.87	0.40
27:BU:20:ILE:HD12	27:BU:95:ALA:O	2.21	0.40
32:Bf:118:ARG:HB2	32:Bf:131:PHE:HD1	1.85	0.40
32:Bf:139:LEU:HD21	32:Bf:150:VAL:HG23	2.03	0.40
38:A1:1110:PSU:H2'	38:A1:1111:U:C6	2.55	0.40
38:A1:2749:G:H2'	38:A1:2750:U:C6	2.56	0.40
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.57	0.40
49:AM:21:VAL:HG12	49:AM:65:LEU:HD23	2.03	0.40
64:Ab:52:LYS:HB2	64:Ab:52:LYS:HE3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	194 (95%)	10 (5%)	0	100	100
2	BB	212/255 (83%)	191 (90%)	21 (10%)	0	100	100
3	BC	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
4	BE	258/261 (99%)	242 (94%)	16 (6%)	0	100	100
5	BG	224/236 (95%)	207 (92%)	17 (8%)	0	100	100
6	BH	182/190 (96%)	166 (91%)	16 (9%)	0	100	100
7	BI	184/200 (92%)	172 (94%)	12 (6%)	0	100	100
8	BJ	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
9	BL	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
10	BN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
11	BO	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
12	BV	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
13	BW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	BX	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
15	BY	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
16	Ba	95/119 (80%)	86 (90%)	9 (10%)	0	100	100
17	Bb	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
18	Be	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
19	BD	221/240 (92%)	209 (95%)	12 (5%)	0	100	100
20	BF	204/225 (91%)	194 (95%)	10 (5%)	0	100	100
21	BK	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
22	BP	122/142 (86%)	115 (94%)	7 (6%)	0	100	100
23	BQ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
24	BR	121/136 (89%)	118 (98%)	3 (2%)	0	100	100
25	BS	143/146 (98%)	134 (94%)	9 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BT	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
27	BU	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
28	BZ	69/108 (64%)	67 (97%)	2 (3%)	0	100	100
29	Bc	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	273 (88%)	37 (12%)	0	100	100
32	Bf	73/152 (48%)	61 (84%)	12 (16%)	0	100	100
33	BM	122/143 (85%)	104 (85%)	18 (15%)	0	100	100
35	AA	245/254 (96%)	233 (95%)	12 (5%)	0	100	100
36	AB	383/387 (99%)	367 (96%)	16 (4%)	0	100	100
37	AC	359/362 (99%)	344 (96%)	15 (4%)	0	100	100
41	AD	290/297 (98%)	268 (92%)	22 (8%)	0	100	100
42	AE	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
43	AF	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
44	AG	228/256 (89%)	216 (95%)	12 (5%)	0	100	100
45	AH	188/191 (98%)	180 (96%)	8 (4%)	0	100	100
46	AI	215/221 (97%)	207 (96%)	8 (4%)	0	100	100
47	AJ	167/174 (96%)	155 (93%)	12 (7%)	0	100	100
48	AL	191/199 (96%)	180 (94%)	11 (6%)	0	100	100
49	AM	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
50	AN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	166 (97%)	5 (3%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	181 (97%)	5 (3%)	0	100	100
55	AS	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
56	AT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
57	AU	98/121 (81%)	89 (91%)	9 (9%)	0	100	100
58	AV	134/137 (98%)	129 (96%)	5 (4%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	114 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AY	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
62	AZ	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
63	Aa	146/149 (98%)	138 (94%)	7 (5%)	1 (1%)	18	7
64	Ab	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
67	Ae	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
68	Af	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
69	Ag	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
70	Ah	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
71	Ai	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
72	Aj	85/88 (97%)	83 (98%)	2 (2%)	0	100	100
73	Ak	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
74	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
75	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
78	Ap	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
All	All	10925/11886 (92%)	10348 (95%)	576 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	Aa	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	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	136 (100%)	0	100	100
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	110 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	62/89 (70%)	62 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	321 (100%)	0	100	100
37	AC	288/289 (100%)	288 (100%)	0	100	100
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	137/153 (90%)	137 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	170 (100%)	0	100	100
46	AI	185/187 (99%)	185 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
All	All	9302/9988 (93%)	9302 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	69	ASN
2	BB	79	HIS
2	BB	211	HIS
3	BC	59	HIS
3	BC	189	GLN
4	BE	67	GLN
4	BE	130	GLN
4	BE	209	HIS
5	BG	22	HIS
6	BH	161	GLN
6	BH	180	GLN
7	BI	116	HIS
7	BI	175	GLN
9	BL	14	GLN
10	BN	36	GLN
12	BV	21	ASN
13	BW	12	ASN
13	BW	39	GLN
15	BY	63	GLN
17	Bb	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	BF	63	GLN
20	BF	158	GLN
21	BK	29	GLN
21	BK	62	GLN
22	BP	103	ASN
23	BQ	8	GLN
23	BQ	83	GLN
23	BQ	139	GLN
25	BS	75	ASN
25	BS	90	ASN
27	BU	15	GLN
27	BU	44	ASN
30	Bd	48	ASN
32	Bf	93	HIS
33	BM	38	HIS
33	BM	142	GLN
35	AA	132	ASN
35	AA	140	ASN
36	AB	121	ASN
37	AC	9	HIS
37	AC	48	GLN
37	AC	116	ASN
37	AC	296	GLN
41	AD	32	GLN
43	AF	48	ASN
43	AF	93	ASN
43	AF	186	HIS
44	AG	95	ASN
44	AG	192	GLN
45	AH	51	GLN
45	AH	157	ASN
46	AI	112	GLN
47	AJ	90	GLN
48	AL	103	ASN
49	AM	27	GLN
49	AM	119	GLN
50	AN	15	GLN
50	AN	32	GLN
51	AO	122[A]	GLN
52	AP	54	HIS
52	AP	55	GLN
52	AP	133	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	AT	5	HIS
57	AU	87	ASN
61	AY	66	GLN
62	AZ	122	HIS
65	Ac	71	GLN
66	Ad	21	HIS
69	Ag	108	GLN
70	Ah	62	GLN
71	Ai	12	ASN
72	Aj	48	ASN
73	Ak	28	ASN
74	Al	19	GLN
77	Ao	105	GLN
78	Ap	32	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1754/1798 (97%)	407 (23%)	18 (1%)
38	A1	3156/3184 (99%)	566 (17%)	50 (1%)
39	A3	120/121 (99%)	11 (9%)	1 (0%)
40	A4	157/158 (99%)	24 (15%)	2 (1%)
All	All	5187/5261 (98%)	1008 (19%)	71 (1%)

All (1008) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	17	C
34	B5	25	C
34	B5	34	G
34	B5	42	G
34	B5	46	A
34	B5	47	A
34	B5	57	G
34	B5	59	C
34	B5	60	U
34	B5	65	A
34	B5	68	A
34	B5	71	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	74	U
34	B5	75	U
34	B5	76	A
34	B5	77	U
34	B5	78	A
34	B5	84	A
34	B5	104	A
34	B5	114	C
34	B5	119	A
34	B5	127	G
34	B5	130	C
34	B5	131	C
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	138	A
34	B5	140	A
34	B5	141	U
34	B5	144	U
34	B5	145	A
34	B5	159	U
34	B5	166	C
34	B5	178	U
34	B5	179	A
34	B5	180	A
34	B5	189	C
34	B5	190	C
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	194	U
34	B5	195	G
34	B5	196	G
34	B5	197	A
34	B5	204	G
34	B5	210	A
34	B5	212	U
34	B5	213	A
34	B5	215	A
34	B5	217	A
34	B5	218	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	220	A
34	B5	221	A
34	B5	223	U
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	227	U
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	231	U
34	B5	233	C
34	B5	234	G
34	B5	235	G
34	B5	238	U
34	B5	239	C
34	B5	240	U
34	B5	241	U
34	B5	242	U
34	B5	243	G
34	B5	249	U
34	B5	252	U
34	B5	260	U
34	B5	261	U
34	B5	265	A
34	B5	272	U
34	B5	275	C
34	B5	276	C
34	B5	278	U
34	B5	280	U
34	B5	314	C
34	B5	316	A
34	B5	322	G
34	B5	337	G
34	B5	338	C
34	B5	352	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	390	G
34	B5	400	A
34	B5	401	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	402	C
34	B5	404	G
34	B5	417	A
34	B5	419	G
34	B5	422	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	434	G
34	B5	439	U
34	B5	444	C
34	B5	448	C
34	B5	452	A
34	B5	468	A
34	B5	477	A
34	B5	478	A
34	B5	481	A
34	B5	482	U
34	B5	483	A
34	B5	484	C
34	B5	486	G
34	B5	487	G
34	B5	488	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	492	A
34	B5	493	U
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	502	U
34	B5	505	A
34	B5	506	A
34	B5	507	U
34	B5	511	A
34	B5	514	G
34	B5	519	C
34	B5	521	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	527	A
34	B5	534	A
34	B5	536	C
34	B5	537	G
34	B5	538	A
34	B5	540	G
34	B5	542	A
34	B5	555	A
34	B5	556	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	565	C
34	B5	571	G
34	B5	574	G
34	B5	578	U
34	B5	594	A
34	B5	595	G
34	B5	597	G
34	B5	606	A
34	B5	619	A
34	B5	620	A
34	B5	623	A
34	B5	648	G
34	B5	649	U
34	B5	650	U
34	B5	652	G
34	B5	653	C
34	B5	655	G
34	B5	656	G
34	B5	657	U
34	B5	658	C
34	B5	677	G
34	B5	678	A
34	B5	679	U
34	B5	680	U
34	B5	681	U
34	B5	682	C
34	B5	683	C
34	B5	694	U
34	B5	697	C
34	B5	698	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	699	U
34	B5	700	C
34	B5	703	G
34	B5	704	C
34	B5	731	C
34	B5	732	G
34	B5	733	A
34	B5	734	A
34	B5	735	C
34	B5	736	C
34	B5	737	A
34	B5	738	G
34	B5	739	G
34	B5	740	A
34	B5	741	C
34	B5	742	U
34	B5	765	G
34	B5	766	PSU
34	B5	771	A
34	B5	774	A
34	B5	778	G
34	B5	779	U
34	B5	780	A
34	B5	782	U
34	B5	783	G
34	B5	787	G
34	B5	789	A
34	B5	794	U
34	B5	807	A
34	B5	810	G
34	B5	812	A
34	B5	814	A
34	B5	819	G
34	B5	823	G
34	B5	824	G
34	B5	825	U
34	B5	826	U
34	B5	827	C
34	B5	828	U
34	B5	829	A
34	B5	830	U
34	B5	831	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	832	U
34	B5	833	U
34	B5	834	G
34	B5	835	U
34	B5	836	U
34	B5	837	G
34	B5	838	G
34	B5	839	U
34	B5	842	C
34	B5	843	U
34	B5	845	G
34	B5	847	A
34	B5	849	C
34	B5	850	A
34	B5	851	U
34	B5	852	C
34	B5	853	G
34	B5	856	A
34	B5	857	U
34	B5	863	A
34	B5	873	U
34	B5	886	U
34	B5	890	C
34	B5	898	A
34	B5	933	A
34	B5	935	U
34	B5	959	U
34	B5	960	U
34	B5	966	A
34	B5	1004	U
34	B5	1021	C
34	B5	1026	A
34	B5	1028	C
34	B5	1031	U
34	B5	1032	G
34	B5	1039	A
34	B5	1052	U
34	B5	1053	G
34	B5	1056	U
34	B5	1057	U
34	B5	1058	U
34	B5	1059	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1063	U
34	B5	1081	A
34	B5	1091	A
34	B5	1092	A
34	B5	1100	G
34	B5	1126	G
34	B5	1138	A
34	B5	1150	G
34	B5	1154	G
34	B5	1158	C
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1217	A
34	B5	1218	G
34	B5	1224	A
34	B5	1238	A
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1250	U
34	B5	1251	U
34	B5	1255	G
34	B5	1256	A
34	B5	1263	G
34	B5	1286	U
34	B5	1290	PSU
34	B5	1291	G
34	B5	1314	U
34	B5	1315	U
34	B5	1321	A
34	B5	1340	U
34	B5	1348	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	1353	U
34	B5	1354	G
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1369	U
34	B5	1370	U
34	B5	1388	A
34	B5	1390	U
34	B5	1398	U
34	B5	1400	A
34	B5	1413	U
34	B5	1414	U
34	B5	1415	PSU
34	B5	1424	A
34	B5	1425	A
34	B5	1427	A
34	B5	1428	G
34	B5	1432	U
34	B5	1433	G
34	B5	1435	G
34	B5	1436	A
34	B5	1459	C
34	B5	1471	A
34	B5	1490	C
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1510	U
34	B5	1514	U
34	B5	1515	A
34	B5	1516	A
34	B5	1521	G
34	B5	1523	G
34	B5	1524	A
34	B5	1537	C
34	B5	1557	U
34	B5	1559	A
34	B5	1575	G7M
34	B5	1576	A
34	B5	1584	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	1590	G
34	B5	1601	G
34	B5	1607	G
34	B5	1611	A
34	B5	1615	C
34	B5	1619	C
34	B5	1631	A
34	B5	1634	C
34	B5	1657	U
34	B5	1658	G
34	B5	1665	U
34	B5	1666	U
34	B5	1683	C
34	B5	1684	U
34	B5	1687	U
34	B5	1688	U
34	B5	1690	G
34	B5	1692	G
34	B5	1693	A
34	B5	1694	A
34	B5	1696	G
34	B5	1697	G
34	B5	1698	G
34	B5	1699	G
34	B5	1700	C
34	B5	1701	A
34	B5	1703	C
34	B5	1704	U
34	B5	1705	C
34	B5	1706	C
34	B5	1707	A
34	B5	1708	U
34	B5	1709	C
34	B5	1711	C
34	B5	1712	A
34	B5	1713	G
34	B5	1714	A
34	B5	1715	G
34	B5	1716	C
34	B5	1731	A
34	B5	1732	A
34	B5	1755	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	1756[A]	A
34	B5	1757	G
34	B5	1760	G
34	B5	1762	A
34	B5	1766	A
34	B5	1768	G
34	B5	1769	U
34	B5	1780	G
34	B5	1782	MA6
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1795	U
34	B5	1796	C
34	B5	1799	U
38	A1	4	U
38	A1	6	A
38	A1	26	A
38	A1	40	A
38	A1	43	A
38	A1	44	U
38	A1	49	A
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	74	G
38	A1	75	G
38	A1	92	G
38	A1	99	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	118	U
38	A1	122	A
38	A1	135	C
38	A1	136	G
38	A1	156	G
38	A1	157	A
38	A1	162	G
38	A1	164	A
38	A1	166	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	170	G
38	A1	171	G
38	A1	172	G
38	A1	173	G
38	A1	174	C
38	A1	175	C
38	A1	178	U
38	A1	181	U
38	A1	187	A
38	A1	190	U
38	A1	200	C
38	A1	210	U
38	A1	211	A
38	A1	219	A
38	A1	231	G
38	A1	240	U
38	A1	241	G
38	A1	242	C
38	A1	243	G
38	A1	244	G
38	A1	245	U
38	A1	246	U
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	254	A
38	A1	259	C
38	A1	260	C
38	A1	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	329	U
38	A1	349	A
38	A1	376	G
38	A1	387	A
38	A1	397	A
38	A1	398	A
38	A1	399	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	402	A
38	A1	403	C
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	439	C
38	A1	440	A
38	A1	441	U
38	A1	442	G
38	A1	443	G
38	A1	444	U
38	A1	445	G
38	A1	446	U
38	A1	447	U
38	A1	448	U
38	A1	449	U
38	A1	450	G
38	A1	451	U
38	A1	487	U
38	A1	488	U
38	A1	489	U
38	A1	490	C
38	A1	493	U
38	A1	494	G
38	A1	495	G
38	A1	520	U
38	A1	521	A
38	A1	536	U
38	A1	542	G
38	A1	543	C
38	A1	544	C
38	A1	545	U
38	A1	546	C
38	A1	547	G
38	A1	548	G
38	A1	552	G
38	A1	554	A
38	A1	557	A
38	A1	558	U
38	A1	559	A
38	A1	567	G
38	A1	569	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	570	A
38	A1	578	A
38	A1	579	G
38	A1	588	G
38	A1	589	A
38	A1	592	A
38	A1	600	G
38	A1	603	A
38	A1	604	G
38	A1	611	A
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	636	C
38	A1	649	A
38	A1	660	A
38	A1	667	C
38	A1	677	A
38	A1	691	A
38	A1	705	A
38	A1	706	A
38	A1	715	A
38	A1	719	U
38	A1	725	G
38	A1	733	G
38	A1	734	C
38	A1	735	A
38	A1	737	G
38	A1	739	G
38	A1	750	G
38	A1	765	C
38	A1	767	U
38	A1	774	G
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	806	A
38	A1	817	A
38	A1	830	A
38	A1	861	C
38	A1	874	U
38	A1	879	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	890	C
38	A1	896	A
38	A1	897	U
38	A1	907	G
38	A1	908	G
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	923	C
38	A1	925	A
38	A1	937	G
38	A1	944	C
38	A1	959	C
38	A1	960	PSU
38	A1	974	G
38	A1	980	A
38	A1	982	C
38	A1	993	G
38	A1	994	G
38	A1	1000	C
38	A1	1001	G
38	A1	1006	A
38	A1	1010	G
38	A1	1014	U
38	A1	1015	U
38	A1	1018	G
38	A1	1019	G
38	A1	1020	G
38	A1	1021	G
38	A1	1022	U
38	A1	1023	C
38	A1	1031	C
38	A1	1032	C
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1036	A
38	A1	1037	C
38	A1	1047	A
38	A1	1064	A
38	A1	1065	A
38	A1	1072	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	1081	U
38	A1	1082	U
38	A1	1083	G
38	A1	1092	C
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1104	G
38	A1	1106	G
38	A1	1117	G
38	A1	1131	G
38	A1	1153	A
38	A1	1159	A
38	A1	1160	C
38	A1	1161	G
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1201	C
38	A1	1208	U
38	A1	1218	U
38	A1	1220	U
38	A1	1221	A
38	A1	1222	G
38	A1	1228	C
38	A1	1229	G
38	A1	1230	G
38	A1	1231	A
38	A1	1232	C
38	A1	1233	G
38	A1	1234	G
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1238	C
38	A1	1239	C
38	A1	1240	A
38	A1	1241	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	1242	G
38	A1	1244	A
38	A1	1245	A
38	A1	1246	G
38	A1	1248	C
38	A1	1249	G
38	A1	1251	A
38	A1	1252	A
38	A1	1253	U
38	A1	1257	C
38	A1	1259	A
38	A1	1260	A
38	A1	1262	G
38	A1	1263	A
38	A1	1264	G
38	A1	1265	U
38	A1	1266	G
38	A1	1268	G
38	A1	1269	U
38	A1	1271	A
38	A1	1272	C
38	A1	1273	A
38	A1	1274	A
38	A1	1275	C
38	A1	1276	U
38	A1	1279	C
38	A1	1280	C
38	A1	1283	C
38	A1	1287	A
38	A1	1292	C
38	A1	1309	U
38	A1	1330	A
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G
38	A1	1355	A
38	A1	1357	G
38	A1	1386	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A
38	A1	1434	G
38	A1	1437	C
38	A1	1446	A
38	A1	1481	A
38	A1	1483	G
38	A1	1527	C
38	A1	1556	C
38	A1	1557	A
38	A1	1561	G
38	A1	1562	C
38	A1	1563	C
38	A1	1564	U
38	A1	1566	A
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1570	U
38	A1	1571	A
38	A1	1572	U
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C
38	A1	1580	A
38	A1	1581	C
38	A1	1582	C
38	A1	1583	A
38	A1	1589	A
38	A1	1620	U
38	A1	1628	C
38	A1	1631	C
38	A1	1642	A
38	A1	1643	A
38	A1	1644	C
38	A1	1645	U
38	A1	1657	C
38	A1	1704	A
38	A1	1724	U
38	A1	1750	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	1751	G
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1797	A
38	A1	1814	A
38	A1	1815	U
38	A1	1816	A
38	A1	1817	G
38	A1	1818	U
38	A1	1819	U
38	A1	1820	U
38	A1	1821	U
38	A1	1842	A
38	A1	1866	C
38	A1	1880	U
38	A1	1906	G
38	A1	1935	G
38	A1	1953	G
38	A1	1954	G
38	A1	2094	C
38	A1	2095	G
38	A1	2099	A
38	A1	2112	U
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2158	A
38	A1	2169	G
38	A1	2188	A
38	A1	2201	G
38	A1	2206	G
38	A1	2207	A
38	A1	2208	A
38	A1	2222	A
38	A1	2223	A
38	A1	2249	G
38	A1	2250	G
38	A1	2251	G
38	A1	2256	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	2260	PSU
38	A1	2265	C
38	A1	2269	U
38	A1	2272	G
38	A1	2273	G
38	A1	2279	A
38	A1	2280	A
38	A1	2281	A
38	A1	2307	G
38	A1	2308	C
38	A1	2310	U
38	A1	2313	A
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2372	A
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2393	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2437	G
38	A1	2438	A
38	A1	2439	A
38	A1	2440	G
38	A1	2441	A
38	A1	2442	G
38	A1	2443	A
38	A1	2444	C
38	A1	2501	U
38	A1	2502	A
38	A1	2503	G
38	A1	2504	U
38	A1	2506	U
38	A1	2507	C
38	A1	2509	U
38	A1	2510	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	2514	U
38	A1	2529	A
38	A1	2530	G
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2541	U
38	A1	2542	U
38	A1	2544	U
38	A1	2545	C
38	A1	2546	C
38	A1	2547	A
38	A1	2548	C
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U
38	A1	2572	C
38	A1	2573	G
38	A1	2574	G
38	A1	2585	G
38	A1	2586	G
38	A1	2593	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2636	A
38	A1	2637	A
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2677	G
38	A1	2681	U
38	A1	2689	A
38	A1	2691	A
38	A1	2694	A
38	A1	2704	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	2729	U
38	A1	2752	U
38	A1	2753	G
38	A1	2762	A
38	A1	2772	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2796	G
38	A1	2799	A
38	A1	2800	G
38	A1	2801	A
38	A1	2802	A
38	A1	2808	A
38	A1	2814	G
38	A1	2817	A
38	A1	2833	A
38	A1	2838	A
38	A1	2839	G
38	A1	2842	U
38	A1	2844	C
38	A1	2845	A
38	A1	2847	A
38	A1	2871	G
38	A1	2875	U
38	A1	2887	A
38	A1	2923	PSU
38	A1	2935	U
38	A1	2936	A
38	A1	2938	G
38	A1	2942	C
38	A1	2947	G
38	A1	2954	U
38	A1	2971	A
38	A1	2983	C
38	A1	2990	G
38	A1	2996	U
38	A1	2997	G
38	A1	3012	A
38	A1	3022	G
38	A1	3023	U
38	A1	3030	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	3056	U
38	A1	3057	U
38	A1	3059	G
38	A1	3078	U
38	A1	3086	A
38	A1	3092	C
38	A1	3101	G
38	A1	3113	A
38	A1	3129	A
38	A1	3130	A
38	A1	3131	U
38	A1	3134	A
38	A1	3142	A
38	A1	3143	C
38	A1	3153	U
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3163	A
38	A1	3165	A
38	A1	3166	C
38	A1	3167	A
38	A1	3168	A
38	A1	3170	A
38	A1	3173	G
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3197	G
38	A1	3198	U
38	A1	3199	G
38	A1	3207	U
38	A1	3208	G
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3225	C
38	A1	3228	C
38	A1	3232	G
38	A1	3234	A
38	A1	3235	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	3243	A
38	A1	3246	G
38	A1	3247	G
38	A1	3259	U
38	A1	3260	G
38	A1	3262	U
38	A1	3268	A
38	A1	3276	G
38	A1	3277	U
38	A1	3284	G
38	A1	3285	C
38	A1	3286	G
38	A1	3287	U
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3307	A
38	A1	3316	A
38	A1	3318	G
38	A1	3319	U
38	A1	3324	C
38	A1	3335	A
38	A1	3341	U
38	A1	3342	A
38	A1	3345	G
38	A1	3348	G
38	A1	3350	C
38	A1	3352	U
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3378	C
38	A1	3396	U
39	A3	22	A
39	A3	23	A
39	A3	24	A
39	A3	38	U
39	A3	42	A
39	A3	54	U
39	A3	55	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	A3	65	G
39	A3	102	A
39	A3	112	G
39	A3	121	U
40	A4	34	U
40	A4	35	C
40	A4	51	G
40	A4	52	A
40	A4	59	A
40	A4	62	C
40	A4	63	G
40	A4	81	U
40	A4	82	U
40	A4	83	C
40	A4	86	U
40	A4	87	G
40	A4	89	A
40	A4	90	U
40	A4	95	G
40	A4	105	A
40	A4	106	C
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	131	A
40	A4	152	G
40	A4	158	U

All (71) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	196	G
34	B5	468	A
34	B5	510	G
34	B5	557	G
34	B5	577	G
34	B5	851	U
34	B5	889	U
34	B5	1091	A
34	B5	1092	A
34	B5	1100	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	B5	1108	G
34	B5	1362	U
34	B5	1363	U
34	B5	1431	C
34	B5	1458	G
34	B5	1683	C
34	B5	1695	G
34	B5	1714	A
38	A1	43	A
38	A1	116	A
38	A1	210	U
38	A1	240	U
38	A1	397	A
38	A1	439	C
38	A1	588	G
38	A1	705	A
38	A1	734	C
38	A1	816	A
38	A1	873	C
38	A1	896	A
38	A1	916	G
38	A1	993	G
38	A1	1033	U
38	A1	1064	A
38	A1	1091	A
38	A1	1160	C
38	A1	1234	G
38	A1	1317	A
38	A1	1560	G
38	A1	1643	A
38	A1	1818	U
38	A1	1841	A
38	A1	1953	G
38	A1	2094	C
38	A1	2222	A
38	A1	2249	G
38	A1	2272	G
38	A1	2372	A
38	A1	2374	C
38	A1	2439	A
38	A1	2441	A
38	A1	2443	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A1	2585	G
38	A1	2656	A
38	A1	2676	A
38	A1	2728	G
38	A1	2772	C
38	A1	2801	A
38	A1	2872	A
38	A1	3022	G
38	A1	3056	U
38	A1	3057	U
38	A1	3154	C
38	A1	3169	U
38	A1	3227	A
38	A1	3242	G
38	A1	3283	U
38	A1	3303	G
39	A3	23	A
40	A4	88	A
40	A4	111	A

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

59 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
38	PSU	A1	2944	79,38	18,21,22	1.40	3 (16%)	21,30,33	2.25	4 (19%)
34	PSU	B5	759	34	18,21,22	1.53	4 (22%)	21,30,33	2.01	3 (14%)
38	UR3	A1	2634	38	19,22,23	0.89	0	26,32,35	1.93	4 (15%)
39	PSU	A3	50	39	18,21,22	1.75	4 (22%)	21,30,33	2.19	4 (19%)
38	PSU	A1	2349	79,38	18,21,22	1.50	3 (16%)	21,30,33	1.98	5 (23%)
34	PSU	B5	1290	34	18,21,22	1.81	4 (22%)	21,30,33	2.93	5 (23%)
34	PSU	B5	120	34	18,21,22	1.48	4 (22%)	21,30,33	2.45	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	MA6	B5	1781	34	23,26,27	1.45	4 (17%)	33,38,41	2.32	11 (33%)
34	PSU	B5	211	34	18,21,22	1.64	3 (16%)	21,30,33	1.81	4 (19%)
38	PSU	A1	2314	38	18,21,22	1.44	3 (16%)	21,30,33	2.07	4 (19%)
34	4AC	B5	1280	34	21,24,25	0.87	1 (4%)	28,34,37	1.59	4 (14%)
34	PSU	B5	1181	34	18,21,22	1.62	4 (22%)	21,30,33	1.90	3 (14%)
34	PSU	B5	302	34	18,21,22	1.69	5 (27%)	21,30,33	1.79	4 (19%)
38	1MA	A1	645	79,38	21,25,26	1.43	5 (23%)	30,37,40	1.67	6 (20%)
38	PSU	A1	966	80,38	18,21,22	1.62	5 (27%)	21,30,33	1.85	4 (19%)
38	PSU	A1	960	38	18,21,22	1.71	6 (33%)	21,30,33	2.24	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.45	3 (15%)	26,32,35	1.28	3 (11%)
34	PSU	B5	1187	34	18,21,22	1.48	3 (16%)	21,30,33	2.17	4 (19%)
34	MA6	B5	1782	34	23,26,27	1.48	5 (21%)	33,38,41	2.31	10 (30%)
38	PSU	A1	2865	38	18,21,22	1.45	4 (22%)	21,30,33	2.10	4 (19%)
34	PSU	B5	632	34	18,21,22	1.75	4 (22%)	21,30,33	1.70	4 (19%)
38	PSU	A1	2880	38	18,21,22	1.38	3 (16%)	21,30,33	1.87	3 (14%)
34	PSU	B5	466	34	18,21,22	1.66	4 (22%)	21,30,33	1.67	4 (19%)
38	1MA	A1	2142	79,38	21,25,26	1.30	5 (23%)	30,37,40	1.74	8 (26%)
38	PSU	A1	1042	38	18,21,22	1.66	5 (27%)	21,30,33	2.23	6 (28%)
38	PSU	A1	1052	38	18,21,22	1.44	4 (22%)	21,30,33	2.10	4 (19%)
36	HIC	AB	243	36	10,11,12	0.46	0	9,14,16	1.08	1 (11%)
38	PSU	A1	2133	38	18,21,22	1.49	3 (16%)	21,30,33	2.18	5 (23%)
34	PSU	B5	999	34	18,21,22	1.48	3 (16%)	21,30,33	2.00	5 (23%)
40	PSU	A4	73	40	18,21,22	1.40	3 (16%)	21,30,33	2.11	4 (19%)
38	PSU	A1	986	38	18,21,22	1.52	4 (22%)	21,30,33	1.69	4 (19%)
38	5MC	A1	2278	79,38	19,22,23	2.06	4 (21%)	26,32,35	1.86	8 (30%)
38	PSU	A1	776	38	18,21,22	1.72	4 (22%)	21,30,33	1.68	4 (19%)
38	PSU	A1	2975	38	18,21,22	1.60	5 (27%)	21,30,33	2.08	5 (23%)
34	B8N	B5	1191	34	25,29,30	1.46	4 (16%)	28,42,45	3.41	6 (21%)
34	PSU	B5	1415	34	18,21,22	1.09	1 (5%)	21,30,33	0.95	1 (4%)
38	PSU	A1	2260	38	18,21,22	1.45	4 (22%)	21,30,33	1.97	5 (23%)
38	PSU	A1	2340	38	18,21,22	1.69	5 (27%)	21,30,33	2.05	4 (19%)
38	PSU	A1	2266	38	18,21,22	1.92	4 (22%)	21,30,33	2.06	6 (28%)
38	PSU	A1	2416	79,38	18,21,22	1.62	4 (22%)	21,30,33	1.79	4 (19%)
38	PSU	A1	2735	38	18,21,22	1.66	4 (22%)	21,30,33	1.77	5 (23%)
38	PSU	A1	2191	38	18,21,22	1.49	3 (16%)	21,30,33	2.10	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	PSU	A1	1004	80,38	18,21,22	1.43	3 (16%)	21,30,33	2.26	5 (23%)
34	G7M	B5	1575	34	23,26,27	2.73	8 (34%)	34,39,42	2.01	9 (26%)
38	PSU	A1	1110	38	18,21,22	1.42	3 (16%)	21,30,33	1.96	4 (19%)
38	OMU	A1	2921	79,38	19,22,23	1.30	3 (15%)	25,31,34	1.88	4 (16%)
38	PSU	A1	2264	38	18,21,22	1.48	4 (22%)	21,30,33	1.67	3 (14%)
38	OMG	A1	2922	38	23,26,27	1.24	4 (17%)	32,38,41	2.00	7 (21%)
34	4AC	B5	1773	34	21,24,25	0.50	0	28,34,37	0.49	0
38	PSU	A1	2129	38	18,21,22	1.40	3 (16%)	21,30,33	2.13	4 (19%)
38	PSU	A1	2826	38	18,21,22	1.41	3 (16%)	21,30,33	2.13	5 (23%)
38	PSU	A1	2923	38	18,21,22	1.49	4 (22%)	21,30,33	2.18	3 (14%)
38	PSU	A1	990	38	18,21,22	1.49	4 (22%)	21,30,33	2.08	3 (14%)
38	PSU	A1	1056	38	18,21,22	1.53	3 (16%)	21,30,33	2.05	3 (14%)
38	PSU	A1	1124	38	18,21,22	1.45	4 (22%)	21,30,33	2.43	3 (14%)
34	PSU	B5	766	34	18,21,22	1.44	4 (22%)	21,30,33	2.09	4 (19%)
38	PSU	A1	2351	38	18,21,22	1.59	4 (22%)	21,30,33	1.75	4 (19%)
38	PSU	A1	2258	38	18,21,22	1.55	5 (27%)	21,30,33	2.66	5 (23%)
34	PSU	B5	106	34	18,21,22	1.50	4 (22%)	21,30,33	2.25	5 (23%)

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
38	PSU	A1	2944	79,38	-	1/7/25/26	0/2/2/2
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	0/7/25/26	0/2/2/2
38	PSU	A1	2349	79,38	-	0/7/25/26	0/2/2/2
34	PSU	B5	1290	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	120	34	-	0/7/25/26	0/2/2/2
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
34	PSU	B5	211	34	-	2/7/25/26	0/2/2/2
38	PSU	A1	2314	38	-	1/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	0/11/29/30	0/2/2/2
34	PSU	B5	1181	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	302	34	-	0/7/25/26	0/2/2/2
38	1MA	A1	645	79,38	-	1/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	966	80,38	-	0/7/25/26	0/2/2/2
38	PSU	A1	960	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
34	PSU	B5	1187	34	-	0/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	3/11/29/30	0/3/3/3
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
38	1MA	A1	2142	79,38	-	1/7/25/26	0/3/3/3
38	PSU	A1	1042	38	-	3/7/25/26	0/2/2/2
38	PSU	A1	1052	38	-	0/7/25/26	0/2/2/2
36	HIC	AB	243	36	-	1/5/6/8	0/1/1/1
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
40	PSU	A4	73	40	-	0/7/25/26	0/2/2/2
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2278	79,38	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
34	B8N	B5	1191	34	-	2/16/34/35	0/2/2/2
34	PSU	B5	1415	34	-	2/7/25/26	0/2/2/2
38	PSU	A1	2260	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	2340	38	-	1/7/25/26	0/2/2/2
38	PSU	A1	2266	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	2416	79,38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1004	80,38	-	0/7/25/26	0/2/2/2
34	G7M	B5	1575	34	2/2/5/5	2/7/25/26	0/3/3/3
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2921	79,38	-	0/9/27/28	0/2/2/2
38	PSU	A1	2264	38	-	0/7/25/26	0/2/2/2
38	OMG	A1	2922	38	-	0/9/27/28	0/3/3/3
34	4AC	B5	1773	34	-	2/11/29/30	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	38	-	3/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	1124	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2351	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O6-C6	7.32	1.37	1.23
38	A1	2278	5MC	C5-C4	6.45	1.49	1.44
34	B5	1575	G7M	C5-N7	-5.78	1.32	1.39
34	B5	1575	G7M	C2-N2	5.40	1.46	1.34
38	A1	2266	PSU	C2-N1	-4.68	1.30	1.36
38	A1	2266	PSU	C4-N3	-4.62	1.30	1.38
34	B5	1781	MA6	C5-C4	4.57	1.47	1.39
39	A3	50	PSU	C6-C5	4.39	1.40	1.35
38	A1	2870	5MC	C5-C4	4.38	1.47	1.44
34	B5	1782	MA6	C5-C4	4.03	1.46	1.39
34	B5	1575	G7M	C8-N7	-4.02	1.26	1.33
38	A1	2278	5MC	O2-C2	-3.86	1.16	1.23
38	A1	1056	PSU	C6-C5	3.81	1.39	1.35
38	A1	2351	PSU	C6-C5	3.79	1.39	1.35
34	B5	466	PSU	C4-N3	-3.78	1.31	1.38
34	B5	632	PSU	C4-N3	-3.78	1.31	1.38
38	A1	2340	PSU	C6-C5	3.69	1.39	1.35
34	B5	1290	PSU	C4-N3	-3.67	1.32	1.38
38	A1	2975	PSU	C6-C5	3.62	1.39	1.35
34	B5	1290	PSU	C2-N3	-3.62	1.31	1.37
34	B5	1415	PSU	C6-C5	3.62	1.39	1.35
34	B5	211	PSU	C6-C5	3.61	1.39	1.35
38	A1	960	PSU	C2-N1	-3.59	1.32	1.36
38	A1	2735	PSU	C2-N1	-3.57	1.32	1.36
38	A1	1042	PSU	C4-N3	-3.57	1.32	1.38
38	A1	776	PSU	C6-C5	3.54	1.39	1.35
34	B5	1290	PSU	C6-C5	3.52	1.39	1.35
34	B5	632	PSU	C6-C5	3.51	1.39	1.35
34	B5	302	PSU	C6-C5	3.51	1.39	1.35
34	B5	1191	B8N	C4-C5	-3.49	1.39	1.47
34	B5	759	PSU	C6-C5	3.48	1.39	1.35
34	B5	302	PSU	C4-N3	-3.47	1.32	1.38
38	A1	1042	PSU	C2-N3	-3.44	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	776	PSU	C4-N3	-3.43	1.32	1.38
38	A1	2129	PSU	C6-C5	3.42	1.39	1.35
34	B5	466	PSU	C2-N3	-3.41	1.31	1.37
34	B5	632	PSU	C2-N3	-3.40	1.31	1.37
38	A1	2314	PSU	C6-C5	3.39	1.39	1.35
34	B5	999	PSU	C6-C5	3.39	1.39	1.35
34	B5	1181	PSU	C4-N3	-3.39	1.32	1.38
38	A1	2191	PSU	C4-N3	-3.37	1.32	1.38
38	A1	966	PSU	C6-C5	3.36	1.39	1.35
38	A1	2349	PSU	C6-C5	3.33	1.39	1.35
34	B5	1575	G7M	CN7-N7	3.31	1.52	1.46
38	A1	2975	PSU	C4-N3	-3.31	1.32	1.38
34	B5	1575	G7M	C6-N1	-3.28	1.32	1.38
34	B5	1191	B8N	C6-C5	3.27	1.39	1.35
38	A1	966	PSU	C4-N3	-3.27	1.32	1.38
38	A1	776	PSU	C2-N3	-3.26	1.32	1.37
34	B5	1187	PSU	C6-C5	3.26	1.38	1.35
38	A1	2880	PSU	C6-C5	3.25	1.38	1.35
34	B5	211	PSU	C4-N3	-3.24	1.32	1.38
38	A1	2349	PSU	C4-N3	-3.23	1.32	1.38
38	A1	2351	PSU	C4-N3	-3.23	1.32	1.38
34	B5	466	PSU	C6-C5	3.23	1.38	1.35
38	A1	2416	PSU	C6-C5	3.22	1.38	1.35
38	A1	990	PSU	C6-C5	3.21	1.38	1.35
38	A1	1124	PSU	C6-C5	3.21	1.38	1.35
38	A1	986	PSU	C6-C5	3.20	1.38	1.35
34	B5	999	PSU	C4-N3	-3.19	1.32	1.38
38	A1	990	PSU	C4-N3	-3.19	1.32	1.38
38	A1	2923	PSU	C6-C5	3.19	1.38	1.35
38	A1	986	PSU	C4-N3	-3.19	1.32	1.38
40	A4	73	PSU	C6-C5	3.17	1.38	1.35
38	A1	2133	PSU	C4-N3	-3.16	1.32	1.38
38	A1	2416	PSU	C4-N3	-3.16	1.32	1.38
38	A1	2735	PSU	C4-N3	-3.14	1.33	1.38
38	A1	2921	OMU	C4-N3	-3.13	1.33	1.38
38	A1	2416	PSU	C2-N1	-3.13	1.32	1.36
38	A1	2258	PSU	C6-C5	3.12	1.38	1.35
34	B5	1187	PSU	C4-N3	-3.12	1.33	1.38
38	A1	2278	5MC	C6-N1	-3.11	1.32	1.38
38	A1	1110	PSU	C6-C5	3.11	1.38	1.35
34	B5	766	PSU	C6-C5	3.09	1.38	1.35
34	B5	759	PSU	C4-N3	-3.07	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2264	PSU	C6-C5	3.07	1.38	1.35
34	B5	106	PSU	C4-N3	-3.05	1.33	1.38
38	A1	2133	PSU	C6-C5	3.05	1.38	1.35
38	A1	2278	5MC	C6-C5	3.05	1.39	1.34
34	B5	1181	PSU	C6-C5	3.04	1.38	1.35
34	B5	1181	PSU	C2-N3	-3.01	1.32	1.37
38	A1	2191	PSU	C6-C5	3.01	1.38	1.35
34	B5	120	PSU	C4-N3	-3.01	1.33	1.38
34	B5	1782	MA6	C5-C6	3.01	1.49	1.41
34	B5	302	PSU	C2-N3	-3.01	1.32	1.37
38	A1	2340	PSU	C4-N3	-2.99	1.33	1.38
38	A1	2865	PSU	C6-C5	2.96	1.38	1.35
38	A1	1004	PSU	C4-N3	-2.95	1.33	1.38
38	A1	2416	PSU	C2-N3	-2.93	1.32	1.37
38	A1	2826	PSU	C6-C5	2.92	1.38	1.35
34	B5	766	PSU	C4-N3	-2.92	1.33	1.38
38	A1	2826	PSU	C4-N3	-2.92	1.33	1.38
38	A1	2944	PSU	C6-C5	2.91	1.38	1.35
38	A1	1004	PSU	C6-C5	2.91	1.38	1.35
38	A1	966	PSU	C2-N1	-2.91	1.32	1.36
39	A3	50	PSU	C4-N3	-2.91	1.33	1.38
38	A1	2735	PSU	C6-C5	2.90	1.38	1.35
38	A1	1124	PSU	C4-N3	-2.90	1.33	1.38
34	B5	632	PSU	C2-N1	-2.89	1.32	1.36
38	A1	1110	PSU	C4-N3	-2.89	1.33	1.38
38	A1	2314	PSU	C4-N3	-2.89	1.33	1.38
38	A1	2735	PSU	C2-N3	-2.88	1.32	1.37
38	A1	986	PSU	C2-N3	-2.87	1.32	1.37
38	A1	2260	PSU	C4-N3	-2.86	1.33	1.38
38	A1	2258	PSU	C2-N1	-2.85	1.32	1.36
38	A1	960	PSU	O4'-C1'	-2.85	1.39	1.43
38	A1	2266	PSU	C2-N3	-2.85	1.32	1.37
34	B5	120	PSU	C6-C5	2.83	1.38	1.35
38	A1	1056	PSU	C4-N3	-2.83	1.33	1.38
38	A1	2340	PSU	C2-N1	-2.81	1.33	1.36
38	A1	2865	PSU	C4-N3	-2.81	1.33	1.38
38	A1	2340	PSU	C6-N1	-2.81	1.31	1.36
40	A4	73	PSU	C4-N3	-2.80	1.33	1.38
38	A1	960	PSU	C4-N3	-2.79	1.33	1.38
38	A1	2260	PSU	C6-C5	2.78	1.38	1.35
38	A1	1042	PSU	C2-N1	-2.78	1.33	1.36
38	A1	2191	PSU	C2-N3	-2.77	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2880	PSU	C4-N3	-2.76	1.33	1.38
38	A1	2944	PSU	C4-N3	-2.76	1.33	1.38
38	A1	2264	PSU	C4-N3	-2.76	1.33	1.38
38	A1	2923	PSU	C4-N3	-2.76	1.33	1.38
38	A1	2351	PSU	C2-N3	-2.75	1.32	1.37
38	A1	645	1MA	C5-C4	2.75	1.46	1.38
34	B5	1781	MA6	C5-C6	2.73	1.48	1.41
38	A1	2142	1MA	C5-C4	2.71	1.46	1.38
38	A1	2921	OMU	C2-N3	-2.70	1.33	1.38
39	A3	50	PSU	C6-N1	-2.70	1.31	1.36
38	A1	2922	OMG	C5-C4	2.69	1.46	1.38
38	A1	1052	PSU	C6-C5	2.69	1.38	1.35
38	A1	1052	PSU	C2-N1	-2.69	1.33	1.36
38	A1	2870	5MC	C6-C5	2.67	1.39	1.34
34	B5	211	PSU	C2-N3	-2.67	1.33	1.37
38	A1	2349	PSU	C2-N3	-2.66	1.33	1.37
34	B5	106	PSU	C6-C5	2.66	1.38	1.35
38	A1	645	1MA	C6-N6	2.64	1.34	1.28
38	A1	776	PSU	C2-N1	-2.62	1.33	1.36
38	A1	1052	PSU	C4-N3	-2.62	1.33	1.38
38	A1	2129	PSU	C4-N3	-2.62	1.33	1.38
38	A1	2264	PSU	C2-N3	-2.61	1.33	1.37
38	A1	2922	OMG	C6-N1	-2.59	1.34	1.38
38	A1	960	PSU	C2-N3	-2.57	1.33	1.37
38	A1	2142	1MA	C5-N7	-2.57	1.33	1.39
34	B5	120	PSU	C2-N1	-2.57	1.33	1.36
38	A1	966	PSU	C2-N3	-2.56	1.33	1.37
38	A1	2922	OMG	C5-N7	-2.55	1.34	1.39
38	A1	2258	PSU	O4'-C1'	-2.54	1.40	1.43
34	B5	1290	PSU	C2-N1	-2.54	1.33	1.36
34	B5	1181	PSU	C2-N1	-2.53	1.33	1.36
39	A3	50	PSU	C2-N1	-2.53	1.33	1.36
38	A1	2975	PSU	C2-N3	-2.53	1.33	1.37
38	A1	990	PSU	C2-N3	-2.51	1.33	1.37
38	A1	645	1MA	C5-N7	-2.51	1.34	1.39
38	A1	2258	PSU	C6-N1	-2.51	1.32	1.36
34	B5	1575	G7M	C4-N9	-2.50	1.31	1.38
38	A1	2922	OMG	C4-N9	-2.49	1.31	1.38
38	A1	2340	PSU	C2-N3	-2.47	1.33	1.37
34	B5	999	PSU	C2-N3	-2.46	1.33	1.37
34	B5	106	PSU	C2-N3	-2.45	1.33	1.37
34	B5	1782	MA6	C4-N9	-2.43	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2923	PSU	O4'-C1'	-2.41	1.40	1.43
38	A1	1110	PSU	C2-N3	-2.37	1.33	1.37
38	A1	645	1MA	C4-N9	-2.36	1.32	1.38
38	A1	2260	PSU	O4'-C1'	-2.35	1.40	1.43
34	B5	1280	4AC	C4-N4	-2.34	1.36	1.39
38	A1	1042	PSU	C6-C5	2.33	1.37	1.35
34	B5	1781	MA6	C5-N7	-2.33	1.34	1.39
38	A1	2975	PSU	C2-N1	-2.33	1.33	1.36
38	A1	2142	1MA	C4-N9	-2.33	1.32	1.38
34	B5	120	PSU	C2-N3	-2.31	1.33	1.37
38	A1	2258	PSU	C4-N3	-2.31	1.34	1.38
34	B5	1575	G7M	C2-N1	-2.30	1.32	1.37
38	A1	1042	PSU	C6-N1	-2.28	1.32	1.36
34	B5	1782	MA6	C5-N7	-2.27	1.34	1.39
34	B5	759	PSU	C2-N3	-2.26	1.33	1.37
34	B5	1187	PSU	C2-N3	-2.25	1.33	1.37
38	A1	2944	PSU	C2-N3	-2.25	1.33	1.37
38	A1	960	PSU	C6-C5	2.24	1.37	1.35
38	A1	960	PSU	C6-N1	-2.23	1.32	1.36
34	B5	1782	MA6	C8-N9	-2.23	1.33	1.37
34	B5	302	PSU	O4'-C1'	-2.21	1.40	1.43
34	B5	759	PSU	C2-N1	-2.20	1.33	1.36
38	A1	2133	PSU	C2-N3	-2.20	1.33	1.37
40	A4	73	PSU	C2-N3	-2.19	1.33	1.37
38	A1	1124	PSU	C6-N1	-2.19	1.32	1.36
38	A1	2142	1MA	C6-N6	2.19	1.33	1.28
38	A1	2351	PSU	C2-N1	-2.18	1.33	1.36
38	A1	2142	1MA	C2-N3	2.17	1.34	1.30
38	A1	2921	OMU	C5-C4	-2.17	1.39	1.43
38	A1	1052	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2975	PSU	C6-N1	-2.17	1.32	1.36
38	A1	2865	PSU	C2-N1	-2.17	1.33	1.36
38	A1	1056	PSU	C2-N3	-2.16	1.33	1.37
38	A1	2870	5MC	C6-N1	-2.15	1.34	1.38
38	A1	2260	PSU	C2-N3	-2.15	1.33	1.37
34	B5	766	PSU	C2-N3	-2.15	1.33	1.37
38	A1	645	1MA	C8-N9	-2.14	1.32	1.37
38	A1	2826	PSU	C2-N3	-2.14	1.33	1.37
38	A1	1124	PSU	C2-N1	-2.14	1.33	1.36
38	A1	2314	PSU	C2-N3	-2.14	1.34	1.37
34	B5	1781	MA6	C8-N9	-2.12	1.33	1.37
34	B5	466	PSU	C2-N1	-2.12	1.33	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1191	B8N	CN1-N1	2.12	1.50	1.46
38	A1	2865	PSU	C2-N3	-2.11	1.34	1.37
38	A1	1004	PSU	C2-N3	-2.11	1.34	1.37
38	A1	2880	PSU	C2-N3	-2.10	1.34	1.37
38	A1	2266	PSU	C6-N1	-2.09	1.32	1.36
34	B5	766	PSU	O4'-C1'	-2.08	1.41	1.43
38	A1	966	PSU	C6-N1	-2.07	1.32	1.36
34	B5	106	PSU	C2-N1	-2.06	1.34	1.36
38	A1	2129	PSU	C2-N1	-2.06	1.34	1.36
34	B5	302	PSU	C2-N1	-2.06	1.34	1.36
38	A1	990	PSU	C2-N1	-2.04	1.34	1.36
38	A1	2923	PSU	C2-N1	-2.02	1.34	1.36
34	B5	1191	B8N	O2-C2	2.01	1.26	1.22
38	A1	986	PSU	C2-N1	-2.00	1.34	1.36
38	A1	2264	PSU	C2-N1	-2.00	1.34	1.36

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C32-C31-N3	-16.34	83.60	112.16
34	B5	1290	PSU	N1-C2-N3	10.10	125.83	115.17
38	A1	2634	UR3	C4-N3-C2	-7.74	118.35	124.58
38	A1	2258	PSU	N1-C2-N3	7.55	123.13	115.17
38	A1	1124	PSU	N1-C2-N3	7.46	123.03	115.17
38	A1	2258	PSU	O2-C2-N1	-7.40	115.16	122.79
34	B5	120	PSU	N1-C2-N3	7.30	122.87	115.17
34	B5	106	PSU	N1-C2-N3	7.29	122.86	115.17
38	A1	1004	PSU	N1-C2-N3	7.09	122.64	115.17
38	A1	960	PSU	N1-C2-N3	7.06	122.61	115.17
38	A1	2133	PSU	N1-C2-N3	7.05	122.60	115.17
34	B5	1187	PSU	N1-C2-N3	6.92	122.47	115.17
38	A1	2923	PSU	N1-C2-N3	6.88	122.43	115.17
38	A1	2944	PSU	N1-C2-N3	6.87	122.41	115.17
39	A3	50	PSU	N1-C2-N3	6.67	122.21	115.17
38	A1	1056	PSU	N1-C2-N3	6.64	122.17	115.17
38	A1	2826	PSU	N1-C2-N3	6.59	122.12	115.17
34	B5	759	PSU	N1-C2-N3	6.44	121.96	115.17
38	A1	2314	PSU	N1-C2-N3	6.43	121.95	115.17
38	A1	990	PSU	N1-C2-N3	6.41	121.92	115.17
38	A1	2191	PSU	N1-C2-N3	6.41	121.92	115.17
38	A1	2129	PSU	N1-C2-N3	6.37	121.89	115.17
34	B5	999	PSU	N1-C2-N3	6.37	121.89	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2865	PSU	N1-C2-N3	6.36	121.88	115.17
40	A4	73	PSU	N1-C2-N3	6.35	121.86	115.17
38	A1	2340	PSU	N1-C2-N3	6.27	121.78	115.17
34	B5	766	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	2975	PSU	N1-C2-N3	6.22	121.73	115.17
38	A1	1110	PSU	N1-C2-N3	6.02	121.52	115.17
38	A1	2260	PSU	N1-C2-N3	6.01	121.51	115.17
38	A1	2349	PSU	N1-C2-N3	5.97	121.46	115.17
34	B5	1782	MA6	C5-C4-N3	-5.96	118.51	126.72
34	B5	1181	PSU	N1-C2-N3	5.93	121.43	115.17
38	A1	1052	PSU	N1-C2-N3	5.85	121.34	115.17
34	B5	120	PSU	O2-C2-N1	-5.80	116.81	122.79
38	A1	2880	PSU	N1-C2-N3	5.79	121.27	115.17
34	B5	211	PSU	N1-C2-N3	5.75	121.24	115.17
34	B5	302	PSU	N1-C2-N3	5.67	121.15	115.17
34	B5	1781	MA6	C2-N1-C6	5.55	125.39	111.83
34	B5	466	PSU	N1-C2-N3	5.45	120.91	115.17
38	A1	2266	PSU	C6-N1-C2	-5.41	117.67	122.69
38	A1	1124	PSU	O2-C2-N1	-5.27	117.36	122.79
38	A1	2264	PSU	N1-C2-N3	5.26	120.72	115.17
38	A1	2922	OMG	C5-C4-N3	-5.25	120.03	128.39
34	B5	1781	MA6	C5-C4-N3	-5.19	119.57	126.72
34	B5	1782	MA6	C4-C5-N7	-5.17	104.67	110.58
38	A1	966	PSU	N1-C2-N3	5.12	120.57	115.17
34	B5	1290	PSU	C4-N3-C2	-5.05	119.42	126.37
38	A1	986	PSU	N1-C2-N3	5.04	120.49	115.17
38	A1	776	PSU	N1-C2-N3	4.97	120.41	115.17
38	A1	2351	PSU	N1-C2-N3	4.97	120.41	115.17
38	A1	2921	OMU	C4-N3-C2	-4.95	120.46	126.61
34	B5	1290	PSU	O2-C2-N3	-4.95	113.07	121.86
38	A1	2142	1MA	C5-C4-N3	-4.92	120.03	127.27
38	A1	2416	PSU	N1-C2-N3	4.90	120.34	115.17
34	B5	632	PSU	N1-C2-N3	4.90	120.34	115.17
38	A1	2278	5MC	N1-C2-N3	4.90	127.30	118.80
38	A1	1124	PSU	C4-N3-C2	-4.83	119.71	126.37
38	A1	2922	OMG	C2-N3-C4	4.75	120.49	112.30
38	A1	2944	PSU	C4-N3-C2	-4.72	119.87	126.37
34	B5	1781	MA6	C4-C5-N7	-4.65	105.26	110.58
34	B5	106	PSU	C4-N3-C2	-4.64	119.97	126.37
34	B5	120	PSU	C4-N3-C2	-4.64	119.98	126.37
34	B5	1280	4AC	C6-C5-C4	4.57	122.50	117.00
38	A1	1042	PSU	C4-N3-C2	-4.57	120.08	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2921	OMU	N3-C2-N1	4.56	120.83	114.89
34	B5	1575	G7M	C2-N3-C4	4.55	120.13	112.30
38	A1	645	1MA	C5-C4-N3	-4.55	120.58	127.27
38	A1	960	PSU	O2-C2-N1	-4.53	118.11	122.79
38	A1	2133	PSU	C4-N3-C2	-4.51	120.15	126.37
38	A1	1042	PSU	N1-C2-N3	4.49	119.91	115.17
38	A1	2191	PSU	C4-N3-C2	-4.49	120.19	126.37
34	B5	1781	MA6	N1-C2-N3	-4.44	121.86	128.58
38	A1	2340	PSU	O2-C2-N1	-4.44	118.21	122.79
38	A1	2865	PSU	C4-N3-C2	-4.44	120.26	126.37
38	A1	1004	PSU	C4-N3-C2	-4.42	120.28	126.37
38	A1	1052	PSU	C4-N3-C2	-4.42	120.28	126.37
34	B5	1187	PSU	C4-N3-C2	-4.41	120.30	126.37
40	A4	73	PSU	C4-N3-C2	-4.39	120.33	126.37
38	A1	2735	PSU	N1-C2-N3	4.37	119.78	115.17
38	A1	645	1MA	C2-N3-C4	4.37	121.09	112.53
38	A1	2314	PSU	C4-N3-C2	-4.36	120.36	126.37
34	B5	1191	B8N	C4-N3-C2	-4.36	120.25	125.62
38	A1	960	PSU	C4-N3-C2	-4.34	120.39	126.37
38	A1	966	PSU	O2-C2-N1	-4.34	118.31	122.79
38	A1	2142	1MA	C2-N3-C4	4.33	121.02	112.53
38	A1	1052	PSU	O2-C2-N1	-4.32	118.33	122.79
38	A1	1004	PSU	O2-C2-N1	-4.32	118.33	122.79
38	A1	2258	PSU	C4-N3-C2	-4.31	120.43	126.37
38	A1	2266	PSU	C6-C5-C4	-4.28	115.29	118.17
34	B5	1782	MA6	C2-N3-C4	4.26	122.24	111.83
39	A3	50	PSU	O2-C2-N1	-4.22	118.43	122.79
34	B5	766	PSU	C4-N3-C2	-4.21	120.56	126.37
38	A1	2870	5MC	C5-C6-N1	-4.21	118.74	123.31
34	B5	1575	G7M	C5-C4-N3	-4.21	120.20	128.15
38	A1	2278	5MC	C5-C6-N1	-4.19	118.76	123.31
38	A1	2826	PSU	C4-N3-C2	-4.17	120.62	126.37
34	B5	1782	MA6	N3-C4-N9	4.15	134.22	127.17
38	A1	2921	OMU	C5-C4-N3	4.12	120.56	114.80
38	A1	2923	PSU	O2-C2-N1	-4.11	118.55	122.79
38	A1	2923	PSU	C4-N3-C2	-4.10	120.72	126.37
34	B5	1781	MA6	N3-C4-N9	4.08	134.11	127.17
38	A1	2129	PSU	C4-N3-C2	-4.08	120.75	126.37
38	A1	1042	PSU	C6-C5-C4	-3.99	115.48	118.17
34	B5	999	PSU	C4-N3-C2	-3.99	120.88	126.37
34	B5	1782	MA6	C2-N1-C6	3.96	121.51	111.83
38	A1	990	PSU	C4-N3-C2	-3.96	120.92	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2865	PSU	O2-C2-N1	-3.90	118.77	122.79
38	A1	2826	PSU	O2-C2-N1	-3.88	118.79	122.79
38	A1	1056	PSU	C4-N3-C2	-3.87	121.03	126.37
34	B5	1191	B8N	C31-N3-C4	3.87	122.65	117.18
34	B5	759	PSU	O2-C2-N1	-3.87	118.80	122.79
38	A1	2922	OMG	C6-C5-N7	3.86	137.31	130.29
38	A1	2416	PSU	C6-C5-C4	-3.85	115.58	118.17
38	A1	2944	PSU	O2-C2-N1	-3.82	118.85	122.79
38	A1	2922	OMG	N9-C4-N3	3.82	133.59	125.95
40	A4	73	PSU	O2-C2-N1	-3.78	118.89	122.79
34	B5	766	PSU	O2-C2-N1	-3.75	118.92	122.79
34	B5	1575	G7M	C5-C6-N1	3.74	119.58	111.84
38	A1	2129	PSU	O2-C2-N1	-3.73	118.94	122.79
34	B5	1181	PSU	O2-C2-N1	-3.72	118.95	122.79
38	A1	2975	PSU	C6-C5-C4	-3.71	115.67	118.17
34	B5	1187	PSU	O2-C2-N1	-3.69	118.99	122.79
38	A1	2278	5MC	C5-C4-N3	-3.69	117.98	121.75
34	B5	1280	4AC	O7-C7-N4	3.69	127.70	121.90
34	B5	759	PSU	C4-N3-C2	-3.65	121.34	126.37
34	B5	1575	G7M	N9-C4-N3	3.64	133.24	125.95
39	A3	50	PSU	C4-N3-C2	-3.64	121.36	126.37
38	A1	2349	PSU	C4-N3-C2	-3.59	121.42	126.37
34	B5	1782	MA6	C5-N7-C8	3.59	109.10	103.45
38	A1	2634	UR3	C5-C4-N3	3.59	119.77	115.04
34	B5	1781	MA6	C2-N3-C4	3.58	120.58	111.83
38	A1	2880	PSU	C4-N3-C2	-3.57	121.46	126.37
38	A1	990	PSU	O2-C2-N1	-3.55	119.12	122.79
34	B5	106	PSU	O2-C2-N1	-3.52	119.16	122.79
38	A1	1110	PSU	C4-N3-C2	-3.51	121.54	126.37
34	B5	1781	MA6	C5-N7-C8	3.50	108.94	103.45
38	A1	2975	PSU	C4-N3-C2	-3.49	121.56	126.37
38	A1	1042	PSU	C6-N1-C2	3.43	125.87	122.69
38	A1	2142	1MA	N9-C4-N3	3.42	134.70	126.90
34	B5	1290	PSU	C6-N1-C2	-3.42	119.51	122.69
38	A1	2260	PSU	C4-N3-C2	-3.42	121.67	126.37
38	A1	2340	PSU	C4-N3-C2	-3.36	121.74	126.37
38	A1	2349	PSU	C6-C5-C4	-3.35	115.91	118.17
34	B5	1575	G7M	CN7-N7-C5	3.34	130.97	126.80
38	A1	2266	PSU	C4-N3-C2	3.33	130.96	126.37
39	A3	50	PSU	C6-C5-C4	-3.32	115.93	118.17
34	B5	1280	4AC	C5-C4-N3	-3.32	117.40	122.60
38	A1	2351	PSU	C6-C5-C4	-3.29	115.96	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2416	PSU	O2-C2-N1	-3.27	119.42	122.79
38	A1	1110	PSU	O2-C2-N1	-3.25	119.44	122.79
38	A1	776	PSU	C6-C5-C4	-3.22	116.00	118.17
34	B5	1782	MA6	N1-C2-N3	-3.22	123.72	128.58
34	B5	1782	MA6	C6-C5-N7	3.21	138.55	133.43
38	A1	1056	PSU	O2-C2-N1	-3.19	119.50	122.79
34	B5	1575	G7M	C5'-C4'-C3'	3.18	126.65	115.21
38	A1	2735	PSU	O2-C2-N1	-3.17	119.52	122.79
38	A1	1042	PSU	C5-C6-N1	-3.15	117.77	122.14
34	B5	1575	G7M	O6-C6-C5	-3.15	120.98	128.01
34	B5	211	PSU	C4-N3-C2	-3.14	122.04	126.37
38	A1	2735	PSU	C6-C5-C4	-3.14	116.06	118.17
38	A1	1042	PSU	O4-C4-N3	-3.14	114.21	120.11
34	B5	1181	PSU	C4-N3-C2	-3.14	122.05	126.37
38	A1	2735	PSU	C4-N3-C2	-3.13	122.05	126.37
34	B5	302	PSU	C4-N3-C2	-3.13	122.06	126.37
38	A1	2260	PSU	O2-C2-N1	-3.12	119.57	122.79
34	B5	1781	MA6	C4-N9-C8	3.07	108.96	105.74
38	A1	2133	PSU	O2-C2-N1	-3.06	119.63	122.79
38	A1	2314	PSU	O2-C2-N1	-3.02	119.68	122.79
38	A1	2264	PSU	O2-C2-N1	-2.98	119.71	122.79
38	A1	2129	PSU	C6-C5-C4	-2.94	116.19	118.17
38	A1	2975	PSU	O2-C2-N1	-2.94	119.76	122.79
38	A1	2266	PSU	C5-C6-N1	2.92	126.20	122.14
38	A1	2351	PSU	O2-C2-N1	-2.92	119.78	122.79
38	A1	966	PSU	C4-N3-C2	-2.91	122.36	126.37
38	A1	2340	PSU	C6-C5-C4	-2.90	116.21	118.17
38	A1	986	PSU	C4-N3-C2	-2.88	122.40	126.37
38	A1	2921	OMU	O4-C4-C5	-2.88	120.20	125.16
34	B5	211	PSU	O2-C2-N1	-2.88	119.82	122.79
38	A1	2351	PSU	C4-N3-C2	-2.85	122.44	126.37
38	A1	2278	5MC	O2-C2-N1	-2.84	113.33	118.90
34	B5	999	PSU	O2-C2-N1	-2.83	119.87	122.79
34	B5	1782	MA6	C4-N9-C8	2.82	108.70	105.74
38	A1	2416	PSU	C4-N3-C2	-2.81	122.50	126.37
38	A1	1052	PSU	C5-C6-N1	-2.78	118.28	122.14
38	A1	645	1MA	C6-C5-N7	2.73	136.98	132.16
38	A1	986	PSU	O2-C2-N1	-2.73	119.97	122.79
34	B5	632	PSU	C5-C6-N1	-2.71	118.38	122.14
38	A1	1110	PSU	C6-C5-C4	-2.68	116.36	118.17
38	A1	645	1MA	C4-C5-N7	-2.67	106.44	110.67
34	B5	302	PSU	C6-C5-C4	-2.67	116.37	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	632	PSU	C4-N3-C2	-2.66	122.70	126.37
38	A1	2264	PSU	C4-N3-C2	-2.66	122.71	126.37
38	A1	2922	OMG	C4-C5-N7	-2.65	106.47	110.67
34	B5	1781	MA6	C6-C5-N7	2.65	137.66	133.43
38	A1	645	1MA	N9-C4-N3	2.64	132.91	126.90
38	A1	2133	PSU	C5-C6-N1	-2.63	118.49	122.14
34	B5	1782	MA6	N9-C8-N7	-2.62	110.22	113.94
38	A1	986	PSU	C6-C5-C4	-2.60	116.42	118.17
38	A1	2278	5MC	CM5-C5-C6	-2.59	119.35	122.85
34	B5	1191	B8N	C1'-C5-C4	2.56	121.48	117.61
34	B5	466	PSU	C5-C6-N1	-2.55	118.59	122.14
38	A1	2258	PSU	C6-N1-C2	-2.50	120.37	122.69
34	B5	999	PSU	C5-C6-N1	-2.48	118.70	122.14
34	B5	1191	B8N	N3-C2-N1	2.48	119.75	116.72
38	A1	2880	PSU	O2-C2-N1	-2.47	120.24	122.79
38	A1	2260	PSU	C6-C5-C4	-2.47	116.51	118.17
38	A1	2349	PSU	O2-C2-N1	-2.47	120.24	122.79
38	A1	2191	PSU	C5-C6-N1	-2.47	118.71	122.14
38	A1	2278	5MC	C4-N3-C2	-2.46	117.40	120.81
38	A1	2191	PSU	O2-C2-N1	-2.44	120.28	122.79
34	B5	1575	G7M	C2-N1-C6	-2.43	120.70	125.11
34	B5	1781	MA6	N9-C8-N7	-2.42	110.50	113.94
38	A1	2314	PSU	C5-C6-N1	-2.40	118.81	122.14
38	A1	1004	PSU	C5-C6-N1	-2.39	118.82	122.14
38	A1	2865	PSU	C5-C6-N1	-2.38	118.84	122.14
38	A1	2826	PSU	C5-C6-N1	-2.38	118.84	122.14
34	B5	211	PSU	C6-C5-C4	-2.38	116.57	118.17
34	B5	1415	PSU	C6-C5-C4	-2.37	116.58	118.17
38	A1	960	PSU	C5-C6-N1	-2.34	118.90	122.14
38	A1	2634	UR3	C6-N1-C2	-2.32	119.90	121.80
38	A1	2922	OMG	O6-C6-C5	-2.32	120.41	126.53
34	B5	1280	4AC	O7-C7-CM7	-2.31	117.94	122.05
38	A1	2133	PSU	O2-C2-N3	-2.31	117.77	121.86
38	A1	2191	PSU	O2-C2-N3	-2.29	117.79	121.86
34	B5	632	PSU	O2-C2-N1	-2.28	120.44	122.79
34	B5	466	PSU	C4-N3-C2	-2.28	123.23	126.37
38	A1	2870	5MC	O2'-C2'-C1'	-2.27	102.28	110.10
34	B5	302	PSU	O2-C2-N1	-2.26	120.45	122.79
38	A1	2142	1MA	C4-C5-N7	-2.26	107.09	110.67
36	AB	243	HIC	NE2-CE1-ND1	-2.22	111.81	112.66
38	A1	776	PSU	O2-C2-N1	-2.21	120.51	122.79
38	A1	2735	PSU	C5-C6-N1	-2.21	119.08	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2142	1MA	C8-N9-C4	2.20	110.15	106.03
34	B5	1191	B8N	O4'-C1'-C2'	2.20	108.19	105.15
34	B5	1575	G7M	O4'-C4'-C5'	2.20	116.38	109.33
38	A1	2142	1MA	C6-C5-N7	2.20	136.04	132.16
34	B5	106	PSU	O2-C2-N3	-2.19	117.98	121.86
38	A1	2260	PSU	O4'-C1'-C2'	2.18	108.17	105.15
38	A1	2826	PSU	O4'-C1'-C2'	2.18	108.16	105.15
38	A1	2634	UR3	C3U-N3-C2	2.16	121.11	117.33
34	B5	1187	PSU	C5-C6-N1	-2.16	119.14	122.14
38	A1	2266	PSU	O4-C4-N3	2.15	124.16	120.11
38	A1	2278	5MC	C6-N1-C2	-2.15	118.09	120.95
40	A4	73	PSU	C6-C5-C4	-2.14	116.73	118.17
38	A1	2944	PSU	C6-C5-C4	-2.13	116.74	118.17
38	A1	2278	5MC	O2-C2-N3	-2.11	119.00	122.33
38	A1	966	PSU	C6-C5-C4	-2.10	116.75	118.17
34	B5	466	PSU	O2-C2-N3	-2.10	118.12	121.86
34	B5	1290	PSU	C5-C6-N1	-2.10	119.23	122.14
34	B5	106	PSU	C5-C6-N1	-2.09	119.24	122.14
38	A1	776	PSU	C4-N3-C2	-2.09	123.49	126.37
38	A1	2266	PSU	O2-C2-N1	-2.08	120.64	122.79
38	A1	2258	PSU	C6-C5-C4	-2.08	116.77	118.17
38	A1	645	1MA	N1-C2-N3	-2.07	123.54	126.00
38	A1	2142	1MA	N9-C8-N7	-2.07	109.57	113.40
38	A1	2142	1MA	C8-N7-C5	2.06	107.92	104.26
34	B5	1781	MA6	N1-C6-N6	2.05	119.36	116.86
38	A1	2870	5MC	C5-C4-N3	-2.05	119.65	121.75
38	A1	2975	PSU	C6-N1-C2	-2.04	120.80	122.69
34	B5	999	PSU	O2-C2-N3	-2.04	118.24	121.86
38	A1	2922	OMG	C5-C6-N1	2.04	118.44	113.25
38	A1	1004	PSU	O4'-C1'-C2'	2.03	107.97	105.15
34	B5	766	PSU	C6-C5-C4	-2.03	116.80	118.17
38	A1	2349	PSU	O2-C2-N3	-2.01	118.30	121.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1575	G7M	C4'
34	B5	1575	G7M	C3'

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	AB	243	HIC	O-C-CA-CB
34	B5	1290	PSU	O4'-C4'-C5'-O5'
34	B5	1773	4AC	N3-C4-N4-C7
34	B5	1773	4AC	C5-C4-N4-C7
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	776	PSU	C2'-C1'-C5-C4
38	A1	1042	PSU	C2'-C1'-C5-C4
38	A1	1042	PSU	O4'-C1'-C5-C4
38	A1	1042	PSU	O4'-C1'-C5-C6
38	A1	2923	PSU	O4'-C4'-C5'-O5'
38	A1	2923	PSU	C4'-C5'-O5'-P
34	B5	1575	G7M	C3'-C4'-C5'-O5'
38	A1	2260	PSU	C3'-C4'-C5'-O5'
38	A1	2260	PSU	O4'-C4'-C5'-O5'
38	A1	2923	PSU	C3'-C4'-C5'-O5'
34	B5	211	PSU	C3'-C4'-C5'-O5'
34	B5	211	PSU	O4'-C4'-C5'-O5'
34	B5	1415	PSU	C3'-C4'-C5'-O5'
34	B5	1575	G7M	O4'-C4'-C5'-O5'
38	A1	2258	PSU	O4'-C4'-C5'-O5'
34	B5	1290	PSU	C3'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
38	A1	2266	PSU	C3'-C4'-C5'-O5'
34	B5	1415	PSU	O4'-C4'-C5'-O5'
38	A1	2266	PSU	O4'-C4'-C5'-O5'
38	A1	2258	PSU	C3'-C4'-C5'-O5'
38	A1	2870	5MC	C2'-C1'-N1-C6
34	B5	1191	B8N	C32-C33-C34-O35
38	A1	2870	5MC	O4'-C1'-N1-C6
38	A1	2314	PSU	C4'-C5'-O5'-P
38	A1	2944	PSU	O4'-C1'-C5-C4
34	B5	1191	B8N	C32-C33-C34-O36
34	B5	1782	MA6	C4'-C5'-O5'-P
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	645	1MA	C2'-C1'-N9-C8
38	A1	776	PSU	O4'-C4'-C5'-O5'
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	2142	1MA	C4'-C5'-O5'-P
38	A1	2340	PSU	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B5	1181	PSU	1	0
38	A1	2880	PSU	1	0
38	A1	2278	5MC	1	0
38	A1	2260	PSU	1	0
38	A1	2266	PSU	2	0
38	A1	1110	PSU	1	0
34	B5	1773	4AC	1	0
38	A1	2258	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 202 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
38	A1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	451:U	O3'	486:A	P	16.51

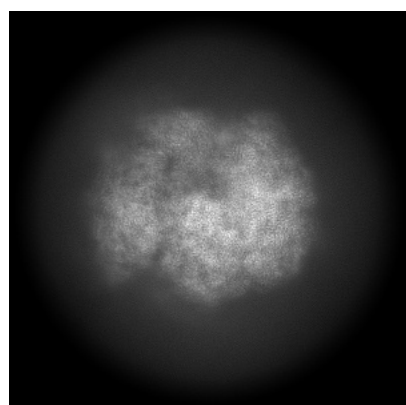
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71745. These allow visual inspection of the internal detail of the map and identification of artifacts.

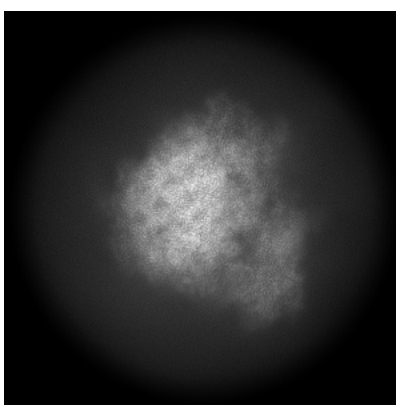
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

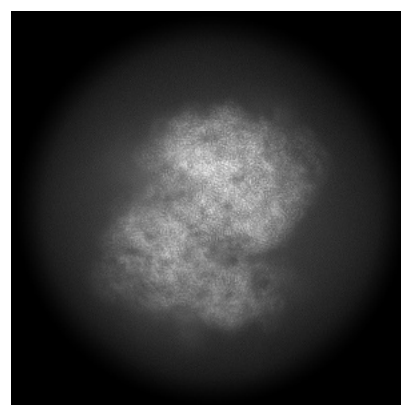
6.1.1 Primary map



X



Y

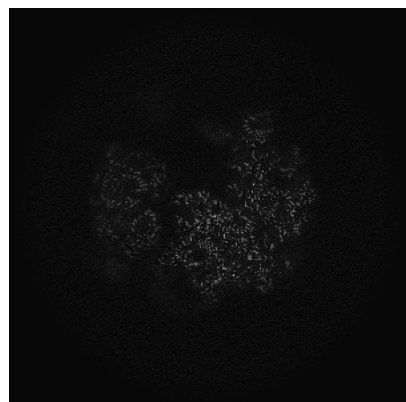


Z

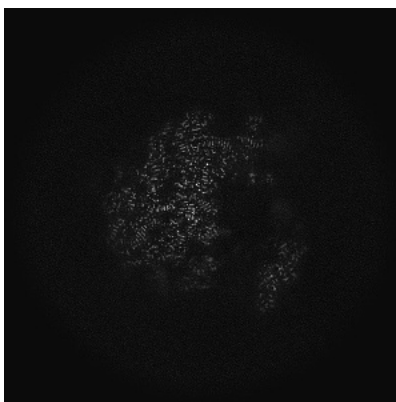
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

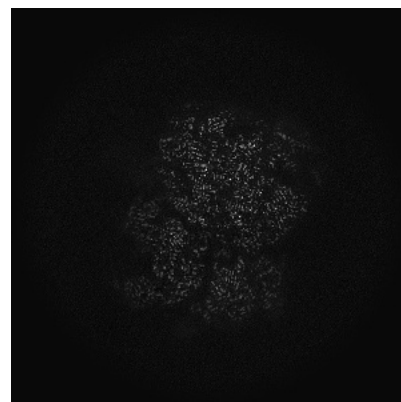
6.2.1 Primary map



X Index: 300



Y Index: 300

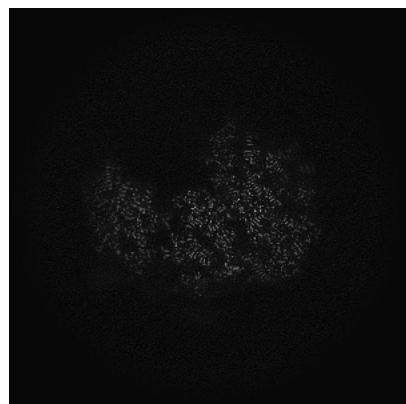


Z Index: 300

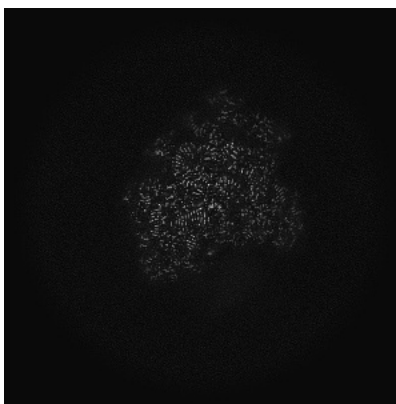
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

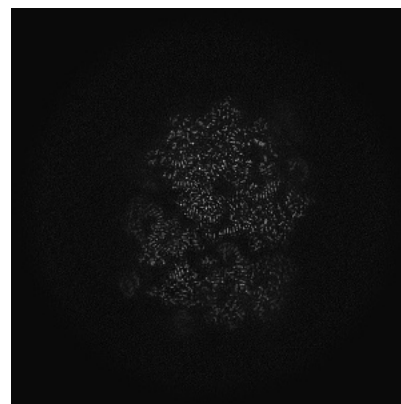
6.3.1 Primary map



X Index: 337



Y Index: 365

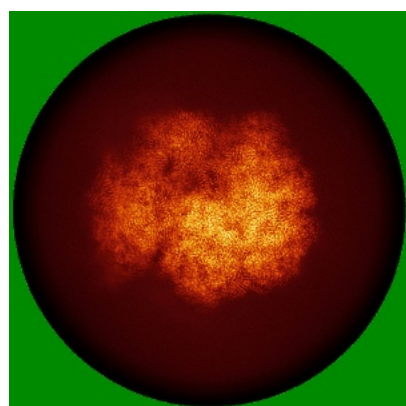


Z Index: 283

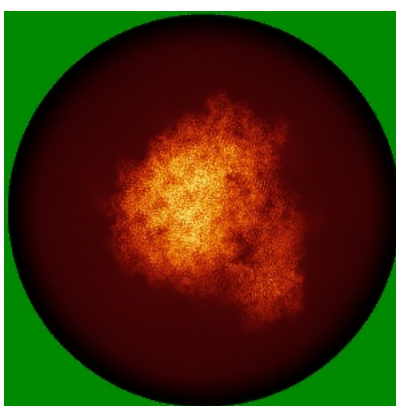
The images above show the largest variance slices of the map in three orthogonal directions.

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

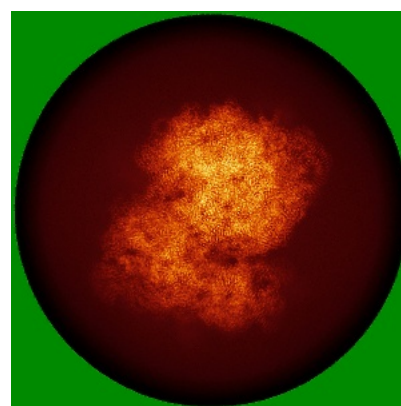
6.4.1 Primary map



X



Y

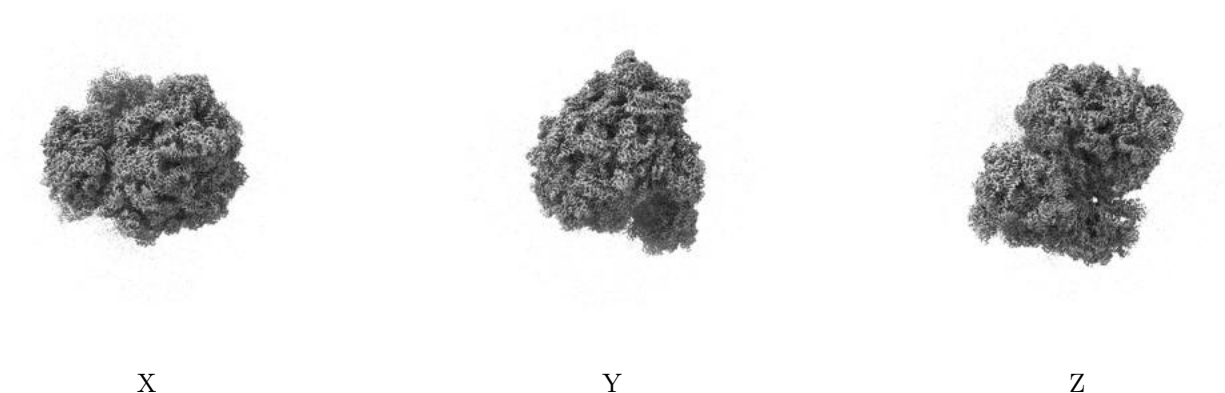


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

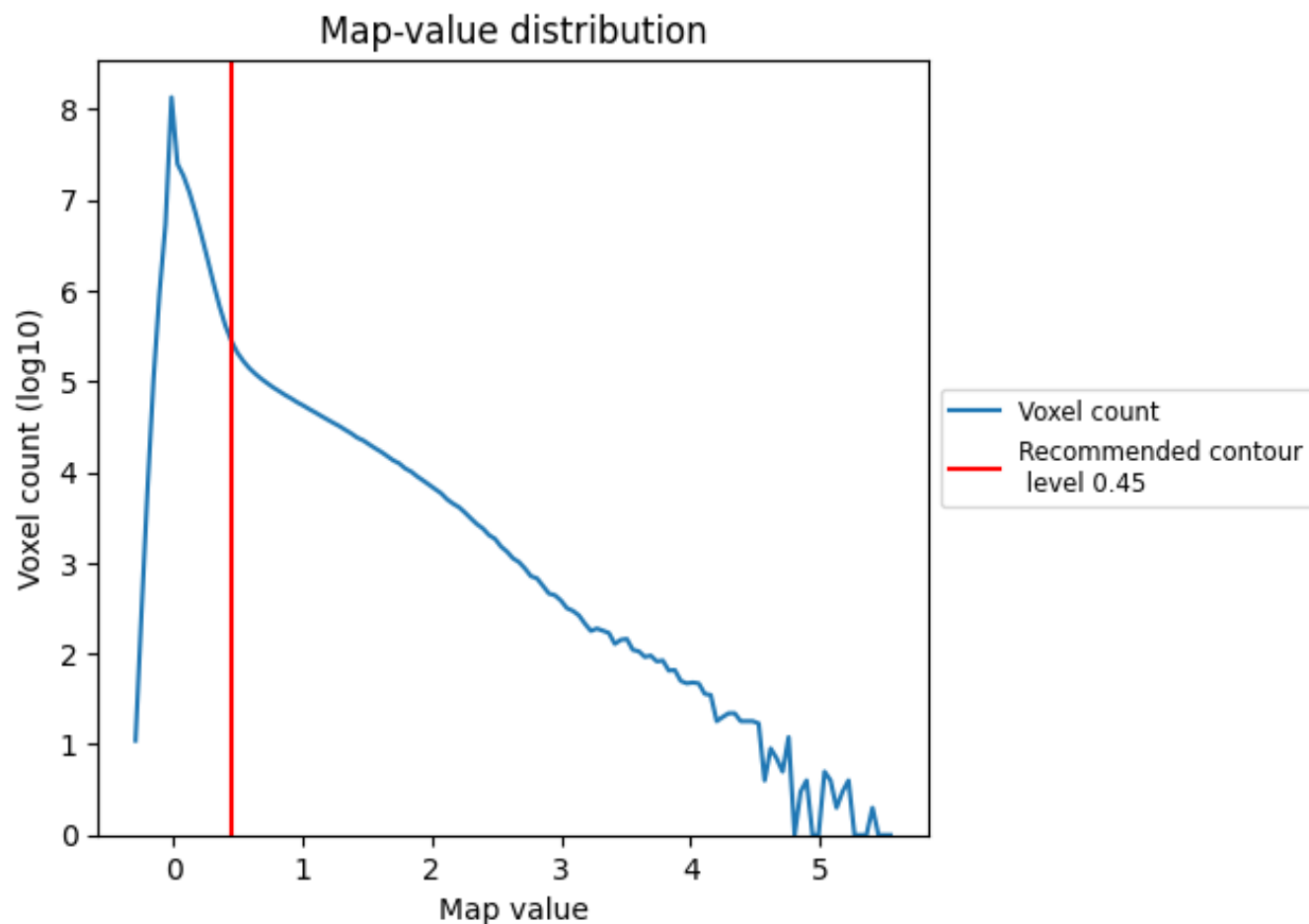
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

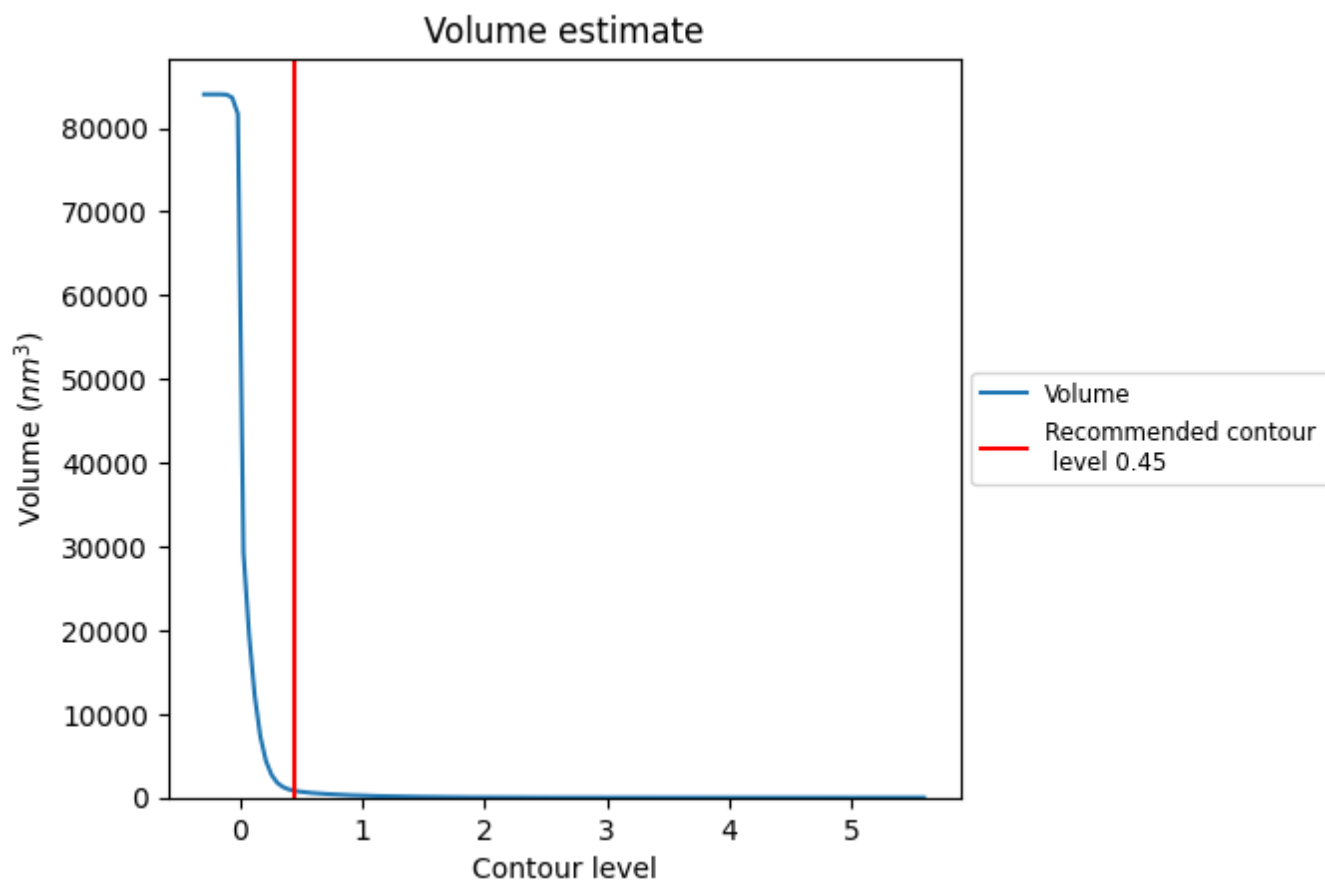
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

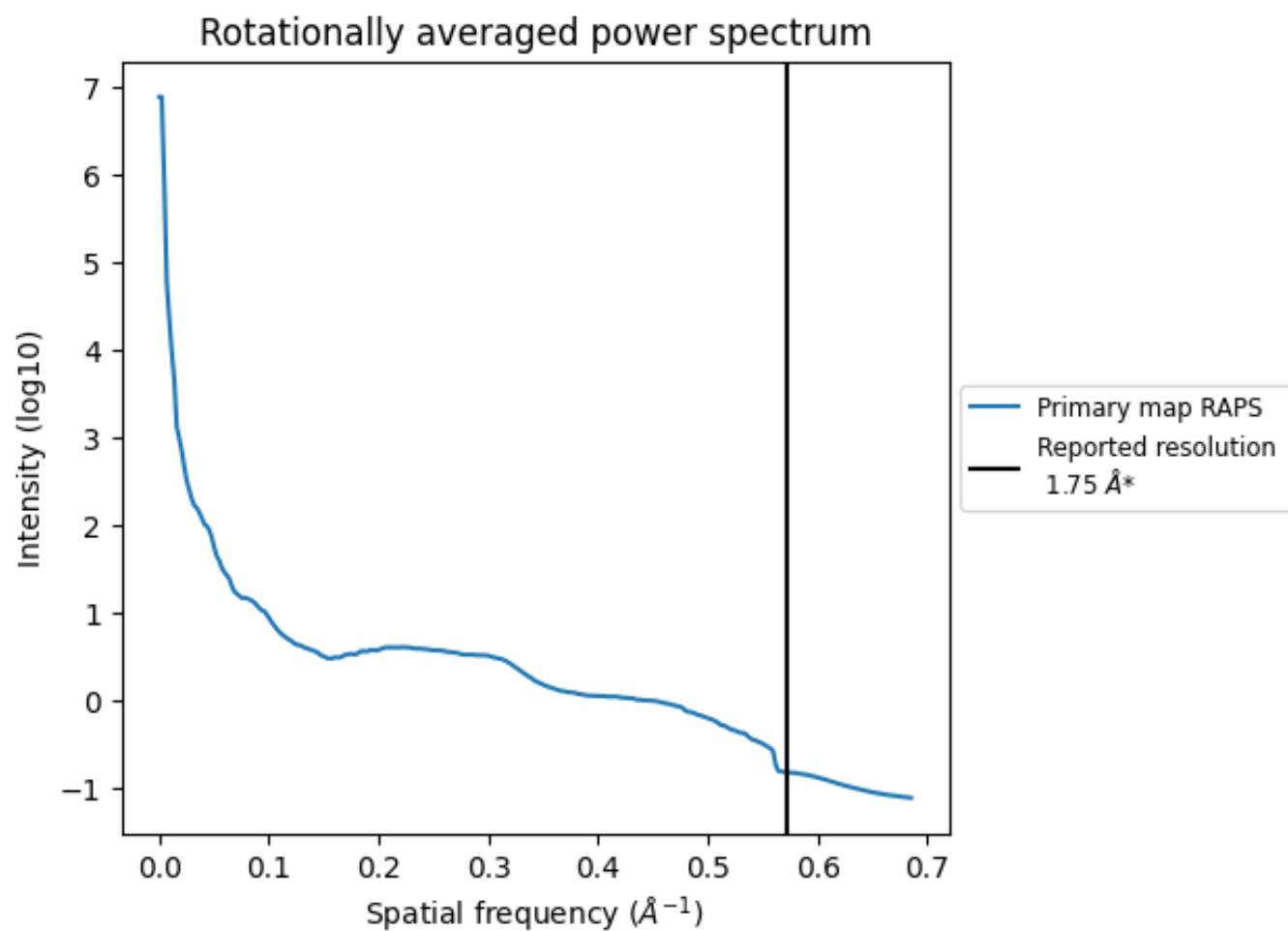
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 724 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 0.571 Å⁻¹

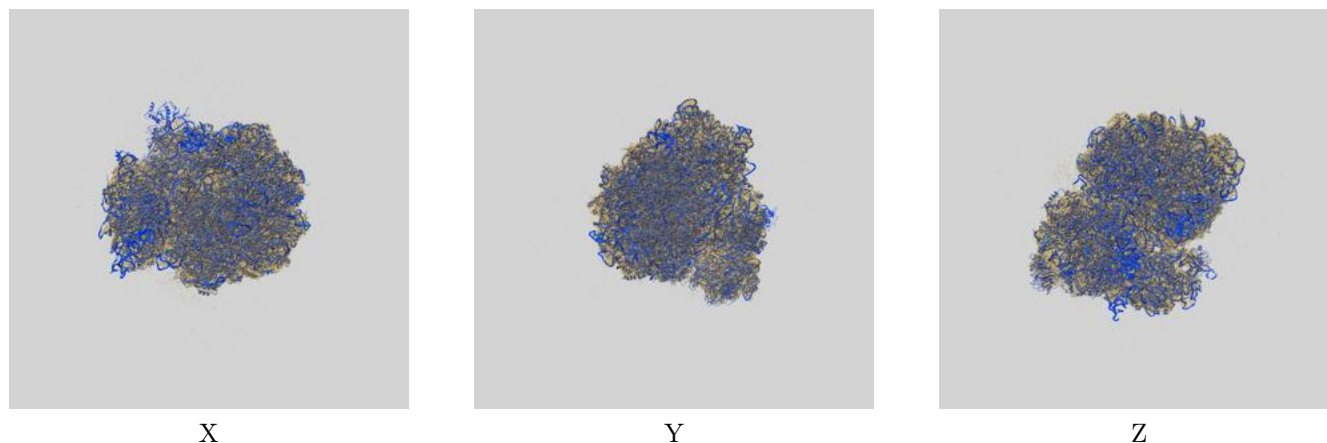
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

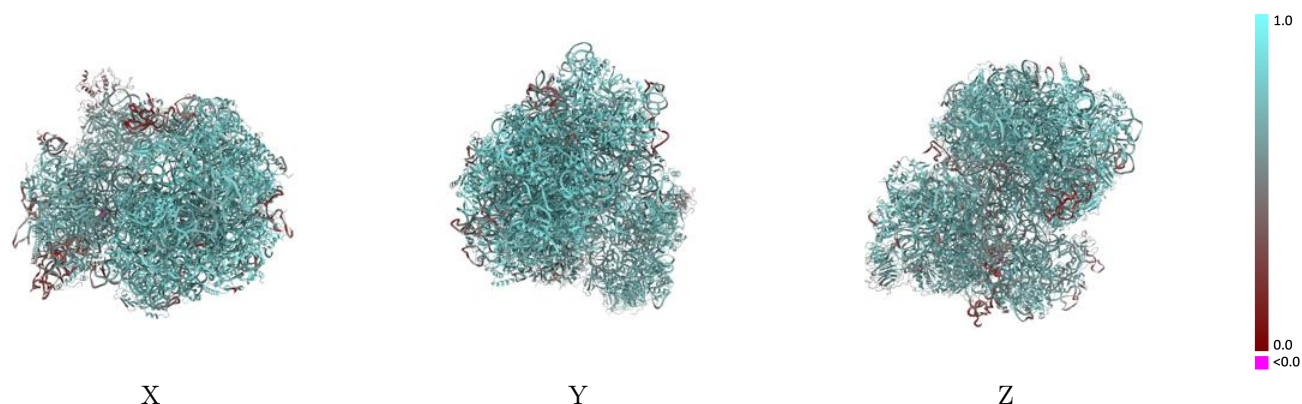
This section contains information regarding the fit between EMDB map EMD-71745 and PDB model 9PN5. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



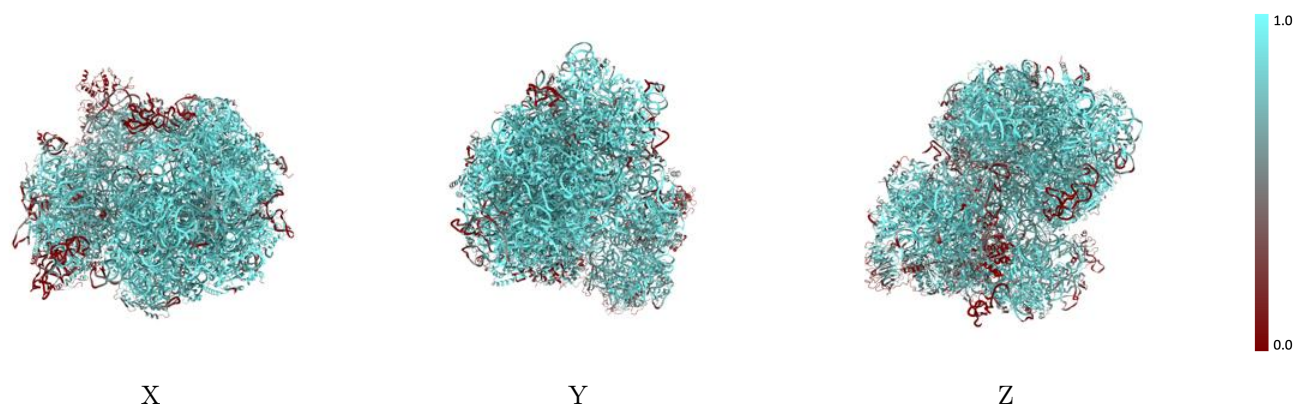
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



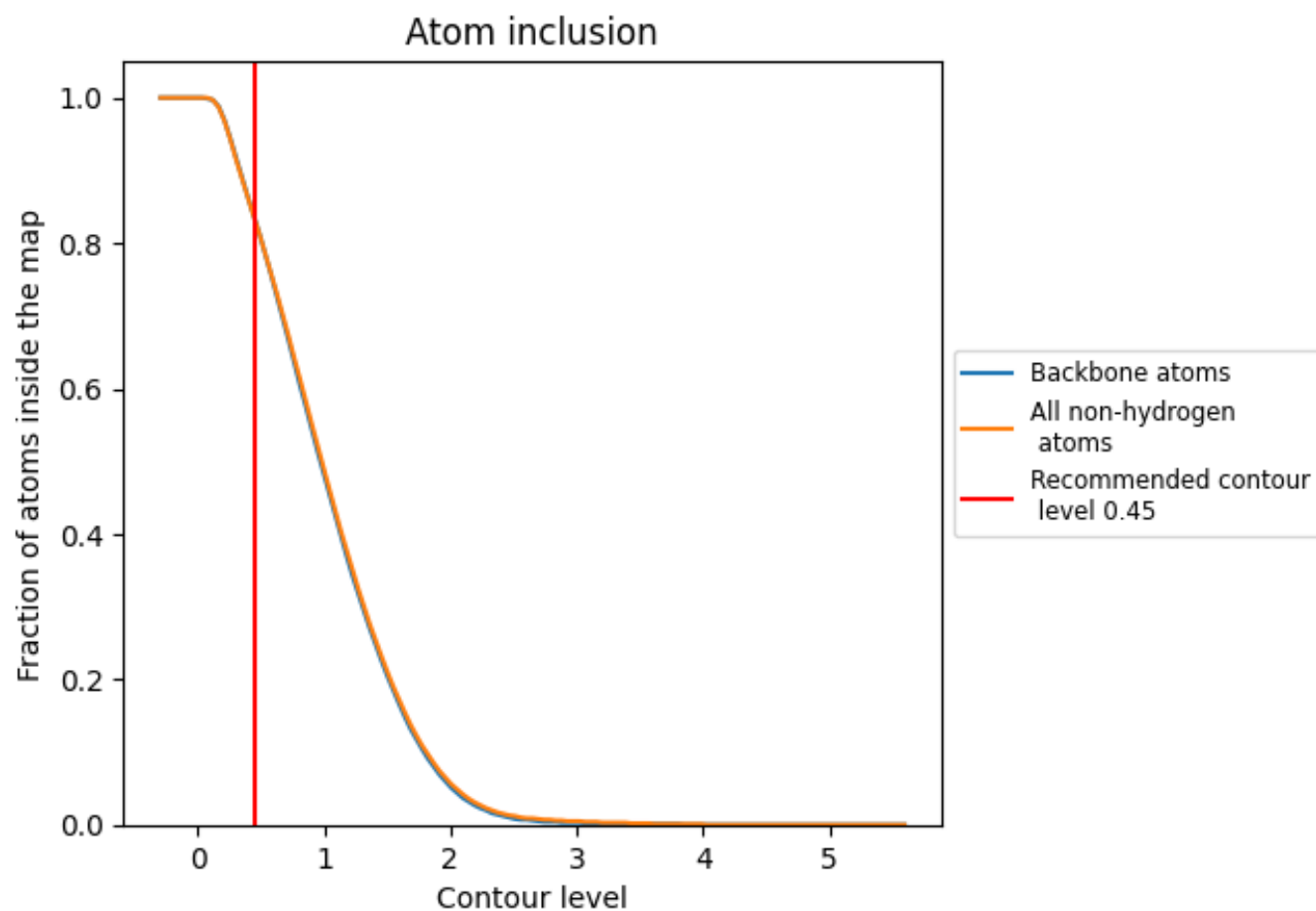
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.7320
A1	 0.8870	 0.7570
A3	 0.9440	 0.7570
A4	 0.9570	 0.7960
AA	 0.9790	 0.8460
AB	 0.9490	 0.8260
AC	 0.9380	 0.8160
AD	 0.7440	 0.7050
AE	 0.8000	 0.7260
AF	 0.9330	 0.8140
AG	 0.8330	 0.7450
AH	 0.8400	 0.7560
AI	 0.8190	 0.7490
AJ	 0.5280	 0.6230
AL	 0.8780	 0.7930
AM	 0.8970	 0.7800
AN	 0.9890	 0.8520
AO	 0.9410	 0.8170
AP	 0.9300	 0.8160
AQ	 0.9700	 0.8350
AR	 0.7630	 0.7250
AS	 0.9290	 0.7980
AT	 0.8980	 0.7850
AU	 0.7260	 0.6830
AV	 0.9300	 0.8100
AW	 0.9310	 0.8160
AX	 0.9120	 0.7970
AY	 0.9260	 0.8060
AZ	 0.8330	 0.7460
Aa	 0.9530	 0.8290
Ab	 0.8410	 0.7470
Ac	 0.8440	 0.7560
Ad	 0.8580	 0.7650
Ae	 0.9500	 0.8330
Af	 0.9720	 0.8350





Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ag	 0.8970	 0.8010
Ah	 0.9070	 0.7880
Ai	 0.8620	 0.7520
Aj	 0.9600	 0.8420
Ak	 0.7030	 0.7050
Al	 0.9690	 0.8240
Am	 0.8410	 0.7710
An	 0.8210	 0.6950
Ao	 0.8290	 0.7690
Ap	 0.9190	 0.8120
B5	 0.7980	 0.6680
BA	 0.7620	 0.6970
BB	 0.7090	 0.6650
BC	 0.8730	 0.7460
BD	 0.5920	 0.6400
BE	 0.8540	 0.7310
BF	 0.7940	 0.7160
BG	 0.5390	 0.6200
BH	 0.4700	 0.5840
BI	 0.8220	 0.7130
BJ	 0.8180	 0.7200
BK	 0.5020	 0.5980
BL	 0.7830	 0.6950
BM	 0.0040	 0.3500
BN	 0.8860	 0.7490
BO	 0.8360	 0.6980
BP	 0.6630	 0.6590
BQ	 0.8940	 0.7570
BR	 0.5180	 0.6230
BS	 0.7940	 0.7060
BT	 0.8680	 0.7360
BU	 0.5570	 0.6220
BV	 0.8250	 0.7300
BW	 0.9590	 0.7870
BX	 0.8480	 0.7380
BY	 0.6960	 0.6800
BZ	 0.6400	 0.6630
Ba	 0.8550	 0.7410
Bb	 0.7210	 0.6870
Bc	 0.5580	 0.6300
Bd	 0.9360	 0.7710
Be	 0.5470	 0.6170

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bf	 0.0120	 0.4370
Bg	 0.5230	 0.6240