



Full wwPDB EM Validation Report ⓘ

Jul 10, 2025 – 02:52 pm BST

PDB ID : 9QQA / pdb_00009qqa
EMDB ID : EMD-53295
Title : Ternary complex of translating ribosome, NAC and NMT1
Authors : Echeverria, B.; Jaskolowski, M.; Scaiola, A.; Ban, N.
Deposited on : 2025-03-31
Resolution : 2.80 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

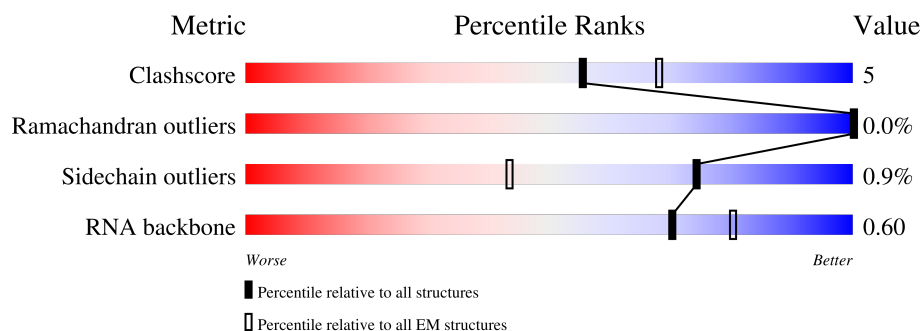
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.





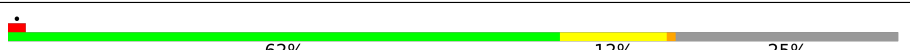
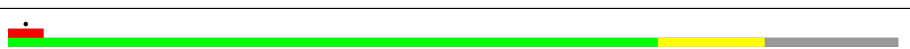

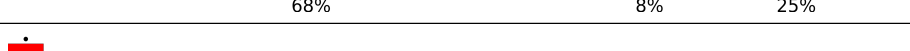
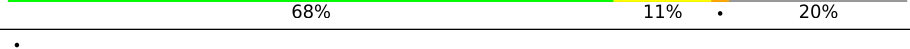





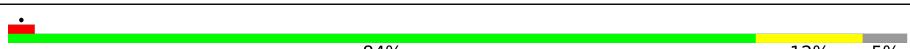











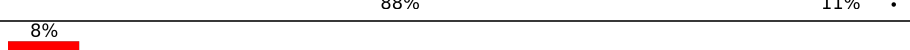
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A2	1870	
2	AA	84	
3	AB	69	
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	




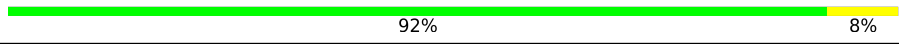


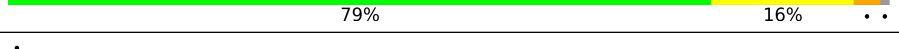
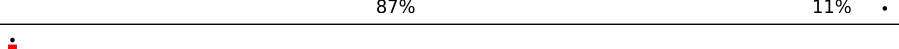
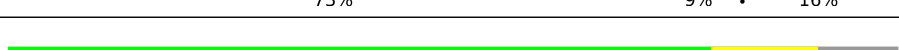


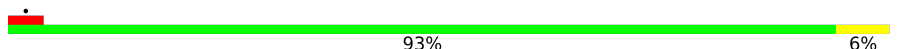



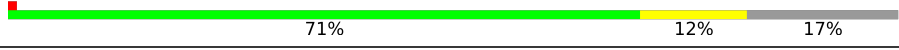
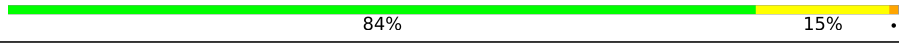

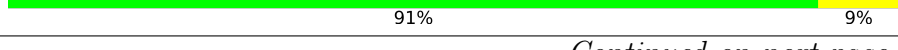
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AG	56	
9	AT	76	
10	AZ	295	
11	Aa	264	
12	Ab	293	
13	Ac	281	
14	Ad	263	
15	Ae	204	
16	Af	249	
17	Ag	432	
18	Ah	208	
19	Ai	194	
20	Aj	165	
21	Ak	158	
22	Al	132	
23	Am	151	
24	An	151	
25	Ao	145	
26	Ap	172	
27	Aq	135	
28	Ar	152	
29	As	145	
30	At	119	
31	Au	84	
32	Av	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Aw	143	
34	Ax	130	
35	Ay	124	
36	Az	25	
37	B5	4808	
38	B7	120	
39	B8	158	
40	BA	257	
41	BB	403	
42	BC	413	
43	BE	291	
44	BF	247	
45	BG	266	
46	BH	192	
47	BI	214	
48	BJ	178	
49	BK	12	
50	BL	211	
51	BM	218	
52	BN	204	
53	BO	203	
54	BP	184	
55	BQ	188	
56	BR	196	
57	BS	176	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	BT	160	
59	BU	128	
60	BV	140	
61	BW	157	
62	BX	156	
63	BY	145	
64	BZ	136	
65	Ba	148	
66	Bb	245	
67	Bc	115	
68	Bd	125	
69	Be	135	
70	Bf	110	
71	Bg	117	
72	Bh	123	
73	Bi	105	
74	Bj	97	
75	Bk	70	
76	Bl	51	
77	Bm	128	
78	Bo	106	
79	Bp	92	
80	Br	137	
81	Bs	318	
82	Bt	165	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	Bv	217	<div><div><div></div><div></div><div></div></div><div>94%75%23%•</div></div>
84	MA	496	<div><div><div></div><div></div><div></div></div><div>33%43%25%•31%</div></div>
85	Nt	215	<div><div><div></div><div></div><div></div></div><div>21%18%11%71%</div></div>
86	Nu	162	<div><div><div></div><div></div><div></div></div><div>41%36%26%••34%</div></div>

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 226637 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

- Molecule 2 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 3 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 4 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 5 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 6 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 7 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 9 is a RNA chain called P site Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AT	76	Total	C	N	O	P	0	0
			1621	724	290	531	76		

- Molecule 10 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AZ	222	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP G1TLT8

- Molecule 11 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	33	ILE	VAL	conflict	UNP O18789
Ab	101	ALA	SER	conflict	UNP O18789

- Molecule 13 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 14 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ad	25	GLY	SER	conflict	UNP G1TK17
Ad	51	ARG	LYS	conflict	UNP G1TK17
Ad	78	THR	ALA	conflict	UNP G1TK17
Ad	156	VAL	MET	conflict	UNP G1TK17

- Molecule 15 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 16 is a protein called 40S ribosomal protein S6.

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

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 18 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 19 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 20 is a protein called S10_ plectin domain-containing protein.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 22 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 23 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	An	122	Total	C	N	O	S	0	0
			899	556	166	171	6		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 27 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 28 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ar	149	Total	C	N	O	S	0	0
			1217	763	245	208	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ar	2	ACE	-	acetylation	UNP G1TPG3

- Molecule 29 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	conflict	UNP G1TN62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	At	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 31 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Au	84	Total	C	N	O	S	0	0
			640	394	117	124	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Au	0	ACE	-	acetylation	UNP G1TM82

- Molecule 32 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 33 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 34 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 35 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 36 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 37 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B5	3706	Total	C	N	O	P	0	0
			79525	35447	14532	25840	3706		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 39 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 40 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 41 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 42 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BC	363	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	2	ACE	-	acetylation	UNP G1SVW5

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 44 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	conflict	UNP G1TUB1
BF	93	ARG	GLY	conflict	UNP G1TUB1
BF	131	MET	VAL	conflict	UNP G1TUB1
BF	153	ILE	VAL	conflict	UNP G1TUB1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	184	LEU	ILE	conflict	UNP P62424

- Molecule 46 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 48 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 49 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BK	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 50 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	74	ARG	HIS	conflict	UNP G1TKB3
BL	190	ARG	HIS	conflict	UNP G1TKB3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 52 is a protein called Ribosomal protein L15.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 54 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BP	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 55 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 56 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	conflict	UNP G1TJR3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BR	64	ARG	GLN	conflict	UNP G1TJR3
BR	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 57 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 58 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 59 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BU	102	Total	C	N	O	S	0	0
			831	531	146	152	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 60 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 61 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 62 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 63 is a protein called Ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 65 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 66 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 68 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bd	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 69 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 70 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 71 is a protein called 60S ribosomal protein L34.

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

- Molecule 72 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 73 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 74 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 75 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 76 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 77 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 79 is a protein called 60S ribosomal protein L37a.

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

- Molecule 80 is a protein called [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Br	127	Total	C	N	O	S	0	0
			1014	629	209	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	2	ACE	-	acetylation	UNP A0A8C0DF35

- Molecule 81 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 82 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 83 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 84 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	MA	341	Total	C	N	O	S	1	0
			2797	1815	475	491	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	180	ALA	TYR	engineered mutation	UNP P30419

- Molecule 85 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Nt	63	Total	C	N	O	S	0	0
			499	316	91	91	1		

- Molecule 86 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Nu	107	Total	C	N	O	S	0	0
			828	518	154	153	3		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	A2	108	Total 108	Mg 108	0
87	Aw	1	Total 1	Mg 1	0
87	B5	273	Total 273	Mg 273	0
87	B7	9	Total 9	Mg 9	0
87	B8	8	Total 8	Mg 8	0
87	BB	3	Total 3	Mg 3	0
87	BI	1	Total 1	Mg 1	0
87	BP	1	Total 1	Mg 1	0
87	BR	1	Total 1	Mg 1	0
87	BV	1	Total 1	Mg 1	0
87	Bj	1	Total 1	Mg 1	0

- Molecule 88 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

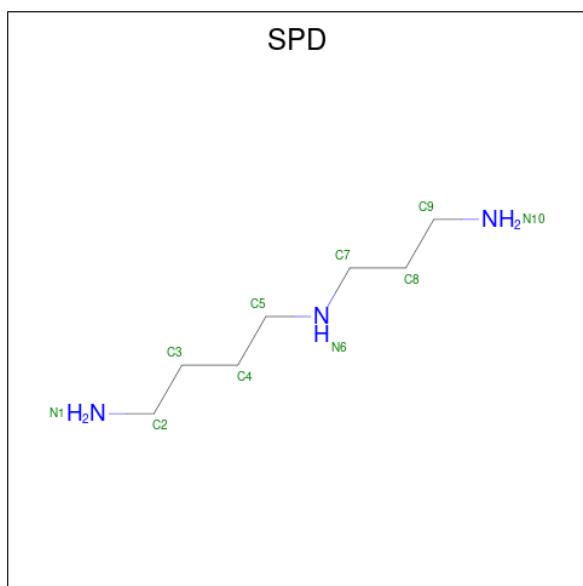
Mol	Chain	Residues	Atoms		AltConf
88	A2	31	Total 31	X 31	0
88	Ad	1	Total 1	X 1	0
88	B5	130	Total 130	X 130	0
88	B7	6	Total 6	X 6	0
88	B8	4	Total 4	X 4	0
88	BA	2	Total 2	X 2	0
88	BH	1	Total 1	X 1	0
88	BI	1	Total 1	X 1	0
88	BL	1	Total 1	X 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	BN	2	Total	X	0
			2	2	
88	BQ	1	Total	X	0
			1	1	
88	BT	1	Total	X	0
			1	1	
88	BY	1	Total	X	0
			1	1	
88	Bb	2	Total	X	0
			2	2	
88	Be	2	Total	X	0
			2	2	
88	Bo	1	Total	X	0
			1	1	

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	
89	A2	1	Total	C	N	0
			10	7	3	

Continued on next page...

Continued from previous page...

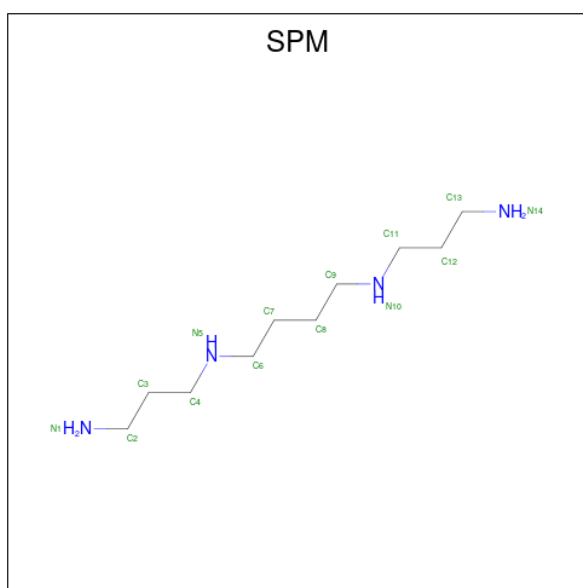
[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
89	B5	1	Total	C	N	0
			10	7	3	
89	B5	1	Total	C	N	0
			10	7	3	
89	B5	1	Total	C	N	0
			10	7	3	
89	B5	1	Total	C	N	0
			10	7	3	
89	B5	1	Total	C	N	0
			10	7	3	

- Molecule 90 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
90	A2	1	Total	C	N	0
			14	10	4	
90	B5	1	Total	C	N	0
			14	10	4	
90	B5	1	Total	C	N	0
			14	10	4	

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	AC	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	AE	1	Total 1	Zn 1	0
91	AG	1	Total 1	Zn 1	0
91	Bg	1	Total 1	Zn 1	0
91	Bj	1	Total 1	Zn 1	0
91	Bm	1	Total 1	Zn 1	0
91	Bo	1	Total 1	Zn 1	0
91	Bp	1	Total 1	Zn 1	0

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	514	Total 514	O 514	0
92	AE	1	Total 1	O 1	0
92	AT	4	Total 4	O 4	0
92	Aa	3	Total 3	O 3	0
92	Af	2	Total 2	O 2	0
92	Ak	2	Total 2	O 2	0
92	An	2	Total 2	O 2	0
92	Ap	1	Total 1	O 1	0
92	Ar	2	Total 2	O 2	0
92	As	2	Total 2	O 2	0
92	At	1	Total 1	O 1	0
92	Aw	4	Total 4	O 4	0

Continued on next page...

Continued from previous page...

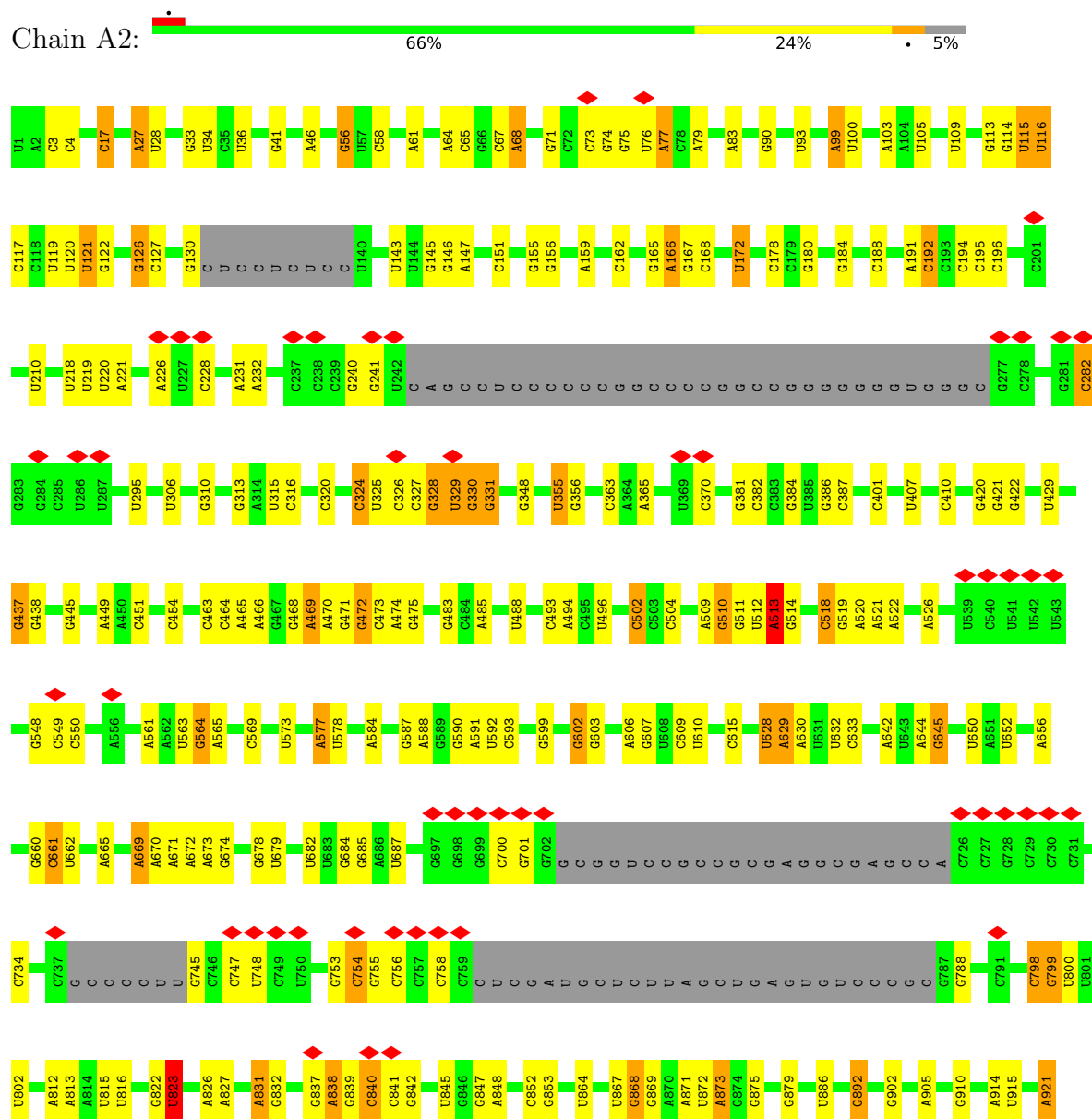
Mol	Chain	Residues	Atoms		AltConf
92	B5	1359	Total 1359	O 1359	0
92	B7	38	Total 38	O 38	0
92	B8	49	Total 49	O 49	0
92	BA	4	Total 4	O 4	0
92	BC	6	Total 6	O 6	0
92	BH	1	Total 1	O 1	0
92	BI	3	Total 3	O 3	0
92	BL	1	Total 1	O 1	0
92	BN	2	Total 2	O 2	0
92	BP	4	Total 4	O 4	0
92	BR	2	Total 2	O 2	0
92	BV	3	Total 3	O 3	0
92	BX	1	Total 1	O 1	0
92	BY	1	Total 1	O 1	0
92	Ba	4	Total 4	O 4	0
92	Bd	1	Total 1	O 1	0
92	Be	3	Total 3	O 3	0
92	Bg	2	Total 2	O 2	0
92	Bj	5	Total 5	O 5	0
92	Bo	1	Total 1	O 1	0

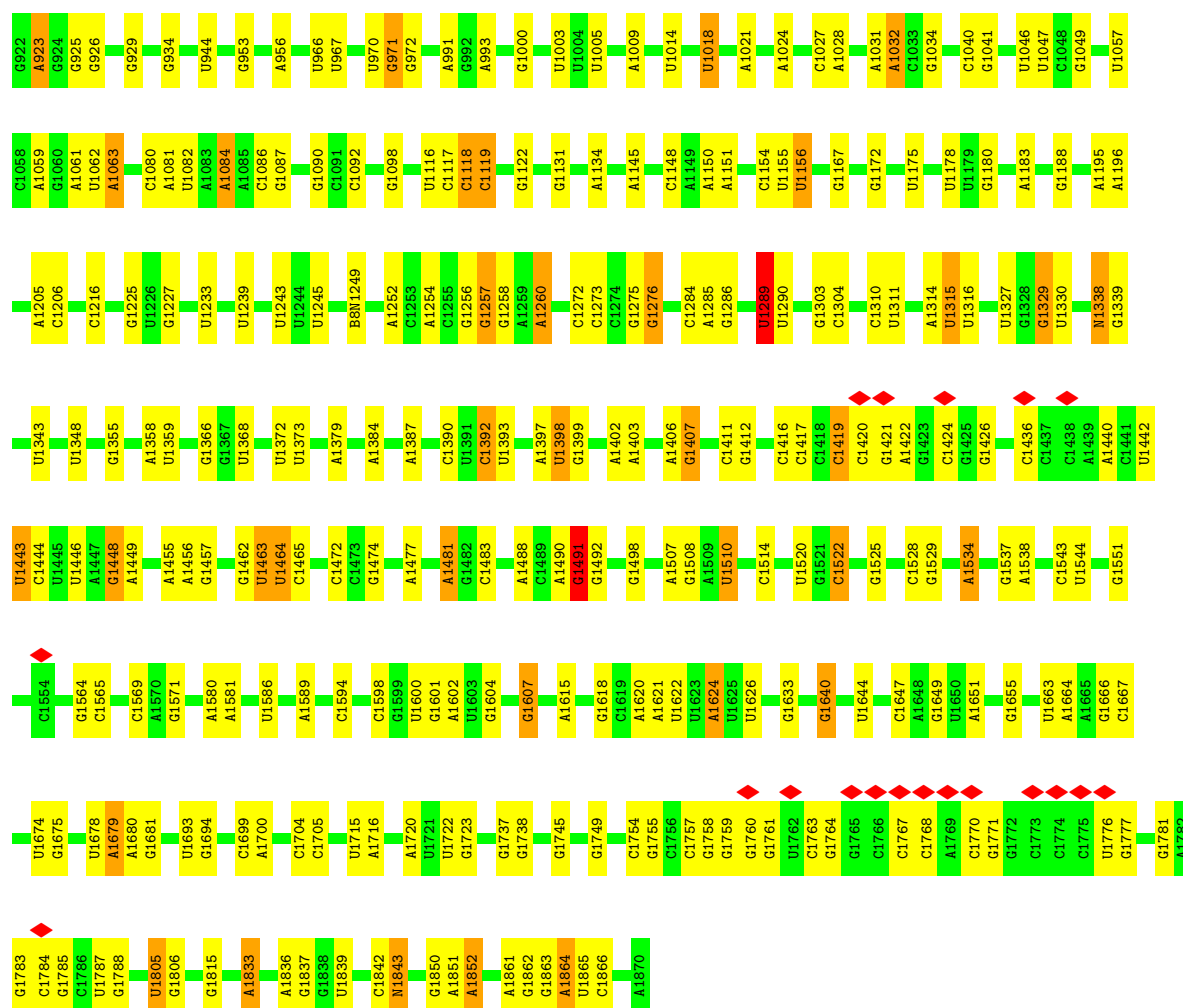
3 Residue-property plots

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

• Molecule 1: 18S rRNA

Chain A2:





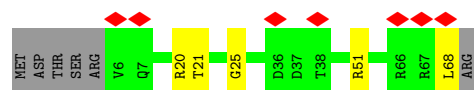
- Molecule 2: Small ribosomal subunit protein eS27

Chain AA: 88% 11% .



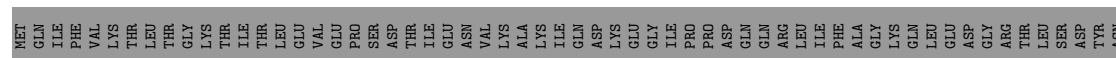
- Molecule 3: Small ribosomal subunit protein eS28

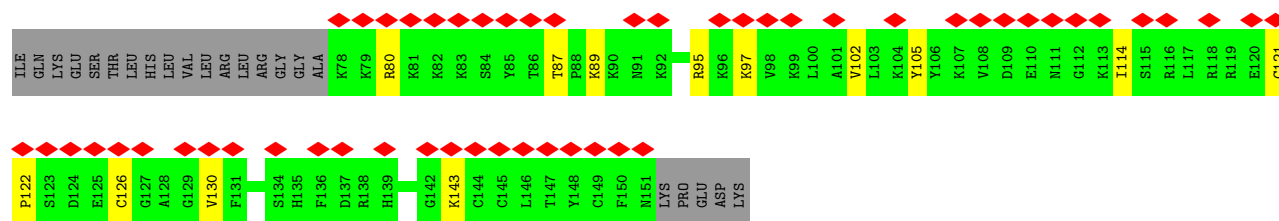
Chain AB: 10% 84% 7% 9%



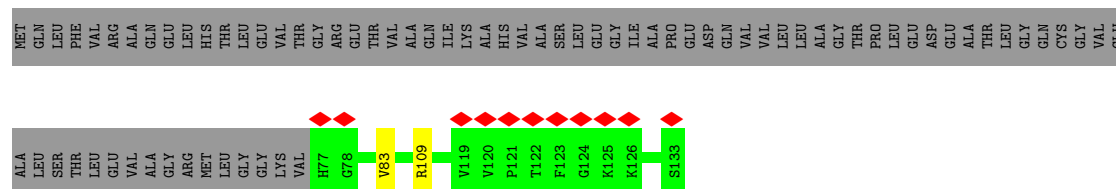
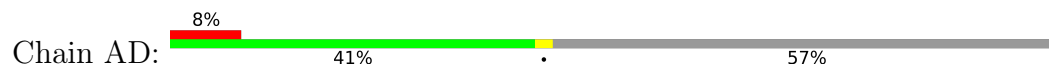
- Molecule 4: Ubiquitin-ribosomal protein eS31 fusion protein

Chain AC: 34% 39% 8% 53%

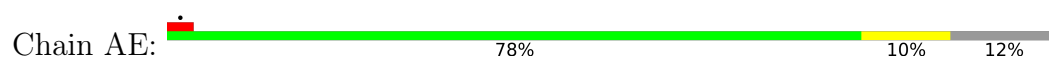




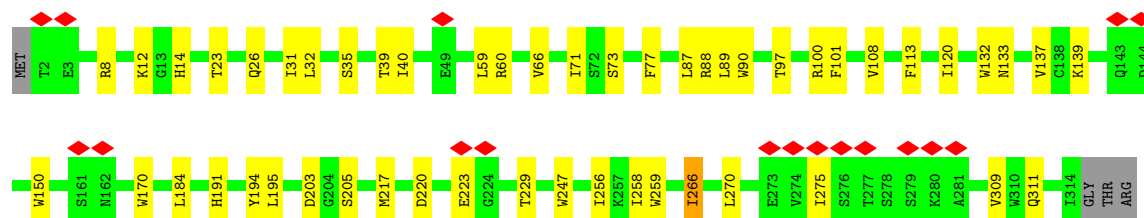
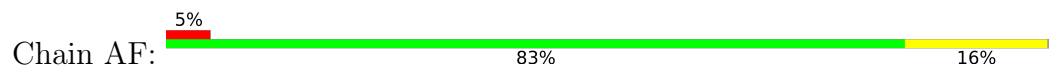
- Molecule 5: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



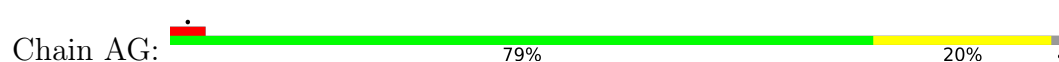
- Molecule 6: eS26



- Molecule 7: Small ribosomal subunit protein RACK1



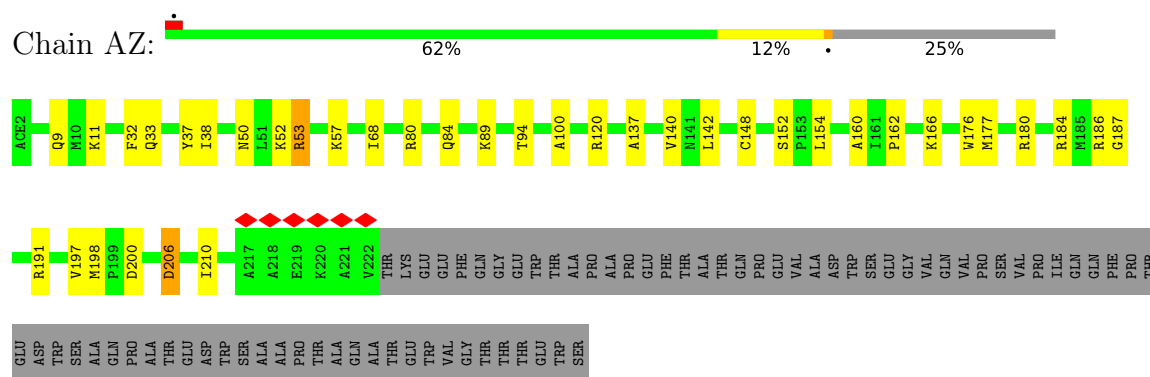
- Molecule 8: Small ribosomal subunit protein uS14



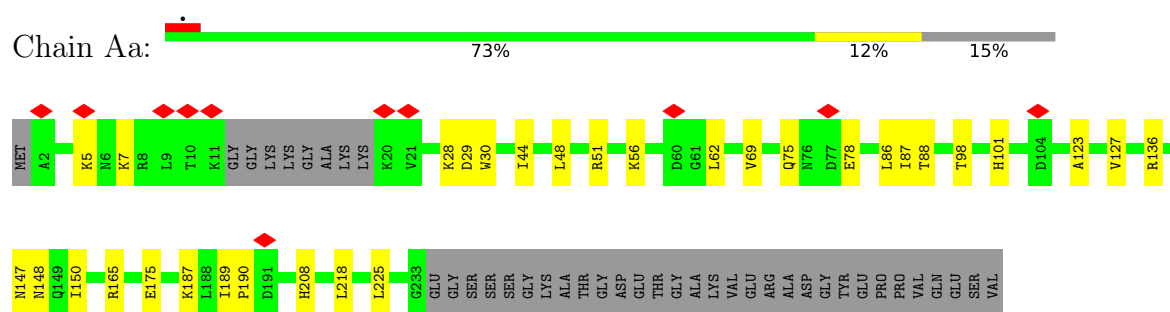
- Molecule 9: P site Phe tRNA



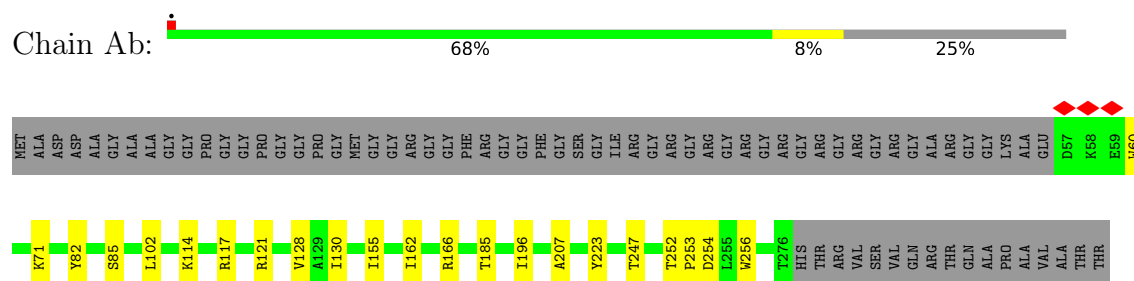
• Molecule 10: Small ribosomal subunit protein uS2



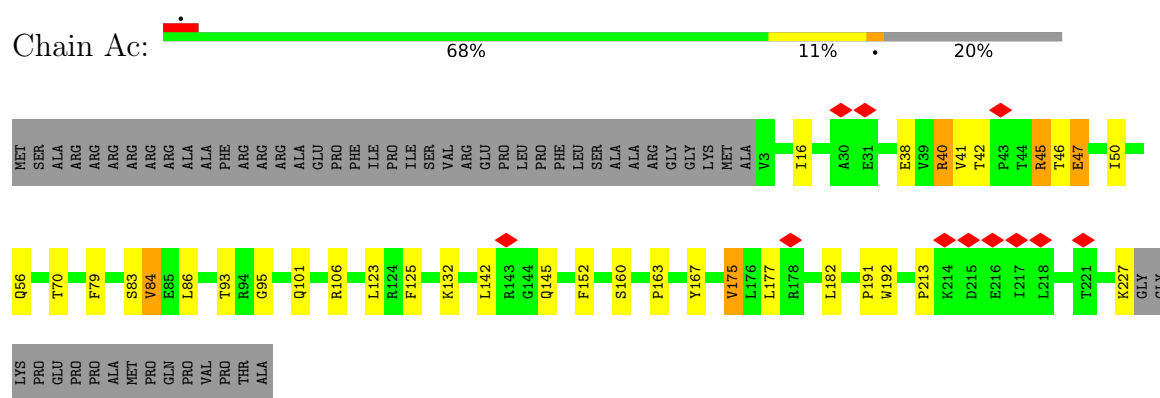
• Molecule 11: 40S ribosomal protein S3a



• Molecule 12: 40S ribosomal protein S2



• Molecule 13: 40S ribosomal protein S3




• Molecule 14: 40S ribosomal protein S4

Chain Ad:  85% 14%



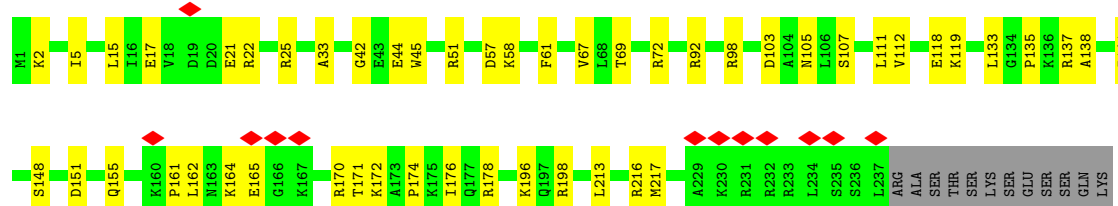
- Molecule 15: Small ribosomal subunit protein uS7

Chain Ae:  5% 84% 10% 6%




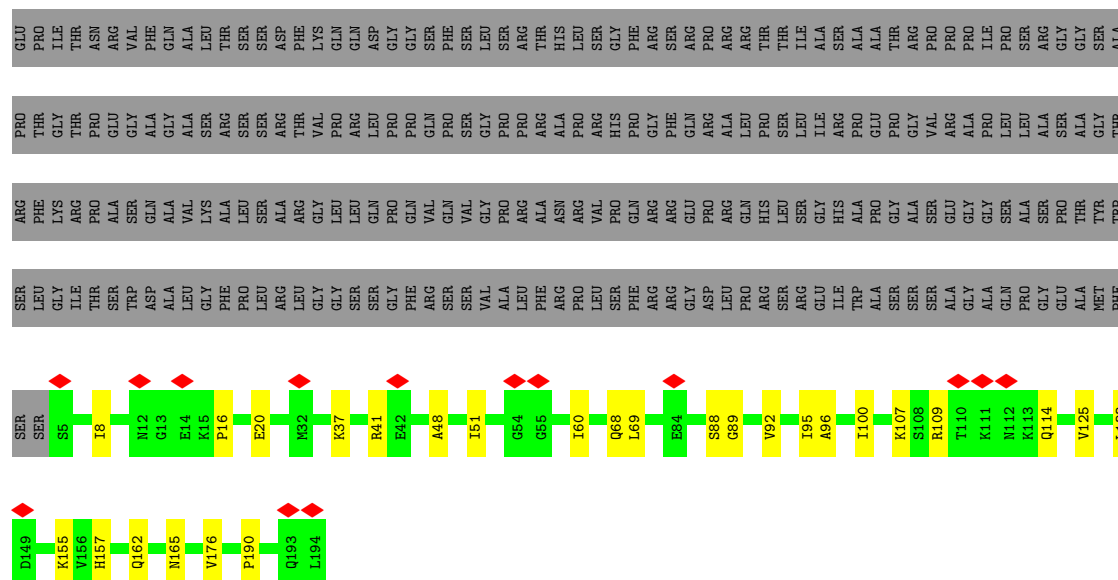
- Molecule 16: 40S ribosomal protein S6

Chain Af:  5% 75% 20% 5%




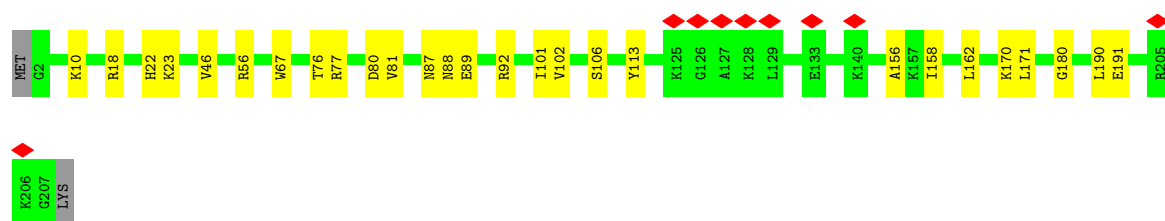
- Molecule 17: 40S ribosomal protein S7

Chain Ag:  38% 6% 56%




- Molecule 18: 40S ribosomal protein S8

Chain Ah:  86% 13%



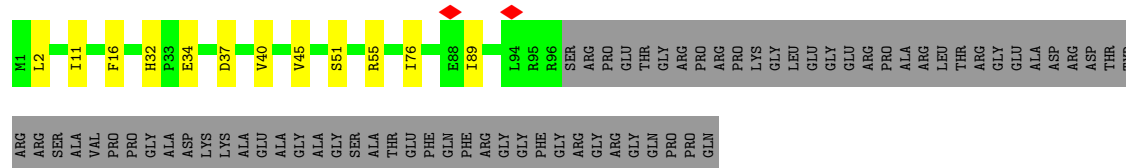
- Molecule 19: Small ribosomal subunit protein uS4

Chain Ai:  84% 12% 5%

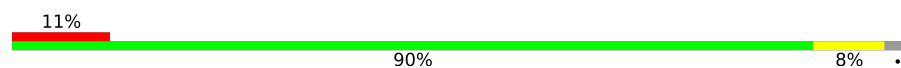


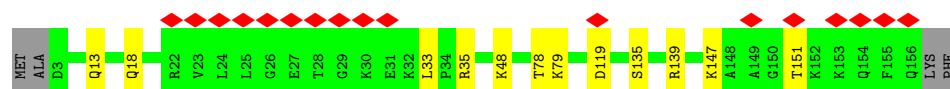
- Molecule 20: S10_ plectin domain-containing protein

Chain Aj:  51% 7% 42%

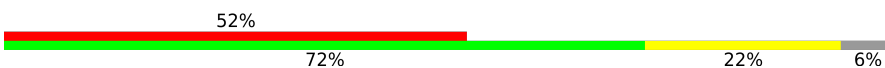


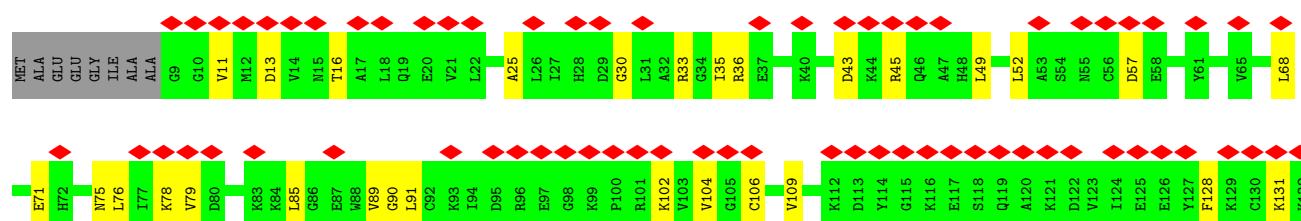
- Molecule 21: Small ribosomal subunit protein uS17

Chain Ak:  11% 90% 8%



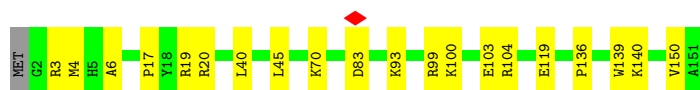
- Molecule 22: Small ribosomal subunit protein eS12

Chain Al:  52% 72% 22% 6%

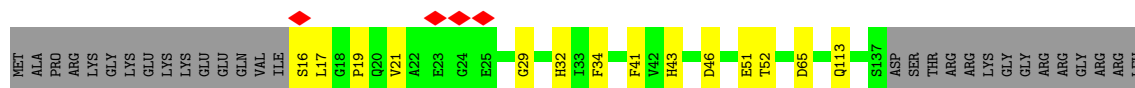
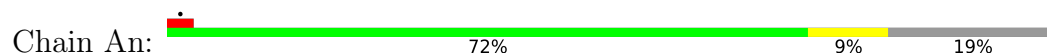


- Molecule 23: Small ribosomal subunit protein uS15

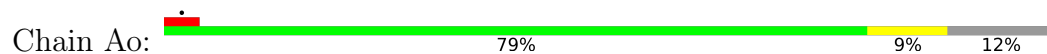
Chain Am:  86% 13%



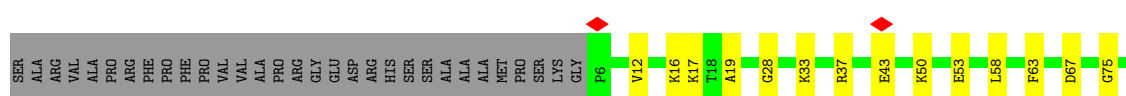
- Molecule 24: Small ribosomal subunit protein uS11



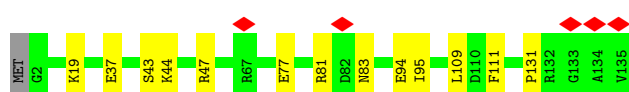
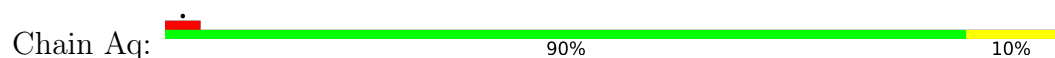
- Molecule 25: Small ribosomal subunit protein uS19



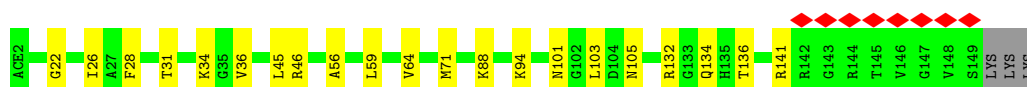
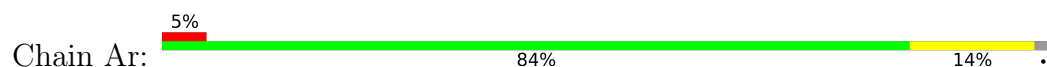
- Molecule 26: Small ribosomal subunit protein uS9



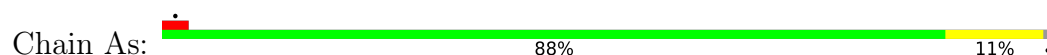
- Molecule 27: Small ribosomal subunit protein eS17



- Molecule 28: Small ribosomal subunit protein uS13

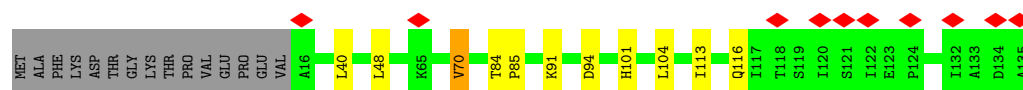
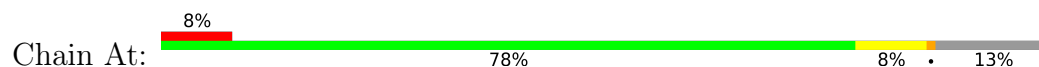


- Molecule 29: 40S ribosomal protein S19

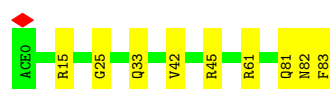
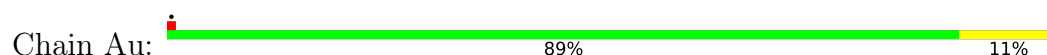




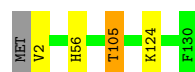
- Molecule 30: Small ribosomal subunit protein uS10



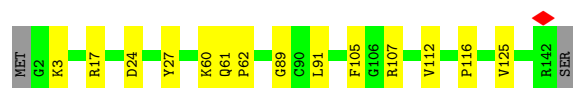
- Molecule 31: Small ribosomal subunit protein eS21



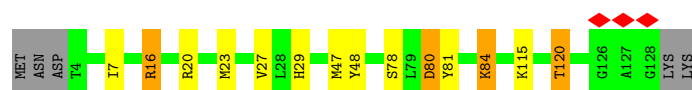
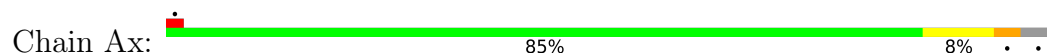
- Molecule 32: Small ribosomal subunit protein uS8



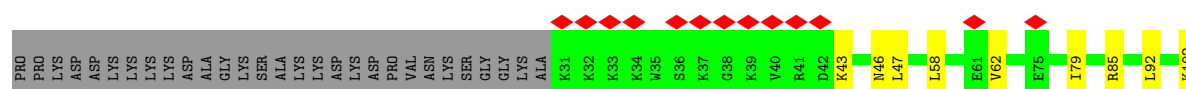
- Molecule 33: 40S ribosomal protein S23

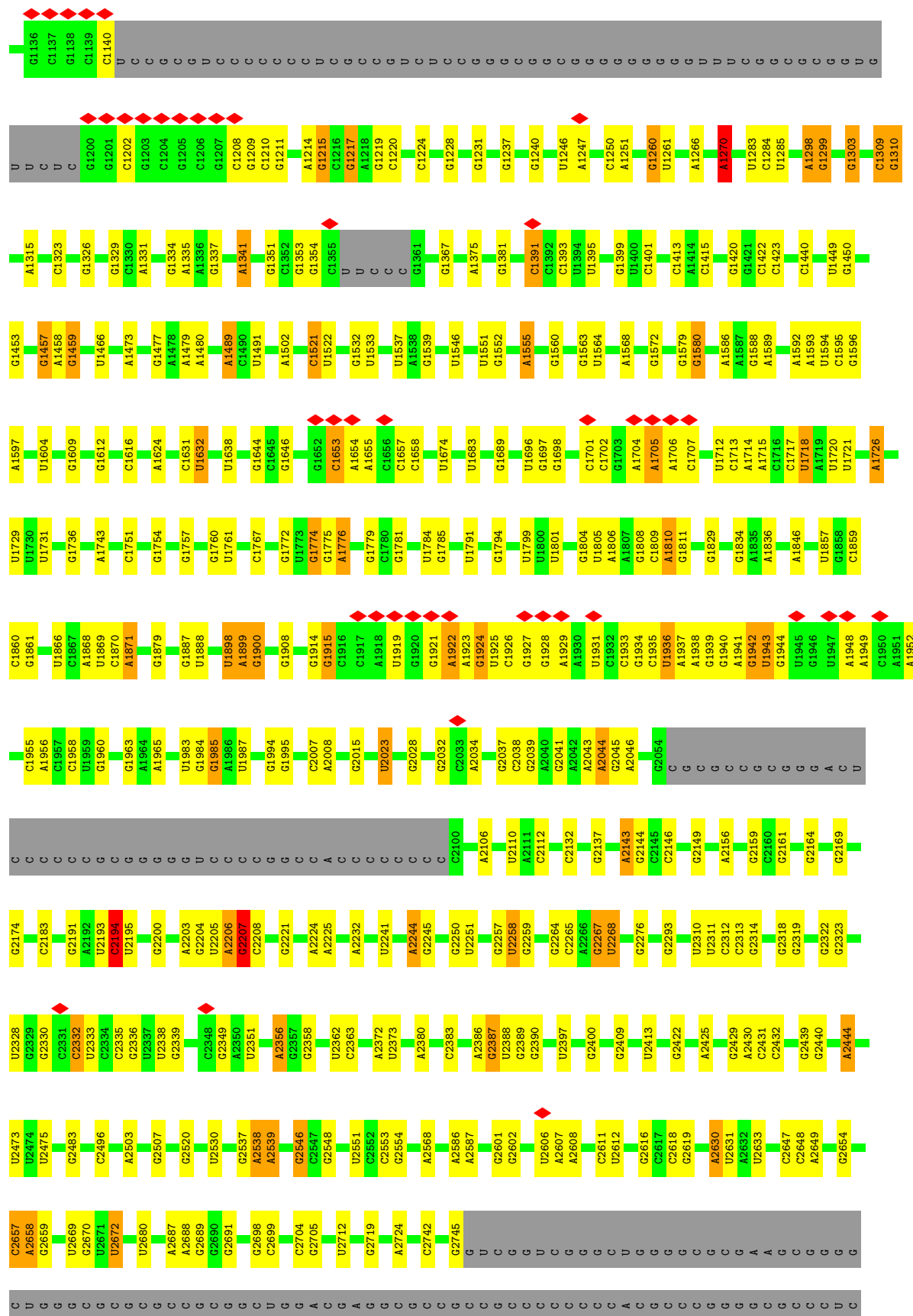


- Molecule 34: 40S ribosomal protein S24

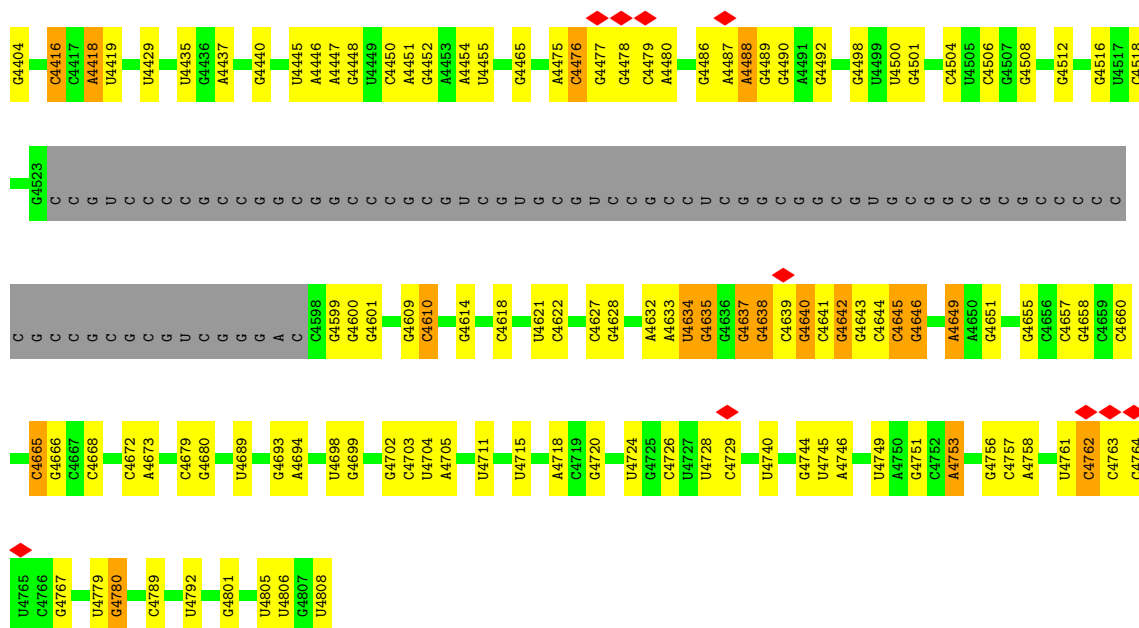


- Molecule 35: Small ribosomal subunit protein eS25

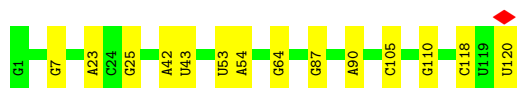
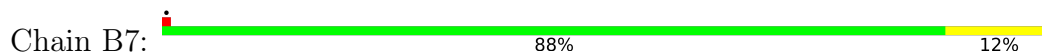




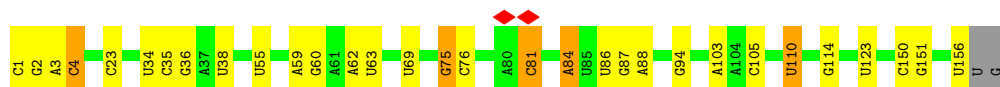
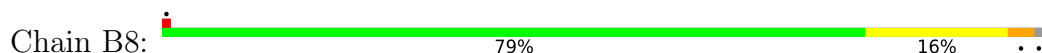




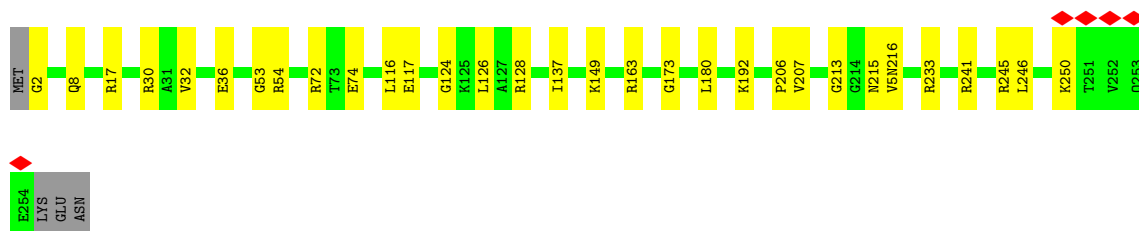
- Molecule 38: 5S rRNA



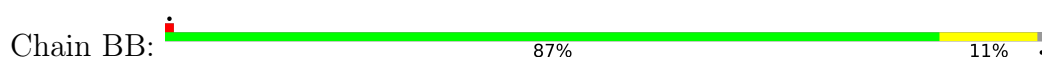
- Molecule 39: 5.8S rRNA



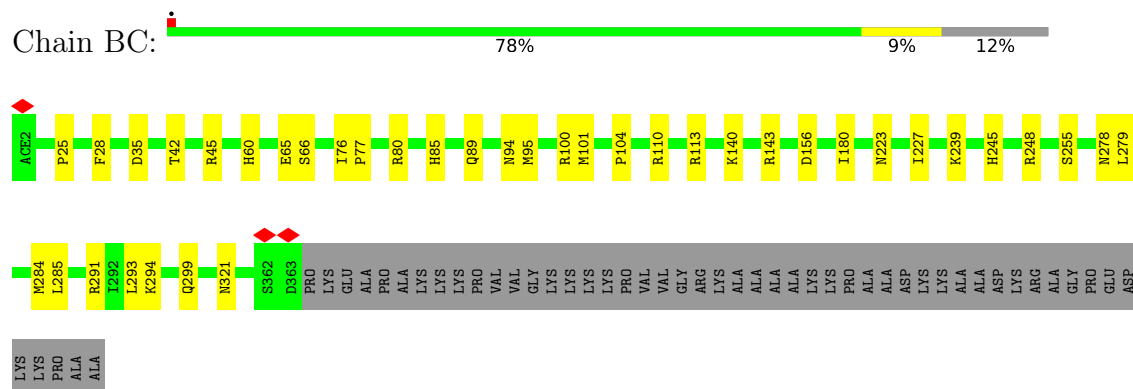
- Molecule 40: Large ribosomal subunit protein uL2



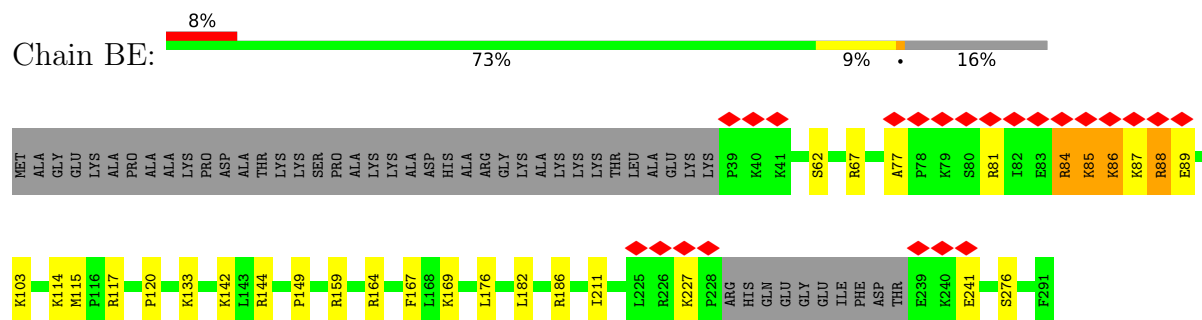
- Molecule 41: Ribosomal protein L3



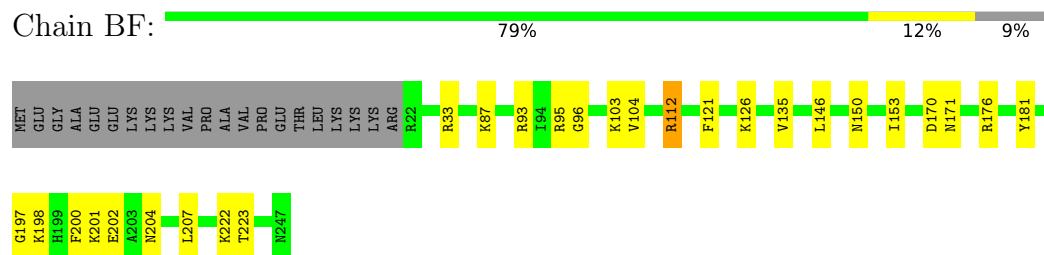
- Molecule 42: Large ribosomal subunit protein uL4



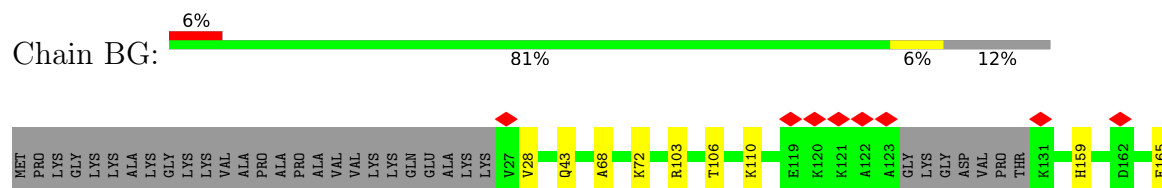
- Molecule 43: 60S ribosomal protein L6

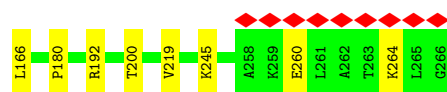


- Molecule 44: Ribosomal Protein uL30

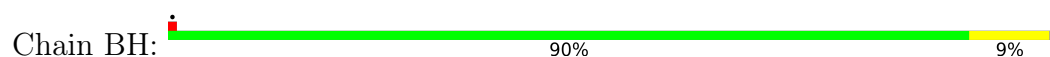


- Molecule 45: 60S ribosomal protein L7a

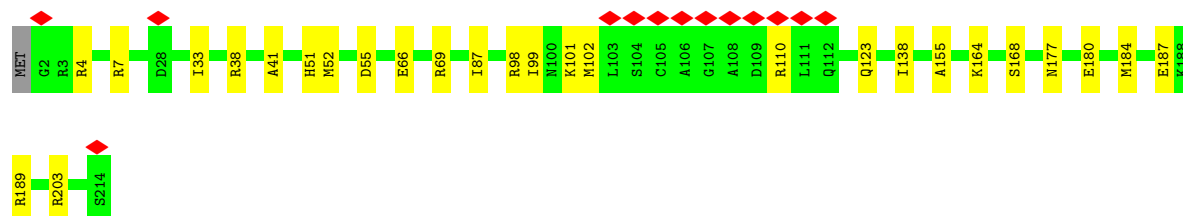
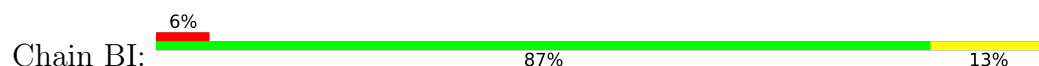




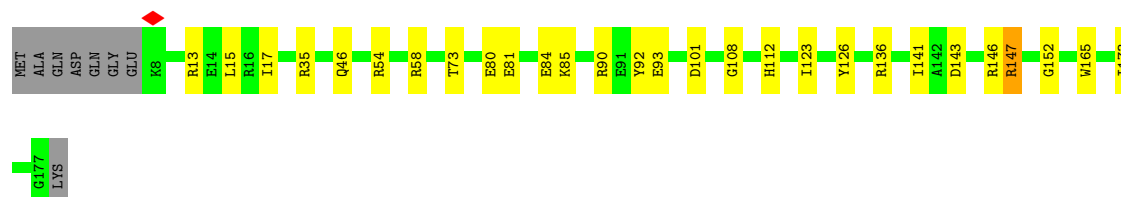
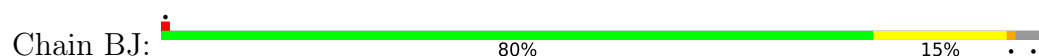
- Molecule 46: 60S ribosomal protein L9



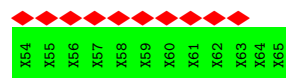
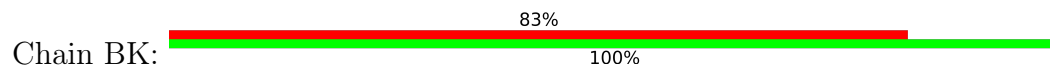
- Molecule 47: 60S ribosomal protein L10



- Molecule 48: 60S ribosomal protein L11



- Molecule 49: Nascent chain

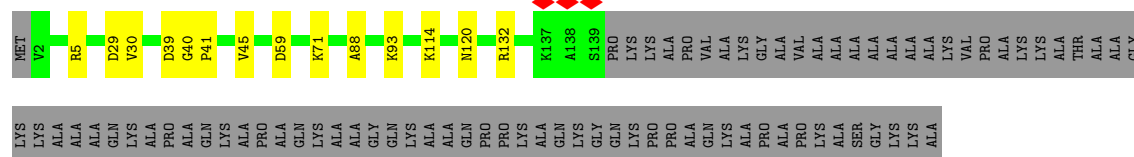


- Molecule 50: Large ribosomal subunit protein eL13

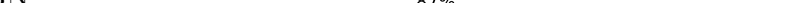


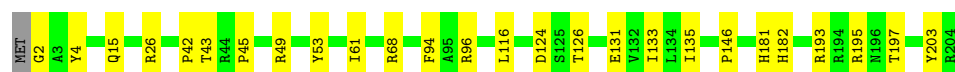
- Molecule 51: 60S ribosomal protein L14

Chain BM: 



- Molecule 52: Ribosomal protein L15

Chain BN:  87% 13%



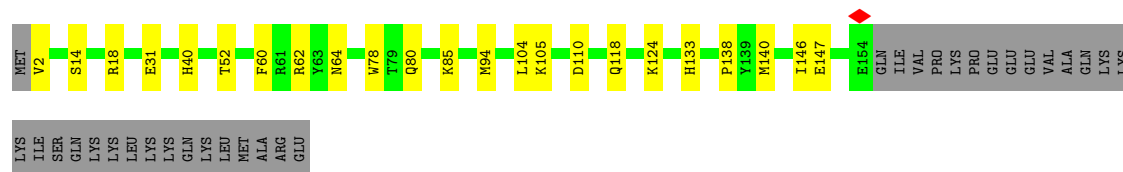
- Molecule 53: Large ribosomal subunit protein uL13

Chain BO: 91% 7%




- Molecule 54: Large ribosomal subunit protein uL22

Chain BP: 71% 12% 17%



- Molecule 55: eL18

Chain BQ:  84% 15%

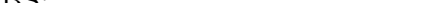


- Molecule 56: Ribosomal protein L19

Chain BR:

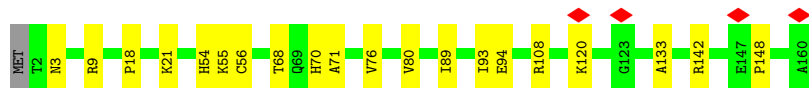


- Molecule 57: Large ribosomal subunit protein eL20

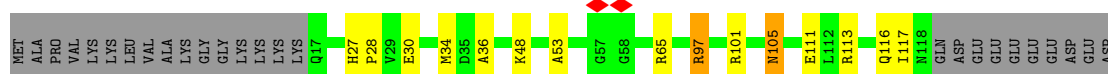
Chain BS:  91% 9%



- Molecule 58: 60S ribosomal protein L21



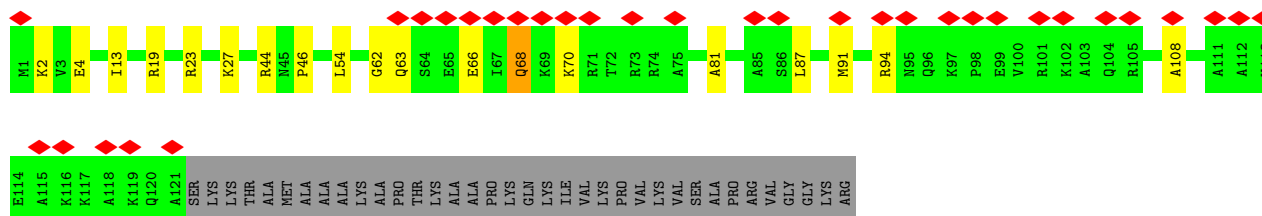
- Molecule 59: 60S ribosomal protein L22



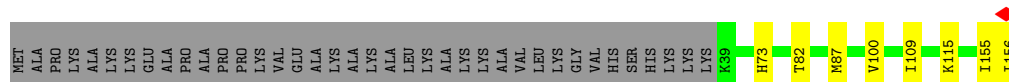
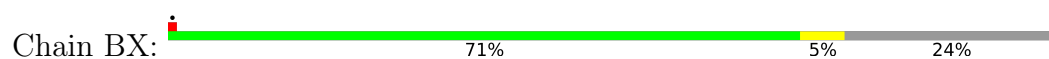
- Molecule 60: Ribosomal protein L23



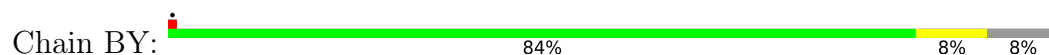
- Molecule 61: Ribosomal protein L24



- Molecule 62: Large ribosomal subunit protein uL23

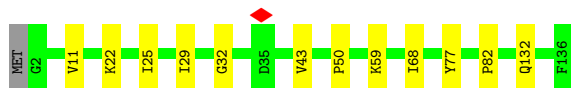
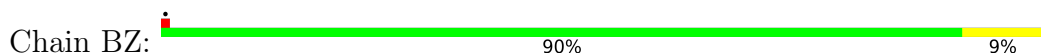


- Molecule 63: Ribosomal protein L26

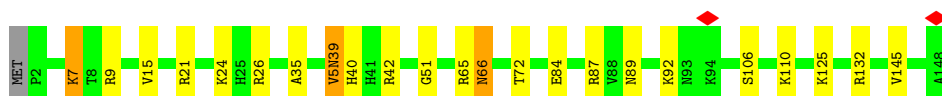
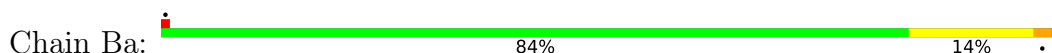




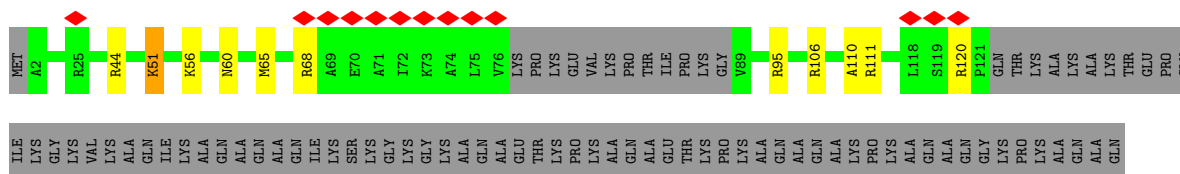
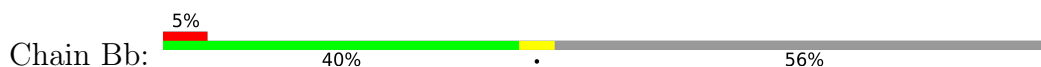
- Molecule 64: 60S ribosomal protein L27



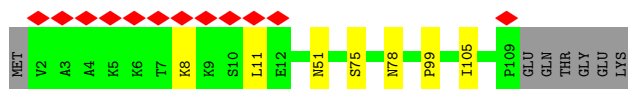
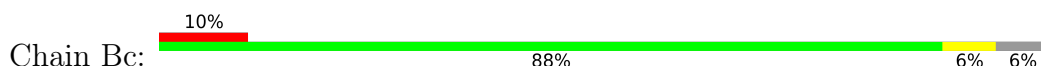
- Molecule 65: 60S ribosomal protein L27a



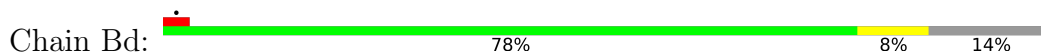
- Molecule 66: 60S ribosomal protein L29



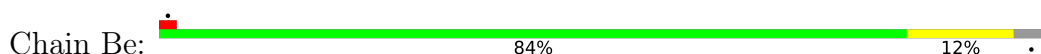
- Molecule 67: 60S ribosomal protein L30



- Molecule 68: 60S ribosomal protein L31



- Molecule 69: Ribosomal protein L32

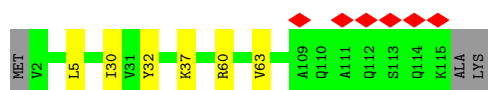




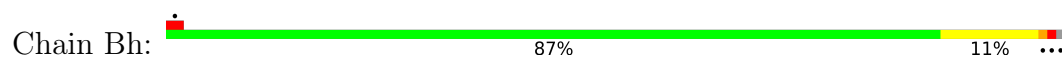
- Molecule 70: 60S ribosomal protein L35a



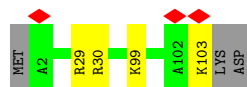
- Molecule 71: 60S ribosomal protein L34



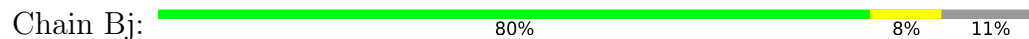
- Molecule 72: 60S ribosomal protein L35



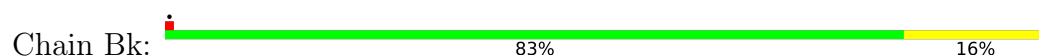
- Molecule 73: 60S ribosomal protein L36




- Molecule 74: Ribosomal protein L37



- Molecule 75: 60S ribosomal protein L38



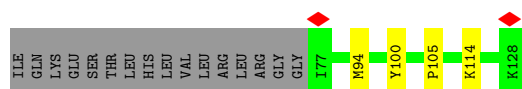
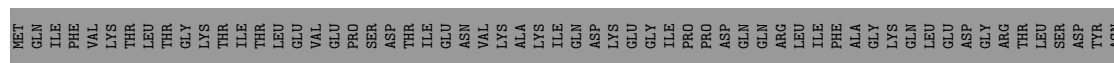
- Molecule 76: 60S ribosomal protein L39-like

Chain Bl:  86% 12%



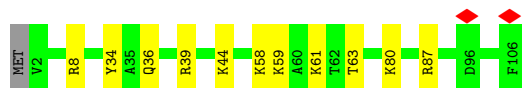
- Molecule 77: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Bm:  38% 59%



- Molecule 78: Large ribosomal subunit protein eL42

Chain Bo:  89% 10%




- Molecule 79: 60S ribosomal protein L37a

Chain Bp:  93% 5%



- Molecule 80: [histone H4]-N-methyl-L-lysine20 N-methyltransferase KMT5B

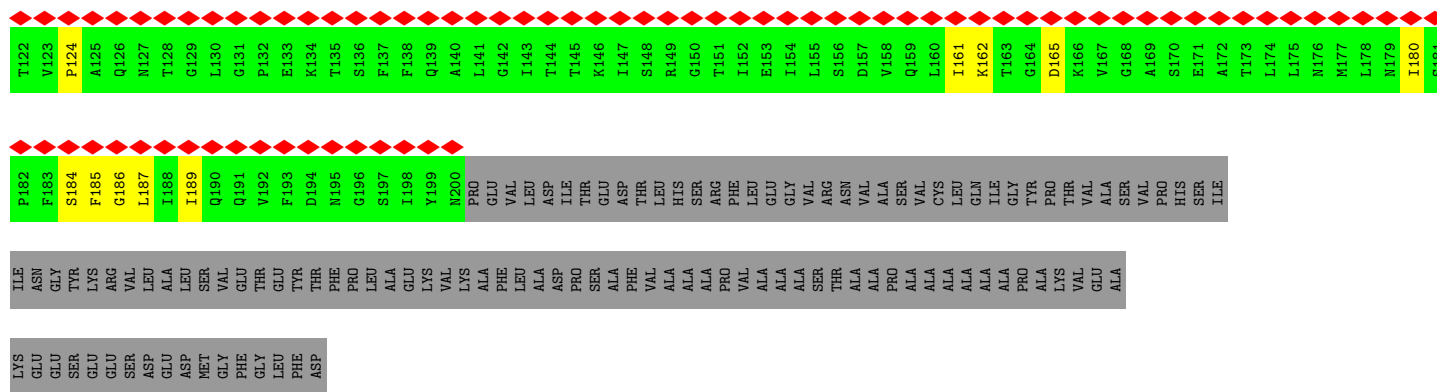
Chain Br:  85% 7% 7%



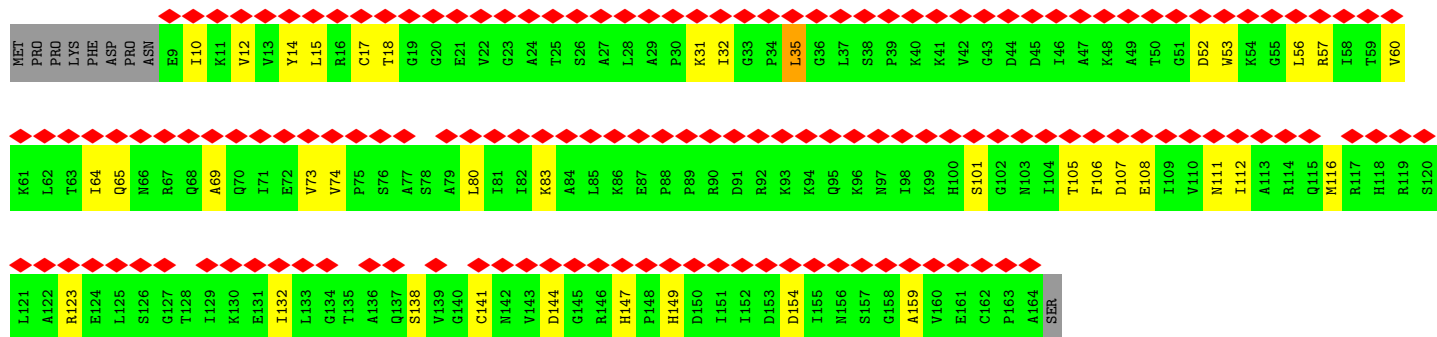
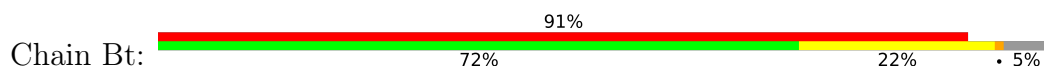
- Molecule 81: Large ribosomal subunit protein uL10

Chain Bs:  59% 49% 12% 38%

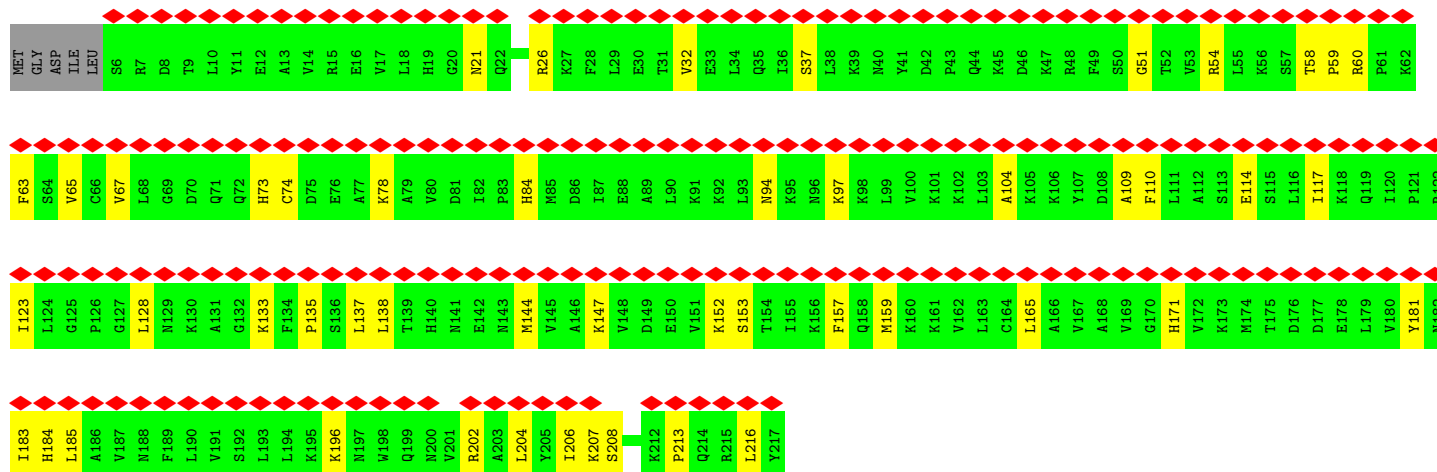
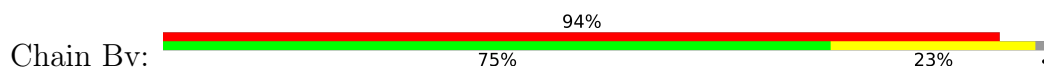




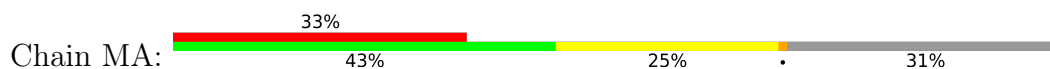
• Molecule 82: 60S ribosomal protein L12

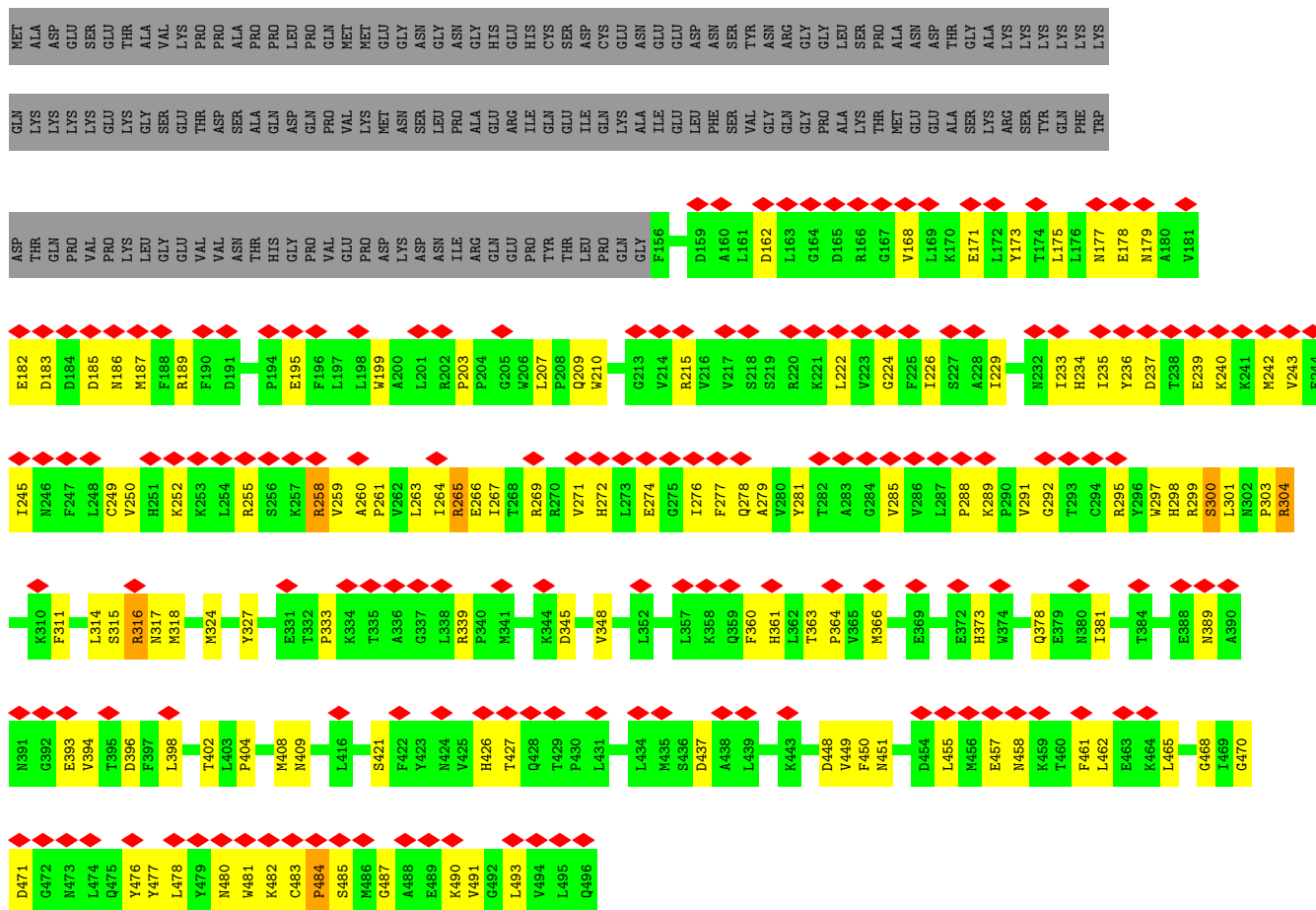


• Molecule 83: Ribosomal protein uL1

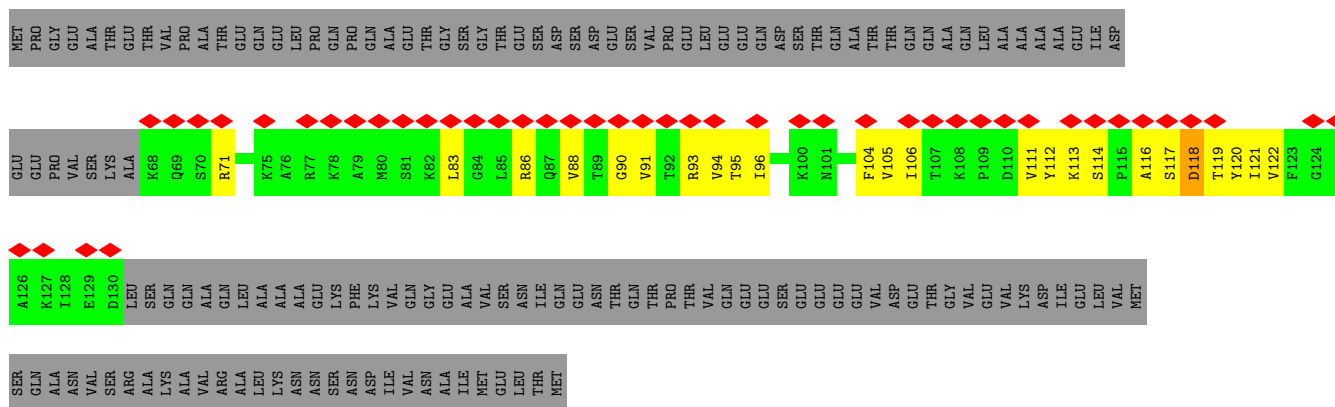


• Molecule 84: Glycylpeptide N-tetradecanoyltransferase 1

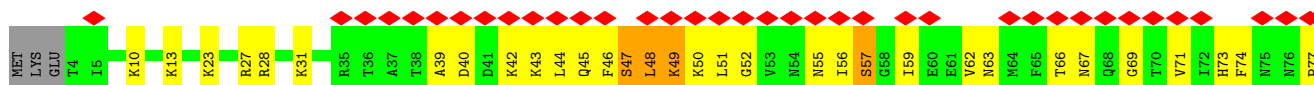




• Molecule 85: Nascent polypeptide-associated complex subunit alpha



• Molecule 86: Isoform 2 of Transcription factor BTF3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87143	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.108	Depositor
Minimum map value	-0.454	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, B8N, SPD, A2M, HY3, 5MC, SPM, MLZ, 5MU, UY1, MG, OMC, MA6, HIC, 1MA, NMM, 4AC, ACE, OMG, OMU, ZN, PSU, G7M, V5N, UR3, 6MZ, M3L

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	A2	0.17	2/40342 (0.0%)	0.19	1/62877 (0.0%)
2	AA	0.08	0/665	0.20	0/891
3	AB	0.07	0/497	0.19	0/666
4	AC	0.07	0/622	0.22	0/822
5	AD	0.09	0/462	0.20	0/607
6	AE	0.09	0/828	0.21	0/1109
7	AF	0.15	0/2493	0.24	0/3394
8	AG	0.08	0/470	0.21	0/623
9	AT	0.17	0/1766	0.22	0/2749
10	AZ	0.13	0/1778	0.26	0/2416
11	Aa	0.09	0/1841	0.21	0/2459
12	Ab	0.08	0/1742	0.21	0/2354
13	Ac	0.22	0/1779	0.37	0/2395
14	Ad	0.15	0/2118	0.30	0/2849
15	Ae	0.09	0/1531	0.26	0/2059
16	Af	0.07	0/1946	0.20	0/2590
17	Ag	0.08	0/1552	0.20	0/2079
18	Ah	0.08	0/1715	0.21	0/2287
19	Ai	0.08	0/1550	0.21	0/2069
20	Aj	0.08	0/834	0.22	0/1125
21	Ak	0.08	0/1284	0.20	0/1717
22	Al	0.07	0/968	0.20	0/1296
23	Am	0.09	0/1232	0.22	0/1656
24	An	0.08	0/912	0.21	0/1230
25	Ao	0.08	0/1069	0.25	0/1429
26	Ap	0.09	0/1142	0.25	0/1528
27	Aq	0.08	0/1094	0.21	0/1469
28	Ar	0.15	0/1233	0.27	0/1653
29	As	0.08	0/1119	0.19	0/1498
30	At	0.08	0/832	0.20	0/1117
31	Au	0.26	0/645	0.34	0/864

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Av	0.09	0/1051	0.20	0/1406
33	Aw	0.09	0/1107	0.21	0/1475
34	Ax	0.35	0/1032	0.50	0/1371
35	Ay	0.07	0/691	0.20	0/922
36	Az	0.07	0/240	0.15	0/305
37	B5	0.17	2/86006 (0.0%)	0.21	0/134179
38	B7	0.27	0/2861	0.37	0/4459
39	B8	0.14	0/3635	0.18	0/5661
40	BA	0.10	0/1965	0.26	0/2633
41	BB	0.09	0/3261	0.23	0/4364
42	BC	0.09	0/2938	0.21	0/3948
43	BE	0.22	0/1998	0.33	0/2673
44	BF	0.24	0/1922	0.37	0/2563
45	BG	0.08	0/1908	0.22	0/2566
46	BH	0.09	0/1535	0.20	0/2063
47	BI	0.08	0/1756	0.21	0/2346
48	BJ	0.30	0/1385	0.42	1/1852 (0.1%)
50	BL	0.26	0/1733	0.42	0/2316
51	BM	0.08	0/1158	0.22	0/1547
52	BN	0.10	0/1746	0.23	0/2338
53	BO	0.09	0/1662	0.20	0/2222
54	BP	0.09	0/1268	0.23	0/1700
55	BQ	0.09	0/1539	0.22	0/2054
56	BR	0.07	0/1524	0.18	0/2013
57	BS	0.10	0/1497	0.23	0/2008
58	BT	0.22	0/1326	0.36	0/1770
59	BU	0.38	0/845	0.54	0/1134
60	BV	0.10	0/1048	0.24	0/1402
61	BW	0.15	0/1006	0.28	0/1334
62	BX	0.09	0/984	0.22	0/1323
63	BY	0.09	0/1132	0.22	0/1504
64	BZ	0.08	0/1130	0.19	0/1507
65	Ba	0.43	0/1179	0.66	3/1572 (0.2%)
66	Bb	0.23	0/884	0.32	0/1169
67	Bc	0.09	0/847	0.20	0/1134
68	Bd	0.09	0/903	0.21	0/1216
69	Be	0.08	0/1088	0.21	0/1451
70	Bf	0.10	0/903	0.22	0/1208
71	Bg	0.08	0/916	0.22	0/1220
72	Bh	0.18	0/1021	0.30	0/1348
73	Bi	0.07	0/841	0.18	0/1112
74	Bj	0.09	0/720	0.24	0/952
75	Bk	0.08	0/575	0.19	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Bl	0.09	0/459	0.20	0/608
77	Bm	0.09	0/426	0.23	0/564
78	Bo	0.09	0/866	0.21	0/1141
79	Bp	0.09	0/718	0.22	0/953
80	Br	0.11	0/1027	0.23	0/1376
81	Bs	0.08	0/1530	0.21	0/2064
82	Bt	0.07	0/1193	0.23	0/1609
83	Bv	0.09	0/1735	0.28	0/2328
84	MA	0.51	2/2876 (0.1%)	0.70	8/3901 (0.2%)
85	Nt	0.12	0/504	0.22	0/672
86	Nu	0.60	0/836	0.88	5/1122 (0.4%)
All	All	0.17	6/234997 (0.0%)	0.25	18/344316 (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
10	AZ	0	1
13	Ac	0	2
14	Ad	0	1
34	Ax	0	1
43	BE	0	3
44	BF	0	1
48	BJ	0	2
50	BL	0	1
59	BU	0	2
65	Ba	0	4
72	Bh	0	1
84	MA	0	4
86	Nu	0	1
All	All	0	24

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	MA	300[A]	SER	C-O	8.21	1.33	1.23
84	MA	300[B]	SER	C-O	8.21	1.33	1.23
37	B5	4052	OMU	O3'-P	5.16	1.61	1.56
1	A2	628	OMU	O3'-P	5.10	1.61	1.56
1	A2	166	A2M	O3'-P	5.08	1.61	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	1270	A2M	O3'-P	5.01	1.61	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	MA	484	PRO	N-CA-C	-13.97	88.32	110.95
84	MA	300[A]	SER	CA-C-O	7.38	129.51	121.02
84	MA	300[B]	SER	CA-C-O	7.38	129.51	121.02
65	Ba	15	VAL	N-CA-C	6.49	117.18	110.36
86	Nu	104	PRO	CB-CA-C	6.45	122.20	111.56
84	MA	300[A]	SER	N-CA-C	6.36	118.81	108.63
84	MA	300[B]	SER	N-CA-C	6.36	118.81	108.63
86	Nu	104	PRO	CA-CB-CG	-6.32	92.49	104.50
86	Nu	104	PRO	CA-N-CD	-5.97	103.64	112.00
86	Nu	98	GLN	CB-CA-C	-5.71	108.99	115.79
1	A2	628	OMU	OP1-P-O3'	5.69	117.72	105.20
48	BJ	152	GLY	CA-C-O	-5.54	117.56	121.88
84	MA	484	PRO	CA-C-N	-5.50	115.41	123.00
84	MA	484	PRO	C-N-CA	-5.50	115.41	123.00
65	Ba	66	ASN	N-CA-C	-5.33	106.15	113.30
84	MA	311	PHE	N-CA-C	-5.26	105.72	111.82
65	Ba	15	VAL	CA-C-O	-5.05	116.02	121.27
86	Nu	47	SER	N-CA-C	-5.04	107.68	113.88

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AZ	53	ARG	Sidechain
13	Ac	40	ARG	Sidechain
13	Ac	45	ARG	Sidechain
14	Ad	68	ARG	Sidechain
34	Ax	20	ARG	Sidechain
43	BE	81	ARG	Sidechain
43	BE	84	ARG	Sidechain
43	BE	88	ARG	Sidechain
44	BF	112	ARG	Sidechain
48	BJ	146	ARG	Sidechain
48	BJ	147	ARG	Sidechain
50	BL	5	ARG	Sidechain
59	BU	101	ARG	Sidechain
59	BU	97	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
65	Ba	21	ARG	Sidechain
65	Ba	26	ARG	Sidechain
65	Ba	65	ARG	Sidechain
65	Ba	9	ARG	Sidechain
72	Bh	112	ARG	Sidechain
84	MA	258	ARG	Sidechain
84	MA	265	ARG	Sidechain
84	MA	304	ARG	Sidechain
84	MA	316	ARG	Sidechain
86	Nu	27	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	A2	37833	0	19168	237	0
2	AA	651	0	672	5	0
3	AB	495	0	523	3	0
4	AC	610	0	634	14	0
5	AD	457	0	502	4	0
6	AE	814	0	863	7	0
7	AF	2436	0	2393	29	0
8	AG	459	0	448	10	0
9	AT	1621	0	823	13	0
10	AZ	1743	0	1748	22	0
11	Aa	1815	0	1908	19	0
12	Ab	1706	0	1796	16	0
13	Ac	1751	0	1846	29	0
14	Ad	2076	0	2177	26	0
15	Ae	1509	0	1563	14	0
16	Af	1923	0	2089	37	0
17	Ag	1529	0	1627	16	0
18	Ah	1686	0	1772	18	0
19	Ai	1525	0	1640	15	0
20	Aj	810	0	836	7	0
21	Ak	1262	0	1335	7	0
22	Al	958	0	993	31	0
23	Am	1208	0	1294	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	An	899	0	912	9	0
25	Ao	1048	0	1093	8	0
26	Ap	1124	0	1193	21	0
27	Aq	1080	0	1135	11	0
28	Ar	1217	0	1279	13	0
29	As	1113	0	1145	14	0
30	At	822	0	887	10	0
31	Au	640	0	633	5	0
32	Av	1034	0	1080	4	0
33	Aw	1099	0	1162	8	0
34	Ax	1015	0	1086	10	0
35	Ay	683	0	761	9	0
36	Az	239	0	289	2	0
37	B5	79525	0	40261	477	0
38	B7	2561	0	1294	4	0
39	B8	3319	0	1684	13	0
40	BA	1940	0	2029	21	0
41	BB	3206	0	3353	32	0
42	BC	2886	0	3057	34	0
43	BE	1960	0	2153	21	0
44	BF	1886	0	2008	25	0
45	BG	1877	0	2023	11	0
46	BH	1516	0	1597	11	0
47	BI	1717	0	1764	17	0
48	BJ	1362	0	1399	14	0
49	BK	60	0	14	0	0
50	BL	1702	0	1820	12	0
51	BM	1137	0	1211	9	0
52	BN	1701	0	1749	18	0
53	BO	1630	0	1778	14	0
54	BP	1242	0	1274	15	0
55	BQ	1515	0	1634	25	0
56	BR	1508	0	1664	12	0
57	BS	1457	0	1492	11	0
58	BT	1298	0	1366	14	0
59	BU	831	0	852	9	0
60	BV	1034	0	1096	10	0
61	BW	991	0	1048	13	0
62	BX	967	0	1040	8	0
63	BY	1115	0	1205	9	0
64	BZ	1107	0	1182	7	0
65	Ba	1163	0	1202	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	Bb	881	0	957	10	0
67	Bc	836	0	888	4	0
68	Bd	888	0	930	6	0
69	Be	1070	0	1164	11	0
70	Bf	884	0	924	8	0
71	Bg	906	0	998	3	0
72	Bh	1013	0	1147	15	0
73	Bi	830	0	916	2	0
74	Bj	705	0	737	7	0
75	Bk	569	0	637	7	0
76	Bl	447	0	480	4	0
77	Bm	432	0	470	3	0
78	Bo	863	0	929	8	0
79	Bp	708	0	756	4	0
80	Br	1014	0	1083	8	0
81	Bs	1507	0	1564	29	0
82	Bt	1178	0	1235	27	0
83	Bv	1707	0	1815	38	0
84	MA	2797	0	2818	147	0
85	Nt	499	0	541	22	0
86	Nu	828	0	874	53	0
87	A2	108	0	0	0	0
87	Aw	1	0	0	0	0
87	B5	273	0	0	0	0
87	B7	9	0	0	0	0
87	B8	8	0	0	0	0
87	BB	3	0	0	0	0
87	BI	1	0	0	0	0
87	BP	1	0	0	0	0
87	BR	1	0	0	0	0
87	BV	1	0	0	0	0
87	Bj	1	0	0	0	0
88	A2	31	0	0	0	0
88	Ad	1	0	0	0	0
88	B5	130	0	0	0	0
88	B7	6	0	0	0	0
88	B8	4	0	0	0	0
88	BA	2	0	0	0	0
88	BH	1	0	0	0	0
88	BI	1	0	0	0	0
88	BL	1	0	0	0	0
88	BN	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	BQ	1	0	0	0	0
88	BT	1	0	0	0	0
88	BY	1	0	0	0	0
88	Bb	2	0	0	0	0
88	Be	2	0	0	0	0
88	Bo	1	0	0	0	0
89	A2	80	0	151	6	0
89	B5	220	0	418	19	0
90	A2	14	0	26	1	0
90	B5	28	0	52	2	0
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	514	0	0	3	0
92	AE	1	0	0	0	0
92	AT	4	0	0	0	0
92	Aa	3	0	0	0	0
92	Af	2	0	0	0	0
92	Ak	2	0	0	0	0
92	An	2	0	0	0	0
92	Ap	1	0	0	0	0
92	Ar	2	0	0	0	0
92	As	2	0	0	0	0
92	At	1	0	0	1	0
92	Aw	4	0	0	0	0
92	B5	1359	0	0	5	0
92	B7	38	0	0	1	0
92	B8	49	0	0	0	0
92	BA	4	0	0	0	0
92	BC	6	0	0	0	0
92	BH	1	0	0	0	0
92	BI	3	0	0	0	0
92	BL	1	0	0	0	0
92	BN	2	0	0	0	0
92	BP	4	0	0	0	0
92	BR	2	0	0	0	0
92	BV	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BX	1	0	0	0	0
92	BY	1	0	0	0	0
92	Ba	4	0	0	0	0
92	Bd	1	0	0	0	0
92	Be	3	0	0	0	0
92	Bg	2	0	0	0	0
92	Bj	5	0	0	0	0
92	Bo	1	0	0	0	0
All	All	226637	0	168064	1661	0

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

All (1661) 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)
84:MA:291:VAL:O	84:MA:485:SER:HB2	1.27	1.29
84:MA:250:VAL:CG1	84:MA:258:ARG:HD3	1.65	1.27
84:MA:250:VAL:HG13	84:MA:258:ARG:CD	1.70	1.19
44:BF:87:LYS:NZ	44:BF:196:VAL:HG23	1.58	1.17
84:MA:291:VAL:HA	84:MA:485:SER:CB	1.72	1.17
84:MA:224:GLY:HA3	84:MA:258:ARG:HH12	1.08	1.12
84:MA:291:VAL:HA	84:MA:485:SER:HB3	1.26	1.12
84:MA:258:ARG:HE	84:MA:263:LEU:CD1	1.65	1.09
84:MA:250:VAL:HG13	84:MA:258:ARG:HD3	1.17	1.06
84:MA:291:VAL:C	84:MA:485:SER:HB2	1.79	1.06
84:MA:314:LEU:HD22	84:MA:318:MET:O	1.57	1.05
84:MA:224:GLY:HA3	84:MA:258:ARG:NH1	1.74	1.03
37:B5:349:A:C6	42:BC:45:ARG:NH1	2.26	1.03
1:A2:1338:4AC:O2'	30:At:84:THR:HG22	1.58	1.02
13:Ac:38:GLU:OE1	13:Ac:40:ARG:HG3	1.58	1.02
44:BF:87:LYS:NZ	44:BF:196:VAL:CG2	2.23	1.02
44:BF:87:LYS:HZ1	44:BF:196:VAL:HG23	1.08	1.00
84:MA:250:VAL:HA	84:MA:258:ARG:HH21	1.22	1.00
84:MA:258:ARG:HE	84:MA:263:LEU:HD11	1.21	1.00
84:MA:250:VAL:HA	84:MA:258:ARG:NH2	1.77	0.99
1:A2:1034:G:H1	1:A2:1081:A:HO2'	1.08	0.99
84:MA:291:VAL:CA	84:MA:485:SER:CB	2.42	0.98
12:Ab:114:LYS:HD3	12:Ab:121:ARG:HH21	1.26	0.97
53:BO:108:ILE:HD13	53:BO:117:ARG:NH1	1.82	0.94
84:MA:224:GLY:CA	84:MA:258:ARG:HH12	1.80	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BX:156:ILE:CG2	84:MA:318:MET:SD	2.58	0.91
84:MA:234:HIS:HB2	84:MA:239:GLU:HG2	1.49	0.91
84:MA:291:VAL:CA	84:MA:485:SER:HB3	2.01	0.91
55:BQ:111:SER:O	55:BQ:115:LYS:HG3	1.70	0.90
37:B5:3374:A:HO2'	74:Bj:2:THR:N	1.70	0.90
62:BX:156:ILE:HG21	84:MA:318:MET:SD	2.16	0.86
44:BF:87:LYS:HZ1	44:BF:196:VAL:CG2	1.83	0.86
84:MA:300[B]:SER:HB3	84:MA:303:PRO:HG3	1.58	0.86
18:Ah:158:ILE:CG2	18:Ah:162:LEU:HD23	2.06	0.85
84:MA:291:VAL:CA	84:MA:485:SER:HB2	2.03	0.84
22:Al:33:ARG:HD3	22:Al:89:VAL:HB	1.59	0.83
12:Ab:114:LYS:CD	12:Ab:121:ARG:HH21	1.91	0.83
1:A2:1092:C:HO2'	32:Av:2:VAL:N	1.77	0.83
84:MA:250:VAL:HG13	84:MA:258:ARG:HD2	1.60	0.83
84:MA:183:ASP:HB3	84:MA:187:MET:H	1.43	0.83
84:MA:300[A]:SER:HB3	84:MA:303:PRO:HG3	1.59	0.82
13:Ac:38:GLU:CD	13:Ac:40:ARG:HG3	2.04	0.82
86:Nu:102:MET:N	86:Nu:102:MET:SD	2.52	0.82
81:Bs:20:LEU:HD12	81:Bs:54:LEU:HD22	1.61	0.82
44:BF:87:LYS:HZ2	44:BF:196:VAL:CG2	1.92	0.81
86:Nu:43:LYS:HD2	86:Nu:46:PHE:HD2	1.44	0.81
84:MA:258:ARG:NE	84:MA:263:LEU:HD11	1.96	0.81
84:MA:234:HIS:CB	84:MA:239:GLU:HG2	2.11	0.81
12:Ab:114:LYS:HD3	12:Ab:121:ARG:NH2	1.96	0.80
84:MA:291:VAL:HG23	84:MA:485:SER:CB	2.10	0.80
86:Nu:102:MET:HA	86:Nu:102:MET:HE3	1.64	0.80
84:MA:250:VAL:HG11	84:MA:258:ARG:HD3	1.64	0.79
84:MA:291:VAL:HG23	84:MA:485:SER:HB3	1.62	0.79
84:MA:175:LEU:HA	84:MA:179:ASN:HD22	1.47	0.79
84:MA:250:VAL:CA	84:MA:258:ARG:HH21	1.96	0.79
84:MA:291:VAL:O	84:MA:485:SER:CB	2.22	0.78
37:B5:755:G:H1	37:B5:800:U:H3	1.28	0.78
37:B5:349:A:N6	42:BC:45:ARG:NH1	2.30	0.78
84:MA:299:ARG:NH1	84:MA:327:TYR:HD1	1.80	0.78
84:MA:299:ARG:NH1	84:MA:327:TYR:CD1	2.51	0.78
84:MA:291:VAL:HG23	84:MA:485:SER:CA	2.14	0.78
37:B5:2023:U:C1'	55:BQ:14:ARG:NH2	2.47	0.78
84:MA:291:VAL:HG23	84:MA:485:SER:HA	1.65	0.77
84:MA:291:VAL:CG2	84:MA:485:SER:HA	2.14	0.77
37:B5:349:A:N6	42:BC:45:ARG:CZ	2.48	0.77
83:Bv:58:THR:HG22	83:Bv:153:SER:N	1.99	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:MA:235:ILE:HG22	84:MA:237:ASP:H	1.48	0.77
1:A2:1758:G:H1	1:A2:1776:U:H3	1.31	0.76
84:MA:258:ARG:NE	84:MA:263:LEU:CD1	2.47	0.76
84:MA:304:ARG:CZ	84:MA:324:MET:SD	2.74	0.75
84:MA:234:HIS:HA	84:MA:239:GLU:HA	1.68	0.75
84:MA:224:GLY:HA2	84:MA:258:ARG:HH22	1.51	0.75
37:B5:2023:U:H1'	55:BQ:14:ARG:HH21	1.51	0.75
84:MA:291:VAL:CG2	84:MA:485:SER:CB	2.64	0.75
84:MA:304:ARG:NH1	84:MA:324:MET:SD	2.60	0.74
13:Ac:42:THR:HG23	13:Ac:47:GLU:CD	2.12	0.74
43:BE:227:LYS:HE2	43:BE:241:GLU:H	1.52	0.73
37:B5:3540:OMC:HM22	37:B5:3541:G:H5'	1.71	0.73
1:A2:1397:A:O2'	1:A2:1399:G:N7	2.21	0.73
18:Ah:158:ILE:HG23	18:Ah:162:LEU:HD23	1.69	0.73
86:Nu:73:HIS:NE2	86:Nu:101:GLU:HG2	2.04	0.73
84:MA:250:VAL:CG1	84:MA:258:ARG:CD	2.45	0.72
37:B5:2704:OMC:HM22	37:B5:2705:G:H5'	1.72	0.72
46:BH:94:SER:HB2	46:BH:142:ASP:HB3	1.72	0.71
86:Nu:69:GLY:O	86:Nu:98:GLN:HA	1.91	0.71
1:A2:1273:C:HO2'	8:AG:2:GLY:N	1.89	0.70
86:Nu:63:ASN:HB2	86:Nu:109:GLN:HE22	1.57	0.70
86:Nu:71:VAL:HG21	86:Nu:102:MET:SD	2.32	0.70
18:Ah:67:TRP:HZ2	18:Ah:162:LEU:HD21	1.56	0.70
37:B5:1810:A2M:HM'2	37:B5:1811:G:H5'	1.73	0.70
50:BL:63:THR:HG21	65:Ba:66:ASN:HD22	1.57	0.70
84:MA:258:ARG:HE	84:MA:263:LEU:HD13	1.53	0.70
7:AF:120:ILE:HB	7:AF:132:TRP:HB2	1.74	0.69
37:B5:1899:A:H1'	81:Bs:63:LYS:HD3	1.74	0.69
81:Bs:65:ILE:HG23	81:Bs:75:LEU:HB3	1.74	0.69
28:Ar:46:ARG:HG2	29:As:35:ASP:HB2	1.74	0.69
37:B5:1237:G:OP2	37:B5:1237:G:N2	2.24	0.69
85:Nt:83:LEU:HD11	86:Nu:47:SER:HB3	1.73	0.69
84:MA:291:VAL:CG2	84:MA:485:SER:HB3	2.21	0.69
37:B5:3555:G:N2	37:B5:3555:G:OP2	2.26	0.69
82:Bt:80:LEU:HD23	82:Bt:83:LYS:HZ3	1.58	0.69
1:A2:926:G:H1	1:A2:1018:U:H3	1.41	0.68
37:B5:1072:C:H1'	37:B5:1074:C:C2	2.29	0.68
37:B5:2143:A:N7	42:BC:143:ARG:NH1	2.42	0.68
50:BL:63:THR:HG23	50:BL:65:ARG:H	1.59	0.68
1:A2:1392:OMC:HM22	1:A2:1393:U:H5'	1.75	0.68
18:Ah:67:TRP:CZ2	18:Ah:162:LEU:HD21	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:308:G:OP2	37:B5:308:G:N2	2.24	0.68
37:B5:2688:A:H61	37:B5:3575:C:H42	1.40	0.68
84:MA:300[B]:SER:CB	84:MA:303:PRO:HG3	2.23	0.68
85:Nt:116:ALA:HB2	86:Nu:40:ASP:HB3	1.75	0.68
1:A2:1009:A:OP2	67:Bc:8:LYS:NZ	2.27	0.67
50:BL:64:VAL:O	50:BL:64:VAL:HG12	1.93	0.67
43:BE:115:MET:O	80:Br:87:ARG:NH1	2.28	0.67
84:MA:175:LEU:HD12	84:MA:179:ASN:HB2	1.76	0.67
1:A2:1338:4AC:O2'	30:At:84:THR:CG2	2.40	0.67
1:A2:745:G:N3	17:Ag:109:ARG:NH2	2.42	0.67
60:BV:69:LYS:HG2	60:BV:71:GLU:HG2	1.76	0.67
37:B5:4304:U:OP2	41:BB:246:ARG:NH2	2.28	0.67
84:MA:315:SER:OG	84:MA:318:MET:HB2	1.94	0.67
1:A2:929:G:H1	1:A2:1014:U:H3	1.42	0.67
2:AA:33:MET:HE2	2:AA:48:SER:HA	1.76	0.67
59:BU:48:LYS:HG2	59:BU:53:ALA:HB2	1.77	0.67
23:Am:136:PRO:HG2	23:Am:139:TRP:HB2	1.76	0.67
1:A2:1285:A:C5	22:Al:91:LEU:HD21	2.31	0.67
22:Al:33:ARG:NH1	22:Al:90:GLY:H	1.92	0.67
84:MA:299:ARG:HH12	84:MA:327:TYR:HB3	1.59	0.67
1:A2:577:A2M:HM'2	1:A2:578:U:H5'	1.78	0.66
22:Al:33:ARG:HD3	22:Al:89:VAL:CB	2.25	0.66
37:B5:223:G:N3	42:BC:223:ASN:ND2	2.43	0.66
84:MA:258:ARG:CG	84:MA:263:LEU:HD11	2.26	0.66
1:A2:1355:G:N2	1:A2:1358:A:OP2	2.25	0.66
1:A2:1624:A:OP2	89:A2:2037:SPD:N1	2.29	0.66
22:Al:33:ARG:NE	22:Al:91:LEU:HG	2.09	0.66
37:B5:3373:U:OP2	37:B5:3378:A:N6	2.28	0.66
37:B5:2548:G:O6	56:BR:46:LYS:NZ	2.29	0.66
82:Bt:108:GLU:HA	82:Bt:111:ASN:HD21	1.60	0.65
84:MA:409:ASN:HB2	86:Nu:78:LYS:HE3	1.77	0.65
37:B5:4202:OMC:HM22	37:B5:4203:PSU:H5''	1.78	0.65
37:B5:4480:A:H61	37:B5:4704:U:H3	1.44	0.65
38:B7:105:C:OP2	47:BI:203:ARG:NH1	2.29	0.65
86:Nu:45:GLN:HA	86:Nu:48:LEU:HB3	1.77	0.65
37:B5:1260:OMG:HM22	37:B5:1261:U:H5'	1.79	0.65
37:B5:2444:A:N6	37:B5:2587:A:OP2	2.30	0.65
37:B5:4366:OMU:HM22	37:B5:4367:C:H5'	1.79	0.65
42:BC:94:ASN:OD1	42:BC:95:MET:N	2.30	0.65
27:Aq:94:GLU:HG2	27:Aq:95:ILE:HG13	1.78	0.64
37:B5:2023:U:N1	55:BQ:14:ARG:NH2	2.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Ay:111:ARG:HD2	35:Ay:114:LYS:HE3	1.78	0.64
37:B5:2106:A:OP1	80:Br:107:ARG:NH2	2.30	0.64
1:A2:1260:A:N6	1:A2:1520:U:OP1	2.29	0.64
19:Ai:134:HIS:ND1	19:Ai:163:SER:OG	2.28	0.64
37:B5:734:G:OP2	51:BM:71:LYS:NZ	2.31	0.64
37:B5:4068:G:N2	37:B5:4071:A:OP2	2.30	0.64
83:Bv:58:THR:HG22	83:Bv:153:SER:CA	2.28	0.64
37:B5:3557:A2M:HM'2	37:B5:3558:C:H5'	1.78	0.64
37:B5:4366:OMU:OP2	37:B5:4416:C:N4	2.30	0.64
47:BI:38:ARG:HD2	47:BI:41:ALA:HB2	1.80	0.64
1:A2:64:A:H2	1:A2:83:A:H62	1.46	0.64
26:Ap:130:LYS:NZ	26:Ap:134:GLY:O	2.30	0.64
37:B5:788:G:H2'	37:B5:789:G:H8	1.62	0.64
37:B5:4416:C:O2'	60:BV:15:ARG:NH2	2.30	0.64
48:BJ:17:ILE:HD12	48:BJ:80:GLU:HG2	1.80	0.64
57:BS:112:ASP:OD1	57:BS:116:ARG:NH1	2.28	0.64
86:Nu:52:GLY:HA2	86:Nu:82:SER:HB2	1.80	0.64
1:A2:1618:G:N1	1:A2:1621:A:OP2	2.31	0.63
85:Nt:120:TYR:HB2	86:Nu:90:ILE:HB	1.79	0.63
1:A2:1289:OMU:OP2	4:AC:97:LYS:NZ	2.31	0.63
37:B5:1415:C:H5''	55:BQ:144:LYS:HG2	1.80	0.63
37:B5:1555:A:H5'	54:BP:133:HIS:HA	1.80	0.63
57:BS:29:ARG:HB2	58:BT:148:PRO:HB2	1.79	0.63
1:A2:642:A:OP1	19:Ai:40:LYS:NZ	2.32	0.63
37:B5:1391:C:O2'	66:Bb:106:ARG:NH2	2.32	0.63
37:B5:1829:G:N2	37:B5:1829:G:OP2	2.30	0.63
37:B5:4634:U:H1'	51:BM:132:ARG:NH1	2.13	0.63
60:BV:13:LYS:HB3	60:BV:128:LEU:HD11	1.80	0.63
1:A2:228:C:H42	1:A2:902:G:H1'	1.62	0.63
62:BX:82:THR:HG22	62:BX:155:ILE:HG23	1.80	0.63
85:Nt:91:VAL:HG22	86:Nu:66:THR:HG22	1.79	0.63
86:Nu:73:HIS:CE1	86:Nu:101:GLU:HG2	2.33	0.63
37:B5:2649:A:O2'	89:B5:5182:SPD:N1	2.31	0.63
44:BF:104:VAL:HG13	44:BF:135:VAL:HG12	1.79	0.63
81:Bs:47:LEU:HB3	81:Bs:51:ALA:HB3	1.80	0.63
83:Bv:32:VAL:HA	83:Bv:208:SER:HA	1.78	0.63
7:AF:247:TRP:HB3	7:AF:258:ILE:HD11	1.81	0.63
37:B5:660:G:O2'	42:BC:291:ARG:NH1	2.31	0.63
66:Bb:65:MET:HG2	66:Bb:68:ARG:HH22	1.64	0.63
86:Nu:10:LYS:HA	86:Nu:13:LYS:HZ3	1.63	0.63
37:B5:1924:G:H1'	37:B5:1942:G:H2'	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Nu:100:THR:O	86:Nu:104:PRO:HD2	1.98	0.62
18:Ah:101:ILE:HD12	18:Ah:190:LEU:HD11	1.82	0.62
55:BQ:72:LEU:HB2	55:BQ:75:ARG:HD2	1.80	0.62
37:B5:758:C:O2'	37:B5:760:C:N4	2.33	0.62
71:Bg:5:LEU:HD21	71:Bg:30:ILE:HG22	1.81	0.62
37:B5:173:C:H1'	72:Bh:112:ARG:HG3	1.82	0.62
84:MA:300[A]:SER:CB	84:MA:303:PRO:HG3	2.23	0.62
37:B5:1334:G:N2	37:B5:1337:G:OP2	2.27	0.62
37:B5:1757:G:N2	37:B5:1757:G:OP2	2.32	0.62
55:BQ:119:LYS:HE3	55:BQ:121:LEU:HD21	1.81	0.61
84:MA:175:LEU:HD12	84:MA:179:ASN:CB	2.30	0.61
22:Al:79:VAL:HG11	22:Al:85:LEU:HB2	1.81	0.61
59:BU:111:GLU:OE2	59:BU:113:ARG:NE	2.30	0.61
4:AC:126:CYS:HB3	4:AC:143:LYS:HD3	1.83	0.61
21:Ak:135:SER:O	21:Ak:139:ARG:NH1	2.34	0.61
37:B5:2422:G:N2	37:B5:2425:A:OP2	2.31	0.61
83:Bv:67:VAL:HG12	83:Bv:84:HIS:HD2	1.64	0.61
84:MA:364:PRO:HG3	84:MA:493:LEU:HD13	1.82	0.61
84:MA:402:THR:HG22	84:MA:404:PRO:HD3	1.81	0.61
15:Ae:47:LYS:NZ	26:Ap:115:TYR:O	2.33	0.61
35:Ay:58:LEU:HD12	35:Ay:62:VAL:HG21	1.83	0.61
37:B5:327:U:O2'	73:Bi:30:ARG:NH1	2.34	0.61
1:A2:953:G:OP1	11:Aa:56:LYS:NZ	2.33	0.61
13:Ac:213:PRO:HG3	27:Aq:19:LYS:HB3	1.81	0.61
53:BO:36:VAL:HG21	53:BO:117:ARG:HD3	1.80	0.61
1:A2:1600:U:OP2	35:Ay:46:ASN:ND2	2.33	0.61
85:Nt:95:THR:HG21	86:Nu:109:GLN:HB3	1.82	0.61
37:B5:2568:A:N6	56:BR:88:ARG:O	2.34	0.61
83:Bv:58:THR:HG21	83:Bv:152:LYS:HB2	1.82	0.61
1:A2:905:A:O2'	21:Ak:48:LYS:NZ	2.33	0.60
11:Aa:44:ILE:HD12	11:Aa:69:VAL:HG21	1.83	0.60
37:B5:1299:G:OP1	55:BQ:108:ARG:NH2	2.34	0.60
37:B5:4779:U:OP2	41:BB:396:ARG:NH2	2.33	0.60
39:B8:81:C:HO2'	72:Bh:2:ALA:N	1.98	0.60
48:BJ:35:ARG:NH1	48:BJ:123:ILE:O	2.34	0.60
65:Ba:72:THR:HG22	65:Ba:110:LYS:HB3	1.82	0.60
81:Bs:39:GLN:HE22	81:Bs:106:LYS:HA	1.64	0.60
1:A2:1598:C:OP2	35:Ay:85:ARG:NH2	2.34	0.60
13:Ac:177:LEU:HD13	13:Ac:182:LEU:HD13	1.83	0.60
37:B5:1005:G:OP1	58:BT:142:ARG:NH1	2.34	0.60
37:B5:1937:A:N3	37:B5:1958:C:O2'	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:3624:U:O2'	54:BP:80:GLN:NE2	2.34	0.60
61:BW:2:LYS:NZ	61:BW:4:GLU:OE2	2.34	0.60
70:Bf:43:LEU:O	70:Bf:109:ARG:NH1	2.32	0.60
44:BF:87:LYS:HZ2	44:BF:196:VAL:HG23	1.52	0.60
83:Bv:74:CYS:SG	83:Bv:78:LYS:NZ	2.67	0.60
29:As:60:THR:HG23	29:As:75:MET:HE2	1.83	0.60
84:MA:482:LYS:HD2	84:MA:484:PRO:HG3	1.83	0.60
86:Nu:43:LYS:HD2	86:Nu:46:PHE:CD2	2.33	0.60
1:A2:1448:OMG:HM22	1:A2:1449:A:H5'	1.83	0.60
37:B5:1915:G:N3	82:Bt:138:SER:OG	2.33	0.60
1:A2:437:OMG:HM22	1:A2:438:G:H5'	1.84	0.60
17:Ag:162:GLN:OE1	17:Ag:165:ASN:ND2	2.34	0.60
37:B5:432:U:H1'	89:B5:5190:SPD:HN6	1.66	0.60
37:B5:1341:A:HO2'	37:B5:1422:C:HO2'	1.50	0.60
37:B5:1604:U:O2	89:B5:5186:SPD:N1	2.35	0.60
37:B5:2169:G:OP1	69:Be:108:ARG:NH2	2.34	0.60
42:BC:110:ARG:O	42:BC:113:ARG:NH1	2.34	0.60
1:A2:1316:U:H4'	20:Aj:2:LEU:HG	1.83	0.60
8:AG:17:GLY:O	8:AG:27:ARG:NH1	2.35	0.60
37:B5:92:C:OP1	89:B5:5176:SPD:N10	2.34	0.60
37:B5:1908:G:H4'	81:Bs:36:GLY:HA2	1.84	0.60
41:BB:215:GLU:OE2	41:BB:349:LYS:NZ	2.35	0.60
51:BM:40:GLY:HA3	51:BM:45:VAL:HB	1.84	0.60
1:A2:121:OMU:HM22	1:A2:122:G:H5'	1.83	0.60
53:BO:108:ILE:CD1	53:BO:117:ARG:NH1	2.62	0.60
75:Bk:57:LYS:NZ	75:Bk:68:GLU:OE2	2.34	0.60
1:A2:1087:G:OP2	6:AE:12:LYS:NZ	2.35	0.60
37:B5:638:G:OP2	50:BL:162:LYS:NZ	2.30	0.60
37:B5:2194:OMC:HM22	37:B5:2195:U:H5'	1.84	0.60
44:BF:197:GLY:HA3	44:BF:200:PHE:HB2	1.82	0.60
1:A2:1508:G:N2	4:AC:87:THR:O	2.34	0.59
43:BE:120:PRO:O	80:Br:112:ARG:NH1	2.35	0.59
60:BV:69:LYS:NZ	60:BV:71:GLU:OE2	2.34	0.59
37:B5:4645:C:O2	37:B5:4655:G:N2	2.34	0.59
54:BP:138:PRO:HB3	54:BP:140:MET:HE2	1.83	0.59
83:Bv:21:ASN:HB2	83:Bv:26:ARG:HD3	1.84	0.59
10:AZ:177:MET:SD	10:AZ:180:ARG:NH2	2.75	0.59
21:Ak:119:ASP:O	21:Ak:147:LYS:NZ	2.34	0.59
22:Al:49:LEU:HG	22:Al:75:ASN:OD1	2.01	0.59
37:B5:230:G:OP1	63:BY:15:ARG:NH1	2.35	0.59
37:B5:375:G:OP2	74:Bj:52:LYS:NZ	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:1399:G:OP2	37:B5:1399:G:N2	2.33	0.59
37:B5:3476:OMG:HM22	37:B5:3477:U:H5'	1.85	0.59
37:B5:3978:U:O4	78:Bo:8:ARG:NH2	2.34	0.59
83:Bv:117:ILE:HD13	83:Bv:137:LEU:HD21	1.83	0.59
8:AG:44:ARG:NH1	30:At:94:ASP:OD2	2.36	0.59
37:B5:1869:U:OP2	53:BO:49:ARG:NH1	2.31	0.59
37:B5:2358:G:OP1	71:Bg:37:LYS:NZ	2.31	0.59
78:Bo:36:GLN:OE1	78:Bo:39:ARG:NH2	2.36	0.59
1:A2:513:A2M:HM'2	1:A2:514:G:H5'	1.85	0.59
1:A2:1285:A:C5	22:Al:91:LEU:CD2	2.85	0.59
1:A2:1491:OMG:HM22	1:A2:1492:G:H5'	1.84	0.59
37:B5:1674:U:H5'	89:B5:5185:SPD:H41	1.84	0.59
81:Bs:39:GLN:HE21	81:Bs:186:GLY:HA2	1.67	0.59
37:B5:2028:G:H1	37:B5:2038:C:H41	1.48	0.59
1:A2:1522:C:OP2	28:Ar:136:THR:OG1	2.21	0.59
1:A2:1679:A2M:OP2	15:Ae:63:LYS:NZ	2.31	0.59
19:Ai:120:ALA:O	19:Ai:125:HIS:ND1	2.32	0.59
21:Ak:78:THR:HG22	21:Ak:79:LYS:HG3	1.85	0.59
50:BL:209:LYS:O	83:Bv:181:TYR:HE1	1.85	0.59
62:BX:156:ILE:HG23	84:MA:318:MET:SD	2.40	0.59
78:Bo:59:LYS:NZ	78:Bo:61:LYS:O	2.35	0.59
1:A2:1289:OMU:HM22	1:A2:1290:U:H5'	1.83	0.59
55:BQ:79:THR:HB	55:BQ:136:THR:HG22	1.85	0.59
83:Bv:63:PHE:O	83:Bv:152:LYS:NZ	2.35	0.59
37:B5:2431:C:OP1	37:B5:2611:C:O2'	2.21	0.59
37:B5:4632:A:OP1	53:BO:188:LYS:NZ	2.36	0.59
37:B5:3812:G:O6	40:BA:72:ARG:NH2	2.36	0.58
56:BR:25:ASP:OD2	86:Nu:31:LYS:NZ	2.36	0.58
10:AZ:184:ARG:HD3	10:AZ:191:ARG:HG2	1.85	0.58
50:BL:130:LYS:HB3	50:BL:133:ALA:HB3	1.84	0.58
78:Bo:34:TYR:O	78:Bo:39:ARG:NH1	2.36	0.58
84:MA:482:LYS:C	84:MA:484:PRO:HD3	2.27	0.58
1:A2:504:C:OP1	14:Ad:62:LYS:NZ	2.35	0.58
1:A2:1864:A:OP2	6:AE:4:LYS:NZ	2.35	0.58
37:B5:4231:C:O2'	77:Bm:114:LYS:NZ	2.36	0.58
2:AA:11:SER:OG	2:AA:14:GLU:OE1	2.22	0.58
37:B5:3541:G:OP2	37:B5:3541:G:N2	2.36	0.58
37:B5:4336:A2M:HM'2	37:B5:4337:U:H5'	1.84	0.58
81:Bs:48:ARG:HD3	82:Bt:123:ARG:HG2	1.85	0.58
1:A2:75:G:O2'	1:A2:77:A:OP1	2.22	0.58
20:Aj:51:SER:OG	20:Aj:55:ARG:NH1	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:40:G:N2	37:B5:4126:A:N7	2.51	0.58
1:A2:966:U:OP1	11:Aa:7:LYS:NZ	2.36	0.58
37:B5:4379:G:OP1	89:B5:5183:SPD:N10	2.37	0.58
14:Ad:68:ARG:NH1	14:Ad:78:THR:CG2	2.66	0.58
25:Ao:18:ARG:NH1	28:Ar:88:LYS:O	2.37	0.58
37:B5:2028:G:OP2	42:BC:294:LYS:NZ	2.37	0.58
37:B5:4445:U:H5	37:B5:4447:A:N7	2.02	0.58
55:BQ:178:ARG:H	65:Ba:51:GLY:HA2	1.69	0.58
86:Nu:102:MET:HA	86:Nu:102:MET:CE	2.28	0.58
23:Am:40:LEU:HB3	23:Am:45:LEU:HD12	1.86	0.58
68:Bd:64:ILE:HG23	68:Bd:68:LEU:HD23	1.86	0.58
85:Nt:94:VAL:HB	85:Nt:106:ILE:HB	1.85	0.58
17:Ag:107:LYS:O	17:Ag:109:ARG:NH2	2.36	0.58
26:Ap:53:GLU:OE1	26:Ap:85:ARG:NH2	2.34	0.58
37:B5:1395:U:OP2	44:BF:33:ARG:NH2	2.36	0.58
37:B5:1772:G:OP1	58:BT:120:LYS:NZ	2.36	0.58
37:B5:4335:A:N1	37:B5:4367:C:O2'	2.37	0.58
39:B8:75:OMG:OP2	63:BY:74:TYR:OH	2.20	0.58
55:BQ:16:LYS:O	55:BQ:33:ARG:NH2	2.36	0.58
83:Bv:207:LYS:HB3	83:Bv:213:PRO:HA	1.86	0.58
13:Ac:70:THR:HG22	13:Ac:86:LEU:HD13	1.86	0.57
41:BB:213:GLN:NE2	41:BB:285:TYR:O	2.34	0.57
1:A2:518:OMC:HM22	1:A2:519:G:H5'	1.86	0.57
37:B5:91:G:OP1	78:Bo:44:LYS:NZ	2.34	0.57
37:B5:2538:A:OP1	75:Bk:35:LYS:NZ	2.37	0.57
37:B5:4018:G:N2	37:B5:4018:G:OP2	2.34	0.57
1:A2:330:G:H2'	1:A2:331:G:O4'	2.04	0.57
37:B5:1420:G:OP1	66:Bb:44:ARG:NH1	2.37	0.57
37:B5:1924:G:N2	37:B5:1924:G:OP1	2.37	0.57
1:A2:753:G:O2'	1:A2:754:C:O2	2.20	0.57
39:B8:1:C:H3'	39:B8:2:G:H8	1.69	0.57
1:A2:1021:A:N7	23:Am:70:LYS:NZ	2.53	0.57
1:A2:1390:C:OP1	27:Aq:43:SER:OG	2.22	0.57
37:B5:1466:U:H5''	65:Ba:7:LYS:HD3	1.86	0.57
39:B8:81:C:O2'	72:Bh:2:ALA:N	2.38	0.57
47:BI:55:ASP:OD2	47:BI:164:LYS:NZ	2.37	0.57
1:A2:840:C:H42	34:Ax:48:TYR:HA	1.70	0.57
37:B5:3909:U:H5'	37:B5:3910:C:H5''	1.86	0.57
84:MA:272:HIS:CE1	84:MA:277:PHE:HA	2.38	0.57
37:B5:3449:A:OP2	37:B5:3467:G:N2	2.32	0.57
37:B5:4218:G:O2'	77:Bm:100:TYR:O	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BA:2:GLY:HA2	40:BA:207:VAL:HG23	1.85	0.57
44:BF:189:LEU:HD21	44:BF:207:LEU:HD21	1.85	0.57
83:Bv:58:THR:HG22	83:Bv:152:LYS:C	2.30	0.57
25:Ao:35:GLN:O	28:Ar:88:LYS:NZ	2.35	0.57
37:B5:1089:G:H2'	37:B5:1091:G:H8	1.70	0.57
7:AF:26:GLN:NE2	7:AF:73:SER:O	2.35	0.57
37:B5:1779:G:H5''	44:BF:112:ARG:HD2	1.87	0.57
1:A2:1329:OMG:HM22	1:A2:1330:U:H5'	1.86	0.56
22:Al:43:ASP:O	22:Al:45:ARG:NH2	2.38	0.56
37:B5:239:C:OP1	63:BY:46:SER:OG	2.23	0.56
1:A2:1402:A:N6	1:A2:1442:U:O2'	2.37	0.56
1:A2:1704:OMC:HM22	1:A2:1705:C:H5'	1.86	0.56
1:A2:1861:A:N7	6:AE:34:LYS:NZ	2.52	0.56
12:Ab:102:LEU:HD22	12:Ab:130:ILE:HG12	1.86	0.56
29:As:90:SER:O	29:As:91:HIS:ND1	2.39	0.56
37:B5:1016:C:O2'	37:B5:1059:G:O4'	2.24	0.56
37:B5:4151:G:OP2	47:BI:7:ARG:NH2	2.39	0.56
86:Nu:62:VAL:HG11	86:Nu:90:ILE:HD13	1.87	0.56
17:Ag:8:ILE:HD13	17:Ag:16:PRO:HB3	1.87	0.56
26:Ap:101:ASP:OD1	26:Ap:102:GLU:N	2.37	0.56
37:B5:1919:U:O4	82:Bt:57:ARG:NH2	2.39	0.56
54:BP:52:THR:HG23	54:BP:85:LYS:HG3	1.88	0.56
1:A2:1286:G:H22	22:Al:57:ASP:HB2	1.71	0.56
1:A2:1564:G:OP1	29:As:121:ARG:NH1	2.39	0.56
6:AE:51:ARG:NH1	6:AE:55:GLU:OE2	2.39	0.56
22:Al:91:LEU:CD1	22:Al:106:CYS:HB2	2.36	0.56
28:Ar:101:ASN:O	28:Ar:105:ASN:ND2	2.37	0.56
37:B5:2023:U:H1'	55:BQ:14:ARG:NH2	2.13	0.56
41:BB:261:ARG:HB2	53:BO:64:THR:HG21	1.87	0.56
47:BI:33:ILE:O	47:BI:69:ARG:NH1	2.36	0.56
10:AZ:52:LYS:HB2	27:Aq:109:LEU:HD13	1.88	0.56
37:B5:1539:G:N7	89:B5:5178:SPD:N10	2.46	0.56
52:BN:181:HIS:O	52:BN:195:ARG:NH2	2.39	0.56
64:BZ:29:ILE:HG22	64:BZ:32:GLY:H	1.71	0.56
82:Bt:147:HIS:HD2	82:Bt:149:HIS:HB2	1.69	0.56
84:MA:243:VAL:HG13	84:MA:276:ILE:HG21	1.87	0.56
1:A2:1594:C:H1'	29:As:12:GLN:HE22	1.70	0.56
1:A2:1651:A:H5''	26:Ap:139:ALA:HB2	1.87	0.56
37:B5:2322:G:H2'	37:B5:2323:G:H8	1.71	0.56
84:MA:389:ASN:HD21	84:MA:393:GLU:HB2	1.71	0.56
37:B5:3958:A:N1	58:BT:3:ASN:ND2	2.47	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BL:209:LYS:O	83:Bv:181:TYR:CE1	2.59	0.56
1:A2:1443:OMU:HM22	1:A2:1444:C:H5'	1.88	0.56
2:AA:84:HIS:OXT	23:Am:19:ARG:NH1	2.38	0.56
17:Ag:143:ARG:HB2	17:Ag:155:LYS:HB2	1.87	0.56
18:Ah:56:ARG:NH1	18:Ah:180:GLY:O	2.38	0.56
19:Ai:170:PRO:O	19:Ai:175:ARG:NH1	2.39	0.56
80:Br:28:GLU:OE2	80:Br:31:ASN:ND2	2.39	0.56
84:MA:378:GLN:HG3	84:MA:381:ILE:HB	1.88	0.56
85:Nt:88:VAL:HB	85:Nt:111:VAL:HB	1.87	0.56
1:A2:1419:C:O2'	1:A2:1421:G:OP2	2.23	0.56
37:B5:1341:A:O2'	37:B5:1422:C:O2'	2.24	0.56
14:Ad:44:LEU:HD21	14:Ad:72:ILE:HD11	1.86	0.55
37:B5:3868:C:H42	37:B5:3889:G:H1	1.54	0.55
47:BI:101:LYS:NZ	47:BI:102:MET:O	2.38	0.55
68:Bd:38:PHE:HB3	68:Bd:78:ARG:HG2	1.87	0.55
1:A2:1276:G:N2	1:A2:1507:A:OP2	2.38	0.55
16:Af:33:ALA:O	61:BW:70:LYS:NZ	2.39	0.55
22:Al:33:ARG:HD3	22:Al:89:VAL:CG2	2.35	0.55
37:B5:4311:C:O2	41:BB:268:ARG:NH2	2.39	0.55
37:B5:4440:G:H4'	46:BH:71:ARG:HH12	1.71	0.55
82:Bt:101:SER:HA	82:Bt:141:CYS:HA	1.88	0.55
84:MA:291:VAL:CG2	84:MA:485:SER:CA	2.80	0.55
2:AA:35:VAL:HG21	2:AA:63:LEU:HD13	1.88	0.55
37:B5:3353:A:HO2'	37:B5:4404:G:HO2'	1.46	0.55
37:B5:4416:C:O2'	37:B5:4418:A:OP2	2.25	0.55
40:BA:36:GLU:OE1	40:BA:163:ARG:NH1	2.36	0.55
65:Ba:84:GLU:OE2	65:Ba:87:ARG:NH2	2.37	0.55
65:Ba:125:LYS:HG2	65:Ba:145:VAL:HB	1.89	0.55
84:MA:278:GLN:HG3	84:MA:481:TRP:HB2	1.87	0.55
85:Nt:114:SER:OG	85:Nt:117:SER:O	2.22	0.55
16:Af:58:LYS:HA	16:Af:107:SER:HB2	1.88	0.55
37:B5:992:C:OP1	37:B5:1106:U:O2'	2.23	0.55
37:B5:2258:OMU:HM22	37:B5:2259:G:H5'	1.88	0.55
42:BC:101:MET:HE2	42:BC:104:PRO:HA	1.89	0.55
84:MA:301:LEU:HB2	84:MA:448:ASP:C	2.30	0.55
7:AF:32:LEU:HB2	7:AF:71:ILE:HD11	1.87	0.55
28:Ar:34:LYS:HG2	28:Ar:103:LEU:HD12	1.87	0.55
37:B5:678:G:H5''	43:BE:103:LYS:HE2	1.87	0.55
37:B5:1458:A:H4'	37:B5:1459:G:H5'	1.88	0.55
74:Bj:2:THR:O	74:Bj:7:SER:OG	2.24	0.55
14:Ad:79:ASP:HB3	14:Ad:82:TYR:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:864:A:HO2'	37:B5:868:C:HO2'	1.50	0.55
37:B5:2110:U:OP1	80:Br:37:SER:OG	2.22	0.55
37:B5:3894:C:OP1	64:BZ:59:LYS:NZ	2.30	0.55
84:MA:261:PRO:HA	84:MA:264:ILE:HD12	1.89	0.55
1:A2:1544:U:H5''	26:Ap:37:ARG:HH12	1.71	0.55
10:AZ:33:GLN:HB3	10:AZ:154:LEU:HD12	1.89	0.55
40:BA:116:LEU:HB3	40:BA:126:LEU:HB2	1.89	0.55
1:A2:1842:C:H2'	1:A2:1843:4AC:H6	1.88	0.55
31:Au:82:ASN:O	31:Au:83:PHE:C	2.50	0.55
48:BJ:112:HIS:HD2	48:BJ:126:TYR:H	1.54	0.55
1:A2:831:A:OP2	1:A2:847:G:N2	2.39	0.55
27:Aq:44:LYS:HG3	27:Aq:47:ARG:HH21	1.71	0.55
67:Bc:11:LEU:HD13	67:Bc:75:SER:HB2	1.89	0.55
1:A2:463:OMC:HM22	1:A2:464:C:H5'	1.88	0.55
1:A2:1090:G:H4'	90:A2:2044:SPM:H111	1.89	0.55
8:AG:22:ARG:HH11	13:Ac:16:ILE:HG21	1.72	0.54
37:B5:859:G:O2'	37:B5:2106:A:N6	2.39	0.54
37:B5:4672:C:H42	37:B5:4673:A:H62	1.55	0.54
70:Bf:40:GLU:O	70:Bf:109:ARG:NH2	2.41	0.54
83:Bv:65:VAL:HG22	83:Bv:109:ALA:HB3	1.88	0.54
84:MA:207:LEU:HD13	84:MA:209:GLN:HE22	1.73	0.54
86:Nu:97:LYS:HB2	86:Nu:101:GLU:HB2	1.89	0.54
16:Af:103:ASP:OD2	16:Af:105:ASN:ND2	2.36	0.54
21:Ak:147:LYS:HD2	21:Ak:151:THR:HG21	1.89	0.54
37:B5:1809:C:H2'	37:B5:1810:A2M:H8	1.87	0.54
37:B5:2363:C:O2	37:B5:2483:G:N2	2.40	0.54
37:B5:4282:OMC:HM22	37:B5:4283:C:H5'	1.89	0.54
22:Al:91:LEU:HD12	22:Al:106:CYS:HB2	1.89	0.54
52:BN:116:LEU:HD22	52:BN:135:ILE:HD11	1.89	0.54
55:BQ:67:ILE:HG12	55:BQ:98:LEU:HD11	1.89	0.54
81:Bs:20:LEU:CD1	81:Bs:54:LEU:HD22	2.35	0.54
81:Bs:68:HIS:HB3	81:Bs:75:LEU:HD22	1.89	0.54
83:Bv:63:PHE:HB2	83:Bv:152:LYS:HG2	1.88	0.54
85:Nt:112:TYR:HB2	85:Nt:121:ILE:HB	1.90	0.54
1:A2:1474:G:N2	1:A2:1477:A:OP2	2.40	0.54
1:A2:1569:C:OP1	29:As:96:SER:OG	2.25	0.54
39:B8:38:U:O2'	72:Bh:86:LYS:NZ	2.34	0.54
1:A2:1663:U:O4	1:A2:1664:A:N6	2.41	0.54
28:Ar:26:ILE:HG13	28:Ar:45:LEU:HD21	1.89	0.54
37:B5:349:A:C6	42:BC:45:ARG:CZ	2.90	0.54
37:B5:784:C:H2'	37:B5:785:G:H8	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:2161:G:N2	37:B5:2164:G:OP2	2.35	0.54
37:B5:4641:C:H2'	37:B5:4642:G:H5'	1.88	0.54
1:A2:165:G:N2	1:A2:165:G:OP2	2.39	0.54
37:B5:2362:U:O2'	37:B5:2373:U:O2	2.25	0.54
11:Aa:5:LYS:NZ	24:An:65:ASP:OD2	2.41	0.54
26:Ap:132:PHE:O	26:Ap:140:ARG:NH2	2.36	0.54
84:MA:298:HIS:O	84:MA:468:GLY:N	2.34	0.54
9:AT:33:U:OP2	26:Ap:146:ARG:NH1	2.39	0.54
37:B5:4120:U:O4	78:Bo:58:LYS:NZ	2.40	0.54
59:BU:28:PRO:HB2	59:BU:34:MET:HG2	1.90	0.54
84:MA:364:PRO:HG2	84:MA:366:MET:HE3	1.89	0.54
86:Nu:100:THR:O	86:Nu:101:GLU:C	2.49	0.54
1:A2:1678:U:H2'	1:A2:1679:A2M:H8	1.90	0.54
7:AF:184:LEU:HD23	13:Ac:227:LYS:HD2	1.89	0.54
37:B5:2705:G:O6	89:B5:5177:SPD:N1	2.41	0.54
37:B5:4666:G:N2	37:B5:4666:G:OP2	2.41	0.54
48:BJ:13:ARG:O	48:BJ:136:ARG:NH1	2.41	0.54
37:B5:2257:G:H2'	37:B5:2258:OMU:H6	1.90	0.54
30:At:40:LEU:HB3	30:At:48:LEU:HD11	1.89	0.53
37:B5:399:G:H2'	37:B5:400:A2M:H8	1.90	0.53
37:B5:1217:G:H4'	43:BE:77:ALA:HB2	1.91	0.53
37:B5:4138:OMG:HM21	37:B5:4140:A:H2'	1.89	0.53
69:Be:9:LYS:NZ	69:Be:71:PRO:O	2.41	0.53
84:MA:242:MET:HB3	84:MA:279:ALA:HA	1.89	0.53
3:AB:20:ARG:NH2	3:AB:25:GLY:O	2.40	0.53
16:Af:98:ARG:NH2	16:Af:103:ASP:OD1	2.40	0.53
37:B5:109:G:OP2	50:BL:74:ARG:NH2	2.41	0.53
37:B5:4004:C:OP2	48:BJ:54:ARG:NH1	2.42	0.53
84:MA:487:GLY:O	84:MA:491:VAL:HG23	2.09	0.53
85:Nt:86:ARG:HB2	85:Nt:113:LYS:HB2	1.91	0.53
1:A2:1456:A:H2'	1:A2:1457:G:H8	1.73	0.53
14:Ad:151:ASP:OD2	16:Af:216:ARG:NH2	2.39	0.53
18:Ah:22:HIS:ND1	18:Ah:23:LYS:O	2.38	0.53
19:Ai:93:LYS:HB2	19:Ai:96:TYR:HD1	1.72	0.53
1:A2:1049:G:N7	92:A2:2205:HOH:O	2.34	0.53
9:AT:13:U:H3	9:AT:22:U:H3	1.57	0.53
37:B5:1931:U:O2'	37:B5:1941:A:OP1	2.26	0.53
37:B5:3450:A2M:HM'2	37:B5:3451:A:H5'	1.90	0.53
37:B5:4516:G:OP1	53:BO:176:ARG:NH1	2.41	0.53
1:A2:1131:G:N2	1:A2:1131:G:OP2	2.41	0.53
1:A2:1760:G:H2'	1:A2:1761:G:H8	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ae:56:TYR:HB3	15:Ae:63:LYS:HA	1.91	0.53
16:Af:67:VAL:HG12	16:Af:69:THR:HG22	1.91	0.53
28:Ar:132:ARG:HB2	28:Ar:134:GLN:HE22	1.73	0.53
37:B5:1093:C:H2'	37:B5:1094:A:H8	1.74	0.53
37:B5:1335:A:N7	89:B5:5193:SPD:N10	2.56	0.53
37:B5:483:G:O2'	37:B5:486:C:OP2	2.25	0.53
37:B5:4328:C:O2'	41:BB:99:LEU:O	2.27	0.53
84:MA:185:ASP:HB2	84:MA:187:MET:HE3	1.91	0.53
1:A2:1080:C:O2'	1:A2:1183:A:N1	2.41	0.53
13:Ac:41:VAL:HG13	13:Ac:46:THR:HG22	1.91	0.53
18:Ah:89:GLU:OE1	18:Ah:92:ARG:NH2	2.42	0.53
37:B5:2601:G:O2'	37:B5:2608:A:N3	2.37	0.53
37:B5:4745:U:H4'	37:B5:4746:A:H5'	1.90	0.53
42:BC:293:LEU:O	42:BC:299:GLN:NE2	2.41	0.53
47:BI:87:ILE:HG12	47:BI:138:ILE:HG12	1.90	0.53
1:A2:282:C:N4	1:A2:892:G:O5'	2.42	0.53
4:AC:102:VAL:HG21	22:Al:35:ILE:HG21	1.91	0.53
16:Af:137:ARG:HD3	16:Af:178:ARG:HH21	1.74	0.53
37:B5:1009:G:N2	37:B5:1093:C:O2	2.34	0.53
40:BA:137:ILE:HD11	40:BA:149:LYS:HB2	1.90	0.53
1:A2:90:G:OP2	89:A2:2038:SPD:N10	2.42	0.53
1:A2:1205:A:N6	1:A2:1694:G:O6	2.41	0.53
7:AF:87:LEU:HB2	7:AF:101:PHE:HB2	1.90	0.53
13:Ac:38:GLU:OE2	13:Ac:40:ARG:HG3	2.08	0.53
37:B5:664:G:H2'	37:B5:665:G:H8	1.74	0.53
37:B5:1449:U:H2'	37:B5:1450:G:H8	1.73	0.53
80:Br:26:SER:OG	80:Br:28:GLU:OE1	2.22	0.53
84:MA:277:PHE:HB3	84:MA:480:ASN:HD22	1.73	0.53
1:A2:602:OMG:HM22	1:A2:603:G:H5'	1.90	0.53
1:A2:1285:A:C6	22:Al:91:LEU:CD2	2.92	0.53
37:B5:395:A:OP2	85:Nt:71:ARG:NH1	2.42	0.53
1:A2:127:C:O2	14:Ad:134:LYS:NZ	2.38	0.52
1:A2:1754:C:H2'	1:A2:1755:G:H8	1.74	0.52
37:B5:4440:G:OP1	37:B5:4440:G:N2	2.41	0.52
81:Bs:124:PRO:HD2	81:Bs:180:ILE:HD13	1.91	0.52
86:Nu:106:ILE:HG23	86:Nu:106:ILE:O	2.08	0.52
1:A2:116:OMU:HM22	1:A2:117:C:H5'	1.91	0.52
37:B5:684:C:OP2	43:BE:114:LYS:NZ	2.42	0.52
37:B5:1846:A:H4'	44:BF:222:LYS:HE3	1.91	0.52
37:B5:1934:G:O6	37:B5:1939:G:N2	2.42	0.52
37:B5:1960:G:OP1	81:Bs:58:ASN:ND2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BF:170:ASP:OD1	44:BF:171:ASN:N	2.42	0.52
65:Ba:89:ASN:OD1	65:Ba:92:LYS:NZ	2.42	0.52
86:Nu:103:LEU:O	86:Nu:104:PRO:C	2.52	0.52
37:B5:1644:G:OP2	90:B5:5142:SPM:N5	2.42	0.52
37:B5:4092:U:H5'	78:Bo:80:LYS:HE2	1.91	0.52
84:MA:291:VAL:CB	84:MA:485:SER:HB3	2.38	0.52
16:Af:57:ASP:OD1	16:Af:61:PHE:N	2.42	0.52
23:Am:99:ARG:NH2	23:Am:119:GLU:OE2	2.42	0.52
37:B5:706:C:OP1	43:BE:142:LYS:NZ	2.34	0.52
39:B8:1:C:H3'	39:B8:2:G:C8	2.44	0.52
41:BB:224:LYS:HE3	41:BB:340:THR:HG22	1.91	0.52
61:BW:81:ALA:HB2	61:BW:87:LEU:HB2	1.90	0.52
75:Bk:13:LEU:HD23	75:Bk:16:ARG:HH21	1.74	0.52
84:MA:234:HIS:HD2	84:MA:239:GLU:HG3	1.73	0.52
1:A2:99:A2M:HM'2	1:A2:100:U:H5'	1.92	0.52
39:B8:110:U:OP2	76:Bl:8:ARG:NH1	2.42	0.52
84:MA:250:VAL:HG22	84:MA:258:ARG:NH2	2.24	0.52
84:MA:278:GLN:CG	84:MA:481:TRP:HB2	2.39	0.52
1:A2:1448:OMG:OP1	30:At:101:HIS:ND1	2.40	0.52
11:Aa:189:ILE:HB	11:Aa:190:PRO:HD3	1.90	0.52
15:Ae:19:LEU:HD21	15:Ae:69:VAL:HG11	1.91	0.52
32:Av:105:THR:HG23	32:Av:124:LYS:HB2	1.91	0.52
37:B5:481:G:O2'	37:B5:483:G:OP1	2.27	0.52
37:B5:2659:G:N2	37:B5:3354:C:O2	2.43	0.52
37:B5:4610:C:N4	57:BS:171:ARG:O	2.43	0.52
53:BO:54:TYR:OH	53:BO:73:PHE:O	2.28	0.52
61:BW:23:ARG:HH21	61:BW:27:LYS:HD2	1.75	0.52
72:Bh:82:ASP:OD1	72:Bh:82:ASP:N	2.34	0.52
82:Bt:154:ASP:HB3	82:Bt:159:ALA:HB3	1.91	0.52
84:MA:292:GLY:O	84:MA:476:TYR:N	2.42	0.52
84:MA:299:ARG:NE	84:MA:465:LEU:O	2.42	0.52
1:A2:869:G:OP2	1:A2:869:G:N2	2.39	0.52
1:A2:1551:G:H3'	1:A2:1580:A:H61	1.74	0.52
22:Al:11:VAL:HG13	22:Al:13:ASP:H	1.74	0.52
37:B5:1804:G:OP2	47:BI:98:ARG:NH2	2.38	0.52
41:BB:224:LYS:O	41:BB:274:TYR:N	2.40	0.52
47:BI:66:GLU:OE2	47:BI:69:ARG:NH2	2.42	0.52
50:BL:64:VAL:O	50:BL:64:VAL:CG1	2.57	0.52
56:BR:12:SER:OG	56:BR:17:CYS:O	2.24	0.52
84:MA:396:ASP:OD1	84:MA:427:THR:N	2.37	0.52
37:B5:1805:U:OP1	47:BI:4:ARG:NH1	2.31	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:1834:G:O2'	37:B5:1846:A:N3	2.41	0.52
37:B5:4287:G:N2	37:B5:4290:A:OP2	2.40	0.52
65:Ba:39:V5N:O2	65:Ba:40:HIS:N	2.41	0.52
84:MA:250:VAL:CB	84:MA:258:ARG:HH21	2.23	0.52
1:A2:1426:G:O3'	26:Ap:33:LYS:NZ	2.41	0.52
37:B5:3631:OMG:HM22	37:B5:3632:G:H5'	1.92	0.52
64:BZ:22:LYS:NZ	64:BZ:132:GLN:O	2.42	0.52
1:A2:1156:U:OP1	12:Ab:185:THR:OG1	2.28	0.52
16:Af:162:LEU:HD11	16:Af:172:LYS:HG3	1.92	0.52
18:Ah:67:TRP:NE1	18:Ah:191:GLU:OE2	2.33	0.52
37:B5:1284:OMC:HM22	37:B5:1285:U:H5'	1.92	0.52
37:B5:1653:C:O2'	44:BF:176:ARG:NH2	2.39	0.52
44:BF:126:LYS:HB2	58:BT:133:ALA:HB3	1.91	0.52
82:Bt:112:ILE:HG22	82:Bt:132:ILE:HD13	1.92	0.52
83:Bv:94:ASN:O	83:Bv:97:LYS:NZ	2.43	0.52
1:A2:679:U:OP2	1:A2:1027:C:N4	2.35	0.51
1:A2:1776:U:H2'	1:A2:1777:G:H8	1.73	0.51
19:Ai:138:ARG:NH1	19:Ai:153:SER:OG	2.42	0.51
27:Aq:109:LEU:HG	27:Aq:111:PHE:HD2	1.73	0.51
28:Ar:22:GLY:HA2	28:Ar:56:ALA:HB3	1.91	0.51
37:B5:1067:C:H2'	37:B5:1068:U:C6	2.45	0.51
37:B5:1934:G:N2	81:Bs:41:GLN:OE1	2.43	0.51
51:BM:29:ASP:OD1	51:BM:30:VAL:N	2.42	0.51
85:Nt:93:ARG:HG3	85:Nt:105:VAL:HG13	1.93	0.51
42:BC:65:GLU:HB3	42:BC:80:ARG:HD3	1.92	0.51
42:BC:284:MET:HE3	55:BQ:124:ASP:HB3	1.92	0.51
86:Nu:39:ALA:HA	86:Nu:42:LYS:HE3	1.92	0.51
86:Nu:106:ILE:O	86:Nu:107:LEU:HD23	2.10	0.51
1:A2:852:C:H5''	1:A2:853:G:H5'	1.91	0.51
42:BC:85:HIS:O	42:BC:89:GLN:NE2	2.44	0.51
86:Nu:71:VAL:CG2	86:Nu:102:MET:SD	2.99	0.51
6:AE:44:ILE:HD12	6:AE:65:PRO:HG2	1.92	0.51
14:Ad:68:ARG:HH12	14:Ad:78:THR:HG21	1.76	0.51
28:Ar:59:LEU:HD23	28:Ar:64:VAL:HG22	1.93	0.51
37:B5:1772:G:N2	37:B5:1774:G:O4'	2.43	0.51
37:B5:1922:A:H1'	37:B5:1949:A:H4'	1.91	0.51
37:B5:2691:G:O2'	37:B5:3570:U:O4	2.24	0.51
37:B5:3442:G:O4'	37:B5:3444:A:N6	2.43	0.51
37:B5:3852:G:N2	45:BG:43:GLN:O	2.44	0.51
1:A2:1031:A:H2'	1:A2:1032:A2M:H8	1.93	0.51
1:A2:1148:C:OP1	6:AE:6:ARG:NH1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Aa:225:LEU:HD23	45:Bg:264:LYS:HG3	1.93	0.51
16:Af:22:ARG:HG2	16:Af:25:ARG:HH22	1.75	0.51
37:B5:856:A:H1'	37:B5:2015:G:H5''	1.90	0.51
52:BN:68:ARG:NH1	52:BN:124:ASP:O	2.36	0.51
84:MA:258:ARG:HG2	84:MA:263:LEU:HD11	1.92	0.51
1:A2:678:G:N1	1:A2:1028:A:OP2	2.32	0.51
37:B5:3391:G:OP1	40:BA:241:ARG:NH1	2.44	0.51
40:BA:173:GLY:O	79:Bp:69:TRP:NE1	2.41	0.51
1:A2:1256:G:OP1	1:A2:1257:G:O2'	2.23	0.51
37:B5:151:G:OP2	52:BN:4:TYR:OH	2.24	0.51
37:B5:3497:G:O2'	37:B5:3499:C:N4	2.43	0.51
37:B5:4744:G:N2	37:B5:4780:G:O2'	2.44	0.51
83:Bv:73:HIS:ND1	83:Bv:144:MET:SD	2.81	0.51
84:MA:250:VAL:HG22	84:MA:258:ARG:HH21	1.75	0.51
1:A2:191:A:H3'	1:A2:192:C:H5''	1.91	0.51
1:A2:1534:A:OP2	15:Ae:164:ARG:NH1	2.44	0.51
13:Ac:132:LYS:HE3	13:Ac:191:PRO:HA	1.92	0.51
15:Ae:124:ASP:OD1	15:Ae:125:SER:N	2.43	0.51
16:Af:2:LYS:HG2	16:Af:17:GLU:HG2	1.92	0.51
37:B5:136:U:O4	72:Bh:79:LYS:NZ	2.34	0.51
37:B5:265:C:H1'	37:B5:266:C:C4	2.46	0.51
37:B5:1283:U:H2'	37:B5:1284:OMC:C6	2.45	0.51
37:B5:2225:A:N1	37:B5:2672:U:O2'	2.41	0.51
83:Bv:128:LEU:HD13	83:Bv:135:PRO:HD3	1.93	0.51
1:A2:355:OMU:HM22	1:A2:356:G:H5'	1.93	0.51
16:Af:51:ARG:HH21	16:Af:112:VAL:HG11	1.75	0.51
37:B5:637:C:N4	37:B5:638:G:O6	2.43	0.51
41:BB:95:THR:OG1	41:BB:98:GLY:O	2.20	0.51
81:Bs:13:TYR:HA	81:Bs:16:LYS:HE2	1.92	0.51
84:MA:426:HIS:NE2	84:MA:457:GLU:OE1	2.41	0.51
1:A2:71:G:O6	16:Af:170:ARG:NH1	2.44	0.50
14:Ad:68:ARG:NH1	14:Ad:78:THR:HG21	2.26	0.50
16:Af:21:GLU:OE1	16:Af:25:ARG:NH2	2.44	0.50
30:At:70:VAL:HG13	30:At:104:LEU:HB2	1.93	0.50
37:B5:74:G:H5'	50:BL:59:VAL:HB	1.93	0.50
37:B5:1089:G:H2'	37:B5:1091:G:C8	2.46	0.50
55:BQ:157:GLY:O	55:BQ:188:ASN:ND2	2.44	0.50
60:BV:106:VAL:HG12	60:BV:112:MET:HA	1.93	0.50
19:Ai:63:LEU:HD11	19:Ai:69:ARG:HH21	1.76	0.50
39:B8:75:OMG:HM22	39:B8:76:C:H5'	1.93	0.50
1:A2:166:A2M:HM'2	1:A2:167:G:H5'	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Ac:50:ILE:HD11	13:Ac:86:LEU:HD23	1.92	0.50
36:Az:23:ARG:NH2	37:B5:3539:A:OP1	2.35	0.50
37:B5:156:G:N2	37:B5:157:U:O4	2.45	0.50
37:B5:3518:U:OP1	37:B5:4296:G:O2'	2.21	0.50
37:B5:3585:PSU:O2'	37:B5:4718:A:N3	2.44	0.50
37:B5:3637:A:N6	92:B5:5772:HOH:O	2.43	0.50
37:B5:4640:G:H2'	37:B5:4641:C:O4'	2.10	0.50
62:BX:73:HIS:CD2	62:BX:115:LYS:HD2	2.47	0.50
84:MA:295:ARG:NH2	84:MA:470:GLY:O	2.44	0.50
1:A2:512:U:O2'	1:A2:577:A2M:N1	2.43	0.50
1:A2:1675:G:N7	26:Ap:17:LYS:NZ	2.54	0.50
15:Ae:40:ALA:HB1	15:Ae:45:TYR:CG	2.47	0.50
37:B5:1674:U:OP2	89:B5:5185:SPD:N6	2.44	0.50
54:BP:94:MET:HE1	54:BP:146:ILE:HB	1.93	0.50
83:Bv:183:ILE:HD13	83:Bv:206:ILE:HD13	1.92	0.50
84:MA:203:PRO:HG3	84:MA:229:ILE:HB	1.93	0.50
10:AZ:89:LYS:NZ	27:Aq:83:ASN:OD1	2.41	0.50
12:Ab:166:ARG:HB3	12:Ab:247:THR:HB	1.93	0.50
29:As:65:TYR:HE1	29:As:128:GLN:HG3	1.76	0.50
81:Bs:48:ARG:HH11	82:Bt:123:ARG:HG2	1.76	0.50
1:A2:1227:G:N1	1:A2:1640:G7M:OP2	2.26	0.50
37:B5:1564:U:O4	89:B5:5178:SPD:N6	2.44	0.50
90:B5:5142:SPM:H21	55:BQ:11:ARG:HB3	1.94	0.50
84:MA:339:ARG:NH1	84:MA:345:ASP:OD2	2.44	0.50
1:A2:1674:U:O2'	15:Ae:84:GLY:O	2.20	0.50
22:Al:76:LEU:O	22:Al:131:LYS:NZ	2.45	0.50
37:B5:1921:G:N2	37:B5:1948:A:O2'	2.45	0.50
37:B5:3430:G:OP2	40:BA:245:ARG:NH2	2.39	0.50
37:B5:3450:A2M:H8	37:B5:3450:A2M:O5'	2.12	0.50
41:BB:17:LEU:HD21	41:BB:235:TRP:HH2	1.77	0.50
41:BB:54:THR:HG22	41:BB:373:LYS:HE3	1.93	0.50
7:AF:39:THR:HG22	7:AF:60:ARG:HG2	1.94	0.50
20:Aj:16:PHE:HE2	20:Aj:89:ILE:HG22	1.77	0.50
24:An:34:PHE:HB3	24:An:41:PHE:HB2	1.92	0.50
27:Aq:77:GLU:OE2	27:Aq:81:ARG:NH2	2.44	0.50
37:B5:394:G:N2	37:B5:397:G:OP2	2.35	0.50
37:B5:440:U:O2'	70:Bf:91:ASN:O	2.27	0.50
37:B5:4429:U:OP2	37:B5:4452:G:N1	2.32	0.50
44:BF:181:TYR:CZ	44:BF:202:GLU:HG2	2.46	0.50
47:BI:177:ASN:HB2	47:BI:180:GLU:HG2	1.93	0.50
84:MA:260:ALA:HB3	84:MA:261:PRO:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1314:A:H1'	1:A2:1315:U:C2	2.47	0.50
23:Am:103:GLU:HG3	23:Am:104:ARG:HG3	1.94	0.50
37:B5:1335:A:OP1	55:BQ:181:ARG:NH2	2.41	0.50
37:B5:2293:G:N7	92:B5:5654:HOH:O	2.35	0.50
37:B5:3611:G:O2'	37:B5:3613:G:OP2	2.24	0.50
37:B5:4397:A:N7	92:B5:5655:HOH:O	2.35	0.50
83:Bv:37:SER:HB2	83:Bv:202:ARG:HB2	1.93	0.50
16:Af:44:GLU:HG3	16:Af:119:LYS:HD3	1.93	0.49
37:B5:4122:A:O2'	65:Ba:42:ARG:NH1	2.45	0.49
40:BA:30:ARG:NH1	40:BA:36:GLU:OE2	2.44	0.49
86:Nu:100:THR:O	86:Nu:104:PRO:CD	2.60	0.49
1:A2:156:G:OP1	16:Af:2:LYS:NZ	2.40	0.49
1:A2:510:OMG:HM22	1:A2:511:G:H5'	1.94	0.49
4:AC:102:VAL:HA	4:AC:105:TYR:HD2	1.77	0.49
7:AF:88:ARG:HH12	7:AF:100:ARG:HH21	1.60	0.49
7:AF:256:ILE:HB	7:AF:270:LEU:HB2	1.94	0.49
37:B5:3650:G:OP2	89:B5:5179:SPD:N10	2.44	0.49
37:B5:4599:G:H2'	37:B5:4600:G:H8	1.77	0.49
38:B7:87:G:N7	92:B7:305:HOH:O	2.35	0.49
46:BH:113:GLU:OE1	46:BH:115:ARG:NH2	2.45	0.49
53:BO:10:ASP:OD2	53:BO:37:ARG:NH2	2.42	0.49
68:Bd:42:ALA:HB3	68:Bd:77:ILE:HG13	1.94	0.49
85:Nt:83:LEU:HD13	86:Nu:44:LEU:HA	1.93	0.49
85:Nt:118:ASP:OD1	85:Nt:118:ASP:N	2.33	0.49
1:A2:1601:G:H4'	35:Ay:43:LYS:HE3	1.93	0.49
37:B5:2267:OMG:HM22	37:B5:2268:U:H5''	1.95	0.49
37:B5:4314:A:O2'	37:B5:4720:G:N7	2.45	0.49
84:MA:291:VAL:HG22	84:MA:485:SER:HA	1.92	0.49
1:A2:1172:G:O2'	1:A2:1188:G:O6	2.28	0.49
1:A2:1456:A:H2'	1:A2:1457:G:C8	2.47	0.49
9:AT:7:G:O2'	9:AT:49:C:O4'	2.30	0.49
37:B5:519:C:H2'	37:B5:520:G:C8	2.48	0.49
83:Bv:204:LEU:HD22	83:Bv:216:LEU:HD23	1.94	0.49
84:MA:250:VAL:CG2	84:MA:258:ARG:HD3	2.40	0.49
85:Nt:96:ILE:HB	85:Nt:104:PHE:HB2	1.94	0.49
24:An:46:ASP:N	24:An:46:ASP:OD1	2.45	0.49
48:BJ:81:GLU:OE2	48:BJ:85:LYS:NZ	2.44	0.49
48:BJ:84:GLU:OE2	48:BJ:92:TYR:OH	2.26	0.49
72:Bh:80:PRO:HD2	72:Bh:83:LEU:HD12	1.94	0.49
10:AZ:84:GLN:HG2	10:AZ:100:ALA:HB1	1.94	0.49
37:B5:3972:G:H2'	37:B5:3973:OMU:H6	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B8:60:G:O6	72:Bh:62:ASN:ND2	2.34	0.49
7:AF:133:ASN:HD21	7:AF:137:VAL:HB	1.77	0.49
12:Ab:114:LYS:CD	12:Ab:121:ARG:NH2	2.64	0.49
37:B5:4698:U:H2'	37:B5:4699:G:H8	1.77	0.49
45:BG:180:PRO:HG2	45:BG:219:VAL:HG13	1.94	0.49
69:Be:114:ARG:NH1	69:Be:117:GLN:OE1	2.45	0.49
84:MA:195:GLU:HB3	84:MA:381:ILE:HD11	1.95	0.49
84:MA:301:LEU:H	84:MA:449:VAL:HA	1.78	0.49
84:MA:471:ASP:OD1	84:MA:471:ASP:N	2.44	0.49
86:Nu:106:ILE:HD11	86:Nu:109:GLN:NE2	2.28	0.49
1:A2:564:G:O6	19:Ai:172:ARG:NH2	2.41	0.49
1:A2:1284:C:H41	22:Al:102:LYS:HE2	1.78	0.49
35:Ay:102:LYS:HD2	35:Ay:107:VAL:HG12	1.95	0.49
37:B5:3619:OMC:HM22	37:B5:3620:G:H5'	1.93	0.49
54:BP:64:ASN:ND2	54:BP:80:GLN:OE1	2.44	0.49
1:A2:813:A:H5''	14:Ad:16:LYS:HD2	1.95	0.49
13:Ac:38:GLU:OE2	13:Ac:40:ARG:CG	2.61	0.49
16:Af:135:PRO:HG2	16:Af:141:ILE:HD13	1.95	0.49
26:Ap:19:ALA:HB2	26:Ap:75:GLY:HA3	1.94	0.49
37:B5:1706:A:C5	37:B5:1707:C:H1'	2.48	0.49
37:B5:4645:C:N4	37:B5:4646:G:O6	2.45	0.49
61:BW:4:GLU:HB2	61:BW:13:ILE:HB	1.94	0.49
1:A2:1843:4AC:O7	36:Az:4:LYS:NZ	2.46	0.49
21:Ak:18:GLN:HG2	21:Ak:33:LEU:HD21	1.95	0.49
34:Ax:7:ILE:HG22	34:Ax:27:VAL:HG22	1.94	0.49
37:B5:4627:C:H2'	37:B5:4628:G:H8	1.78	0.49
45:BG:260:GLU:O	45:BG:264:LYS:N	2.45	0.49
52:BN:193:ARG:O	52:BN:197:THR:OG1	2.26	0.49
12:Ab:252:THR:OG1	12:Ab:254:ASP:OD1	2.25	0.48
16:Af:148:SER:N	16:Af:151:ASP:OD2	2.41	0.48
17:Ag:95:ILE:HD11	17:Ag:133:LEU:HD13	1.95	0.48
45:BG:103:ARG:NH2	45:BG:192:ARG:O	2.45	0.48
63:BY:112:ASP:OD1	63:BY:112:ASP:N	2.46	0.48
84:MA:162:ASP:H	84:MA:168:VAL:HG11	1.78	0.48
1:A2:1462:G:H3'	1:A2:1464:U:H3	1.78	0.48
7:AF:40:ILE:HD11	7:AF:66:VAL:HG11	1.94	0.48
37:B5:4724:U:OP1	41:BB:175:GLN:NE2	2.46	0.48
67:Bc:51:ASN:ND2	67:Bc:78:ASN:OD1	2.37	0.48
1:A2:1529:G:O2'	1:A2:1667:C:OP1	2.29	0.48
10:AZ:198:MET:HG2	10:AZ:200:ASP:H	1.76	0.48
12:Ab:60:TRP:O	12:Ab:71:LYS:NZ	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:369:G:N2	37:B5:372:A:OP2	2.39	0.48
37:B5:1208:C:H2'	37:B5:1209:G:H8	1.78	0.48
84:MA:171:GLU:OE1	84:MA:215:ARG:NH1	2.45	0.48
84:MA:182:GLU:N	84:MA:252:LYS:HZ1	2.11	0.48
84:MA:234:HIS:CD2	84:MA:239:GLU:CG	2.96	0.48
85:Nt:91:VAL:HA	86:Nu:66:THR:HA	1.95	0.48
9:AT:24:A:O2'	37:B5:3502:PSU:OP1	2.31	0.48
15:Ae:131:ALA:HB2	15:Ae:135:ARG:HH21	1.78	0.48
37:B5:985:G:OP2	43:BE:67:ARG:NH1	2.45	0.48
37:B5:1955:C:H2'	37:B5:1956:A:H8	1.77	0.48
38:B7:23:A:N3	38:B7:118:C:O2'	2.46	0.48
51:BM:5:ARG:NE	51:BM:59:ASP:OD1	2.37	0.48
71:Bg:60:ARG:HB2	71:Bg:63:VAL:HG23	1.96	0.48
84:MA:175:LEU:HD22	84:MA:222:LEU:HG	1.94	0.48
84:MA:226:ILE:HD13	84:MA:267:ILE:HG21	1.95	0.48
14:Ad:112:HIS:NE2	14:Ad:237:SER:O	2.47	0.48
37:B5:2293:G:OP1	40:BA:17:ARG:NH1	2.47	0.48
37:B5:2338:U:H2'	37:B5:2339:G:C8	2.48	0.48
37:B5:4346:G:O2'	37:B5:4355:G:O6	2.28	0.48
52:BN:43:THR:OG1	52:BN:131:GLU:OE2	2.31	0.48
53:BO:108:ILE:HD13	53:BO:117:ARG:CZ	2.41	0.48
13:Ac:93:THR:HG22	13:Ac:95:GLY:H	1.78	0.48
37:B5:1927:G:H2'	37:B5:1928:G:H8	1.78	0.48
55:BQ:122:THR:OG1	55:BQ:124:ASP:OD1	2.25	0.48
18:Ah:81:VAL:HG22	18:Ah:102:VAL:HG12	1.94	0.48
23:Am:20:ARG:HH21	32:Av:56:HIS:HB3	1.79	0.48
37:B5:115:C:OP1	52:BN:2:GLY:N	2.47	0.48
37:B5:3676:OMG:HM22	37:B5:3677:A:H5'	1.95	0.48
60:BV:92:ASP:OD1	60:BV:92:ASP:N	2.46	0.48
82:Bt:80:LEU:HA	82:Bt:83:LYS:HG2	1.95	0.48
1:A2:798:C:H2'	1:A2:799:G:C4	2.48	0.48
1:A2:1760:G:H2'	1:A2:1761:G:C8	2.48	0.48
4:AC:114:ILE:HD12	22:Al:71:GLU:HG2	1.95	0.48
25:Ao:22:LEU:HD22	25:Ao:109:PRO:HB3	1.96	0.48
37:B5:1624:A:N3	37:B5:1791:U:O2'	2.40	0.48
37:B5:1726:A:N3	37:B5:3956:U:O2'	2.46	0.48
37:B5:2383:C:N4	92:B5:5666:HOH:O	2.36	0.48
83:Bv:104:ALA:O	83:Bv:133:LYS:NZ	2.38	0.48
85:Nt:121:ILE:HG12	86:Nu:89:THR:HG22	1.96	0.48
37:B5:152:U:OP2	52:BN:49:ARG:NH2	2.39	0.48
37:B5:2647:OMC:HM22	37:B5:2648:C:H5'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B8:84:A:O4'	72:Bh:3:LYS:NZ	2.47	0.48
7:AF:23:THR:HG23	7:AF:31:ILE:HG22	1.95	0.48
37:B5:4450:C:H2'	37:B5:4451:A:H8	1.79	0.48
81:Bs:19:GLN:NE2	81:Bs:23:ASP:OD2	2.46	0.48
83:Bv:159:MET:HB3	83:Bv:165:LEU:HD11	1.96	0.48
86:Nu:71:VAL:HG21	86:Nu:102:MET:HE2	1.95	0.48
86:Nu:103:LEU:HB2	86:Nu:104:PRO:CD	2.44	0.48
6:AE:38:LYS:HG2	6:AE:40:VAL:HG23	1.96	0.47
8:AG:54:LYS:NZ	30:At:94:ASP:OD1	2.39	0.47
37:B5:330:G:N7	89:B5:5175:SPD:N10	2.62	0.47
37:B5:349:A:C5	42:BC:45:ARG:NH1	2.79	0.47
37:B5:373:G:OP2	74:Bj:36:LYS:NZ	2.35	0.47
37:B5:398:A2M:H8	37:B5:398:A2M:O5'	2.13	0.47
37:B5:823:C:OP1	37:B5:825:G:O2'	2.31	0.47
37:B5:864:A:O2'	37:B5:868:C:O2'	2.22	0.47
37:B5:1210:C:H2'	37:B5:1211:G:H8	1.79	0.47
37:B5:1696:U:H2'	37:B5:1697:G:C8	2.49	0.47
37:B5:4383:OMG:HM22	37:B5:4384:U:H5'	1.96	0.47
59:BU:36:ALA:HB3	59:BU:65:ARG:HH21	1.78	0.47
16:Af:42:GLY:HA3	16:Af:45:TRP:HD1	1.78	0.47
37:B5:1095:C:H2'	37:B5:1096:G:H8	1.79	0.47
37:B5:2232:A:H5'	68:Bd:70:LYS:HE2	1.95	0.47
37:B5:4500:U:OP1	70:Bf:8:LYS:NZ	2.42	0.47
46:BH:48:LEU:HD11	46:BH:56:ARG:HH11	1.78	0.47
37:B5:194:C:O2	63:BY:121:ARG:NH2	2.48	0.47
37:B5:2043:A:N6	37:B5:2044:A:N1	2.61	0.47
37:B5:4703:C:N4	37:B5:4704:U:O4	2.48	0.47
46:BH:92:MET:HE2	46:BH:179:ILE:HG22	1.96	0.47
7:AF:8:ARG:NE	7:AF:311:GLN:OE1	2.42	0.47
10:AZ:94:THR:HG23	10:AZ:186:ARG:HH12	1.80	0.47
13:Ac:106:ARG:HG3	13:Ac:175:VAL:HB	1.96	0.47
37:B5:150:U:OP2	45:BG:200:THR:OG1	2.24	0.47
37:B5:2007:C:OP1	70:Bf:15:LYS:NZ	2.45	0.47
47:BI:51:HIS:CD2	47:BI:168:SER:HB2	2.50	0.47
56:BR:44:LEU:HD22	56:BR:49:LEU:HD12	1.95	0.47
57:BS:74:ARG:HH21	57:BS:76:LYS:HD3	1.79	0.47
7:AF:217:MET:HG2	7:AF:229:THR:HG22	1.96	0.47
30:At:113:ILE:O	30:At:116:GLN:NE2	2.48	0.47
37:B5:2207:OMG:HM22	37:B5:2208:OMC:H5''	1.97	0.47
37:B5:3422:U:O2'	37:B5:3549:A:N3	2.44	0.47
37:B5:3456:A2M:HM'2	37:B5:3457:G:H5'	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BA:53:GLY:O	40:BA:192:LYS:NZ	2.37	0.47
61:BW:63:GLN:HG3	61:BW:68:GLN:HE21	1.79	0.47
85:Nt:111:VAL:HG22	85:Nt:122:VAL:HG22	1.96	0.47
1:A2:496:U:H4'	14:Ad:24:THR:HG22	1.96	0.47
1:A2:875:G:N3	17:Ag:114:GLN:NE2	2.57	0.47
37:B5:409:G:OP2	54:BP:2:VAL:N	2.48	0.47
37:B5:439:G:O3'	70:Bf:91:ASN:ND2	2.47	0.47
37:B5:2328:U:H3	37:B5:2336:G:H1	1.63	0.47
37:B5:4693:G:H2'	37:B5:4694:A:C8	2.50	0.47
45:BG:166:LEU:HD21	52:BN:45:PRO:HG2	1.96	0.47
1:A2:921:A:O2'	1:A2:923:A:OP1	2.28	0.47
4:AC:126:CYS:HB2	4:AC:130:VAL:HB	1.96	0.47
13:Ac:101:GLN:HE22	13:Ac:125:PHE:HE2	1.62	0.47
33:Aw:24:ASP:HB3	33:Aw:27:TYR:HB3	1.97	0.47
37:B5:511:A:N6	65:Ba:106:SER:OG	2.48	0.47
37:B5:1224:C:O2'	42:BC:321:ASN:OD1	2.31	0.47
37:B5:3400:C:OP1	40:BA:8:GLN:NE2	2.46	0.47
37:B5:3562:A2M:HM'2	37:B5:3563:U:H5'	1.97	0.47
37:B5:4371:C:OP1	41:BB:224:LYS:HG3	2.15	0.47
41:BB:206:PRO:HG2	41:BB:209:GLN:HG3	1.97	0.47
42:BC:35:ASP:N	42:BC:35:ASP:OD1	2.47	0.47
69:Be:89:LEU:HD13	69:Be:118:LEU:HD22	1.96	0.47
84:MA:189:ARG:NH1	84:MA:408:MET:SD	2.88	0.47
86:Nu:71:VAL:HG11	86:Nu:102:MET:HE2	1.96	0.47
1:A2:823:PSU:HN3	1:A2:827:A:H62	1.63	0.47
11:Aa:123:ALA:HB2	11:Aa:165:ARG:HG3	1.97	0.47
17:Ag:51:ILE:HD11	17:Ag:176:VAL:HG22	1.95	0.47
18:Ah:80:ASP:OD1	18:Ah:81:VAL:N	2.48	0.47
34:Ax:29:HIS:ND1	34:Ax:29:HIS:O	2.48	0.47
37:B5:1936:U:N3	37:B5:1939:G:OP2	2.45	0.47
37:B5:2654:G:N2	37:B5:2657:C:OP2	2.44	0.47
37:B5:3421:G:O2'	37:B5:3550:UY1:OP2	2.27	0.47
37:B5:3524:OMG:HM22	37:B5:3525:U:H5'	1.96	0.47
44:BF:153:ILE:HD12	44:BF:190:ILE:HG12	1.97	0.47
63:BY:2:LYS:HE3	63:BY:2:LYS:HB3	1.81	0.47
83:Bv:54:ARG:NH1	83:Bv:153:SER:OG	2.47	0.47
85:Nt:119:THR:HG22	86:Nu:91:THR:HG22	1.97	0.47
86:Nu:97:LYS:CB	86:Nu:101:GLU:HB2	2.45	0.47
86:Nu:103:LEU:HB2	86:Nu:104:PRO:HD2	1.95	0.47
1:A2:27:A2M:HM'2	1:A2:28:U:H5'	1.96	0.47
1:A2:1206:C:N4	92:A2:2251:HOH:O	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AD:83:VAL:HG12	33:Aw:89:GLY:HA2	1.95	0.47
7:AF:88:ARG:HH11	7:AF:97:THR:HG21	1.80	0.47
11:Aa:87:ILE:HG22	11:Aa:101:HIS:HB2	1.97	0.47
16:Af:161:PRO:HA	16:Af:171:THR:HG22	1.96	0.47
37:B5:82:U:HO2'	37:B5:1326:G:HO2'	1.63	0.47
37:B5:382:G:N1	37:B5:385:A:OP2	2.47	0.47
37:B5:857:G:OP1	69:Be:65:LYS:NZ	2.40	0.47
37:B5:1612:G:OP2	65:Ba:24:LYS:NZ	2.47	0.47
37:B5:3882:G:H2'	37:B5:3883:G:C8	2.50	0.47
37:B5:4379:G:OP2	89:B5:5183:SPD:N1	2.48	0.47
37:B5:4668:C:H5''	51:BM:114:LYS:HD2	1.96	0.47
42:BC:278:ASN:OD1	42:BC:279:LEU:N	2.47	0.47
52:BN:124:ASP:OD1	52:BN:126:THR:N	2.38	0.47
64:BZ:25:ILE:HA	64:BZ:43:VAL:HG12	1.97	0.47
66:Bb:56:LYS:O	66:Bb:60:ASN:ND2	2.38	0.47
1:A2:628:OMU:H1'	1:A2:628:OMU:HM22	1.51	0.47
1:A2:1180:G:N2	1:A2:1183:A:OP2	2.46	0.47
1:A2:1757:C:H2'	1:A2:1758:G:C8	2.50	0.47
23:Am:3:ARG:HB2	23:Am:6:ALA:HB3	1.97	0.47
37:B5:2553:C:OP1	56:BR:39:GLN:NE2	2.42	0.47
37:B5:4194:G:H5''	37:B5:4195:A:H5''	1.96	0.47
37:B5:4450:C:H2'	37:B5:4451:A:C8	2.49	0.47
86:Nu:43:LYS:HA	86:Nu:46:PHE:CD2	2.50	0.47
1:A2:454:C:O2'	16:Af:92:ARG:O	2.26	0.46
13:Ac:142:LEU:HD21	13:Ac:182:LEU:HD21	1.97	0.46
37:B5:1933:C:H2'	37:B5:1934:G:H8	1.81	0.46
37:B5:2400:G:H1	37:B5:2413:U:H3	1.61	0.46
37:B5:4635:G:N2	37:B5:4665:C:H41	2.12	0.46
43:BE:182:LEU:HD12	43:BE:186:ARG:HA	1.97	0.46
1:A2:468:G:O5'	16:Af:72:ARG:NH2	2.48	0.46
22:Al:25:ALA:O	22:Al:30:GLY:N	2.34	0.46
31:Au:15:ARG:NH1	31:Au:33:GLN:OE1	2.48	0.46
40:BA:117:GLU:HG2	40:BA:124:GLY:H	1.80	0.46
40:BA:246:LEU:HD21	40:BA:250:LYS:HB2	1.97	0.46
41:BB:291:TYR:HB3	41:BB:298:LEU:HD11	1.97	0.46
42:BC:66:SER:HA	42:BC:77:PRO:HA	1.97	0.46
68:Bd:123:ASP:OD1	68:Bd:123:ASP:N	2.48	0.46
84:MA:252:LYS:HA	84:MA:255:ARG:HG2	1.95	0.46
1:A2:1416:C:O2'	29:As:132:ASP:OD2	2.30	0.46
1:A2:1680:A:H2'	15:Ae:60:ARG:HD2	1.97	0.46
1:A2:1763:C:H2'	1:A2:1764:G:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AC:114:ILE:HD13	22:Al:68:LEU:HD23	1.96	0.46
9:AT:75:C:OP2	47:BI:110:ARG:NH2	2.48	0.46
10:AZ:57:LYS:NZ	10:AZ:160:ALA:O	2.44	0.46
16:Af:44:GLU:HG3	16:Af:119:LYS:NZ	2.31	0.46
37:B5:305:A:P	52:BN:15:GLN:HE22	2.38	0.46
37:B5:4649:A:H4'	41:BB:95:THR:HG22	1.96	0.46
54:BP:78:TRP:CD1	54:BP:80:GLN:H	2.33	0.46
84:MA:199:TRP:NE1	84:MA:373:HIS:O	2.39	0.46
8:AG:22:ARG:NH1	13:Ac:16:ILE:HG21	2.29	0.46
37:B5:1310:G:N2	37:B5:1315:A:OP2	2.48	0.46
37:B5:3412:U:OP1	40:BA:54:ARG:NH2	2.33	0.46
52:BN:146:PRO:HB2	72:Bh:104:THR:HG23	1.96	0.46
81:Bs:161:ILE:HB	81:Bs:165:ASP:HB2	1.97	0.46
84:MA:299:ARG:CZ	84:MA:327:TYR:HD1	2.28	0.46
1:A2:1620:A:OP2	25:Ao:47:ARG:NH2	2.45	0.46
8:AG:3:HIS:HB3	8:AG:6:LEU:HB2	1.96	0.46
37:B5:293:G:O6	52:BN:182:HIS:NE2	2.48	0.46
82:Bt:147:HIS:CD2	82:Bt:149:HIS:HB2	2.49	0.46
1:A2:1525:G:N7	28:Ar:141:ARG:NH2	2.57	0.46
9:AT:20:U:OP1	48:BJ:58:ARG:NH2	2.42	0.46
15:Ae:49:LEU:HD12	26:Ap:50:LYS:HG2	1.96	0.46
17:Ag:100:ILE:HG12	17:Ag:125:VAL:HG21	1.96	0.46
37:B5:135:G:N2	72:Bh:95:LEU:O	2.36	0.46
37:B5:2338:U:H2'	37:B5:2339:G:H8	1.79	0.46
41:BB:56:ILE:HG22	41:BB:368:ILE:HA	1.96	0.46
41:BB:322:HIS:O	41:BB:342:LYS:NZ	2.37	0.46
85:Nt:90:GLY:O	86:Nu:67:ASN:N	2.46	0.46
1:A2:328:G:H2'	1:A2:329:U:H4'	1.97	0.46
1:A2:1510:U:O4'	4:AC:80:ARG:NH1	2.48	0.46
1:A2:1715:U:H2'	1:A2:1716:A:C8	2.51	0.46
37:B5:527:G:H1	37:B5:628:U:H3	1.63	0.46
37:B5:1712:U:H2'	37:B5:1713:C:C6	2.51	0.46
37:B5:2539:A:H62	75:Bk:35:LYS:NZ	2.13	0.46
44:BF:95:ARG:HH21	44:BF:223:THR:HA	1.81	0.46
56:BR:15:LEU:HD13	56:BR:52:ARG:HB2	1.98	0.46
68:Bd:37:GLY:O	68:Bd:41:ARG:HG3	2.15	0.46
76:Bl:44:TRP:O	76:Bl:48:LYS:NZ	2.48	0.46
83:Bv:181:TYR:CZ	83:Bv:185:LEU:HD11	2.51	0.46
84:MA:178:GLU:HA	84:MA:189:ARG:HE	1.81	0.46
1:A2:1787:U:H2'	1:A2:1788:G:H8	1.81	0.46
7:AF:150:TRP:NE1	27:Aq:37:GLU:OE1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Ad:199:GLU:OE2	14:Ad:209:HIS:NE2	2.42	0.46
23:Am:93:LYS:HA	23:Am:150:VAL:HG21	1.97	0.46
37:B5:184:U:H3	37:B5:253:G:H1	1.64	0.46
37:B5:1353:G:H2'	37:B5:1354:G:C8	2.51	0.46
37:B5:2602:G:H1'	37:B5:2607:A:H2	1.81	0.46
82:Bt:53:TRP:HD1	82:Bt:56:LEU:HB2	1.81	0.46
1:A2:1059:A:OP1	9:AT:38:C:O2'	2.34	0.46
11:Aa:30:TRP:CG	24:An:19:PRO:HB3	2.51	0.46
13:Ac:42:THR:CG2	13:Ac:47:GLU:CD	2.87	0.46
37:B5:757:A:N6	37:B5:759:G:O6	2.49	0.46
37:B5:1888:U:H5'	46:BH:65:LYS:HE2	1.98	0.46
38:B7:87:G:N2	38:B7:90:A:OP2	2.49	0.46
40:BA:180:LEU:HD21	79:Bp:22:LEU:HB3	1.98	0.46
83:Bv:58:THR:CG2	83:Bv:153:SER:HB3	2.46	0.46
84:MA:233:ILE:O	84:MA:240:LYS:N	2.48	0.46
86:Nu:57:SER:C	86:Nu:59:ILE:H	2.24	0.46
1:A2:68:A:OP2	16:Af:164:LYS:NZ	2.42	0.46
1:A2:758:C:O2	1:A2:788:G:N2	2.33	0.46
89:A2:2042:SPD:HN6	12:Ab:117:ARG:HH21	1.63	0.46
37:B5:423:G:OP1	54:BP:62:ARG:NH1	2.41	0.46
37:B5:778:C:H2'	37:B5:779:G:C8	2.51	0.46
37:B5:2205:U:H2'	37:B5:2206:A2M:H8	1.98	0.46
42:BC:294:LYS:HA	42:BC:299:GLN:HE21	1.80	0.46
52:BN:42:PRO:HG3	52:BN:61:ILE:HG13	1.98	0.46
59:BU:105:ASN:N	59:BU:105:ASN:OD1	2.47	0.46
77:Bm:94:MET:HG2	77:Bm:105:PRO:HA	1.98	0.46
7:AF:259:TRP:HD1	7:AF:266:ILE:HA	1.81	0.45
37:B5:3609:A:N3	37:B5:4147:G:O2'	2.46	0.45
37:B5:4757:C:H2'	37:B5:4758:A:H8	1.81	0.45
44:BF:146:LEU:O	44:BF:150:ASN:ND2	2.44	0.45
84:MA:245:ILE:HB	84:MA:281:TYR:HB3	1.97	0.45
14:Ad:211:LYS:NZ	14:Ad:215:GLY:O	2.49	0.45
15:Ae:58:ALA:HB3	15:Ae:62:ARG:NH2	2.32	0.45
17:Ag:60:ILE:HB	17:Ag:92:VAL:HG22	1.98	0.45
37:B5:469:C:OP2	37:B5:678:G:N1	2.42	0.45
37:B5:515:U:H4'	37:B5:516:U:H5''	1.99	0.45
37:B5:1105:C:O2'	37:B5:1106:U:OP1	2.33	0.45
37:B5:1736:G:OP1	44:BF:103:LYS:NZ	2.49	0.45
37:B5:1925:U:O4	37:B5:1952:A:N6	2.49	0.45
37:B5:2618:C:H2'	37:B5:2619:G:C8	2.51	0.45
55:BQ:82:VAL:HG13	55:BQ:102:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:MA:243:VAL:HG21	84:MA:271:VAL:HG11	1.98	0.45
84:MA:288:PRO:HA	84:MA:289:LYS:HA	1.49	0.45
84:MA:315:SER:O	84:MA:316:ARG:C	2.60	0.45
16:Af:164:LYS:HG2	16:Af:165:GLU:H	1.81	0.45
47:BI:52:MET:HE1	47:BI:155:ALA:HB3	1.97	0.45
83:Bv:114:GLU:HA	83:Bv:137:LEU:HD22	1.98	0.45
84:MA:266:GLU:OE2	84:MA:269:ARG:NH2	2.49	0.45
84:MA:285:VAL:O	84:MA:477:TYR:OH	2.33	0.45
1:A2:99:A2M:H8	1:A2:99:A2M:O5'	2.16	0.45
55:BQ:178:ARG:N	65:Ba:51:GLY:HA2	2.30	0.45
83:Bv:138:LEU:HD21	83:Bv:147:LYS:HG2	1.99	0.45
84:MA:210:TRP:CZ2	84:MA:274:GLU:HG3	2.50	0.45
84:MA:235:ILE:CD1	84:MA:478:LEU:HD13	2.46	0.45
84:MA:360:PHE:HB2	84:MA:363:THR:HG23	1.99	0.45
1:A2:126:G:O6	16:Af:196:LYS:NZ	2.31	0.45
7:AF:203:ASP:OD1	7:AF:205:SER:OG	2.32	0.45
37:B5:114:G:N2	37:B5:158:A:H61	2.14	0.45
37:B5:364:G:O6	74:Bj:55:ARG:NH2	2.39	0.45
43:BE:144:ARG:NH2	70:Bf:110:ILE:O	2.49	0.45
46:BH:137:SER:HB2	46:BH:145:VAL:HG23	1.97	0.45
54:BP:118:GLN:NE2	54:BP:147:GLU:OE2	2.50	0.45
83:Bv:60:ARG:O	83:Bv:171:HIS:ND1	2.46	0.45
84:MA:234:HIS:CG	84:MA:239:GLU:HG2	2.52	0.45
84:MA:458:ASN:O	84:MA:462:LEU:HG	2.16	0.45
1:A2:661:C:OP2	33:Aw:3:LYS:NZ	2.42	0.45
30:At:91:LYS:NZ	92:At:201:HOH:O	2.44	0.45
37:B5:3548:A:OP1	37:B5:3550:UY1:N1	2.50	0.45
37:B5:3805:A:N1	37:B5:3917:C:N4	2.64	0.45
41:BB:19:ARG:HB2	41:BB:234:ARG:NH2	2.32	0.45
84:MA:224:GLY:HA2	84:MA:258:ARG:NH2	2.27	0.45
84:MA:421:SER:HB2	84:MA:450:PHE:HZ	1.82	0.45
86:Nu:62:VAL:HB	86:Nu:74:PHE:HB2	1.99	0.45
1:A2:469:A2M:HM'2	1:A2:470:A:H5'	1.99	0.45
12:Ab:128:VAL:HG11	12:Ab:155:ILE:HG12	1.99	0.45
28:Ar:36:VAL:HG21	28:Ar:71:MET:HE3	1.98	0.45
37:B5:1654:A:H2'	37:B5:1655:A:C8	2.51	0.45
44:BF:87:LYS:NZ	44:BF:196:VAL:HG22	2.22	0.45
54:BP:14:SER:O	54:BP:105:LYS:NZ	2.36	0.45
1:A2:115:U:O2'	1:A2:382:C:O2	2.28	0.45
8:AG:40:ARG:NH2	30:At:85:PRO:O	2.48	0.45
37:B5:4627:C:H2'	37:B5:4628:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BS:99:ASP:OD1	57:BS:100:LEU:N	2.44	0.45
86:Nu:71:VAL:HG21	86:Nu:102:MET:CE	2.46	0.45
1:A2:1118:C:O2'	1:A2:1119:C:O4'	2.35	0.45
26:Ap:16:LYS:HG3	26:Ap:17:LYS:H	1.82	0.45
37:B5:515:U:O2'	37:B5:634:C:O4'	2.31	0.45
37:B5:639:G:H2'	37:B5:640:G:H8	1.82	0.45
37:B5:1068:U:H2'	37:B5:1069:G:C8	2.52	0.45
37:B5:1572:G:H1'	37:B5:2356:A:N6	2.32	0.45
44:BF:87:LYS:HD2	44:BF:196:VAL:HG22	1.97	0.45
19:Ai:83:ARG:HH21	19:Ai:150:ARG:NH1	2.15	0.45
34:Ax:23:MET:N	34:Ax:23:MET:SD	2.90	0.45
37:B5:260:C:H2'	37:B5:261:G:H8	1.82	0.45
37:B5:1458:A:H62	55:BQ:87:THR:HG21	1.82	0.45
37:B5:1806:A:N3	37:B5:4149:PSU:O2'	2.47	0.45
37:B5:2473:U:OP1	59:BU:48:LYS:NZ	2.33	0.45
42:BC:140:LYS:HE3	42:BC:245:HIS:HB2	1.99	0.45
82:Bt:17:CYS:SG	82:Bt:18:THR:N	2.90	0.45
84:MA:458:ASN:HA	84:MA:461:PHE:CE2	2.52	0.45
1:A2:151:C:OP1	34:Ax:120:THR:OG1	2.27	0.44
1:A2:165:G:H2'	1:A2:166:A2M:H8	1.99	0.44
1:A2:599:G:O2'	1:A2:606:A:N1	2.47	0.44
1:A2:925:G:H5'	23:Am:4:MET:HE3	1.98	0.44
1:A2:1528:C:OP1	26:Ap:142:GLN:NE2	2.50	0.44
1:A2:1754:C:O2	1:A2:1781:G:N2	2.50	0.44
12:Ab:85:SER:OG	31:Au:25:GLY:O	2.35	0.44
20:Aj:16:PHE:HE1	20:Aj:76:ILE:HG23	1.82	0.44
37:B5:793:C:N3	37:B5:794:G:N1	2.65	0.44
42:BC:60:HIS:NE2	42:BC:100:ARG:HD3	2.32	0.44
58:BT:9:ARG:O	58:BT:55:LYS:NZ	2.46	0.44
59:BU:27:HIS:O	59:BU:30:GLU:HG2	2.17	0.44
59:BU:105:ASN:HD21	59:BU:111:GLU:HB3	1.81	0.44
83:Bv:51:GLY:O	83:Bv:157:PHE:N	2.40	0.44
1:A2:220:U:H2'	1:A2:221:A:H8	1.82	0.44
10:AZ:140:VAL:HG23	10:AZ:142:LEU:HB2	1.99	0.44
14:Ad:124:CYS:HB3	14:Ad:141:THR:HB	1.99	0.44
25:Ao:64:LYS:NZ	25:Ao:92:SER:OG	2.31	0.44
37:B5:1532:G:OP1	79:Bp:17:ARG:NH2	2.50	0.44
37:B5:1701:C:H2'	37:B5:1702:C:C6	2.52	0.44
37:B5:1938:A:OP1	81:Bs:9:TRP:NE1	2.48	0.44
37:B5:1943:U:H2'	37:B5:1944:G:C8	2.52	0.44
37:B5:4073:C:OP1	58:BT:70:HIS:NE2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B8:36:G:C5	72:Bh:89:ARG:HD3	2.52	0.44
41:BB:46:PHE:HE2	41:BB:81:THR:HB	1.81	0.44
41:BB:90:VAL:HG22	41:BB:104:THR:HG23	1.99	0.44
42:BC:76:ILE:HD12	42:BC:77:PRO:HD2	1.98	0.44
42:BC:94:ASN:OD1	42:BC:95:MET:HE3	2.17	0.44
74:Bj:21:ARG:NH2	74:Bj:37:CYS:O	2.50	0.44
80:Br:90:LEU:HD22	80:Br:111:ILE:HG23	1.99	0.44
82:Bt:105:THR:HB	82:Bt:108:GLU:HG3	1.98	0.44
83:Bv:58:THR:HG23	83:Bv:153:SER:HB3	1.99	0.44
37:B5:218:A:O2'	37:B5:219:G:H5'	2.18	0.44
37:B5:521:C:H2'	37:B5:522:U:C6	2.51	0.44
37:B5:4698:U:H2'	37:B5:4699:G:C8	2.52	0.44
40:BA:30:ARG:HG2	40:BA:74:GLU:HG3	1.98	0.44
52:BN:94:PHE:CE2	52:BN:96:ARG:HB2	2.52	0.44
1:A2:120:U:H2'	1:A2:121:OMU:H6	1.99	0.44
1:A2:1607:G:N2	1:A2:1633:G:H1'	2.32	0.44
37:B5:1779:G:OP2	44:BF:201:LYS:NZ	2.50	0.44
37:B5:4361:C:H5''	41:BB:357:ARG:HE	1.82	0.44
55:BQ:88:ASP:HB2	55:BQ:109:ALA:HB2	2.00	0.44
58:BT:94:GLU:OE1	58:BT:94:GLU:N	2.46	0.44
81:Bs:14:PHE:HE1	81:Bs:64:ALA:HA	1.82	0.44
85:Nt:86:ARG:N	85:Nt:113:LYS:O	2.41	0.44
1:A2:1833:6MZ:H8	1:A2:1833:6MZ:O5'	2.17	0.44
12:Ab:196:ILE:HB	12:Ab:223:TYR:HB2	2.00	0.44
13:Ac:42:THR:HG23	13:Ac:47:GLU:OE1	2.18	0.44
35:Ay:47:LEU:HB2	35:Ay:79:ILE:HG22	2.00	0.44
37:B5:435:A:O2'	69:Be:26:ASP:OD2	2.33	0.44
37:B5:2658:A2M:HM'2	37:B5:2659:G:H5'	2.00	0.44
37:B5:4488:A:H2'	37:B5:4689:U:H3	1.82	0.44
47:BI:187:GLU:HG3	47:BI:189:ARG:HG3	1.99	0.44
48:BJ:101:ASP:OD1	48:BJ:101:ASP:N	2.50	0.44
74:Bj:2:THR:HB	74:Bj:6:SER:HB3	2.00	0.44
84:MA:333:PRO:HB3	84:MA:437:ASP:HB3	1.98	0.44
85:Nt:95:THR:OG1	86:Nu:63:ASN:O	2.29	0.44
1:A2:192:C:H4'	1:A2:192:C:OP1	2.18	0.44
1:A2:1290:U:OP2	4:AC:95:ARG:NE	2.38	0.44
18:Ah:76:THR:OG1	18:Ah:77:ARG:N	2.50	0.44
20:Aj:11:ILE:HD13	20:Aj:45:VAL:HA	2.00	0.44
37:B5:458:C:OP2	43:BE:117:ARG:NH1	2.51	0.44
37:B5:1072:C:H4'	37:B5:1073:C:C4	2.53	0.44
37:B5:2023:U:C2	55:BQ:14:ARG:NH2	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:4268:G:H5'	37:B5:4270:G:N7	2.33	0.44
60:BV:87:SER:HB3	61:BW:19:ARG:HH21	1.82	0.44
81:Bs:39:GLN:NE2	81:Bs:185:PHE:O	2.51	0.44
84:MA:240:LYS:HB2	84:MA:242:MET:HE3	1.99	0.44
3:AB:21:THR:HB	3:AB:68:LEU:HD21	1.99	0.44
13:Ac:123:LEU:HD22	13:Ac:152:PHE:HB3	1.99	0.44
14:Ad:68:ARG:HH12	14:Ad:78:THR:CG2	2.31	0.44
37:B5:1697:G:H2'	37:B5:1698:G:C8	2.53	0.44
37:B5:1784:U:H2'	37:B5:1785:G:C8	2.52	0.44
37:B5:2183:C:O2'	42:BC:45:ARG:NH2	2.50	0.44
37:B5:3341:G:H2'	37:B5:3342:A:H8	1.83	0.44
37:B5:4751:G:O2'	37:B5:4753:A:OP1	2.29	0.44
41:BB:19:ARG:HB2	41:BB:234:ARG:HH21	1.82	0.44
48:BJ:46:GLN:NE2	48:BJ:73:THR:O	2.43	0.44
1:A2:381:G:N1	1:A2:384:G:OP2	2.35	0.44
10:AZ:176:TRP:HE1	10:AZ:197:VAL:HG23	1.83	0.44
22:Al:33:ARG:HE	22:Al:91:LEU:HG	1.82	0.44
37:B5:1211:G:O6	66:Bb:111:ARG:NH2	2.47	0.44
37:B5:2200:G:N7	92:B5:5668:HOH:O	2.36	0.44
37:B5:4599:G:H2'	37:B5:4600:G:C8	2.53	0.44
42:BC:285:LEU:N	55:BQ:124:ASP:OD2	2.50	0.44
61:BW:91:MET:SD	61:BW:94:ARG:NH2	2.89	0.44
83:Bv:94:ASN:OD1	83:Bv:97:LYS:NZ	2.36	0.44
84:MA:297:TRP:CD2	84:MA:462:LEU:HD13	2.53	0.44
1:A2:521:A:O2'	1:A2:826:A:N3	2.40	0.44
7:AF:77:PHE:HB3	7:AF:89:LEU:HD11	1.99	0.44
19:Ai:170:PRO:HB3	19:Ai:174:LYS:HE3	1.99	0.44
31:Au:81:GLN:H	31:Au:81:GLN:HG2	1.62	0.44
37:B5:2183:C:H4'	42:BC:42:THR:HG23	2.00	0.44
37:B5:2712:U:O2'	37:B5:2724:A:N7	2.46	0.44
46:BH:113:GLU:HG2	46:BH:125:ARG:HG2	2.00	0.44
51:BM:39:ASP:C	51:BM:41:PRO:HD3	2.42	0.44
64:BZ:11:VAL:HG12	64:BZ:82:PRO:HA	2.00	0.44
1:A2:1481:A:O2'	8:AG:56:ASP:OXT	2.28	0.43
12:Ab:253:PRO:HA	12:Ab:256:TRP:CE2	2.53	0.43
16:Af:155:GLN:HE22	61:BW:108:ALA:HA	1.83	0.43
29:As:96:SER:HB3	29:As:99:VAL:HG22	2.00	0.43
37:B5:1250:C:H2'	37:B5:1251:A:C8	2.53	0.43
37:B5:1729:U:C5	89:B5:5185:SPD:H72	2.52	0.43
37:B5:4805:U:H2'	37:B5:4806:U:C6	2.53	0.43
48:BJ:15:LEU:HD12	48:BJ:165:TRP:HB2	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BS:97:TYR:OH	57:BS:112:ASP:OD2	2.34	0.43
61:BW:46:PRO:HB2	61:BW:54:LEU:HD12	2.00	0.43
84:MA:260:ALA:O	84:MA:261:PRO:C	2.61	0.43
37:B5:1697:G:H2'	37:B5:1698:G:H8	1.83	0.43
37:B5:2546:G:OP1	59:BU:113:ARG:NH1	2.50	0.43
37:B5:3386:G:O2'	37:B5:3425:U:OP1	2.37	0.43
57:BS:30:MET:HE2	57:BS:30:MET:HB3	1.94	0.43
69:Be:35:TRP:CZ2	69:Be:56:PRO:HD2	2.53	0.43
84:MA:210:TRP:NE1	84:MA:274:GLU:HG3	2.33	0.43
84:MA:409:ASN:OD1	86:Nu:77:PRO:HA	2.18	0.43
1:A2:700:C:H2'	1:A2:701:G:C8	2.53	0.43
1:A2:1366:G:N2	1:A2:1463:U:O4	2.37	0.43
37:B5:754:G:H5'	46:BH:50:LYS:HE2	2.00	0.43
37:B5:1001:C:H2'	37:B5:1002:A:H8	1.83	0.43
37:B5:2439:G:H2'	37:B5:2440:G:H8	1.81	0.43
37:B5:4292:A:N7	40:BA:215:ASN:ND2	2.66	0.43
84:MA:482:LYS:HB3	84:MA:484:PRO:HD3	2.00	0.43
20:Aj:37:ASP:OD1	20:Aj:37:ASP:N	2.51	0.43
22:Al:52:LEU:HD23	22:Al:78:LYS:HZ3	1.84	0.43
37:B5:3632:G:OP1	37:B5:3633:A:O2'	2.33	0.43
82:Bt:106:PHE:N	82:Bt:144:ASP:OD1	2.51	0.43
84:MA:186:ASN:C	84:MA:408:MET:HE3	2.42	0.43
86:Nu:28:ARG:HE	86:Nu:28:ARG:HB2	1.54	0.43
1:A2:219:U:H2'	1:A2:220:U:C6	2.54	0.43
14:Ad:95:THR:HG22	34:Ax:16:ARG:HD2	2.00	0.43
17:Ag:88:SER:OG	17:Ag:89:GLY:N	2.45	0.43
22:Al:11:VAL:HG11	22:Al:16:THR:HB	2.01	0.43
34:Ax:84:LYS:H	34:Ax:84:LYS:HG3	1.70	0.43
37:B5:1208:C:OP1	66:Bb:95:ARG:HD3	2.19	0.43
37:B5:2689:G:O2'	60:BV:19:GLY:O	2.33	0.43
37:B5:3823:G:O2'	37:B5:3825:G:OP1	2.36	0.43
37:B5:4049:C:O2'	37:B5:4050:A:H2'	2.18	0.43
37:B5:4633:A:H5'	37:B5:4635:G:H5'	2.00	0.43
41:BB:56:ILE:HD13	41:BB:365:LEU:HD22	2.01	0.43
43:BE:85:LYS:HB3	43:BE:85:LYS:HE2	1.58	0.43
43:BE:169:LYS:HE3	43:BE:211:ILE:HD12	1.99	0.43
44:BF:121:PHE:O	44:BF:204:ASN:ND2	2.51	0.43
67:Bc:99:PRO:HG3	67:Bc:105:ILE:HG13	2.01	0.43
81:Bs:72:ASN:N	81:Bs:72:ASN:OD1	2.51	0.43
1:A2:845:U:OP1	14:Ad:240:ARG:NH2	2.47	0.43
1:A2:873:A:H5'	56:BR:170:ARG:HH22	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:173:C:H2'	37:B5:174:C:C6	2.54	0.43
37:B5:1067:C:H2'	37:B5:1068:U:H6	1.82	0.43
37:B5:3545:A:N3	37:B5:4284:G:O2'	2.44	0.43
37:B5:4224:G:N2	37:B5:4354:G:O2'	2.52	0.43
58:BT:18:PRO:HG2	58:BT:21:LYS:HB2	2.01	0.43
81:Bs:30:VAL:HG12	81:Bs:189:ILE:HA	2.00	0.43
1:A2:126:G:OP2	16:Af:198:ARG:NH2	2.42	0.43
37:B5:226:G:OP2	63:BY:1:MET:N	2.40	0.43
37:B5:522:U:H2'	37:B5:523:C:C6	2.54	0.43
37:B5:664:G:H2'	37:B5:665:G:C8	2.54	0.43
37:B5:4138:OMG:N3	37:B5:4193:5MC:HM52	2.34	0.43
44:BF:93:ARG:NH2	44:BF:96:GLY:O	2.43	0.43
63:BY:55:VAL:HG12	63:BY:106:ILE:HG12	2.01	0.43
84:MA:173:TYR:O	84:MA:177:ASN:N	2.51	0.43
1:A2:421:G:O2'	1:A2:661:C:N3	2.51	0.43
1:A2:1411:C:H2'	1:A2:1412:G:C8	2.54	0.43
9:AT:62:C:H2'	9:AT:63:G:C8	2.54	0.43
14:Ad:31:PRO:HG3	14:Ad:43:PRO:HG3	2.01	0.43
16:Af:213:LEU:HG	16:Af:217:MET:HE2	2.00	0.43
37:B5:639:G:H2'	37:B5:640:G:C8	2.54	0.43
37:B5:1776:A:OP1	58:BT:108:ARG:NH1	2.51	0.43
37:B5:1935:C:H42	37:B5:1939:G:H22	1.67	0.43
37:B5:3819:G:H1	37:B5:3904:C:H42	1.67	0.43
37:B5:4012:G:N3	37:B5:4012:G:H2'	2.34	0.43
42:BC:25:PRO:HG2	42:BC:28:PHE:HD1	1.84	0.43
48:BJ:93:GLU:HG2	48:BJ:173:ILE:HB	2.00	0.43
56:BR:106:LEU:HB3	56:BR:120:TYR:CE1	2.54	0.43
84:MA:224:GLY:CA	84:MA:258:ARG:NH1	2.55	0.43
84:MA:250:VAL:CG2	84:MA:258:ARG:HH21	2.32	0.43
2:AA:28:PRO:HG3	23:Am:17:PRO:HG3	1.99	0.43
9:AT:66:C:H2'	9:AT:67:G:H8	1.83	0.43
26:Ap:58:LEU:HB2	26:Ap:63:PHE:HE1	1.83	0.43
33:Aw:60:LYS:HG3	33:Aw:116:PRO:HG3	2.00	0.43
35:Ay:47:LEU:H	35:Ay:79:ILE:HA	1.84	0.43
37:B5:629:G:H2'	37:B5:630:G:C8	2.54	0.43
37:B5:1270:A2M:OP2	37:B5:4191:U:O2'	2.32	0.43
37:B5:2221:G:N2	37:B5:2224:A:OP2	2.50	0.43
37:B5:3461:U:H2'	37:B5:3462:PSU:H6	1.83	0.43
37:B5:4642:G:H2'	37:B5:4643:G:C8	2.54	0.43
61:BW:66:GLU:HG3	61:BW:68:GLN:HE22	1.84	0.43
86:Nu:79:VAL:HG22	86:Nu:90:ILE:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1092:C:O2'	32:Av:2:VAL:N	2.47	0.43
1:A2:1407:G:O6	1:A2:1440:A:N6	2.52	0.43
29:As:35:ASP:OD1	29:As:35:ASP:N	2.47	0.43
37:B5:268:G:H2'	37:B5:269:G:H8	1.83	0.43
37:B5:709:G:OP1	42:BC:321:ASN:ND2	2.52	0.43
37:B5:1381:G:N1	37:B5:1413:C:OP2	2.45	0.43
37:B5:4637:G:H3'	37:B5:4638:G:H8	1.83	0.43
75:Bk:33:LYS:HG2	75:Bk:46:VAL:HG22	2.01	0.43
76:Bl:30:LYS:HB2	76:Bl:33:ASN:HB2	2.01	0.43
1:A2:195:C:H2'	1:A2:196:C:C6	2.54	0.42
7:AF:87:LEU:HD21	7:AF:108:VAL:HG11	2.01	0.42
14:Ad:85:GLY:N	14:Ad:88:ASP:OD2	2.45	0.42
17:Ag:37:LYS:O	17:Ag:41:ARG:HG3	2.19	0.42
18:Ah:87:ASN:OD1	18:Ah:88:ASN:N	2.52	0.42
37:B5:1714:A:H2'	37:B5:1715:A:C8	2.54	0.42
37:B5:3432:C:H2'	37:B5:3478:A:H61	1.83	0.42
37:B5:3973:OMU:HM22	37:B5:3974:OMG:H5'	2.01	0.42
57:BS:147:ASP:HB3	57:BS:150:ILE:HB	2.01	0.42
58:BT:68:THR:OG1	58:BT:71:ALA:O	2.33	0.42
66:Bb:51:LYS:H	66:Bb:51:LYS:HG3	1.48	0.42
84:MA:249:CYS:O	84:MA:258:ARG:NH2	2.52	0.42
1:A2:61:A:HO2'	1:A2:316:C:HO2'	1.64	0.42
1:A2:953:G:H21	24:An:52:THR:HG21	1.83	0.42
1:A2:1315:U:H2'	1:A2:1316:U:C6	2.54	0.42
14:Ad:151:ASP:HB3	14:Ad:154:ILE:HG13	2.00	0.42
15:Ae:14:THR:HB	15:Ae:15:PRO:HD3	2.01	0.42
33:Aw:107:ARG:HD3	33:Aw:112:VAL:HG22	2.01	0.42
37:B5:1303:G:H4'	52:BN:203:TYR:HB2	2.00	0.42
37:B5:2318:G:H4'	37:B5:2319:G:H8	1.85	0.42
37:B5:2742:C:P	56:BR:108:ARG:HH22	2.41	0.42
42:BC:180:ILE:HD11	42:BC:227:ILE:HD11	2.01	0.42
43:BE:149:PRO:HA	43:BE:167:PHE:HD2	1.84	0.42
43:BE:167:PHE:HE1	43:BE:176:LEU:HD22	1.85	0.42
56:BR:106:LEU:HB3	56:BR:120:TYR:HE1	1.83	0.42
84:MA:291:VAL:HB	84:MA:483:CYS:HB3	2.01	0.42
1:A2:324:C:N4	1:A2:328:G:OP2	2.50	0.42
1:A2:1720:A:N6	1:A2:1815:G:O2'	2.52	0.42
1:A2:1805:OMU:HM22	1:A2:1806:G:H5'	2.01	0.42
10:AZ:137:ALA:HB1	10:AZ:142:LEU:HB3	2.01	0.42
23:Am:83:ASP:OD1	23:Am:83:ASP:N	2.51	0.42
37:B5:1125:C:H5	43:BE:62:SER:HB2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:1784:U:H2'	37:B5:1785:G:H8	1.85	0.42
37:B5:4046:U:H4'	58:BT:89:ILE:HG22	2.01	0.42
42:BC:156:ASP:OD1	42:BC:255:SER:N	2.42	0.42
54:BP:40:HIS:NE2	54:BP:110:ASP:O	2.49	0.42
82:Bt:52:ASP:OD1	82:Bt:52:ASP:N	2.43	0.42
84:MA:265:ARG:O	84:MA:266:GLU:C	2.62	0.42
1:A2:145:G:H2'	1:A2:146:G:C8	2.54	0.42
1:A2:1311:U:H5''	4:AC:130:VAL:HG13	2.01	0.42
1:A2:1338:4AC:H2'	1:A2:1339:G:H8	1.85	0.42
9:AT:62:C:H2'	9:AT:63:G:H8	1.85	0.42
16:Af:5:ILE:HG12	16:Af:111:LEU:HB2	2.02	0.42
17:Ag:20:GLU:HG2	17:Ag:48:ALA:HB3	2.01	0.42
18:Ah:10:LYS:O	18:Ah:18:ARG:NH1	2.51	0.42
37:B5:1260:OMG:OP1	69:Be:43:ASN:HB2	2.20	0.42
37:B5:3347:G:O2'	61:BW:44:ARG:NH2	2.51	0.42
80:Br:46:ARG:HH22	80:Br:67:ARG:HG3	1.84	0.42
84:MA:182:GLU:HB3	84:MA:189:ARG:NH1	2.35	0.42
86:Nu:101:GLU:O	86:Nu:104:PRO:HB2	2.19	0.42
1:A2:629:A:O2'	13:Ac:145:GLN:NE2	2.52	0.42
21:Ak:13:GLN:HE22	21:Ak:35:ARG:HD2	1.85	0.42
37:B5:1941:A:N1	82:Bt:138:SER:HB2	2.34	0.42
41:BB:92:TYR:HB2	41:BB:159:VAL:HB	2.01	0.42
54:BP:18:ARG:NH1	54:BP:147:GLU:OE1	2.51	0.42
84:MA:259:VAL:HG12	84:MA:261:PRO:HD2	2.02	0.42
11:Aa:48:LEU:O	24:An:51:GLU:HG3	2.19	0.42
16:Af:118:GLU:H	16:Af:118:GLU:HG3	1.68	0.42
24:An:29:GLY:HA2	24:An:46:ASP:O	2.19	0.42
37:B5:260:C:H2'	37:B5:261:G:C8	2.54	0.42
89:B5:5195:SPD:H102	57:BS:166:ARG:HB3	1.84	0.42
54:BP:31:GLU:HG3	54:BP:60:PHE:CD2	2.55	0.42
82:Bt:112:ILE:O	82:Bt:116:MET:HG2	2.19	0.42
1:A2:502:C:OP1	89:A2:2041:SPD:N6	2.53	0.42
1:A2:519:G:H2'	1:A2:520:A:H8	1.84	0.42
1:A2:660:G:H21	33:Aw:17:ARG:NH2	2.17	0.42
7:AF:191:HIS:CE1	7:AF:195:LEU:HD11	2.54	0.42
10:AZ:68:ILE:HD12	10:AZ:120:ARG:HE	1.84	0.42
11:Aa:75:GLN:HB3	11:Aa:78:GLU:HG3	2.02	0.42
11:Aa:136:ARG:HB2	11:Aa:218:LEU:HD11	2.00	0.42
14:Ad:86:PHE:CD2	14:Ad:87:MET:HG2	2.54	0.42
23:Am:140:LYS:HD2	23:Am:140:LYS:HA	1.85	0.42
37:B5:1059:G:H2'	37:B5:1060:G:H8	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:1215:G:H5''	66:Bb:110:ALA:HB1	2.01	0.42
37:B5:2387:G:O2'	37:B5:2389:G:H3'	2.19	0.42
37:B5:3413:G:OP2	40:BA:128:ARG:NH2	2.52	0.42
39:B8:84:A:C5	39:B8:88:A:H4'	2.54	0.42
48:BJ:112:HIS:CD2	48:BJ:126:TYR:H	2.36	0.42
53:BO:36:VAL:HG21	53:BO:117:ARG:CD	2.48	0.42
82:Bt:10:ILE:HG12	82:Bt:65:GLN:HG2	2.02	0.42
7:AF:14:HIS:ND1	7:AF:35:SER:HB2	2.35	0.42
9:AT:51:C:H2'	9:AT:52:G:H8	1.85	0.42
9:AT:63:G:H2'	9:AT:64:G:C8	2.55	0.42
11:Aa:150:ILE:HG23	27:Aq:131:PRO:HA	2.01	0.42
11:Aa:175:GLU:O	11:Aa:187:LYS:NZ	2.37	0.42
37:B5:519:C:H2'	37:B5:520:G:H8	1.85	0.42
37:B5:1898:U:H1'	37:B5:1900:G:C2	2.54	0.42
37:B5:2146:C:H5''	69:Be:104:SER:HB3	2.02	0.42
37:B5:3651:C:H2'	37:B5:3652:PSU:H6	1.85	0.42
37:B5:4641:C:C2'	37:B5:4642:G:H5'	2.49	0.42
42:BC:25:PRO:HG2	42:BC:28:PHE:CD1	2.55	0.42
43:BE:103:LYS:HE2	43:BE:103:LYS:HB2	1.94	0.42
46:BH:41:ILE:HG22	46:BH:43:VAL:HG13	2.02	0.42
81:Bs:66:ARG:HA	81:Bs:69:LEU:HG	2.01	0.42
83:Bv:196:LYS:HD2	83:Bv:196:LYS:HA	1.87	0.42
1:A2:17:C:O2'	1:A2:1195:A:N1	2.52	0.42
1:A2:65:C:C6	16:Af:174:PRO:HB3	2.54	0.42
1:A2:1310:C:H5'	4:AC:105:TYR:HE1	1.84	0.42
14:Ad:11:ARG:HA	14:Ad:28:ALA:HB2	2.01	0.42
22:Al:52:LEU:HB3	22:Al:76:LEU:HD11	2.01	0.42
22:Al:75:ASN:OD1	22:Al:75:ASN:O	2.37	0.42
37:B5:1309:C:N4	89:B5:5188:SPD:H101	2.17	0.42
37:B5:1717:C:H2'	37:B5:1718:PSU:H6	1.84	0.42
37:B5:1760:G:H4'	37:B5:1761:U:H5''	2.01	0.42
53:BO:108:ILE:CD1	53:BO:117:ARG:CZ	2.98	0.42
1:A2:56:G:OP2	34:Ax:115:LYS:NZ	2.32	0.42
1:A2:172:OMU:H6	1:A2:315:U:H1'	2.02	0.42
1:A2:324:C:H2'	1:A2:325:U:O4'	2.20	0.42
1:A2:1040:C:H2'	1:A2:1041:G:H8	1.84	0.42
3:AB:51:ARG:HB3	15:Ae:61:PHE:CE2	2.55	0.42
10:AZ:9:GLN:O	10:AZ:11:LYS:NZ	2.44	0.42
10:AZ:50:ASN:HB3	10:AZ:53:ARG:HG3	2.01	0.42
22:Al:33:ARG:HG2	22:Al:109:VAL:HG12	2.02	0.42
24:An:32:HIS:HB2	24:An:43:HIS:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:180:C:H42	37:B5:256:G:H1	1.67	0.42
37:B5:1928:G:H2'	37:B5:1929:A:C8	2.55	0.42
37:B5:3561:G:H2'	37:B5:3562:A2M:H8	2.02	0.42
37:B5:4726:C:OP1	41:BB:176:LYS:NZ	2.45	0.42
54:BP:124:LYS:HE2	54:BP:140:MET:HB3	2.02	0.42
65:Ba:7:LYS:HE3	65:Ba:7:LYS:HB3	1.64	0.42
69:Be:124:ASN:OD1	69:Be:124:ASN:N	2.52	0.42
82:Bt:14:TYR:O	82:Bt:31:LYS:NZ	2.53	0.42
84:MA:236:TYR:N	84:MA:361:HIS:O	2.48	0.42
10:AZ:80:ARG:HH22	10:AZ:166:LYS:HA	1.85	0.41
11:Aa:62:LEU:O	11:Aa:88:THR:OG1	2.28	0.41
37:B5:685:C:H2'	37:B5:686:A:C8	2.55	0.41
37:B5:1298:A:H62	37:B5:1457:G:HO2'	1.65	0.41
37:B5:1563:G:N7	89:B5:5178:SPD:H52	2.34	0.41
45:BG:68:ALA:O	45:BG:72:LYS:NZ	2.48	0.41
51:BM:88:ALA:O	51:BM:93:LYS:NZ	2.53	0.41
1:A2:65:C:C2	16:Af:133:LEU:HD22	2.56	0.41
1:A2:587:G:H2'	19:Ai:172:ARG:HH12	1.86	0.41
7:AF:170:TRP:HA	7:AF:194:TYR:HB2	2.02	0.41
10:AZ:37:TYR:CD1	10:AZ:162:PRO:HG3	2.55	0.41
11:Aa:147:ASN:OD1	11:Aa:148:ASN:N	2.53	0.41
29:As:5:THR:OG1	29:As:6:VAL:N	2.53	0.41
37:B5:3941:G:OP1	37:B5:3967:C:O2'	2.36	0.41
52:BN:53:TYR:HB2	52:BN:133:ILE:HD13	2.02	0.41
58:BT:80:VAL:HG23	58:BT:80:VAL:O	2.20	0.41
82:Bt:64:ILE:HG23	82:Bt:69:ALA:HB2	2.02	0.41
86:Nu:99:LEU:HA	86:Nu:102:MET:HB2	2.02	0.41
1:A2:77:A:N3	16:Af:176:ILE:HG22	2.35	0.41
1:A2:420:G:N2	1:A2:662:U:O2	2.53	0.41
1:A2:1770:C:H2'	1:A2:1771:G:H8	1.84	0.41
7:AF:220:ASP:HB3	7:AF:223:GLU:HG2	2.01	0.41
10:AZ:210:ILE:HG21	27:Aq:81:ARG:HD3	2.03	0.41
26:Ap:12:VAL:HG21	26:Ap:91:ALA:HA	2.02	0.41
37:B5:707:C:O2	43:BE:133:LYS:NZ	2.53	0.41
37:B5:3867:C:H2'	37:B5:3868:C:C6	2.55	0.41
73:Bi:99:LYS:HG2	73:Bi:103:LYS:HE2	2.02	0.41
81:Bs:106:LYS:HB3	81:Bs:184:SER:HB3	2.01	0.41
1:A2:325:U:N3	1:A2:328:G:OP2	2.51	0.41
1:A2:445:G:H4'	89:A2:2038:SPD:H91	2.02	0.41
1:A2:838:A:C5	34:Ax:47:MET:HE3	2.56	0.41
1:A2:1649:G:O2'	1:A2:1675:G:O6	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AT:51:C:H2'	9:AT:52:G:C8	2.55	0.41
19:Ai:152:ASP:OD1	19:Ai:152:ASP:N	2.47	0.41
26:Ap:129:SER:O	26:Ap:131:LYS:NZ	2.48	0.41
37:B5:1868:A:C8	37:B5:1871:A:H1'	2.56	0.41
37:B5:2616:G:H5'	75:Bk:17:ARG:HH21	1.84	0.41
37:B5:3385:A:N6	37:B5:3423:G:O2'	2.50	0.41
40:BA:206:PRO:HG3	40:BA:213:GLY:HA3	2.02	0.41
47:BI:99:ILE:HG22	47:BI:123:GLN:HB2	2.02	0.41
48:BJ:90:ARG:NH2	48:BJ:108:GLY:O	2.53	0.41
53:BO:125:LYS:HG2	53:BO:129:LEU:HD12	2.02	0.41
60:BV:21:PRO:HA	60:BV:54:ALA:HA	2.02	0.41
82:Bt:32:ILE:HB	82:Bt:35:LEU:HD11	2.01	0.41
84:MA:236:TYR:CG	84:MA:361:HIS:HD2	2.39	0.41
84:MA:250:VAL:CB	84:MA:258:ARG:HD3	2.43	0.41
1:A2:1537:G:H2'	1:A2:1538:A:C8	2.56	0.41
1:A2:1737:G:H2'	1:A2:1738:G:C8	2.55	0.41
5:AD:109:ARG:HD2	19:Ai:124:HIS:CD2	2.55	0.41
7:AF:32:LEU:HD22	7:AF:71:ILE:HG12	2.03	0.41
11:Aa:86:LEU:HB3	11:Aa:98:THR:HB	2.02	0.41
13:Ac:46:THR:OG1	13:Ac:84:VAL:HA	2.20	0.41
13:Ac:132:LYS:HE3	13:Ac:192:TRP:H	1.85	0.41
26:Ap:28:GLY:HA3	26:Ap:67:ASP:CG	2.45	0.41
37:B5:158:A:N1	37:B5:276:C:O2'	2.50	0.41
37:B5:1113:A:O2'	37:B5:1120:G:OP1	2.32	0.41
37:B5:1866:U:OP1	37:B5:1888:U:O2'	2.31	0.41
37:B5:2330:G:OP2	37:B5:2332:C:N4	2.53	0.41
37:B5:2687:A:O2'	37:B5:4377:G:H4'	2.20	0.41
37:B5:3681:A:N3	37:B5:3792:C:N4	2.68	0.41
37:B5:3911:C:OP1	45:BG:245:LYS:NZ	2.51	0.41
37:B5:4314:A:O3'	41:BB:21:ARG:NH2	2.53	0.41
41:BB:55:HIS:NE2	41:BB:369:ASP:OD2	2.53	0.41
57:BS:45:TRP:HA	57:BS:48:VAL:HG22	2.02	0.41
63:BY:54:GLU:HB2	63:BY:108:ARG:HB3	2.02	0.41
72:Bh:13:LYS:HE2	72:Bh:13:LYS:HB2	1.93	0.41
81:Bs:48:ARG:HD3	82:Bt:123:ARG:HA	2.02	0.41
82:Bt:107:ASP:O	82:Bt:111:ASN:ND2	2.53	0.41
1:A2:437:OMG:OP2	1:A2:472:G:O2'	2.37	0.41
1:A2:1398:U:O4	26:Ap:12:VAL:HA	2.20	0.41
7:AF:59:LEU:HD23	7:AF:90:TRP:CD2	2.55	0.41
16:Af:2:LYS:HB3	16:Af:15:LEU:HD11	2.03	0.41
18:Ah:113:TYR:OH	18:Ah:156:ALA:O	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Aj:32:HIS:CD2	20:Aj:34:GLU:HB2	2.55	0.41
28:Ar:28:PHE:O	28:Ar:31:THR:OG1	2.29	0.41
37:B5:1127:G:H21	66:Bb:120:ARG:NH1	2.17	0.41
37:B5:1298:A:N1	37:B5:1329:G:O2'	2.52	0.41
81:Bs:20:LEU:HD22	81:Bs:52:VAL:HG11	2.03	0.41
1:A2:665:A:O2'	1:A2:671:A:N1	2.48	0.41
1:A2:1084:A:N7	1:A2:1842:C:O2'	2.50	0.41
1:A2:1338:4AC:H2'	1:A2:1339:G:C8	2.55	0.41
13:Ac:45:ARG:HB3	13:Ac:83:SER:O	2.21	0.41
13:Ac:56:GLN:H	13:Ac:56:GLN:HG3	1.72	0.41
16:Af:44:GLU:CG	16:Af:119:LYS:HD3	2.49	0.41
25:Ao:75:VAL:HG21	25:Ao:104:GLN:HG2	2.03	0.41
37:B5:126:C:OP1	72:Bh:78:TYR:OH	2.38	0.41
37:B5:2335:C:H2'	37:B5:2336:G:C8	2.56	0.41
37:B5:3642:C:O2'	37:B5:3942:OMG:N2	2.39	0.41
37:B5:4057:A:H2'	37:B5:4058:PSU:H6	1.84	0.41
37:B5:4476:C:O2'	37:B5:4479:C:N3	2.53	0.41
83:Bv:110:PHE:HB3	83:Bv:135:PRO:HG3	2.02	0.41
1:A2:1098:G:H4'	10:AZ:32:PHE:CD1	2.55	0.41
1:A2:1417:C:OP1	29:As:129:ARG:NH1	2.54	0.41
1:A2:1483:C:N3	92:A2:2215:HOH:O	2.35	0.41
7:AF:40:ILE:HB	7:AF:59:LEU:HB2	2.01	0.41
26:Ap:112:LEU:HD22	26:Ap:119:LEU:HD13	2.01	0.41
35:Ay:92:LEU:HD22	35:Ay:109:TYR:HE1	1.86	0.41
37:B5:1423:C:OP1	65:Ba:132:ARG:NH2	2.53	0.41
37:B5:2204:G:O2'	37:B5:3591:G:O6	2.32	0.41
37:B5:3572:U:H2'	37:B5:3573:OMC:O4'	2.21	0.41
1:A2:4:C:H4'	12:Ab:207:ALA:HB2	2.03	0.41
1:A2:194:C:H2'	1:A2:195:C:C6	2.56	0.41
1:A2:220:U:H2'	1:A2:221:A:C8	2.55	0.41
1:A2:563:U:H2'	1:A2:564:G:C8	2.56	0.41
1:A2:868:OMG:HM22	1:A2:869:G:H5'	2.02	0.41
1:A2:1598:C:H4'	1:A2:1604:G:C6	2.56	0.41
5:AD:83:VAL:HG21	33:Aw:91:LEU:HD23	2.01	0.41
5:AD:83:VAL:HG11	33:Aw:91:LEU:HB3	2.02	0.41
14:Ad:19:MET:HE2	14:Ad:51:ARG:NH2	2.35	0.41
14:Ad:171:ASP:OD1	14:Ad:172:PHE:N	2.53	0.41
37:B5:38:A:H5''	65:Ba:35:ALA:HB2	2.03	0.41
37:B5:121:A:OP1	45:BG:110:LYS:NZ	2.47	0.41
37:B5:257:C:H2'	37:B5:258:G:H8	1.86	0.41
37:B5:632:G:H5''	37:B5:633:U:H5'	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:702:G:OP1	70:Bf:89:ARG:NH2	2.54	0.41
37:B5:1208:C:H2'	37:B5:1209:G:C8	2.56	0.41
37:B5:3599:A2M:HM'3	37:B5:3599:A2M:H1'	1.86	0.41
37:B5:3882:G:H2'	37:B5:3883:G:H8	1.86	0.41
37:B5:3930:G:H5'	40:BA:233:ARG:HB2	2.03	0.41
37:B5:4037:G:H5'	37:B5:4039:PSU:C6	2.56	0.41
37:B5:4600:G:H2'	37:B5:4601:G:H8	1.86	0.41
42:BC:239:LYS:O	42:BC:248:ARG:NH1	2.40	0.41
43:BE:85:LYS:O	43:BE:86:LYS:C	2.63	0.41
46:BH:177:ASP:OD1	46:BH:177:ASP:N	2.52	0.41
55:BQ:177:ALA:O	55:BQ:184:ARG:HB2	2.20	0.41
66:Bb:65:MET:HA	66:Bb:68:ARG:HH12	1.84	0.41
75:Bk:61:PRO:HA	75:Bk:62:PRO:HD3	1.97	0.41
78:Bo:63:THR:O	78:Bo:87:ARG:NH1	2.53	0.41
82:Bt:116:MET:HG3	82:Bt:132:ILE:HD11	2.02	0.41
83:Bv:59:PRO:HB2	83:Bv:171:HIS:CE1	2.56	0.41
1:A2:522:A:OP1	19:Ai:45:ARG:NH1	2.41	0.41
1:A2:970:U:OP1	1:A2:971:G:O2'	2.27	0.41
1:A2:1411:C:H2'	1:A2:1412:G:H8	1.85	0.41
12:Ab:82:TYR:OH	12:Ab:162:ILE:O	2.37	0.41
37:B5:58:G:H4'	37:B5:59:A:H4'	2.03	0.41
37:B5:2244:A2M:HM'2	37:B5:2245:G:O5'	2.21	0.41
37:B5:4643:G:N2	37:B5:4657:C:O2	2.53	0.41
43:BE:164:ARG:NH1	43:BE:276:SER:OG	2.54	0.41
56:BR:28:GLU:HG3	56:BR:49:LEU:HD22	2.03	0.41
61:BW:62:GLY:O	61:BW:66:GLU:HG2	2.21	0.41
83:Bv:94:ASN:HB2	83:Bv:123:ILE:HB	2.02	0.41
84:MA:298:HIS:ND1	84:MA:451:ASN:OD1	2.50	0.41
84:MA:348:VAL:HG21	84:MA:394:VAL:HB	2.03	0.41
1:A2:1040:C:H2'	1:A2:1041:G:C8	2.56	0.40
1:A2:1770:C:H2'	1:A2:1771:G:C8	2.55	0.40
16:Af:138:ALA:HA	16:Af:176:ILE:HD11	2.02	0.40
18:Ah:10:LYS:HE3	18:Ah:10:LYS:HB3	1.92	0.40
18:Ah:170:LYS:HE3	37:B5:4762:C:H41	1.87	0.40
22:Al:11:VAL:HG21	22:Al:16:THR:HG21	2.03	0.40
22:Al:75:ASN:HB3	22:Al:128:PHE:CD1	2.57	0.40
37:B5:385:A:H4'	37:B5:386:A:H5'	2.02	0.40
37:B5:1983:U:C2	41:BB:259:PRO:HG3	2.55	0.40
37:B5:3341:G:H2'	37:B5:3342:A:C8	2.55	0.40
37:B5:3942:OMG:HM22	37:B5:3943:G:H5'	2.03	0.40
37:B5:4403:U:H3	89:B5:5183:SPD:H82	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:4618:C:OP1	51:BM:120:ASN:ND2	2.49	0.40
37:B5:4679:C:OP1	43:BE:159:ARG:NH1	2.55	0.40
37:B5:4764:C:O2'	37:B5:4767:G:N3	2.50	0.40
45:BG:165:GLU:OE2	52:BN:26:ARG:NH1	2.55	0.40
53:BO:128:ARG:NH1	57:BS:162:GLN:OE1	2.54	0.40
62:BX:82:THR:HG21	72:Bh:37:THR:HG22	2.03	0.40
86:Nu:48:LEU:O	86:Nu:49:LYS:C	2.64	0.40
1:A2:240:G:H2'	1:A2:241:G:C8	2.55	0.40
1:A2:588:A:H5'	1:A2:593:C:H41	1.86	0.40
1:A2:1457:G:N2	1:A2:1472:C:C2	2.89	0.40
1:A2:1508:G:C5	4:AC:89:LYS:HB2	2.56	0.40
7:AF:8:ARG:HB3	7:AF:309:VAL:HG23	2.03	0.40
10:AZ:148:CYS:HB3	10:AZ:152:SER:HB2	2.02	0.40
13:Ac:46:THR:HG21	13:Ac:79:PHE:CE2	2.57	0.40
14:Ad:87:MET:HE2	14:Ad:123:LEU:HB2	2.03	0.40
18:Ah:106:SER:HB3	18:Ah:171:LEU:HG	2.03	0.40
22:Al:36:ARG:HA	22:Al:36:ARG:HE	1.86	0.40
37:B5:2250:G:N2	76:Bl:51:LEU:OXT	2.54	0.40
37:B5:3642:C:HO2'	37:B5:3942:OMG:HN22	1.63	0.40
37:B5:3866:C:H2'	37:B5:3867:C:C6	2.56	0.40
62:BX:100:VAL:HG21	62:BX:109:ILE:HD11	2.03	0.40
69:Be:37:LYS:HD2	69:Be:38:PRO:HD2	2.02	0.40
79:Bp:62:LYS:HE3	79:Bp:62:LYS:HB2	1.94	0.40
1:A2:1063:A:OP1	89:A2:2039:SPD:H52	2.22	0.40
1:A2:1565:C:P	29:As:121:ARG:HH22	2.44	0.40
1:A2:1758:G:H2'	1:A2:1759:G:C8	2.56	0.40
10:AZ:206:ASP:OD1	10:AZ:206:ASP:N	2.35	0.40
23:Am:100:LYS:O	23:Am:103:GLU:HG2	2.21	0.40
25:Ao:34:MET:HB3	25:Ao:42:ARG:HG3	2.03	0.40
37:B5:1984:G:O2'	37:B5:1985:G:H5''	2.21	0.40
37:B5:2507:G:H4'	37:B5:2520:G:H4'	2.03	0.40
39:B8:3:A:H3'	39:B8:4:C:C6	2.57	0.40
50:BL:60:ARG:HD3	50:BL:67:HIS:O	2.21	0.40
60:BV:91:LYS:HD3	60:BV:91:LYS:HA	1.80	0.40
64:BZ:50:PRO:HD3	64:BZ:68:ILE:HG12	2.04	0.40
64:BZ:77:TYR:HD1	64:BZ:77:TYR:HA	1.77	0.40
84:MA:235:ILE:HD13	84:MA:478:LEU:HD13	2.03	0.40
84:MA:361:HIS:ND1	84:MA:490:LYS:HB3	2.36	0.40
1:A2:120:U:H1'	14:Ad:33:THR:O	2.21	0.40
1:A2:231:A:H2'	1:A2:232:A:C8	2.56	0.40
10:AZ:187:GLY:HA2	31:Au:45:ARG:HE	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Aa:28:LYS:HB3	11:Aa:48:LEU:HD11	2.04	0.40
13:Ac:163:PRO:O	13:Ac:167:TYR:HB2	2.22	0.40
17:Ag:68:GLN:H	17:Ag:68:GLN:HG2	1.77	0.40
17:Ag:69:LEU:HD13	17:Ag:96:ALA:HB2	2.03	0.40
17:Ag:157:HIS:HB3	17:Ag:190:PRO:HD3	2.04	0.40
19:Ai:61:LEU:HA	19:Ai:70:ARG:HH12	1.86	0.40
24:An:16:SER:OG	24:An:17:LEU:N	2.51	0.40
29:As:71:GLY:O	29:As:75:MET:HG2	2.21	0.40
37:B5:741:A:N6	37:B5:810:U:O2	2.55	0.40
37:B5:999:C:H2'	37:B5:1000:C:C6	2.57	0.40
37:B5:1095:C:H2'	37:B5:1096:G:C8	2.57	0.40
37:B5:1521:C:H2'	37:B5:1522:U:C6	2.57	0.40
41:BB:231:VAL:HG21	41:BB:251:VAL:HG23	2.04	0.40
41:BB:317:LEU:HB2	41:BB:372:SER:HB2	2.03	0.40
58:BT:54:HIS:ND1	58:BT:56:CYS:SG	2.82	0.40
81:Bs:30:VAL:HG21	81:Bs:187:LEU:HD13	2.03	0.40
82:Bt:53:TRP:CD1	82:Bt:56:LEU:HB2	2.57	0.40
84:MA:242:MET:HE2	84:MA:278:GLN:HB3	2.04	0.40
86:Nu:63:ASN:OD1	86:Nu:73:HIS:ND1	2.32	0.40
1:A2:1387:A:OP2	13:Ac:160:SER:OG	2.27	0.40
1:A2:1514:C:P	8:AG:12:ARG:HH22	2.45	0.40
1:A2:1543:C:O2'	26:Ap:43:GLU:OE2	2.37	0.40
1:A2:1615:A:OP2	25:Ao:42:ARG:NH2	2.45	0.40
1:A2:1767:C:H4'	1:A2:1768:C:H5	1.87	0.40
4:AC:121:CYS:HA	4:AC:122:PRO:HD3	1.91	0.40
7:AF:133:ASN:HB3	7:AF:139:LYS:HE3	2.01	0.40
11:Aa:29:ASP:OD1	11:Aa:51:ARG:NH2	2.54	0.40
22:Al:33:ARG:HD2	22:Al:91:LEU:CD1	2.51	0.40
34:Ax:80:ASP:O	34:Ax:81:TYR:C	2.63	0.40
37:B5:176:G:H2'	37:B5:177:G:C8	2.56	0.40
37:B5:1704:A:C5	37:B5:1705:A:H1'	2.56	0.40
47:BI:184:MET:HA	47:BI:187:GLU:HG2	2.03	0.40
50:BL:208:GLU:HB2	83:Bv:184:HIS:CD2	2.56	0.40
62:BX:87:MET:HE3	84:MA:317:ASN:HB2	2.04	0.40
81:Bs:58:ASN:O	81:Bs:62:ARG:HG3	2.22	0.40
81:Bs:120:GLU:HG3	81:Bs:162:LYS:HA	2.03	0.40
83:Bv:59:PRO:HB2	83:Bv:171:HIS:ND1	2.36	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	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
5	AD	55/133 (41%)	55 (100%)	0	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
10	AZ	220/295 (75%)	217 (99%)	3 (1%)	0	100	100
11	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
12	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
13	Ac	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
14	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
15	Ae	189/204 (93%)	187 (99%)	2 (1%)	0	100	100
16	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
17	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
18	Ah	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
19	Ai	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
20	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
21	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
22	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
23	Am	148/151 (98%)	148 (100%)	0	0	100	100
24	An	120/151 (80%)	117 (98%)	3 (2%)	0	100	100
25	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
26	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
27	Aq	132/135 (98%)	132 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ar	147/152 (97%)	143 (97%)	4 (3%)	0	100	100
29	As	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
30	At	102/119 (86%)	102 (100%)	0	0	100	100
31	Au	82/84 (98%)	82 (100%)	0	0	100	100
32	Av	127/130 (98%)	127 (100%)	0	0	100	100
33	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
34	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
35	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
36	Az	23/25 (92%)	23 (100%)	0	0	100	100
40	BA	250/257 (97%)	245 (98%)	5 (2%)	0	100	100
41	BB	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
42	BC	361/413 (87%)	358 (99%)	3 (1%)	0	100	100
43	BE	239/291 (82%)	236 (99%)	3 (1%)	0	100	100
44	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
45	BG	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
46	BH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
47	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
48	BJ	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
50	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
51	BM	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
52	BN	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
53	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
54	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
55	BQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
56	BR	178/196 (91%)	178 (100%)	0	0	100	100
57	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
58	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
59	BU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
60	BV	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
61	BW	119/157 (76%)	119 (100%)	0	0	100	100
62	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
64	BZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
65	Ba	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
66	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
67	Bc	106/115 (92%)	106 (100%)	0	0	100	100
68	Bd	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
69	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
70	Bf	108/110 (98%)	108 (100%)	0	0	100	100
71	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
72	Bh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
73	Bi	100/105 (95%)	100 (100%)	0	0	100	100
74	Bj	84/97 (87%)	84 (100%)	0	0	100	100
75	Bk	67/70 (96%)	67 (100%)	0	0	100	100
76	Bl	48/51 (94%)	48 (100%)	0	0	100	100
77	Bm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
78	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
79	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
80	Br	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
81	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
82	Bt	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
83	Bv	210/217 (97%)	200 (95%)	10 (5%)	0	100	100
84	MA	340/496 (68%)	322 (95%)	18 (5%)	0	100	100
85	Nt	61/215 (28%)	59 (97%)	2 (3%)	0	100	100
86	Nu	105/162 (65%)	94 (90%)	9 (9%)	2 (2%)	6	23
All	All	12113/14414 (84%)	11903 (98%)	208 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
86	Nu	104	PRO
86	Nu	98	GLN

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	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	65	88
3	AB	56/62 (90%)	56 (100%)	0	100	100
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	47/106 (44%)	47 (100%)	0	100	100
6	AE	88/98 (90%)	87 (99%)	1 (1%)	70	90
7	AF	272/275 (99%)	268 (98%)	4 (2%)	60	86
8	AG	48/49 (98%)	48 (100%)	0	100	100
10	AZ	183/243 (75%)	181 (99%)	2 (1%)	70	90
11	Aa	203/231 (88%)	201 (99%)	2 (1%)	73	91
12	Ab	185/223 (83%)	185 (100%)	0	100	100
13	Ac	189/232 (82%)	186 (98%)	3 (2%)	58	85
14	Ad	224/225 (100%)	222 (99%)	2 (1%)	75	92
15	Ae	161/170 (95%)	161 (100%)	0	100	100
16	Af	207/218 (95%)	207 (100%)	0	100	100
17	Ag	170/360 (47%)	170 (100%)	0	100	100
18	Ah	178/180 (99%)	177 (99%)	1 (1%)	84	95
19	Ai	161/168 (96%)	160 (99%)	1 (1%)	84	95
20	Aj	87/136 (64%)	86 (99%)	1 (1%)	70	90
21	Ak	139/142 (98%)	139 (100%)	0	100	100
22	Al	104/108 (96%)	103 (99%)	1 (1%)	73	91
23	Am	130/131 (99%)	130 (100%)	0	100	100
24	An	95/119 (80%)	93 (98%)	2 (2%)	48	80
25	Ao	114/130 (88%)	112 (98%)	2 (2%)	54	83
26	Ap	117/140 (84%)	117 (100%)	0	100	100
27	Aq	120/121 (99%)	120 (100%)	0	100	100
28	Ar	128/131 (98%)	127 (99%)	1 (1%)	79	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	As	112/114 (98%)	112 (100%)	0	100	100
30	At	94/107 (88%)	93 (99%)	1 (1%)	70	90
31	Au	68/68 (100%)	66 (97%)	2 (3%)	37	71
32	Av	112/113 (99%)	111 (99%)	1 (1%)	75	92
33	Aw	112/114 (98%)	109 (97%)	3 (3%)	40	74
34	Ax	107/112 (96%)	102 (95%)	5 (5%)	22	54
35	Ay	75/102 (74%)	75 (100%)	0	100	100
36	Az	24/24 (100%)	24 (100%)	0	100	100
40	BA	194/198 (98%)	193 (100%)	1 (0%)	86	95
41	BB	344/347 (99%)	344 (100%)	0	100	100
42	BC	302/336 (90%)	302 (100%)	0	100	100
43	BE	216/251 (86%)	210 (97%)	6 (3%)	38	72
44	BF	197/215 (92%)	196 (100%)	1 (0%)	86	95
45	BG	199/223 (89%)	196 (98%)	3 (2%)	60	86
46	BH	169/171 (99%)	169 (100%)	0	100	100
47	BI	180/181 (99%)	180 (100%)	0	100	100
48	BJ	143/149 (96%)	140 (98%)	3 (2%)	48	80
50	BL	175/176 (99%)	174 (99%)	1 (1%)	84	95
51	BM	117/161 (73%)	117 (100%)	0	100	100
52	BN	171/172 (99%)	171 (100%)	0	100	100
53	BO	171/173 (99%)	170 (99%)	1 (1%)	84	95
54	BP	134/163 (82%)	133 (99%)	1 (1%)	81	94
55	BQ	164/165 (99%)	163 (99%)	1 (1%)	84	95
56	BR	159/175 (91%)	158 (99%)	1 (1%)	84	95
57	BS	154/154 (100%)	154 (100%)	0	100	100
58	BT	139/140 (99%)	137 (99%)	2 (1%)	62	87
59	BU	91/113 (80%)	87 (96%)	4 (4%)	24	56
60	BV	106/107 (99%)	106 (100%)	0	100	100
61	BW	100/126 (79%)	99 (99%)	1 (1%)	73	91
62	BX	106/134 (79%)	106 (100%)	0	100	100
63	BY	124/135 (92%)	123 (99%)	1 (1%)	79	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	BZ	117/118 (99%)	117 (100%)	0	100	100
65	Ba	118/119 (99%)	117 (99%)	1 (1%)	79	93
66	Bb	87/183 (48%)	86 (99%)	1 (1%)	70	90
67	Bc	92/98 (94%)	92 (100%)	0	100	100
68	Bd	98/110 (89%)	98 (100%)	0	100	100
69	Be	116/121 (96%)	116 (100%)	0	100	100
70	Bf	89/89 (100%)	89 (100%)	0	100	100
71	Bg	98/100 (98%)	97 (99%)	1 (1%)	73	91
72	Bh	109/110 (99%)	107 (98%)	2 (2%)	54	83
73	Bi	86/89 (97%)	85 (99%)	1 (1%)	67	89
74	Bj	73/80 (91%)	73 (100%)	0	100	100
75	Bk	64/65 (98%)	63 (98%)	1 (2%)	58	85
76	Bl	47/48 (98%)	47 (100%)	0	100	100
77	Bm	47/115 (41%)	47 (100%)	0	100	100
78	Bo	92/93 (99%)	92 (100%)	0	100	100
79	Bp	74/75 (99%)	73 (99%)	1 (1%)	62	87
80	Br	110/120 (92%)	109 (99%)	1 (1%)	75	92
81	Bs	164/258 (64%)	163 (99%)	1 (1%)	84	95
82	Bt	128/137 (93%)	122 (95%)	6 (5%)	22	54
83	Bv	191/195 (98%)	191 (100%)	0	100	100
84	MA	310/442 (70%)	308 (99%)	2 (1%)	84	95
85	Nt	56/183 (31%)	55 (98%)	1 (2%)	54	83
86	Nu	91/136 (67%)	81 (89%)	10 (11%)	5	17
All	All	10564/12217 (86%)	10472 (99%)	92 (1%)	74	92

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
6	AE	75	VAL
7	AF	12	LYS
7	AF	113	PHE
7	AF	266	ILE
7	AF	275	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	AZ	38	ILE
10	AZ	206	ASP
11	Aa	127	VAL
11	Aa	208	HIS
13	Ac	47	GLU
13	Ac	84	VAL
13	Ac	175	VAL
14	Ad	93	ASP
14	Ad	165	GLU
18	Ah	46	VAL
19	Ai	55	LYS
20	Aj	40	VAL
22	Al	104	VAL
24	An	21	VAL
24	An	113	GLN
25	Ao	105	VAL
25	Ao	133	ILE
28	Ar	94	LYS
30	At	70	VAL
31	Au	42	VAL
31	Au	61	ARG
32	Av	105	THR
33	Aw	61	GLN
33	Aw	105	PHE
33	Aw	125	VAL
34	Ax	16	ARG
34	Ax	78	SER
34	Ax	80	ASP
34	Ax	84	LYS
34	Ax	120	THR
40	BA	32	VAL
43	BE	84	ARG
43	BE	85	LYS
43	BE	86	LYS
43	BE	87	LYS
43	BE	88	ARG
43	BE	89	GLU
44	BF	198	LYS
45	BG	28	VAL
45	BG	106	THR
45	BG	159	HIS
48	BJ	141	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	BJ	143	ASP
48	BJ	147	ARG
50	BL	63	THR
53	BO	126	VAL
54	BP	104	LEU
55	BQ	82	VAL
56	BR	3	MET
58	BT	76	VAL
58	BT	93	ILE
59	BU	97	ARG
59	BU	105	ASN
59	BU	116	GLN
59	BU	117	ILE
61	BW	68	GLN
63	BY	113	LYS
65	Ba	7	LYS
66	Bb	51	LYS
71	Bg	32	TYR
72	Bh	82	ASP
72	Bh	112	ARG
73	Bi	29	ARG
75	Bk	36	VAL
79	Bp	52	VAL
80	Br	28	GLU
81	Bs	78	LEU
82	Bt	12	VAL
82	Bt	15	LEU
82	Bt	35	LEU
82	Bt	60	VAL
82	Bt	73	VAL
82	Bt	74	VAL
84	MA	398	LEU
84	MA	455	LEU
85	Nt	118	ASP
86	Nu	23	LYS
86	Nu	48	LEU
86	Nu	49	LYS
86	Nu	50	LYS
86	Nu	51	LEU
86	Nu	55	ASN
86	Nu	56	ILE
86	Nu	57	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
86	Nu	102	MET
86	Nu	104	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	9	HIS
5	AD	113	ASN
7	AF	222	ASN
8	AG	37	ASN
11	Aa	95	ASN
11	Aa	158	HIS
11	Aa	160	GLN
12	Ab	115	GLN
12	Ab	136	HIS
13	Ac	4	GLN
13	Ac	101	GLN
13	Ac	145	GLN
14	Ad	67	GLN
14	Ad	98	ASN
14	Ad	179	ASN
16	Af	56	ASN
16	Af	155	GLN
17	Ag	126	HIS
18	Ah	52	ASN
20	Aj	50	GLN
20	Aj	61	GLN
21	Ak	39	ASN
23	Am	5	HIS
25	Ao	137	HIS
28	Ar	19	ASN
30	At	34	HIS
30	At	63	ASN
31	Au	35	ASN
32	Av	120	HIS
33	Aw	92	ASN
34	Ax	94	HIS
35	Ay	64	ASN
40	BA	139	HIS
41	BB	376	HIS
42	BC	21	ASN
42	BC	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	BC	48	ASN
42	BC	116	ASN
42	BC	212	ASN
42	BC	276	ASN
42	BC	299	GLN
42	BC	329	ASN
44	BF	98	ASN
44	BF	247	ASN
45	BG	153	GLN
45	BG	236	HIS
46	BH	98	HIS
47	BI	166	HIS
48	BJ	112	HIS
48	BJ	167	GLN
51	BM	34	ASN
51	BM	48	GLN
52	BN	90	ASN
53	BO	143	HIS
53	BO	180	GLN
53	BO	184	ASN
54	BP	137	ASN
55	BQ	7	HIS
55	BQ	44	ASN
55	BQ	57	ASN
55	BQ	125	GLN
56	BR	34	ASN
56	BR	36	ASN
56	BR	118	HIS
58	BT	127	GLN
58	BT	131	GLN
61	BW	68	GLN
63	BY	56	GLN
63	BY	96	HIS
64	BZ	28	ASN
65	Ba	19	HIS
65	Ba	28	HIS
65	Ba	34	ASN
65	Ba	62	HIS
65	Ba	66	ASN
66	Bb	11	ASN
68	Bd	18	ASN
70	Bf	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
70	Bf	56	ASN
72	Bh	98	HIS
81	Bs	39	GLN
81	Bs	127	ASN
81	Bs	179	ASN
81	Bs	195	ASN
82	Bt	111	ASN
82	Bt	118	HIS
83	Bv	184	HIS
84	MA	179	ASN
84	MA	186	ASN
84	MA	234	HIS
84	MA	480	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1870 (94%)	231 (13%)	0
37	B5	3694/4808 (76%)	477 (12%)	7 (0%)
38	B7	119/120 (99%)	9 (7%)	0
39	B8	155/158 (98%)	20 (12%)	0
9	AT	75/76 (98%)	12 (16%)	0
All	All	5807/7032 (82%)	749 (12%)	7 (0%)

All (749) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	3	C
1	A2	17	C
1	A2	33	G
1	A2	41	G
1	A2	46	A
1	A2	56	G
1	A2	58	C
1	A2	67	C
1	A2	68	A
1	A2	73	C
1	A2	74	G
1	A2	76	U
1	A2	77	A
1	A2	79	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	103	A
1	A2	113	G
1	A2	114	G
1	A2	115	U
1	A2	126	G
1	A2	130	G
1	A2	143	U
1	A2	147	A
1	A2	155	G
1	A2	162	C
1	A2	168	C
1	A2	178	C
1	A2	180	G
1	A2	184	G
1	A2	188	C
1	A2	192	C
1	A2	226	A
1	A2	282	C
1	A2	295	U
1	A2	306	U
1	A2	310	G
1	A2	313	G
1	A2	320	C
1	A2	324	C
1	A2	326	C
1	A2	327	C
1	A2	328	G
1	A2	329	U
1	A2	330	G
1	A2	331	G
1	A2	348	G
1	A2	363	C
1	A2	365	A
1	A2	370	C
1	A2	386	G
1	A2	387	C
1	A2	401	C
1	A2	410	C
1	A2	422	G
1	A2	449	A
1	A2	451	C
1	A2	465	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	466	A
1	A2	471	G
1	A2	472	G
1	A2	473	C
1	A2	474	A
1	A2	475	G
1	A2	483	G
1	A2	488	U
1	A2	493	C
1	A2	494	A
1	A2	502	C
1	A2	509	A
1	A2	513	A2M
1	A2	526	A
1	A2	548	G
1	A2	549	C
1	A2	550	C
1	A2	561	A
1	A2	564	G
1	A2	565	A
1	A2	569	C
1	A2	584	A
1	A2	590	G
1	A2	592	U
1	A2	607	G
1	A2	609	C
1	A2	615	C
1	A2	629	A
1	A2	630	A
1	A2	632	U
1	A2	633	C
1	A2	644	A
1	A2	645	OMG
1	A2	656	A
1	A2	661	C
1	A2	669	A2M
1	A2	670	A
1	A2	672	A
1	A2	673	A
1	A2	674	G
1	A2	685	G
1	A2	734	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	747	C
1	A2	748	U
1	A2	754	C
1	A2	755	G
1	A2	756	C
1	A2	798	C
1	A2	799	G
1	A2	800	U
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G
1	A2	837	G
1	A2	838	A
1	A2	839	G
1	A2	840	C
1	A2	841	C
1	A2	842	G
1	A2	848	A
1	A2	871	A
1	A2	872	U
1	A2	873	A
1	A2	879	G
1	A2	886	U
1	A2	892	G
1	A2	910	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
1	A2	934	G
1	A2	944	U
1	A2	956	A
1	A2	971	G
1	A2	972	G
1	A2	991	A
1	A2	993	A
1	A2	1000	G
1	A2	1003	U
1	A2	1018	U
1	A2	1024	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	1061	A
1	A2	1062	U
1	A2	1063	A
1	A2	1084	A
1	A2	1086	C
1	A2	1116	U
1	A2	1117	C
1	A2	1118	C
1	A2	1119	C
1	A2	1122	G
1	A2	1134	A
1	A2	1145	A
1	A2	1150	A
1	A2	1151	A
1	A2	1154	C
1	A2	1155	U
1	A2	1156	U
1	A2	1167	G
1	A2	1196	A
1	A2	1216	C
1	A2	1225	G
1	A2	1243	U
1	A2	1252	A
1	A2	1254	A
1	A2	1257	G
1	A2	1258	G
1	A2	1260	A
1	A2	1272	C
1	A2	1275	G
1	A2	1276	G
1	A2	1289	OMU
1	A2	1303	G
1	A2	1304	C
1	A2	1315	U
1	A2	1343	U
1	A2	1359	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1398	U
1	A2	1403	A
1	A2	1406	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	1407	G
1	A2	1419	C
1	A2	1420	C
1	A2	1422	A
1	A2	1424	C
1	A2	1436	C
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U
1	A2	1465	C
1	A2	1481	A
1	A2	1488	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1498	G
1	A2	1510	U
1	A2	1522	C
1	A2	1534	A
1	A2	1571	G
1	A2	1581	A
1	A2	1586	U
1	A2	1589	A
1	A2	1602	A
1	A2	1607	G
1	A2	1622	U
1	A2	1624	A
1	A2	1647	C
1	A2	1655	G
1	A2	1666	G
1	A2	1681	G
1	A2	1699	C
1	A2	1700	A
1	A2	1722	U
1	A2	1723	G
1	A2	1745	G
1	A2	1749	G
1	A2	1783	G
1	A2	1784	C
1	A2	1785	G
1	A2	1836	A
1	A2	1837	G
1	A2	1839	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A2	1850	G
1	A2	1852	MA6
1	A2	1862	G
1	A2	1863	G
1	A2	1864	A
1	A2	1865	U
1	A2	1866	C
9	AT	2	U
9	AT	3	U
9	AT	16	U
9	AT	17	G
9	AT	18	G
9	AT	20	U
9	AT	22	U
9	AT	23	C
9	AT	46	G
9	AT	47	U
9	AT	48	C
9	AT	76	A
37	B5	14	C
37	B5	25	A
37	B5	39	A
37	B5	42	A
37	B5	58	G
37	B5	59	A
37	B5	64	A
37	B5	65	A
37	B5	70	A
37	B5	71	C
37	B5	72	C
37	B5	74	G
37	B5	85	G
37	B5	91	G
37	B5	98	A
37	B5	109	G
37	B5	119	G
37	B5	132	G
37	B5	135	G
37	B5	136	U
37	B5	144	G
37	B5	151	G
37	B5	159	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	171	U
37	B5	172	C
37	B5	173	C
37	B5	181	C
37	B5	184	U
37	B5	185	C
37	B5	187	U
37	B5	188	G
37	B5	200	U
37	B5	201	C
37	B5	209	U
37	B5	218	A
37	B5	219	G
37	B5	220	C
37	B5	233	U
37	B5	234	G
37	B5	263	G
37	B5	264	C
37	B5	265	C
37	B5	266	C
37	B5	268	G
37	B5	297	U
37	B5	309	C
37	B5	315	G
37	B5	316	U
37	B5	322	C
37	B5	334	A
37	B5	340	C
37	B5	363	A
37	B5	386	A
37	B5	387	G
37	B5	409	G
37	B5	412	G
37	B5	413	G
37	B5	440	U
37	B5	449	C
37	B5	450	G
37	B5	452	A
37	B5	453	G
37	B5	454	U
37	B5	468	U
37	B5	482	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	483	G
37	B5	484	G
37	B5	485	U
37	B5	486	C
37	B5	488	G
37	B5	493	U
37	B5	497	G
37	B5	499	C
37	B5	502	U
37	B5	503	C
37	B5	504	U
37	B5	505	C
37	B5	512	U
37	B5	515	U
37	B5	516	U
37	B5	517	C
37	B5	628	U
37	B5	634	C
37	B5	635	G
37	B5	660	G
37	B5	661	A
37	B5	682	U
37	B5	691	G
37	B5	698	C
37	B5	699	G
37	B5	724	G
37	B5	725	G
37	B5	732	C
37	B5	734	G
37	B5	739	G
37	B5	758	C
37	B5	759	G
37	B5	760	C
37	B5	790	G
37	B5	791	C
37	B5	792	G
37	B5	794	G
37	B5	795	A
37	B5	797	C
37	B5	798	C
37	B5	810	U
37	B5	812	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	814	A
37	B5	815	G
37	B5	824	C
37	B5	825	G
37	B5	831	A
37	B5	832	G
37	B5	833	C
37	B5	834	A
37	B5	835	G
37	B5	843	A
37	B5	844	A
37	B5	845	U
37	B5	856	A
37	B5	860	A
37	B5	861	G
37	B5	866	A
37	B5	867	C
37	B5	868	C
37	B5	869	U
37	B5	870	G
37	B5	884	U
37	B5	983	G
37	B5	985	G
37	B5	987	C
37	B5	1069	G
37	B5	1071	C
37	B5	1072	C
37	B5	1073	C
37	B5	1074	C
37	B5	1090	U
37	B5	1091	G
37	B5	1102	G
37	B5	1105	C
37	B5	1106	U
37	B5	1124	A
37	B5	1127	G
37	B5	1133	C
37	B5	1140	C
37	B5	1202	C
37	B5	1214	A
37	B5	1215	G
37	B5	1217	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	1219	G
37	B5	1220	C
37	B5	1228	G
37	B5	1231	G
37	B5	1240	G
37	B5	1246	U
37	B5	1247	A
37	B5	1270	A2M
37	B5	1298	A
37	B5	1299	G
37	B5	1303	G
37	B5	1309	C
37	B5	1310	G
37	B5	1323	C
37	B5	1331	A
37	B5	1341	A
37	B5	1351	G
37	B5	1367	G
37	B5	1375	A
37	B5	1391	C
37	B5	1393	C
37	B5	1401	C
37	B5	1440	C
37	B5	1453	G
37	B5	1457	G
37	B5	1459	G
37	B5	1473	A
37	B5	1480	A
37	B5	1489	A2M
37	B5	1502	A
37	B5	1521	C
37	B5	1533	U
37	B5	1546	U
37	B5	1551	U
37	B5	1552	G
37	B5	1555	A
37	B5	1560	G
37	B5	1568	A
37	B5	1579	G
37	B5	1580	OMG
37	B5	1586	A
37	B5	1588	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	1589	A
37	B5	1592	A
37	B5	1593	A
37	B5	1594	U
37	B5	1595	C
37	B5	1596	G
37	B5	1597	A
37	B5	1609	G
37	B5	1616	C
37	B5	1631	C
37	B5	1632	PSU
37	B5	1646	G
37	B5	1653	C
37	B5	1657	C
37	B5	1658	C
37	B5	1689	G
37	B5	1705	A
37	B5	1726	A
37	B5	1743	A
37	B5	1751	C
37	B5	1754	G
37	B5	1767	C
37	B5	1774	G
37	B5	1775	G
37	B5	1776	A
37	B5	1781	G
37	B5	1794	G
37	B5	1808	G
37	B5	1836	A
37	B5	1857	U
37	B5	1859	C
37	B5	1860	C
37	B5	1861	G
37	B5	1870	C
37	B5	1871	A
37	B5	1879	G
37	B5	1887	G
37	B5	1898	U
37	B5	1899	A
37	B5	1900	G
37	B5	1914	G
37	B5	1915	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	1922	A
37	B5	1923	A
37	B5	1924	G
37	B5	1926	C
37	B5	1936	U
37	B5	1940	G
37	B5	1942	G
37	B5	1943	U
37	B5	1963	G
37	B5	1965	A
37	B5	1985	G
37	B5	1987	U
37	B5	1994	G
37	B5	1995	G
37	B5	2008	A
37	B5	2023	U
37	B5	2032	G
37	B5	2034	A
37	B5	2037	G
37	B5	2039	G
37	B5	2041	G
37	B5	2044	A
37	B5	2045	G
37	B5	2046	A
37	B5	2112	C
37	B5	2132	C
37	B5	2137	G
37	B5	2143	A
37	B5	2144	G
37	B5	2149	G
37	B5	2156	A
37	B5	2159	G
37	B5	2174	G
37	B5	2191	G
37	B5	2193	U
37	B5	2194	OMC
37	B5	2203	A
37	B5	2207	OMG
37	B5	2241	U
37	B5	2251	U
37	B5	2264	G
37	B5	2268	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	2276	G
37	B5	2310	U
37	B5	2311	U
37	B5	2312	C
37	B5	2313	C
37	B5	2314	G
37	B5	2332	C
37	B5	2333	U
37	B5	2349	G
37	B5	2356	A
37	B5	2372	A
37	B5	2380	A
37	B5	2386	A
37	B5	2387	G
37	B5	2388	U
37	B5	2390	G
37	B5	2397	U
37	B5	2409	G
37	B5	2429	G
37	B5	2430	A
37	B5	2432	C
37	B5	2444	A
37	B5	2496	C
37	B5	2503	A
37	B5	2530	U
37	B5	2537	G
37	B5	2538	A
37	B5	2539	A
37	B5	2546	G
37	B5	2551	U
37	B5	2554	G
37	B5	2586	A
37	B5	2606	U
37	B5	2612	U
37	B5	2630	A2M
37	B5	2631	U
37	B5	2633	U
37	B5	2657	C
37	B5	2669	U
37	B5	2670	G
37	B5	2672	U
37	B5	2698	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	2699	C
37	B5	2745	G
37	B5	3329	G
37	B5	3347	G
37	B5	3350	C
37	B5	3358	G
37	B5	3362	A
37	B5	3367	A
37	B5	3378	A
37	B5	3394	A
37	B5	3396	G
37	B5	3428	C
37	B5	3443	A
37	B5	3444	A
37	B5	3485	G
37	B5	3492	A2M
37	B5	3493	C
37	B5	3498	A
37	B5	3508	G
37	B5	3509	G
37	B5	3516	A
37	B5	3517	A2M
37	B5	3543	G
37	B5	3546	U
37	B5	3549	A
37	B5	3551	G
37	B5	3572	U
37	B5	3609	A
37	B5	3610	C
37	B5	3611	G
37	B5	3629	G
37	B5	3630	G
37	B5	3633	A
37	B5	3638	A
37	B5	3639	G
37	B5	3640	A
37	B5	3647	U
37	B5	3670	G
37	B5	3671	G
37	B5	3804	G
37	B5	3812	G
37	B5	3823	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	3824	C
37	B5	3825	G
37	B5	3832	G
37	B5	3833	A
37	B5	3834	G
37	B5	3847	C
37	B5	3849	G
37	B5	3850	G
37	B5	3855	A
37	B5	3869	G
37	B5	3875	C
37	B5	3891	C
37	B5	3892	G
37	B5	3916	A
37	B5	3929	G
37	B5	3930	G
37	B5	3937	G
37	B5	3949	A
37	B5	3975	U
37	B5	3979	A
37	B5	3997	A
37	B5	4000	G
37	B5	4012	G
37	B5	4014	A
37	B5	4017	A
37	B5	4019	A
37	B5	4027	A
37	B5	4051	G
37	B5	4052	OMU
37	B5	4075	G
37	B5	4076	G
37	B5	4078	C
37	B5	4096	C
37	B5	4100	U
37	B5	4119	G
37	B5	4121	C
37	B5	4123	G
37	B5	4124	A
37	B5	4133	C
37	B5	4140	A
37	B5	4168	A
37	B5	4194	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	4210	A
37	B5	4212	C
37	B5	4237	G
37	B5	4258	U
37	B5	4259	A
37	B5	4265	C
37	B5	4270	G
37	B5	4294	A
37	B5	4306	C
37	B5	4313	G
37	B5	4321	G
37	B5	4336	A2M
37	B5	4370	A
37	B5	4381	A
37	B5	4382	PSU
37	B5	4416	C
37	B5	4418	A
37	B5	4437	A
37	B5	4446	A
37	B5	4448	G
37	B5	4454	A
37	B5	4455	U
37	B5	4465	G
37	B5	4475	A
37	B5	4476	C
37	B5	4477	G
37	B5	4478	G
37	B5	4486	G
37	B5	4487	A
37	B5	4488	A
37	B5	4489	G
37	B5	4490	G
37	B5	4492	G
37	B5	4498	G
37	B5	4501	G
37	B5	4504	C
37	B5	4506	C
37	B5	4508	G
37	B5	4512	G
37	B5	4518	C
37	B5	4609	G
37	B5	4610	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	B5	4614	G
37	B5	4621	U
37	B5	4622	C
37	B5	4634	U
37	B5	4635	G
37	B5	4637	G
37	B5	4638	G
37	B5	4639	C
37	B5	4640	G
37	B5	4642	G
37	B5	4644	C
37	B5	4645	C
37	B5	4646	G
37	B5	4649	A
37	B5	4651	G
37	B5	4658	G
37	B5	4660	C
37	B5	4665	C
37	B5	4680	G
37	B5	4702	G
37	B5	4705	A
37	B5	4715	U
37	B5	4728	U
37	B5	4729	C
37	B5	4753	A
37	B5	4756	G
37	B5	4761	U
37	B5	4762	C
37	B5	4763	C
37	B5	4780	G
37	B5	4789	C
37	B5	4792	U
37	B5	4801	G
37	B5	4808	U
38	B7	7	G
38	B7	25	G
38	B7	42	A
38	B7	43	U
38	B7	53	U
38	B7	54	A
38	B7	64	G
38	B7	110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	B7	120	U
39	B8	4	C
39	B8	23	C
39	B8	34	U
39	B8	35	C
39	B8	59	A
39	B8	62	A
39	B8	63	U
39	B8	81	C
39	B8	84	A
39	B8	86	U
39	B8	87	G
39	B8	94	G
39	B8	103	A
39	B8	105	C
39	B8	110	U
39	B8	114	G
39	B8	123	U
39	B8	150	C
39	B8	151	G
39	B8	156	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	B5	70	A
37	B5	171	U
37	B5	1588	G
37	B5	2310	U
37	B5	2313	C
37	B5	4486	G
37	B5	4634	U

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

219 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	$\# Z > 2$
37	PSU	B5	1638	37	18,21,22	0.85	1 (5%)	22,30,33	0.69	0
1	A2M	A2	485	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
37	OMG	B5	3631	87,37	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
37	PSU	B5	1537	37	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
37	PSU	B5	3462	37	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	A2M	B5	2244	87,37	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
37	A2M	B5	3456	37	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
29	NMM	As	67	29	9,11,12	0.59	0	6,12,14	0.42	0
37	PSU	B5	1632	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
1	OMU	A2	355	1	19,22,23	1.23	2 (10%)	26,31,34	1.72	4 (15%)
37	A2M	B5	3599	37	18,25,26	0.99	1 (5%)	18,36,39	1.28	2 (11%)
1	PSU	A2	1057	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	109	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
37	OMG	B5	3359	37	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
78	MLZ	Bo	53	78	8,9,10	0.49	0	4,9,11	0.14	0
33	HY3	Aw	62	33	6,8,9	6.51	4 (66%)	5,10,12	0.96	0
1	OMC	A2	1704	1	19,22,23	0.82	0	26,31,34	0.80	0
37	OMG	B5	2207	37	18,26,27	0.90	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
37	OMG	B5	3942	9,37	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
1	PSU	A2	1082	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
37	PSU	B5	1718	37	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	116	1	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	1720	37	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
37	OMU	B5	2680	37	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
37	PSU	B5	3496	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
37	OMG	B5	3974	37	18,26,27	0.91	1 (5%)	19,38,41	1.10	2 (10%)
37	OMG	B5	1260	37	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	A2	645	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
1	OMG	A2	868	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
37	OMU	B5	2258	37	19,22,23	1.22	3 (15%)	26,31,34	1.68	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	V5N	BA	216	40	4,11,12	0.77	0	5,14,16	1.52	1 (20%)
1	OMC	A2	1392	1	19,22,23	0.83	0	26,31,34	0.87	1 (3%)
1	A2M	A2	513	1	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
37	OMU	B5	4052	37	19,22,23	0.21	0	26,31,34	0.50	0
39	PSU	B8	69	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	4169	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	3500	37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	A2M	B5	2658	87,37	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
37	PSU	B5	4374	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4177	37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	687	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	823	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
37	5MC	B5	3514	87,37	18,22,23	0.97	2 (11%)	26,32,35	1.18	3 (11%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	105	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	967	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
37	OMC	B5	3619	37	19,22,23	0.81	0	26,31,34	0.82	0
37	PSU	B5	3447	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
77	M3L	Bm	98	77	10,11,12	0.83	0	9,14,16	0.55	0
37	A2M	B5	1810	87,37	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	93	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	PSU	B5	4099	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
37	OMG	B5	4364	37	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	A2	1289	1	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
37	PSU	B5	1799	37	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	OMC	B5	1284	37	19,22,23	0.82	0	26,31,34	0.83	0
37	PSU	B5	4267	37	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	A2	166	1	18,25,26	1.04	1 (5%)	18,36,39	1.27	2 (11%)
1	OMU	A2	1805	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
37	PSU	B5	3369	37	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
37	OMU	B5	3657	37	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	OMG	A2	1448	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
37	PSU	B5	4322	37	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
37	OMC	B5	1820	87,37	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	A2M	B5	3450	37	18,25,26	1.01	1 (5%)	18,36,39	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	B5	4435	37	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	4AC	A2	1843	1	21,24,25	1.11	2 (9%)	29,34,37	1.29	3 (10%)
37	PSU	B5	3427	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
37	OMC	B5	2647	37	19,22,23	0.82	0	26,31,34	0.80	0
1	PSU	A2	1239	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
37	OMG	B5	4240	37	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
37	OMC	B5	3601	37	19,22,23	0.81	0	26,31,34	0.84	0
37	OMC	B5	2194	87,37	19,22,23	0.82	0	26,31,34	0.91	1 (3%)
1	PSU	A2	610	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	OMG	B5	3476	37	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
37	A2M	B5	4269	87,37	18,25,26	0.62	0	18,36,39	0.79	1 (5%)
37	OMG	B5	2719	37	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
37	OMG	B5	1477	37	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
37	PSU	B5	4058	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	1032	1	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
37	OMG	B5	1580	37	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	MA6	A2	1852	1	18,26,27	1.10	2 (11%)	19,38,41	1.93	3 (15%)
37	OMC	B5	2208	87,37	19,22,23	0.81	0	26,31,34	0.78	0
1	PSU	A2	1368	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	469	1	18,25,26	1.05	1 (5%)	18,36,39	1.25	2 (11%)
37	PSU	B5	4042	37	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	A2	1491	1,87	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
37	A2M	B5	3492	1,37	18,25,26	1.02	1 (5%)	18,36,39	1.37	2 (11%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	1683	37	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	577	1	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
37	OMU	B5	4244	37	19,22,23	1.20	2 (10%)	26,31,34	1.70	5 (19%)
37	PSU	B5	4039	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	4278	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	119	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1046	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	1644	1,87	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
37	OMC	B5	3433	37	19,22,23	0.79	0	26,31,34	0.77	0
37	A2M	B5	2630	87,37	18,25,26	0.99	1 (5%)	18,36,39	1.33	2 (11%)
37	PSU	B5	3554	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
37	1MA	B5	1266	37	16,25,26	1.57	2 (12%)	18,37,40	1.04	2 (11%)
37	OMG	B5	4383	37	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
37	PSU	B5	4749	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	A2	172	1	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
37	PSU	B5	1801	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	1384	1	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
1	PSU	A2	816	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	A2	510	1,87	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	A2M	A2	1679	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
37	A2M	B5	2206	87,37	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
37	A2M	B5	400	37	18,25,26	1.01	1 (5%)	18,36,39	1.23	2 (11%)
37	A2M	B5	398	37	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
66	MLZ	Bb	5	66	8,9,10	0.49	0	4,9,11	0.18	0
37	6MZ	B5	3966	37	18,25,26	0.87	1 (5%)	16,36,39	2.00	4 (25%)
1	A2M	A2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
37	OMC	B5	3540	37	19,22,23	0.82	0	26,31,34	0.80	0
37	PSU	B5	4740	37	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
37	OMU	B5	4366	37	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
37	PSU	B5	3502	37	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
37	OMG	B5	4116	37	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
1	A2M	A2	591	1	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
65	V5N	Ba	39	65	4,11,12	0.76	0	5,14,16	1.49	1 (20%)
1	OMU	A2	628	1	19,22,23	0.24	0	26,31,34	0.51	0
37	PSU	B5	3616	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
37	PSU	B5	3576	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
37	PSU	B5	3490	37	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
37	PSU	B5	4298	37	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
37	PSU	B5	4711	37	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
41	HIC	BB	245	41	8,11,12	0.88	0	6,14,16	0.84	0
1	OMG	A2	602	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	A2	867	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	UR3	B5	4276	37	19,22,23	0.98	0	26,32,35	1.42	1 (3%)
37	5MC	B5	4193	37	18,22,23	1.00	2 (11%)	26,32,35	1.19	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	B5	4045	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4166	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	573	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
37	A2M	B5	3562	37	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
37	PSU	B5	3652	87,37	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
37	PSU	B5	4325	37	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
37	OMC	B5	2704	37	19,22,23	0.81	0	26,31,34	0.81	0
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	3371	37	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
37	OMC	B5	2667	37	19,22,23	0.82	0	26,31,34	0.79	0
1	PSU	A2	1693	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
37	PSU	B5	3585	87,37	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	A2	174	1,87	19,22,23	0.81	0	26,31,34	0.81	0
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
37	A2M	B5	4336	37	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
37	PSU	B5	1721	37	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
37	UY1	B5	3550	37	19,22,23	1.36	3 (15%)	22,31,34	1.90	5 (22%)
37	PSU	B5	3466	37	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	682	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
37	OMC	B5	4282	87,37	19,22,23	0.81	0	26,31,34	0.82	0
39	OMG	B8	75	39	18,26,27	0.94	1 (5%)	19,38,41	1.05	2 (10%)
37	PSU	B5	4203	37	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
37	OMG	B5	4369	37	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
37	PSU	B5	1731	37	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
37	OMU	B5	3973	37	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
37	PSU	B5	1491	37	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	2351	37	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
9	PSU	AT	55	9	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	1327	1,87	19,22,23	1.17	2 (10%)	26,31,34	1.71	5 (19%)
37	PSU	B5	4149	37	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	218	1	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A2	802	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	B8N	A2	1249	1	24,29,30	1.28	3 (12%)	29,42,45	1.28	3 (10%)
37	A2M	B5	3517	37	18,25,26	0.96	1 (5%)	18,36,39	1.32	2 (11%)
39	PSU	B8	55	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMG	B5	3524	37	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	34	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	99	1,87	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
1	OMC	A2	518	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	PSU	A2	1233	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	OMG	B5	4245	37	18,26,27	0.92	1 (5%)	19,38,41	1.05	2 (10%)
1	OMU	A2	429	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
37	PSU	B5	4382	37	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
37	PSU	B5	3494	37	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	A2	669	1,87	18,25,26	0.97	1 (5%)	18,36,39	1.35	2 (11%)
1	PSU	A2	1175	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1005	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
37	OMG	B5	4138	37	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
9	5MU	AT	54	9	19,22,23	1.40	6 (31%)	28,32,35	2.05	6 (21%)
37	PSU	B5	4246	37	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
37	PSU	B5	3583	37	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
37	PSU	B5	4419	37	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	27	1,87	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
37	A2M	B5	1479	37	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
37	A2M	B5	3557	37	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
37	A2M	B5	4317	37	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	A2	210	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
37	OMG	B5	3676	37	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	OMU	A2	1443	1,87	19,22,23	1.23	4 (21%)	26,31,34	1.69	5 (19%)
37	OMC	B5	4202	37	19,22,23	0.82	0	26,31,34	0.83	0
37	A2M	B5	1489	87,37	18,25,26	0.99	1 (5%)	18,36,39	1.35	2 (11%)
37	PSU	B5	2475	37	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	G7M	A2	1640	1,9	20,26,27	2.99	7 (35%)	17,39,42	0.96	1 (5%)
37	A2M	B5	1270	37	18,25,26	0.98	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	A2	1348	1	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.17	3 (10%)
37	OMG	B5	2267	37	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
37	PSU	B5	4188	37	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
37	PSU	B5	4217	37	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	A2	437	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
1	OMC	A2	463	1	19,22,23	0.83	0	26,31,34	0.84	0
37	OMC	B5	3573	37	19,22,23	0.81	0	26,31,34	0.93	1 (3%)
1	MA6	A2	1851	1	18,26,27	1.10	2 (11%)	19,38,41	2.00	3 (15%)
37	OMC	B5	2265	87,37	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
37	PSU	B5	4107	37	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	OMG	A2	1329	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	A2	815	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1245	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	6MZ	A2	1833	1,87	18,25,26	0.92	1 (5%)	16,36,39	1.86	4 (25%)

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
37	PSU	B5	1638	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	1/5/27/28	0/3/3/3
37	OMG	B5	3631	87,37	-	1/5/27/28	0/3/3/3
37	PSU	B5	1537	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3462	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	2244	87,37	-	0/5/27/28	0/3/3/3
37	A2M	B5	3456	37	-	0/5/27/28	0/3/3/3
29	NMM	As	67	29	-	0/9/11/13	-
37	PSU	B5	1632	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	1/9/27/28	0/2/2/2
37	A2M	B5	3599	37	-	0/5/27/28	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	3359	37	-	0/5/27/28	0/3/3/3
78	MLZ	Bo	53	78	-	0/7/8/10	-
33	HY3	Aw	62	33	-	1/1/12/14	0/1/1/1
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
37	OMG	B5	2207	37	-	2/5/27/28	0/3/3/3
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
37	OMG	B5	3942	9,37	-	0/5/27/28	0/3/3/3
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
37	PSU	B5	1718	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	1720	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	2680	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	3496	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	3974	37	-	0/5/27/28	0/3/3/3
37	OMG	B5	1260	37	-	0/5/27/28	0/3/3/3
1	OMG	A2	645	1	-	3/5/27/28	0/3/3/3
1	OMG	A2	868	1	-	1/5/27/28	0/3/3/3
37	OMU	B5	2258	37	-	0/9/27/28	0/2/2/2
40	V5N	BA	216	40	-	1/5/10/12	0/1/1/1
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	513	1	-	2/5/27/28	0/3/3/3
37	OMU	B5	4052	37	-	0/9/27/28	0/2/2/2
39	PSU	B8	69	39	-	0/7/25/26	0/2/2/2
37	PSU	B5	4169	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3500	37	-	0/7/25/26	0/2/2/2
37	A2M	B5	2658	87,37	-	0/5/27/28	0/3/3/3
37	PSU	B5	4374	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4177	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
37	5MC	B5	3514	87,37	-	0/7/25/26	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	3619	37	-	2/9/27/28	0/2/2/2
37	PSU	B5	3447	37	-	0/7/25/26	0/2/2/2
77	M3L	Bm	98	77	-	0/9/10/12	-
37	A2M	B5	1810	87,37	-	0/5/27/28	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	4099	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	4364	37	-	0/5/27/28	0/3/3/3
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
37	PSU	B5	1799	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	1284	37	-	1/9/27/28	0/2/2/2
37	PSU	B5	4267	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
37	PSU	B5	3369	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	3657	37	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A2	1448	1	-	2/5/27/28	0/3/3/3
37	PSU	B5	4322	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	1820	87,37	-	1/9/27/28	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
37	A2M	B5	3450	37	-	0/5/27/28	0/3/3/3
37	PSU	B5	4435	37	-	0/7/25/26	0/2/2/2
1	4AC	A2	1843	1	-	4/11/29/30	0/2/2/2
37	PSU	B5	3427	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	2647	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	4240	37	-	0/5/27/28	0/3/3/3
37	OMC	B5	3601	37	-	0/9/27/28	0/2/2/2
37	OMC	B5	2194	87,37	-	2/9/27/28	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	3476	37	-	1/5/27/28	0/3/3/3
37	A2M	B5	4269	87,37	-	1/5/27/28	0/3/3/3
37	OMG	B5	2719	37	-	0/5/27/28	0/3/3/3
37	OMG	B5	1477	37	-	0/5/27/28	0/3/3/3
37	PSU	B5	4058	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	0/5/27/28	0/3/3/3
37	OMG	B5	1580	37	-	0/5/27/28	0/3/3/3
1	MA6	A2	1852	1	-	2/7/29/30	0/3/3/3
37	OMC	B5	2208	87,37	-	0/9/27/28	0/2/2/2
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
37	PSU	B5	4042	37	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,87	-	0/5/27/28	0/3/3/3
37	A2M	B5	3492	1,37	-	1/5/27/28	0/3/3/3
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	1683	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	577	1	-	0/5/27/28	0/3/3/3
37	OMU	B5	4244	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	4039	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4278	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1644	1,87	-	0/7/25/26	0/2/2/2
37	OMC	B5	3433	37	-	4/9/27/28	0/2/2/2
37	A2M	B5	2630	87,37	-	0/5/27/28	0/3/3/3
37	PSU	B5	3554	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	1MA	B5	1266	37	-	0/3/25/26	0/3/3/3
37	OMG	B5	4383	37	-	1/5/27/28	0/3/3/3
37	PSU	B5	4749	37	-	0/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
37	PSU	B5	1801	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	510	1,87	-	1/5/27/28	0/3/3/3
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
37	A2M	B5	2206	87,37	-	0/5/27/28	0/3/3/3
37	A2M	B5	400	37	-	0/5/27/28	0/3/3/3
37	A2M	B5	398	37	-	2/5/27/28	0/3/3/3
66	MLZ	Bb	5	66	-	1/7/8/10	-
37	6MZ	B5	3966	37	-	0/5/27/28	0/3/3/3
1	A2M	A2	159	1	-	1/5/27/28	0/3/3/3
37	OMC	B5	3540	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	4740	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	4366	37	-	1/9/27/28	0/2/2/2
37	PSU	B5	3502	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	4116	37	-	0/5/27/28	0/3/3/3
1	A2M	A2	591	1	-	1/5/27/28	0/3/3/3
65	V5N	Ba	39	65	-	0/5/10/12	0/1/1/1
1	OMU	A2	628	1	-	1/9/27/28	0/2/2/2
37	PSU	B5	3616	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	3576	37	-	1/7/25/26	0/2/2/2
37	PSU	B5	3490	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4298	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4711	37	-	0/7/25/26	0/2/2/2
41	HIC	BB	245	41	-	2/5/6/8	0/1/1/1
1	OMG	A2	602	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
37	UR3	B5	4276	37	-	0/7/25/26	0/2/2/2
37	5MC	B5	4193	37	-	4/7/25/26	0/2/2/2
37	PSU	B5	4045	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4166	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
37	A2M	B5	3562	37	-	0/5/27/28	0/3/3/3
37	PSU	B5	3652	87,37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4325	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	2704	37	-	0/9/27/28	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	B5	3371	37	-	0/7/25/26	0/2/2/2
37	OMC	B5	2667	37	-	3/9/27/28	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
37	PSU	B5	3585	87,37	-	0/7/25/26	0/2/2/2
1	OMC	A2	174	1,87	-	0/9/27/28	0/2/2/2
1	OMG	A2	684	1	-	2/5/27/28	0/3/3/3
37	A2M	B5	4336	37	-	1/5/27/28	0/3/3/3
37	PSU	B5	1721	37	-	0/7/25/26	0/2/2/2
37	UY1	B5	3550	37	-	1/9/27/28	0/2/2/2
37	PSU	B5	3466	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
37	OMC	B5	4282	87,37	-	1/9/27/28	0/2/2/2
39	OMG	B8	75	39	-	2/5/27/28	0/3/3/3
37	PSU	B5	4203	37	-	0/7/25/26	0/2/2/2
37	OMG	B5	4369	37	-	0/5/27/28	0/3/3/3
37	PSU	B5	1731	37	-	0/7/25/26	0/2/2/2
37	OMU	B5	3973	37	-	0/9/27/28	0/2/2/2
37	PSU	B5	1491	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	2351	37	-	0/7/25/26	0/2/2/2
9	PSU	AT	55	9	-	0/7/25/26	0/2/2/2
1	OMU	A2	1327	1,87	-	0/9/27/28	0/2/2/2
37	PSU	B5	4149	37	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
37	A2M	B5	3517	37	-	2/5/27/28	0/3/3/3
39	PSU	B8	55	39	-	0/7/25/26	0/2/2/2
37	OMG	B5	3524	37	-	0/5/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	99	1,87	-	1/5/27/28	0/3/3/3
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	4245	37	-	0/5/27/28	0/3/3/3
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
37	PSU	B5	4382	37	-	4/7/25/26	0/2/2/2
37	PSU	B5	3494	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	1,87	-	2/5/27/28	0/3/3/3
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	B5	4138	37	-	0/5/27/28	0/3/3/3
9	5MU	AT	54	9	-	0/7/25/26	0/2/2/2
37	PSU	B5	4246	37	-	1/7/25/26	0/2/2/2
37	PSU	B5	3583	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4419	37	-	0/7/25/26	0/2/2/2
1	A2M	A2	27	1,87	-	0/5/27/28	0/3/3/3
37	A2M	B5	1479	37	-	0/5/27/28	0/3/3/3
37	A2M	B5	3557	37	-	0/5/27/28	0/3/3/3
37	A2M	B5	4317	37	-	0/5/27/28	0/3/3/3
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
37	OMG	B5	3676	37	-	1/5/27/28	0/3/3/3
1	OMU	A2	1443	1,87	-	0/9/27/28	0/2/2/2
37	OMC	B5	4202	37	-	0/9/27/28	0/2/2/2
37	A2M	B5	1489	87,37	-	2/5/27/28	0/3/3/3
37	PSU	B5	2475	37	-	0/7/25/26	0/2/2/2
1	G7M	A2	1640	1,9	-	2/3/25/26	0/3/3/3
37	A2M	B5	1270	37	-	0/5/27/28	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
37	OMG	B5	2267	37	-	0/5/27/28	0/3/3/3
37	PSU	B5	4188	37	-	0/7/25/26	0/2/2/2
37	PSU	B5	4217	37	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	1/5/27/28	0/3/3/3
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
37	OMC	B5	3573	37	-	1/9/27/28	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
37	OMC	B5	2265	87,37	-	1/9/27/28	0/2/2/2
37	PSU	B5	4107	37	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
1	6MZ	A2	1833	1,87	-	0/5/27/28	0/3/3/3

All (331) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Aw	62	HY3	C4-C3	-11.35	1.32	1.52
33	Aw	62	HY3	C3-CA	10.43	1.65	1.55
1	A2	1640	G7M	C5-C4	7.39	1.53	1.39
1	A2	1640	G7M	O6-C6	7.32	1.38	1.23
37	B5	1266	1MA	C2-N3	4.82	1.34	1.29
1	A2	1640	G7M	C2-N2	4.48	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C2-N1	3.84	1.47	1.37
37	B5	3550	UY1	C6-C5	3.57	1.39	1.35
1	A2	1640	G7M	C8-N9	3.45	1.39	1.33
1	A2	1851	MA6	C5-N7	3.36	1.51	1.39
1	A2	1348	PSU	C6-C5	3.35	1.39	1.35
1	A2	1852	MA6	C5-N7	3.31	1.51	1.39
1	A2	1640	G7M	C2-N3	3.28	1.41	1.33
37	B5	4166	PSU	C6-C5	3.28	1.39	1.35
37	B5	1638	PSU	C6-C5	3.25	1.39	1.35
1	A2	1640	G7M	C6-N1	3.24	1.42	1.37
37	B5	1266	1MA	C6-N6	3.22	1.35	1.27
1	A2	210	PSU	C6-C5	3.21	1.39	1.35
9	AT	55	PSU	C6-C5	3.19	1.39	1.35
37	B5	3500	PSU	C6-C5	3.17	1.39	1.35
37	B5	3494	PSU	C6-C5	3.17	1.39	1.35
1	A2	652	PSU	C6-C5	3.16	1.39	1.35
37	B5	3496	PSU	C6-C5	3.16	1.39	1.35
37	B5	4382	PSU	C6-C5	3.16	1.39	1.35
1	A2	1239	PSU	C6-C5	3.15	1.39	1.35
37	B5	1799	PSU	C6-C5	3.15	1.39	1.35
37	B5	1632	PSU	C6-C5	3.15	1.39	1.35
37	B5	4177	PSU	C6-C5	3.15	1.39	1.35
1	A2	1626	PSU	C6-C5	3.15	1.39	1.35
1	A2	610	PSU	C6-C5	3.14	1.39	1.35
1	A2	802	PSU	C6-C5	3.14	1.39	1.35
1	A2	816	PSU	C6-C5	3.14	1.39	1.35
1	A2	1368	PSU	C6-C5	3.13	1.39	1.35
1	A2	1175	PSU	C6-C5	3.13	1.39	1.35
37	B5	1537	PSU	C6-C5	3.13	1.39	1.35
37	B5	3371	PSU	C6-C5	3.13	1.39	1.35
37	B5	3462	PSU	C6-C5	3.12	1.39	1.35
1	A2	119	PSU	C6-C5	3.12	1.39	1.35
1	A2	218	PSU	C6-C5	3.12	1.39	1.35
37	B5	4169	PSU	C6-C5	3.12	1.39	1.35
37	B5	4107	PSU	C6-C5	3.11	1.38	1.35
37	B5	3447	PSU	C6-C5	3.11	1.38	1.35
1	A2	682	PSU	C6-C5	3.11	1.38	1.35
1	A2	1233	PSU	C6-C5	3.11	1.38	1.35
1	A2	864	PSU	C6-C5	3.11	1.38	1.35
37	B5	3466	PSU	C6-C5	3.11	1.38	1.35
37	B5	4099	PSU	C6-C5	3.11	1.38	1.35
37	B5	4322	PSU	C6-C5	3.10	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	4749	PSU	C6-C5	3.10	1.38	1.35
37	B5	4740	PSU	C6-C5	3.10	1.38	1.35
1	A2	1005	PSU	C6-C5	3.10	1.38	1.35
37	B5	4278	PSU	C6-C5	3.10	1.38	1.35
37	B5	1491	PSU	C6-C5	3.10	1.38	1.35
1	A2	105	PSU	C6-C5	3.10	1.38	1.35
1	A2	815	PSU	C6-C5	3.09	1.38	1.35
37	B5	4325	PSU	C6-C5	3.09	1.38	1.35
1	A2	687	PSU	C6-C5	3.09	1.38	1.35
1	A2	823	PSU	C6-C5	3.09	1.38	1.35
1	A2	1047	PSU	C6-C5	3.09	1.38	1.35
37	B5	2351	PSU	C6-C5	3.09	1.38	1.35
1	A2	867	PSU	C6-C5	3.09	1.38	1.35
1	A2	1446	PSU	C6-C5	3.09	1.38	1.35
37	B5	3502	PSU	C6-C5	3.08	1.38	1.35
1	A2	109	PSU	C6-C5	3.08	1.38	1.35
37	B5	3583	PSU	C6-C5	3.08	1.38	1.35
1	A2	1178	PSU	C6-C5	3.08	1.38	1.35
37	B5	4267	PSU	C6-C5	3.08	1.38	1.35
37	B5	4045	PSU	C6-C5	3.08	1.38	1.35
37	B5	1683	PSU	C6-C5	3.08	1.38	1.35
37	B5	1721	PSU	C6-C5	3.08	1.38	1.35
39	B8	69	PSU	C6-C5	3.07	1.38	1.35
1	A2	34	PSU	C6-C5	3.07	1.38	1.35
37	B5	3576	PSU	C6-C5	3.07	1.38	1.35
1	A2	1249	B8N	C4-N3	-3.07	1.34	1.40
1	A2	967	PSU	C6-C5	3.07	1.38	1.35
37	B5	3554	PSU	C6-C5	3.07	1.38	1.35
37	B5	4217	PSU	C6-C5	3.07	1.38	1.35
37	B5	4711	PSU	C6-C5	3.07	1.38	1.35
37	B5	1720	PSU	C6-C5	3.06	1.38	1.35
37	B5	1731	PSU	C6-C5	3.06	1.38	1.35
1	A2	1245	PSU	C6-C5	3.06	1.38	1.35
39	B8	55	PSU	C6-C5	3.06	1.38	1.35
37	B5	3427	PSU	C6-C5	3.05	1.38	1.35
1	A2	1082	PSU	C6-C5	3.05	1.38	1.35
37	B5	4298	PSU	C6-C5	3.05	1.38	1.35
37	B5	4039	PSU	C6-C5	3.05	1.38	1.35
1	A2	1057	PSU	C6-C5	3.04	1.38	1.35
37	B5	2475	PSU	C6-C5	3.04	1.38	1.35
37	B5	4203	PSU	C6-C5	3.04	1.38	1.35
1	A2	573	PSU	C6-C5	3.04	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1046	PSU	C6-C5	3.04	1.38	1.35
1	A2	1644	PSU	C6-C5	3.04	1.38	1.35
1	A2	650	PSU	C6-C5	3.04	1.38	1.35
37	B5	3490	PSU	C6-C5	3.04	1.38	1.35
1	A2	93	PSU	C6-C5	3.04	1.38	1.35
1	A2	407	PSU	C6-C5	3.03	1.38	1.35
37	B5	4419	PSU	C6-C5	3.03	1.38	1.35
37	B5	4246	PSU	C6-C5	3.03	1.38	1.35
37	B5	4374	PSU	C6-C5	3.03	1.38	1.35
1	A2	1693	PSU	C6-C5	3.03	1.38	1.35
37	B5	3585	PSU	C6-C5	3.03	1.38	1.35
37	B5	4149	PSU	C6-C5	3.03	1.38	1.35
37	B5	1801	PSU	C6-C5	3.03	1.38	1.35
33	Aw	62	HY3	C4-C5	3.02	1.57	1.53
37	B5	4058	PSU	C6-C5	3.02	1.38	1.35
37	B5	1718	PSU	C6-C5	3.01	1.38	1.35
37	B5	4435	PSU	C6-C5	3.01	1.38	1.35
1	A2	36	PSU	C6-C5	3.00	1.38	1.35
37	B5	4188	PSU	C6-C5	3.00	1.38	1.35
37	B5	3369	PSU	C6-C5	2.97	1.38	1.35
37	B5	4042	PSU	C6-C5	2.97	1.38	1.35
1	A2	1843	4AC	C4-N4	-2.96	1.35	1.39
37	B5	3616	PSU	C6-C5	2.96	1.38	1.35
37	B5	3652	PSU	C6-C5	2.95	1.38	1.35
1	A2	1249	B8N	C6-C5	2.95	1.39	1.34
1	A2	1338	4AC	C4-N4	-2.89	1.35	1.39
37	B5	4193	5MC	C6-C5	2.83	1.39	1.34
37	B5	1491	PSU	C4-N3	-2.77	1.33	1.38
37	B5	3550	UY1	C2-N1	2.76	1.40	1.36
37	B5	3514	5MC	C6-C5	2.76	1.39	1.34
1	A2	1046	PSU	C4-N3	-2.76	1.33	1.38
37	B5	4188	PSU	C4-N3	-2.75	1.33	1.38
37	B5	4325	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.73	1.33	1.38
37	B5	4419	PSU	C4-N3	-2.73	1.33	1.38
37	B5	4435	PSU	C4-N3	-2.73	1.33	1.38
37	B5	4039	PSU	C4-N3	-2.73	1.33	1.38
37	B5	3369	PSU	C4-N3	-2.72	1.33	1.38
37	B5	3490	PSU	C4-N3	-2.72	1.33	1.38
37	B5	3652	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4246	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4711	PSU	C4-N3	-2.72	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	4177	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4298	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4058	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4267	PSU	C4-N3	-2.72	1.33	1.38
37	B5	4374	PSU	C4-N3	-2.71	1.33	1.38
1	A2	650	PSU	C4-N3	-2.71	1.33	1.38
37	B5	3616	PSU	C4-N3	-2.71	1.33	1.38
1	A2	105	PSU	C4-N3	-2.71	1.33	1.38
37	B5	3585	PSU	C4-N3	-2.71	1.33	1.38
37	B5	3576	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1178	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1175	PSU	C4-N3	-2.71	1.33	1.38
37	B5	4149	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1693	PSU	C4-N3	-2.71	1.33	1.38
1	A2	864	PSU	C4-N3	-2.70	1.33	1.38
37	B5	4042	PSU	C4-N3	-2.70	1.33	1.38
37	B5	2351	PSU	C4-N3	-2.70	1.33	1.38
37	B5	4203	PSU	C4-N3	-2.70	1.33	1.38
1	A2	119	PSU	C4-N3	-2.70	1.33	1.38
1	A2	36	PSU	C4-N3	-2.69	1.33	1.38
1	A2	93	PSU	C4-N3	-2.69	1.33	1.38
1	A2	652	PSU	C4-N3	-2.69	1.33	1.38
37	B5	4107	PSU	C4-N3	-2.69	1.33	1.38
1	A2	815	PSU	C4-N3	-2.69	1.33	1.38
37	B5	1801	PSU	C4-N3	-2.69	1.33	1.38
9	AT	54	5MU	C6-C5	2.68	1.39	1.34
1	A2	816	PSU	C4-N3	-2.68	1.33	1.38
37	B5	4099	PSU	C4-N3	-2.68	1.33	1.38
37	B5	1799	PSU	C4-N3	-2.68	1.33	1.38
1	A2	682	PSU	C4-N3	-2.68	1.33	1.38
1	A2	867	PSU	C4-N3	-2.68	1.33	1.38
1	A2	407	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1047	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.68	1.33	1.38
37	B5	3583	PSU	C4-N3	-2.68	1.33	1.38
37	B5	4382	PSU	C4-N3	-2.67	1.33	1.38
37	B5	4740	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1446	PSU	C4-N3	-2.67	1.33	1.38
1	A2	573	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.67	1.33	1.38
37	B5	1721	PSU	C4-N3	-2.67	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	34	PSU	C4-N3	-2.67	1.33	1.38
37	B5	4217	PSU	C4-N3	-2.67	1.33	1.38
37	B5	1720	PSU	C4-N3	-2.67	1.33	1.38
37	B5	1683	PSU	C4-N3	-2.66	1.33	1.38
37	B5	3496	PSU	C4-N3	-2.66	1.33	1.38
37	B5	3502	PSU	C4-N3	-2.66	1.33	1.38
37	B5	3371	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1368	PSU	C4-N3	-2.66	1.33	1.38
37	B5	3554	PSU	C4-N3	-2.66	1.33	1.38
37	B5	4045	PSU	C4-N3	-2.66	1.33	1.38
1	A2	802	PSU	C4-N3	-2.66	1.33	1.38
1	A2	218	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.66	1.33	1.38
37	B5	3447	PSU	C4-N3	-2.66	1.33	1.38
37	B5	1537	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1245	PSU	C4-N3	-2.65	1.33	1.38
37	B5	4749	PSU	C4-N3	-2.65	1.33	1.38
1	A2	1239	PSU	C4-N3	-2.65	1.33	1.38
1	A2	687	PSU	C4-N3	-2.65	1.33	1.38
37	B5	1731	PSU	C4-N3	-2.65	1.33	1.38
37	B5	4278	PSU	C4-N3	-2.65	1.33	1.38
37	B5	2475	PSU	C4-N3	-2.64	1.33	1.38
37	B5	3500	PSU	C4-N3	-2.64	1.33	1.38
37	B5	4169	PSU	C4-N3	-2.64	1.33	1.38
39	B8	69	PSU	C4-N3	-2.64	1.33	1.38
37	B5	3462	PSU	C4-N3	-2.64	1.33	1.38
37	B5	3427	PSU	C4-N3	-2.64	1.33	1.38
37	B5	4166	PSU	C4-N3	-2.63	1.34	1.38
37	B5	4322	PSU	C4-N3	-2.63	1.34	1.38
1	A2	967	PSU	C4-N3	-2.63	1.34	1.38
39	B8	55	PSU	C4-N3	-2.63	1.34	1.38
1	A2	1626	PSU	C4-N3	-2.63	1.34	1.38
1	A2	610	PSU	C4-N3	-2.63	1.34	1.38
9	AT	55	PSU	C4-N3	-2.63	1.34	1.38
1	A2	109	PSU	C4-N3	-2.62	1.34	1.38
37	B5	1718	PSU	C4-N3	-2.62	1.34	1.38
1	A2	823	PSU	C4-N3	-2.62	1.34	1.38
37	B5	3494	PSU	C4-N3	-2.61	1.34	1.38
1	A2	210	PSU	C4-N3	-2.60	1.34	1.38
37	B5	1632	PSU	C4-N3	-2.60	1.34	1.38
37	B5	4366	OMU	C4-N3	-2.59	1.33	1.38
1	A2	429	OMU	C4-N3	-2.58	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	3466	PSU	C4-N3	-2.57	1.34	1.38
37	B5	3973	OMU	C4-N3	-2.56	1.34	1.38
9	AT	54	5MU	C4-N3	-2.56	1.34	1.38
37	B5	3657	OMU	C4-N3	-2.55	1.34	1.38
37	B5	1477	OMG	C6-N1	-2.55	1.34	1.37
37	B5	4244	OMU	C4-N3	-2.55	1.34	1.38
1	A2	355	OMU	C4-N3	-2.54	1.34	1.38
37	B5	2680	OMU	C4-N3	-2.53	1.34	1.38
37	B5	2258	OMU	C4-N3	-2.52	1.34	1.38
37	B5	2719	OMG	C6-N1	-2.52	1.34	1.37
1	A2	591	A2M	C5-C4	2.52	1.47	1.40
37	B5	3942	OMG	C6-N1	-2.52	1.34	1.37
37	B5	1580	OMG	C6-N1	-2.51	1.34	1.37
1	A2	172	OMU	C4-N3	-2.51	1.34	1.38
1	A2	1491	OMG	C6-N1	-2.51	1.34	1.37
37	B5	4138	OMG	C6-N1	-2.50	1.34	1.37
1	A2	1443	OMU	C4-N3	-2.50	1.34	1.38
1	A2	1805	OMU	C4-N3	-2.50	1.34	1.38
37	B5	4364	OMG	C6-N1	-2.50	1.34	1.37
1	A2	469	A2M	C5-C4	2.50	1.47	1.40
1	A2	121	OMU	C4-N3	-2.49	1.34	1.38
37	B5	2267	OMG	C6-N1	-2.49	1.34	1.37
1	A2	116	OMU	C4-N3	-2.48	1.34	1.38
37	B5	3492	A2M	C5-C4	2.48	1.47	1.40
39	B8	75	OMG	C6-N1	-2.48	1.34	1.37
1	A2	510	OMG	C6-N1	-2.48	1.34	1.37
37	B5	4116	OMG	C6-N1	-2.47	1.34	1.37
1	A2	645	OMG	C6-N1	-2.46	1.34	1.37
37	B5	4369	OMG	C6-N1	-2.46	1.34	1.37
1	A2	1833	6MZ	C5-C4	2.46	1.47	1.40
37	B5	2658	A2M	C5-C4	2.45	1.47	1.40
37	B5	3359	OMG	C6-N1	-2.45	1.34	1.37
1	A2	159	A2M	C5-C4	2.45	1.47	1.40
37	B5	3599	A2M	C5-C4	2.45	1.47	1.40
1	A2	1289	OMU	C4-N3	-2.45	1.34	1.38
37	B5	3524	OMG	C6-N1	-2.45	1.34	1.37
1	A2	577	A2M	C5-C4	2.45	1.47	1.40
37	B5	1260	OMG	C6-N1	-2.45	1.34	1.37
1	A2	485	A2M	C5-C4	2.44	1.47	1.40
1	A2	27	A2M	C5-C4	2.44	1.47	1.40
1	A2	437	OMG	C6-N1	-2.44	1.34	1.37
37	B5	4317	A2M	C5-C4	2.44	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1384	A2M	C5-C4	2.44	1.47	1.40
37	B5	3974	OMG	C6-N1	-2.44	1.34	1.37
1	A2	1249	B8N	C2-N3	-2.44	1.34	1.38
1	A2	1329	OMG	C6-N1	-2.44	1.34	1.37
1	A2	602	OMG	C6-N1	-2.43	1.34	1.37
37	B5	3631	OMG	C6-N1	-2.43	1.34	1.37
37	B5	4240	OMG	C6-N1	-2.43	1.34	1.37
37	B5	3456	A2M	C5-C4	2.43	1.47	1.40
37	B5	2244	A2M	C5-C4	2.43	1.47	1.40
37	B5	2630	A2M	C5-C4	2.43	1.47	1.40
1	A2	513	A2M	C5-C4	2.43	1.47	1.40
37	B5	3450	A2M	C5-C4	2.43	1.47	1.40
37	B5	400	A2M	C5-C4	2.43	1.47	1.40
1	A2	1032	A2M	C5-C4	2.42	1.47	1.40
37	B5	4245	OMG	C6-N1	-2.42	1.34	1.37
37	B5	1479	A2M	C5-C4	2.42	1.47	1.40
37	B5	3966	6MZ	C5-C4	2.42	1.47	1.40
1	A2	684	OMG	C6-N1	-2.42	1.34	1.37
1	A2	99	A2M	C5-C4	2.42	1.47	1.40
1	A2	1327	OMU	C4-N3	-2.42	1.34	1.38
37	B5	3557	A2M	C5-C4	2.41	1.47	1.40
37	B5	4383	OMG	C6-N1	-2.41	1.34	1.37
1	A2	166	A2M	C5-C4	2.41	1.47	1.40
37	B5	398	A2M	C5-C4	2.41	1.47	1.40
37	B5	2207	OMG	C6-N1	-2.41	1.34	1.37
37	B5	3676	OMG	C6-N1	-2.40	1.34	1.37
37	B5	3562	A2M	C5-C4	2.40	1.47	1.40
37	B5	4336	A2M	C5-C4	2.40	1.47	1.40
1	A2	1679	A2M	C5-C4	2.40	1.47	1.40
37	B5	1810	A2M	C5-C4	2.39	1.47	1.40
37	B5	3476	OMG	C6-N1	-2.39	1.34	1.37
1	A2	669	A2M	C5-C4	2.38	1.47	1.40
37	B5	2206	A2M	C5-C4	2.38	1.47	1.40
1	A2	1448	OMG	C6-N1	-2.37	1.34	1.37
37	B5	1270	A2M	C5-C4	2.37	1.47	1.40
37	B5	1489	A2M	C5-C4	2.36	1.47	1.40
9	AT	54	5MU	C4-C5	2.36	1.48	1.44
1	A2	868	OMG	C6-N1	-2.36	1.34	1.37
37	B5	3517	A2M	C5-C4	2.34	1.47	1.40
33	Aw	62	HY3	C5-N	2.32	1.57	1.49
37	B5	3514	5MC	C6-N1	-2.30	1.34	1.38
37	B5	4193	5MC	C6-N1	-2.29	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	3657	OMU	C2-N3	-2.27	1.33	1.38
1	A2	355	OMU	C2-N3	-2.23	1.34	1.38
37	B5	2680	OMU	C2-N3	-2.22	1.34	1.38
1	A2	1843	4AC	C7-N4	-2.22	1.33	1.37
37	B5	3973	OMU	C2-N3	-2.22	1.34	1.38
9	AT	54	5MU	C6-N1	-2.20	1.34	1.38
37	B5	2258	OMU	C2-N3	-2.20	1.34	1.38
1	A2	121	OMU	C2-N3	-2.19	1.34	1.38
37	B5	4366	OMU	C2-N3	-2.18	1.34	1.38
1	A2	116	OMU	C2-N3	-2.18	1.34	1.38
9	AT	54	5MU	C2-N1	2.18	1.41	1.38
1	A2	172	OMU	C2-N3	-2.18	1.34	1.38
1	A2	1851	MA6	C4-N3	-2.17	1.32	1.35
37	B5	4244	OMU	C2-N3	-2.14	1.34	1.38
1	A2	1805	OMU	C2-N3	-2.14	1.34	1.38
37	B5	3550	UY1	C6-N1	-2.14	1.32	1.36
1	A2	429	OMU	C2-N3	-2.12	1.34	1.38
1	A2	1443	OMU	C2-N3	-2.12	1.34	1.38
1	A2	1805	OMU	C2-N1	2.12	1.41	1.38
1	A2	1289	OMU	C2-N1	2.11	1.41	1.38
1	A2	1852	MA6	C4-N3	-2.11	1.32	1.35
1	A2	1289	OMU	C2-N3	-2.11	1.34	1.38
1	A2	1338	4AC	C7-N4	-2.11	1.33	1.37
1	A2	1327	OMU	C2-N3	-2.09	1.34	1.38
1	A2	429	OMU	C2-N1	2.08	1.41	1.38
1	A2	1443	OMU	C2-N1	2.07	1.41	1.38
37	B5	3973	OMU	C2-N1	2.02	1.41	1.38
37	B5	2258	OMU	C2-N1	2.01	1.41	1.38
1	A2	121	OMU	C5-C4	-2.01	1.39	1.43
9	AT	54	5MU	C2-N3	-2.01	1.34	1.38
1	A2	1443	OMU	C5-C4	-2.00	1.39	1.43

All (528) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	3369	PSU	N1-C2-N3	6.11	122.06	115.13
37	B5	4435	PSU	N1-C2-N3	6.09	122.03	115.13
37	B5	4325	PSU	N1-C2-N3	6.09	122.03	115.13
37	B5	4298	PSU	N1-C2-N3	6.08	122.02	115.13
37	B5	4246	PSU	N1-C2-N3	6.08	122.02	115.13
1	A2	967	PSU	N1-C2-N3	6.07	122.01	115.13
37	B5	2351	PSU	N1-C2-N3	6.05	121.99	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4749	PSU	N1-C2-N3	6.04	121.97	115.13
37	B5	1683	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	652	PSU	N1-C2-N3	6.02	121.96	115.13
37	B5	4149	PSU	N1-C2-N3	6.02	121.95	115.13
1	A2	610	PSU	N1-C2-N3	6.01	121.94	115.13
37	B5	3447	PSU	N1-C2-N3	6.01	121.94	115.13
37	B5	4042	PSU	N1-C2-N3	6.01	121.94	115.13
37	B5	3616	PSU	N1-C2-N3	6.00	121.93	115.13
37	B5	4039	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	573	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	682	PSU	N1-C2-N3	6.00	121.92	115.13
39	B8	69	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	105	PSU	N1-C2-N3	5.99	121.92	115.13
37	B5	3494	PSU	N1-C2-N3	5.99	121.91	115.13
1	A2	1178	PSU	N1-C2-N3	5.99	121.91	115.13
37	B5	2475	PSU	N1-C2-N3	5.99	121.91	115.13
1	A2	109	PSU	N1-C2-N3	5.99	121.91	115.13
1	A2	1368	PSU	N1-C2-N3	5.98	121.91	115.13
37	B5	3371	PSU	N1-C2-N3	5.98	121.91	115.13
37	B5	3500	PSU	N1-C2-N3	5.98	121.91	115.13
39	B8	55	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	1175	PSU	N1-C2-N3	5.98	121.91	115.13
37	B5	4711	PSU	N1-C2-N3	5.98	121.90	115.13
37	B5	3585	PSU	N1-C2-N3	5.98	121.90	115.13
1	A2	650	PSU	N1-C2-N3	5.98	121.90	115.13
37	B5	4177	PSU	N1-C2-N3	5.98	121.90	115.13
37	B5	3427	PSU	N1-C2-N3	5.97	121.90	115.13
1	A2	687	PSU	N1-C2-N3	5.97	121.90	115.13
1	A2	1005	PSU	N1-C2-N3	5.97	121.90	115.13
37	B5	4267	PSU	N1-C2-N3	5.97	121.90	115.13
37	B5	4419	PSU	N1-C2-N3	5.97	121.90	115.13
37	B5	4278	PSU	N1-C2-N3	5.97	121.89	115.13
37	B5	1801	PSU	N1-C2-N3	5.97	121.89	115.13
37	B5	3583	PSU	N1-C2-N3	5.97	121.89	115.13
1	A2	93	PSU	N1-C2-N3	5.97	121.89	115.13
37	B5	4188	PSU	N1-C2-N3	5.97	121.89	115.13
1	A2	1057	PSU	N1-C2-N3	5.96	121.89	115.13
37	B5	4374	PSU	N1-C2-N3	5.96	121.89	115.13
1	A2	36	PSU	N1-C2-N3	5.96	121.89	115.13
37	B5	4045	PSU	N1-C2-N3	5.96	121.88	115.13
37	B5	4169	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	802	PSU	N1-C2-N3	5.96	121.88	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	3502	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	34	PSU	N1-C2-N3	5.96	121.88	115.13
37	B5	3576	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	1245	PSU	N1-C2-N3	5.95	121.88	115.13
37	B5	3554	PSU	N1-C2-N3	5.95	121.88	115.13
37	B5	4058	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	864	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	1446	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	1047	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	407	PSU	N1-C2-N3	5.95	121.87	115.13
37	B5	1491	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	1644	PSU	N1-C2-N3	5.95	121.87	115.13
37	B5	4099	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	1239	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	1233	PSU	N1-C2-N3	5.94	121.86	115.13
37	B5	1720	PSU	N1-C2-N3	5.93	121.85	115.13
37	B5	3462	PSU	N1-C2-N3	5.93	121.85	115.13
37	B5	1537	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	119	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	1046	PSU	N1-C2-N3	5.93	121.85	115.13
37	B5	1718	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	867	PSU	N1-C2-N3	5.93	121.85	115.13
37	B5	3466	PSU	N1-C2-N3	5.92	121.84	115.13
37	B5	3490	PSU	N1-C2-N3	5.92	121.84	115.13
37	B5	4217	PSU	N1-C2-N3	5.92	121.84	115.13
37	B5	4276	UR3	C4-N3-C2	-5.92	118.99	124.56
37	B5	1632	PSU	N1-C2-N3	5.92	121.83	115.13
37	B5	4166	PSU	N1-C2-N3	5.92	121.83	115.13
37	B5	1721	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	816	PSU	N1-C2-N3	5.91	121.83	115.13
37	B5	3496	PSU	N1-C2-N3	5.91	121.82	115.13
37	B5	1731	PSU	N1-C2-N3	5.91	121.82	115.13
1	A2	1626	PSU	N1-C2-N3	5.90	121.82	115.13
37	B5	4107	PSU	N1-C2-N3	5.90	121.81	115.13
37	B5	4740	PSU	N1-C2-N3	5.90	121.81	115.13
9	AT	55	PSU	N1-C2-N3	5.90	121.81	115.13
37	B5	1799	PSU	N1-C2-N3	5.90	121.81	115.13
37	B5	3652	PSU	N1-C2-N3	5.90	121.81	115.13
37	B5	4382	PSU	N1-C2-N3	5.90	121.81	115.13
1	A2	815	PSU	N1-C2-N3	5.90	121.81	115.13
1	A2	1693	PSU	N1-C2-N3	5.90	121.81	115.13
37	B5	4322	PSU	N1-C2-N3	5.88	121.79	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1082	PSU	N1-C2-N3	5.87	121.78	115.13
37	B5	3966	6MZ	C2-N1-C6	5.87	121.62	116.59
1	A2	218	PSU	N1-C2-N3	5.86	121.77	115.13
37	B5	4203	PSU	N1-C2-N3	5.86	121.76	115.13
1	A2	823	PSU	N1-C2-N3	5.85	121.76	115.13
1	A2	210	PSU	N1-C2-N3	5.84	121.75	115.13
1	A2	1851	MA6	C4-C5-N7	-5.80	103.35	109.40
1	A2	1833	6MZ	C2-N1-C6	5.67	121.45	116.59
1	A2	1852	MA6	C4-C5-N7	-5.54	103.62	109.40
37	B5	3550	UY1	C4-N3-C2	-5.20	118.85	126.34
9	AT	54	5MU	C4-N3-C2	-5.14	120.70	127.35
9	AT	54	5MU	N3-C2-N1	4.90	121.40	114.89
1	A2	1843	4AC	N4-C4-N3	4.71	121.76	113.85
1	A2	1327	OMU	C4-N3-C2	-4.58	120.54	126.58
37	B5	3657	OMU	C4-N3-C2	-4.53	120.60	126.58
37	B5	4244	OMU	C4-N3-C2	-4.48	120.67	126.58
1	A2	1851	MA6	C1'-N9-C4	-4.47	118.79	126.64
1	A2	172	OMU	C4-N3-C2	-4.46	120.69	126.58
37	B5	2680	OMU	C4-N3-C2	-4.46	120.70	126.58
1	A2	355	OMU	C4-N3-C2	-4.43	120.74	126.58
37	B5	4366	OMU	C4-N3-C2	-4.43	120.74	126.58
1	A2	121	OMU	C4-N3-C2	-4.42	120.75	126.58
37	B5	2258	OMU	C4-N3-C2	-4.39	120.78	126.58
1	A2	1805	OMU	C4-N3-C2	-4.39	120.79	126.58
9	AT	54	5MU	C5-C4-N3	4.37	119.05	115.31
37	B5	3973	OMU	C4-N3-C2	-4.37	120.81	126.58
1	A2	429	OMU	C4-N3-C2	-4.34	120.86	126.58
1	A2	116	OMU	C4-N3-C2	-4.32	120.89	126.58
1	A2	1289	OMU	C4-N3-C2	-4.31	120.90	126.58
1	A2	1338	4AC	N4-C4-N3	4.31	121.08	113.85
1	A2	1443	OMU	C4-N3-C2	-4.30	120.91	126.58
1	A2	1851	MA6	N3-C2-N1	-4.27	122.00	128.68
1	A2	1852	MA6	N3-C2-N1	-4.23	122.07	128.68
37	B5	4244	OMU	N3-C2-N1	4.16	120.41	114.89
1	A2	1852	MA6	C1'-N9-C4	-4.15	119.34	126.64
1	A2	355	OMU	N3-C2-N1	4.15	120.40	114.89
37	B5	3550	UY1	N1-C2-N3	4.14	119.82	115.13
37	B5	3657	OMU	N3-C2-N1	4.14	120.38	114.89
37	B5	2680	OMU	N3-C2-N1	4.10	120.33	114.89
1	A2	1805	OMU	N3-C2-N1	4.10	120.33	114.89
37	B5	4366	OMU	N3-C2-N1	4.09	120.32	114.89
1	A2	172	OMU	N3-C2-N1	4.08	120.31	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1327	OMU	N3-C2-N1	4.07	120.30	114.89
1	A2	121	OMU	N3-C2-N1	4.07	120.29	114.89
37	B5	3973	OMU	N3-C2-N1	4.07	120.29	114.89
1	A2	429	OMU	N3-C2-N1	4.06	120.29	114.89
37	B5	2258	OMU	N3-C2-N1	4.04	120.25	114.89
37	B5	4149	PSU	C4-N3-C2	-4.01	120.56	126.34
37	B5	4419	PSU	C4-N3-C2	-4.01	120.57	126.34
1	A2	116	OMU	N3-C2-N1	4.00	120.20	114.89
37	B5	4325	PSU	C4-N3-C2	-4.00	120.58	126.34
37	B5	4267	PSU	C4-N3-C2	-4.00	120.58	126.34
1	A2	1443	OMU	N3-C2-N1	3.99	120.19	114.89
1	A2	1289	OMU	N3-C2-N1	3.98	120.18	114.89
37	B5	4711	PSU	C4-N3-C2	-3.98	120.61	126.34
37	B5	4246	PSU	C4-N3-C2	-3.97	120.62	126.34
37	B5	4042	PSU	C4-N3-C2	-3.97	120.62	126.34
37	B5	3369	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	652	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	105	PSU	C4-N3-C2	-3.96	120.64	126.34
1	A2	1178	PSU	C4-N3-C2	-3.95	120.64	126.34
37	B5	3576	PSU	C4-N3-C2	-3.95	120.64	126.34
37	B5	4298	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	573	PSU	C4-N3-C2	-3.95	120.65	126.34
37	B5	4749	PSU	C4-N3-C2	-3.95	120.65	126.34
37	B5	1731	PSU	C4-N3-C2	-3.94	120.66	126.34
37	B5	4039	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	1046	PSU	C4-N3-C2	-3.94	120.66	126.34
37	B5	4188	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	1175	PSU	C4-N3-C2	-3.94	120.67	126.34
1	A2	36	PSU	C4-N3-C2	-3.93	120.67	126.34
37	B5	1799	PSU	C4-N3-C2	-3.93	120.67	126.34
1	A2	1233	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B8	55	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B8	69	PSU	C4-N3-C2	-3.93	120.68	126.34
37	B5	4058	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A2	93	PSU	C4-N3-C2	-3.93	120.68	126.34
37	B5	2351	PSU	C4-N3-C2	-3.92	120.69	126.34
37	B5	3554	PSU	C4-N3-C2	-3.92	120.69	126.34
37	B5	4193	5MC	C5-C6-N1	-3.92	119.31	123.34
37	B5	1721	PSU	C4-N3-C2	-3.92	120.69	126.34
37	B5	3616	PSU	C4-N3-C2	-3.92	120.70	126.34
37	B5	1720	PSU	C4-N3-C2	-3.91	120.70	126.34
9	AT	54	5MU	O4-C4-C5	-3.91	120.37	124.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	1683	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	687	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	650	PSU	C4-N3-C2	-3.90	120.71	126.34
9	AT	55	PSU	C4-N3-C2	-3.90	120.71	126.34
37	B5	3371	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	967	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	119	PSU	C4-N3-C2	-3.90	120.72	126.34
37	B5	4217	PSU	C4-N3-C2	-3.90	120.73	126.34
37	B5	4435	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	1057	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	1245	PSU	C4-N3-C2	-3.89	120.73	126.34
37	B5	3427	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	109	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	407	PSU	C4-N3-C2	-3.88	120.75	126.34
37	B5	3502	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	610	PSU	C4-N3-C2	-3.88	120.75	126.34
37	B5	4169	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	1644	PSU	C4-N3-C2	-3.87	120.76	126.34
37	B5	1801	PSU	C4-N3-C2	-3.87	120.76	126.34
1	A2	682	PSU	C4-N3-C2	-3.87	120.76	126.34
37	B5	2475	PSU	C4-N3-C2	-3.87	120.76	126.34
37	B5	3500	PSU	C4-N3-C2	-3.87	120.77	126.34
1	A2	34	PSU	C4-N3-C2	-3.87	120.77	126.34
37	B5	3496	PSU	C4-N3-C2	-3.87	120.77	126.34
1	A2	816	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	864	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	867	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	1368	PSU	C4-N3-C2	-3.86	120.78	126.34
37	B5	1718	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	1005	PSU	C4-N3-C2	-3.86	120.78	126.34
37	B5	4045	PSU	C4-N3-C2	-3.85	120.79	126.34
37	B5	4177	PSU	C4-N3-C2	-3.85	120.79	126.34
37	B5	3585	PSU	C4-N3-C2	-3.85	120.79	126.34
37	B5	4278	PSU	C4-N3-C2	-3.85	120.80	126.34
1	A2	1446	PSU	C4-N3-C2	-3.85	120.80	126.34
37	B5	3462	PSU	C4-N3-C2	-3.84	120.80	126.34
37	B5	4374	PSU	C4-N3-C2	-3.84	120.80	126.34
37	B5	3466	PSU	C4-N3-C2	-3.84	120.81	126.34
37	B5	3447	PSU	C4-N3-C2	-3.83	120.82	126.34
37	B5	1491	PSU	C4-N3-C2	-3.82	120.83	126.34
37	B5	4099	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A2	1693	PSU	C4-N3-C2	-3.82	120.83	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4166	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A2	802	PSU	C4-N3-C2	-3.82	120.84	126.34
1	A2	218	PSU	C4-N3-C2	-3.82	120.84	126.34
1	A2	1082	PSU	C4-N3-C2	-3.82	120.84	126.34
1	A2	1047	PSU	C4-N3-C2	-3.82	120.84	126.34
1	A2	815	PSU	C4-N3-C2	-3.81	120.84	126.34
37	B5	3583	PSU	C4-N3-C2	-3.81	120.85	126.34
37	B5	3490	PSU	C4-N3-C2	-3.81	120.85	126.34
37	B5	3652	PSU	C4-N3-C2	-3.81	120.86	126.34
1	A2	1239	PSU	C4-N3-C2	-3.80	120.86	126.34
37	B5	4203	PSU	C4-N3-C2	-3.80	120.87	126.34
37	B5	4322	PSU	C4-N3-C2	-3.79	120.88	126.34
37	B5	4740	PSU	C4-N3-C2	-3.79	120.88	126.34
37	B5	4382	PSU	C4-N3-C2	-3.77	120.91	126.34
37	B5	1632	PSU	C4-N3-C2	-3.77	120.91	126.34
37	B5	1537	PSU	C4-N3-C2	-3.77	120.91	126.34
37	B5	3494	PSU	C4-N3-C2	-3.76	120.92	126.34
1	A2	1626	PSU	C4-N3-C2	-3.75	120.93	126.34
37	B5	4107	PSU	C4-N3-C2	-3.75	120.94	126.34
1	A2	210	PSU	C4-N3-C2	-3.69	121.02	126.34
9	AT	54	5MU	C5-C6-N1	-3.67	119.56	123.34
1	A2	823	PSU	C4-N3-C2	-3.66	121.07	126.34
1	A2	1327	OMU	C5-C4-N3	3.65	120.31	114.84
37	B5	2680	OMU	C5-C4-N3	3.60	120.23	114.84
37	B5	3657	OMU	C5-C4-N3	3.60	120.22	114.84
1	A2	172	OMU	C5-C4-N3	3.59	120.21	114.84
1	A2	121	OMU	C5-C4-N3	3.58	120.19	114.84
1	A2	429	OMU	C5-C4-N3	3.57	120.18	114.84
37	B5	4366	OMU	C5-C4-N3	3.57	120.18	114.84
37	B5	4244	OMU	C5-C4-N3	3.56	120.17	114.84
37	B5	3973	OMU	C5-C4-N3	3.56	120.17	114.84
37	B5	2258	OMU	C5-C4-N3	3.56	120.16	114.84
1	A2	1289	OMU	C5-C4-N3	3.55	120.15	114.84
1	A2	1805	OMU	C5-C4-N3	3.55	120.15	114.84
1	A2	355	OMU	C5-C4-N3	3.53	120.11	114.84
37	B5	3585	PSU	O2-C2-N1	-3.51	118.92	122.79
1	A2	116	OMU	C5-C4-N3	3.51	120.09	114.84
1	A2	1443	OMU	C5-C4-N3	3.50	120.08	114.84
37	B5	3514	5MC	C5-C6-N1	-3.49	119.75	123.34
37	B5	4435	PSU	O2-C2-N1	-3.48	118.96	122.79
1	A2	407	PSU	O2-C2-N1	-3.48	118.96	122.79
37	B5	4325	PSU	O2-C2-N1	-3.47	118.97	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B8	55	PSU	O2-C2-N1	-3.47	118.97	122.79
37	B5	3616	PSU	O2-C2-N1	-3.47	118.97	122.79
37	B5	4149	PSU	O2-C2-N1	-3.46	118.98	122.79
37	B5	1683	PSU	O2-C2-N1	-3.46	118.98	122.79
37	B5	3447	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	1005	PSU	O2-C2-N1	-3.45	119.00	122.79
37	B5	4267	PSU	O2-C2-N1	-3.45	119.00	122.79
37	B5	3500	PSU	O2-C2-N1	-3.45	119.00	122.79
37	B5	1632	PSU	O2-C2-N1	-3.44	119.00	122.79
1	A2	864	PSU	O2-C2-N1	-3.44	119.00	122.79
37	B5	4169	PSU	O2-C2-N1	-3.44	119.00	122.79
37	B5	3369	PSU	O2-C2-N1	-3.44	119.01	122.79
37	B5	3494	PSU	O2-C2-N1	-3.43	119.01	122.79
37	B5	4246	PSU	O2-C2-N1	-3.43	119.02	122.79
1	A2	573	PSU	O2-C2-N1	-3.42	119.02	122.79
37	B5	3583	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	967	PSU	O2-C2-N1	-3.42	119.03	122.79
37	B5	4058	PSU	O2-C2-N1	-3.42	119.03	122.79
37	B5	3466	PSU	O2-C2-N1	-3.42	119.03	122.79
37	B5	4042	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	652	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	1693	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A2	1446	PSU	O2-C2-N1	-3.41	119.03	122.79
37	B5	2475	PSU	O2-C2-N1	-3.40	119.04	122.79
1	A2	650	PSU	O2-C2-N1	-3.40	119.04	122.79
37	B5	3576	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A2	1368	PSU	O2-C2-N1	-3.40	119.05	122.79
37	B5	4177	PSU	O2-C2-N1	-3.40	119.05	122.79
37	B5	4749	PSU	O2-C2-N1	-3.40	119.05	122.79
37	B5	4298	PSU	O2-C2-N1	-3.39	119.05	122.79
1	A2	210	PSU	O2-C2-N1	-3.39	119.05	122.79
1	A2	823	PSU	O2-C2-N1	-3.39	119.05	122.79
37	B5	3496	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A2	109	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A2	1626	PSU	O2-C2-N1	-3.39	119.06	122.79
37	B5	3371	PSU	O2-C2-N1	-3.38	119.06	122.79
37	B5	4099	PSU	O2-C2-N1	-3.38	119.06	122.79
37	B5	4045	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A2	802	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1175	PSU	O2-C2-N1	-3.38	119.07	122.79
37	B5	4107	PSU	O2-C2-N1	-3.38	119.07	122.79
37	B5	1491	PSU	O2-C2-N1	-3.38	119.07	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4711	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1047	PSU	O2-C2-N1	-3.38	119.07	122.79
37	B5	1799	PSU	O2-C2-N1	-3.38	119.07	122.79
37	B5	2351	PSU	O2-C2-N1	-3.37	119.08	122.79
37	B5	3427	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1057	PSU	O2-C2-N1	-3.37	119.08	122.79
37	B5	3652	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	36	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	119	PSU	O2-C2-N1	-3.37	119.08	122.79
37	B5	1720	PSU	O2-C2-N1	-3.37	119.08	122.79
37	B5	4188	PSU	O2-C2-N1	-3.37	119.08	122.79
37	B5	1718	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	610	PSU	O2-C2-N1	-3.36	119.09	122.79
37	B5	3490	PSU	O2-C2-N1	-3.36	119.09	122.79
37	B5	3462	PSU	O2-C2-N1	-3.36	119.09	122.79
37	B5	4419	PSU	O2-C2-N1	-3.36	119.09	122.79
37	B5	3502	PSU	O2-C2-N1	-3.35	119.10	122.79
37	B5	4278	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1046	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1644	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1245	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1233	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1239	PSU	O2-C2-N1	-3.35	119.11	122.79
39	B8	69	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A2	687	PSU	O2-C2-N1	-3.34	119.11	122.79
37	B5	4166	PSU	O2-C2-N1	-3.34	119.11	122.79
37	B5	4374	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A2	1249	B8N	C4-N3-C2	-3.34	121.23	125.46
37	B5	4382	PSU	O2-C2-N1	-3.34	119.11	122.79
37	B5	4740	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A2	105	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A2	682	PSU	O2-C2-N1	-3.34	119.12	122.79
37	B5	1721	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	815	PSU	O2-C2-N1	-3.33	119.12	122.79
37	B5	1537	PSU	O2-C2-N1	-3.33	119.12	122.79
37	B5	4322	PSU	O2-C2-N1	-3.33	119.13	122.79
1	A2	34	PSU	O2-C2-N1	-3.32	119.13	122.79
9	AT	55	PSU	O2-C2-N1	-3.32	119.13	122.79
37	B5	1801	PSU	O2-C2-N1	-3.32	119.14	122.79
37	B5	1731	PSU	O2-C2-N1	-3.32	119.14	122.79
37	B5	3554	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	1082	PSU	O2-C2-N1	-3.31	119.15	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4217	PSU	O2-C2-N1	-3.31	119.15	122.79
1	A2	218	PSU	O2-C2-N1	-3.30	119.15	122.79
1	A2	816	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A2	1178	PSU	O2-C2-N1	-3.30	119.16	122.79
37	B5	4203	PSU	O2-C2-N1	-3.29	119.17	122.79
37	B5	4039	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	93	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	867	PSU	O2-C2-N1	-3.26	119.20	122.79
37	B5	1489	A2M	N3-C2-N1	-3.24	123.62	128.68
37	B5	3517	A2M	N3-C2-N1	-3.23	123.64	128.68
1	A2	513	A2M	N3-C2-N1	-3.23	123.64	128.68
37	B5	1270	A2M	N3-C2-N1	-3.22	123.64	128.68
37	B5	3456	A2M	N3-C2-N1	-3.22	123.64	128.68
37	B5	398	A2M	N3-C2-N1	-3.22	123.65	128.68
1	A2	1032	A2M	N3-C2-N1	-3.22	123.65	128.68
1	A2	1679	A2M	N3-C2-N1	-3.21	123.66	128.68
37	B5	3562	A2M	N3-C2-N1	-3.21	123.66	128.68
1	A2	27	A2M	N3-C2-N1	-3.21	123.66	128.68
37	B5	1479	A2M	N3-C2-N1	-3.21	123.67	128.68
37	B5	4336	A2M	N3-C2-N1	-3.21	123.67	128.68
1	A2	1384	A2M	N3-C2-N1	-3.20	123.68	128.68
1	A2	166	A2M	N3-C2-N1	-3.20	123.68	128.68
37	B5	3966	6MZ	C9-N6-C6	-3.19	120.13	122.87
37	B5	2658	A2M	N3-C2-N1	-3.19	123.70	128.68
1	A2	485	A2M	N3-C2-N1	-3.18	123.70	128.68
37	B5	4317	A2M	N3-C2-N1	-3.18	123.70	128.68
37	B5	3599	A2M	N3-C2-N1	-3.18	123.71	128.68
37	B5	3492	A2M	N3-C2-N1	-3.18	123.71	128.68
1	A2	669	A2M	N3-C2-N1	-3.18	123.71	128.68
1	A2	159	A2M	N3-C2-N1	-3.17	123.72	128.68
1	A2	591	A2M	N3-C2-N1	-3.17	123.73	128.68
37	B5	400	A2M	N3-C2-N1	-3.17	123.73	128.68
1	A2	577	A2M	N3-C2-N1	-3.17	123.73	128.68
37	B5	1810	A2M	N3-C2-N1	-3.16	123.73	128.68
37	B5	3557	A2M	N3-C2-N1	-3.15	123.75	128.68
1	A2	469	A2M	N3-C2-N1	-3.15	123.75	128.68
37	B5	2244	A2M	N3-C2-N1	-3.15	123.76	128.68
37	B5	2630	A2M	N3-C2-N1	-3.15	123.76	128.68
37	B5	2206	A2M	N3-C2-N1	-3.14	123.76	128.68
1	A2	99	A2M	N3-C2-N1	-3.14	123.77	128.68
37	B5	3966	6MZ	N3-C2-N1	-3.13	123.78	128.68
37	B5	3450	A2M	N3-C2-N1	-3.12	123.81	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1833	6MZ	N3-C2-N1	-3.05	123.91	128.68
1	A2	429	OMU	O4-C4-C5	-3.03	119.84	125.16
1	A2	1249	B8N	N3-C2-N1	3.02	121.02	116.76
1	A2	116	OMU	O4-C4-C5	-3.00	119.89	125.16
1	A2	1289	OMU	O4-C4-C5	-2.99	119.90	125.16
37	B5	4366	OMU	O4-C4-C5	-2.99	119.90	125.16
37	B5	2680	OMU	O4-C4-C5	-2.99	119.90	125.16
1	A2	1327	OMU	O4-C4-C5	-2.99	119.90	125.16
1	A2	1443	OMU	O4-C4-C5	-2.99	119.91	125.16
1	A2	355	OMU	O4-C4-C5	-2.97	119.93	125.16
37	B5	3973	OMU	O4-C4-C5	-2.96	119.95	125.16
1	A2	172	OMU	O4-C4-C5	-2.96	119.95	125.16
37	B5	3657	OMU	O4-C4-C5	-2.95	119.96	125.16
1	A2	1640	G7M	C2-N1-C6	-2.95	119.67	125.10
37	B5	2258	OMU	O4-C4-C5	-2.95	119.98	125.16
1	A2	121	OMU	O4-C4-C5	-2.95	119.98	125.16
37	B5	4244	OMU	O4-C4-C5	-2.94	119.99	125.16
1	A2	1805	OMU	O4-C4-C5	-2.94	119.99	125.16
1	A2	166	A2M	C4-C5-N7	-2.84	106.44	109.40
37	B5	1489	A2M	C4-C5-N7	-2.84	106.44	109.40
37	B5	2206	A2M	C4-C5-N7	-2.78	106.50	109.40
37	B5	2244	A2M	C4-C5-N7	-2.74	106.54	109.40
37	B5	4336	A2M	C4-C5-N7	-2.73	106.56	109.40
1	A2	159	A2M	C4-C5-N7	-2.73	106.56	109.40
1	A2	469	A2M	C4-C5-N7	-2.71	106.57	109.40
37	B5	1810	A2M	C4-C5-N7	-2.71	106.58	109.40
1	A2	669	A2M	C4-C5-N7	-2.69	106.59	109.40
1	A2	1679	A2M	C4-C5-N7	-2.68	106.61	109.40
37	B5	3599	A2M	C4-C5-N7	-2.67	106.61	109.40
37	B5	1270	A2M	C4-C5-N7	-2.67	106.61	109.40
1	A2	1032	A2M	C4-C5-N7	-2.67	106.62	109.40
1	A2	99	A2M	C4-C5-N7	-2.66	106.62	109.40
1	A2	27	A2M	C4-C5-N7	-2.66	106.62	109.40
1	A2	513	A2M	C4-C5-N7	-2.66	106.63	109.40
37	B5	3557	A2M	C4-C5-N7	-2.66	106.63	109.40
37	B5	398	A2M	C4-C5-N7	-2.65	106.64	109.40
1	A2	485	A2M	C4-C5-N7	-2.65	106.64	109.40
37	B5	1479	A2M	C4-C5-N7	-2.65	106.64	109.40
37	B5	3456	A2M	C4-C5-N7	-2.65	106.64	109.40
37	B5	2658	A2M	C4-C5-N7	-2.65	106.64	109.40
37	B5	400	A2M	C4-C5-N7	-2.64	106.64	109.40
37	B5	3966	6MZ	C4-C5-N7	-2.64	106.65	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4317	A2M	C4-C5-N7	-2.63	106.66	109.40
37	B5	3550	UY1	CM2-O2'-C2'	-2.63	107.62	114.52
37	B5	3492	A2M	C4-C5-N7	-2.63	106.66	109.40
1	A2	1384	A2M	C4-C5-N7	-2.61	106.68	109.40
1	A2	577	A2M	C4-C5-N7	-2.60	106.69	109.40
37	B5	3450	A2M	C4-C5-N7	-2.59	106.70	109.40
37	B5	3562	A2M	C4-C5-N7	-2.59	106.70	109.40
1	A2	1843	4AC	C5-C4-N4	-2.57	118.45	122.92
37	B5	2630	A2M	C4-C5-N7	-2.57	106.72	109.40
37	B5	3514	5MC	C5-C4-N3	-2.56	118.92	121.67
1	A2	1833	6MZ	C9-N6-C6	-2.55	120.68	122.87
37	B5	3550	UY1	C6-C5-C4	2.54	119.98	118.20
37	B5	3517	A2M	C4-C5-N7	-2.54	106.75	109.40
37	B5	4193	5MC	C5-C4-N3	-2.53	118.95	121.67
1	A2	591	A2M	C4-C5-N7	-2.51	106.78	109.40
40	BA	216	V5N	O-C-CA	-2.43	118.41	124.78
37	B5	3476	OMG	C8-N7-C5	2.37	107.50	102.99
1	A2	684	OMG	C8-N7-C5	2.37	107.50	102.99
37	B5	3631	OMG	C8-N7-C5	2.36	107.49	102.99
37	B5	1260	OMG	C8-N7-C5	2.35	107.47	102.99
37	B5	3359	OMG	C8-N7-C5	2.35	107.46	102.99
37	B5	3524	OMG	C8-N7-C5	2.35	107.46	102.99
37	B5	4369	OMG	C8-N7-C5	2.34	107.46	102.99
37	B5	3524	OMG	C5-C6-N1	2.34	118.08	113.95
1	A2	1329	OMG	C8-N7-C5	2.34	107.45	102.99
37	B5	3514	5MC	O2-C2-N3	-2.33	118.53	122.33
37	B5	4245	OMG	C8-N7-C5	2.33	107.44	102.99
37	B5	3573	OMC	O2-C2-N3	-2.33	118.54	122.33
37	B5	1477	OMG	C8-N7-C5	2.33	107.43	102.99
1	A2	437	OMG	C8-N7-C5	2.33	107.43	102.99
37	B5	1266	1MA	C5-C6-N1	2.33	117.37	113.90
1	A2	645	OMG	C8-N7-C5	2.33	107.42	102.99
37	B5	1580	OMG	C5-C6-N1	2.32	118.06	113.95
37	B5	1266	1MA	C8-N7-C5	2.32	107.42	102.99
65	Ba	39	V5N	O-C-CA	-2.32	118.69	124.78
37	B5	1260	OMG	C5-C6-N1	2.32	118.05	113.95
1	A2	645	OMG	C5-C6-N1	2.32	118.05	113.95
39	B8	75	OMG	C8-N7-C5	2.32	107.42	102.99
37	B5	4383	OMG	C8-N7-C5	2.32	107.41	102.99
37	B5	4138	OMG	C8-N7-C5	2.32	107.41	102.99
37	B5	2207	OMG	C5-C6-N1	2.32	118.05	113.95
1	A2	602	OMG	C8-N7-C5	2.32	107.41	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	2267	OMG	C5-C6-N1	2.32	118.04	113.95
37	B5	3676	OMG	C8-N7-C5	2.32	107.40	102.99
1	A2	1833	6MZ	C4-C5-N7	-2.31	106.99	109.40
37	B5	3631	OMG	C5-C6-N1	2.31	118.04	113.95
1	A2	437	OMG	C5-C6-N1	2.31	118.04	113.95
37	B5	4116	OMG	C8-N7-C5	2.31	107.39	102.99
37	B5	3550	UY1	O2-C2-N1	-2.31	120.25	122.79
37	B5	3942	OMG	C5-C6-N1	2.31	118.02	113.95
37	B5	2267	OMG	C8-N7-C5	2.30	107.38	102.99
37	B5	3942	OMG	C8-N7-C5	2.30	107.38	102.99
37	B5	1580	OMG	C8-N7-C5	2.30	107.38	102.99
1	A2	510	OMG	C8-N7-C5	2.30	107.38	102.99
37	B5	4383	OMG	C5-C6-N1	2.30	118.01	113.95
37	B5	4138	OMG	C5-C6-N1	2.30	118.01	113.95
1	A2	868	OMG	C8-N7-C5	2.29	107.36	102.99
1	A2	1448	OMG	C5-C6-N1	2.29	118.00	113.95
1	A2	1843	4AC	C6-C5-C4	2.29	119.77	116.96
37	B5	2719	OMG	C8-N7-C5	2.29	107.36	102.99
1	A2	1491	OMG	C8-N7-C5	2.29	107.36	102.99
37	B5	3974	OMG	C5-C6-N1	2.29	117.99	113.95
37	B5	4240	OMG	C8-N7-C5	2.29	107.35	102.99
37	B5	2207	OMG	C8-N7-C5	2.29	107.34	102.99
1	A2	1338	4AC	C5-C4-N4	-2.28	118.95	122.92
37	B5	2719	OMG	C5-C6-N1	2.28	117.98	113.95
1	A2	1448	OMG	C8-N7-C5	2.28	107.34	102.99
37	B5	1477	OMG	C5-C6-N1	2.28	117.98	113.95
37	B5	4364	OMG	C8-N7-C5	2.28	107.33	102.99
1	A2	1327	OMU	O2-C2-N1	-2.28	119.76	122.79
37	B5	3974	OMG	C8-N7-C5	2.28	107.33	102.99
39	B8	75	OMG	C5-C6-N1	2.27	117.97	113.95
1	A2	1329	OMG	C5-C6-N1	2.27	117.96	113.95
1	A2	1491	OMG	C5-C6-N1	2.27	117.96	113.95
37	B5	4245	OMG	C5-C6-N1	2.26	117.95	113.95
1	A2	684	OMG	C5-C6-N1	2.26	117.95	113.95
37	B5	4240	OMG	C5-C6-N1	2.26	117.94	113.95
1	A2	602	OMG	C5-C6-N1	2.26	117.94	113.95
37	B5	3476	OMG	C5-C6-N1	2.26	117.94	113.95
1	A2	1338	4AC	C6-C5-C4	2.26	119.72	116.96
37	B5	3359	OMG	C5-C6-N1	2.26	117.94	113.95
37	B5	4116	OMG	C5-C6-N1	2.25	117.93	113.95
37	B5	3676	OMG	C5-C6-N1	2.25	117.92	113.95
1	A2	510	OMG	C5-C6-N1	2.25	117.92	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B5	4369	OMG	C5-C6-N1	2.23	117.89	113.95
37	B5	4364	OMG	C5-C6-N1	2.23	117.89	113.95
1	A2	868	OMG	C5-C6-N1	2.23	117.88	113.95
9	AT	54	5MU	O2-C2-N1	-2.22	119.83	122.79
37	B5	4244	OMU	O2-C2-N1	-2.22	119.84	122.79
37	B5	2265	OMC	O2-C2-N3	-2.22	118.73	122.33
1	A2	1443	OMU	C1'-N1-C2	2.20	121.55	117.57
37	B5	2194	OMC	O2-C2-N3	-2.16	118.82	122.33
1	A2	1249	B8N	C5-C4-N3	2.13	120.12	116.17
37	B5	1632	PSU	O4'-C1'-C2'	2.10	108.10	105.14
1	A2	1392	OMC	O2-C2-N3	-2.06	118.98	122.33
1	A2	518	OMC	O2-C2-N3	-2.05	119.00	122.33
37	B5	4269	A2M	C5-C6-N6	2.05	123.47	120.35
1	A2	105	PSU	C5-C6-N1	-2.04	119.05	122.11
1	A2	1046	PSU	C5-C6-N1	-2.02	119.08	122.11
37	B5	3576	PSU	C5-C6-N1	-2.01	119.10	122.11
1	A2	1805	OMU	C1'-N1-C2	2.00	121.19	117.57

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Aw	62	HY3	O-C-CA-C3
37	B5	1489	A2M	O4'-C4'-C5'-O5'
37	B5	2207	OMG	O4'-C4'-C5'-O5'
37	B5	3433	OMC	C2'-C1'-N1-C2
37	B5	3433	OMC	C2'-C1'-N1-C6
37	B5	4269	A2M	C1'-C2'-O2'-CM'
37	B5	4336	A2M	C4'-C5'-O5'-P
37	B5	4382	PSU	O4'-C1'-C5-C4
37	B5	4382	PSU	O4'-C1'-C5-C6
37	B5	4382	PSU	C3'-C4'-C5'-O5'
40	BA	216	V5N	O-C-CA-CB
41	BB	245	HIC	CA-CB-CG-ND1
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	628	OMU	C1'-C2'-O2'-CM2
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	1249	B8N	N34-C33-C34-O35
1	A2	1338	4AC	N3-C4-N4-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A2	1338	4AC	C5-C4-N4-C7
1	A2	1338	4AC	O7-C7-N4-C4
1	A2	1338	4AC	CM7-C7-N4-C4
1	A2	1448	OMG	C3'-C4'-C5'-O5'
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1843	4AC	C5-C4-N4-C7
1	A2	1843	4AC	O7-C7-N4-C4
1	A2	1843	4AC	CM7-C7-N4-C4
1	A2	429	OMU	O4'-C1'-N1-C2
37	B5	398	A2M	O4'-C4'-C5'-O5'
37	B5	2207	OMG	C3'-C4'-C5'-O5'
37	B5	3517	A2M	O4'-C4'-C5'-O5'
37	B5	3517	A2M	C3'-C4'-C5'-O5'
1	A2	513	A2M	C3'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	669	A2M	C3'-C4'-C5'-O5'
37	B5	1489	A2M	C3'-C4'-C5'-O5'
1	A2	1249	B8N	N34-C33-C34-O36
37	B5	4193	5MC	C2'-C1'-N1-C6
1	A2	429	OMU	O4'-C1'-N1-C6
37	B5	398	A2M	C3'-C4'-C5'-O5'
37	B5	4382	PSU	O4'-C4'-C5'-O5'
1	A2	1448	OMG	O4'-C4'-C5'-O5'
1	A2	1640	G7M	O4'-C4'-C5'-O5'
1	A2	645	OMG	C4'-C5'-O5'-P
1	A2	1704	OMC	C3'-C2'-O2'-CM2
37	B5	4193	5MC	O4'-C1'-N1-C6
1	A2	1640	G7M	C3'-C4'-C5'-O5'
37	B5	3433	OMC	O4'-C1'-N1-C6
1	A2	1249	B8N	C32-C33-C34-O36
37	B5	4193	5MC	C2'-C1'-N1-C2
37	B5	3576	PSU	C4'-C5'-O5'-P
1	A2	1289	OMU	C4'-C5'-O5'-P
1	A2	1852	MA6	C4'-C5'-O5'-P
1	A2	684	OMG	O4'-C4'-C5'-O5'
37	B5	1284	OMC	C3'-C2'-O2'-CM2
37	B5	3476	OMG	C3'-C2'-O2'-CM2
37	B5	3619	OMC	C3'-C2'-O2'-CM2
37	B5	4282	OMC	C3'-C2'-O2'-CM2
37	B5	4383	OMG	C3'-C2'-O2'-CM2
66	Bb	5	MLZ	N-CA-CB-CG
1	A2	1249	B8N	C32-C33-C34-O35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	B5	4246	PSU	C4'-C5'-O5'-P
37	B5	4193	5MC	O4'-C1'-N1-C2
1	A2	1082	PSU	C4'-C5'-O5'-P
37	B5	3550	UY1	C4'-C5'-O5'-P
1	A2	469	A2M	O4'-C4'-C5'-O5'
37	B5	1820	OMC	C3'-C2'-O2'-CM2
37	B5	3676	OMG	C3'-C2'-O2'-CM2
1	A2	437	OMG	C3'-C2'-O2'-CM2
1	A2	868	OMG	C3'-C2'-O2'-CM2
37	B5	3433	OMC	O4'-C1'-N1-C2
37	B5	3619	OMC	C4'-C5'-O5'-P
37	B5	3492	A2M	O4'-C4'-C5'-O5'
37	B5	2194	OMC	O4'-C4'-C5'-O5'
37	B5	2265	OMC	C3'-C2'-O2'-CM2
37	B5	4366	OMU	C3'-C2'-O2'-CM2
1	A2	591	A2M	C3'-C4'-C5'-O5'
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	159	A2M	O4'-C4'-C5'-O5'
1	A2	485	A2M	O4'-C4'-C5'-O5'
1	A2	510	OMG	O4'-C4'-C5'-O5'
1	A2	1852	MA6	C3'-C4'-C5'-O5'
37	B5	2667	OMC	C1'-C2'-O2'-CM2
39	B8	75	OMG	C1'-C2'-O2'-CM2
37	B5	2667	OMC	C3'-C2'-O2'-CM2
39	B8	75	OMG	C3'-C2'-O2'-CM2
37	B5	2667	OMC	O4'-C4'-C5'-O5'
1	A2	116	OMU	O4'-C4'-C5'-O5'
1	A2	1704	OMC	O4'-C4'-C5'-O5'
37	B5	3631	OMG	C3'-C2'-O2'-CM2
1	A2	355	OMU	C3'-C2'-O2'-CM2
1	A2	684	OMG	C3'-C4'-C5'-O5'
41	BB	245	HIC	CA-CB-CG-CD2
37	B5	2194	OMC	C2'-C1'-N1-C2
37	B5	3573	OMC	C2'-C1'-N1-C2

There are no ring outliers.

82 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	3631	OMG	1	0
37	B5	3462	PSU	1	0
37	B5	2244	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	3456	A2M	1	0
1	A2	355	OMU	1	0
37	B5	3599	A2M	1	0
1	A2	1704	OMC	1	0
37	B5	2207	OMG	1	0
1	A2	121	OMU	2	0
37	B5	3942	OMG	3	0
37	B5	1718	PSU	1	0
1	A2	116	OMU	1	0
37	B5	3974	OMG	1	0
37	B5	1260	OMG	2	0
1	A2	868	OMG	1	0
37	B5	2258	OMU	2	0
1	A2	1392	OMC	1	0
1	A2	513	A2M	1	0
37	B5	2658	A2M	1	0
1	A2	823	PSU	1	0
37	B5	3619	OMC	1	0
37	B5	1810	A2M	2	0
1	A2	1289	OMU	2	0
37	B5	1284	OMC	2	0
1	A2	166	A2M	2	0
1	A2	1805	OMU	1	0
1	A2	1448	OMG	2	0
37	B5	3450	A2M	2	0
1	A2	1843	4AC	2	0
37	B5	2647	OMC	1	0
37	B5	2194	OMC	1	0
37	B5	3476	OMG	1	0
37	B5	4058	PSU	1	0
1	A2	1032	A2M	1	0
37	B5	2208	OMC	1	0
1	A2	469	A2M	1	0
1	A2	1491	OMG	1	0
1	A2	577	A2M	2	0
37	B5	4039	PSU	1	0
37	B5	4383	OMG	1	0
1	A2	172	OMU	1	0
1	A2	510	OMG	1	0
1	A2	1679	A2M	2	0
37	B5	2206	A2M	1	0
37	B5	400	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B5	398	A2M	1	0
37	B5	3540	OMC	1	0
37	B5	4366	OMU	2	0
37	B5	3502	PSU	1	0
65	Ba	39	V5N	1	0
1	A2	628	OMU	1	0
1	A2	602	OMG	1	0
37	B5	4193	5MC	1	0
37	B5	3562	A2M	2	0
37	B5	3652	PSU	1	0
37	B5	2704	OMC	1	0
37	B5	3585	PSU	1	0
37	B5	4336	A2M	1	0
37	B5	3550	UY1	2	0
37	B5	4282	OMC	1	0
39	B8	75	OMG	2	0
37	B5	4203	PSU	1	0
37	B5	3973	OMU	2	0
37	B5	4149	PSU	1	0
37	B5	3524	OMG	1	0
1	A2	99	A2M	2	0
1	A2	518	OMC	1	0
37	B5	4138	OMG	2	0
1	A2	27	A2M	1	0
37	B5	3557	A2M	1	0
37	B5	3676	OMG	1	0
1	A2	1443	OMU	1	0
37	B5	4202	OMC	1	0
1	A2	1640	G7M	1	0
37	B5	1270	A2M	1	0
1	A2	1338	4AC	4	0
37	B5	2267	OMG	1	0
1	A2	437	OMG	2	0
1	A2	463	OMC	1	0
37	B5	3573	OMC	1	0
1	A2	1329	OMG	1	0
1	A2	1833	6MZ	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 635 ligands modelled in this entry, 415 are monoatomic and 187 are unknown - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	B5	5178	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	A2	2036	-	9,9,9	0.15	0	8,8,8	0.15	0
89	SPD	B5	5194	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	A2	2043	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5184	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5181	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	B5	5188	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	B5	5191	-	9,9,9	0.15	0	8,8,8	0.14	0
89	SPD	B5	5180	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5192	-	9,9,9	0.16	0	8,8,8	0.17	0
89	SPD	B5	5179	-	9,9,9	0.15	0	8,8,8	0.16	0
90	SPM	A2	2044	-	13,13,13	0.15	0	12,12,12	0.14	0
89	SPD	A2	2039	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5190	-	9,9,9	0.16	0	8,8,8	0.17	0
90	SPM	B5	5143	-	13,13,13	0.14	0	12,12,12	0.15	0
89	SPD	B5	5186	-	9,9,9	0.15	0	8,8,8	0.21	0
90	SPM	B5	5142	-	13,13,13	0.15	0	12,12,12	0.24	0
89	SPD	B5	5185	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5182	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	B5	5176	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5177	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	A2	2041	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	A2	2038	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	A2	2040	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	A2	2042	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5183	-	9,9,9	0.15	0	8,8,8	0.19	0
89	SPD	A2	2037	-	9,9,9	0.15	0	8,8,8	0.20	0
89	SPD	B5	5175	-	9,9,9	0.15	0	8,8,8	0.18	0
89	SPD	B5	5187	-	9,9,9	0.15	0	8,8,8	0.17	0
89	SPD	B5	5196	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5195	-	9,9,9	0.15	0	8,8,8	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	SPD	B5	5189	-	9,9,9	0.16	0	8,8,8	0.18	0
89	SPD	B5	5193	-	9,9,9	0.15	0	8,8,8	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	B5	5178	-	-	0/7/7/7	-
89	SPD	A2	2036	-	-	0/7/7/7	-
89	SPD	B5	5194	-	-	0/7/7/7	-
89	SPD	A2	2043	-	-	0/7/7/7	-
89	SPD	B5	5184	-	-	0/7/7/7	-
89	SPD	B5	5181	-	-	0/7/7/7	-
89	SPD	B5	5188	-	-	1/7/7/7	-
89	SPD	B5	5191	-	-	1/7/7/7	-
89	SPD	B5	5180	-	-	0/7/7/7	-
89	SPD	B5	5192	-	-	2/7/7/7	-
89	SPD	B5	5179	-	-	1/7/7/7	-
90	SPM	A2	2044	-	-	1/11/11/11	-
89	SPD	A2	2039	-	-	0/7/7/7	-
89	SPD	B5	5190	-	-	1/7/7/7	-
90	SPM	B5	5143	-	-	0/11/11/11	-
89	SPD	B5	5186	-	-	0/7/7/7	-
90	SPM	B5	5142	-	-	1/11/11/11	-
89	SPD	B5	5185	-	-	0/7/7/7	-
89	SPD	B5	5182	-	-	0/7/7/7	-
89	SPD	B5	5176	-	-	0/7/7/7	-
89	SPD	B5	5177	-	-	0/7/7/7	-
89	SPD	A2	2041	-	-	1/7/7/7	-
89	SPD	A2	2038	-	-	0/7/7/7	-
89	SPD	A2	2040	-	-	0/7/7/7	-
89	SPD	A2	2042	-	-	1/7/7/7	-
89	SPD	B5	5183	-	-	0/7/7/7	-
89	SPD	A2	2037	-	-	0/7/7/7	-
89	SPD	B5	5175	-	-	0/7/7/7	-
89	SPD	B5	5187	-	-	0/7/7/7	-
89	SPD	B5	5196	-	-	1/7/7/7	-
89	SPD	B5	5195	-	-	1/7/7/7	-
89	SPD	B5	5189	-	-	0/7/7/7	-
89	SPD	B5	5193	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	A2	2044	SPM	C8-C9-N10-C11
89	B5	5190	SPD	C2-C3-C4-C5
90	B5	5142	SPM	C8-C9-N10-C11
89	B5	5192	SPD	C2-C3-C4-C5
89	A2	2041	SPD	C2-C3-C4-C5
89	B5	5195	SPD	C2-C3-C4-C5
89	B5	5191	SPD	C2-C3-C4-C5
89	B5	5196	SPD	C2-C3-C4-C5
89	B5	5193	SPD	C2-C3-C4-C5
89	A2	2042	SPD	C2-C3-C4-C5
89	B5	5192	SPD	C4-C5-N6-C7
89	B5	5179	SPD	C2-C3-C4-C5
89	B5	5188	SPD	C2-C3-C4-C5

There are no ring outliers.

20 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B5	5178	SPD	3	0
89	B5	5188	SPD	1	0
89	B5	5179	SPD	1	0
90	A2	2044	SPM	1	0
89	A2	2039	SPD	1	0
89	B5	5190	SPD	1	0
89	B5	5186	SPD	1	0
90	B5	5142	SPM	2	0
89	B5	5185	SPD	3	0
89	B5	5182	SPD	1	0
89	B5	5176	SPD	1	0
89	B5	5177	SPD	1	0
89	A2	2041	SPD	1	0
89	A2	2038	SPD	2	0
89	A2	2042	SPD	1	0
89	B5	5183	SPD	3	0
89	A2	2037	SPD	1	0
89	B5	5175	SPD	1	0
89	B5	5195	SPD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	B5	5193	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

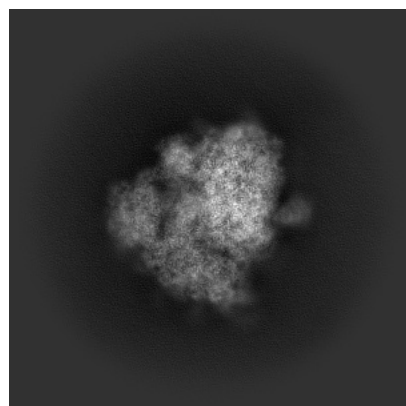
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53295. These allow visual inspection of the internal detail of the map and identification of artifacts.

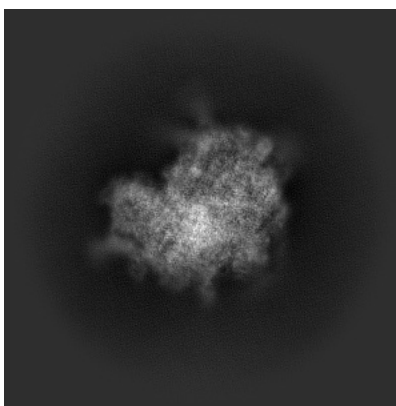
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

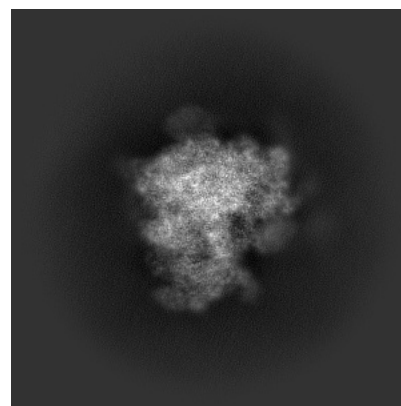
6.1.1 Primary map



X

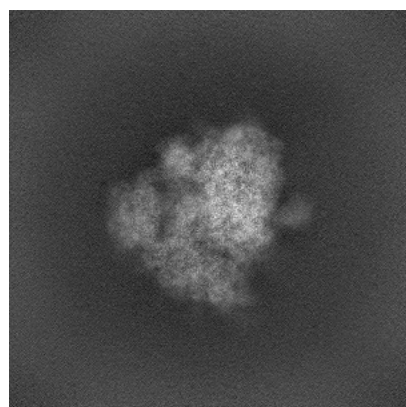


Y

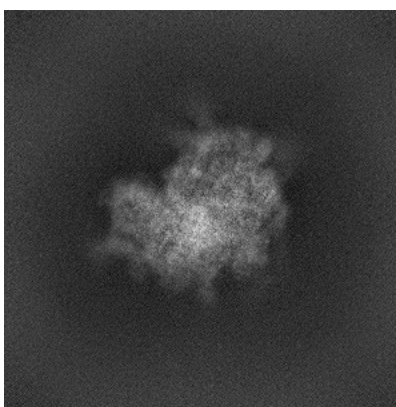


Z

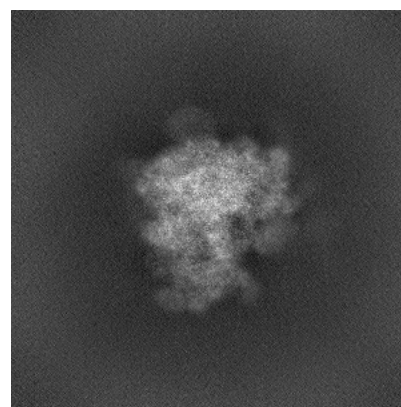
6.1.2 Raw map



X



Y

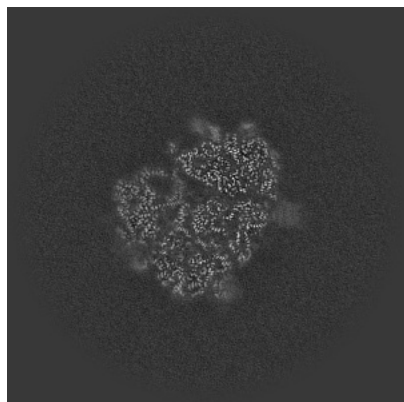


Z

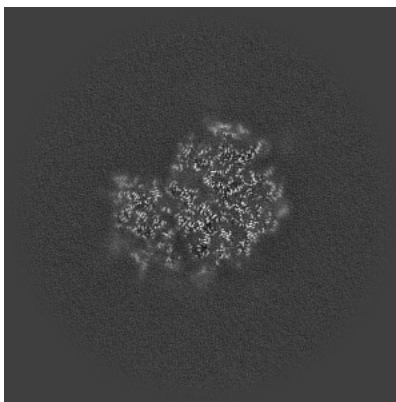
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

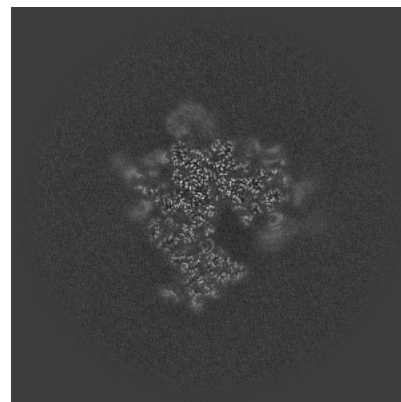
6.2.1 Primary map



X Index: 280

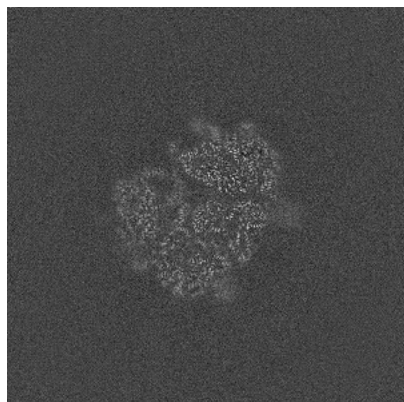


Y Index: 280

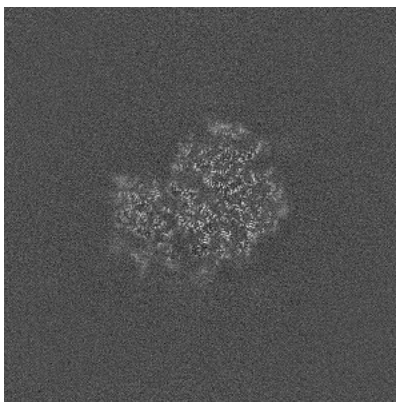


Z Index: 280

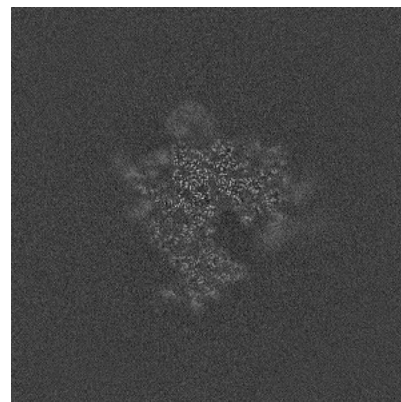
6.2.2 Raw map



X Index: 280



Y Index: 280

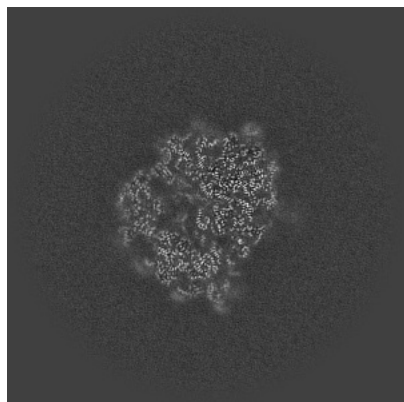


Z Index: 280

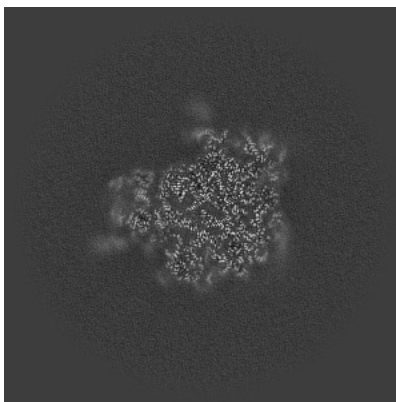
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

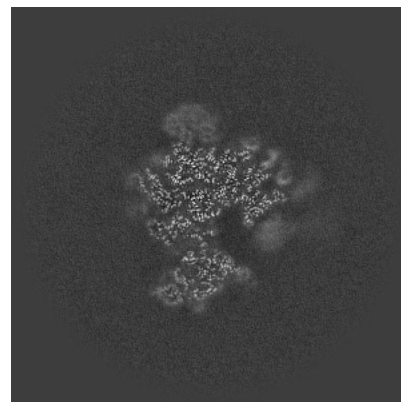
6.3.1 Primary map



X Index: 288

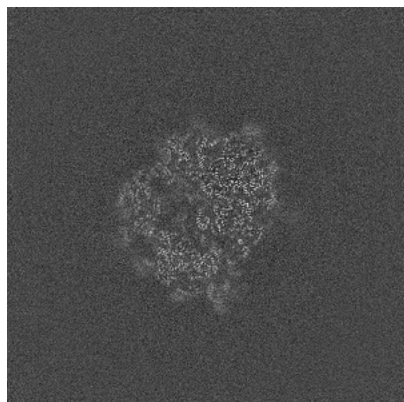


Y Index: 313

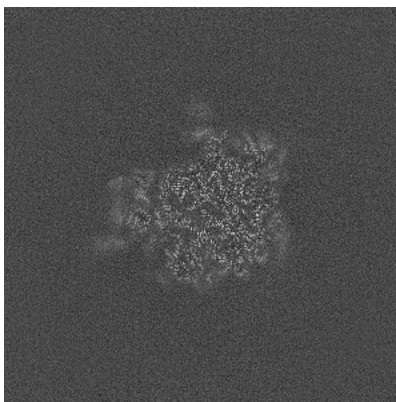


Z Index: 272

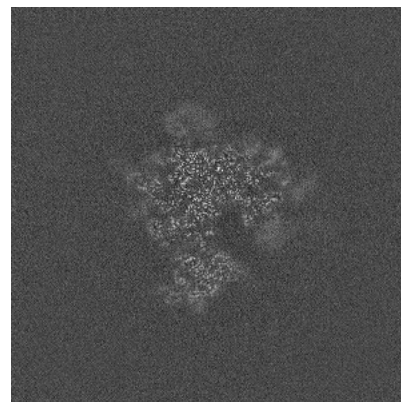
6.3.2 Raw map



X Index: 288



Y Index: 313

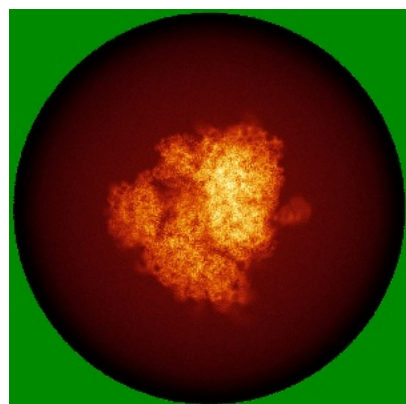


Z Index: 275

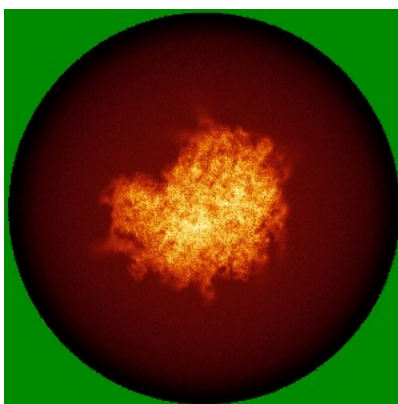
The images above show the largest variance slices of the map in three orthogonal directions.

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

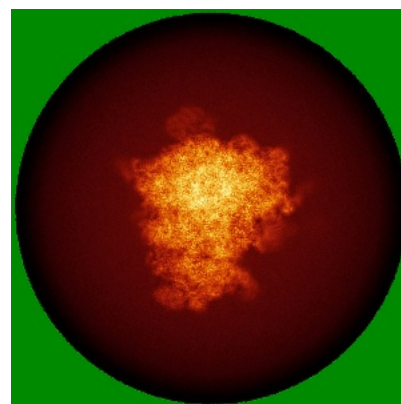
6.4.1 Primary map



X

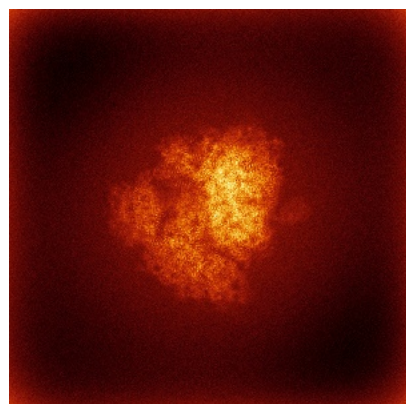


Y

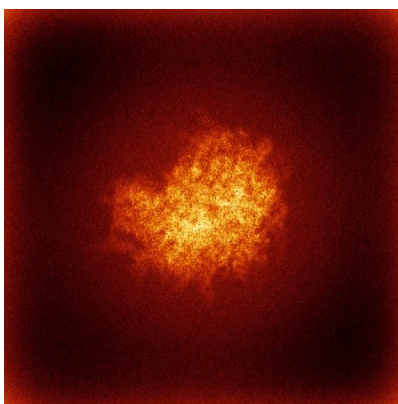


Z

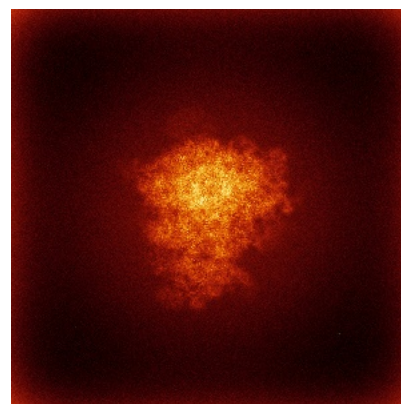
6.4.2 Raw map



X



Y

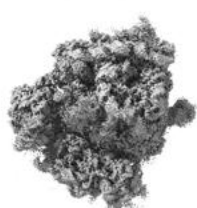


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



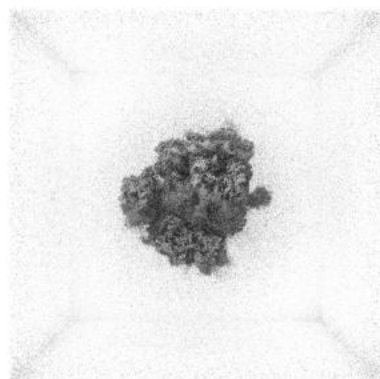
Y



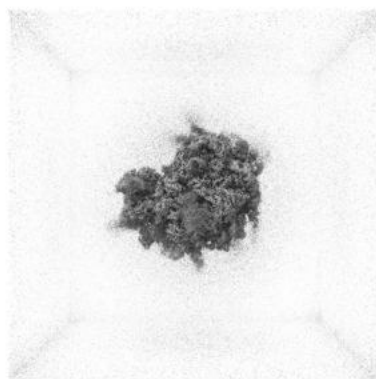
Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

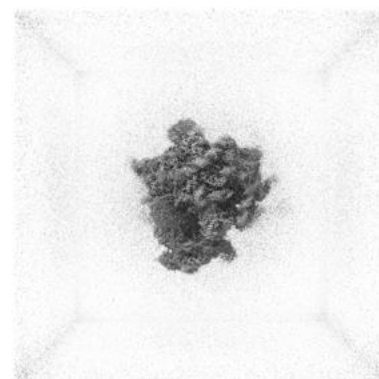
6.5.2 Raw map



X



Y



Z

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

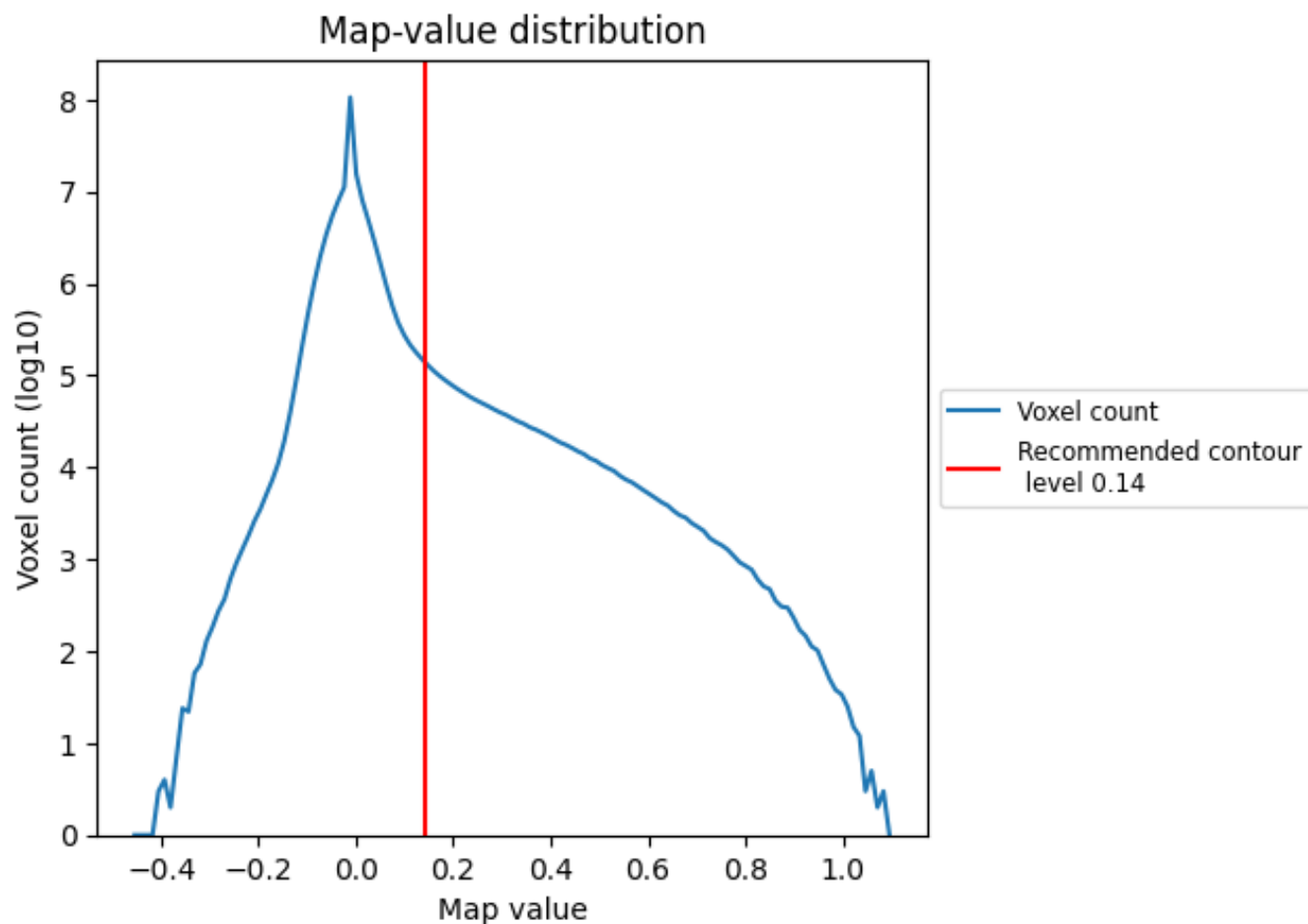
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

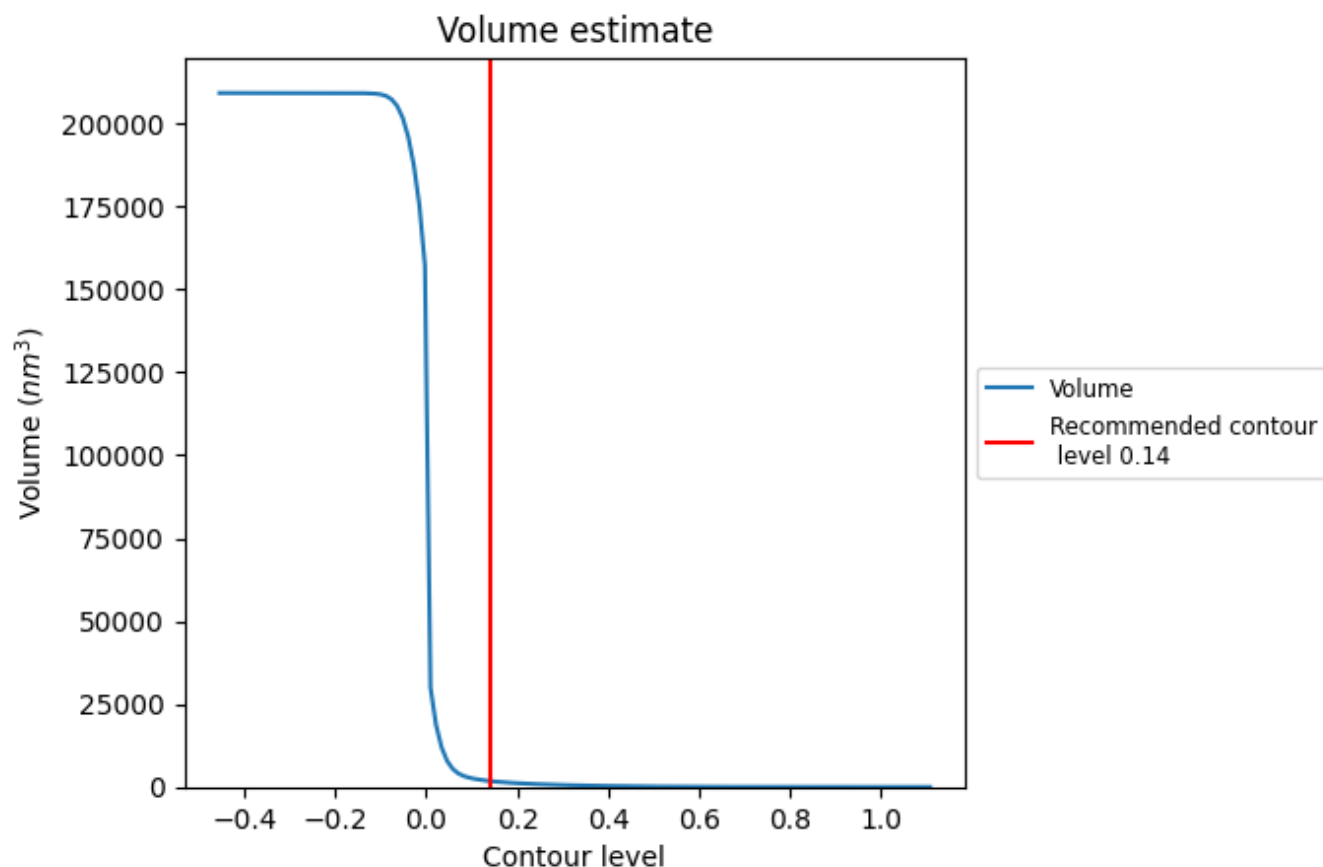
This section contains the results of statistical analysis of the map.

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.

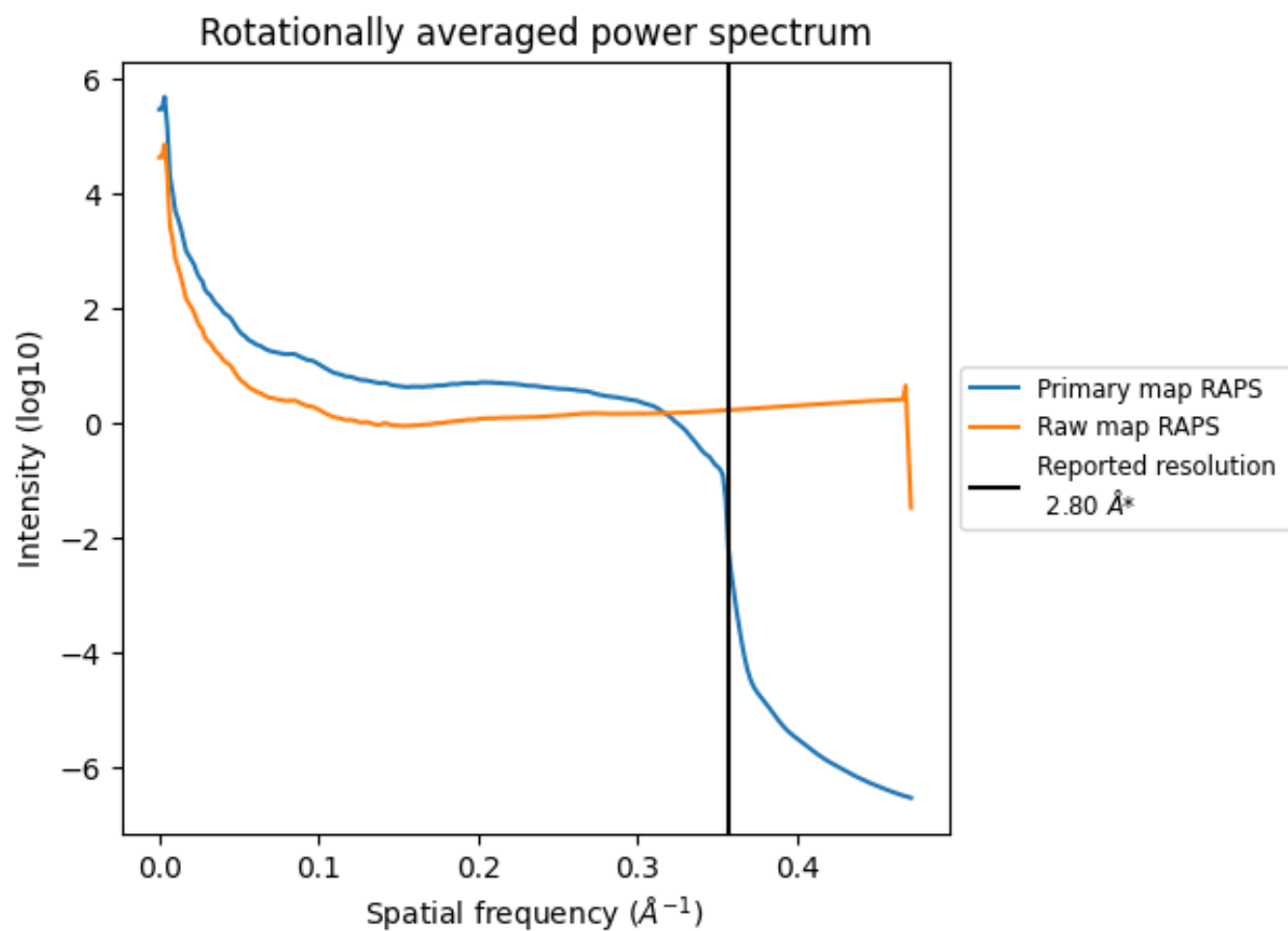
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1787 nm^3 ; this corresponds to an approximate mass of 1614 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 ⓘ

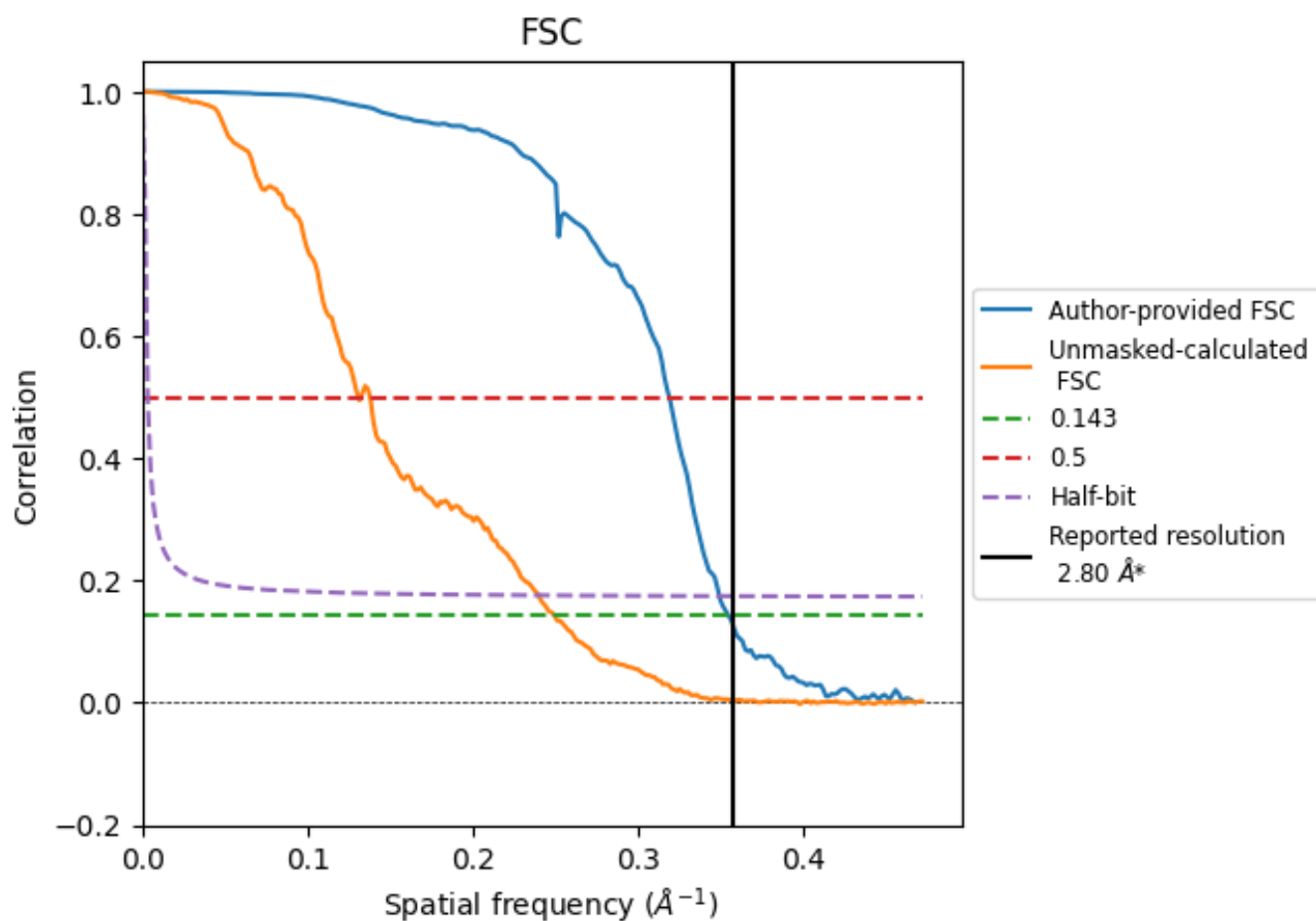


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

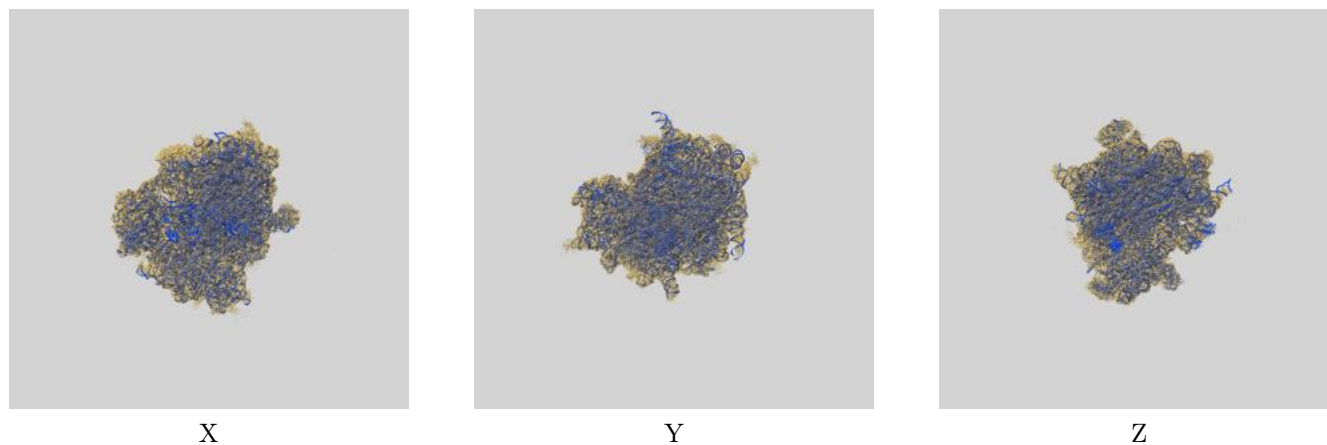
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.14	2.87
Unmasked-calculated*	4.01	7.65	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

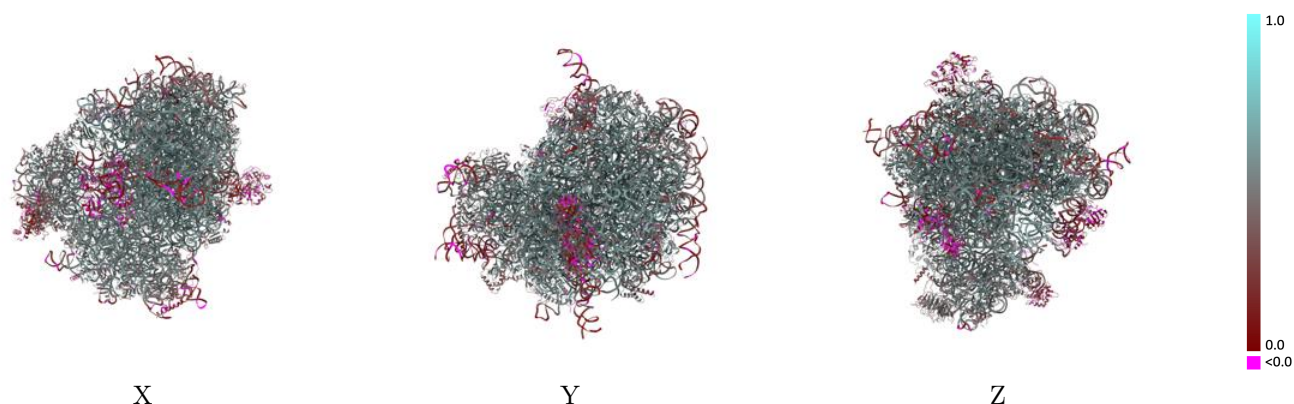
This section contains information regarding the fit between EMDB map EMD-53295 and PDB model 9QQA. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

9.1 Map-model overlay [i](#)



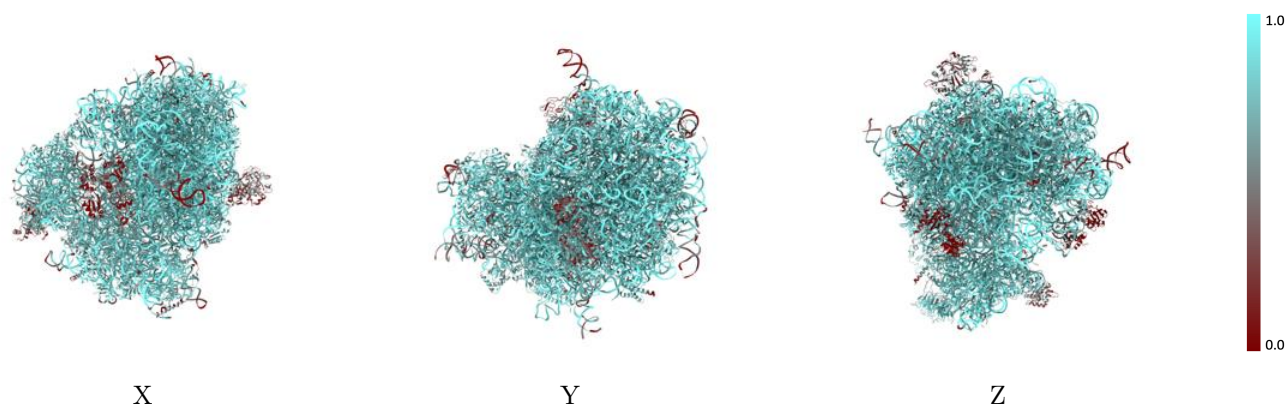
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



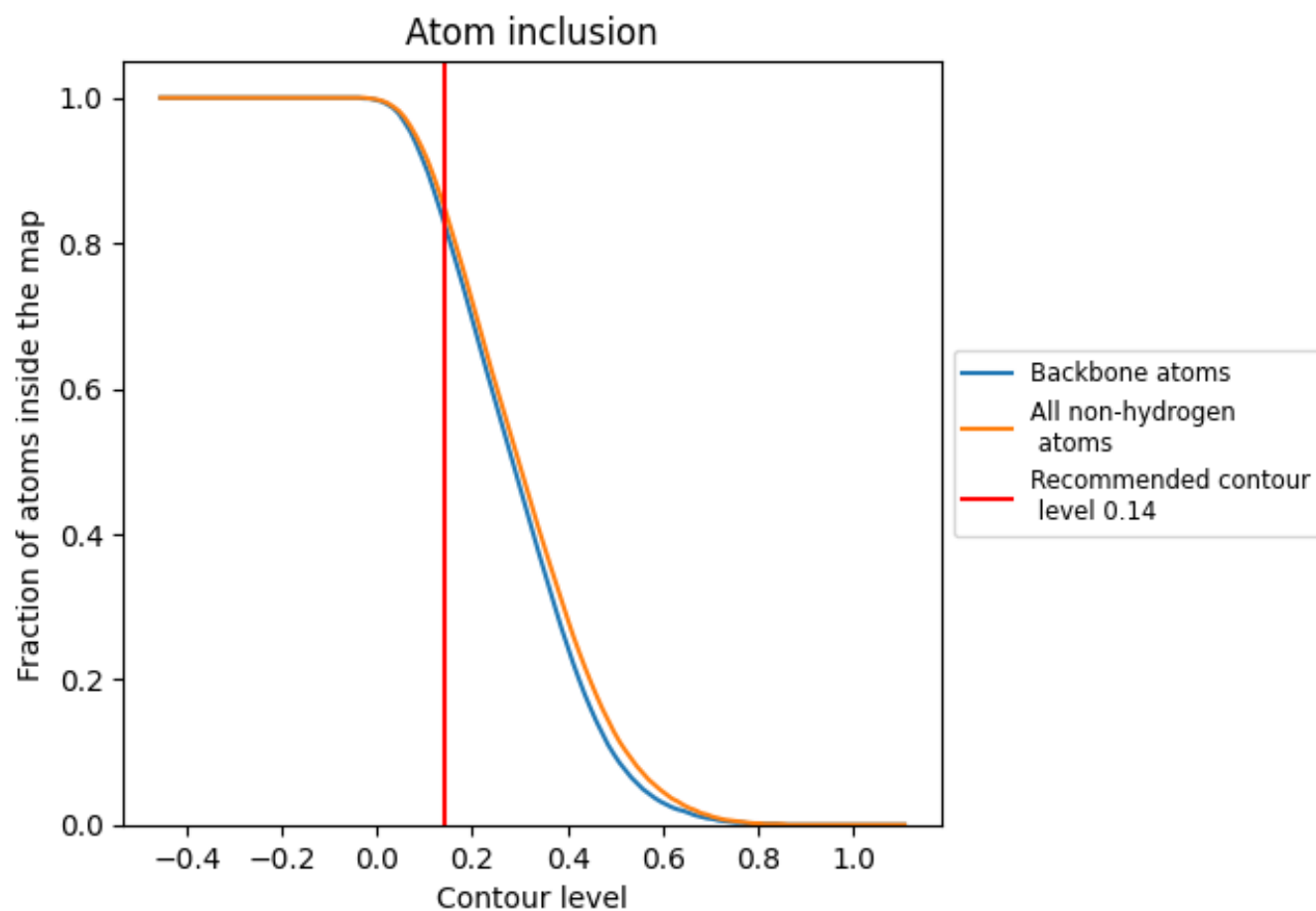
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.4920
A2	 0.9200	 0.4970
AA	 0.7950	 0.4760
AB	 0.7250	 0.4680
AC	 0.2860	 0.1350
AD	 0.6590	 0.4430
AE	 0.8450	 0.5290
AF	 0.7700	 0.3990
AG	 0.8640	 0.5070
AT	 0.7720	 0.4740
AZ	 0.8400	 0.4960
Aa	 0.8070	 0.5000
Ab	 0.8420	 0.5200
Ac	 0.7470	 0.4420
Ad	 0.8450	 0.5090
Ae	 0.7730	 0.4710
Af	 0.7810	 0.4290
Ag	 0.7480	 0.4250
Ah	 0.8320	 0.4910
Ai	 0.8420	 0.4960
Aj	 0.7960	 0.4200
Ak	 0.7860	 0.5040
Al	 0.3630	 0.1640
Am	 0.8400	 0.5270
An	 0.8360	 0.5130
Ao	 0.7730	 0.4340
Ap	 0.8280	 0.4930
Aq	 0.7750	 0.4520
Ar	 0.7920	 0.4690
As	 0.8380	 0.4860
At	 0.7250	 0.4110
Au	 0.8160	 0.5130
Av	 0.8530	 0.5510
Aw	 0.8500	 0.5360
Ax	 0.8160	 0.4780























Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ay	 0.6840	 0.4380
Az	 0.8490	 0.5460
B5	 0.9180	 0.5130
B7	 0.9870	 0.5790
B8	 0.9540	 0.5440
BA	 0.8770	 0.5700
BB	 0.8850	 0.5490
BC	 0.8940	 0.5540
BE	 0.7980	 0.4810
BF	 0.8790	 0.5550
BG	 0.8140	 0.4850
BH	 0.8540	 0.5260
BI	 0.8400	 0.5360
BJ	 0.8340	 0.4970
BK	 0.1670	 0.2710
BL	 0.8510	 0.5220
BM	 0.8870	 0.5290
BN	 0.9290	 0.5830
BO	 0.9000	 0.5570
BP	 0.8920	 0.5580
BQ	 0.8840	 0.5580
BR	 0.8510	 0.5110
BS	 0.9080	 0.5580
BT	 0.8460	 0.5360
BU	 0.8340	 0.4840
BV	 0.8250	 0.5280
BW	 0.6570	 0.3630
BX	 0.8560	 0.5330
BY	 0.8810	 0.5320
BZ	 0.8840	 0.5340
Ba	 0.9260	 0.5760
Bb	 0.7410	 0.4680
Bc	 0.7700	 0.4810
Bd	 0.8750	 0.5420
Be	 0.8550	 0.5580
Bf	 0.9120	 0.5720
Bg	 0.8580	 0.5330
Bh	 0.8550	 0.5160
Bi	 0.8330	 0.5090
Bj	 0.9240	 0.5750
Bk	 0.7920	 0.4730
Bl	 0.8600	 0.5490

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bm	 0.8520	 0.5380
Bo	 0.8320	 0.5340
Bp	 0.8260	 0.5380
Br	 0.8950	 0.5600
Bs	 0.0770	 0.0650
Bt	 0.0560	 0.0430
Bv	 0.0600	 0.0550
MA	 0.4200	 0.1470
Nt	 0.2480	 0.1120
Nu	 0.3780	 0.2430