



Full wwPDB EM Validation Report ⓘ

Dec 9, 2025 – 01:42 am GMT

PDB ID : 9SYR / pdb_00009syr
EMDB ID : EMD-55351
Title : Human quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatD
Authors : Yudin, D.; Jaskolowski, M.; Scaiola, A.; Ban, N.
Deposited on : 2025-10-13
Resolution : 3.55 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.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

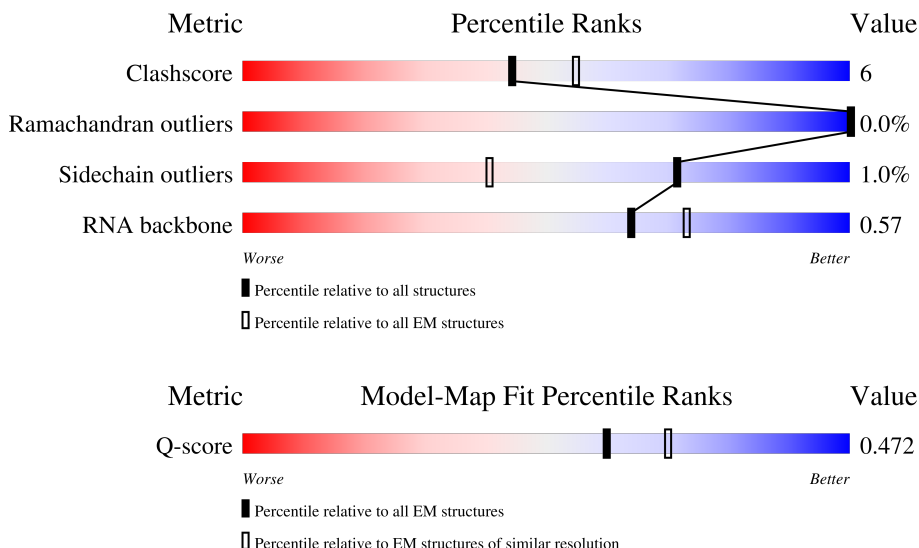
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




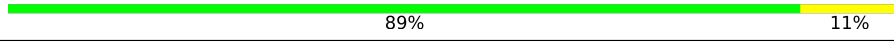
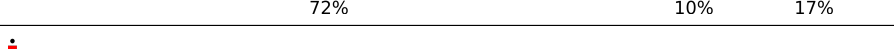
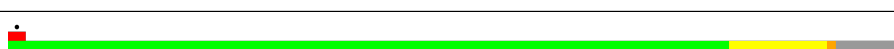



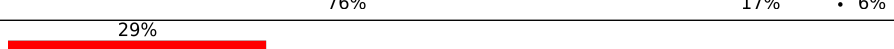



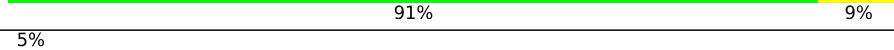

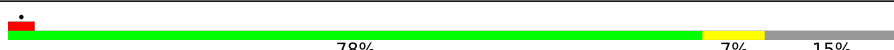


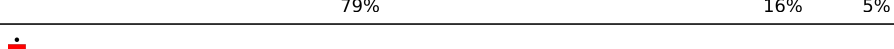







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	12819 (3.05 - 4.05)

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	L1	5070	
2	Lc	427	
3	Ld	297	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Le	288	
5	Lf	199	
6	Lg	184	
7	Lh	188	
8	Li	196	
9	Lj	176	
10	Lk	160	
11	Ll	128	
12	Lm	140	
13	Ln	157	
14	Lo	156	
15	Lp	145	
16	Lq	136	
17	Lr	148	
18	Ls	159	
19	Lt	115	
20	Lu	125	
21	Lv	135	
22	Lw	110	
23	Lx	117	
24	Ly	123	
25	Lz	105	
26	Na	238	
27	Nb	162	
28	Nd	365	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Nm	386	
30	S1	1869	
31	S2	1824	
32	S3	76	
33	SA	208	
34	SB	194	
35	SC	204	
36	SD	158	
37	SE	165	
38	SF	151	
39	SG	151	
40	SH	132	
41	Sa	152	
42	Sb	135	
43	Sc	146	
44	Sd	152	
45	Se	84	
46	Sf	130	
47	Sg	143	
48	L2	121	
49	Sh	131	
50	Si	145	
51	Sj	115	
52	Sk	84	
53	Sl	119	



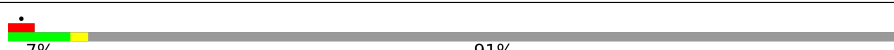
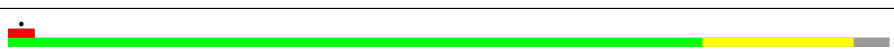

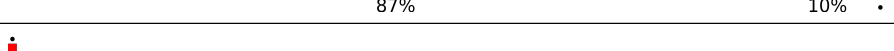
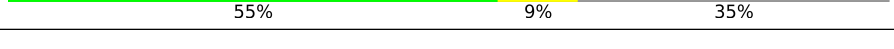

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Sm	125	
55	Sn	133	
56	So	69	
57	Sp	56	
58	Sq	25	
59	Sr	156	
60	Ss	317	
61	St	295	
62	Su	264	
63	Sv	293	
64	Sw	263	
65	Sx	243	
66	Sy	249	
67	Sz	194	
68	L3	157	
69	LA	97	
70	LB	70	
71	LC	51	
72	LD	99	
73	LE	106	
74	LF	92	
75	LG	137	
76	LH	204	
77	LI	248	
78	LJ	266	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	LK	192	
80	LM	214	
81	LN	414	
82	LO	178	
83	LP	211	
84	LQ	215	
85	La	257	
86	Lb	403	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 217377 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	3403	Total	C	N	O	P	1	0
			73061	32575	13368	23714	3404		

- Molecule 2 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Lc	363	Total	C	N	O	S	0	0
			2890	1818	577	482	13		

- Molecule 3 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ld	292	Total	C	N	O	S	0	0
			2372	1503	431	424	14		

- Molecule 4 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Le	218	Total	C	N	O	S	0	0
			1752	1128	333	287	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Lf	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 6 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Lg	152	Total	C	N	O	S	0	0
			1233	771	240	213	9		

- Molecule 7 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Lh	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 8 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Li	180	Total	C	N	O	S	0	0
			1501	929	327	236	9		

- Molecule 9 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Lj	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 10 is a protein called 60S ribosomal protein L21.

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

- Molecule 11 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ll	102	Total	C	N	O	S	0	0
			833	533	146	152	2		

- Molecule 12 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Lm	132	Total	C	N	O	S	0	0
			985	621	185	174	5		

- Molecule 13 is a protein called 60S ribosomal protein L24.

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

- Molecule 14 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Lo	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 15 is a protein called 60S ribosomal protein L26.

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

- Molecule 16 is a protein called 60S ribosomal protein L27.

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

- Molecule 17 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Lr	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 18 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ls	99	Total	C	N	O	S	0	0
			806	500	177	125	4		

- Molecule 19 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Lt	100	Total	C	N	O	S	0	0
			772	490	136	139	7		

- Molecule 20 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Lu	106	Total	C	N	O	S	0	0
			868	551	170	145	2		

- Molecule 21 is a protein called 60S ribosomal protein L32.

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

- Molecule 22 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Lw	109	Total	C	N	O	S	1	0
			879	557	174	144	4		

- Molecule 23 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Lx	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 24 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ly	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 25 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Lz	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 26 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Na	108	Total	C	N	O	S	0	0
			840	524	153	159	4		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Na	-22	MET	-	initiating methionine	UNP Q13765
Na	-21	GLY	-	expression tag	UNP Q13765
Na	-20	SER	-	expression tag	UNP Q13765
Na	-19	SER	-	expression tag	UNP Q13765
Na	-18	HIS	-	expression tag	UNP Q13765
Na	-17	HIS	-	expression tag	UNP Q13765

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Na	-16	HIS	-	expression tag	UNP Q13765
Na	-15	HIS	-	expression tag	UNP Q13765
Na	-14	HIS	-	expression tag	UNP Q13765
Na	-13	HIS	-	expression tag	UNP Q13765
Na	-12	SER	-	expression tag	UNP Q13765
Na	-11	SER	-	expression tag	UNP Q13765
Na	-10	GLY	-	expression tag	UNP Q13765
Na	-9	LEU	-	expression tag	UNP Q13765
Na	-8	GLU	-	expression tag	UNP Q13765
Na	-7	VAL	-	expression tag	UNP Q13765
Na	-6	LEU	-	expression tag	UNP Q13765
Na	-5	PHE	-	expression tag	UNP Q13765
Na	-4	GLN	-	expression tag	UNP Q13765
Na	-3	GLY	-	expression tag	UNP Q13765
Na	-2	PRO	-	expression tag	UNP Q13765
Na	-1	SER	-	expression tag	UNP Q13765
Na	0	GLY	-	expression tag	UNP Q13765

- Molecule 27 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Nb	120	Total	C	N	O	S	0	0
			934	580	168	182	4		

- Molecule 28 is a protein called Ubiquitin-like protein SMT3,N-alpha-acetyltransferase 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Nd	236	Total	C	N	O	S	0	0
			1890	1182	337	353	18		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Nd	-127	MET	-	initiating methionine	UNP Q12306
Nd	-126	GLY	-	expression tag	UNP Q12306
Nd	-125	SER	-	expression tag	UNP Q12306
Nd	-124	SER	-	expression tag	UNP Q12306
Nd	-123	HIS	-	expression tag	UNP Q12306
Nd	-122	HIS	-	expression tag	UNP Q12306
Nd	-121	HIS	-	expression tag	UNP Q12306
Nd	-120	HIS	-	expression tag	UNP Q12306
Nd	-119	HIS	-	expression tag	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Nd	-118	HIS	-	expression tag	UNP Q12306
Nd	-117	SER	-	expression tag	UNP Q12306
Nd	-116	SER	-	expression tag	UNP Q12306
Nd	-115	GLY	-	expression tag	UNP Q12306
Nd	-114	LEU	-	expression tag	UNP Q12306
Nd	-113	VAL	-	expression tag	UNP Q12306
Nd	-112	PRO	-	expression tag	UNP Q12306
Nd	-111	ARG	-	expression tag	UNP Q12306
Nd	-110	GLY	-	expression tag	UNP Q12306
Nd	-109	SER	-	expression tag	UNP Q12306
Nd	-108	HIS	-	expression tag	UNP Q12306
Nd	-107	MET	-	expression tag	UNP Q12306
Nd	-106	ALA	-	expression tag	UNP Q12306
Nd	-105	SER	-	expression tag	UNP Q12306
Nd	-104	MET	-	expression tag	UNP Q12306
Nd	-103	THR	-	expression tag	UNP Q12306
Nd	-102	GLY	-	expression tag	UNP Q12306
Nd	-101	GLY	-	expression tag	UNP Q12306
Nd	-100	GLN	-	expression tag	UNP Q12306
Nd	-99	GLN	-	expression tag	UNP Q12306
Nd	-98	MET	-	expression tag	UNP Q12306
Nd	-97	GLY	-	expression tag	UNP Q12306
Nd	-96	ARG	-	expression tag	UNP Q12306
Nd	-95	GLY	-	expression tag	UNP Q12306
Nd	-94	SER	-	expression tag	UNP Q12306

- Molecule 29 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Nm	380	Total	C	N	O	S	0	0
			2984	1870	532	558	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Nm	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 30 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S1	1771	Total	C	N	O	P	0	0
			37855	16922	6786	12376	1771		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S2	7	Total	C	N	O	P	0	0
			148	66	24	51	7		

- Molecule 32 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S3	74	Total	C	N	O	P	0	0
			1579	704	284	517	74		

- Molecule 33 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 34 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SB	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 35 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SC	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 36 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SD	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 37 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SE	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 38 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SF	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 39 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SG	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SG	138	IAS	ASP	conflict	UNP P62263

- Molecule 40 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SH	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 41 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Sa	124	Total	C	N	O	S	0	0
			1016	644	192	173	7		

- Molecule 42 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Sb	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 43 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Sc	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Sd	146	Total	C	N	O	S	0	0
			1200	753	242	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sd	2	ACE	-	acetylation	UNP P62269

- Molecule 45 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Se	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Se	0	ACE	-	acetylation	UNP P63220

- Molecule 46 is a protein called 40S ribosomal protein S15a.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 48 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L2	118	Total	C	N	O	P	0	0
			2518	1122	449	829	118		

- Molecule 49 is a protein called Isoform 3 of Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Sh	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 50 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Si	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 51 is a protein called 40S ribosomal protein S26.

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

- Molecule 52 is a protein called 40S ribosomal protein S27.

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

- Molecule 53 is a protein called 40S ribosomal protein S20.

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

- Molecule 54 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Sm	83	Total	C	N	O	S	0	0
			670	431	125	113	1		

- Molecule 55 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

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

- Molecule 56 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	So	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 57 is a protein called 40S ribosomal protein S29.

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

- Molecule 58 is a protein called 60S ribosomal protein L41.

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

- Molecule 59 is a protein called Ubiquitin.

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

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ss	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 61 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	St	223	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
St	2	ACE	-	acetylation	UNP P08865

- Molecule 62 is a protein called 40S ribosomal protein S3a.

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

- Molecule 63 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sv	223	Total	C	N	O	S	1	0
			1741	1124	300	307	10		

- Molecule 64 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 65 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sx	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 66 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sy	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 67 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sz	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 68 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	L3	148	Total	C	N	O	P	0	0
			3156	1408	563	1037	148		

- Molecule 69 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	LA	86	Total	C	N	O	S	1	0
			713	442	155	111	5		

- Molecule 70 is a protein called 60S ribosomal protein L38.

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

- Molecule 71 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	LC	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 72 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	LD	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 73 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	LE	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 74 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	LF	92	Total	C	N	O	S	0	0
			716	450	137	121	8		

- Molecule 75 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	LG	124	Total	C	N	O	S	0	0
			992	615	206	167	4		

- Molecule 76 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	LH	203	Total	C	N	O	S	1	0
			1708	1077	360	267	4		

- Molecule 77 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	LI	223	Total	C	N	O	S	0	0
			1851	1189	355	298	9		

- Molecule 78 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	LJ	223	Total	C	N	O	S	0	0
			1809	1153	349	303	4		

- Molecule 79 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	LK	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 80 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LM	213	Total	C	N	O	S	0	0
			1716	1086	331	285	14		

- Molecule 81 is a protein called Green fluorescent protein,Small ubiquitin-related modifier 1,Green fluorescent protein,Small ubiquitin-related modifier 1,Histone H4,X-box-binding protein 1,X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	LN	39	Total	C	N	O	S	0	0
			316	203	62	48	3		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LN	-4	MET	-	initiating methionine	UNP P42212
LN	-3	ALA	-	expression tag	UNP P42212
LN	-2	ALA	-	expression tag	UNP P42212
LN	-1	ALA	-	expression tag	UNP P42212
LN	0	THR	-	expression tag	UNP P42212
LN	1	MET	-	expression tag	UNP P42212
LN	2	VAL	-	expression tag	UNP P42212
LN	65	LEU	PHE	conflict	UNP P42212
LN	66	THR	SER	conflict	UNP P42212
LN	222	LYS	LEU	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LN	232	GLY	-	linker	UNP P42212
LN	233	SER	-	linker	UNP P42212
LN	234	GLY	-	linker	UNP P42212
LN	235	SER	-	linker	UNP P42212
LN	236	GLY	-	linker	UNP P42212
LN	237	SER	-	linker	UNP P42212
LN	238	GLY	-	linker	UNP P42212
LN	239	SER	-	linker	UNP P42212
LN	240	GLY	-	linker	UNP P42212
LN	241	SER	-	linker	UNP P42212
LN	242	GLY	-	linker	UNP P42212
LN	243	SER	-	linker	UNP P42212
LN	244	GLY	-	linker	UNP P42212
LN	245	SER	-	linker	UNP P42212
LN	246	GLY	-	linker	UNP P42212
LN	247	SER	-	linker	UNP P42212
LN	248	GLY	-	linker	UNP P42212
LN	249	SER	-	linker	UNP P42212
LN	250	GLY	-	linker	UNP P42212
LN	251	SER	-	linker	UNP P42212
LN	252	GLY	-	linker	UNP P42212
LN	253	SER	-	linker	UNP P42212
LN	254	SER	-	linker	UNP P42212
LN	255	ALA	-	linker	UNP P42212
LN	256	ALA	-	linker	UNP P42212
LN	257	GLY	-	linker	UNP P42212
LN	312	LYS	ASN	conflict	UNP P55857
LN	319	LYS	ASP	conflict	UNP P55857
LN	325	ALA	GLY	conflict	UNP P55857
LN	327	ARG	GLN	conflict	UNP P55857
LN	403	CYS	PRO	conflict	UNP B1AHH2
LN	404	ALA	SER	conflict	UNP B1AHH2

- Molecule 82 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	LO	170	Total	C	N	O	S	0	0
			1358	858	253	241	6		

- Molecule 83 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	LP	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 84 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	LQ	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 85 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	La	246	Total	C	N	O	S	0	0
			1887	1183	387	311	6		

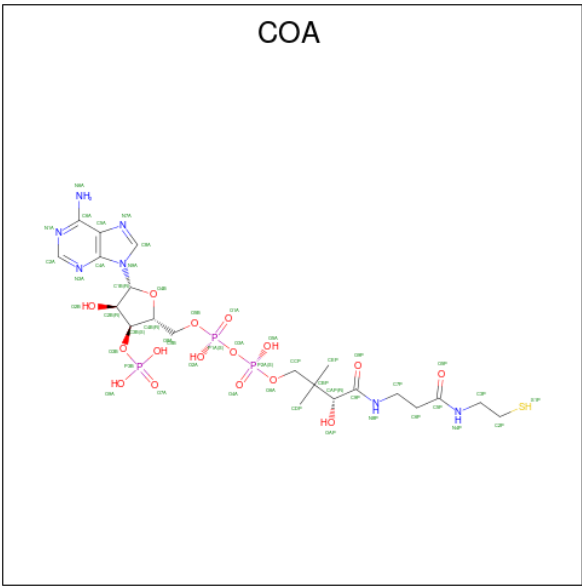
- Molecule 86 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Lb	395	Total	C	N	O	S	1	0
			3194	2034	600	545	15		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

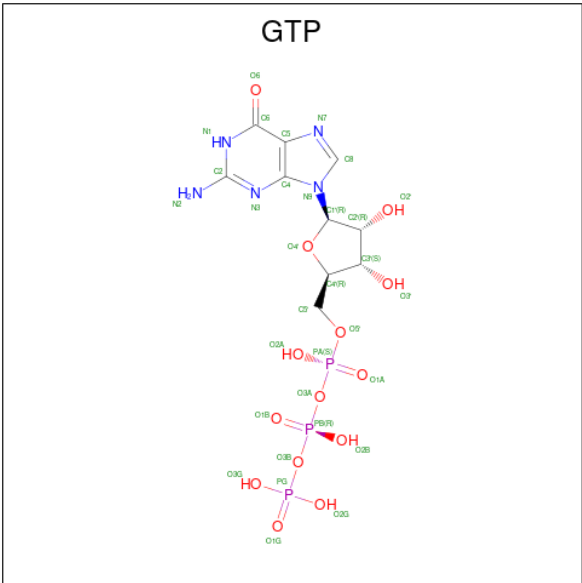
Mol	Chain	Residues	Atoms		AltConf
87	Lx	1	Total	Zn	0
			1	1	
87	Nm	2	Total	Zn	0
			2	2	
87	Sj	1	Total	Zn	0
			1	1	
87	Sp	1	Total	Zn	0
			1	1	
87	Sr	1	Total	Zn	0
			1	1	
87	LA	1	Total	Zn	0
			1	1	
87	LD	1	Total	Zn	0
			1	1	
87	LE	1	Total	Zn	0
			1	1	
87	LF	1	Total	Zn	0
			1	1	

- Molecule 88 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						AltConf
88	Nd	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 89 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

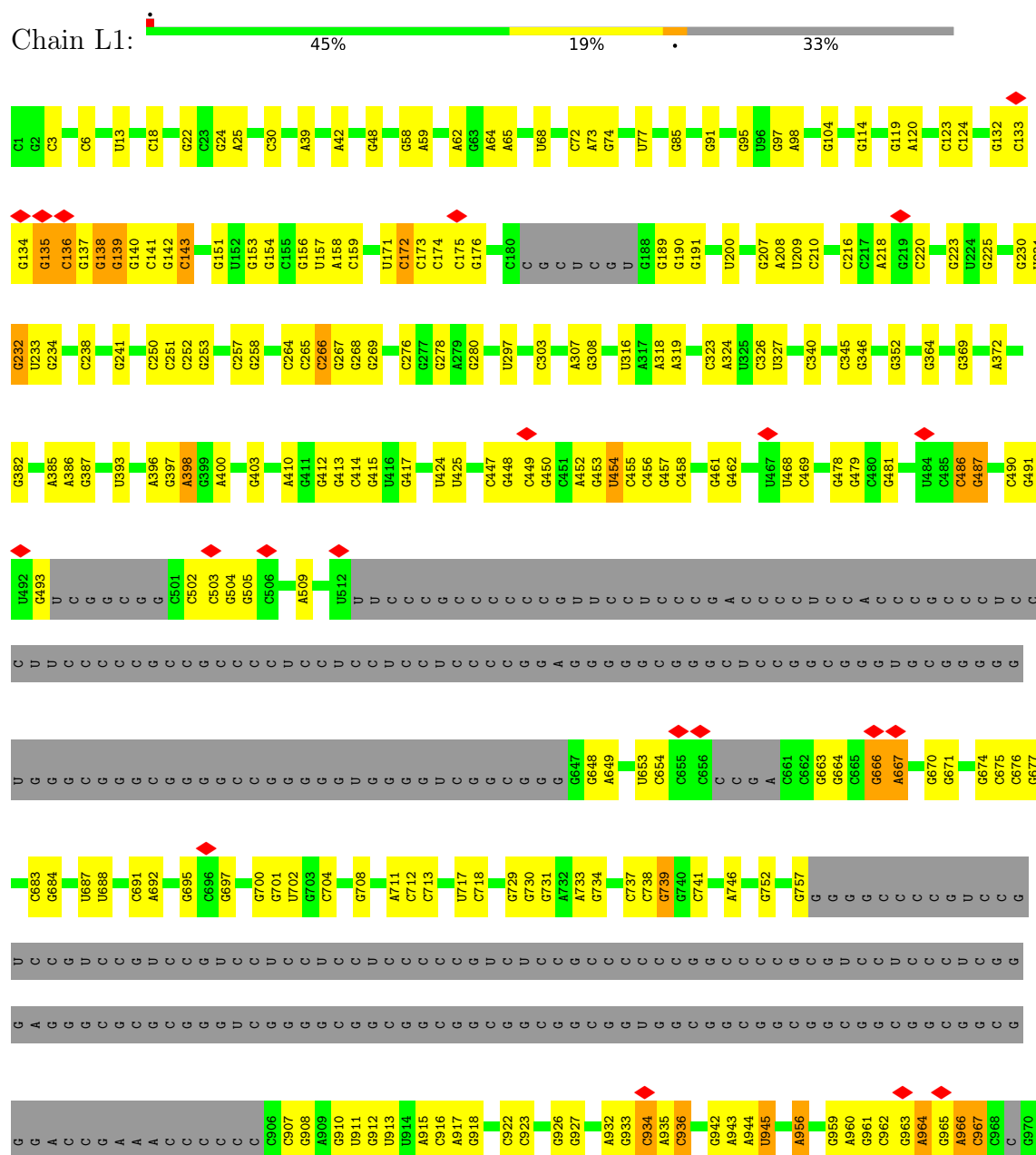


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
89	L2	1	32	10	5	14	3	0

3 Residue-property plots

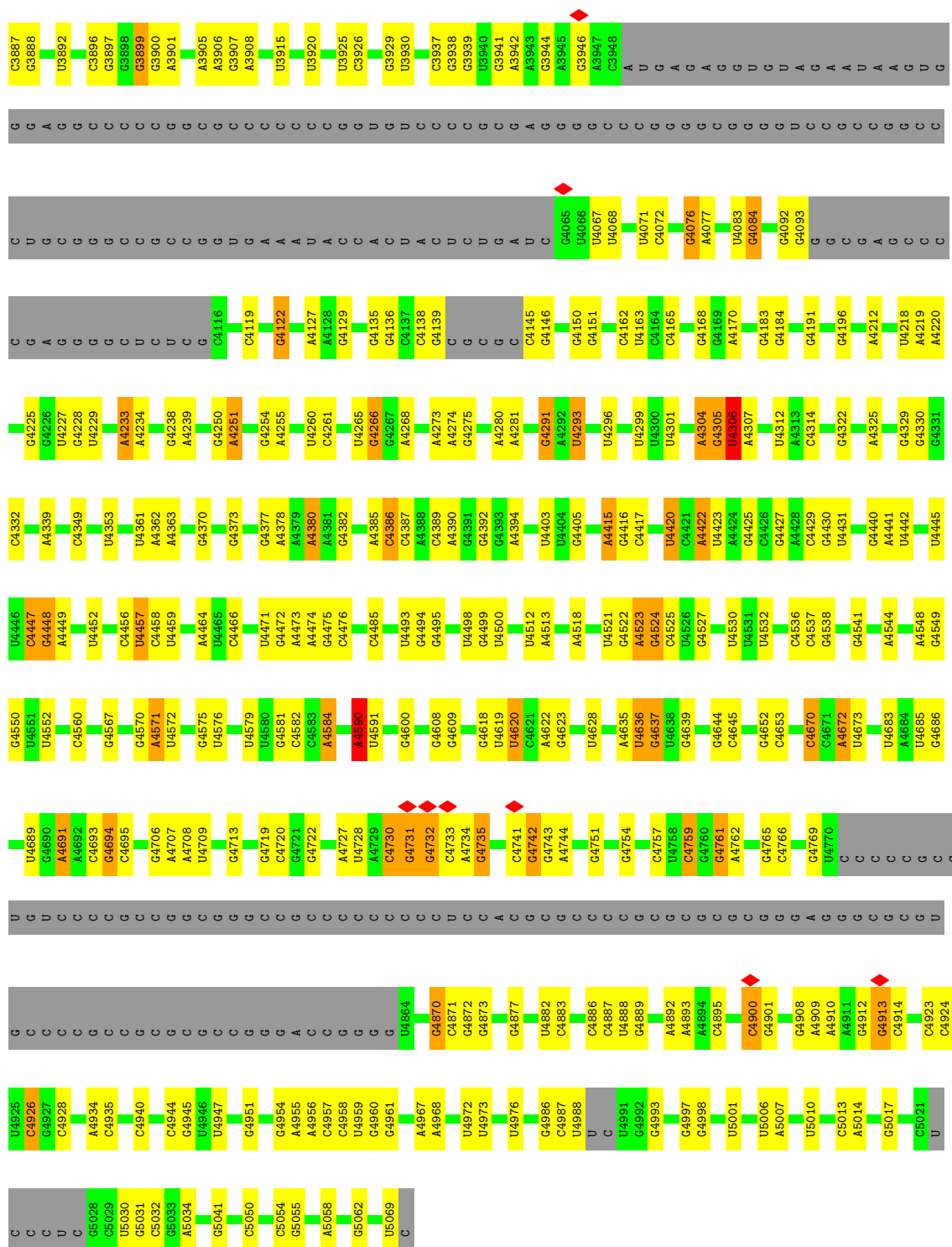
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S rRNA





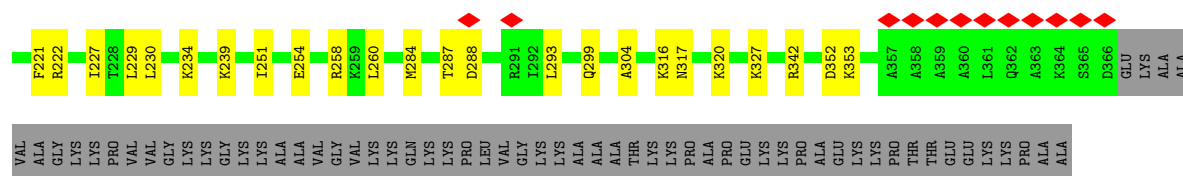




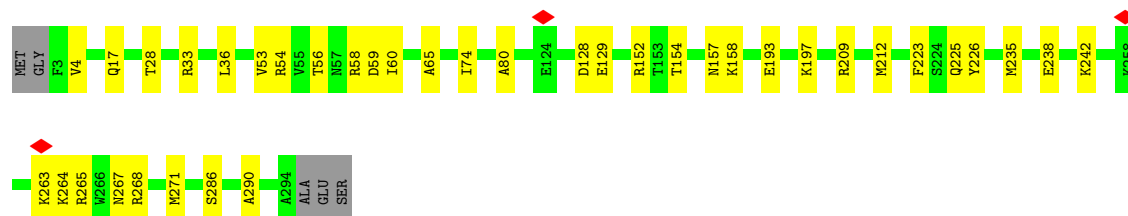
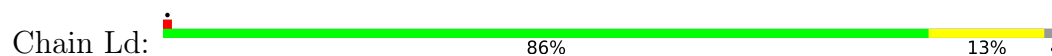
• Molecule 2: 60S ribosomal protein L4

Chain Lc:

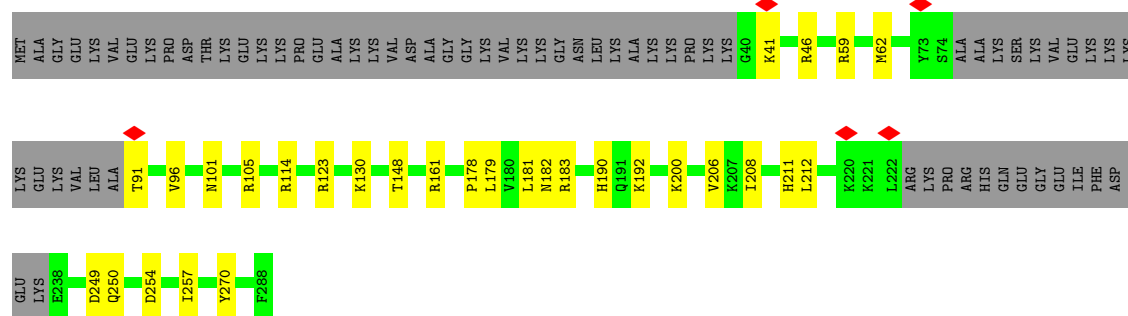




• Molecule 3: 60S ribosomal protein L5



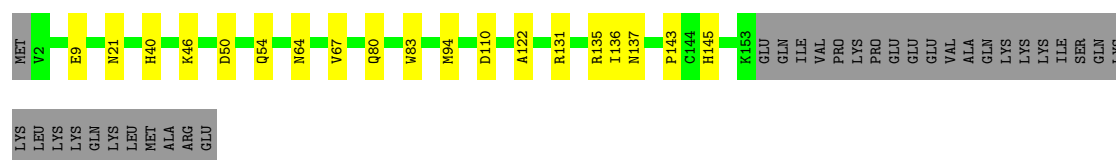
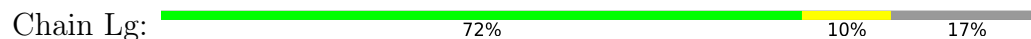
• Molecule 4: Large ribosomal subunit protein eL6




• Molecule 5: Large ribosomal subunit protein uL13



• Molecule 6: 60S ribosomal protein L17




• Molecule 7: 60S ribosomal protein L18

Chain Lh:  87% 12% ..




- Molecule 8: 60S ribosomal protein L19

Chain Li:  81% 11% . 8%




- Molecule 9: 60S ribosomal protein L18a

Chain Lj:  89% 11%



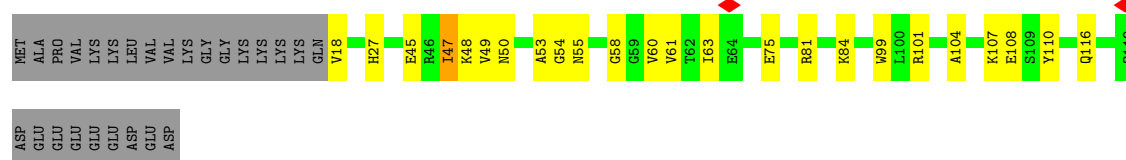
- Molecule 10: 60S ribosomal protein L21

Chain Lk:  82% 17% .




- Molecule 11: 60S ribosomal protein L22

Chain Ll:  61% 18% . 20%



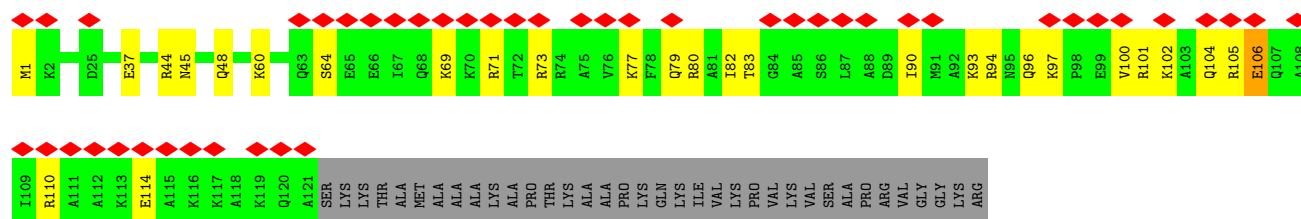
- Molecule 12: 60S ribosomal protein L23

Chain Lm:  76% 17% . 6%

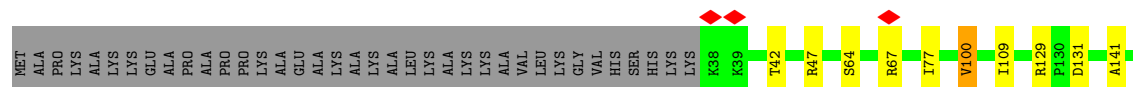


- Molecule 13: 60S ribosomal protein L24

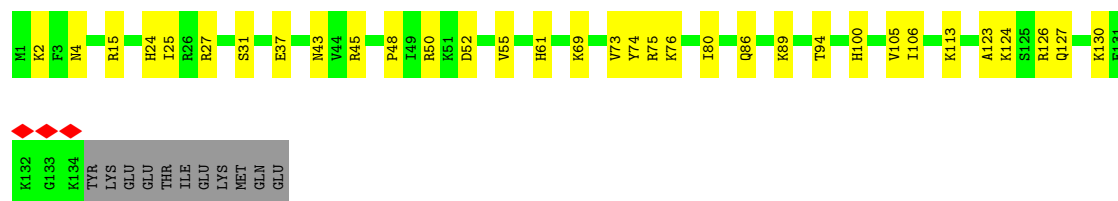
Chain Ln:  29% 59% 17% . 23%



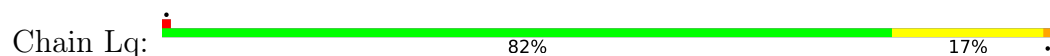
- Molecule 14: 60S ribosomal protein L23a



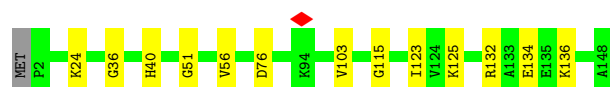
- Molecule 15: 60S ribosomal protein L26



- Molecule 16: 60S ribosomal protein L27

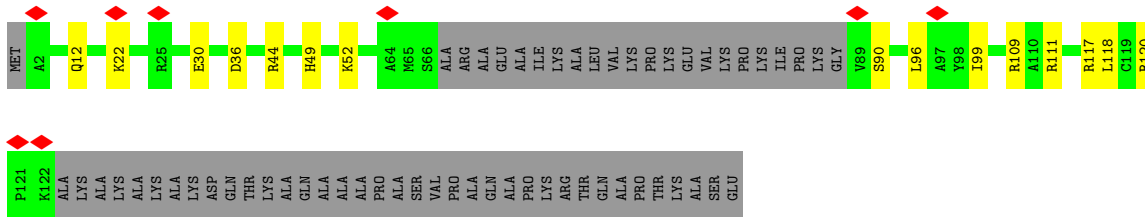


- Molecule 17: 60S ribosomal protein L27a

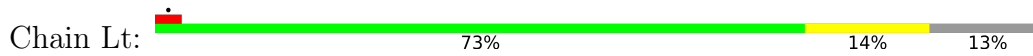


- Molecule 18: 60S ribosomal protein L29

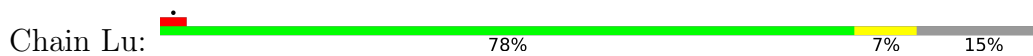




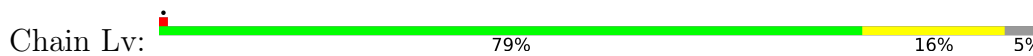
- Molecule 19: 60S ribosomal protein L30



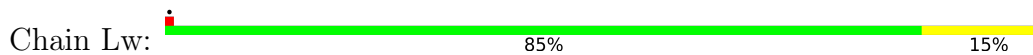
- Molecule 20: 60S ribosomal protein L31



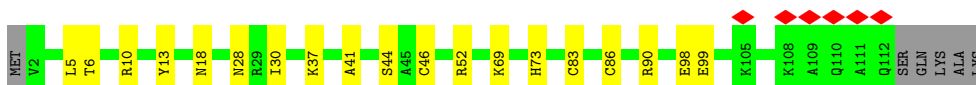
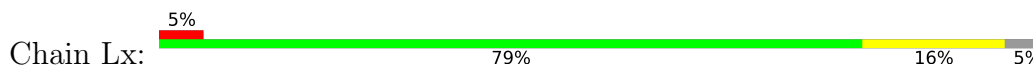
- Molecule 21: 60S ribosomal protein L32



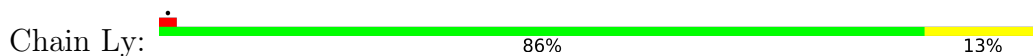
- Molecule 22: 60S ribosomal protein L35a



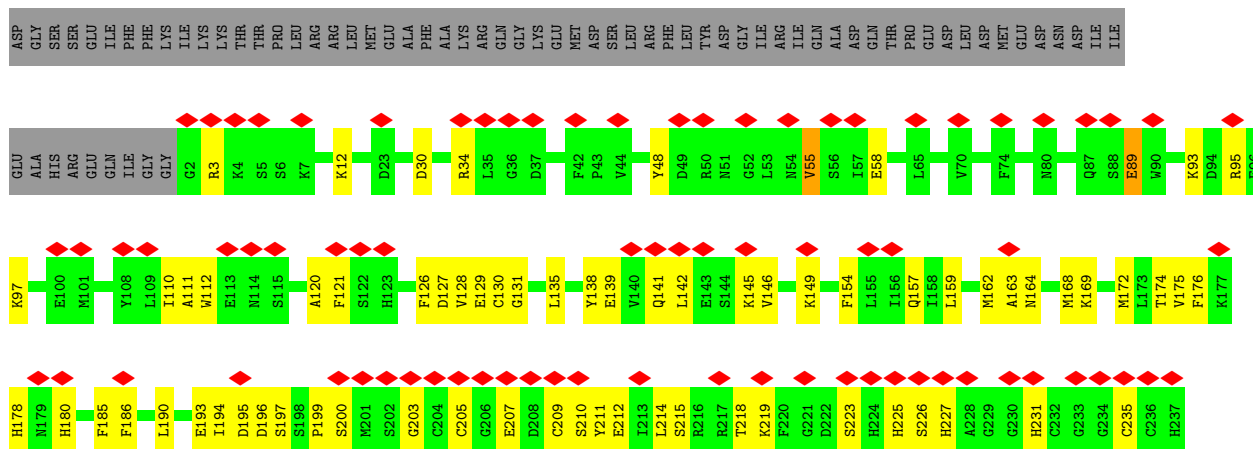
- Molecule 23: 60S ribosomal protein L34



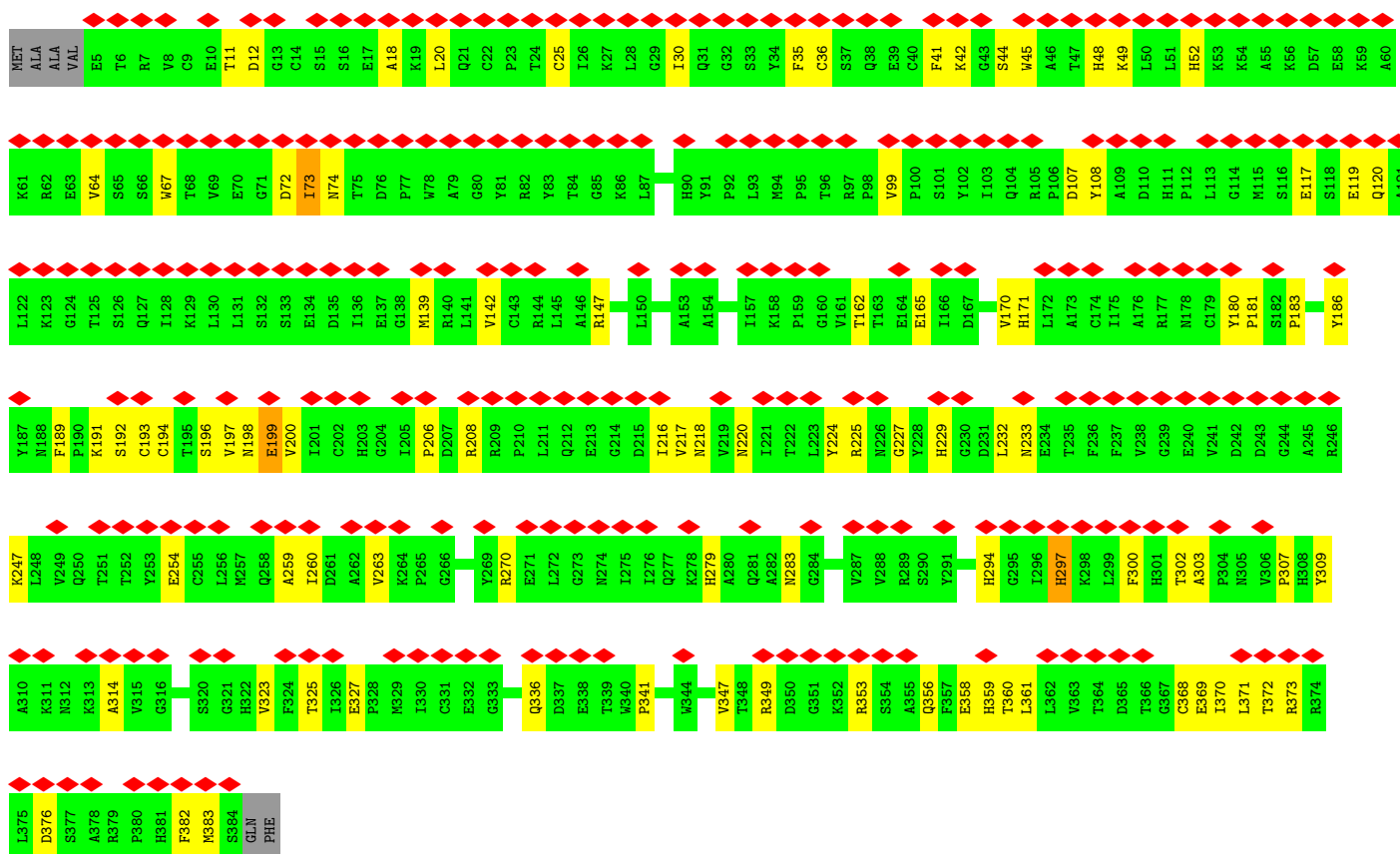
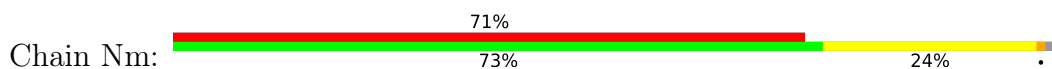
- Molecule 24: 60S ribosomal protein L35





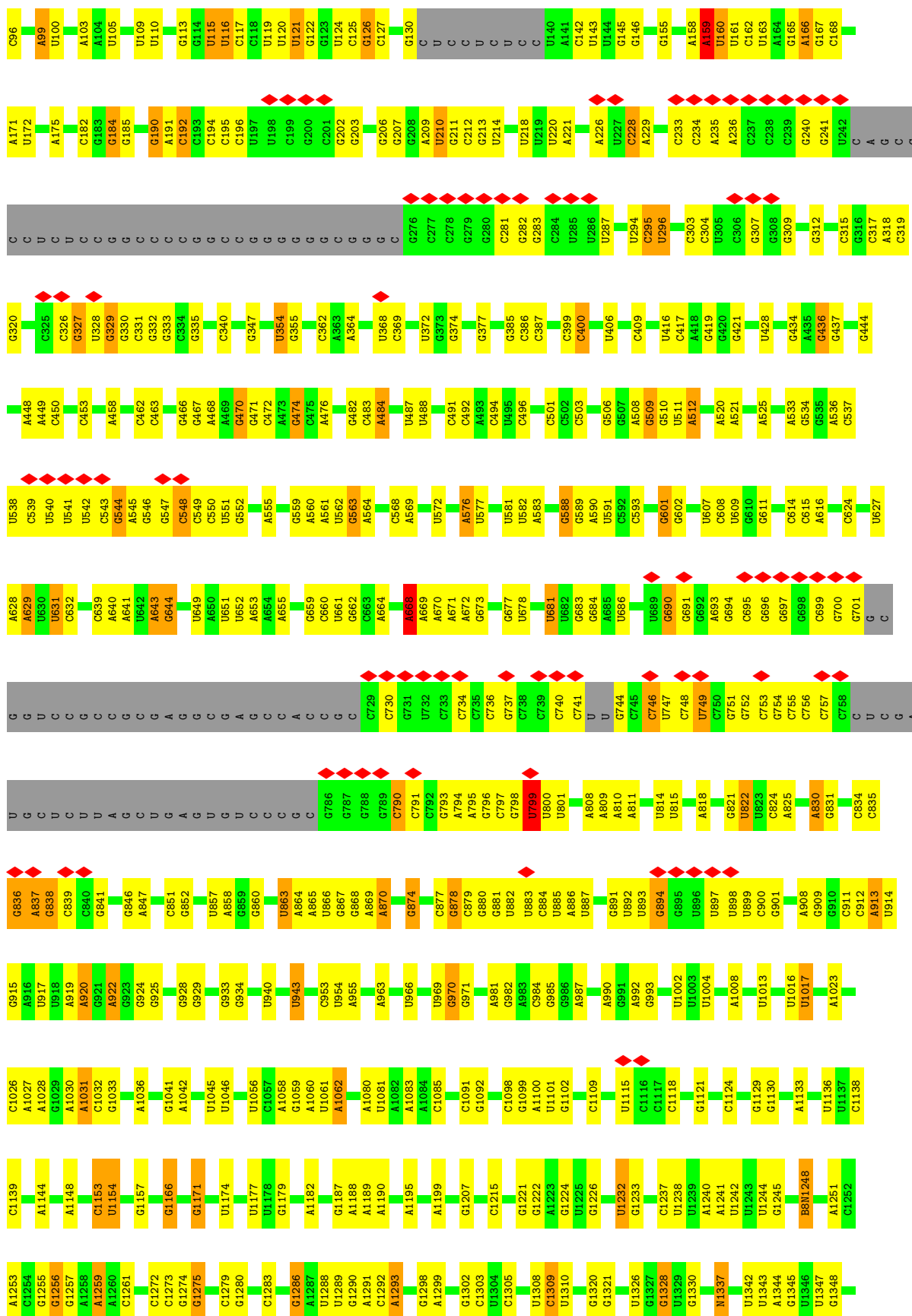


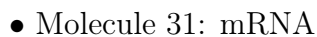
• Molecule 29: Methionine aminopeptidase 1



• Molecule 30: 18S rRNA

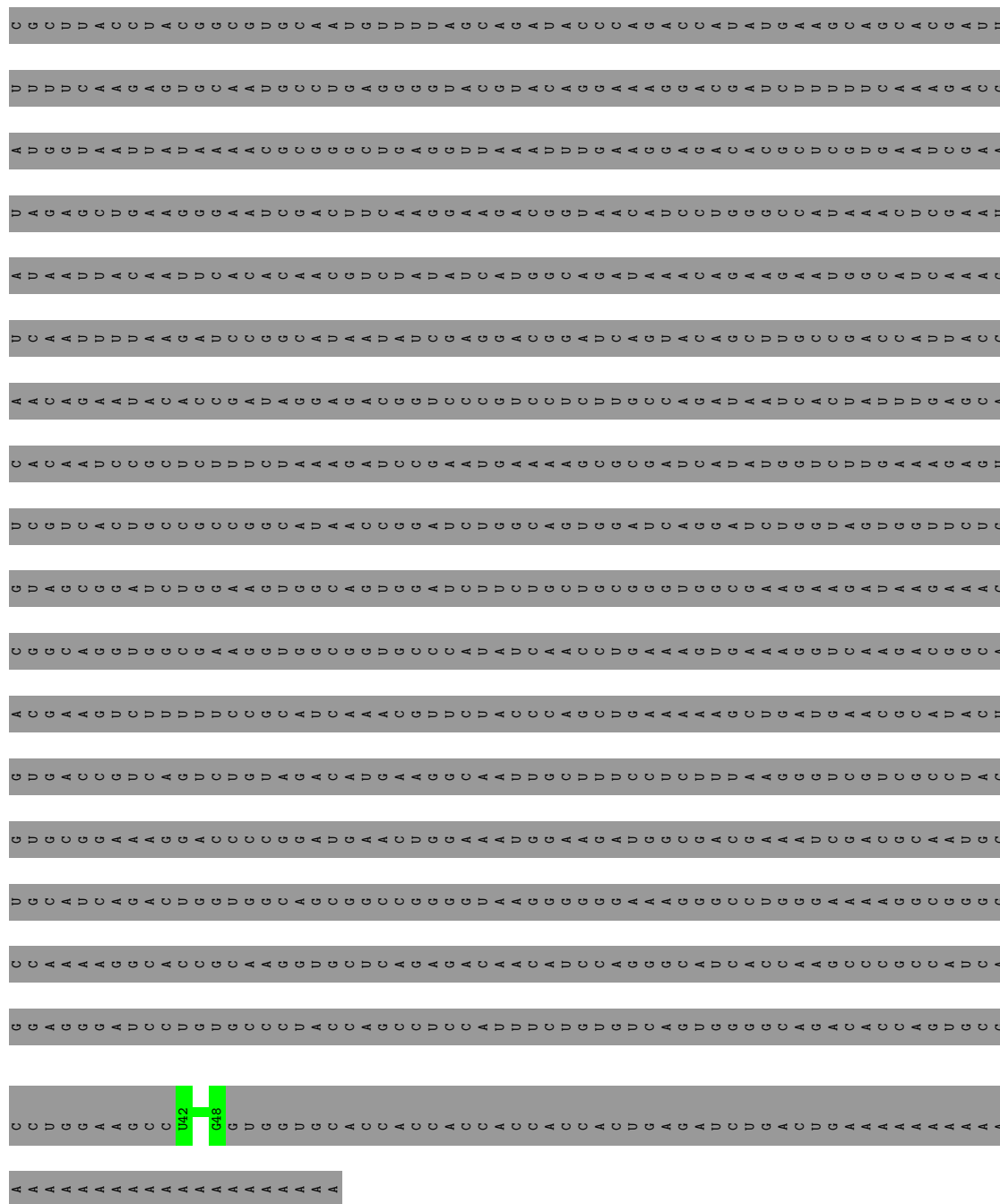






100%

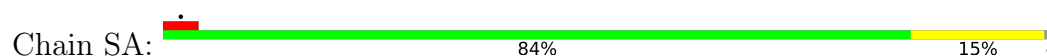




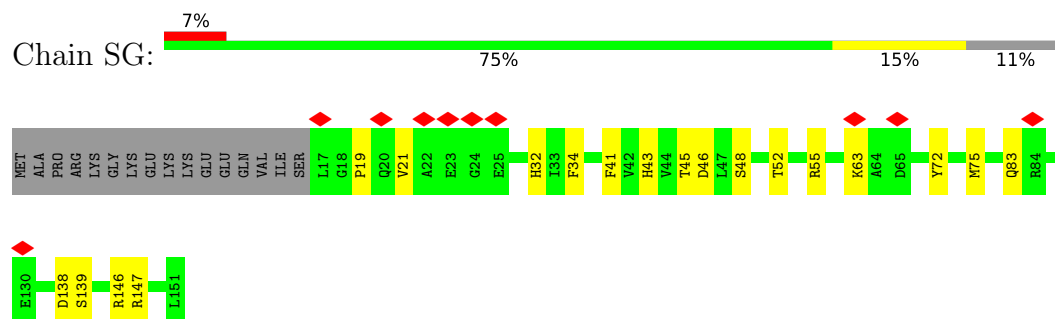
- Molecule 32: tRNA



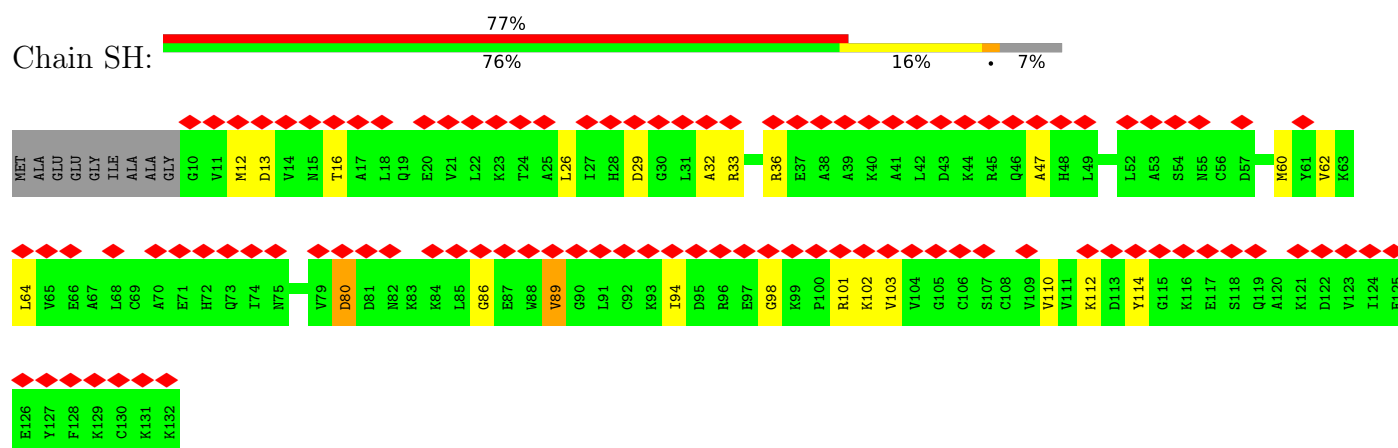
- Molecule 33: 40S ribosomal protein S8



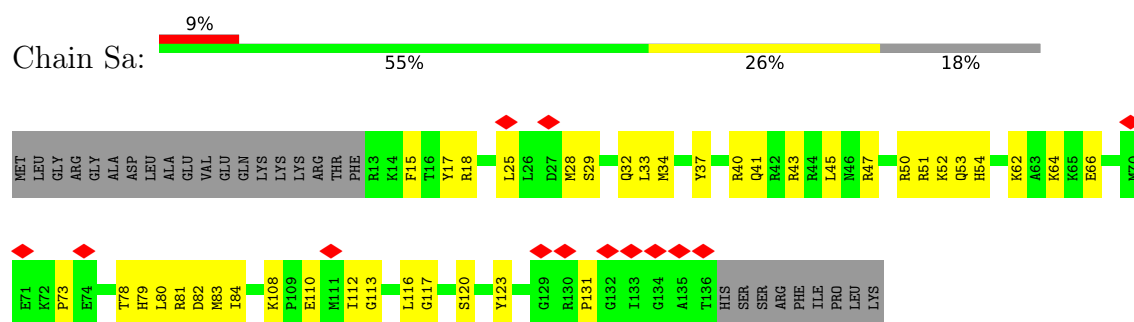
- Molecule 39: 40S ribosomal protein S14



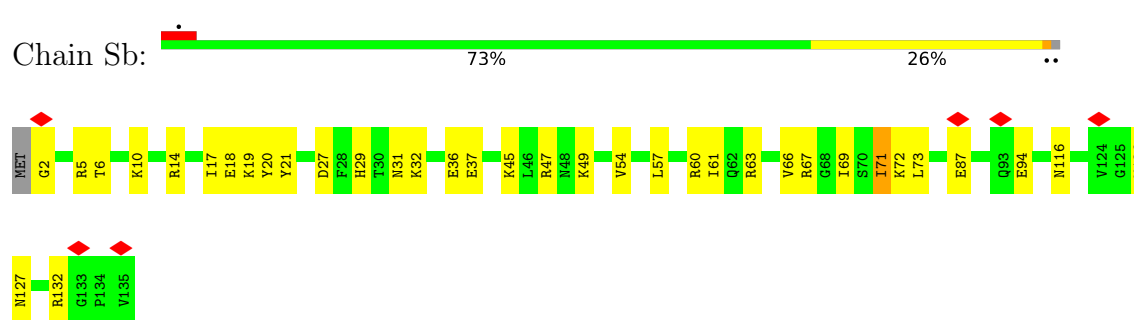
- Molecule 40: 40S ribosomal protein S12




- Molecule 41: 40S ribosomal protein S15

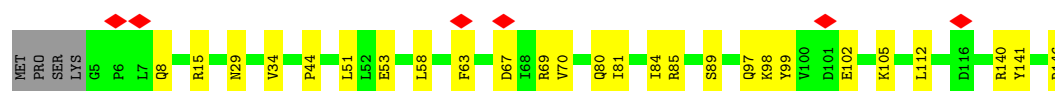


- Molecule 42: 40S ribosomal protein S17




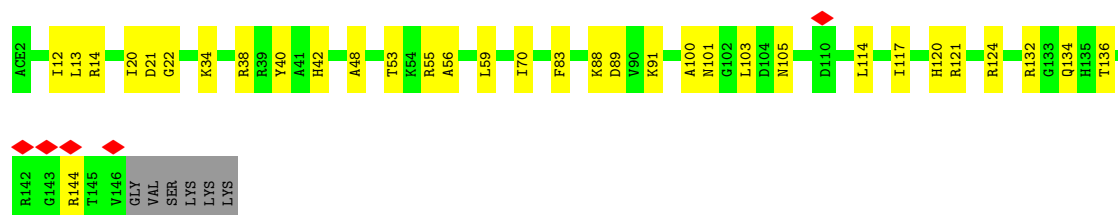
- Molecule 43: 40S ribosomal protein S16

Chain Sc:  79% 18%




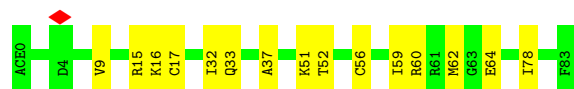
- Molecule 44: Small ribosomal subunit protein uS13

Chain Sd:  74% 22%




- Molecule 45: Small ribosomal subunit protein eS21

Chain Se:  82% 18%




- Molecule 46: 40S ribosomal protein S15a

Chain Sf:  81% 18%




- Molecule 47: Small ribosomal subunit protein uS12

Chain Sg:  88% 10%




- Molecule 48: 5S rRNA

Chain L2:  74% 21%

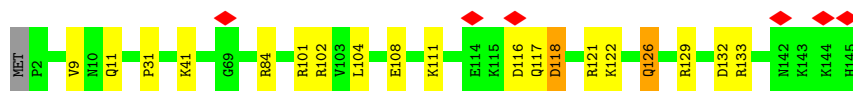
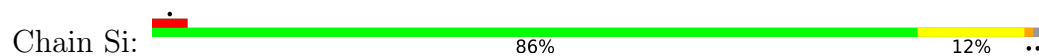


- Molecule 49: Isoform 3 of Small ribosomal subunit protein eS24

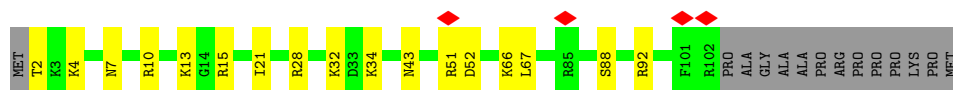
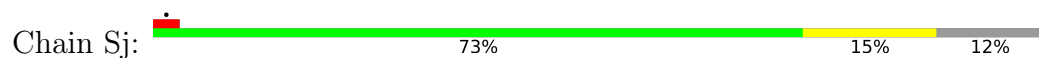
Chain Sh:  79% 15% 5%



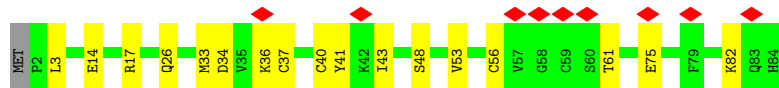
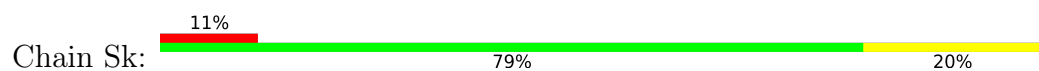
- Molecule 50: Small ribosomal subunit protein eS19



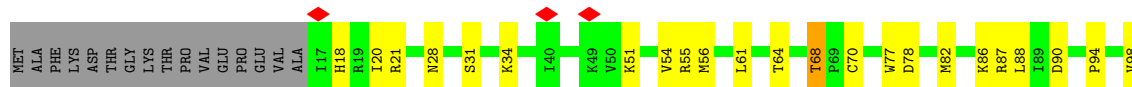
- Molecule 51: 40S ribosomal protein S26



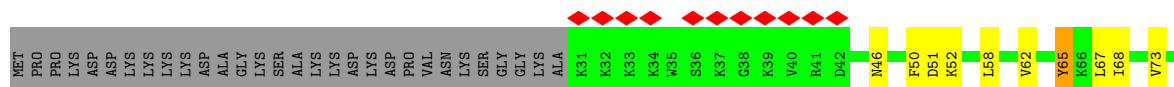
- Molecule 52: 40S ribosomal protein S27



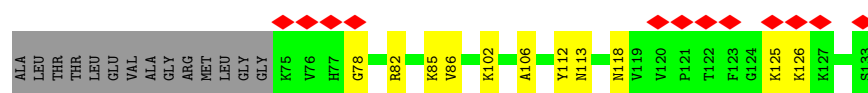
- Molecule 53: 40S ribosomal protein S20



- Molecule 54: 40S ribosomal protein S25



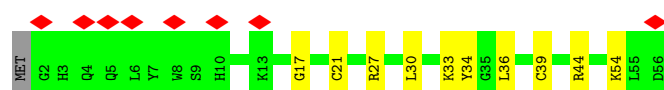
- Molecule 55: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



- Chain So: 

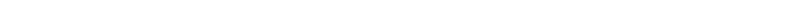


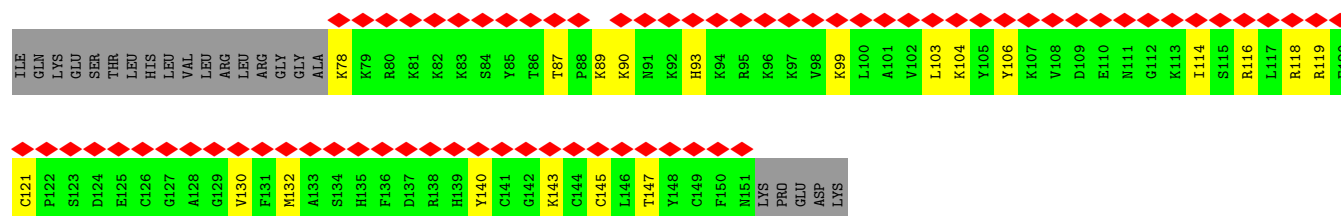
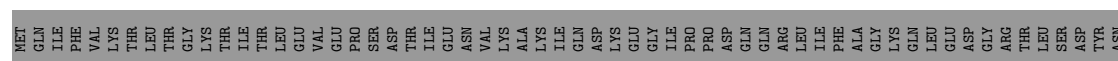
- Chain Sp: 14% 80% 18%

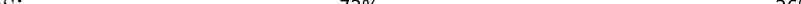


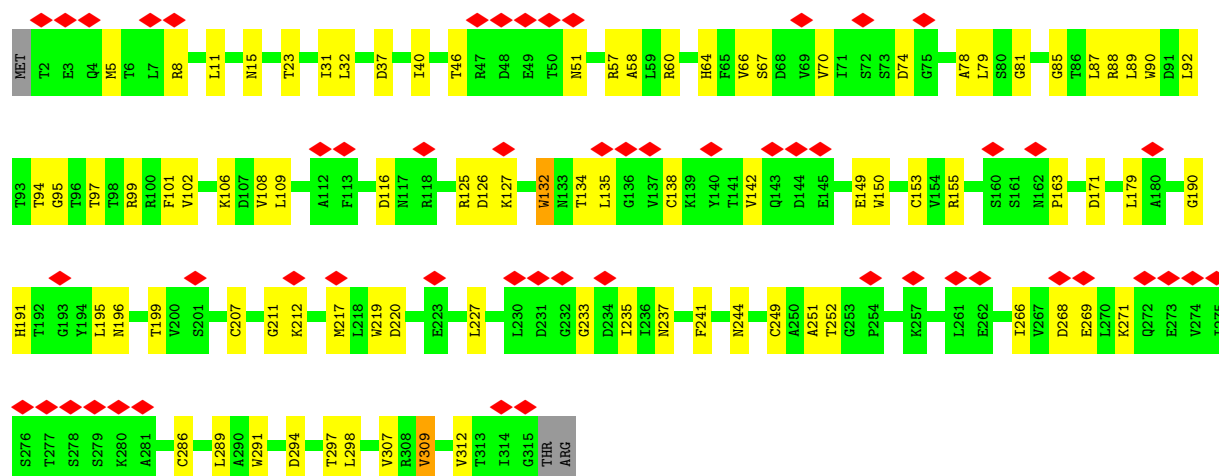
- Chain Sq: 12% 68% 32%



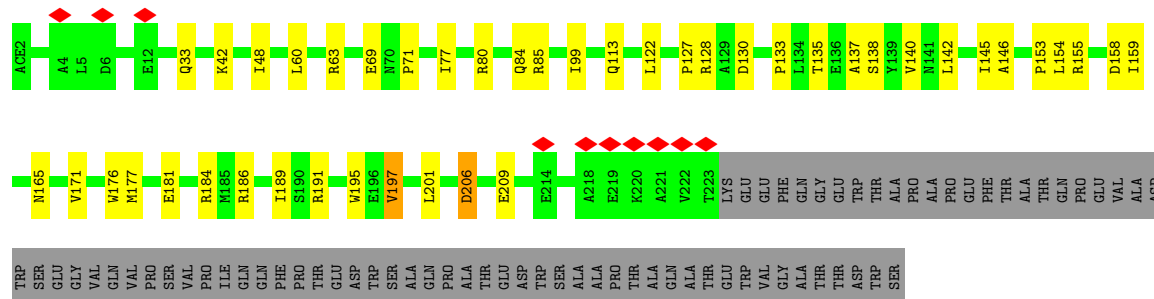
- Chain Sr: 



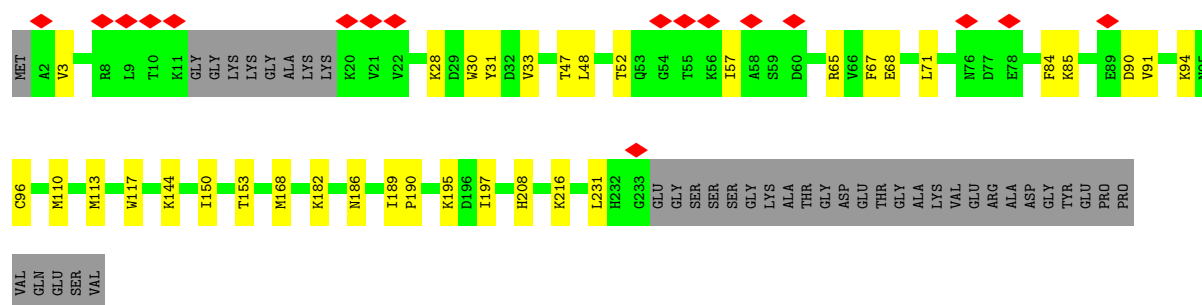
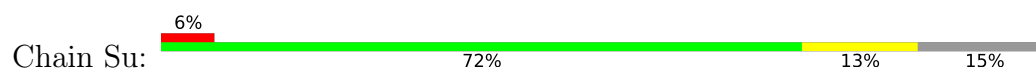
- Chain Ss:  17% 72% 26%



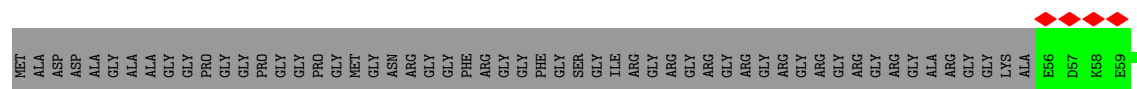
- Molecule 61: Small ribosomal subunit protein uS2

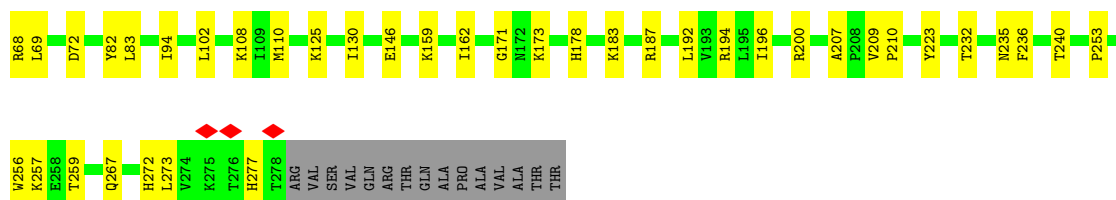


- Molecule 62: 40S ribosomal protein S3a



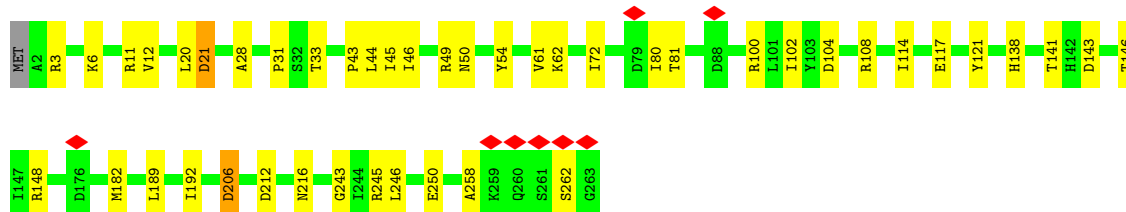
- Molecule 63: 40S ribosomal protein S2





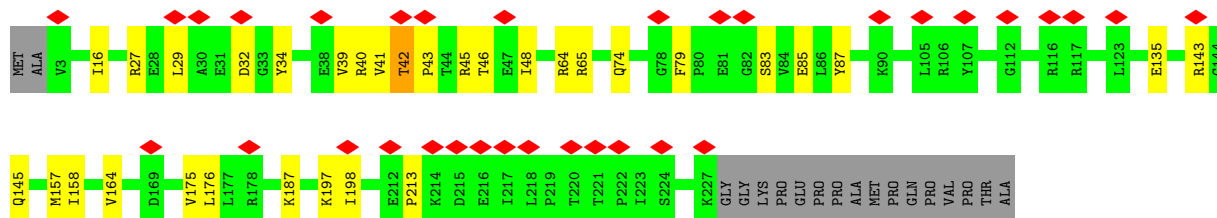
- Molecule 64: Small ribosomal subunit protein eS4, X isoform

Chain Sw: 83% 16%



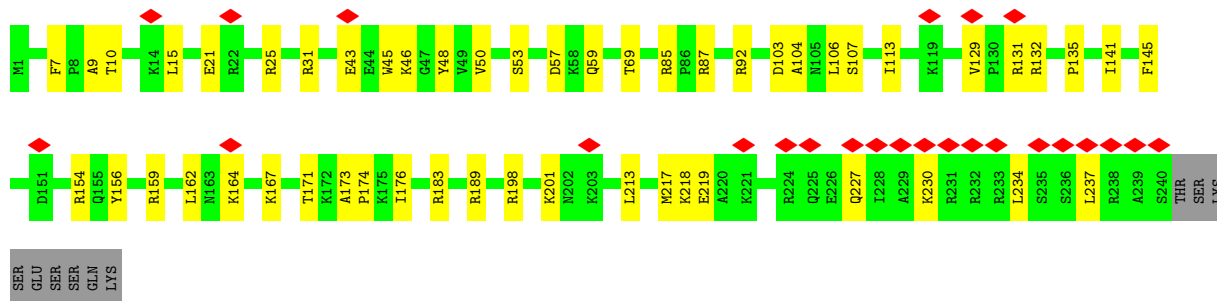
- Molecule 65: 40S ribosomal protein S3

Chain Sx: 14% 79% 13% 7%



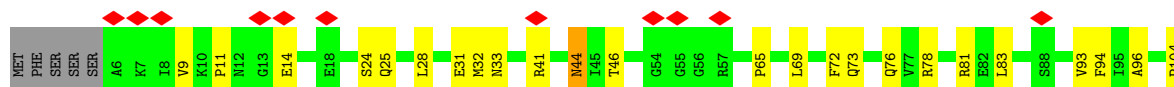
- Molecule 66: 40S ribosomal protein S6

Chain Sy: 10% 76% 21%

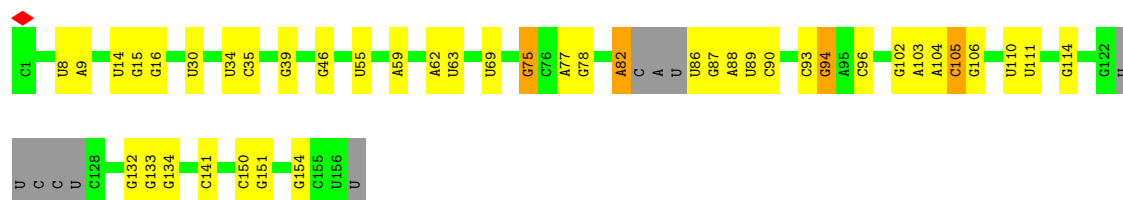


- Molecule 67: 40S ribosomal protein S7

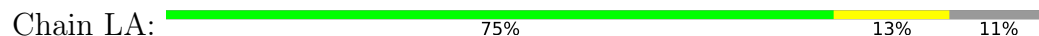
Chain Sz: 10% 77% 20%



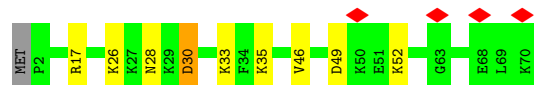
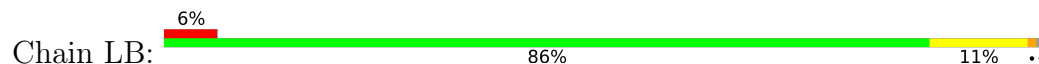
- Molecule 68: 5.8S rRNA



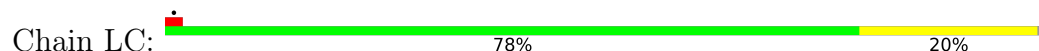
- Molecule 69: Large ribosomal subunit protein eL37



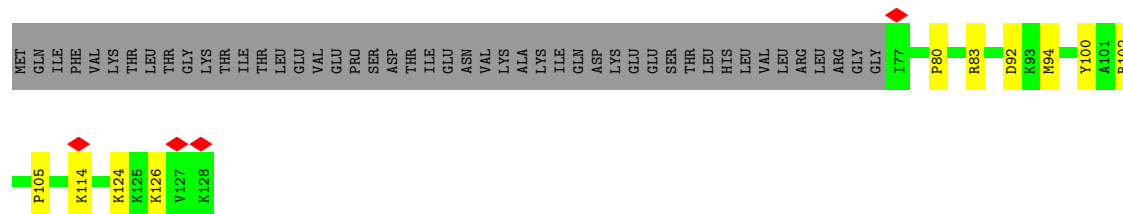
- Molecule 70: 60S ribosomal protein L38




- Molecule 71: 60S ribosomal protein L39

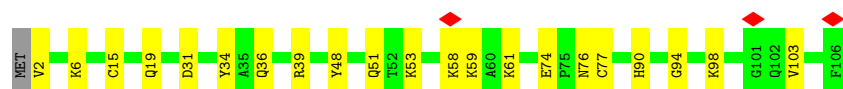


- Molecule 72: Ubiquitin-60S ribosomal protein L40




- Molecule 73: 60S ribosomal protein L36a

Chain LE:  79% 20%




- Molecule 74: 60S ribosomal protein L37a

Chain LF:  5% 87% 13%




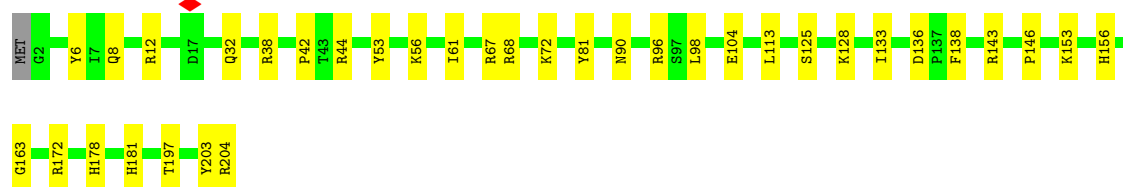
- Molecule 75: 60S ribosomal protein L28

Chain LG:  82% 9% 9%




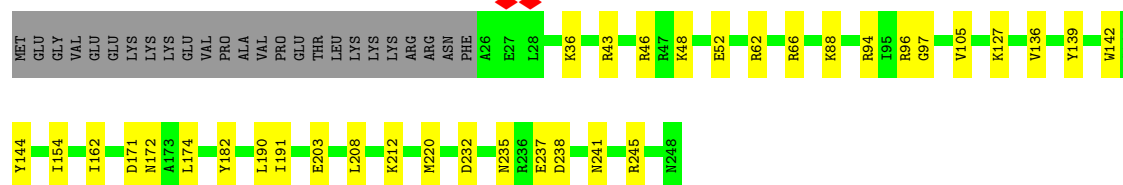
- Molecule 76: 60S ribosomal protein L15

Chain LH:  82% 17%




- Molecule 77: Large ribosomal subunit protein uL30

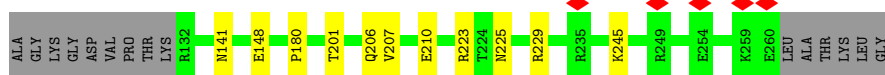
Chain LI:  76% 14% 10%



- Molecule 78: 60S ribosomal protein L7a

Chain LJ:  74% 10% 16%





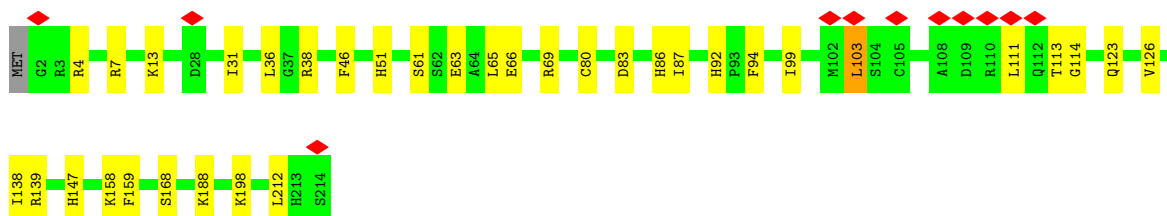
- Molecule 79: 60S ribosomal protein L9

Chain LK: 86% 12%



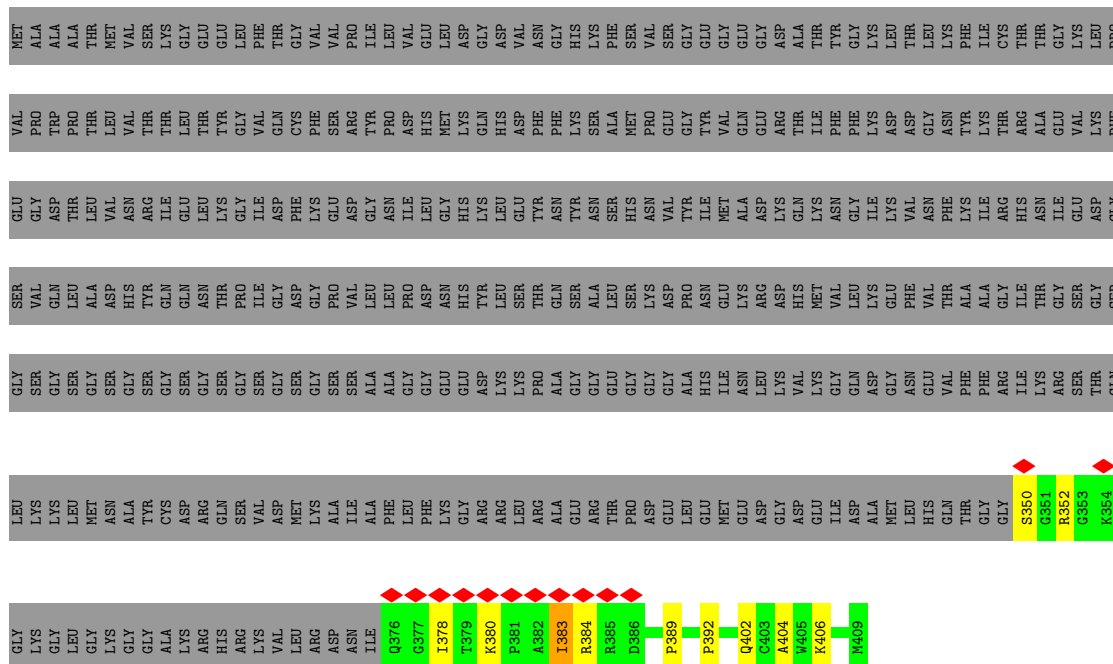
- Molecule 80: 60S ribosomal protein L10

Chain LM: 5% 83% 16%




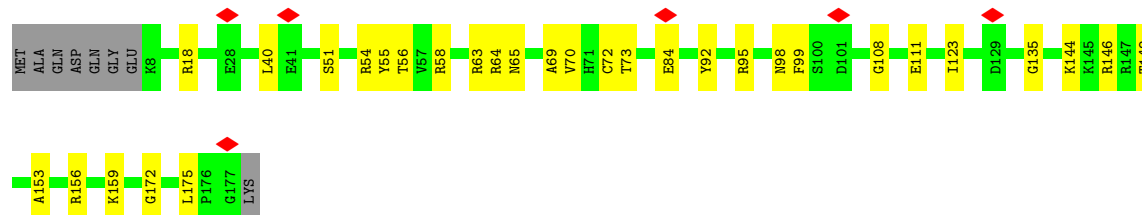
- Molecule 81: Green fluorescent protein, Small ubiquitin-related modifier 1, Green fluorescent protein, Small ubiquitin-related modifier 1, Histone H4, X-box-binding protein 1, X-box-binding protein 1

Chain LN: 7% 91%




- Molecule 82: 60S ribosomal protein L11

Chain LO:  78% 17%



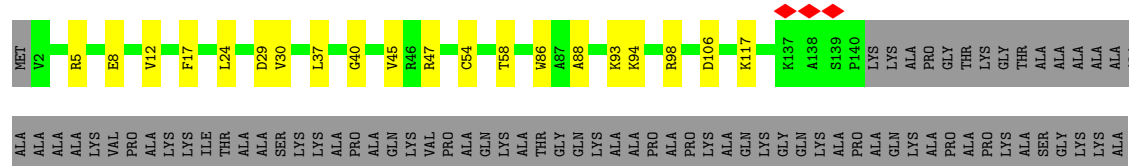
- Molecule 83: Large ribosomal subunit protein eL13

Chain LP:  87% 10%




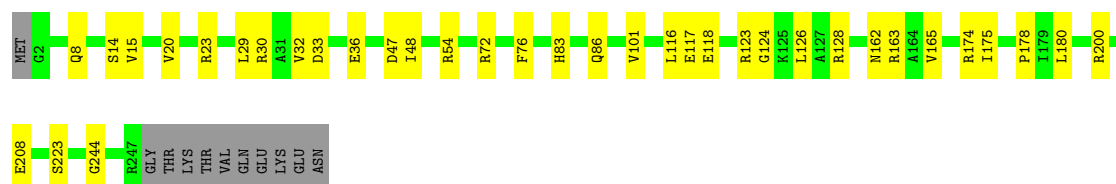
- Molecule 84: 60S ribosomal protein L14

Chain LQ:  55% 9% 35%




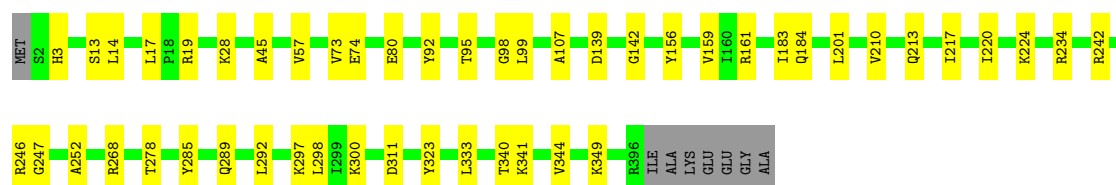
- Molecule 85: 60S ribosomal protein L8

Chain La:  82% 14%



- Molecule 86: 60S ribosomal protein L3

Chain Lb:  86% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11206	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.022	Depositor
Minimum map value	-0.502	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IAS, 5MC, 1MA, ZN, UR3, UY1, HY3, OMU, OMC, B8N, PSU, OMG, A2M, 4AC, GTP, COA, ACE, NMM, MA6, G7M, 6MZ

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	L1	0.19	1/78858 (0.0%)	0.19	0/122991
2	Lc	0.16	0/2944	0.24	0/3954
3	Ld	0.14	0/2418	0.22	0/3239
4	Le	0.14	0/1786	0.25	0/2395
5	Lf	0.17	0/1666	0.23	0/2228
6	Lg	0.16	0/1259	0.24	0/1689
7	Lh	0.17	0/1537	0.25	0/2052
8	Li	0.14	0/1517	0.21	0/2005
9	Lj	0.16	0/1501	0.23	0/2013
10	Lk	0.16	0/1326	0.23	0/1770
11	Ll	0.16	0/847	0.29	0/1137
12	Lm	0.17	0/999	0.23	0/1340
13	Ln	0.13	0/1006	0.23	0/1334
14	Lo	0.15	0/993	0.21	0/1334
15	Lp	0.15	0/1132	0.24	0/1504
16	Lq	0.15	0/1130	0.22	0/1507
17	Lr	0.16	0/1191	0.24	0/1591
18	Ls	0.13	0/819	0.22	0/1081
19	Lt	0.15	0/783	0.21	0/1052
20	Lu	0.15	0/883	0.23	0/1190
21	Lv	0.17	0/1071	0.24	0/1429
22	Lw	0.17	0/901	0.24	0/1206
23	Lx	0.16	0/892	0.25	0/1189
24	Ly	0.14	0/1023	0.19	0/1351
25	Lz	0.12	0/843	0.20	0/1115
26	Na	0.10	0/844	0.23	0/1128
27	Nb	0.13	0/942	0.30	0/1264
28	Nd	0.10	0/1931	0.26	0/2589
29	Nm	0.10	0/3057	0.26	0/4144
30	S1	0.19	1/40280 (0.0%)	0.18	0/62782
31	S2	0.13	0/164	0.22	0/253

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	S3	0.12	0/1763	0.20	0/2742
33	SA	0.14	0/1711	0.25	0/2282
34	SB	0.13	0/1524	0.21	0/2035
35	SC	0.13	0/1539	0.27	0/2071
36	SD	0.15	0/1250	0.22	0/1673
37	SE	0.11	0/840	0.23	0/1133
38	SF	0.15	0/1226	0.24	0/1649
39	SG	0.15	0/1014	0.23	0/1358
40	SH	0.10	0/963	0.28	0/1291
41	Sa	0.12	0/1035	0.22	0/1383
42	Sb	0.31	0/1097	0.40	0/1474
43	Sc	0.13	0/1146	0.24	0/1534
44	Sd	0.14	0/1216	0.25	0/1630
45	Se	0.15	0/644	0.24	0/862
46	Sf	0.16	0/1051	0.25	0/1406
47	Sg	0.19	0/1107	0.26	0/1475
48	L2	0.16	0/2813	0.16	0/4384
49	Sh	0.12	0/1031	0.21	0/1370
50	Si	0.12	0/1130	0.22	0/1513
51	Sj	0.15	0/828	0.24	0/1109
52	Sk	0.13	0/664	0.26	0/891
53	Sl	0.13	0/813	0.26	0/1092
54	Sm	0.13	0/678	0.26	0/906
55	Sn	0.12	0/473	0.24	0/623
56	So	0.12	0/514	0.21	0/688
57	Sp	0.13	0/469	0.22	0/623
58	Sq	0.15	0/240	0.22	0/305
59	Sr	0.09	0/622	0.26	0/822
60	Ss	0.12	0/2497	0.27	0/3399
61	St	0.15	0/1785	0.25	0/2426
62	Su	0.14	0/1841	0.25	0/2459
63	Sv	0.15	0/1781	0.24	0/2405
64	Sw	0.13	0/2118	0.23	0/2849
65	Sx	0.13	0/1780	0.24	0/2397
66	Sy	0.11	0/1968	0.22	0/2619
67	Sz	0.13	0/1546	0.25	0/2071
68	L3	0.17	0/3453	0.16	0/5376
69	LA	0.17	0/732	0.25	0/968
70	LB	0.13	0/575	0.22	0/761
71	LC	0.17	0/454	0.22	0/599
72	LD	0.13	0/435	0.25	0/575
73	LE	0.14	0/876	0.23	0/1156
74	LF	0.16	0/726	0.25	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	LG	0.16	0/1007	0.23	0/1351
76	LH	0.18	0/1753	0.24	0/2348
77	LI	0.17	0/1885	0.23	0/2512
78	LJ	0.14	0/1840	0.23	0/2476
79	LK	0.15	0/1537	0.23	0/2066
80	LM	0.16	0/1755	0.26	0/2344
81	LN	0.17	0/327	0.34	0/441
82	LO	0.14	0/1381	0.28	0/1848
83	LP	0.15	0/1695	0.24	0/2270
84	LQ	0.14	0/1161	0.20	0/1554
85	La	0.17	0/1925	0.26	0/2581
86	Lb	0.16	0/3265	0.24	0/4369
All	All	0.17	2/228042 (0.0%)	0.21	0/333363

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
42	Sb	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S1	1288	OMU	O3'-P	5.06	1.61	1.56
1	L1	3785	A2M	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	Sb	67	ARG	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	73061	0	37008	588	0
2	Lc	2890	0	3063	42	0
3	Ld	2372	0	2403	28	0
4	Le	1752	0	1904	21	0
5	Lf	1634	0	1779	13	0
6	Lg	1233	0	1263	13	0
7	Lh	1513	0	1628	16	0
8	Li	1501	0	1651	19	0
9	Lj	1461	0	1502	14	0
10	Lk	1298	0	1366	20	0
11	Ll	833	0	856	21	0
12	Lm	985	0	1044	16	0
13	Ln	991	0	1048	27	0
14	Lo	976	0	1053	10	0
15	Lp	1115	0	1205	24	0
16	Lq	1107	0	1182	17	0
17	Lr	1162	0	1213	11	0
18	Ls	806	0	865	13	0
19	Lt	772	0	808	10	0
20	Lu	868	0	913	6	0
21	Lv	1053	0	1147	18	0
22	Lw	879	0	917	10	0
23	Lx	882	0	972	13	0
24	Ly	1015	0	1148	14	0
25	Lz	832	0	917	7	0
26	Na	840	0	898	28	0
27	Nb	934	0	963	40	0
28	Nd	1890	0	1819	55	0
29	Nm	2984	0	2908	63	0
30	S1	37855	0	19186	432	0
31	S2	148	0	75	0	0
32	S3	1579	0	801	20	0
33	SA	1682	0	1769	25	0
34	SB	1499	0	1618	19	0
35	SC	1517	0	1569	18	0
36	SD	1229	0	1302	15	0
37	SE	816	0	841	10	0
38	SF	1202	0	1289	11	0
39	SG	1010	0	1033	14	0
40	SH	953	0	990	14	0
41	Sa	1016	0	1066	32	0
42	Sb	1082	0	1137	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Sc	1128	0	1195	21	0
44	Sd	1200	0	1262	23	0
45	Se	639	0	638	13	0
46	Sf	1034	0	1080	17	0
47	Sg	1099	0	1162	11	0
48	L2	2518	0	1274	22	0
49	Sh	1014	0	1082	18	0
50	Si	1123	0	1152	15	0
51	Sj	814	0	863	11	0
52	Sk	650	0	672	9	0
53	Sl	803	0	873	17	0
54	Sm	670	0	745	11	0
55	Sn	467	0	516	8	0
56	So	512	0	541	13	0
57	Sp	458	0	448	8	0
58	Sq	239	0	289	8	0
59	Sr	610	0	634	17	0
60	Ss	2440	0	2396	51	0
61	St	1750	0	1755	28	0
62	Su	1815	0	1908	22	0
63	Sv	1741	0	1827	31	0
64	Sw	2076	0	2177	31	0
65	Sx	1752	0	1848	20	0
66	Sy	1945	0	2112	42	0
67	Sz	1523	0	1622	26	0
68	L3	3156	0	1602	20	0
69	LA	713	0	746	11	0
70	LB	569	0	637	6	0
71	LC	444	0	483	9	0
72	LD	429	0	465	8	0
73	LE	862	0	929	13	0
74	LF	716	0	768	9	0
75	LG	992	0	1052	8	0
76	LH	1708	0	1757	29	0
77	LI	1851	0	1981	26	0
78	LJ	1809	0	1941	21	0
79	LK	1518	0	1601	16	0
80	LM	1716	0	1765	23	0
81	LN	316	0	318	12	0
82	LO	1358	0	1388	18	0
83	LP	1664	0	1773	19	0
84	LQ	1138	0	1204	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	La	1887	0	1983	27	0
86	Lb	3194	0	3336	33	0
87	LA	1	0	0	0	0
87	LD	1	0	0	0	0
87	LE	1	0	0	0	0
87	LF	1	0	0	0	0
87	Lx	1	0	0	0	0
87	Nm	2	0	0	0	0
87	Sj	1	0	0	0	0
87	Sp	1	0	0	0	0
87	Sr	1	0	0	0	0
88	Nd	48	0	32	5	0
89	L2	32	0	11	1	0
All	All	217377	0	163962	2122	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 6.

All (2122) 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)
1:L1:3642:A:HO2'	69:LA:2:THR:N	1.54	1.06
88:Nd:301:COA:HS1	81:LN:350:SER:N	1.59	0.97
42:Sb:71:ILE:HD11	42:Sb:73:LEU:HG	1.54	0.88
30:S1:1757:G:H1	30:S1:1775:U:H3	1.21	0.87
27:Nb:53:VAL:HG12	27:Nb:80:GLN:HB3	1.59	0.83
1:L1:737:C:O2	1:L1:926:G:N2	2.13	0.81
30:S1:165:G:H2'	30:S1:166:A2M:H8	1.62	0.81
1:L1:1754:U:H3	1:L1:1776:A:H61	1.30	0.80
60:Ss:87:LEU:HB2	60:Ss:101:PHE:HB2	1.64	0.79
30:S1:116:OMU:HN3	30:S1:347:G:H1	1.27	0.79
1:L1:3717:A:OP2	1:L1:3735:G:N2	2.16	0.79
30:S1:576:A2M:HM'2	30:S1:577:U:H5'	1.67	0.77
1:L1:1447:C:O2	1:L1:2098:G:N2	2.17	0.77
11:L1:27:HIS:HE1	27:Nb:1:MET:N	1.83	0.77
23:Lx:83:CYS:HB2	23:Lx:86:CYS:SG	2.26	0.76
30:S1:867:G:H1	67:Sz:109:ARG:HH21	1.32	0.75
28:Nd:185:PHE:HD1	88:Nd:301:COA:H8A	1.52	0.75
1:L1:3946:G:H1	1:L1:4067:U:H3	1.35	0.74
29:Nm:196:SER:HB2	29:Nm:218:ASN:HB3	1.69	0.74
29:Nm:180:TYR:HB3	29:Nm:224:TYR:HB3	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3830:A2M:HM'2	1:L1:3831:U:H5'	1.70	0.73
30:S1:581:U:OP1	34:SB:133:ARG:NH2	2.22	0.73
30:S1:496:C:OP1	64:Sw:49:ARG:NH2	2.22	0.73
59:Sr:130:VAL:HG21	59:Sr:143:LYS:HD2	1.71	0.73
53:Sl:56:MET:HB2	53:Sl:86:LYS:HB3	1.71	0.73
30:S1:984:C:HO2'	39:SG:139:SER:N	1.86	0.72
1:L1:2377:C:OP1	26:Na:82:LYS:NZ	2.23	0.72
8:Li:173:ARG:HH12	30:S1:911:C:H41	1.38	0.72
30:S1:387:C:OP2	33:SA:10:LYS:NZ	2.22	0.72
30:S1:1757:G:N2	30:S1:1775:U:O2	2.19	0.72
30:S1:1091:C:HO2'	46:Sf:2:VAL:N	1.86	0.72
1:L1:3808:OMC:HM22	1:L1:3809:G:H5'	1.69	0.72
39:SG:34:PHE:HB3	39:SG:41:PHE:HB2	1.71	0.72
13:Ln:69:LYS:HB2	30:S1:1783:C:H41	1.55	0.71
1:L1:3641:U:OP2	1:L1:3646:A:N6	2.24	0.71
73:LE:34:TYR:O	73:LE:39:ARG:NH1	2.24	0.71
1:L1:223:G:N7	2:Lc:165:LYS:NZ	2.37	0.71
1:L1:3937:C:H1'	76:LH:125:SER:HB3	1.71	0.71
33:SA:11:ARG:O	36:SD:136:LYS:NZ	2.23	0.71
1:L1:3823:G:OP2	1:L1:3823:G:N2	2.24	0.70
3:Ld:268:ARG:NH2	48:L2:60:G:O2'	2.22	0.70
28:Nd:176:PHE:HA	28:Nd:211:TYR:HA	1.72	0.70
85:La:30:ARG:NH1	85:La:36:GLU:OE2	2.24	0.70
30:S1:659:G:H21	47:Sg:17:ARG:HH22	1.40	0.70
30:S1:1033:G:H1	30:S1:1080:A:HO2'	1.33	0.70
1:L1:369:G:N2	1:L1:372:A:OP2	2.25	0.70
11:Ll:18:VAL:HG12	11:Ll:75:GLU:HB3	1.73	0.70
29:Nm:232:LEU:HD13	29:Nm:372:THR:HB	1.74	0.70
1:L1:1459:A:OP1	7:Lh:65:ARG:NH1	2.25	0.70
1:L1:666:G:N2	2:Lc:288:ASP:OD2	2.25	0.69
1:L1:2483:G:H1	1:L1:2495:U:H3	1.40	0.69
11:Ll:27:HIS:HE1	27:Nb:1:MET:H2	1.39	0.69
61:St:184:ARG:HD2	61:St:191:ARG:HG2	1.73	0.69
53:Sl:54:VAL:HB	53:Sl:88:LEU:HB2	1.75	0.69
5:Lf:42:ASN:HD22	5:Lf:125:LYS:HD3	1.57	0.69
30:S1:744:G:N2	30:S1:797:OMC:O2	2.23	0.69
49:Sh:8:ARG:HB3	49:Sh:26:ASP:HB2	1.73	0.69
1:L1:2300:A:N7	2:Lc:143:ARG:NH1	2.40	0.69
1:L1:3887:OMC:HM22	1:L1:3888:G:H5'	1.73	0.69
26:Na:190:VAL:HG21	26:Na:213:LEU:HD13	1.74	0.69
5:Lf:54:TYR:OH	5:Lf:73:PHE:O	2.11	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:230:G:OP1	15:Lp:15:ARG:NH1	2.26	0.69
1:L1:4924:C:O2'	1:L1:4926:C:O2	2.10	0.69
30:S1:1522:A:OP1	44:Sd:144:ARG:NH2	2.26	0.68
19:Lt:13:SER:OG	19:Lt:17:ARG:NH1	2.25	0.68
64:Sw:100:ARG:NH2	64:Sw:121:TYR:O	2.26	0.68
65:Sx:29:LEU:HB2	65:Sx:34:TYR:HB2	1.75	0.68
80:LM:103:LEU:HD11	80:LM:111:LEU:HB3	1.75	0.68
86:Lb:213:GLN:NE2	86:Lb:285:TYR:O	2.27	0.68
30:S1:235:A:N6	30:S1:892:U:O4	2.27	0.68
30:S1:1283:C:H42	40:SH:102:LYS:HE3	1.56	0.68
1:L1:1364:U:OP2	83:LP:36:ARG:NH2	2.24	0.68
1:L1:2838:G:H5'	86:Lb:247:GLY:HA2	1.75	0.68
30:S1:1153:C:OP2	46:Sf:71:LYS:NZ	2.27	0.68
61:St:71:PRO:HB3	61:St:186:ARG:HH22	1.57	0.67
30:S1:506:G:OP1	49:Sh:108:LYS:NZ	2.27	0.67
30:S1:1753:C:H2'	30:S1:1754:G:H8	1.59	0.67
38:SF:4:MET:SD	38:SF:124:ARG:NH1	2.67	0.67
1:L1:2845:A:H61	1:L1:3843:C:H42	1.42	0.67
1:L1:664:G:H21	1:L1:667:A:H61	1.41	0.67
1:L1:4751:G:N7	22:Lw:52:LYS:NZ	2.39	0.67
1:L1:1199:G:O6	9:Lj:15:ARG:NH1	2.27	0.67
1:L1:4732:G:N2	1:L1:4734:A:N7	2.43	0.67
27:Nb:100:THR:HA	27:Nb:103:LEU:HG	1.77	0.67
30:S1:746:C:H4'	30:S1:747:U:H5'	1.77	0.67
41:Sa:81:ARG:NH1	41:Sa:120:SER:OG	2.28	0.67
30:S1:641:A:OP1	34:SB:40:LYS:NZ	2.28	0.67
39:SG:72:TYR:HA	56:So:63:ARG:HE	1.59	0.67
44:Sd:38:ARG:O	44:Sd:42:HIS:ND1	2.25	0.67
30:S1:1617:G:N1	30:S1:1620:A:OP2	2.28	0.66
41:Sa:28:MET:HB3	41:Sa:32:GLN:HB2	1.77	0.66
30:S1:228:C:O2'	30:S1:887:U:O2	2.12	0.66
38:SF:99:ARG:NH2	38:SF:119:GLU:OE2	2.27	0.66
45:Se:15:ARG:NH1	63:Sv:83:LEU:O	2.28	0.66
53:Sl:51:LYS:HB2	53:Sl:90:ASP:HB2	1.77	0.66
1:L1:4541:G:N2	1:L1:4544:A:OP2	2.25	0.66
50:Si:9:VAL:O	50:Si:11:GLN:NE2	2.29	0.66
79:LK:113:GLU:HG2	79:LK:125:ARG:HG2	1.76	0.66
80:LM:188:LYS:HB3	80:LM:212:LEU:HD21	1.77	0.66
1:L1:4250:G:OP1	82:LO:98:ASN:ND2	2.28	0.66
68:L3:46:G:OP1	71:LC:18:LYS:NZ	2.28	0.66
67:Sz:78:ARG:HH21	67:Sz:81:ARG:HH22	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Sb:21:TYR:CE2	42:Sb:71:ILE:HD13	2.31	0.66
62:Su:190:PRO:O	62:Su:195:LYS:NZ	2.29	0.66
30:S1:1166:G:N7	47:Sg:25:LYS:NZ	2.44	0.66
67:Sz:104:PRO:O	67:Sz:109:ARG:NH1	2.28	0.66
1:L1:2861:OMC:HM22	1:L1:2862:G:H5'	1.77	0.65
1:L1:4670:C:O2'	1:L1:4672:A:OP2	2.14	0.65
15:Lp:24:HIS:HD1	68:L3:90:C:HO2'	1.44	0.65
29:Nm:41:PHE:HE1	29:Nm:48:HIS:HD2	1.44	0.65
29:Nm:194:CYS:HB2	29:Nm:220:ASN:HB3	1.77	0.65
1:L1:134:G:O6	24:Ly:74:LYS:NZ	2.27	0.65
30:S1:659:G:HO2'	30:S1:662:G:HO2'	1.44	0.65
3:Ld:268:ARG:HH21	48:L2:60:G:HO2'	1.42	0.65
42:Sb:37:GLU:OE2	60:Ss:106:LYS:NZ	2.29	0.65
1:L1:4620:OMU:OP2	1:L1:4670:C:N4	2.28	0.65
1:L1:2725:A:N6	8:Li:88:ARG:O	2.29	0.65
1:L1:1316:OMG:HM22	1:L1:1317:U:H5'	1.78	0.65
1:L1:4380:A:OP1	73:LE:58:LYS:NZ	2.30	0.65
19:Lt:72:HIS:ND1	19:Lt:108:MET:SD	2.70	0.65
30:S1:185:G:H1	30:S1:214:U:H3	1.42	0.65
43:Sc:98:LYS:O	60:Ss:57:ARG:NH2	2.30	0.65
60:Ss:132:TRP:HB3	60:Ss:138:CYS:HA	1.78	0.65
30:S1:320:G:N2	30:S1:331:C:O2	2.30	0.64
1:L1:713:C:O2	4:Le:130:LYS:NZ	2.28	0.64
25:Lz:45:ARG:NH1	25:Lz:49:GLY:O	2.30	0.64
40:SH:80:ASP:N	40:SH:80:ASP:OD1	2.30	0.64
30:S1:1677:U:H2'	30:S1:1678:A2M:H8	1.80	0.64
83:LP:64:VAL:HA	83:LP:67:HIS:CD2	2.32	0.64
52:Sk:14:GLU:HG2	52:Sk:17:ARG:HH12	1.61	0.64
63:Sv:196:ILE:HB	63:Sv:223:TYR:HB2	1.79	0.64
1:L1:4742:G:OP1	1:L1:4900:C:N4	2.31	0.64
28:Nd:139:GLU:OE1	81:LN:350:SER:OG	2.14	0.64
30:S1:754:G:O6	30:S1:790:C:N4	2.20	0.64
3:Ld:264:LYS:NZ	3:Ld:265:ARG:O	2.31	0.64
33:SA:191:GLU:O	36:SD:19:ASN:ND2	2.30	0.64
56:So:44:ARG:NH2	56:So:60:GLU:O	2.28	0.64
1:L1:1100:U:H3	1:L1:1195:G:H1	1.46	0.64
23:Lx:41:ALA:O	23:Lx:52:ARG:NH1	2.31	0.64
1:L1:2431:A:OP1	71:LC:41:ARG:NH1	2.31	0.64
26:Na:98:LYS:HB3	26:Na:102:ILE:HB	1.79	0.64
30:S1:1292:C:O2'	59:Sr:147:THR:OG1	2.16	0.64
48:L2:27:G:OP1	82:LO:146:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4322:G:N2	1:L1:4325:A:OP2	2.28	0.63
60:Ss:251:ALA:HB2	60:Ss:289:LEU:HD22	1.80	0.63
64:Sw:21:ASP:N	64:Sw:21:ASP:OD1	2.31	0.63
40:SH:26:LEU:HD21	40:SH:33:ARG:HH12	1.63	0.63
1:L1:1870:C:H2'	1:L1:1871:A2M:H8	1.79	0.63
28:Nd:174:THR:O	81:LN:350:SER:N	2.30	0.63
45:Se:60:ARG:NH1	61:St:158:ASP:OD1	2.31	0.63
53:Sl:78:ASP:OD2	57:Sp:44:ARG:NH1	2.30	0.63
30:S1:165:G:OP2	30:S1:165:G:N2	2.24	0.63
30:S1:503:C:OP1	64:Sw:62:LYS:NZ	2.30	0.63
1:L1:1268:G:N7	18:Ls:111:ARG:NH2	2.39	0.63
30:S1:1597:C:OP2	54:Sm:85:ARG:NH2	2.31	0.63
76:LH:32:GLN:O	78:LJ:59:ARG:NH2	2.31	0.63
37:SE:80:ARG:HH22	37:SE:90:VAL:HG12	1.62	0.63
74:LF:88:GLU:O	74:LF:92:GLN:NE2	2.32	0.63
83:LP:80:GLU:OE2	83:LP:113:ASN:ND2	2.31	0.63
30:S1:436:OMG:HM22	30:S1:437:G:H5'	1.79	0.63
30:S1:690:G:H2'	30:S1:691:G:H8	1.64	0.63
9:Lj:99:ASP:OD1	9:Lj:100:LEU:N	2.32	0.63
30:S1:1703:OMC:HM22	30:S1:1704:C:H5'	1.80	0.63
76:LH:6:TYR:OH	78:LJ:148:GLU:OE2	2.15	0.63
78:LJ:85:GLN:HE22	78:LJ:229:ARG:HH12	1.46	0.63
1:L1:4693:C:O2	1:L1:4695:C:N4	2.31	0.62
29:Nm:327:GLU:HB2	29:Nm:356:GLN:HE21	1.63	0.62
1:L1:4472:G:O2'	72:LD:100:TYR:O	2.17	0.62
27:Nb:53:VAL:CG1	27:Nb:80:GLN:HB3	2.30	0.62
30:S1:1298:G:H4'	41:Sa:78:THR:HA	1.80	0.62
32:S3:33:U:OP2	43:Sc:146:ARG:NH2	2.32	0.62
1:L1:3680:U:OP1	85:La:54:ARG:NH2	2.30	0.62
1:L1:3713:U:H1'	1:L1:3714:G:H5'	1.82	0.62
1:L1:3642:A:O2'	69:LA:2:THR:N	2.28	0.62
30:S1:1092:G:OP2	38:SF:9:LYS:NZ	2.32	0.62
57:Sp:17:GLY:O	57:Sp:27:ARG:NH1	2.33	0.62
1:L1:393:U:OP2	26:Na:68:LYS:NZ	2.32	0.62
30:S1:520:A:O2'	30:S1:825:A:N3	2.30	0.62
30:S1:1396:A:O2'	30:S1:1398:G:N7	2.29	0.62
3:Ld:238:GLU:HG3	3:Ld:242:LYS:HE2	1.81	0.62
4:Le:161:ARG:O	4:Le:182:ASN:ND2	2.33	0.62
4:Le:179:LEU:HD12	4:Le:183:ARG:HA	1.82	0.62
13:Ln:110:ARG:NH2	13:Ln:114:GLU:OE2	2.31	0.62
30:S1:92:A:H4'	64:Sw:3:ARG:HH21	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:1490:OMG:HM22	30:S1:1491:G:H5'	1.81	0.62
21:Lv:101:HIS:O	21:Lv:128:ARG:NH2	2.32	0.62
30:S1:1033:G:N1	30:S1:1080:A:O2'	2.27	0.62
30:S1:1507:G:N2	59:Sr:87:THR:O	2.33	0.62
30:S1:1599:U:OP2	54:Sm:46:ASN:ND2	2.33	0.62
3:Ld:193:GLU:OE2	3:Ld:197:LYS:NZ	2.32	0.62
6:Lg:40:HIS:NE2	6:Lg:110:ASP:O	2.26	0.62
30:S1:1380:C:O2'	61:St:113:GLN:NE2	2.33	0.62
54:Sm:73:VAL:HG21	54:Sm:88:LEU:HD11	1.82	0.62
26:Na:77:ARG:NH1	26:Na:110:ASP:OD2	2.33	0.61
60:Ss:244:ASN:ND2	60:Ss:294:ASP:O	2.32	0.61
62:Su:182:LYS:O	62:Su:186:ASN:ND2	2.33	0.61
1:L1:252:C:H2'	1:L1:253:G:H8	1.65	0.61
1:L1:2385:U:OP1	8:Li:5:ARG:NH2	2.33	0.61
1:L1:4683:U:OP2	1:L1:4706:G:N1	2.25	0.61
30:S1:142:C:N4	30:S1:329:G:OP1	2.32	0.61
42:Sb:17:ILE:HG13	42:Sb:57:LEU:HD23	1.81	0.61
67:Sz:69:LEU:HD22	67:Sz:96:ALA:HB2	1.82	0.61
30:S1:476:A:N3	30:S1:488:U:O2'	2.29	0.61
43:Sc:102:GLU:OE2	60:Ss:58:ALA:N	2.31	0.61
44:Sd:22:GLY:HA2	44:Sd:56:ALA:HB3	1.82	0.61
13:Ln:94:ARG:HG2	66:Sy:145:PHE:HA	1.81	0.61
41:Sa:123:TYR:OH	44:Sd:124:ARG:NH1	2.33	0.61
70:LB:30:ASP:OD1	70:LB:30:ASP:N	2.30	0.61
13:Ln:79:GLN:NE2	13:Ln:80:ARG:O	2.33	0.61
26:Na:94:VAL:HB	26:Na:106:ILE:HB	1.83	0.61
30:S1:678:U:OP2	30:S1:1026:C:N4	2.25	0.61
60:Ss:11:LEU:HB2	60:Ss:307:VAL:HB	1.81	0.61
85:La:101:VAL:HG22	85:La:165:VAL:HG22	1.82	0.61
26:Na:85:LEU:HD22	26:Na:114:SER:HA	1.82	0.61
26:Na:100:LYS:HB3	28:Nd:205:CYS:HB2	1.81	0.61
32:S3:23:C:H2'	32:S3:24:G:C8	2.35	0.61
61:St:85:ARG:HH21	61:St:201:LEU:HD12	1.64	0.61
1:L1:1077:C:OP1	1:L1:1215:C:O2'	2.18	0.61
21:Lv:117:GLN:O	75:LG:119:ARG:NH2	2.34	0.61
54:Sm:68:ILE:HB	54:Sm:109:TYR:HB2	1.83	0.61
1:L1:2527:A:OP1	8:Li:38:ARG:NH2	2.34	0.61
1:L1:3760:A:N6	30:S1:1824:A:C4	2.69	0.61
10:Lk:133:ALA:HB3	77:LI:127:LYS:HB2	1.83	0.61
30:S1:229:A:H62	30:S1:887:U:H3	1.48	0.61
33:SA:80:ASP:OD1	33:SA:81:VAL:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:L2:28:C:H1'	48:L2:54:A:H61	1.65	0.61
1:L1:1802:A:O2'	10:Lk:108:ARG:NH2	2.33	0.61
1:L1:4769:G:H5''	5:Lf:176:ARG:HD3	1.83	0.61
30:S1:818:A:OP1	34:SB:80:ARG:NH1	2.33	0.61
1:L1:4429:C:N3	80:LM:158:LYS:NZ	2.48	0.60
1:L1:4527:G:N2	1:L1:4527:G:OP2	2.34	0.60
35:SC:123:GLU:OE1	35:SC:204:ARG:NH2	2.33	0.60
84:LQ:88:ALA:O	84:LQ:93:LYS:NZ	2.34	0.60
1:L1:2351:OMC:HM22	1:L1:2352:U:H5'	1.81	0.60
1:L1:3616:U:OP2	1:L1:3617:G:N2	2.34	0.60
3:Ld:225:GLN:HE21	48:L2:49:A:H3'	1.66	0.60
79:LK:43:VAL:HG12	79:LK:59:LYS:HD3	1.83	0.60
13:Ln:80:ARG:NH2	66:Sy:10:THR:O	2.31	0.60
30:S1:540:U:O2'	30:S1:543:C:N4	2.31	0.60
1:L1:664:G:N2	1:L1:667:A:H61	1.99	0.60
1:L1:1573:G:OP1	8:Li:92:LYS:NZ	2.34	0.60
36:SD:111:VAL:HG12	36:SD:140:PHE:HB2	1.82	0.60
64:Sw:182:MET:HE2	64:Sw:192:ILE:HD11	1.84	0.60
1:L1:4145:C:H2'	1:L1:4146:G:H8	1.66	0.60
30:S1:744:G:H1'	67:Sz:108:SER:HB3	1.82	0.60
30:S1:1226:G:N1	30:S1:1639:G7M:OP2	2.30	0.60
1:L1:4590:A2M:HM'2	1:L1:4591:U:H5'	1.82	0.60
3:Ld:58:ARG:NH2	48:L2:27:G:N7	2.47	0.60
28:Nd:129:GLU:OE1	81:LN:352:ARG:NH2	2.32	0.60
47:Sg:66:ILE:HD13	55:Sn:78:GLY:HA3	1.84	0.60
1:L1:327:U:O2'	25:Lz:30:ARG:NH1	2.34	0.60
1:L1:2588:C:OP1	1:L1:2768:C:O2'	2.20	0.60
1:L1:2693:G:OP1	70:LB:35:LYS:NZ	2.35	0.60
30:S1:546:G:O2'	30:S1:548:C:OP1	2.15	0.60
30:S1:1199:A:OP1	51:Sj:2:THR:OG1	2.18	0.60
30:S1:1498:A:OP2	65:Sx:27:ARG:NH2	2.35	0.60
39:SG:147:ARG:HA	51:Sj:28:ARG:HH11	1.66	0.60
9:Lj:80:ILE:HG12	9:Lj:129:VAL:HG22	1.83	0.60
30:S1:1030:A:H2'	30:S1:1031:A2M:H8	1.84	0.60
30:S1:1291:A:O2'	59:Sr:145:CYS:SG	2.59	0.60
30:S1:1619:A:OP1	41:Sa:47:ARG:NE	2.35	0.60
27:Nb:149:LEU:HB3	29:Nm:20:LEU:HB3	1.83	0.60
30:S1:1842:4AC:O7	58:Sq:4:LYS:NZ	2.27	0.60
51:Sj:51:ARG:NH2	56:So:39:SER:OG	2.34	0.60
11:Ll:27:HIS:CE1	27:Nb:1:MET:N	2.68	0.59
26:Na:99:SER:N	27:Nb:58:GLY:O	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:879:C:H2'	30:S1:880:G:H8	1.67	0.59
40:SH:33:ARG:NH1	40:SH:89:VAL:O	2.35	0.59
67:Sz:119:SER:OG	67:Sz:120:ARG:NH1	2.35	0.59
78:LJ:58:PRO:HD2	78:LJ:61:ILE:HD12	1.83	0.59
1:L1:2045:G:N2	1:L1:2046:G:N7	2.46	0.59
1:L1:2706:G:N2	1:L1:2706:G:OP2	2.34	0.59
30:S1:509:OMG:HM22	30:S1:510:G:H5'	1.84	0.59
26:Na:96:ILE:HB	26:Na:104:PHE:HB2	1.83	0.59
30:S1:1124:C:H5''	62:Su:150:ILE:HG12	1.83	0.59
61:St:69:GLU:OE2	63:Sv:267:GLN:NE2	2.35	0.59
1:L1:1890:G:OP2	1:L1:1890:G:N2	2.36	0.59
1:L1:2414:G:H2'	1:L1:2415:OMU:H6	1.85	0.59
1:L1:1179:U:O2	3:Ld:290:ALA:HB2	2.02	0.59
1:L1:1390:G:N2	1:L1:1393:G:OP2	2.33	0.59
1:L1:1398:A:OP1	17:Lr:136:LYS:NZ	2.36	0.59
30:S1:1369:A:OP1	42:Sb:2:GLY:N	2.36	0.59
30:S1:1464:C:OP1	42:Sb:63:ARG:NH2	2.26	0.59
55:Sn:125:LYS:NZ	55:Sn:126:LYS:O	2.32	0.59
1:L1:2262:G:OP2	75:LG:98:ARG:NH2	2.36	0.59
14:Lo:77:ILE:HD13	14:Lo:100:VAL:HG23	1.84	0.59
35:SC:78:MET:HB3	35:SC:79:HIS:HD2	1.68	0.59
60:Ss:149:GLU:HG2	60:Ss:171:ASP:HB3	1.84	0.59
62:Su:47:THR:OG1	62:Su:65:ARG:NH1	2.35	0.59
80:LM:87:ILE:HG12	80:LM:138:ILE:HG12	1.85	0.59
10:Lk:121:GLU:OE2	10:Lk:122:LYS:NZ	2.36	0.59
29:Nm:191:LYS:HG3	29:Nm:206:PRO:HD2	1.83	0.59
30:S1:1753:C:H2'	30:S1:1754:G:C8	2.38	0.59
1:L1:977:C:OP2	4:Le:59:ARG:NH2	2.25	0.59
30:S1:1679:A:OP1	56:So:20:ARG:NH2	2.36	0.59
39:SG:45:THR:HG22	39:SG:52:THR:HA	1.84	0.59
60:Ss:23:THR:HG22	60:Ss:31:ILE:HG23	1.84	0.59
74:LF:42:CYS:SG	74:LF:59:SER:OG	2.57	0.59
77:LI:238:ASP:O	77:LI:241:ASN:ND2	2.36	0.59
1:L1:114:G:N2	1:L1:158:A:H61	2.01	0.59
16:Lq:88:ASP:OD1	16:Lq:121:ARG:NH2	2.36	0.59
60:Ss:269:GLU:O	60:Ss:271:LYS:NZ	2.36	0.59
64:Sw:45:ILE:HA	64:Sw:61:VAL:HG11	1.84	0.59
1:L1:1741:G:O6	48:L2:103:A:O2'	2.16	0.59
1:L1:2415:OMU:HM22	1:L1:2416:G:H5'	1.85	0.59
1:L1:4582:C:O2'	86:Lb:99:LEU:O	2.18	0.59
39:SG:63:LYS:HG2	62:Su:3:VAL:HB	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Sd:101:ASN:O	44:Sd:105:ASN:ND2	2.36	0.59
30:S1:681:PSU:H4'	47:Sg:9:THR:HG22	1.85	0.58
30:S1:1275:G:N2	30:S1:1506:A:OP2	2.34	0.58
30:S1:1605:G:OP1	50:Si:84:ARG:NH2	2.36	0.58
42:Sb:37:GLU:HG3	60:Ss:150:TRP:HZ2	1.68	0.58
84:LQ:40:GLY:HA3	84:LQ:45:VAL:HB	1.85	0.58
1:L1:4993:G:H22	1:L1:5058:A:H2	1.50	0.58
17:Lr:76:ASP:HB3	17:Lr:115:GLY:HA3	1.84	0.58
30:S1:987:A:OP1	51:Sj:32:LYS:NZ	2.34	0.58
41:Sa:41:GLN:OE1	41:Sa:41:GLN:N	2.34	0.58
62:Su:71:LEU:HD21	62:Su:189:ILE:HG23	1.85	0.58
1:L1:2607:C:H2'	1:L1:2608:G:H8	1.68	0.58
30:S1:1354:G:N2	30:S1:1357:A:OP2	2.35	0.58
30:S1:1846:G:N7	58:Sq:8:LYS:NZ	2.49	0.58
36:SD:13:GLN:OE1	36:SD:35:ARG:NH1	2.36	0.58
78:LJ:210:GLU:OE1	78:LJ:210:GLU:N	2.33	0.58
85:La:117:GLU:O	85:La:162:ASN:ND2	2.34	0.58
1:L1:382:G:N1	1:L1:385:A:OP2	2.35	0.58
1:L1:1326:A2M:OP2	1:L1:4445:U:O2'	2.20	0.58
1:L1:1818:G:O2'	1:L1:1822:U:O2	2.21	0.58
11:Ll:49:VAL:HG12	11:Ll:50:ASN:HD22	1.69	0.58
30:S1:372:U:OP1	36:SD:136:LYS:NZ	2.30	0.58
10:Lk:46:GLY:O	10:Lk:49:GLN:NE2	2.37	0.58
26:Na:106:ILE:HG12	26:Na:126:ALA:HA	1.86	0.58
30:S1:1419:C:O2	30:S1:1420:G:N1	2.37	0.58
30:S1:1644:C:H4'	43:Sc:140:ARG:HB2	1.84	0.58
1:L1:2400:G:H21	23:Lx:6:THR:HG22	1.69	0.58
1:L1:4639:G:OP2	1:L1:4639:G:N2	2.34	0.58
45:Se:51:LYS:HD2	45:Se:78:ILE:HD11	1.84	0.58
82:LO:54:ARG:NH2	82:LO:55:TYR:OH	2.37	0.58
1:L1:1809:C:H2'	1:L1:1810:G:H8	1.68	0.58
33:SA:4:SER:OG	33:SA:6:ASP:OD2	2.20	0.58
52:Sk:33:MET:HE2	52:Sk:48:SER:HA	1.86	0.58
1:L1:4420:PSU:O2	1:L1:4475:G:N2	2.36	0.58
46:Sf:11:LEU:HD12	46:Sf:74:VAL:HB	1.85	0.58
66:Sy:135:PRO:HG2	66:Sy:141:ILE:HD13	1.86	0.58
16:Lq:68:ILE:O	16:Lq:115:LYS:NZ	2.32	0.58
29:Nm:147:ARG:HH21	29:Nm:359:HIS:HE1	1.50	0.58
30:S1:94:G:OP1	64:Sw:6:LYS:NZ	2.34	0.58
30:S1:125:C:OP1	30:S1:127:C:N4	2.37	0.58
52:Sk:36:LYS:HB2	52:Sk:43:ILE:HG12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1238:A:O2'	77:LI:52:GLU:OE2	2.21	0.58
26:Na:96:ILE:HG12	27:Nb:62:VAL:HG13	1.86	0.58
29:Nm:220:ASN:HA	29:Nm:233:ASN:HB3	1.85	0.58
67:Sz:9:VAL:HG23	67:Sz:24:SER:HB3	1.85	0.58
68:L3:30:U:OP1	83:LP:34:ARG:NH2	2.36	0.58
1:L1:318:A:H2'	1:L1:319:A:H8	1.69	0.57
1:L1:2406:G:N7	71:LC:2:SER:N	2.52	0.57
30:S1:190:G:N2	30:S1:210:PSU:O2	2.37	0.57
54:Sm:51:ASP:OD1	54:Sm:52:LYS:N	2.37	0.57
30:S1:1289:U:H2'	30:S1:1290:G:C8	2.39	0.57
30:S1:1863:A:OP2	51:Sj:4:LYS:NZ	2.36	0.57
41:Sa:53:GLN:OE1	41:Sa:53:GLN:N	2.37	0.57
61:St:33:GLN:HB3	61:St:154:LEU:HD12	1.86	0.57
68:L3:141:C:OP1	76:LH:38:ARG:NH1	2.36	0.57
1:L1:3825:A2M:HM'2	1:L1:3826:C:H5'	1.84	0.57
1:L1:265:C:O2'	24:Ly:112:ARG:NH2	2.37	0.57
11:Ll:54:GLY:O	11:Ll:55:ASN:ND2	2.36	0.57
26:Na:96:ILE:HG23	27:Nb:62:VAL:HG22	1.85	0.57
30:S1:1482:C:OP1	57:Sp:54:LYS:NZ	2.37	0.57
72:LD:94:MET:HG2	72:LD:105:PRO:HA	1.85	0.57
82:LO:144:LYS:O	82:LO:148:THR:OG1	2.23	0.57
1:L1:505:G:H1	1:L1:653:U:H3	1.51	0.57
30:S1:160:U:O2'	30:S1:162:C:OP2	2.21	0.57
30:S1:746:C:H1'	30:S1:747:U:H5	1.69	0.57
32:S3:47:U:H4'	32:S3:48:C:H5''	1.85	0.57
4:Le:250:GLN:NE2	4:Le:254:ASP:OD2	2.38	0.57
44:Sd:13:LEU:HB2	44:Sd:20:ILE:HB	1.85	0.57
79:LK:103:VAL:HG11	79:LK:144:LEU:HD11	1.87	0.57
1:L1:4415:A:N6	1:L1:4427:G:O2'	2.38	0.57
2:Lc:60:HIS:HE1	2:Lc:100:ARG:HH11	1.52	0.57
18:Ls:118:LEU:HD13	18:Ls:120:ARG:HE	1.69	0.57
30:S1:1013:U:OP1	30:S1:1129:G:O2'	2.22	0.57
73:LE:15:CYS:SG	73:LE:19:GLN:NE2	2.77	0.57
24:Ly:70:ARG:NH2	68:L3:96:C:OP1	2.36	0.57
88:Nd:301:COA:S1P	81:LN:350:SER:N	2.73	0.57
30:S1:115:U:H2'	30:S1:116:OMU:H6	1.87	0.57
30:S1:304:C:OP1	33:SA:75:LYS:NZ	2.38	0.57
27:Nb:56:ILE:HD11	27:Nb:81:ALA:HB2	1.85	0.57
28:Nd:145:LYS:HG3	28:Nd:146:VAL:HG13	1.86	0.57
85:La:116:LEU:HB3	85:La:126:LEU:HB2	1.87	0.57
1:L1:2267:U:OP1	75:LG:37:SER:OG	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4314:C:O2'	18:Ls:36:ASP:OD1	2.23	0.57
3:Ld:65:ALA:HB2	3:Ld:74:ILE:HD13	1.86	0.57
62:Su:33:VAL:HG12	62:Su:96:CYS:HB2	1.87	0.57
67:Sz:46:THR:HG23	67:Sz:65:PRO:HD3	1.85	0.57
1:L1:1397:A:HO2'	1:L1:1467:C:HO2'	1.53	0.56
1:L1:3748:A:O2'	85:La:223:SER:OG	2.23	0.56
1:L1:4083:U:OP1	85:La:123:ARG:NH1	2.38	0.56
2:Lc:293:LEU:O	2:Lc:299:GLN:NE2	2.36	0.56
79:LK:186:THR:O	79:LK:189:GLN:NE2	2.37	0.56
15:Lp:43:ASN:OD1	15:Lp:127:GLN:NE2	2.38	0.56
19:Lt:99:PRO:HG3	19:Lt:105:ILE:HG13	1.87	0.56
23:Lx:5:LEU:HD21	23:Lx:30:ILE:HG22	1.87	0.56
30:S1:751:G:H2'	30:S1:752:G:C8	2.40	0.56
30:S1:1662:U:O4	30:S1:1663:A:N6	2.38	0.56
41:Sa:41:GLN:NE2	41:Sa:113:GLY:O	2.33	0.56
59:Sr:121:CYS:HA	59:Sr:132:MET:HE3	1.86	0.56
69:LA:14:LYS:NZ	71:LC:51:LEU:OXT	2.37	0.56
1:L1:133:C:N3	1:L1:136:C:N4	2.53	0.56
1:L1:137:G:H2'	1:L1:138:G:H8	1.70	0.56
1:L1:208:A:OP1	28:Nd:12:LYS:NZ	2.39	0.56
1:L1:2815:A2M:HM'2	1:L1:2816:G:H5'	1.86	0.56
1:L1:3809:G:OP2	1:L1:3809:G:N2	2.31	0.56
1:L1:4523:A2M:H5''	1:L1:4524:G:H5'	1.86	0.56
6:Lg:135:ARG:HG2	81:LN:392:PRO:HB3	1.86	0.56
30:S1:377:G:H5'	33:SA:98:LYS:HB3	1.88	0.56
30:S1:1544:C:O2'	43:Sc:80:GLN:NE2	2.38	0.56
63:Sv:187[B]:ARG:HE	63:Sv:192:LEU:HD13	1.70	0.56
64:Sw:11:ARG:HA	64:Sw:28:ALA:HB2	1.87	0.56
66:Sy:103:ASP:OD1	66:Sy:104:ALA:N	2.38	0.56
86:Lb:80:GLU:OE1	86:Lb:323:TYR:OH	2.21	0.56
15:Lp:76:LYS:HE3	71:LC:31:THR:HB	1.88	0.56
30:S1:61:A:HO2'	30:S1:315:C:HO2'	1.50	0.56
6:Lg:136:ILE:HD12	81:LN:389:PRO:HB3	1.87	0.56
16:Lq:22:LYS:NZ	16:Lq:129:TRP:O	2.35	0.56
30:S1:1563:G:OP1	50:Si:121:ARG:NH1	2.37	0.56
30:S1:1678:A2M:OP2	35:SC:63:LYS:NZ	2.32	0.56
32:S3:58:A:O2'	32:S3:61:C:N4	2.38	0.56
65:Sx:42:THR:HB	65:Sx:43:PRO:HD3	1.86	0.56
65:Sx:74:GLN:HA	65:Sx:79:PHE:HB2	1.87	0.56
1:L1:2811:G:N1	1:L1:2814:C:OP2	2.38	0.56
8:Li:151:ARG:HH22	36:SD:119:ASP:HB2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ly:86:LYS:O	24:Ly:92:ARG:NH1	2.32	0.56
29:Nm:18:ALA:HA	29:Nm:36:CYS:HA	1.88	0.56
30:S1:1292:C:H2'	30:S1:1293:A:H8	1.71	0.56
30:S1:1748:G:H1	30:S1:1786:U:H3	1.52	0.56
1:L1:959:G:C8	4:Le:123:ARG:HG2	2.40	0.56
1:L1:1432:G:O2'	1:L1:1452:A:N6	2.39	0.56
5:Lf:118:MET:HG2	9:Lj:169:THR:HG22	1.88	0.56
11:Ll:75:GLU:OE1	11:Ll:75:GLU:N	2.39	0.56
40:SH:32:ALA:HB3	40:SH:110:VAL:HB	1.87	0.56
51:Sj:7:ASN:ND2	51:Sj:10:ARG:O	2.38	0.56
1:L1:1266:G:N7	18:Ls:90:SER:OG	2.38	0.56
1:L1:5006:U:H4'	1:L1:5007:A:H5'	1.88	0.56
30:S1:1615:U:O4	41:Sa:40:ARG:NH2	2.39	0.56
1:L1:1194:G:H2'	1:L1:1195:G:H8	1.71	0.56
15:Lp:113:LYS:NZ	68:L3:86:U:O4	2.39	0.56
34:SB:18:ARG:O	34:SB:24:ARG:NH1	2.38	0.56
1:L1:729:G:OP1	9:Lj:63:TYR:OH	2.23	0.56
1:L1:2306:G:O6	28:Nd:3:ARG:NH2	2.39	0.56
1:L1:4474:A:OP2	72:LD:124:LYS:NZ	2.38	0.56
28:Nd:227:HIS:O	28:Nd:231:HIS:ND1	2.39	0.56
60:Ss:116:ASP:OD1	60:Ss:116:ASP:N	2.35	0.56
1:L1:4304:A:OP2	1:L1:4305:G:N2	2.40	0.55
2:Lc:221:PHE:HB3	2:Lc:227:ILE:HG21	1.88	0.55
24:Ly:103:LYS:O	24:Ly:108:GLN:NE2	2.36	0.55
35:SC:168:THR:HB	35:SC:171:GLU:HG3	1.87	0.55
64:Sw:100:ARG:HB2	64:Sw:114:ILE:HD13	1.87	0.55
1:L1:68:U:OP1	76:LH:178:HIS:ND1	2.27	0.55
3:Ld:223:PHE:HB3	3:Ld:226:TYR:HB2	1.88	0.55
18:Ls:49:HIS:HB3	18:Ls:52:LYS:HE2	1.87	0.55
30:S1:374:G:OP1	36:SD:59:LYS:NZ	2.38	0.55
37:SE:90:VAL:O	37:SE:95:ARG:NH2	2.36	0.55
46:Sf:91:ASN:O	63:Sv:183:LYS:NZ	2.39	0.55
1:L1:4456:OMC:HM22	1:L1:4457:PSU:H5''	1.88	0.55
32:S3:35:A:OP2	43:Sc:146:ARG:NH1	2.38	0.55
35:SC:128:ILE:HG21	56:So:68:LEU:HB3	1.87	0.55
60:Ss:153:CYS:SG	60:Ss:155:ARG:NH1	2.79	0.55
64:Sw:80:ILE:HG13	64:Sw:81:THR:HG23	1.88	0.55
1:L1:4873:G:N7	5:Lf:179:LYS:NZ	2.55	0.55
13:Ln:83:THR:HA	66:Sy:131:ARG:HD2	1.88	0.55
26:Na:94:VAL:HG23	26:Na:109:PRO:HG3	1.89	0.55
28:Nd:196:ASP:OD1	28:Nd:196:ASP:N	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S3:4:U:H3	32:S3:69:G:H1	1.55	0.55
74:LF:26:VAL:HG11	85:La:180:LEU:HD11	1.88	0.55
10:Lk:88:ARG:NH2	18:Ls:30:GLU:OE2	2.39	0.55
13:Ln:104:GLN:OE1	66:Sy:156:TYR:OH	2.18	0.55
34:SB:110:LEU:HB2	34:SB:147:PHE:HB3	1.88	0.55
50:Si:108:GLU:OE2	50:Si:121:ARG:NE	2.36	0.55
1:L1:252:C:H2'	1:L1:253:G:C8	2.42	0.55
1:L1:3681:G:OP2	85:La:128:ARG:NH2	2.38	0.55
14:Lo:42:THR:HB	78:LJ:48:LYS:HD2	1.88	0.55
86:Lb:74:GLU:OE1	86:Lb:285:TYR:OH	2.20	0.55
1:L1:2848:G:O2'	1:L1:3838:U:O4	2.24	0.55
1:L1:2706:G:O6	1:L1:2710:C:N4	2.40	0.55
1:L1:3760:A:N1	30:S1:1824:A:H2'	2.22	0.55
1:L1:4872:G:OP2	84:LQ:94:LYS:NZ	2.37	0.55
30:S1:677:G:H21	30:S1:1028:A:H62	1.53	0.55
30:S1:1059:G:O6	30:S1:1060:A:N6	2.39	0.55
30:S1:1757:G:H2'	30:S1:1758:G:C8	2.42	0.55
47:Sg:68:LYS:HB3	47:Sg:91:LEU:HD22	1.89	0.55
74:LF:26:VAL:HG12	85:La:178:PRO:HD2	1.88	0.55
1:L1:268:G:H2'	1:L1:269:G:H8	1.71	0.55
16:Lq:125:GLY:HA3	78:LJ:30:PRO:HB2	1.89	0.55
29:Nm:233:ASN:ND2	29:Nm:358:GLU:OE1	2.40	0.55
64:Sw:31:PRO:HG3	64:Sw:43:PRO:HG3	1.89	0.55
29:Nm:294:HIS:O	29:Nm:325:THR:OG1	2.25	0.55
30:S1:116:OMU:HM22	30:S1:117:C:H5'	1.88	0.55
30:S1:155:G:H4'	66:Sy:15:LEU:HD22	1.89	0.55
30:S1:1310:U:OP1	40:SH:36:ARG:NH2	2.40	0.55
30:S1:1604:G:OP2	44:Sd:38:ARG:NH2	2.40	0.55
70:LB:33:LYS:HG2	70:LB:46:VAL:HG22	1.89	0.55
72:LD:80:PRO:HA	72:LD:83:ARG:HB3	1.89	0.55
1:L1:942:G:OP1	77:LI:245:ARG:NH2	2.38	0.54
1:L1:1577:G:H5'	1:L1:1578:U:H5''	1.88	0.54
1:L1:3816:A:O2'	1:L1:3819:G:N3	2.36	0.54
7:Lh:157:GLY:O	7:Lh:188:ASN:ND2	2.33	0.54
7:Lh:172:ARG:NH1	17:Lr:56:VAL:O	2.40	0.54
9:Lj:98:ARG:NH2	84:LQ:30:VAL:O	2.40	0.54
16:Lq:50:PRO:HD3	16:Lq:68:ILE:HG12	1.88	0.54
30:S1:444:G:O6	33:SA:26:LYS:NZ	2.25	0.54
73:LE:2:VAL:N	73:LE:90:HIS:O	2.40	0.54
1:L1:1468:C:OP1	17:Lr:132:ARG:NH2	2.39	0.54
1:L1:2318:G:N2	1:L1:2321:G:OP2	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2759:G:H1'	1:L1:2764:A:H2	1.73	0.54
30:S1:99:A2M:H8	30:S1:99:A2M:O5'	2.06	0.54
30:S1:145:G:H2'	30:S1:146:G:C8	2.42	0.54
30:S1:920:A:O2'	30:S1:922:A:OP1	2.23	0.54
43:Sc:51:LEU:HD13	43:Sc:81:ILE:HG23	1.88	0.54
45:Se:16:LYS:H	63:Sv:259:THR:HG21	1.72	0.54
62:Su:117:TRP:HB3	62:Su:153:THR:HG22	1.89	0.54
73:LE:74:GLU:HB3	73:LE:77:CYS:HB3	1.89	0.54
16:Lq:10:VAL:O	16:Lq:83:THR:OG1	2.20	0.54
28:Nd:226:SER:HB2	28:Nd:231:HIS:NE2	2.22	0.54
63:Sv:187[A]:ARG:HE	63:Sv:192:LEU:HD13	1.70	0.54
1:L1:4967:A:H2'	1:L1:4968:A:C8	2.42	0.54
8:Li:172:ARG:NH1	30:S1:908:A:H5''	2.21	0.54
13:Ln:102:LYS:HG2	13:Ln:105:ARG:HE	1.71	0.54
77:LI:190:LEU:HD21	77:LI:208:LEU:HD21	1.88	0.54
28:Nd:138:TYR:OH	81:LN:352:ARG:NH1	2.41	0.54
30:S1:664:A:O2'	30:S1:670:A:N1	2.34	0.54
54:Sm:102:LYS:HA	54:Sm:107:VAL:HG12	1.88	0.54
86:Lb:224:LYS:HG2	86:Lb:340:THR:HB	1.89	0.54
6:Lg:64:ASN:ND2	6:Lg:80:GLN:OE1	2.39	0.54
19:Lt:34:THR:HG23	19:Lt:95:ALA:HB2	1.89	0.54
34:SB:21:GLU:HG2	34:SB:24:ARG:H	1.73	0.54
60:Ss:88:ARG:HH11	60:Ss:97:THR:HG21	1.71	0.54
1:L1:156:G:OP2	24:Ly:106:LYS:NZ	2.39	0.54
1:L1:3712:A:O2'	1:L1:3713:U:O5'	2.25	0.54
29:Nm:197:VAL:HG12	29:Nm:198:ASN:HD22	1.73	0.54
30:S1:51:U:H2'	30:S1:52:G:C8	2.43	0.54
30:S1:96:C:H1'	30:S1:474:G:H5'	1.88	0.54
30:S1:1453:C:H2'	30:S1:1454:A:H4'	1.87	0.54
30:S1:1466:G:OP2	42:Sb:5:ARG:NH1	2.37	0.54
37:SE:55:ARG:NH1	37:SE:78:TYR:OH	2.40	0.54
1:L1:2325:C:P	21:Lv:101:HIS:HD1	2.30	0.54
1:L1:4233:A:H4'	73:LE:98:LYS:HD2	1.89	0.54
1:L1:4954:G:H2'	1:L1:4955:A:C8	2.43	0.54
8:Li:61:ALA:HA	8:Li:64:ARG:HD3	1.90	0.54
28:Nd:48:TYR:OH	28:Nd:149:LYS:O	2.23	0.54
36:SD:31:GLU:OE1	36:SD:31:GLU:N	2.40	0.54
51:Sj:43:ASN:OD1	51:Sj:66:LYS:NZ	2.40	0.54
59:Sr:119:ARG:O	59:Sr:132:MET:N	2.40	0.54
86:Lb:210:VAL:O	86:Lb:349:LYS:NZ	2.36	0.54
1:L1:4405:G:OP2	80:LM:7:ARG:NH2	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4694:G:OP1	1:L1:4694:G:N2	2.39	0.54
21:Lv:78:LEU:O	75:LG:20:ARG:NH1	2.41	0.54
30:S1:1757:G:H2'	30:S1:1758:G:H8	1.72	0.54
38:SF:63:VAL:HG21	38:SF:71:ILE:HD11	1.90	0.54
65:Sx:32:ASP:OD2	65:Sx:65:ARG:NH1	2.40	0.54
1:L1:2096:G:N2	1:L1:2097:U:O4	2.41	0.54
1:L1:2486:G:H1	1:L1:2492:C:H42	1.56	0.54
1:L1:3941:G:H2'	1:L1:3942:A:H8	1.73	0.54
1:L1:4522:G:O2'	1:L1:4525:C:OP2	2.18	0.54
29:Nm:25:CYS:HB3	29:Nm:30:ILE:HB	1.89	0.54
41:Sa:62:LYS:NZ	41:Sa:66:GLU:OE2	2.33	0.54
43:Sc:53:GLU:OE1	43:Sc:85:ARG:NH2	2.41	0.54
66:Sy:10:THR:HA	66:Sy:129:VAL:HG12	1.90	0.54
86:Lb:289:GLN:HE21	86:Lb:292:LEU:HD11	1.73	0.54
1:L1:1290:G:H2'	1:L1:1291:G:H8	1.73	0.53
15:Lp:52:ASP:O	15:Lp:69:LYS:NZ	2.41	0.53
30:S1:161:U:O2'	66:Sy:87:ARG:NH2	2.41	0.53
30:S1:458:A:N6	30:S1:470:G:O6	2.41	0.53
30:S1:1413:G:H2'	30:S1:1414:A:H8	1.73	0.53
30:S1:1599:U:C5	35:SC:166:ILE:HB	2.43	0.53
30:S1:1745:A:O3'	66:Sy:31:ARG:NH1	2.38	0.53
65:Sx:197:LYS:HG2	65:Sx:198:ILE:HG23	1.90	0.53
75:LG:90:LEU:HD22	75:LG:111:ILE:HG23	1.90	0.53
16:Lq:94:THR:O	16:Lq:97:ASN:ND2	2.41	0.53
30:S1:1858:G:N7	39:SG:146:ARG:NH2	2.57	0.53
50:Si:111:LYS:O	50:Si:126:GLN:NE2	2.42	0.53
60:Ss:57:ARG:HD3	60:Ss:95:GLY:HA3	1.90	0.53
62:Su:28:LYS:HB3	62:Su:48:LEU:HD11	1.89	0.53
1:L1:135:G:H1	24:Ly:97:LYS:HD3	1.73	0.53
1:L1:308:G:OP2	1:L1:308:G:N2	2.24	0.53
1:L1:648:G:H2'	1:L1:649:A:H8	1.73	0.53
1:L1:2607:C:H2'	1:L1:2608:G:C8	2.44	0.53
1:L1:4570:G:H2'	1:L1:4571:A2M:H8	1.89	0.53
28:Nd:55:VAL:HG11	28:Nd:111:ALA:HB1	1.88	0.53
28:Nd:195:ASP:OD2	28:Nd:197:SER:OG	2.17	0.53
30:S1:551:U:H2'	30:S1:552:G:C8	2.44	0.53
37:SE:73:ASN:OD1	65:Sx:64:ARG:NH1	2.40	0.53
60:Ss:163:PRO:HB2	60:Ss:179:LEU:HB3	1.89	0.53
1:L1:1082:C:H2'	1:L1:1083:U:O4'	2.09	0.53
1:L1:4306:OMU:HM22	1:L1:4307:A:H5'	1.90	0.53
1:L1:4960:G:H2'	1:L1:4961:G:H8	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Lg:21:ASN:H	6:Lg:145:HIS:CE1	2.27	0.53
30:S1:206:G:H2'	30:S1:207:G:H8	1.73	0.53
30:S1:511:U:H2'	30:S1:512:A2M:H8	1.89	0.53
49:Sh:14:THR:HG23	49:Sh:21:LYS:HG2	1.89	0.53
60:Ss:109:LEU:HD11	60:Ss:125:ARG:HE	1.74	0.53
79:LK:141:LYS:NZ	79:LK:142:ASP:OD2	2.34	0.53
1:L1:1418:C:H2'	1:L1:1419:G:O4'	2.08	0.53
1:L1:1426:G:N1	1:L1:1458:C:OP2	2.38	0.53
1:L1:2698:G:H21	23:Lx:28:ASN:HD21	1.56	0.53
48:L2:38:U:N3	48:L2:41:G:OP2	2.34	0.53
73:LE:59:LYS:NZ	73:LE:61:LYS:O	2.30	0.53
1:L1:1340:OMC:HM22	1:L1:1341:U:H5'	1.91	0.53
1:L1:1844:G:OP1	18:Ls:22:LYS:NZ	2.41	0.53
1:L1:2856:C:O2	86:Lb:242:ARG:NH2	2.42	0.53
13:Ln:83:THR:OG1	66:Sy:131:ARG:NH1	2.41	0.53
16:Lq:35:ASP:OD1	16:Lq:35:ASP:N	2.30	0.53
30:S1:601:OMG:HM22	30:S1:602:G:H5'	1.90	0.53
30:S1:652:U:H2'	30:S1:653:A:H8	1.73	0.53
30:S1:874:G:N3	67:Sz:114:GLN:NE2	2.57	0.53
30:S1:1036:A:N3	30:S1:1844:U:O2'	2.42	0.53
30:S1:1606:G:N2	30:S1:1632:G:H1'	2.23	0.53
33:SA:62:VAL:HA	33:SA:77:ARG:HA	1.91	0.53
62:Su:52:THR:HG23	62:Su:57:ILE:HA	1.90	0.53
79:LK:120:GLU:OE1	79:LK:124:ARG:NH2	2.38	0.53
1:L1:114:G:N2	1:L1:276:C:O2'	2.42	0.53
1:L1:2403:A:OP1	23:Lx:10:ARG:NH1	2.42	0.53
10:Lk:66:ASN:O	10:Lk:73:GLY:N	2.36	0.53
14:Lo:64:SER:HB2	24:Ly:69:LEU:HD13	1.90	0.53
30:S1:202:G:H2'	30:S1:203:G:H8	1.73	0.53
42:Sb:45:LYS:HG2	42:Sb:49:LYS:HE2	1.91	0.53
60:Ss:196:ASN:HB2	60:Ss:211:GLY:HA2	1.90	0.53
1:L1:1591:U:OP2	1:L1:2856:C:O2'	2.24	0.53
60:Ss:106:LYS:HB2	60:Ss:126:ASP:HB2	1.89	0.53
77:LI:105:VAL:HG13	77:LI:136:VAL:HG12	1.91	0.53
78:LJ:225:ASN:O	78:LJ:229:ARG:NH1	2.41	0.53
17:Lr:134:GLU:OE2	83:LP:178:ALA:N	2.40	0.53
26:Na:110:ASP:HB2	26:Na:123:PHE:HB2	1.91	0.53
30:S1:436:OMG:OP2	30:S1:471:G:O2'	2.27	0.53
86:Lb:57:VAL:HG22	86:Lb:73:VAL:HG22	1.91	0.53
1:L1:1950:U:O2'	9:Lj:116:ARG:NH1	2.41	0.52
1:L1:2503:G:N2	1:L1:4084:G:O4'	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2702:C:OP1	11:L1:101:ARG:NH2	2.42	0.52
30:S1:699:C:N4	30:S1:700:G:O6	2.42	0.52
30:S1:1601:A:OP2	30:S1:1636:G:N2	2.38	0.52
30:S1:1656:G:H1	30:S1:1668:U:H3	1.56	0.52
33:SA:81:VAL:HG22	33:SA:102:VAL:HG12	1.90	0.52
44:Sd:34:LYS:HG2	44:Sd:103:LEU:HD23	1.91	0.52
58:Sq:7:LYS:HA	58:Sq:10:MET:HE2	1.90	0.52
63:Sv:68:ARG:HG2	63:Sv:277:HIS:HB2	1.90	0.52
68:L3:102:G:OP2	68:L3:104:A:O2'	2.27	0.52
75:LG:26:SER:OG	75:LG:28:GLU:OE1	2.19	0.52
82:LO:99:PHE:O	82:LO:159:LYS:NZ	2.42	0.52
1:L1:138:G:H2'	1:L1:139:G:C8	2.43	0.52
27:Nb:66:THR:OG1	27:Nb:70:THR:OG1	2.21	0.52
41:Sa:18:ARG:NH1	44:Sd:88:LYS:O	2.43	0.52
55:Sn:102:LYS:HD3	55:Sn:106:ALA:HB1	1.90	0.52
62:Su:144:LYS:HD2	62:Su:208:HIS:HB3	1.90	0.52
64:Sw:246:LEU:HB3	64:Sw:250:GLU:HG3	1.90	0.52
1:L1:737:C:C5	1:L1:739:G:H5''	2.45	0.52
1:L1:2601:A:N6	1:L1:2744:A:OP2	2.38	0.52
26:Na:97:ARG:HD3	27:Nb:61:GLU:HG2	1.91	0.52
28:Nd:89:GLU:OE1	28:Nd:210:SER:OG	2.28	0.52
30:S1:1280:G:OP1	40:SH:101:ARG:NH2	2.43	0.52
30:S1:1550:G:H3'	30:S1:1579:A:H61	1.74	0.52
37:SE:80:ARG:NH1	37:SE:87:PRO:O	2.42	0.52
1:L1:956:A:H1'	1:L1:2076:G:H5''	1.92	0.52
9:Lj:147:ASP:HB3	9:Lj:150:ILE:HB	1.91	0.52
30:S1:546:G:H2'	30:S1:548:C:H5	1.73	0.52
32:S3:58:A:O2'	32:S3:60:C:OP2	2.21	0.52
44:Sd:89:ASP:OD1	44:Sd:91:LYS:N	2.36	0.52
83:LP:116:ARG:NH2	83:LP:155:MET:O	2.42	0.52
1:L1:963:G:H2'	1:L1:964:A:O4'	2.09	0.52
1:L1:4305:G:N7	10:Lk:87:LYS:NZ	2.54	0.52
30:S1:860:G:N2	46:Sf:107:SER:OG	2.40	0.52
30:S1:1628:C:H2'	30:S1:1629:C:C6	2.45	0.52
30:S1:1769:C:H2'	30:S1:1770:G:C8	2.44	0.52
30:S1:1782:G:H3'	30:S1:1783:C:H4'	1.92	0.52
53:Sl:34:LYS:NZ	53:Sl:107:GLU:OE1	2.43	0.52
1:L1:1428:U:H5''	7:Lh:42:THR:HB	1.92	0.52
30:S1:67:C:N4	66:Sy:164:LYS:H	2.07	0.52
30:S1:282:G:H2'	30:S1:283:G:O4'	2.09	0.52
30:S1:303:C:H4'	33:SA:75:LYS:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SE:32:HIS:HB3	37:SE:35:LEU:HB2	1.91	0.52
1:L1:1465:G:OP1	18:Ls:44:ARG:NH1	2.43	0.52
1:L1:2479:G:H2'	1:L1:2480:G:C8	2.45	0.52
1:L1:2485:U:H2'	1:L1:2486:G:C8	2.45	0.52
30:S1:799:OMU:HM22	30:S1:800:U:H5'	1.91	0.52
32:S3:68:G:H2'	32:S3:69:G:H8	1.74	0.52
52:Sk:40:CYS:SG	52:Sk:41:TYR:N	2.83	0.52
67:Sz:106:ARG:HA	67:Sz:109:ARG:HB2	1.91	0.52
1:L1:3896:C:O2'	86:Lb:268:ARG:NH2	2.43	0.52
27:Nb:82:SER:N	27:Nb:87:THR:O	2.41	0.52
30:S1:120:U:H2'	30:S1:121:OMU:H6	1.92	0.52
30:S1:121:OMU:HM22	30:S1:122:G:H5'	1.92	0.52
30:S1:582:U:H2'	30:S1:583:A:C8	2.45	0.52
30:S1:1748:G:H2'	30:S1:1749:G:H8	1.75	0.52
43:Sc:29:ASN:N	43:Sc:67:ASP:OD1	2.43	0.52
79:LK:93:ARG:NH1	79:LK:140:GLN:OE1	2.43	0.52
1:L1:1867:A:OP1	80:LM:13:LYS:NZ	2.36	0.52
1:L1:4280:A:N6	3:Ld:28:THR:O	2.39	0.52
13:Ln:73:ARG:NH1	30:S1:1780:G:OP2	2.43	0.52
16:Lq:36:ARG:NH1	16:Lq:38:TYR:OH	2.43	0.52
26:Na:94:VAL:HG13	27:Nb:64:MET:HE1	1.92	0.52
30:S1:1610:G:N7	44:Sd:132:ARG:NH2	2.58	0.52
60:Ss:32:LEU:HD21	60:Ss:92:LEU:HD21	1.92	0.52
66:Sy:154:ARG:HG2	66:Sy:176:ILE:HD12	1.92	0.52
1:L1:934:C:H5'	1:L1:936:C:H5''	1.91	0.52
1:L1:4960:G:H2'	1:L1:4961:G:C8	2.45	0.52
30:S1:191:A:H3'	30:S1:192:C:H5''	1.92	0.52
30:S1:1060:A:O2'	30:S1:1062:A:N7	2.43	0.52
35:SC:43:GLU:CD	35:SC:43:GLU:H	2.18	0.52
4:Le:211:HIS:NE2	4:Le:249:ASP:OD2	2.42	0.51
30:S1:538:U:H2'	30:S1:539:C:C6	2.45	0.51
30:S1:1528:G:O2'	30:S1:1666:C:OP1	2.25	0.51
30:S1:1792:G:H2'	30:S1:1793:A:H8	1.75	0.51
61:St:135:THR:O	61:St:138:SER:OG	2.26	0.51
64:Sw:141:THR:OG1	64:Sw:143:ASP:OD1	2.23	0.51
66:Sy:57:ASP:O	66:Sy:107:SER:OG	2.27	0.51
85:La:47:ASP:OD1	85:La:48:ILE:N	2.43	0.51
1:L1:2380:G:N2	1:L1:2425:U:OP1	2.36	0.51
1:L1:4645:C:OP2	8:Li:62:ARG:NH1	2.43	0.51
2:Lc:352:ASP:OD1	2:Lc:353:LYS:N	2.43	0.51
30:S1:212:C:H2'	30:S1:213:G:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:1574:C:H2'	30:S1:1575:G:H8	1.75	0.51
1:L1:190:G:H2'	1:L1:191:G:H8	1.75	0.51
1:L1:1093:C:H2'	1:L1:1094:G:H8	1.76	0.51
30:S1:1344:A:N1	30:S1:1385:G:O2'	2.39	0.51
65:Sx:39:VAL:HG22	65:Sx:48:ILE:HG12	1.92	0.51
86:Lb:300:LYS:NZ	86:Lb:311:ASP:OD2	2.43	0.51
1:L1:137:G:H2'	1:L1:138:G:C8	2.45	0.51
1:L1:364:G:O6	69:LA:55:ARG:NH2	2.42	0.51
1:L1:2845:A:H61	1:L1:3843:C:N4	2.07	0.51
1:L1:4923:C:H2'	1:L1:4924:C:C6	2.46	0.51
13:Ln:1:MET:HG3	86:Lb:57:VAL:HG11	1.90	0.51
29:Nm:224:TYR:CZ	29:Nm:227:GLY:HA2	2.45	0.51
30:S1:740:C:H2'	30:S1:741:C:C6	2.45	0.51
63:Sv:69:LEU:HG	63:Sv:273:LEU:HD21	1.92	0.51
1:L1:3661:G:H4'	1:L1:3662:A:H5'	1.91	0.51
24:Ly:80:PRO:HD2	24:Ly:83:LEU:HD12	1.91	0.51
30:S1:690:G:N2	30:S1:741:C:N3	2.58	0.51
60:Ss:249:CYS:SG	60:Ss:291:TRP:NE1	2.84	0.51
61:St:176:TRP:HE1	61:St:197:VAL:HG13	1.75	0.51
1:L1:3668:C:OP1	85:La:8:GLN:NE2	2.43	0.51
30:S1:690:G:H2'	30:S1:691:G:C8	2.44	0.51
73:LE:31:ASP:OD1	73:LE:31:ASP:N	2.40	0.51
4:Le:178:PRO:HD2	4:Le:181:LEU:HD12	1.93	0.51
5:Lf:81:TRP:HB2	5:Lf:104:VAL:HG21	1.92	0.51
30:S1:1179:G:N2	30:S1:1182:A:OP2	2.44	0.51
30:S1:1616:U:OP2	41:Sa:43:ARG:NH2	2.34	0.51
84:LQ:29:ASP:OD1	84:LQ:30:VAL:N	2.43	0.51
1:L1:398:A2M:H8	1:L1:398:A2M:O5'	2.10	0.51
1:L1:1872:G:O2'	1:L1:4219:A:N3	2.38	0.51
1:L1:3690:U:H5	85:La:200:ARG:HD3	1.75	0.51
1:L1:4693:C:OP1	79:LK:64:ARG:NH2	2.43	0.51
30:S1:520:A:H2'	30:S1:521:A:H8	1.75	0.51
30:S1:953:C:O2	39:SG:55:ARG:NH2	2.44	0.51
32:S3:63:C:H2'	32:S3:64:A:H8	1.76	0.51
35:SC:71:ARG:NH2	35:SC:148:ASN:OD1	2.43	0.51
42:Sb:37:GLU:HG3	60:Ss:150:TRP:CZ2	2.46	0.51
64:Sw:117:GLU:OE1	64:Sw:117:GLU:N	2.44	0.51
1:L1:2479:G:H2'	1:L1:2480:G:H8	1.76	0.51
28:Nd:121:PHE:CE1	28:Nd:141:GLN:HB2	2.46	0.51
29:Nm:99:VAL:HG22	29:Nm:171:HIS:HE1	1.75	0.51
30:S1:122:G:H21	64:Sw:146:THR:HG21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:1850:MA6:H8	30:S1:1850:MA6:O5'	2.10	0.51
55:Sn:113:ASN:O	55:Sn:118:ASN:ND2	2.44	0.51
1:L1:4301:U:OP1	10:Lk:78:LYS:NZ	2.43	0.50
1:L1:4957:C:H2'	1:L1:4958:C:C6	2.46	0.50
3:Ld:60:ILE:HB	3:Ld:80:ALA:HB2	1.93	0.50
14:Lo:129:ARG:NH2	14:Lo:131:ASP:OD2	2.44	0.50
15:Lp:123:ALA:O	15:Lp:127:GLN:HG2	2.10	0.50
29:Nm:181:PRO:HB2	29:Nm:192:SER:HB3	1.92	0.50
30:S1:560:A:OP2	34:SB:177:ASN:ND2	2.39	0.50
1:L1:4908:G:H21	1:L1:4913:G:H5'	1.74	0.50
14:Lo:100:VAL:HG21	14:Lo:109:ILE:HG12	1.93	0.50
30:S1:491:C:H3'	49:Sh:104:ARG:HD2	1.92	0.50
82:LO:56:THR:HG23	82:LO:63:ARG:HA	1.92	0.50
13:Ln:106:GLU:O	13:Ln:110:ARG:N	2.40	0.50
16:Lq:92:ASP:OD1	16:Lq:94:THR:OG1	2.26	0.50
26:Na:122:VAL:O	27:Nb:88:PHE:N	2.43	0.50
30:S1:65:C:C6	66:Sy:174:PRO:HB3	2.47	0.50
43:Sc:8:GLN:HB2	43:Sc:99:TYR:CZ	2.47	0.50
60:Ss:191:HIS:CD2	60:Ss:195:LEU:HD21	2.45	0.50
63:Sv:108:LYS:HE2	63:Sv:110:MET:HB3	1.94	0.50
1:L1:3671:G:OP1	76:LH:72:LYS:NZ	2.44	0.50
2:Lc:186:SER:O	2:Lc:188:ARG:NH1	2.42	0.50
13:Ln:45:ASN:HB3	13:Ln:48:GLN:HG2	1.92	0.50
30:S1:746:C:H1'	30:S1:747:U:C5	2.46	0.50
30:S1:835:C:H4'	30:S1:836:G:N7	2.26	0.50
33:SA:64:ASN:HA	33:SA:75:LYS:HA	1.93	0.50
41:Sa:37:TYR:HB3	41:Sa:41:GLN:HB2	1.93	0.50
86:Lb:340:THR:OG1	86:Lb:341:LYS:N	2.44	0.50
1:L1:143:C:OP1	78:LJ:111:LYS:NZ	2.43	0.50
1:L1:4135:G:H2'	1:L1:4136:G:H8	1.77	0.50
1:L1:4759:C:OP1	5:Lf:116:LYS:NZ	2.42	0.50
30:S1:1272:OMC:HM22	30:S1:1273:C:H5'	1.93	0.50
63:Sv:194:ARG:HD3	63:Sv:196:ILE:HD11	1.92	0.50
1:L1:1359:G:H5'	2:Lc:114:ARG:HE	1.76	0.50
1:L1:3718:A2M:HM'2	1:L1:3719:A:H5'	1.93	0.50
1:L1:4145:C:H2'	1:L1:4146:G:C8	2.45	0.50
2:Lc:230:LEU:HD21	2:Lc:239:LYS:HG3	1.94	0.50
26:Na:202:ASN:ND2	26:Na:212:GLU:OE1	2.36	0.50
30:S1:61:A:O2'	30:S1:315:C:O2'	2.19	0.50
30:S1:824:C:H1'	34:SB:144:ILE:HG21	1.93	0.50
80:LM:86:HIS:HB3	80:LM:139:ARG:HG2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:4525:C:OP1	86:Lb:246:ARG:NH2	2.41	0.50
30:S1:1608:U:OP1	44:Sd:134:GLN:NE2	2.44	0.50
39:SG:83:GLN:NE2	39:SG:87:GLU:OE2	2.45	0.50
1:L1:250:C:H2'	1:L1:251:C:C6	2.47	0.50
1:L1:1378:C:C6	83:LP:158:ARG:HD2	2.47	0.50
1:L1:1559:G:OP1	8:Li:126:LYS:NZ	2.44	0.50
1:L1:1617:G:H1'	1:L1:2513:A:N6	2.27	0.50
1:L1:1833:G:N2	1:L1:1835:G:O4'	2.45	0.50
1:L1:2804:OMC:HM22	1:L1:2805:C:H5'	1.92	0.50
2:Lc:144:ILE:HD12	2:Lc:150:LEU:HD11	1.93	0.50
3:Ld:152:ARG:HG3	3:Ld:154:THR:HG23	1.93	0.50
11:Ll:18:VAL:HA	11:Ll:75:GLU:HA	1.93	0.50
11:Ll:55:ASN:OD1	11:Ll:58:GLY:N	2.36	0.50
30:S1:145:G:H2'	30:S1:146:G:H8	1.77	0.50
35:SC:100:ILE:O	35:SC:104:THR:OG1	2.26	0.50
86:Lb:139:ASP:OD2	86:Lb:142:GLY:N	2.42	0.50
1:L1:1486:C:H2'	1:L1:1487:G:C8	2.47	0.50
1:L1:3607:U:H2'	1:L1:3608:A:H8	1.76	0.50
29:Nm:370:ILE:O	29:Nm:373:ARG:NH1	2.34	0.50
30:S1:629:A:O2'	30:S1:631:U:OP1	2.30	0.50
66:Sy:43:GLU:HA	66:Sy:46:LYS:HE3	1.93	0.50
85:La:117:GLU:HG2	85:La:124:GLY:H	1.77	0.50
1:L1:139:G:H2'	1:L1:140:G:H8	1.77	0.49
1:L1:1703:C:O3'	77:Li:43:ARG:NH2	2.44	0.49
1:L1:2101:C:H2'	1:L1:2102:G:C8	2.47	0.49
28:Nd:194:ILE:HA	28:Nd:214:LEU:HD23	1.94	0.49
29:Nm:35:PHE:HE2	29:Nm:44:SER:HB2	1.76	0.49
29:Nm:197:VAL:HG12	29:Nm:198:ASN:ND2	2.26	0.49
30:S1:652:U:H2'	30:S1:653:A:C8	2.47	0.49
30:S1:796:G:H2'	30:S1:797:OMC:C6	2.47	0.49
30:S1:919:A:OP2	38:SF:64:ARG:NH2	2.24	0.49
30:S1:1415:C:O2'	50:Si:132:ASP:OD2	2.24	0.49
80:LM:111:LEU:HD21	80:LM:113:THR:HG23	1.94	0.49
1:L1:2313:A:H5'	1:L1:2314:G:OP2	2.12	0.49
1:L1:4967:A:H2'	1:L1:4968:A:H8	1.77	0.49
2:Lc:209:ILE:HD13	2:Lc:251:ILE:HB	1.94	0.49
27:Nb:79:VAL:HG22	27:Nb:90:ILE:HG23	1.93	0.49
29:Nm:370:ILE:HB	29:Nm:373:ARG:HB3	1.93	0.49
30:S1:1171:G:O2'	30:S1:1187:G:O6	2.25	0.49
1:L1:729:G:O6	9:Lj:70:LYS:NZ	2.45	0.49
1:L1:1645:C:OP1	2:Lc:80:ARG:NH2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2318:G:OP2	21:Lv:14:LYS:NZ	2.45	0.49
1:L1:3748:A:HO2'	85:La:223:SER:HG	1.57	0.49
3:Ld:271:MET:HE2	48:L2:61:G:H5''	1.93	0.49
27:Nb:103:LEU:HA	27:Nb:106:ILE:HG22	1.93	0.49
29:Nm:73:ILE:HG13	29:Nm:74:ASN:H	1.78	0.49
34:SB:67:ASP:HB3	34:SB:70:ARG:HB3	1.93	0.49
60:Ss:70:VAL:N	60:Ss:79:LEU:O	2.42	0.49
61:St:77:ILE:HG12	61:St:99:ILE:HB	1.94	0.49
1:L1:24:G:N7	69:LA:46:LYS:NZ	2.61	0.49
25:Lz:96:ALA:HA	25:Lz:99:LYS:HE2	1.95	0.49
30:S1:166:A2M:HM'2	30:S1:167:G:H5'	1.95	0.49
30:S1:864:A:H2'	30:S1:865:A:H8	1.77	0.49
33:SA:141:ARG:HB2	33:SA:146:GLN:HG2	1.93	0.49
40:SH:60:MET:HG3	59:Sr:103:LEU:HD22	1.92	0.49
60:Ss:85:GLY:HA2	60:Ss:108:VAL:HG23	1.94	0.49
84:LQ:12:VAL:O	84:LQ:58:THR:OG1	2.20	0.49
1:L1:1249:C:H2'	1:L1:1250:C:C6	2.47	0.49
1:L1:1484:G:O2'	83:LP:195:ARG:NH2	2.45	0.49
1:L1:2739:C:O2	85:La:174:ARG:NH1	2.45	0.49
1:L1:4135:G:H2'	1:L1:4136:G:C8	2.47	0.49
30:S1:1286:G:OP1	59:Sr:99:LYS:NZ	2.34	0.49
30:S1:1291:A:N3	59:Sr:140:TYR:OH	2.40	0.49
49:Sh:118:ARG:HH11	66:Sy:85:ARG:HH21	1.61	0.49
80:LM:51:HIS:CD2	80:LM:168:SER:HB2	2.48	0.49
29:Nm:183:PRO:O	29:Nm:189:PHE:HB3	2.12	0.49
30:S1:1832:6MZ:H8	30:S1:1832:6MZ:O5'	2.12	0.49
40:SH:94:ILE:HG23	40:SH:98:GLY:HA2	1.94	0.49
46:Sf:30:CYS:SG	46:Sf:31:SER:N	2.85	0.49
62:Su:30:TRP:CD2	62:Su:48:LEU:HD13	2.46	0.49
64:Sw:192:ILE:HB	64:Sw:243:GLY:HA3	1.93	0.49
1:L1:318:A:H2'	1:L1:319:A:C8	2.48	0.49
1:L1:1899:G:O2'	21:Lv:57:ASN:OD1	2.28	0.49
1:L1:4274:A:H2'	1:L1:4275:G:C8	2.48	0.49
1:L1:4892:A:H2'	1:L1:4893:A:O4'	2.12	0.49
30:S1:54:A:OP1	49:Sh:111:LYS:NZ	2.38	0.49
30:S1:1118:C:O2'	52:Sk:75:GLU:OE1	2.28	0.49
30:S1:1761:U:H2'	30:S1:1762:C:C6	2.47	0.49
41:Sa:82:ASP:OD1	41:Sa:82:ASP:N	2.45	0.49
84:LQ:17:PHE:CE1	84:LQ:54:CYS:HB3	2.47	0.49
1:L1:3746:A:H5''	85:La:244:GLY:HA3	1.95	0.49
30:S1:1648:G:O2'	30:S1:1674:G:O6	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:1668:U:OP2	43:Sc:141:TYR:OH	2.25	0.49
79:LK:111:LEU:HD11	79:LK:125:ARG:HB3	1.95	0.49
1:L1:2091:C:C2	1:L1:2094:G:H4'	2.48	0.49
29:Nm:224:TYR:HD2	29:Nm:229:HIS:CE1	2.30	0.49
30:S1:851:C:H5''	30:S1:852:G:H5'	1.93	0.49
45:Se:16:LYS:N	63:Sv:259:THR:HG21	2.28	0.49
74:LF:59:SER:OG	74:LF:60:CYS:N	2.46	0.49
1:L1:670:G:H2'	1:L1:671:G:H8	1.77	0.49
1:L1:4441:A:H5''	80:LM:114:GLY:HA2	1.93	0.49
11:Ll:48:LYS:HG2	11:Ll:53:ALA:HB2	1.95	0.49
12:Lm:56:GLY:N	12:Lm:59:ASP:OD2	2.44	0.49
29:Nm:254:GLU:OE1	29:Nm:279:HIS:NE2	2.25	0.49
30:S1:206:G:H2'	30:S1:207:G:C8	2.47	0.49
30:S1:1566:G:N7	50:Si:101:ARG:NH2	2.59	0.49
37:SE:35:LEU:HD13	37:SE:40:VAL:HG11	1.95	0.49
40:SH:47:ALA:HA	40:SH:112:LYS:HA	1.95	0.49
45:Se:32:ILE:HD13	45:Se:60:ARG:HH11	1.78	0.49
82:LO:40:LEU:HD12	82:LO:70:VAL:HG12	1.95	0.49
83:LP:64:VAL:HA	83:LP:67:HIS:HD2	1.75	0.49
1:L1:135:G:C6	24:Ly:97:LYS:HB2	2.48	0.48
1:L1:1696:C:O2'	1:L1:1719:A:N6	2.46	0.48
1:L1:2822:G:OP2	8:Li:21:LYS:NZ	2.34	0.48
2:Lc:218:ILE:HA	2:Lc:229:LEU:HD13	1.94	0.48
16:Lq:84:ARG:NH2	23:Lx:99:GLU:OE1	2.45	0.48
22:Lw:57:THR:HG21	22:Lw:68:ARG:HG2	1.95	0.48
29:Nm:139:MET:HE2	29:Nm:323:VAL:HG11	1.95	0.48
30:S1:1402:A:N6	30:S1:1441:U:O2'	2.45	0.48
30:S1:1780:G:H2'	30:S1:1781:A:C8	2.47	0.48
50:Si:118:ASP:N	50:Si:118:ASP:OD1	2.46	0.48
85:La:20:VAL:HG12	85:La:23:ARG:HD2	1.95	0.48
86:Lb:92:TYR:HB3	86:Lb:99:LEU:HD22	1.95	0.48
1:L1:3:C:H42	68:L3:154:G:H1	1.61	0.48
1:L1:4485:C:O2'	72:LD:114:LYS:NZ	2.46	0.48
15:Lp:74:TYR:OH	68:L3:75:OMG:OP2	2.21	0.48
21:Lv:85:LEU:HD21	21:Lv:115:ALA:HB2	1.95	0.48
30:S1:747:U:H3'	30:S1:749:U:H5''	1.95	0.48
30:S1:1292:C:H2'	30:S1:1293:A:C8	2.48	0.48
57:Sp:21:CYS:HA	57:Sp:30:LEU:HD21	1.95	0.48
65:Sx:145:GLN:OE1	65:Sx:145:GLN:N	2.39	0.48
82:LO:84:GLU:OE2	82:LO:92:TYR:OH	2.28	0.48
1:L1:151:G:N7	78:LJ:141:ASN:ND2	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Nb:41:ASP:HB3	27:Nb:45:GLN:NE2	2.29	0.48
27:Nb:146:VAL:HG21	29:Nm:42:LYS:HE2	1.94	0.48
30:S1:377:G:H5'	33:SA:98:LYS:HD3	1.93	0.48
30:S1:1404:U:OP1	53:Sl:21:ARG:NH2	2.45	0.48
30:S1:1442:OMU:HM22	30:S1:1443:C:H5'	1.95	0.48
41:Sa:50:ARG:O	41:Sa:54:HIS:ND1	2.43	0.48
1:L1:1617:G:H1'	1:L1:2513:A:H61	1.78	0.48
1:L1:2407:G:N2	1:L1:2407:G:OP2	2.46	0.48
1:L1:2519:U:H1'	1:L1:2520:C:C6	2.47	0.48
57:Sp:33:LYS:HE2	57:Sp:34:TYR:CZ	2.49	0.48
60:Ss:297:THR:HG23	60:Ss:309:VAL:HG23	1.95	0.48
61:St:184:ARG:HG2	61:St:189:ILE:HG13	1.96	0.48
1:L1:172:C:N4	1:L1:264:C:O2	2.46	0.48
1:L1:1494:U:H2'	1:L1:1495:G:H8	1.78	0.48
1:L1:1705:G:OP1	77:LI:46:ARG:NH1	2.47	0.48
1:L1:2730:U:H2'	1:L1:2731:C:C6	2.48	0.48
30:S1:969:U:O2	30:S1:971:G:N1	2.46	0.48
36:SD:13:GLN:NE2	36:SD:36:TYR:HB3	2.29	0.48
43:Sc:89:SER:HB3	43:Sc:112:LEU:HD13	1.94	0.48
46:Sf:86:LEU:HD21	46:Sf:113:HIS:HB2	1.96	0.48
60:Ss:99:ARG:NH1	60:Ss:135:LEU:O	2.46	0.48
1:L1:4251:A:H5''	82:LO:108:GLY:HA3	1.96	0.48
30:S1:756:C:H2'	30:S1:757:C:C6	2.48	0.48
30:S1:1292:C:H5'	59:Sr:145:CYS:HB3	1.95	0.48
84:LQ:24:LEU:HD11	84:LQ:86:TRP:CG	2.49	0.48
1:L1:700:G:H2'	1:L1:701:G:H8	1.78	0.48
19:Lt:13:SER:O	19:Lt:16:SER:OG	2.28	0.48
30:S1:568:C:H2'	30:S1:569:A:C8	2.49	0.48
30:S1:1031:A2M:HM'2	30:S1:1032:C:H5'	1.96	0.48
53:Sl:108:PRO:HB3	65:Sx:40:ARG:HG2	1.96	0.48
1:L1:700:G:H2'	1:L1:701:G:C8	2.49	0.48
1:L1:982:U:H2'	1:L1:983:C:O4'	2.14	0.48
1:L1:1290:G:H2'	1:L1:1291:G:C8	2.49	0.48
28:Nd:135:LEU:HD21	28:Nd:159:LEU:HD13	1.96	0.48
30:S1:212:C:H2'	30:S1:213:G:H8	1.78	0.48
30:S1:1098:C:H2'	30:S1:1099:G:C8	2.49	0.48
30:S1:1279:C:H2'	30:S1:1280:G:H8	1.78	0.48
38:SF:83:ASP:N	38:SF:83:ASP:OD1	2.46	0.48
50:Si:116:ASP:OD1	50:Si:117:GLN:N	2.45	0.48
56:So:18:LEU:HD12	56:So:29:GLN:HG2	1.95	0.48
1:L1:1279:A:O2'	1:L1:1281:G:N7	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:3760:A:C6	30:S1:1824:A:H2'	2.49	0.48
1:L1:3777:G:O2'	1:L1:3815:G:O6	2.22	0.48
30:S1:581:U:H4'	49:Sh:66:GLY:HA2	1.95	0.48
30:S1:868:G:OP2	30:S1:868:G:N2	2.34	0.48
30:S1:1430:C:H3'	30:S1:1431:G:H21	1.78	0.48
53:Sl:107:GLU:HG3	53:Sl:108:PRO:HD2	1.96	0.48
1:L1:175:C:H2'	1:L1:176:G:H8	1.78	0.48
1:L1:2083:C:OP2	7:Lh:14:ARG:NH2	2.46	0.48
1:L1:2374:A:H2'	1:L1:2375:A:C8	2.49	0.48
1:L1:2893:U:H4'	33:SA:88:ASN:HD21	1.79	0.48
19:Lt:78:ASN:OD1	19:Lt:78:ASN:N	2.46	0.48
30:S1:1101:U:H2'	30:S1:1102:G:C8	2.49	0.48
32:S3:18:G:N2	32:S3:57:G:H2'	2.28	0.48
33:SA:135:GLU:O	33:SA:139:LYS:HB2	2.14	0.48
67:Sz:163:GLN:O	67:Sz:167:GLU:HB2	2.14	0.48
86:Lb:161:ARG:HG2	86:Lb:184:GLN:HA	1.95	0.48
1:L1:653:U:H2'	1:L1:654:C:C6	2.49	0.47
1:L1:674:G:H2'	1:L1:675:C:C6	2.49	0.47
2:Lc:114:ARG:HD2	76:LH:203:TYR:HB3	1.96	0.47
39:SG:48:SER:HB3	62:Su:67:PHE:CE1	2.49	0.47
42:Sb:17:ILE:HD11	42:Sb:54:VAL:HG13	1.96	0.47
54:Sm:58:LEU:HD12	54:Sm:62:VAL:HG21	1.96	0.47
61:St:128:ARG:HH21	61:St:153:PRO:HD3	1.79	0.47
76:LH:96:ARG:NH2	76:LH:104:GLU:OE1	2.47	0.47
82:LO:95:ARG:HG2	82:LO:175:LEU:HD12	1.95	0.47
11:Ll:27:HIS:CE1	27:Nb:1:MET:H2	2.27	0.47
13:Ln:97:LYS:HB2	13:Ln:100:VAL:HG23	1.96	0.47
27:Nb:19:ARG:NH2	27:Nb:21:GLY:O	2.47	0.47
28:Nd:93:LYS:HG3	28:Nd:95:ARG:HG2	1.96	0.47
30:S1:67:C:C5	66:Sy:162:LEU:HB3	2.48	0.47
30:S1:1549:U:OP1	57:Sp:34:TYR:OH	2.21	0.47
62:Su:68:GLU:OE2	62:Su:85:LYS:NZ	2.46	0.47
67:Sz:11:PRO:HB2	67:Sz:14:GLU:H	1.78	0.47
1:L1:4238:G:H2'	1:L1:4239:A:C8	2.49	0.47
1:L1:4908:G:N2	1:L1:4913:G:H5'	2.29	0.47
1:L1:4928:C:O3'	84:LQ:117:LYS:NZ	2.47	0.47
30:S1:893:U:H2'	30:S1:894:G:C8	2.49	0.47
30:S1:1100:A:H5''	42:Sb:132:ARG:CZ	2.45	0.47
33:SA:155:ASN:O	36:SD:21:LYS:NZ	2.39	0.47
42:Sb:29:HIS:HA	42:Sb:32:LYS:HE2	1.96	0.47
54:Sm:50:PHE:HE1	54:Sm:79:ILE:HG13	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Sz:76:GLN:HE22	67:Sz:94:PHE:HB2	1.80	0.47
1:L1:72:C:O4'	25:Lz:15:HIS:HB3	2.14	0.47
1:L1:2482:C:H2'	1:L1:2483:G:C8	2.49	0.47
3:Ld:56:THR:HG21	48:L2:26:C:H5''	1.95	0.47
13:Ln:96:GLN:HE21	13:Ln:100:VAL:HG12	1.80	0.47
13:Ln:97:LYS:O	13:Ln:101:ARG:N	2.37	0.47
30:S1:167:G:O2'	66:Sy:132:ARG:NH2	2.48	0.47
30:S1:533:A:H2'	30:S1:534:G:C8	2.49	0.47
30:S1:834:C:O2	30:S1:838:G:N2	2.48	0.47
49:Sh:49:LYS:HE2	49:Sh:49:LYS:HB2	1.70	0.47
50:Si:129:ARG:HD3	50:Si:133:ARG:CZ	2.45	0.47
60:Ss:15:ASN:HB2	60:Ss:37:ASP:HB3	1.96	0.47
60:Ss:196:ASN:HD22	60:Ss:237:ASN:HA	1.80	0.47
78:LJ:206:GLN:NE2	78:LJ:207:VAL:O	2.36	0.47
86:Lb:14:LEU:HD22	86:Lb:17:LEU:HD11	1.95	0.47
1:L1:153:G:H2'	1:L1:154:G:H8	1.79	0.47
2:Lc:65:GLU:HG2	2:Lc:80:ARG:HD3	1.95	0.47
30:S1:561:A:O2'	34:SB:134:HIS:NE2	2.47	0.47
30:S1:1357:A:OP1	63:Sv:125:LYS:NZ	2.45	0.47
30:S1:1400:U:O4	30:S1:1401:A:N6	2.46	0.47
30:S1:1444:U:P	43:Sc:15:ARG:HH22	2.37	0.47
82:LO:51:SER:HB2	82:LO:69:ALA:HB3	1.96	0.47
1:L1:156:G:N2	1:L1:157:U:O4	2.48	0.47
1:L1:4457:PSU:OP1	12:Lm:50:ASN:ND2	2.41	0.47
17:Lr:24:LYS:H	17:Lr:24:LYS:HD2	1.79	0.47
23:Lx:13:TYR:O	23:Lx:18:ASN:ND2	2.43	0.47
27:Nb:146:VAL:HG21	29:Nm:42:LYS:HG2	1.97	0.47
30:S1:86:C:O2'	30:S1:171:A:N1	2.35	0.47
30:S1:419:G:N2	30:S1:661:U:O2	2.48	0.47
39:SG:121:ARG:NH2	51:Sj:52:ASP:OD2	2.47	0.47
41:Sa:52:LYS:HG2	41:Sa:80:LEU:HD11	1.97	0.47
42:Sb:19:LYS:HE3	65:Sx:213:PRO:HD3	1.97	0.47
46:Sf:83:LEU:HD11	46:Sf:117:ARG:HD3	1.95	0.47
60:Ss:220:ASP:HB2	60:Ss:227:LEU:HD11	1.96	0.47
65:Sx:45:ARG:NH2	65:Sx:87:TYR:OH	2.48	0.47
1:L1:1088:C:H2'	1:L1:1089:G:C8	2.50	0.47
1:L1:1486:C:H2'	1:L1:1487:G:H8	1.80	0.47
1:L1:3617:G:OP1	13:Ln:44:ARG:NH1	2.48	0.47
1:L1:4743:G:H2'	1:L1:4744:A:C8	2.49	0.47
6:Lg:9:GLU:OE1	6:Lg:9:GLU:N	2.44	0.47
13:Ln:71:ARG:HG2	30:S1:1783:C:N3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Ln:102:LYS:HA	13:Ln:105:ARG:HB2	1.97	0.47
15:Lp:24:HIS:ND1	68:L3:90:C:O2'	2.39	0.47
19:Lt:64:ALA:O	19:Lt:68:LYS:N	2.47	0.47
25:Lz:55:ARG:O	25:Lz:59:GLU:HG2	2.15	0.47
29:Nm:297:HIS:CE1	29:Nm:302:THR:HG21	2.49	0.47
30:S1:220:U:H2'	30:S1:221:A:C8	2.49	0.47
30:S1:1189:A:H2'	30:S1:1190:A:H8	1.80	0.47
37:SE:80:ARG:HD3	37:SE:87:PRO:HA	1.95	0.47
49:Sh:45:ALA:HB2	49:Sh:55:ILE:HG13	1.97	0.47
58:Sq:2:ARG:HD3	58:Sq:5:TRP:NE1	2.30	0.47
61:St:177:MET:O	61:St:181:GLU:HG2	2.15	0.47
63:Sv:209:VAL:HB	63:Sv:210:PRO:HD3	1.96	0.47
66:Sy:45:TRP:HA	66:Sy:48:TYR:HD2	1.80	0.47
85:La:83:HIS:CE1	85:La:86:GLN:HB2	2.50	0.47
1:L1:74:G:H5'	83:LP:59:VAL:HB	1.97	0.47
1:L1:1866:U:O4'	80:LM:4:ARG:NH1	2.48	0.47
1:L1:2573:A:H1'	16:Lq:112:ARG:HH12	1.80	0.47
4:Le:270:TYR:OH	84:LQ:106:ASP:OD2	2.27	0.47
19:Lt:50:ASN:OD1	19:Lt:51:ASN:N	2.48	0.47
21:Lv:114:ARG:NH1	21:Lv:117:GLN:OE1	2.36	0.47
28:Nd:130:CYS:HB3	28:Nd:231:HIS:CE1	2.49	0.47
30:S1:51:U:H2'	30:S1:52:G:H8	1.79	0.47
40:SH:64:LEU:HD22	59:Sr:103:LEU:HD23	1.96	0.47
42:Sb:36:GLU:OE1	42:Sb:47:ARG:NH1	2.47	0.47
42:Sb:61:ILE:HD11	42:Sb:66:VAL:HG22	1.97	0.47
42:Sb:94:GLU:O	42:Sb:116:ASN:ND2	2.46	0.47
46:Sf:96:SER:OG	46:Sf:97:ARG:N	2.48	0.47
66:Sy:218:LYS:NZ	66:Sy:219:GLU:OE2	2.47	0.47
1:L1:1198:G:O2'	1:L1:1200:G:O4'	2.29	0.47
1:L1:1332:C:H2'	1:L1:1333:A:C8	2.49	0.47
1:L1:2303:C:O2'	1:L1:2332:A:N1	2.43	0.47
1:L1:2373:C:H5'	20:Lu:46:LEU:HD23	1.97	0.47
1:L1:3786:U:OP1	1:L1:4550:G:O2'	2.26	0.47
1:L1:4473:A:P	72:LD:102:ARG:HH21	2.38	0.47
1:L1:4475:G:H5''	1:L1:4476:C:H5''	1.95	0.47
1:L1:4887:C:H2'	1:L1:4888:U:O4'	2.15	0.47
4:Le:148:THR:HA	4:Le:200:LYS:HG2	1.96	0.47
12:Lm:45:ILE:HG21	12:Lm:53:PRO:HB3	1.96	0.47
27:Nb:82:SER:HB3	27:Nb:87:THR:HB	1.97	0.47
28:Nd:111:ALA:HB3	28:Nd:120:ALA:HB3	1.97	0.47
32:S3:63:C:H2'	32:S3:64:A:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Su:110:MET:HA	62:Su:113:MET:HE2	1.97	0.47
63:Sv:68:ARG:HE	63:Sv:277:HIS:CD2	2.33	0.47
66:Sy:7:PHE:CE2	66:Sy:9:ALA:HB3	2.50	0.47
1:L1:171:U:H5''	83:LP:135:LYS:HE2	1.97	0.47
1:L1:257:C:H2'	1:L1:258:G:H8	1.80	0.47
1:L1:461:G:H2'	1:L1:462:G:H8	1.80	0.47
1:L1:667:A:C8	2:Lc:4:ALA:HB3	2.50	0.47
8:Li:44:LEU:HD22	8:Li:49:LEU:HD12	1.96	0.47
27:Nb:55:ASN:HA	27:Nb:80:GLN:HA	1.96	0.47
30:S1:210:PSU:H2'	30:S1:211:G:C8	2.50	0.47
30:S1:317:C:OP2	66:Sy:183:ARG:NH2	2.30	0.47
30:S1:332:G:O6	66:Sy:189:ARG:NH2	2.37	0.47
30:S1:462:OMC:HM22	30:S1:463:C:H5'	1.97	0.47
32:S3:73:A:H5''	32:S3:74:C:H5'	1.96	0.47
50:Si:104:LEU:HD13	50:Si:121:ARG:HD2	1.97	0.47
77:LI:142:TRP:CZ2	77:LI:235:ASN:HB2	2.49	0.47
1:L1:280:G:OP2	76:LH:44:ARG:NH2	2.33	0.46
1:L1:2520:C:H2'	1:L1:2521:G:H8	1.79	0.46
1:L1:4266:G:H2'	1:L1:4266:G:N3	2.31	0.46
2:Lc:76:ILE:HG12	2:Lc:96:CYS:SG	2.55	0.46
24:Ly:119:TYR:HB2	83:LP:124:LEU:HD11	1.96	0.46
29:Nm:196:SER:O	29:Nm:218:ASN:N	2.30	0.46
39:SG:19:PRO:HG3	62:Su:30:TRP:CD2	2.50	0.46
44:Sd:14:ARG:NH1	82:LO:111:GLU:OE1	2.48	0.46
66:Sy:164:LYS:HD3	66:Sy:167:LYS:HD2	1.97	0.46
80:LM:80:CYS:SG	80:LM:147:HIS:ND1	2.66	0.46
1:L1:4260:U:H2'	1:L1:4261:C:C6	2.50	0.46
12:Lm:43:LYS:HG3	12:Lm:60:MET:HG2	1.96	0.46
30:S1:799:OMU:H5	67:Sz:109:ARG:HE	1.80	0.46
30:S1:943:U:OP2	62:Su:216:LYS:NZ	2.47	0.46
36:SD:15:THR:O	36:SD:15:THR:OG1	2.33	0.46
42:Sb:127:ASN:N	42:Sb:127:ASN:OD1	2.48	0.46
61:St:80:ARG:O	61:St:84:GLN:HG3	2.15	0.46
72:LD:92:ASP:OD1	72:LD:126:LYS:NZ	2.48	0.46
86:Lb:19:ARG:HB2	86:Lb:234:ARG:HH21	1.79	0.46
1:L1:345:C:H2'	1:L1:346:G:H8	1.81	0.46
1:L1:746:A:N6	1:L1:913:U:O2	2.48	0.46
1:L1:1301:C:C2	21:Lv:17:THR:HG21	2.49	0.46
1:L1:2092:G:OP1	1:L1:2094:G:N2	2.37	0.46
3:Ld:59:ASP:OD1	3:Ld:60:ILE:N	2.48	0.46
48:L2:4:U:H2'	48:L2:5:A:H8	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:2073:C:OP1	77:LI:212:LYS:HE3	2.16	0.46
1:L1:3700:C:H2'	1:L1:3746:A:H61	1.79	0.46
1:L1:4685:U:H2'	1:L1:4686:G:H8	1.81	0.46
7:Lh:177:ALA:O	7:Lh:184:ARG:HB2	2.15	0.46
21:Lv:100:ALA:HB3	21:Lv:103:VAL:HG23	1.98	0.46
29:Nm:260:ILE:HG12	29:Nm:361:LEU:HD11	1.96	0.46
30:S1:295:C:H2'	30:S1:296:PSU:H6	1.80	0.46
30:S1:879:C:H2'	30:S1:880:G:C8	2.47	0.46
30:S1:1232:PSU:H2'	30:S1:1233:G:H8	1.81	0.46
30:S1:1351:G:O2'	30:S1:1378:A:N1	2.40	0.46
30:S1:1786:U:H2'	30:S1:1787:G:H8	1.80	0.46
43:Sc:8:GLN:HB2	43:Sc:99:TYR:CE2	2.49	0.46
44:Sd:34:LYS:HB3	44:Sd:100:ALA:HA	1.97	0.46
58:Sq:2:ARG:HB3	58:Sq:5:TRP:CD1	2.50	0.46
75:LG:117:ILE:O	75:LG:120:SER:OG	2.31	0.46
76:LH:153:LYS:HB2	76:LH:156:HIS:HD2	1.80	0.46
82:LO:64:ARG:NH1	82:LO:65:ASN:OD1	2.49	0.46
86:Lb:19:ARG:HB2	86:Lb:234:ARG:NH2	2.31	0.46
1:L1:454:U:H3	1:L1:702:U:H3	1.62	0.46
1:L1:907:C:H2'	1:L1:908:G:H8	1.79	0.46
1:L1:1730:U:H1'	10:Lk:101:SER:HB3	1.97	0.46
1:L1:2486:G:H1	1:L1:2492:C:N4	2.13	0.46
1:L1:2822:G:H5''	8:Li:18:GLY:HA3	1.98	0.46
66:Sy:159:ARG:HB3	66:Sy:171:THR:HB	1.98	0.46
1:L1:663:G:H2'	1:L1:664:G:H8	1.79	0.46
1:L1:1179:U:O2	1:L1:1179:U:H2'	2.16	0.46
1:L1:2482:C:H2'	1:L1:2483:G:H8	1.79	0.46
11:Ll:107:LYS:O	11:Ll:108:GLU:HG2	2.15	0.46
15:Lp:31:SER:HA	15:Lp:48:PRO:HA	1.97	0.46
24:Ly:19:LYS:NZ	24:Ly:23:ASP:OD1	2.48	0.46
30:S1:190:G:O2'	30:S1:209:A:N6	2.48	0.46
30:S1:611:G:H1	30:S1:632:C:H42	1.63	0.46
30:S1:693:A:H2'	30:S1:694:G:H8	1.80	0.46
30:S1:925:G:H1	30:S1:1017:U:H3	1.62	0.46
30:S1:1621:U:O2'	30:S1:1622:U:H2'	2.15	0.46
34:SB:53:ILE:HD13	34:SB:81:LEU:HD21	1.96	0.46
60:Ss:70:VAL:HB	60:Ss:79:LEU:HB3	1.98	0.46
73:LE:48:TYR:OH	76:LH:90:ASN:O	2.27	0.46
86:Lb:95:THR:OG1	86:Lb:98:GLY:O	2.25	0.46
1:L1:2090:U:H4'	1:L1:2091:C:H5''	1.98	0.46
1:L1:3710:G:H2'	1:L1:3711:A:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Nb:80:GLN:O	27:Nb:89:THR:N	2.45	0.46
28:Nd:172:MET:HG2	28:Nd:215:SER:HB3	1.97	0.46
45:Se:33:GLN:HE21	45:Se:52:THR:HG21	1.81	0.46
68:L3:132:G:H2'	68:L3:133:G:H8	1.81	0.46
1:L1:396:A:H2'	1:L1:397:G:C8	2.50	0.46
1:L1:1281:G:OP1	2:Lc:316:LYS:NZ	2.48	0.46
1:L1:1704:C:P	77:LI:43:ARG:HH21	2.39	0.46
1:L1:2480:G:H2'	1:L1:2481:G:H8	1.80	0.46
1:L1:2611:A:H5'	1:L1:2688:G:H4'	1.97	0.46
1:L1:3724:A2M:HM'2	1:L1:3725:G:H5'	1.97	0.46
18:Ls:117:ARG:HG3	18:Ls:118:LEU:N	2.31	0.46
19:Lt:13:SER:HG	19:Lt:17:ARG:HH12	1.59	0.46
26:Na:98:LYS:HG2	26:Na:99:SER:H	1.81	0.46
28:Nd:110:ILE:HA	28:Nd:121:PHE:HA	1.97	0.46
30:S1:126:G:OP1	66:Sy:198:ARG:NH1	2.49	0.46
30:S1:453:C:O2'	66:Sy:92:ARG:O	2.30	0.46
30:S1:537:C:H2'	30:S1:538:U:C6	2.51	0.46
30:S1:877:C:H2'	30:S1:878:G:C8	2.50	0.46
30:S1:1603:G:H4'	44:Sd:38:ARG:NH2	2.31	0.46
40:SH:12:MET:HG3	40:SH:16:THR:HB	1.97	0.46
45:Se:59:ILE:HG23	45:Se:64:GLU:HB2	1.96	0.46
53:Sl:99:LYS:O	53:Sl:103:SER:OG	2.30	0.46
64:Sw:44:LEU:HD13	64:Sw:72:ILE:HD11	1.97	0.46
65:Sx:157:MET:HE2	65:Sx:187:LYS:HD3	1.96	0.46
1:L1:190:G:H2'	1:L1:191:G:C8	2.51	0.46
1:L1:907:C:H2'	1:L1:908:G:C8	2.49	0.46
1:L1:1245:C:H2'	1:L1:1246:G:H8	1.81	0.46
1:L1:3690:U:O2'	1:L1:3817:A:N3	2.42	0.46
2:Lc:260:LEU:HD23	2:Lc:260:LEU:HA	1.81	0.46
12:Lm:89:ARG:HB2	12:Lm:95:PHE:CE2	2.50	0.46
27:Nb:61:GLU:HB2	27:Nb:73:HIS:CE1	2.51	0.46
28:Nd:186:PHE:HD1	28:Nd:190:LEU:HD12	1.80	0.46
30:S1:15:U:H2'	30:S1:16:G:O4'	2.16	0.46
30:S1:808:A:H3'	30:S1:809:A:H8	1.81	0.46
41:Sa:108:LYS:HB2	44:Sd:117:ILE:HD11	1.97	0.46
45:Se:17:CYS:HB2	45:Se:56:CYS:HB3	1.97	0.46
67:Sz:44:ASN:OD1	67:Sz:44:ASN:N	2.49	0.46
82:LO:72:CYS:SG	82:LO:73:THR:N	2.88	0.46
1:L1:989:U:O2	1:L1:1064:G:N2	2.49	0.46
26:Na:73:GLU:OE2	26:Na:77:ARG:NH2	2.49	0.46
28:Nd:131:GLY:HA3	28:Nd:227:HIS:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:92:A:C4'	64:Sw:3:ARG:HH21	2.28	0.46
30:S1:969:U:OP1	30:S1:970:G:O2'	2.26	0.46
30:S1:1391:OMC:HM22	30:S1:1392:U:H5'	1.98	0.46
30:S1:1748:G:H2'	30:S1:1749:G:C8	2.51	0.46
65:Sx:46:THR:OG1	65:Sx:83:SER:O	2.29	0.46
1:L1:352:G:N7	2:Lc:197:ARG:NH2	2.60	0.45
1:L1:1447:C:H2'	1:L1:1448:G:H8	1.80	0.45
1:L1:4238:G:H2'	1:L1:4239:A:H8	1.80	0.45
1:L1:4872:G:O6	84:LQ:98:ARG:NH1	2.49	0.45
21:Lv:67:LYS:HG2	21:Lv:68:HIS:CD2	2.51	0.45
30:S1:77:A:H1'	66:Sy:176:ILE:HG13	1.98	0.45
30:S1:546:G:H2'	30:S1:548:C:C5	2.50	0.45
30:S1:1597:C:H4'	30:S1:1603:G:C6	2.51	0.45
32:S3:11:C:N4	32:S3:12:G:O6	2.49	0.45
1:L1:268:G:H2'	1:L1:269:G:C8	2.49	0.45
1:L1:1566:C:H2'	1:L1:1567:U:C6	2.50	0.45
1:L1:1628:C:OP1	85:La:14:SER:OG	2.32	0.45
1:L1:4870:G:OP2	84:LQ:5:ARG:NH2	2.38	0.45
5:Lf:75:ALA:HB3	5:Lf:78:ARG:HG2	1.98	0.45
20:Lu:37:GLY:O	20:Lu:41:ARG:HG3	2.17	0.45
20:Lu:64:ILE:HG23	20:Lu:68:LEU:HD23	1.97	0.45
27:Nb:143:ASP:HA	29:Nm:45:TRP:HZ2	1.82	0.45
29:Nm:142:VAL:HB	29:Nm:225:ARG:HB3	1.97	0.45
29:Nm:186:TYR:O	29:Nm:189:PHE:HB2	2.17	0.45
30:S1:317:C:H2'	30:S1:318:A:C8	2.51	0.45
30:S1:693:A:H2	30:S1:737:G:H1	1.63	0.45
30:S1:917:U:O4'	67:Sz:118:ARG:HG3	2.16	0.45
30:S1:1407:U:H2'	30:S1:1408:U:C6	2.52	0.45
30:S1:1574:C:H2'	30:S1:1575:G:C8	2.51	0.45
30:S1:1588:A:H2'	30:S1:1589:A:C8	2.51	0.45
41:Sa:83:MET:HB3	41:Sa:116:LEU:HD12	1.98	0.45
45:Se:16:LYS:NZ	63:Sv:257:LYS:O	2.35	0.45
46:Sf:98:GLN:NE2	63:Sv:171:GLY:O	2.50	0.45
67:Sz:25:GLN:HA	67:Sz:28:LEU:HD12	1.98	0.45
1:L1:135:G:N1	24:Ly:97:LYS:HD3	2.31	0.45
1:L1:478:G:H2'	1:L1:479:G:H8	1.81	0.45
1:L1:3712:A:O2'	1:L1:3713:U:H6	1.99	0.45
2:Lc:317:ASN:HD22	2:Lc:320:LYS:HE2	1.81	0.45
28:Nd:178:HIS:CE1	28:Nd:210:SER:HB2	2.51	0.45
30:S1:233:C:H2'	30:S1:234:C:C6	2.51	0.45
30:S1:900:C:H2'	30:S1:901:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:L2:32:A:O2'	48:L2:41:G:N7	2.38	0.45
51:Sj:88:SER:O	51:Sj:92:ARG:HG3	2.16	0.45
1:L1:417:G:H1'	68:L3:16:G:N2	2.31	0.45
1:L1:1234:G:H2'	1:L1:1235:G:H8	1.82	0.45
1:L1:1401:C:H2'	1:L1:1402:C:C6	2.52	0.45
1:L1:2717:G:OP1	11:L1:107:LYS:NZ	2.49	0.45
1:L1:3744:OMG:HM22	1:L1:3745:U:H5'	1.98	0.45
1:L1:3941:G:H2'	1:L1:3942:A:C8	2.50	0.45
27:Nb:55:ASN:OD1	27:Nb:80:GLN:HG3	2.16	0.45
30:S1:434:G:OP2	33:SA:25:ARG:NH2	2.50	0.45
64:Sw:189:LEU:O	64:Sw:245:ARG:NH2	2.49	0.45
85:La:33:ASP:OD1	85:La:33:ASP:N	2.48	0.45
1:L1:2808:G:O2'	8:Li:60:ARG:NH1	2.50	0.45
1:L1:4425:G:OP1	72:LD:100:TYR:OH	2.28	0.45
2:Lc:152:LEU:HD23	2:Lc:251:ILE:HG12	1.98	0.45
11:L1:27:HIS:ND1	27:Nb:3:GLU:OE1	2.50	0.45
56:So:17:VAL:HA	56:So:30:VAL:HG12	1.99	0.45
82:LO:18:ARG:HG3	82:LO:135:GLY:HA3	1.99	0.45
86:Lb:220:ILE:HG12	86:Lb:278:THR:HG23	1.98	0.45
1:L1:1169:G:H2'	1:L1:1170:G:H8	1.81	0.45
1:L1:1298:C:H2'	1:L1:1299:G:C8	2.52	0.45
1:L1:1949:U:H2'	1:L1:1950:U:C6	2.52	0.45
1:L1:4076:G:OP1	78:LJ:73:ARG:NH2	2.50	0.45
7:Lh:178:ARG:N	17:Lr:51:GLY:HA2	2.31	0.45
9:Lj:74:ARG:O	9:Lj:76:LYS:NZ	2.49	0.45
26:Na:215:MET:SD	28:Nd:219:LYS:HD3	2.55	0.45
30:S1:165:G:H21	30:S1:165:G:P	2.38	0.45
30:S1:940:U:H3	30:S1:1002:U:H3	1.63	0.45
30:S1:953:C:H2'	30:S1:954:U:O4'	2.17	0.45
30:S1:1667:U:H2'	30:S1:1668:U:C6	2.52	0.45
35:SC:42:LYS:HD3	35:SC:42:LYS:HA	1.84	0.45
36:SD:3:ASP:OD1	36:SD:3:ASP:N	2.50	0.45
41:Sa:41:GLN:HG3	41:Sa:84:ILE:HD13	1.98	0.45
80:LM:46:PHE:HB2	80:LM:139:ARG:NH1	2.31	0.45
1:L1:490:C:H2'	1:L1:491:G:C8	2.52	0.45
1:L1:670:G:H2'	1:L1:671:G:C8	2.50	0.45
1:L1:1218:G:H2'	1:L1:1219:G:H8	1.80	0.45
1:L1:2326:G:OP1	21:Lv:108:ARG:NH2	2.49	0.45
1:L1:2713:C:H2'	1:L1:2714:G:H8	1.82	0.45
1:L1:3689:G:O2'	1:L1:3818:UY1:OP2	2.33	0.45
13:Ln:82:ILE:HG12	13:Ln:90:ILE:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Lw:47[B]:CYS:SG	22:Lw:74:VAL:HG23	2.57	0.45
29:Nm:270:ARG:NH2	29:Nm:314:ALA:O	2.43	0.45
30:S1:561:A:HO2'	34:SB:134:HIS:HE2	1.65	0.45
30:S1:1189:A:H2'	30:S1:1190:A:C8	2.52	0.45
1:L1:1834:U:OP1	10:Lk:120:LYS:NZ	2.40	0.45
1:L1:1921:C:H1'	9:Lj:160:ARG:HB3	1.98	0.45
1:L1:2773:G:H5'	70:LB:17:ARG:HH21	1.81	0.45
1:L1:4537:C:H2'	1:L1:4538:G:C8	2.52	0.45
8:Li:168:GLU:O	8:Li:172:ARG:HG3	2.17	0.45
30:S1:240:G:H2'	30:S1:241:G:C8	2.52	0.45
30:S1:1221:G:O2'	30:S1:1676:U:O2	2.33	0.45
45:Se:62:MET:HB2	45:Se:64:GLU:HG2	1.98	0.45
66:Sy:57:ASP:HA	66:Sy:106:LEU:HA	1.99	0.45
83:LP:128:PRO:HG3	83:LP:138:ASP:HB3	1.98	0.45
1:L1:481:G:OP2	1:L1:481:G:N2	2.41	0.45
1:L1:945:U:OP1	2:Lc:342:ARG:NH2	2.49	0.45
1:L1:2620:G:H2'	1:L1:2621:A:H8	1.81	0.45
1:L1:4305:G:O5'	10:Lk:83:LYS:NZ	2.50	0.45
28:Nd:180:HIS:CD2	29:Nm:12:ASP:HB2	2.51	0.45
30:S1:78:C:H5'	66:Sy:173:ALA:HB3	1.98	0.45
30:S1:159:A2M:N1	30:S1:467:G:O2'	2.50	0.45
30:S1:236:A:N1	30:S1:892:U:N3	2.65	0.45
39:SG:32:HIS:HB2	39:SG:43:HIS:HB3	1.97	0.45
42:Sb:27:ASP:O	42:Sb:31:ASN:ND2	2.49	0.45
48:L2:83:A:O2'	48:L2:85:G:OP1	2.31	0.45
56:So:20:ARG:NH1	56:So:25:GLY:O	2.50	0.45
61:St:42:LYS:HB3	61:St:48:ILE:HD11	1.99	0.45
63:Sv:253:PRO:HA	63:Sv:256:TRP:CE2	2.52	0.45
64:Sw:104:ASP:OD1	64:Sw:108:ARG:N	2.33	0.45
67:Sz:93:VAL:HG11	67:Sz:133:LEU:HD12	1.97	0.45
1:L1:4571:A2M:HM'2	1:L1:4572:U:H5'	1.98	0.45
1:L1:4600:G:O2'	1:L1:4609:G:O6	2.32	0.45
2:Lc:145:GLU:OE1	2:Lc:145:GLU:N	2.50	0.45
30:S1:1406:G:H2'	30:S1:1407:U:C6	2.52	0.45
30:S1:1458:G:H2'	30:S1:1459:G:C8	2.52	0.45
30:S1:1679:A:H2'	35:SC:60:ARG:HD2	1.99	0.45
49:Sh:10:ARG:NE	49:Sh:26:ASP:OD2	2.31	0.45
57:Sp:21:CYS:HB2	57:Sp:39:CYS:HB3	1.99	0.45
63:Sv:253:PRO:HA	63:Sv:256:TRP:NE1	2.31	0.45
69:LA:27:TYR:HA	69:LA:34:CYS:HA	1.99	0.45
80:LM:66:GLU:CD	80:LM:69:ARG:HH21	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1088:C:H2'	1:L1:1089:G:H8	1.83	0.44
1:L1:2693:G:H2'	1:L1:2694:G:C2	2.52	0.44
29:Nm:99:VAL:HG22	29:Nm:171:HIS:CE1	2.51	0.44
30:S1:67:C:H41	66:Sy:164:LYS:H	1.65	0.44
35:SC:119:SER:HB2	35:SC:150:ALA:HB1	1.99	0.44
56:So:7:GLN:OE1	56:So:10:LYS:NZ	2.45	0.44
61:St:127:PRO:HG3	61:St:146:ALA:HB1	1.99	0.44
63:Sv:102:LEU:HD13	63:Sv:130:ILE:HD11	1.98	0.44
77:LI:94:ARG:NH2	77:LI:97:GLY:O	2.43	0.44
1:L1:386:A:OP2	15:Lp:89:LYS:NZ	2.40	0.44
1:L1:691:C:H2'	1:L1:692:A:C8	2.52	0.44
1:L1:1503:A:H4'	1:L1:1504:G:H5'	1.97	0.44
1:L1:1702:C:N3	77:LI:36:LYS:NZ	2.64	0.44
1:L1:2581:A:N3	1:L1:2654:C:O2'	2.40	0.44
1:L1:4691:A:OP1	79:LK:75:SER:OG	2.30	0.44
6:Lg:46:LYS:NZ	6:Lg:50:ASP:OD2	2.50	0.44
15:Lp:126:ARG:O	15:Lp:130:LYS:HG2	2.17	0.44
30:S1:39:A:OP2	34:SB:5:ARG:NH1	2.50	0.44
30:S1:544:G:H2'	30:S1:545:A:H8	1.81	0.44
44:Sd:40:TYR:HA	44:Sd:83:PHE:HE1	1.82	0.44
60:Ss:207:CYS:SG	60:Ss:219:TRP:HB2	2.58	0.44
1:L1:303:C:OP2	76:LH:68:ARG:NH2	2.45	0.44
1:L1:910:G:H2'	1:L1:911:U:H6	1.81	0.44
1:L1:1534:A2M:H8	69:LA:15:THR:OG1	2.17	0.44
1:L1:2407:G:O6	71:LC:2:SER:N	2.51	0.44
1:L1:2845:A:N6	1:L1:3843:C:H42	2.13	0.44
1:L1:3681:G:N1	85:La:118:GLU:OE2	2.51	0.44
28:Nd:154:PHE:O	28:Nd:157:GLN:HG2	2.17	0.44
30:S1:643:A:OP1	34:SB:38:ARG:NH2	2.32	0.44
30:S1:874:G:H21	67:Sz:114:GLN:HE21	1.65	0.44
33:SA:101:ILE:HD12	33:SA:190:LEU:HD11	1.99	0.44
46:Sf:101:PHE:HA	46:Sf:113:HIS:CE1	2.53	0.44
51:Sj:13:LYS:O	51:Sj:15:ARG:NH1	2.50	0.44
61:St:128:ARG:NH2	61:St:153:PRO:HD3	2.33	0.44
79:LK:41:ILE:HG22	79:LK:43:VAL:HG13	1.98	0.44
1:L1:757:G:O6	1:L1:907:C:N4	2.50	0.44
1:L1:2092:G:OP2	1:L1:2092:G:H4'	2.18	0.44
1:L1:2563:C:H3'	1:L1:2564:G:H8	1.82	0.44
15:Lp:55:VAL:HG12	15:Lp:106:ILE:HA	1.98	0.44
26:Na:178:VAL:HA	26:Na:181:ILE:HD12	1.98	0.44
28:Nd:197:SER:HB3	28:Nd:231:HIS:CD2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Nm:162:THR:N	29:Nm:165:GLU:OE1	2.39	0.44
29:Nm:199:GLU:HA	29:Nm:353:ARG:HA	1.99	0.44
30:S1:857:U:H2'	30:S1:858:A:C8	2.52	0.44
30:S1:1240:A:N6	30:S1:1241:A:N1	2.66	0.44
30:S1:1245:G:O2'	30:S1:1492:U:OP1	2.29	0.44
41:Sa:17:TYR:HB3	41:Sa:25:LEU:HD11	1.99	0.44
44:Sd:55:ARG:NH2	54:Sm:82:SER:OG	2.50	0.44
47:Sg:24:ASP:HB3	47:Sg:27:TYR:HB3	1.99	0.44
52:Sk:56:CYS:HB3	52:Sk:61:THR:H	1.81	0.44
76:LH:178:HIS:HA	76:LH:181:HIS:NE2	2.32	0.44
1:L1:4713:G:OP1	5:Lf:148:LYS:NZ	2.31	0.44
1:L1:4973:U:H1'	1:L1:4986:G:C2	2.52	0.44
9:Lj:20:PRO:HA	9:Lj:23:HIS:CE1	2.53	0.44
12:Lm:87:SER:HA	12:Lm:97:TYR:HB3	2.00	0.44
28:Nd:127:ASP:OD1	28:Nd:128:VAL:N	2.50	0.44
29:Nm:200:VAL:HA	29:Nm:347:VAL:HG12	2.00	0.44
30:S1:14:C:O2'	30:S1:668:A2M:N1	2.45	0.44
30:S1:483:C:H2'	30:S1:484:A2M:O4'	2.18	0.44
30:S1:790:C:H2'	30:S1:791:C:O4'	2.17	0.44
30:S1:793:G:C2	30:S1:794:A:C4	3.06	0.44
30:S1:897:U:H2'	30:S1:898:U:C6	2.52	0.44
33:SA:190:LEU:HB2	33:SA:195:LEU:HD13	2.00	0.44
60:Ss:233:GLY:HA3	60:Ss:252:THR:HG21	1.98	0.44
1:L1:910:G:H2'	1:L1:911:U:C6	2.52	0.44
1:L1:966:A:O2'	1:L1:2092:G:N2	2.50	0.44
1:L1:3725:G:N2	1:L1:3728:A:OP2	2.43	0.44
1:L1:4945:G:N1	22:Lw:3:GLY:O	2.34	0.44
7:Lh:176:ARG:HA	7:Lh:180:ARG:HG3	1.99	0.44
11:Ll:47:ILE:HD12	11:Ll:63:ILE:HD11	2.00	0.44
13:Ln:80:ARG:HD3	66:Sy:132:ARG:CZ	2.47	0.44
30:S1:934:G:OP2	30:S1:993:G:N2	2.43	0.44
42:Sb:66:VAL:HG23	42:Sb:69:ILE:H	1.83	0.44
61:St:137:ALA:HB1	61:St:142:LEU:HB3	1.99	0.44
61:St:195:TRP:CD2	61:St:197:VAL:HG12	2.53	0.44
67:Sz:28:LEU:O	67:Sz:32:MET:HG2	2.18	0.44
80:LM:103:LEU:HD21	80:LM:111:LEU:HD22	2.00	0.44
1:L1:238:C:OP2	15:Lp:45:ARG:NH2	2.51	0.44
1:L1:1363:C:OP2	83:LP:39:ARG:NH2	2.40	0.44
1:L1:4138:C:H2'	1:L1:4139:G:C8	2.53	0.44
4:Le:46:ARG:HB2	4:Le:62:MET:HE1	2.00	0.44
5:Lf:10:ASP:OD2	5:Lf:37:ARG:NH2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Na:95:THR:OG1	27:Nb:109:GLN:OE1	2.22	0.44
29:Nm:247:LYS:HE2	29:Nm:283:ASN:HB3	2.00	0.44
30:S1:615:C:O2	55:Sn:85:LYS:NZ	2.40	0.44
30:S1:1520:G:H2'	30:S1:1520:G:N3	2.32	0.44
47:Sg:77:ASN:OD1	47:Sg:77:ASN:N	2.50	0.44
86:Lb:92:TYR:HB2	86:Lb:159:VAL:HB	2.00	0.44
1:L1:701:G:H2'	1:L1:702:U:C6	2.53	0.44
1:L1:2520:C:H2'	1:L1:2521:G:C8	2.52	0.44
1:L1:2622:G:O6	11:L1:81:ARG:NH2	2.51	0.44
1:L1:4265:U:N3	3:Ld:17:GLN:O	2.48	0.44
1:L1:4909:A:OP2	86:Lb:156:TYR:OH	2.25	0.44
28:Nd:97:LYS:NZ	28:Nd:139:GLU:OE2	2.39	0.44
29:Nm:368:CYS:SG	29:Nm:369:GLU:N	2.91	0.44
30:S1:466:G:O2'	66:Sy:59:GLN:NE2	2.50	0.44
30:S1:886:A:H62	30:S1:900:C:H42	1.65	0.44
30:S1:1308:U:H2'	30:S1:1309:C:C6	2.53	0.44
45:Se:62:MET:O	61:St:33:GLN:NE2	2.44	0.44
46:Sf:68:ARG:HD3	63:Sv:256:TRP:CD2	2.53	0.44
76:LH:53:TYR:HB2	76:LH:133:ILE:HD13	2.00	0.44
77:LI:220:MET:HB3	77:LI:232:ASP:OD2	2.18	0.44
1:L1:1399:G:H2'	1:L1:1400:G:H8	1.83	0.44
1:L1:4549:G:H2'	1:L1:4550:G:H8	1.82	0.44
30:S1:303:C:H2'	30:S1:304:C:O4'	2.17	0.44
30:S1:624:C:H41	47:Sg:63:ASN:CG	2.25	0.44
30:S1:1711:U:H2'	30:S1:1712:A:H8	1.83	0.44
63:Sv:72:ASP:OD2	63:Sv:272:HIS:NE2	2.42	0.44
68:L3:93:C:O2'	68:L3:94:G:H8	2.01	0.44
73:LE:6:LYS:HE3	73:LE:94:GLY:HA3	2.00	0.44
78:LJ:81:ASN:O	78:LJ:84:THR:OG1	2.28	0.44
1:L1:207:G:OP1	28:Nd:3:ARG:NH1	2.52	0.43
1:L1:1348:U:H2'	1:L1:1349:G:C8	2.53	0.43
1:L1:1378:C:H5	83:LP:158:ARG:HB3	1.83	0.43
1:L1:1485:C:O4'	1:L1:4349:C:N4	2.51	0.43
5:Lf:43:ILE:HD11	5:Lf:138:LEU:HD13	1.99	0.43
7:Lh:155:ALA:HB3	7:Lh:158:THR:HG23	1.99	0.43
11:Ll:104:ALA:HA	11:Ll:110:TYR:HD1	1.83	0.43
30:S1:283:G:H1	30:S1:892:U:H4'	1.81	0.43
30:S1:563:G:O2'	30:S1:564:A:H8	2.01	0.43
30:S1:794:A:H2'	30:S1:795:A:C8	2.53	0.43
30:S1:928:G:H2'	30:S1:929:G:C8	2.53	0.43
30:S1:1124:C:O2'	42:Sb:126:MET:O	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:1413:G:H2'	30:S1:1414:A:C8	2.52	0.43
41:Sa:79:HIS:O	41:Sa:81:ARG:N	2.51	0.43
42:Sb:14:ARG:CB	42:Sb:69:ILE:HD11	2.48	0.43
60:Ss:5:MET:HG2	60:Ss:312:VAL:HG22	2.00	0.43
64:Sw:212:ASP:OD1	64:Sw:216:ASN:N	2.51	0.43
70:LB:26:LYS:NZ	70:LB:28:ASN:OD1	2.31	0.43
1:L1:1084:C:H2'	1:L1:1085:C:C6	2.53	0.43
1:L1:1477:C:H2'	1:L1:1478:C:C6	2.53	0.43
1:L1:1577:G:O2'	1:L1:1612:G:H4'	2.18	0.43
1:L1:2515:G:OP1	23:Lx:37:LYS:NZ	2.39	0.43
1:L1:4635:A:H3'	1:L1:4636:U:H4'	2.00	0.43
30:S1:694:G:H2'	30:S1:695:C:C6	2.53	0.43
30:S1:1255:G:OP1	30:S1:1256:G:O2'	2.27	0.43
30:S1:1403:C:N4	30:S1:1433:C:OP2	2.52	0.43
30:S1:1673:U:O2'	35:SC:84:GLY:O	2.28	0.43
36:SD:35:ARG:NE	36:SD:53:GLY:O	2.34	0.43
43:Sc:97:GLN:HE22	60:Ss:60:ARG:HH21	1.64	0.43
49:Sh:77:ASP:HB2	49:Sh:81:TYR:CD2	2.52	0.43
62:Su:30:TRP:CE2	62:Su:48:LEU:HD13	2.53	0.43
65:Sx:45:ARG:HH12	65:Sx:85:GLU:HB3	1.84	0.43
84:LQ:37:LEU:HD21	84:LQ:47:ARG:HD3	2.00	0.43
1:L1:964:A:H2'	1:L1:2093:A:N1	2.33	0.43
1:L1:1245:C:H2'	1:L1:1246:G:C8	2.53	0.43
1:L1:2485:U:H2'	1:L1:2486:G:H8	1.83	0.43
1:L1:2504:C:OP1	14:Lo:47:ARG:NH2	2.47	0.43
1:L1:2521:G:H5'	1:L1:2640:G:H1'	2.00	0.43
1:L1:4129:G:OP1	16:Lq:55:ALA:N	2.50	0.43
1:L1:4458:C:H2'	1:L1:4459:U:C6	2.53	0.43
2:Lc:192:GLY:O	2:Lc:195:LYS:NZ	2.41	0.43
2:Lc:209:ILE:HB	2:Lc:229:LEU:HD23	1.99	0.43
7:Lh:69:LYS:O	7:Lh:75:ARG:NH1	2.51	0.43
30:S1:751:G:C2	30:S1:752:G:C5	3.06	0.43
77:LI:241:ASN:O	77:LI:245:ARG:HG2	2.19	0.43
78:LJ:113:ARG:HH21	78:LJ:114:LEU:HD21	1.82	0.43
1:L1:1699:A:H3'	1:L1:1699:A:N3	2.33	0.43
1:L1:2579:G:N2	1:L1:2582:A:OP2	2.42	0.43
1:L1:2770:C:H2'	1:L1:2771:G:H8	1.83	0.43
1:L1:2809:G:O2'	1:L1:4644:G:OP1	2.34	0.43
1:L1:3732:A:H2'	1:L1:3733:A:C8	2.53	0.43
1:L1:3784:A:O2'	1:L1:3785:A2M:H3'	2.18	0.43
1:L1:3856:A:H5''	6:Lg:83:TRP:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:5031:G:H2'	1:L1:5032:C:C6	2.52	0.43
10:Lk:118:GLU:O	10:Lk:121:GLU:HG2	2.18	0.43
28:Nd:175:VAL:O	28:Nd:212:GLU:N	2.31	0.43
29:Nm:307:PRO:HD2	29:Nm:314:ALA:HB2	1.99	0.43
1:L1:1080:C:H2'	1:L1:1081:C:C6	2.53	0.43
1:L1:1700:G:H8	1:L1:1703:C:H42	1.67	0.43
1:L1:2045:G:O2'	1:L1:2046:G:H5''	2.19	0.43
1:L1:2088:A:OP1	7:Lh:38:ARG:NH1	2.52	0.43
1:L1:3599:A:H2'	1:L1:3600:G:C8	2.54	0.43
6:Lg:94:MET:HE3	6:Lg:94:MET:HB2	1.94	0.43
10:Lk:41:ASP:OD1	10:Lk:61:THR:OG1	2.23	0.43
12:Lm:75:LYS:HE3	12:Lm:77:HIS:CE1	2.53	0.43
26:Na:74:LYS:HG2	26:Na:78:LYS:HE3	2.00	0.43
27:Nb:73:HIS:HB3	27:Nb:95:GLU:HB2	1.99	0.43
29:Nm:11:THR:HA	29:Nm:44:SER:OG	2.18	0.43
30:S1:4:C:H4'	63:Sv:207:ALA:HB2	1.98	0.43
30:S1:60:A:N6	30:S1:61:A:N1	2.67	0.43
30:S1:520:A:H2'	30:S1:521:A:C8	2.53	0.43
30:S1:551:U:H2'	30:S1:552:G:H8	1.84	0.43
30:S1:615:C:O2'	55:Sn:82:ARG:NE	2.47	0.43
42:Sb:18:GLU:HG3	42:Sb:69:ILE:HD12	2.01	0.43
43:Sc:97:GLN:HB2	43:Sc:105:LYS:HD2	2.01	0.43
60:Ss:40:ILE:HG12	60:Ss:66:VAL:HG11	2.00	0.43
60:Ss:78:ALA:HB3	60:Ss:90:TRP:HB2	2.00	0.43
76:LH:163:GLY:O	76:LH:172:ARG:NH1	2.40	0.43
80:LM:92:HIS:HB2	80:LM:94:PHE:CE2	2.53	0.43
1:L1:413:G:N2	71:LC:36:ARG:HD2	2.34	0.43
1:L1:1177:U:H2'	1:L1:1178:G:C8	2.53	0.43
1:L1:1259:G:H2'	1:L1:1260:G:C8	2.53	0.43
1:L1:1298:C:H2'	1:L1:1299:G:H8	1.83	0.43
1:L1:1948:G:O3'	79:LK:65:LYS:NZ	2.52	0.43
1:L1:2562:G:H1'	1:L1:2566:G:C2	2.54	0.43
1:L1:4620:OMU:OP1	12:Lm:51:ARG:NH1	2.51	0.43
6:Lg:54:GLN:HA	6:Lg:83:TRP:CD1	2.53	0.43
10:Lk:121:GLU:HG3	10:Lk:122:LYS:HG3	2.00	0.43
22:Lw:71:TRP:HB2	22:Lw:89:ARG:HE	1.83	0.43
29:Nm:180:TYR:O	29:Nm:224:TYR:N	2.52	0.43
30:S1:213:G:C6	30:S1:214:U:C4	3.07	0.43
30:S1:659:G:N2	47:Sg:17:ARG:HH12	2.17	0.43
30:S1:755:C:H2'	30:S1:756:C:O4'	2.18	0.43
30:S1:1862:G:H4'	30:S1:1863:A:OP1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:SA:132:GLU:O	33:SA:135:GLU:HG2	2.18	0.43
37:SE:16:PHE:CD1	37:SE:79:LEU:HD22	2.53	0.43
38:SF:19:ARG:HH21	67:Sz:138:GLU:CD	2.26	0.43
39:SG:46:ASP:OD2	39:SG:48:SER:OG	2.31	0.43
41:Sa:64:LYS:HA	41:Sa:73:PRO:HB3	2.01	0.43
43:Sc:51:LEU:HD11	43:Sc:84:ILE:HB	2.00	0.43
43:Sc:58:LEU:HB2	43:Sc:63:PHE:HE1	1.83	0.43
57:Sp:36:LEU:HD23	65:Sx:16:ILE:HD11	2.01	0.43
60:Ss:268:ASP:OD1	60:Ss:269:GLU:N	2.52	0.43
64:Sw:206:ASP:N	64:Sw:206:ASP:OD1	2.49	0.43
65:Sx:158:ILE:HG22	65:Sx:164:VAL:HG22	2.00	0.43
73:LE:74:GLU:HG3	73:LE:76:ASN:H	1.84	0.43
1:L1:1194:G:H2'	1:L1:1195:G:C8	2.52	0.43
1:L1:1218:G:H2'	1:L1:1219:G:C8	2.54	0.43
1:L1:1365:C:H41	2:Lc:234:LYS:HD3	1.83	0.43
1:L1:4934:A:H2'	1:L1:4935:C:C6	2.53	0.43
16:Lq:10:VAL:HG11	16:Lq:129:TRP:HZ3	1.82	0.43
27:Nb:146:VAL:HG11	29:Nm:42:LYS:HG2	2.00	0.43
30:S1:639:C:H2'	30:S1:640:A:C8	2.54	0.43
30:S1:1736:G:H2'	30:S1:1737:G:C8	2.54	0.43
52:Sk:34:ASP:OD1	52:Sk:82:LYS:HD2	2.19	0.43
68:L3:88:A:H2'	68:L3:89:U:O4'	2.19	0.43
77:LI:182:TYR:CZ	77:LI:203:GLU:HG2	2.54	0.43
1:L1:683:C:H2'	1:L1:684:G:O4'	2.18	0.43
1:L1:1273:G:OP2	18:Ls:117:ARG:NH1	2.44	0.43
1:L1:1530:G:O6	1:L1:1643:A:N6	2.52	0.43
1:L1:3723:A:H2'	1:L1:3724:A2M:H8	2.01	0.43
3:Ld:157:ASN:OD1	3:Ld:158:LYS:N	2.52	0.43
4:Le:161:ARG:HD3	4:Le:270:TYR:CE2	2.54	0.43
7:Lh:18:PRO:HG2	7:Lh:29:VAL:HG21	2.00	0.43
16:Lq:76:ASN:OD1	16:Lq:77:TYR:N	2.50	0.43
17:Lr:36:GLY:HA3	17:Lr:40:HIS:CE1	2.53	0.43
19:Lt:65:MET:HE3	19:Lt:65:MET:HB3	1.95	0.43
26:Na:76:ALA:HA	27:Nb:51:LEU:HD22	2.00	0.43
28:Nd:200:SER:HB3	28:Nd:209:CYS:HB2	2.00	0.43
29:Nm:259:ALA:O	29:Nm:263:VAL:HG23	2.19	0.43
30:S1:1041:G:H2'	30:S1:1042:A:H8	1.83	0.43
44:Sd:48:ALA:HB2	44:Sd:70:ILE:HD12	2.01	0.43
64:Sw:258:ALA:O	64:Sw:262:SER:N	2.41	0.43
71:LC:15:LYS:HE2	71:LC:19:GLN:HE21	1.84	0.43
1:L1:62:A:N3	1:L1:77:U:O2'	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1625:OMG:HM23	76:LH:81:TYR:HE1	1.84	0.43
1:L1:2324:C:O2'	21:Lv:98:GLU:OE1	2.34	0.43
8:Li:176:ARG:NH2	30:S1:909:G:OP1	2.39	0.43
27:Nb:95:GLU:HB3	27:Nb:97:LYS:HE3	1.99	0.43
28:Nd:169:LYS:NZ	28:Nd:223:SER:OG	2.52	0.43
30:S1:616:A:H1'	55:Sn:86:VAL:HG23	2.01	0.43
32:S3:61:C:H2'	32:S3:62:U:H6	1.83	0.43
41:Sa:81:ARG:NH2	41:Sa:117:GLY:O	2.52	0.43
70:LB:49:ASP:HB2	70:LB:52:LYS:HD3	2.00	0.43
75:LG:39:ARG:NH1	75:LG:105:ASP:OD2	2.51	0.43
76:LH:138:PHE:HA	76:LH:143:ARG:HD2	2.00	0.43
77:LI:36:LYS:HD3	77:LI:36:LYS:HA	1.85	0.43
1:L1:648:G:H2'	1:L1:649:A:C8	2.53	0.43
1:L1:4291:G:H5'	1:L1:4293:PSU:C6	2.54	0.43
2:Lc:67:TRP:HE3	2:Lc:73:VAL:HG21	1.84	0.43
2:Lc:108:TRP:O	76:LH:204:ARG:NH2	2.52	0.43
3:Ld:209:ARG:HA	3:Ld:212:MET:HG2	2.00	0.43
15:Lp:73:VAL:HG13	15:Lp:80:ILE:HG22	2.00	0.43
17:Lr:123:ILE:HD11	83:LP:169:ILE:HG12	2.01	0.43
26:Na:190:VAL:HG11	26:Na:213:LEU:HD22	2.00	0.43
29:Nm:117:GLU:HA	29:Nm:120:GLN:HB2	2.01	0.43
30:S1:536:A:N6	30:S1:546:G:O6	2.52	0.43
30:S1:696:G:H1	30:S1:734:C:H42	1.67	0.43
30:S1:1109:C:N3	42:Sb:126:MET:HG2	2.33	0.43
30:S1:1279:C:H2'	30:S1:1280:G:C8	2.54	0.43
30:S1:1841:C:H2'	30:S1:1842:4AC:H6	2.00	0.43
53:Sl:18:HIS:NE2	53:Sl:94:PRO:HA	2.33	0.43
63:Sv:236:PHE:O	63:Sv:240:THR:HG22	2.19	0.43
73:LE:51:GLN:HE21	73:LE:53:LYS:H	1.66	0.43
81:LN:380:LYS:HD3	81:LN:380:LYS:HA	1.86	0.43
82:LO:153:ALA:HA	82:LO:156:ARG:HE	1.84	0.43
1:L1:2480:G:H2'	1:L1:2481:G:C8	2.54	0.42
1:L1:4165:C:OP1	78:LJ:245:LYS:NZ	2.51	0.42
1:L1:4582:C:OP2	86:Lb:28:LYS:NZ	2.43	0.42
1:L1:4731:G:H1'	1:L1:4732:G:C8	2.54	0.42
21:Lv:124:ASN:N	21:Lv:124:ASN:OD1	2.52	0.42
22:Lw:16:ARG:NH2	22:Lw:18:LEU:O	2.51	0.42
28:Nd:199:PRO:O	28:Nd:207:GLU:HG2	2.19	0.42
29:Nm:302:THR:OG1	29:Nm:303:ALA:N	2.52	0.42
30:S1:1041:G:H2'	30:S1:1042:A:C8	2.54	0.42
33:SA:80:ASP:OD1	33:SA:94:LYS:HE3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:L2:110:G:H2'	48:L2:111:C:C6	2.53	0.42
49:Sh:77:ASP:HB2	49:Sh:81:TYR:HD2	1.84	0.42
50:Si:31:PRO:HG3	50:Si:102:ARG:HD2	2.01	0.42
53:Sl:28:ASN:ND2	53:Sl:31:SER:H	2.17	0.42
69:LA:39:TYR:CG	69:LA:40:PRO:HA	2.54	0.42
80:LM:63:GLU:OE1	80:LM:63:GLU:N	2.40	0.42
80:LM:99:ILE:HG22	80:LM:123:GLN:HB2	2.02	0.42
83:LP:87:HIS:HB3	83:LP:90:VAL:HG23	2.01	0.42
85:La:14:SER:OG	85:La:15:VAL:N	2.53	0.42
1:L1:153:G:OP1	76:LH:56:LYS:NZ	2.50	0.42
1:L1:717:U:H2'	1:L1:718:C:C6	2.54	0.42
1:L1:1399:G:H2'	1:L1:1400:G:C8	2.55	0.42
1:L1:2538:U:H2'	1:L1:2539:C:C6	2.54	0.42
1:L1:2557:G:H1	1:L1:2570:U:H3	1.67	0.42
1:L1:4584:A:OP1	5:Lf:149:TYR:OH	2.33	0.42
1:L1:4653:C:OP1	20:Lu:79:ASN:ND2	2.53	0.42
1:L1:4955:A:H2'	1:L1:4956:A:H8	1.83	0.42
1:L1:4959:U:H2'	1:L1:4960:G:H8	1.84	0.42
11:Ll:99:TRP:CZ3	27:Nb:11:LEU:HB3	2.54	0.42
12:Lm:55:ALA:HB1	12:Lm:59:ASP:HB2	2.00	0.42
12:Lm:71:GLU:OE1	12:Lm:71:GLU:N	2.45	0.42
15:Lp:27:ARG:HB2	15:Lp:75:ARG:CZ	2.50	0.42
30:S1:912:C:H3'	30:S1:913:A:H5''	2.02	0.42
30:S1:1522:A:N6	41:Sa:131:PRO:HG3	2.34	0.42
35:SC:34:SER:HA	56:So:55:VAL:HB	2.00	0.42
60:Ss:212:LYS:HA	60:Ss:235:ILE:HG23	2.01	0.42
62:Su:168:MET:HG2	62:Su:197:ILE:HD13	1.99	0.42
63:Sv:102:LEU:HD22	63:Sv:130:ILE:HG12	2.01	0.42
66:Sy:50:VAL:HG12	66:Sy:113:ILE:HG12	2.00	0.42
1:L1:18:C:H4'	76:LH:138:PHE:CE2	2.55	0.42
1:L1:307:A:OP1	25:Lz:86:LYS:NZ	2.52	0.42
1:L1:478:G:H2'	1:L1:479:G:C8	2.55	0.42
1:L1:956:A:N6	1:L1:1283:G:H1'	2.35	0.42
1:L1:4447:5MC:H6	1:L1:4447:5MC:H2'	1.67	0.42
10:Lk:146:LYS:HE3	10:Lk:146:LYS:HB2	1.84	0.42
27:Nb:44:LEU:O	27:Nb:47:SER:OG	2.28	0.42
30:S1:190:G:OP1	33:SA:149:TYR:OH	2.23	0.42
30:S1:809:A:H2'	30:S1:810:A:O4'	2.19	0.42
42:Sb:87:GLU:CD	42:Sb:87:GLU:H	2.26	0.42
53:Sl:55:ARG:HG2	53:Sl:87:ARG:HD2	2.00	0.42
56:So:13:ARG:HE	56:So:53:GLY:HA2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Su:31:TYR:CD2	62:Su:94:LYS:HA	2.54	0.42
67:Sz:116:ARG:NH2	67:Sz:121:THR:HG23	2.34	0.42
77:LI:62:ARG:HG3	77:LI:66:ARG:HE	1.84	0.42
81:LN:402:GLN:HE21	81:LN:404:ALA:HB2	1.84	0.42
1:L1:257:C:H2'	1:L1:258:G:C8	2.54	0.42
1:L1:461:G:H2'	1:L1:462:G:C8	2.54	0.42
1:L1:676:C:H2'	1:L1:677:G:H8	1.84	0.42
1:L1:967:C:H2'	1:L1:2092:G:H1	1.83	0.42
1:L1:1098:G:H2'	1:L1:1099:C:C6	2.55	0.42
1:L1:1170:G:H2'	1:L1:1171:G:H8	1.83	0.42
1:L1:2495:U:H2'	1:L1:2496:G:C8	2.54	0.42
1:L1:2815:A2M:P	1:L1:2815:A2M:H8	2.59	0.42
1:L1:4071:U:H2'	1:L1:4072:C:C6	2.54	0.42
7:Lh:50:ARG:HH12	7:Lh:140:SER:HB2	1.84	0.42
7:Lh:151:HIS:ND1	7:Lh:164:LYS:O	2.39	0.42
30:S1:195:C:H2'	30:S1:196:C:H6	1.83	0.42
30:S1:882:U:H2'	30:S1:883:U:H6	1.84	0.42
30:S1:893:U:H2'	30:S1:894:G:H8	1.85	0.42
30:S1:1016:U:H5'	38:SF:15:ALA:O	2.19	0.42
30:S1:1337:4AC:N3	30:S1:1490:OMG:N1	2.50	0.42
35:SC:165:ASN:OD1	35:SC:166:ILE:N	2.52	0.42
41:Sa:15:PHE:CE2	41:Sa:112:ILE:HD12	2.54	0.42
49:Sh:11:LYS:HD2	49:Sh:24:VAL:HG21	2.00	0.42
63:Sv:94:ILE:HG13	63:Sv:159:LYS:O	2.19	0.42
1:L1:1259:G:H2'	1:L1:1260:G:H8	1.84	0.42
1:L1:2258:C:O2	4:Le:91:THR:N	2.51	0.42
1:L1:3899:OMG:HM22	1:L1:3900:G:H5'	2.01	0.42
1:L1:4218:U:OP2	10:Lk:9:ARG:NH2	2.53	0.42
1:L1:4734:A:H2'	1:L1:4735:G:C8	2.55	0.42
1:L1:4761:G:H2'	1:L1:4762:A:C8	2.55	0.42
27:Nb:54:ASN:O	27:Nb:81:ALA:N	2.42	0.42
29:Nm:170:VAL:HG11	29:Nm:193:CYS:HB3	2.01	0.42
30:S1:695:C:N4	30:S1:696:G:O6	2.52	0.42
30:S1:830:A:OP2	30:S1:846:G:N2	2.53	0.42
33:SA:178:ARG:CZ	33:SA:181:GLN:HG3	2.49	0.42
34:SB:21:GLU:HB3	34:SB:24:ARG:NH1	2.35	0.42
41:Sa:15:PHE:HE2	41:Sa:112:ILE:HD12	1.85	0.42
60:Ss:190:GLY:HA3	60:Ss:217:MET:HE1	2.01	0.42
77:LI:162:ILE:HD11	77:LI:174:LEU:HB3	2.01	0.42
86:Lb:217:ILE:HD11	86:Lb:333:LEU:HD21	2.02	0.42
1:L1:123:C:H2'	1:L1:124:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:174:C:H2'	1:L1:175:C:C6	2.53	0.42
1:L1:2859:G:N2	1:L1:3837:C:O2	2.39	0.42
1:L1:4685:U:H2'	1:L1:4686:G:C8	2.54	0.42
22:Lw:36:ARG:NH1	22:Lw:79:GLY:O	2.43	0.42
30:S1:399:C:H3'	30:S1:400:C:H5'	2.00	0.42
30:S1:934:G:H22	30:S1:1008:A:H2	1.68	0.42
30:S1:1464:C:O3'	42:Sb:60:ARG:NH1	2.52	0.42
32:S3:28:C:H2'	32:S3:29:A:H8	1.85	0.42
48:L2:77:A:H62	48:L2:99:G:H21	1.68	0.42
52:Sk:37:CYS:SG	52:Sk:40:CYS:HB3	2.59	0.42
60:Ss:74:ASP:OD1	60:Ss:74:ASP:N	2.52	0.42
64:Sw:45:ILE:N	64:Sw:80:ILE:O	2.52	0.42
68:L3:77:A:H2'	68:L3:78:G:O4'	2.20	0.42
80:LM:61:SER:HA	80:LM:126:VAL:HG12	2.02	0.42
1:L1:173:C:H2'	1:L1:174:C:C6	2.55	0.42
1:L1:711:A:H2'	1:L1:712:C:C6	2.54	0.42
1:L1:2529:A:O2'	1:L1:2531:C:OP2	2.38	0.42
1:L1:2634:C:H2'	1:L1:2635:U:H6	1.83	0.42
1:L1:2890:C:H42	1:L1:3611:A:H61	1.67	0.42
1:L1:3782:5MC:P	58:Sq:23:ARG:HH22	2.43	0.42
1:L1:4150:G:H2'	1:L1:4151:G:H8	1.85	0.42
1:L1:4719:G:O2'	1:L1:4720:C:H5''	2.19	0.42
1:L1:4761:G:N2	1:L1:4766:C:O3'	2.52	0.42
3:Ld:33:ARG:NH1	48:L2:7:G:O5'	2.52	0.42
28:Nd:163:ALA:O	28:Nd:168:MET:N	2.53	0.42
29:Nm:64:VAL:HA	29:Nm:67:TRP:CZ3	2.55	0.42
29:Nm:119:GLU:OE2	29:Nm:300:PHE:N	2.52	0.42
30:S1:562:U:O4	34:SB:172:ARG:NH1	2.53	0.42
30:S1:1402:A:H5'	53:Sl:51:LYS:NZ	2.33	0.42
30:S1:1787:G:H2'	30:S1:1788:A:C8	2.54	0.42
35:SC:78:MET:O	35:SC:159:ARG:NH1	2.53	0.42
53:Sl:64:THR:HG22	53:Sl:77:TRP:HE3	1.84	0.42
86:Lb:107:ALA:HB2	86:Lb:201:LEU:HD22	2.01	0.42
1:L1:278:G:H5''	76:LH:8:GLN:NE2	2.35	0.42
1:L1:455:C:N3	1:L1:456:C:N4	2.68	0.42
1:L1:1487:G:H2'	1:L1:1488:G:H8	1.85	0.42
1:L1:4619:U:H2'	1:L1:4620:OMU:H6	2.01	0.42
2:Lc:284:MET:HE2	2:Lc:287:THR:HA	2.01	0.42
3:Ld:267:ASN:ND2	48:L2:59:G:O2'	2.49	0.42
14:Lo:147:LEU:HD12	14:Lo:147:LEU:HA	1.88	0.42
15:Lp:50:ARG:NH2	68:L3:82:A:N1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Nd:223:SER:HB2	28:Nd:225:HIS:CE1	2.54	0.42
29:Nm:360:THR:HG22	29:Nm:371:LEU:HD12	2.02	0.42
38:SF:64:ARG:HD3	38:SF:70:LYS:HG3	2.01	0.42
42:Sb:20:TYR:CE1	65:Sx:213:PRO:HB3	2.54	0.42
43:Sc:44:PRO:HD2	43:Sc:81:ILE:HD11	2.02	0.42
49:Sh:111:LYS:HB3	49:Sh:111:LYS:HE2	1.87	0.42
62:Su:71:LEU:HD22	62:Su:84:PHE:HE1	1.84	0.42
63:Sv:82:TYR:OH	63:Sv:162:ILE:O	2.28	0.42
79:LK:115:ARG:HG2	79:LK:123:ILE:HG12	2.02	0.42
1:L1:141:C:H2'	1:L1:142:G:C8	2.54	0.42
1:L1:988:C:N4	1:L1:1064:G:O6	2.52	0.42
1:L1:1437:C:H2'	1:L1:1438:U:O4'	2.19	0.42
12:Lm:40:ILE:HG12	12:Lm:62:MET:O	2.20	0.42
12:Lm:112:MET:HE1	12:Lm:117:ILE:HG12	2.01	0.42
15:Lp:124:LYS:HE2	15:Lp:124:LYS:HB3	1.82	0.42
28:Nd:30:ASP:O	28:Nd:34:ARG:HG3	2.20	0.42
30:S1:327:G:H8	30:S1:327:G:OP2	2.03	0.42
30:S1:837:A:N1	49:Sh:8:ARG:HA	2.35	0.42
30:S1:884:C:H2'	30:S1:885:U:C6	2.55	0.42
30:S1:1447:OMG:HM22	30:S1:1448:A:O4'	2.20	0.42
30:S1:1677:U:H2'	30:S1:1678:A2M:C8	2.49	0.42
30:S1:1754:G:C6	30:S1:1779:G:C6	3.08	0.42
38:SF:114:ARG:HD3	38:SF:114:ARG:HA	1.89	0.42
41:Sa:110:GLU:HB2	44:Sd:117:ILE:HD13	2.02	0.42
48:L2:28:C:O2'	48:L2:54:A:N1	2.53	0.42
53:Sl:61:LEU:HB2	53:Sl:82:MET:HB3	2.00	0.42
63:Sv:173:LYS:HB2	63:Sv:173:LYS:HE3	1.86	0.42
1:L1:1178:G:O2'	3:Ld:286:SER:OG	2.29	0.42
1:L1:1179:U:C2	3:Ld:290:ALA:HB2	2.54	0.42
1:L1:3761:C:H2'	1:L1:3762:U:O4'	2.20	0.42
1:L1:4389:C:H2'	1:L1:4390:A:C8	2.54	0.42
1:L1:4448:G:H5''	1:L1:4449:A:H5''	2.02	0.42
1:L1:4536:OMC:HM22	1:L1:4537:C:H5'	2.02	0.42
13:Ln:73:ARG:HH22	30:S1:1779:G:H5''	1.84	0.42
14:Lo:141:ALA:HB3	14:Lo:144:TYR:HD1	1.85	0.42
18:Ls:96:LEU:HD21	77:Li:48:LYS:HE3	2.02	0.42
28:Nd:58:GLU:OE2	28:Nd:112:TRP:NE1	2.53	0.42
28:Nd:142:LEU:HD13	88:Nd:301:COA:H132	2.00	0.42
29:Nm:49:LYS:HA	29:Nm:52:HIS:HD1	1.85	0.42
29:Nm:72:ASP:O	29:Nm:208:ARG:NH2	2.53	0.42
29:Nm:107:ASP:OD1	29:Nm:108:TYR:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Nm:197:VAL:HG13	29:Nm:217:VAL:HG22	2.02	0.42
30:S1:5:U:H2'	30:S1:6:G:H8	1.84	0.42
30:S1:1453:C:H4'	42:Sb:49:LYS:HA	2.00	0.42
34:SB:136:ARG:HD3	34:SB:160:SER:HA	2.02	0.42
41:Sa:34:MET:HE2	41:Sa:45:LEU:HB3	2.02	0.42
59:Sr:106:TYR:HE1	59:Sr:116:ARG:HG3	1.84	0.42
77:LI:88:LYS:HE3	77:LI:88:LYS:HB2	1.89	0.42
1:L1:687:U:H2'	4:Le:96:VAL:HG12	2.02	0.41
1:L1:1865:G:N2	1:L1:1868:A:OP2	2.51	0.41
1:L1:2101:C:H2'	1:L1:2102:G:H8	1.84	0.41
1:L1:2712:G:C6	1:L1:2713:C:C4	3.08	0.41
1:L1:2878:G:H4'	1:L1:3825:A2M:H5''	2.02	0.41
1:L1:4622:A:H4'	86:Lb:13:SER:HB2	2.01	0.41
1:L1:4727:A:H2'	1:L1:4728:U:O4'	2.19	0.41
1:L1:4957:C:H2'	1:L1:4958:C:H6	1.83	0.41
3:Ld:53:VAL:O	3:Ld:54:ARG:NH1	2.43	0.41
4:Le:206:VAL:HG11	4:Le:257:ILE:HD11	2.02	0.41
12:Lm:97:TYR:OH	13:Ln:37:GLU:OE2	2.23	0.41
23:Lx:69:LYS:HG2	23:Lx:73:HIS:CD2	2.55	0.41
30:S1:124:U:H3	30:S1:340:C:H42	1.68	0.41
30:S1:158:A:H2'	30:S1:159:A2M:O4'	2.20	0.41
40:SH:86:GLY:O	40:SH:89:VAL:HG12	2.20	0.41
53:Sl:20:ILE:HD12	53:Sl:98:VAL:HG21	2.02	0.41
60:Ss:127:LYS:HG2	60:Ss:149:GLU:C	2.44	0.41
61:St:60:LEU:HG	61:St:159:ILE:HD13	2.02	0.41
1:L1:1284:G:O2'	1:L1:1285:U:H5''	2.20	0.41
1:L1:5031:G:H2'	1:L1:5032:C:H6	1.85	0.41
6:Lg:131:ARG:HG3	6:Lg:137:ASN:OD1	2.20	0.41
7:Lh:178:ARG:H	17:Lr:51:GLY:HA2	1.85	0.41
16:Lq:25:ILE:HG12	16:Lq:43:VAL:HG12	2.03	0.41
28:Nd:130:CYS:HB3	28:Nd:231:HIS:NE2	2.35	0.41
28:Nd:199:PRO:HA	28:Nd:235:CYS:HA	2.03	0.41
30:S1:14:C:O2	30:S1:668:A2M:H2	2.20	0.41
30:S1:1365:G:H2'	30:S1:1366:G:C8	2.55	0.41
32:S3:2:C:H2'	32:S3:3:C:C6	2.55	0.41
46:Sf:3:ARG:HD3	46:Sf:6:VAL:HG22	2.02	0.41
49:Sh:77:ASP:OD1	49:Sh:77:ASP:N	2.52	0.41
58:Sq:7:LYS:HE2	58:Sq:11:ARG:HH21	1.84	0.41
60:Ss:89:LEU:HB3	60:Ss:99:ARG:HB3	2.02	0.41
61:St:122:LEU:O	61:St:145:ILE:N	2.53	0.41
64:Sw:46:ILE:HG23	64:Sw:50:ASN:HD22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Sx:135:GLU:HB3	65:Sx:187:LYS:HB2	2.02	0.41
77:LI:171:ASP:OD1	77:LI:172:ASN:N	2.54	0.41
78:LJ:111:LYS:HE2	78:LJ:111:LYS:HB3	1.83	0.41
1:L1:308:G:O6	76:LH:12:ARG:NH1	2.53	0.41
1:L1:413:G:C2	71:LC:36:ARG:HD2	2.55	0.41
1:L1:486:C:O2'	1:L1:487:G:O5'	2.37	0.41
1:L1:1076:C:H2'	1:L1:1077:C:C6	2.55	0.41
1:L1:1809:C:H2'	1:L1:1810:G:C8	2.53	0.41
1:L1:3654:G:O2'	1:L1:3693:U:OP1	2.33	0.41
1:L1:4886:C:H2'	1:L1:4887:C:H6	1.86	0.41
4:Le:208:ILE:HG23	4:Le:212:LEU:HD12	2.02	0.41
8:Li:171:LYS:O	8:Li:175:GLU:HG2	2.20	0.41
13:Ln:83:THR:HA	66:Sy:131:ARG:HB2	2.02	0.41
22:Lw:15:LYS:HB3	22:Lw:25:THR:HB	2.03	0.41
23:Lx:44:SER:OG	23:Lx:46:CYS:SG	2.70	0.41
28:Nd:126:PHE:HE1	28:Nd:135:LEU:HD12	1.85	0.41
30:S1:354:OMU:HM22	30:S1:355:G:O4'	2.19	0.41
30:S1:1259:A:O2'	30:S1:1261:C:OP2	2.28	0.41
30:S1:1418:C:N4	30:S1:1421:A:O2'	2.53	0.41
30:S1:1597:C:H4'	30:S1:1603:G:O6	2.21	0.41
44:Sd:12:ILE:HD13	44:Sd:21:ASP:HA	2.02	0.41
44:Sd:114:LEU:HD13	44:Sd:121:ARG:HD2	2.01	0.41
48:L2:19:C:H2'	48:L2:20:U:H6	1.84	0.41
81:LN:402:GLN:O	81:LN:406:LYS:HE2	2.21	0.41
82:LO:92:TYR:HB3	82:LO:172:GLY:HA2	2.03	0.41
1:L1:1520:C:O2'	2:Lc:94:ASN:OD1	2.37	0.41
2:Lc:138:MET:HE3	2:Lc:138:MET:HB3	1.99	0.41
9:Lj:151:LYS:HB2	84:LQ:8:GLU:HB3	2.01	0.41
16:Lq:60:LYS:HE2	16:Lq:60:LYS:HB2	1.94	0.41
30:S1:693:A:H2'	30:S1:694:G:C8	2.55	0.41
30:S1:1139:C:H4'	46:Sf:20:ARG:HH12	1.86	0.41
56:So:4:SER:OG	56:So:5:ARG:N	2.52	0.41
59:Sr:106:TYR:HB3	59:Sr:114:ILE:HG23	2.03	0.41
78:LJ:120:LYS:HB2	78:LJ:120:LYS:HE3	1.81	0.41
79:LK:14:GLU:H	79:LK:14:GLU:CD	2.28	0.41
1:L1:323:C:H2'	1:L1:324:A:C8	2.55	0.41
1:L1:963:G:H3'	1:L1:963:G:N3	2.35	0.41
1:L1:2562:G:H1'	1:L1:2566:G:N1	2.35	0.41
1:L1:2896:G:P	8:Li:136:ARG:HH21	2.43	0.41
3:Ld:263:LYS:NZ	89:L2:201:GTP:O1A	2.39	0.41
4:Le:190:HIS:CE1	4:Le:192:LYS:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Lf:181:ALA:O	5:Lf:185:VAL:HG22	2.21	0.41
15:Lp:86:GLN:HB2	15:Lp:94:THR:HG22	2.02	0.41
23:Lx:86:CYS:O	23:Lx:90:ARG:HG3	2.20	0.41
24:Ly:104:THR:HG23	76:LH:146:PRO:HB2	2.03	0.41
30:S1:416:U:H2'	30:S1:417:C:O4'	2.21	0.41
30:S1:588:G:OP2	30:S1:588:G:N2	2.35	0.41
30:S1:1232:PSU:H2'	30:S1:1233:G:C8	2.56	0.41
30:S1:1237:C:H5'	41:Sa:131:PRO:HA	2.01	0.41
30:S1:1298:G:C6	30:S1:1299:A:C6	3.08	0.41
30:S1:1305:C:OP2	59:Sr:93:HIS:ND1	2.54	0.41
30:S1:1787:G:H2'	30:S1:1788:A:H8	1.86	0.41
60:Ss:8:ARG:HA	60:Ss:8:ARG:HD2	1.95	0.41
80:LM:198:LYS:HE3	80:LM:198:LYS:HB2	1.87	0.41
1:L1:469:C:N3	4:Le:105:ARG:NH2	2.55	0.41
1:L1:733:A:H2'	1:L1:734:G:O4'	2.20	0.41
1:L1:1094:G:H2'	1:L1:1095:A:H8	1.86	0.41
1:L1:1476:C:H2'	1:L1:1477:C:C6	2.55	0.41
12:Lm:37:LEU:HB3	12:Lm:63:ALA:HB1	2.02	0.41
14:Lo:67:ARG:NH2	68:L3:134:G:OP2	2.51	0.41
29:Nm:382:PHE:CZ	29:Nm:383:MET:HG3	2.55	0.41
30:S1:701:G:N2	30:S1:730:C:N3	2.68	0.41
30:S1:898:U:H2'	30:S1:899:U:C6	2.55	0.41
30:S1:924:G:H5'	38:SF:4:MET:HE3	2.03	0.41
30:S1:1171:G:H22	30:S1:1188:A:P	2.43	0.41
41:Sa:51:ARG:HE	41:Sa:51:ARG:HB3	1.64	0.41
60:Ss:46:THR:OG1	60:Ss:51:ASN:O	2.38	0.41
66:Sy:234:LEU:HD23	66:Sy:237:LEU:HB2	2.03	0.41
77:LI:96:ARG:HD2	77:LI:139:TYR:HA	2.02	0.41
78:LJ:108:GLN:O	78:LJ:112:GLN:HG2	2.20	0.41
85:La:29:LEU:HA	85:La:76:PHE:CE1	2.56	0.41
1:L1:1174:G:N2	1:L1:1188:C:N3	2.69	0.41
1:L1:1440:U:H2'	1:L1:1441:C:H6	1.86	0.41
1:L1:2458:C:OP1	76:LH:67:ARG:HD3	2.20	0.41
1:L1:4084:G:O6	85:La:72:ARG:NH2	2.53	0.41
2:Lc:254:GLU:OE2	2:Lc:258:ARG:NH2	2.40	0.41
6:Lg:122:ALA:HB3	6:Lg:143:PRO:HG2	2.03	0.41
10:Lk:80:VAL:O	10:Lk:83:LYS:HG2	2.20	0.41
13:Ln:60:LYS:O	13:Ln:64:SER:OG	2.33	0.41
20:Lu:117:LEU:HD23	20:Lu:117:LEU:HA	1.89	0.41
22:Lw:36:ARG:HB2	22:Lw:80:ASN:HA	2.02	0.41
28:Nd:185:PHE:CD1	88:Nd:301:COA:H8A	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S1:234:C:H2'	30:S1:235:A:C8	2.56	0.41
30:S1:538:U:O2	30:S1:546:G:N2	2.54	0.41
30:S1:863:PSU:O3'	46:Sf:78:ARG:NH1	2.53	0.41
30:S1:1437:C:H5''	30:S1:1438:A:H5'	2.03	0.41
34:SB:33:GLY:HA3	55:Sn:112:TYR:CG	2.56	0.41
41:Sa:29:SER:O	41:Sa:33:LEU:HG	2.21	0.41
47:Sg:124:LYS:HG2	47:Sg:129:SER:HA	2.02	0.41
80:LM:38:ARG:HD3	80:LM:83:ASP:HB3	2.03	0.41
1:L1:225:G:OP1	2:Lc:222:ARG:NE	2.52	0.41
1:L1:1705:G:H5''	77:LI:46:ARG:HH12	1.84	0.41
1:L1:4067:U:H2'	1:L1:4068:U:C6	2.55	0.41
3:Ld:128:ASP:OD1	3:Ld:129:GLU:N	2.53	0.41
4:Le:101:ASN:OD1	4:Le:105:ARG:NH2	2.45	0.41
11:Ll:60:VAL:HG23	11:Ll:61:VAL:HG23	2.01	0.41
17:Lr:103:VAL:HG22	17:Lr:125:LYS:O	2.20	0.41
30:S1:753:C:H2'	30:S1:754:G:H8	1.86	0.41
30:S1:1154:U:OP2	63:Sv:187[B]:ARG:NH2	2.54	0.41
30:S1:1275:G:O4'	30:S1:1506:A:N6	2.53	0.41
30:S1:1782:G:N7	30:S1:1783:C:O2'	2.45	0.41
30:S1:1860:A:N7	51:Sj:34:LYS:NZ	2.68	0.41
50:Si:116:ASP:HA	50:Si:122:LYS:HE2	2.03	0.41
59:Sr:89:LYS:HG2	59:Sr:90:LYS:H	1.86	0.41
64:Sw:100:ARG:HG2	64:Sw:102:ILE:HG12	2.02	0.41
66:Sy:227:GLN:HA	66:Sy:230:LYS:HD2	2.02	0.41
1:L1:232:G:O6	15:Lp:61:HIS:N	2.45	0.41
1:L1:266:C:H2'	1:L1:267:G:H8	1.86	0.41
1:L1:447:C:H2'	1:L1:448:G:C8	2.55	0.41
1:L1:922:C:O2'	1:L1:923:C:H5'	2.21	0.41
1:L1:1326:A2M:HM'3	1:L1:1326:A2M:H1'	1.71	0.41
1:L1:1359:G:H4'	76:LH:203:TYR:HB2	2.02	0.41
1:L1:1909:G:H2'	1:L1:1910:G:O4'	2.20	0.41
1:L1:2319:C:OP2	21:Lv:62:SER:OG	2.29	0.41
1:L1:2459:G:N2	1:L1:2462:C:OP2	2.52	0.41
1:L1:2521:G:H2'	1:L1:2522:G:H8	1.86	0.41
1:L1:2674:A:N6	74:LF:42:CYS:HA	2.35	0.41
1:L1:3707:U:H2'	1:L1:3708:C:C6	2.55	0.41
1:L1:4417:C:N4	1:L1:4422:A:O2'	2.52	0.41
1:L1:4452:U:OP2	1:L1:4522:G:N1	2.31	0.41
1:L1:4524:G:C2	86:Lb:252:ALA:HB1	2.56	0.41
1:L1:4886:C:H2'	1:L1:4887:C:C6	2.56	0.41
2:Lc:94:ASN:HA	2:Lc:100:ARG:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Lj:49:SER:O	48:L2:75:G:H5''	2.21	0.41
12:Lm:128:LEU:HD12	12:Lm:128:LEU:HA	1.91	0.41
15:Lp:2:LYS:HD3	15:Lp:4:ASN:O	2.21	0.41
26:Na:133:GLN:HA	28:Nd:203:GLY:O	2.20	0.41
28:Nd:164:ASN:OD1	28:Nd:218:THR:HB	2.21	0.41
28:Nd:193:GLU:N	28:Nd:215:SER:O	2.52	0.41
29:Nm:307:PRO:HB3	29:Nm:309:TYR:CZ	2.56	0.41
30:S1:549:C:H2'	30:S1:550:C:C6	2.56	0.41
30:S1:736:C:H2'	30:S1:737:G:C8	2.56	0.41
30:S1:1138:C:OP1	61:St:155:ARG:NH1	2.46	0.41
30:S1:1328:OMG:OP1	59:Sr:78:LYS:NZ	2.44	0.41
30:S1:1560:U:H2'	30:S1:1561:A:H8	1.85	0.41
32:S3:9:A:O2'	32:S3:10:G:N7	2.51	0.41
42:Sb:71:ILE:HD12	42:Sb:72:LYS:N	2.36	0.41
46:Sf:42:MET:HE1	67:Sz:146:VAL:HG12	2.03	0.41
48:L2:4:U:H2'	48:L2:5:A:C8	2.56	0.41
59:Sr:104:LYS:O	59:Sr:118:ARG:NH2	2.51	0.41
60:Ss:199:THR:HG23	60:Ss:241:PHE:CE1	2.55	0.41
60:Ss:289:LEU:HG	60:Ss:298:LEU:HD11	2.03	0.41
61:St:130:ASP:O	61:St:133:PRO:HD2	2.21	0.41
64:Sw:138:HIS:CD2	64:Sw:148:ARG:HG2	2.56	0.41
66:Sy:59:GLN:OE1	66:Sy:59:GLN:N	2.54	0.41
67:Sz:31:GLU:O	67:Sz:41:ARG:NH2	2.54	0.41
68:L3:105:C:H4'	68:L3:106:G:H5''	2.02	0.41
74:LF:84:ARG:HE	74:LF:84:ARG:HB3	1.67	0.41
77:LI:154:ILE:HD12	77:LI:191:ILE:HG12	2.03	0.41
78:LJ:48:LYS:HD3	78:LJ:48:LYS:HA	1.89	0.41
78:LJ:70:LEU:HD23	78:LJ:70:LEU:HA	1.95	0.41
86:Lb:297:LYS:HD3	86:Lb:297:LYS:HA	1.93	0.41
1:L1:22:G:OP1	69:LA:44:LYS:N	2.50	0.41
1:L1:458:C:OP1	4:Le:114:ARG:HG2	2.21	0.41
1:L1:752:G:O6	1:L1:912:G:N2	2.54	0.41
1:L1:1689:G:OP1	7:Lh:11:ARG:NH2	2.53	0.41
1:L1:2622:G:OP2	11:Ll:84:LYS:NZ	2.49	0.41
1:L1:4122:G:N1	23:Lx:98:GLU:OE2	2.47	0.41
10:Lk:119:ALA:HB1	10:Lk:124:THR:O	2.21	0.41
12:Lm:85:ARG:NH1	12:Lm:99:GLU:O	2.44	0.41
30:S1:494:C:N4	30:S1:509:OMG:HN22	2.17	0.41
30:S1:1439:A:H2'	30:S1:1440:C:C6	2.56	0.41
30:S1:1520:G:H3'	30:S1:1521:C:H6	1.86	0.41
30:S1:1740:C:OP1	33:SA:44:HIS:ND1	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SD:57:ASP:HB2	36:SD:84:ARG:NH1	2.36	0.41
42:Sb:5:ARG:O	42:Sb:10:LYS:NZ	2.54	0.41
61:St:206:ASP:HB3	61:St:209:GLU:CD	2.46	0.41
69:LA:28:HIS:HE1	69:LA:30:GLN:HB2	1.85	0.41
1:L1:424:U:H2'	1:L1:425:U:C6	2.56	0.40
1:L1:1392:A:H2'	1:L1:1393:G:C8	2.55	0.40
1:L1:1701:A:H5'	2:Lc:304:ALA:HB3	2.03	0.40
1:L1:2685:C:H2'	1:L1:2686:G:O4'	2.20	0.40
1:L1:3607:U:H2'	1:L1:3608:A:C8	2.56	0.40
1:L1:3929:G:H2'	1:L1:3930:U:O4'	2.22	0.40
1:L1:4743:G:H2'	1:L1:4744:A:H8	1.86	0.40
1:L1:5030:U:H2'	1:L1:5031:G:C8	2.56	0.40
6:Lg:67:VAL:O	6:Lg:80:GLN:NE2	2.39	0.40
10:Lk:94:GLU:OE1	10:Lk:94:GLU:N	2.48	0.40
25:Lz:7:MET:HE3	25:Lz:7:MET:HB2	1.95	0.40
29:Nm:376:ASP:OD1	29:Nm:376:ASP:N	2.54	0.40
30:S1:240:G:H2'	30:S1:241:G:H8	1.85	0.40
30:S1:928:G:H1	30:S1:1013:U:H3	1.68	0.40
42:Sb:71:ILE:HD11	42:Sb:73:LEU:CG	2.38	0.40
46:Sf:57:ARG:HD2	52:Sk:26:GLN:NE2	2.36	0.40
49:Sh:15:ASN:ND2	64:Sw:54:TYR:O	2.54	0.40
49:Sh:38:THR:O	49:Sh:42:GLU:HG2	2.21	0.40
54:Sm:65:TYR:C	54:Sm:67:LEU:H	2.29	0.40
60:Ss:67:SER:N	60:Ss:81:GLY:O	2.53	0.40
63:Sv:178:HIS:HD2	63:Sv:200:ARG:NH2	2.19	0.40
68:L3:8:U:H2'	68:L3:9:A:C8	2.56	0.40
69:LA:52:LYS:HE3	69:LA:52:LYS:HB2	1.92	0.40
1:L1:231:U:H4'	15:Lp:100:HIS:CD2	2.57	0.40
1:L1:1670:G:OP1	18:Ls:12:GLN:NE2	2.54	0.40
1:L1:2096:G:N3	1:L1:2096:G:H2'	2.36	0.40
1:L1:4385:A:H4'	1:L1:4386:C:H5''	2.03	0.40
1:L1:4997:G:H2'	1:L1:4998:G:H8	1.87	0.40
2:Lc:35:ASP:OD1	2:Lc:35:ASP:N	2.55	0.40
2:Lc:230:LEU:HD11	2:Lc:239:LYS:HB2	2.03	0.40
2:Lc:327:LYS:HE2	2:Lc:327:LYS:HB3	1.86	0.40
3:Ld:235:MET:HE2	3:Ld:235:MET:HB2	2.01	0.40
4:Le:192:LYS:HD3	22:Lw:107:PRO:HB3	2.04	0.40
15:Lp:24:HIS:CE1	15:Lp:25:ILE:HG13	2.57	0.40
18:Ls:99:ILE:HG23	18:Ls:109:ARG:HG3	2.04	0.40
21:Lv:88:LEU:HB2	21:Lv:120:ILE:HD13	2.03	0.40
27:Nb:21:GLY:HA3	27:Nb:25:THR:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Nd:110:ILE:HG12	28:Nd:121:PHE:HB2	2.01	0.40
30:S1:28:U:H2'	30:S1:29:G:H8	1.86	0.40
30:S1:165:G:H4'	66:Sy:53:SER:HB3	2.03	0.40
30:S1:184:G:H2'	30:S1:185:G:O4'	2.21	0.40
30:S1:1058:A:OP1	32:S3:38:A:O2'	2.38	0.40
30:S1:1344:A:H4'	30:S1:1345:G:H5'	2.03	0.40
30:S1:1569:A:H5'	50:Si:41:LYS:HD3	2.04	0.40
30:S1:1763:G:H2'	30:S1:1764:G:C8	2.56	0.40
37:SE:49:MET:HE1	37:SE:58:VAL:HG11	2.03	0.40
50:Si:111:LYS:HD3	50:Si:111:LYS:HA	1.91	0.40
53:Sl:68:THR:OG1	53:Sl:70:CYS:O	2.39	0.40
58:Sq:7:LYS:HE2	58:Sq:11:ARG:NH2	2.37	0.40
64:Sw:108:ARG:HE	64:Sw:108:ARG:HB2	1.74	0.40
66:Sy:21:GLU:O	66:Sy:25:ARG:HG2	2.21	0.40
76:LH:113:LEU:HD22	76:LH:136:ASP:HA	2.03	0.40
78:LJ:180:PRO:HG3	78:LJ:223:ARG:CZ	2.51	0.40
1:L1:97:G:N7	83:LP:13:HIS:NE2	2.66	0.40
1:L1:1346:C:H2'	1:L1:1347:G:H8	1.86	0.40
1:L1:1929:A:C8	1:L1:1932:A:H1'	2.56	0.40
1:L1:2563:C:H3'	1:L1:2564:G:C8	2.57	0.40
1:L1:3870:C:H2'	1:L1:3871:A:C8	2.57	0.40
1:L1:4362:A:H2'	1:L1:4363:A:H8	1.86	0.40
2:Lc:204:ARG:HE	2:Lc:204:ARG:HB2	1.75	0.40
8:Li:145:LEU:HD23	8:Li:145:LEU:HA	1.90	0.40
10:Lk:71:ALA:HA	10:Lk:92:ARG:HA	2.03	0.40
13:Ln:77:LYS:H	30:S1:1778:C:P	2.44	0.40
13:Ln:77:LYS:N	30:S1:1778:C:OP1	2.54	0.40
21:Lv:26:ASP:OD1	21:Lv:26:ASP:N	2.42	0.40
28:Nd:154:PHE:HA	28:Nd:157:GLN:CD	2.47	0.40
29:Nm:336:GLN:HB3	29:Nm:349:ARG:HD3	2.03	0.40
30:S1:1426:U:P	43:Sc:69:ARG:HH21	2.44	0.40
30:S1:1451:G:OP1	42:Sb:32:LYS:NZ	2.41	0.40
30:S1:1622:U:OP1	44:Sd:120:HIS:ND1	2.44	0.40
32:S3:20:C:N4	82:LO:58:ARG:HG3	2.36	0.40
36:SD:135:SER:OG	36:SD:136:LYS:N	2.54	0.40
45:Se:37:ALA:O	61:St:63:ARG:HD3	2.21	0.40
63:Sv:232:THR:HG22	63:Sv:235:ASN:H	1.87	0.40
65:Sx:143:ARG:HA	65:Sx:143:ARG:HD2	1.85	0.40
74:LF:22:LEU:HB3	85:La:180:LEU:HD21	2.03	0.40
76:LH:98:LEU:HD12	76:LH:128:LYS:HD2	2.03	0.40
1:L1:1093:C:H2'	1:L1:1094:G:C8	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1217:G:H2'	1:L1:1218:G:H8	1.85	0.40
1:L1:4691:A:O2'	79:LK:68:ALA:O	2.32	0.40
2:Lc:25:PRO:HB2	2:Lc:27:VAL:HG12	2.04	0.40
21:Lv:92:ASN:OD1	21:Lv:92:ASN:N	2.54	0.40
27:Nb:95:GLU:HA	29:Nm:341:PRO:O	2.22	0.40
30:S1:981:A:H2'	30:S1:982:G:C8	2.57	0.40
30:S1:1221:G:H2'	30:S1:1222:G:H8	1.85	0.40
30:S1:1536:G:H2'	30:S1:1537:A:C8	2.56	0.40
34:SB:94:LEU:HD12	34:SB:94:LEU:HA	1.90	0.40
35:SC:99:ILE:HD11	54:Sm:106:GLN:HE21	1.85	0.40
35:SC:200:ALA:O	35:SC:204:ARG:HG3	2.21	0.40
43:Sc:34:VAL:HG22	43:Sc:70:VAL:HB	2.03	0.40
56:So:64:GLU:HG2	56:So:65:ALA:H	1.87	0.40
60:Ss:237:ASN:ND2	60:Ss:286:CYS:O	2.47	0.40
61:St:140:VAL:HG23	61:St:142:LEU:HB2	2.04	0.40
61:St:165:ASN:HA	61:St:171:VAL:HG22	2.02	0.40
64:Sw:20:LEU:HD21	64:Sw:46:ILE:HD12	2.03	0.40
67:Sz:180:LEU:HD23	67:Sz:180:LEU:HA	1.82	0.40
68:L3:14:U:O4	68:L3:15:G:N1	2.55	0.40
77:LI:144:TYR:CE2	77:LI:237:GLU:HA	2.56	0.40
80:LM:36:LEU:HD13	80:LM:69:ARG:HH11	1.87	0.40
1:L1:926:G:H2'	1:L1:927:G:C8	2.57	0.40
1:L1:2274:C:H2'	1:L1:2275:G:H8	1.86	0.40
1:L1:2504:C:P	14:Lo:47:ARG:HH22	2.44	0.40
1:L1:2890:C:H2'	1:L1:2891:U:C6	2.56	0.40
1:L1:4363:A:H5''	73:LE:36:GLN:HG2	2.03	0.40
1:L1:4730:C:H2'	1:L1:4732:G:H1'	2.03	0.40
3:Ld:28:THR:OG1	48:L2:7:G:OP2	2.40	0.40
15:Lp:37:GLU:H	15:Lp:37:GLU:CD	2.29	0.40
20:Lu:18:ASN:O	20:Lu:90:ARG:NH2	2.54	0.40
28:Nd:135:LEU:HD11	28:Nd:159:LEU:HD22	2.04	0.40
28:Nd:159:LEU:HA	28:Nd:162:MET:HB2	2.02	0.40
30:S1:870:A:H62	30:S1:915:G:H2'	1.86	0.40
30:S1:954:U:C4	30:S1:971:G:C2	3.10	0.40
30:S1:1320:G:H2'	30:S1:1321:G:O4'	2.22	0.40
32:S3:21:A:N6	32:S3:46:G:H2'	2.36	0.40
40:SH:13:ASP:OD1	40:SH:13:ASP:N	2.54	0.40
41:Sa:50:ARG:HB2	41:Sa:53:GLN:HE22	1.86	0.40
47:Sg:73:GLN:OE1	47:Sg:80:LYS:NZ	2.55	0.40
60:Ss:125:ARG:HG3	60:Ss:150:TRP:CD2	2.56	0.40
62:Su:90:ASP:OD1	62:Su:91:VAL:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sy:213:LEU:HD11	66:Sy:217:MET:HE2	2.03	0.40
67:Sz:69:LEU:O	67:Sz:73:GLN:HG2	2.22	0.40
74:LF:38:THR:HA	74:LF:45:THR:HA	2.04	0.40
76:LH:42:PRO:HG3	76:LH:61:ILE:HG13	2.03	0.40
76:LH:197:THR:HG23	83:LP:21:ARG:O	2.22	0.40
79:LK:94:SER:HB2	79:LK:142:ASP:HB3	2.03	0.40
80:LM:65:LEU:HD23	80:LM:159:PHE:HZ	1.87	0.40
81:LN:383:ILE:H	81:LN:383:ILE:HG12	1.62	0.40
85:La:36:GLU:OE1	85:La:163:ARG:NH1	2.52	0.40
86:Lb:45:ALA:HB3	86:Lb:183:ILE:HG23	2.03	0.40
86:Lb:292:LEU:O	86:Lb:298:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Lc	361/427 (84%)	351 (97%)	10 (3%)	0	100	100
3	Ld	290/297 (98%)	284 (98%)	6 (2%)	0	100	100
4	Le	212/288 (74%)	202 (95%)	10 (5%)	0	100	100
5	Lf	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
6	Lg	150/184 (82%)	147 (98%)	3 (2%)	0	100	100
7	Lh	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
8	Li	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
9	Lj	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
10	Lk	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
11	Ll	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
12	Lm	130/140 (93%)	127 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Ln	119/157 (76%)	115 (97%)	4 (3%)	0	100	100
14	Lo	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
15	Lp	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
16	Lq	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
17	Lr	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
18	Ls	95/159 (60%)	94 (99%)	1 (1%)	0	100	100
19	Lt	98/115 (85%)	98 (100%)	0	0	100	100
20	Lu	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
21	Lv	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
22	Lw	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
23	Lx	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
24	Ly	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
25	Lz	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
26	Na	104/238 (44%)	100 (96%)	4 (4%)	0	100	100
27	Nb	116/162 (72%)	115 (99%)	1 (1%)	0	100	100
28	Nd	234/365 (64%)	226 (97%)	8 (3%)	0	100	100
29	Nm	378/386 (98%)	369 (98%)	8 (2%)	1 (0%)	37	67
33	SA	203/208 (98%)	198 (98%)	5 (2%)	0	100	100
34	SB	178/194 (92%)	174 (98%)	4 (2%)	0	100	100
35	SC	190/204 (93%)	183 (96%)	7 (4%)	0	100	100
36	SD	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
37	SE	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
38	SF	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
39	SG	131/151 (87%)	127 (97%)	4 (3%)	0	100	100
40	SH	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
41	Sa	122/152 (80%)	117 (96%)	5 (4%)	0	100	100
42	Sb	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
43	Sc	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
44	Sd	144/152 (95%)	138 (96%)	6 (4%)	0	100	100
45	Se	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
46	Sf	127/130 (98%)	125 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Sg	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
49	Sh	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
50	Si	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
51	Sj	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
52	Sk	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
53	Sl	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
54	Sm	81/125 (65%)	78 (96%)	3 (4%)	0	100	100
55	Sn	57/133 (43%)	54 (95%)	3 (5%)	0	100	100
56	So	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
57	Sp	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
58	Sq	23/25 (92%)	23 (100%)	0	0	100	100
59	Sr	72/156 (46%)	65 (90%)	7 (10%)	0	100	100
60	Ss	312/317 (98%)	295 (95%)	17 (5%)	0	100	100
61	St	221/295 (75%)	216 (98%)	5 (2%)	0	100	100
62	Su	220/264 (83%)	215 (98%)	5 (2%)	0	100	100
63	Sv	222/293 (76%)	218 (98%)	4 (2%)	0	100	100
64	Sw	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
65	Sx	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	30	62
66	Sy	238/249 (96%)	234 (98%)	4 (2%)	0	100	100
67	Sz	187/194 (96%)	184 (98%)	3 (2%)	0	100	100
69	LA	85/97 (88%)	85 (100%)	0	0	100	100
70	LB	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
71	LC	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
72	LD	50/99 (50%)	50 (100%)	0	0	100	100
73	LE	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
74	LF	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
75	LG	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
76	LH	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
77	LI	221/248 (89%)	214 (97%)	7 (3%)	0	100	100
78	LJ	219/266 (82%)	213 (97%)	6 (3%)	0	100	100
79	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	LM	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	25	59
81	LN	35/414 (8%)	32 (91%)	3 (9%)	0	100	100
82	LO	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
83	LP	204/211 (97%)	200 (98%)	4 (2%)	0	100	100
84	LQ	137/215 (64%)	135 (98%)	2 (2%)	0	100	100
85	La	244/257 (95%)	229 (94%)	15 (6%)	0	100	100
86	Lb	394/403 (98%)	385 (98%)	9 (2%)	0	100	100
All	All	12133/14300 (85%)	11816 (97%)	314 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	Nm	297	HIS
65	Sx	42	THR
80	LM	103	LEU

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	Lc	302/348 (87%)	301 (100%)	1 (0%)	91	96
3	Ld	245/250 (98%)	243 (99%)	2 (1%)	79	89
4	Le	193/252 (77%)	192 (100%)	1 (0%)	86	93
5	Lf	171/171 (100%)	170 (99%)	1 (1%)	84	92
6	Lg	133/163 (82%)	133 (100%)	0	100	100
7	Lh	164/165 (99%)	162 (99%)	2 (1%)	67	83
8	Li	157/175 (90%)	156 (99%)	1 (1%)	84	92
9	Lj	157/157 (100%)	157 (100%)	0	100	100
10	Lk	139/140 (99%)	137 (99%)	2 (1%)	62	80
11	Ll	92/115 (80%)	89 (97%)	3 (3%)	33	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Lm	102/107 (95%)	101 (99%)	1 (1%)	73	85
13	Ln	100/126 (79%)	98 (98%)	2 (2%)	50	72
14	Lo	107/133 (80%)	105 (98%)	2 (2%)	52	73
15	Lp	124/135 (92%)	123 (99%)	1 (1%)	79	89
16	Lq	117/118 (99%)	116 (99%)	1 (1%)	75	87
17	Lr	120/121 (99%)	120 (100%)	0	100	100
18	Ls	82/126 (65%)	82 (100%)	0	100	100
19	Lt	84/97 (87%)	83 (99%)	1 (1%)	67	83
20	Lu	93/110 (84%)	93 (100%)	0	100	100
21	Lv	114/121 (94%)	114 (100%)	0	100	100
22	Lw	89/89 (100%)	89 (100%)	0	100	100
23	Lx	95/100 (95%)	95 (100%)	0	100	100
24	Ly	109/110 (99%)	109 (100%)	0	100	100
25	Lz	86/89 (97%)	85 (99%)	1 (1%)	67	83
26	Na	95/202 (47%)	94 (99%)	1 (1%)	70	84
27	Nb	104/136 (76%)	99 (95%)	5 (5%)	21	51
28	Nd	200/314 (64%)	198 (99%)	2 (1%)	73	85
29	Nm	326/330 (99%)	323 (99%)	3 (1%)	75	87
33	SA	178/180 (99%)	177 (99%)	1 (1%)	84	92
34	SB	160/168 (95%)	160 (100%)	0	100	100
35	SC	162/170 (95%)	160 (99%)	2 (1%)	67	83
36	SD	135/142 (95%)	134 (99%)	1 (1%)	81	90
37	SE	88/136 (65%)	87 (99%)	1 (1%)	70	84
38	SF	130/131 (99%)	129 (99%)	1 (1%)	79	89
39	SG	104/118 (88%)	101 (97%)	3 (3%)	37	64
40	SH	104/108 (96%)	98 (94%)	6 (6%)	17	45
41	Sa	110/134 (82%)	110 (100%)	0	100	100
42	Sb	121/122 (99%)	119 (98%)	2 (2%)	56	76
43	Sc	117/121 (97%)	117 (100%)	0	100	100
44	Sd	126/131 (96%)	123 (98%)	3 (2%)	44	68
45	Se	67/67 (100%)	66 (98%)	1 (2%)	60	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Sf	112/113 (99%)	111 (99%)	1 (1%)	75	87
47	Sg	112/114 (98%)	112 (100%)	0	100	100
49	Sh	108/113 (96%)	108 (100%)	0	100	100
50	Si	113/114 (99%)	111 (98%)	2 (2%)	54	74
51	Sj	88/98 (90%)	86 (98%)	2 (2%)	45	69
52	Sk	75/76 (99%)	73 (97%)	2 (3%)	40	65
53	Sl	93/107 (87%)	92 (99%)	1 (1%)	70	84
54	Sm	74/103 (72%)	73 (99%)	1 (1%)	62	80
55	Sn	48/104 (46%)	48 (100%)	0	100	100
56	So	58/62 (94%)	57 (98%)	1 (2%)	56	76
57	Sp	48/49 (98%)	48 (100%)	0	100	100
58	Sq	24/24 (100%)	24 (100%)	0	100	100
59	Sr	67/140 (48%)	67 (100%)	0	100	100
60	Ss	272/275 (99%)	264 (97%)	8 (3%)	37	64
61	St	184/242 (76%)	182 (99%)	2 (1%)	70	84
62	Su	203/231 (88%)	202 (100%)	1 (0%)	86	93
63	Sv	190/225 (84%)	189 (100%)	1 (0%)	86	93
64	Sw	224/225 (100%)	220 (98%)	4 (2%)	54	74
65	Sx	189/202 (94%)	186 (98%)	3 (2%)	58	77
66	Sy	209/218 (96%)	207 (99%)	2 (1%)	73	85
67	Sz	169/174 (97%)	165 (98%)	4 (2%)	44	68
69	LA	74/80 (92%)	74 (100%)	0	100	100
70	LB	64/65 (98%)	63 (98%)	1 (2%)	58	77
71	LC	47/48 (98%)	45 (96%)	2 (4%)	25	54
72	LD	48/91 (53%)	48 (100%)	0	100	100
73	LE	93/94 (99%)	92 (99%)	1 (1%)	70	84
74	LF	75/75 (100%)	73 (97%)	2 (3%)	40	65
75	LG	107/121 (88%)	107 (100%)	0	100	100
76	LH	172/172 (100%)	172 (100%)	0	100	100
77	LI	192/215 (89%)	192 (100%)	0	100	100
78	LJ	193/223 (86%)	192 (100%)	1 (0%)	86	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	LK	169/171 (99%)	169 (100%)	0	100	100
80	LM	180/181 (99%)	179 (99%)	1 (1%)	84	92
81	LN	33/336 (10%)	30 (91%)	3 (9%)	7	31
82	LO	142/149 (95%)	141 (99%)	1 (1%)	81	90
83	LP	172/177 (97%)	172 (100%)	0	100	100
84	LQ	118/161 (73%)	118 (100%)	0	100	100
85	La	189/199 (95%)	186 (98%)	3 (2%)	58	77
86	Lb	345/349 (99%)	343 (99%)	2 (1%)	84	92
All	All	10575/12144 (87%)	10469 (99%)	106 (1%)	71	85

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Lc	94	ASN
3	Ld	4	VAL
3	Ld	36	LEU
4	Le	41	LYS
5	Lf	126	VAL
7	Lh	42	THR
7	Lh	82	VAL
8	Li	136	ARG
10	Lk	76	VAL
10	Lk	136	ARG
11	Ll	45	GLU
11	Ll	47	ILE
11	Ll	116	GLN
12	Lm	77	HIS
13	Ln	93	LYS
13	Ln	106	GLU
14	Lo	100	VAL
14	Lo	156	ILE
15	Lp	105	VAL
16	Lq	35	ASP
19	Lt	94	LEU
25	Lz	60	LEU
26	Na	215	MET
27	Nb	38	THR
27	Nb	53	VAL
27	Nb	80	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Nb	142	ASP
27	Nb	146	VAL
28	Nd	55	VAL
28	Nd	89	GLU
29	Nm	73	ILE
29	Nm	199	GLU
29	Nm	216	ILE
33	SA	119	LEU
35	SC	44	LYS
35	SC	128	ILE
36	SD	119	ASP
37	SE	72	THR
38	SF	124	ARG
39	SG	21	VAL
39	SG	75	MET
39	SG	100	THR
40	SH	29	ASP
40	SH	62	VAL
40	SH	80	ASP
40	SH	89	VAL
40	SH	103	VAL
40	SH	114	TYR
42	Sb	6	THR
42	Sb	71	ILE
44	Sd	53	THR
44	Sd	59	LEU
44	Sd	136	THR
45	Se	9	VAL
46	Sf	105	THR
50	Si	118	ASP
50	Si	126	GLN
51	Sj	21	ILE
51	Sj	67	LEU
52	Sk	3	LEU
52	Sk	53	VAL
53	Sl	68	THR
54	Sm	65	TYR
56	So	32	VAL
60	Ss	64	HIS
60	Ss	94	THR
60	Ss	102	VAL
60	Ss	132	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	Ss	134	THR
60	Ss	142	VAL
60	Ss	266	ILE
60	Ss	309	VAL
61	St	197	VAL
61	St	206	ASP
62	Su	231	LEU
63	Sv	146	GLU
64	Sw	12	VAL
64	Sw	21	ASP
64	Sw	33	THR
64	Sw	206	ASP
65	Sx	41	VAL
65	Sx	175	VAL
65	Sx	176	LEU
66	Sy	69	THR
66	Sy	201	LYS
67	Sz	33	ASN
67	Sz	44	ASN
67	Sz	72	PHE
67	Sz	83	LEU
70	LB	30	ASP
71	LC	23	ILE
71	LC	47	THR
73	LE	103	VAL
74	LF	3	LYS
74	LF	52	VAL
78	LJ	201	THR
80	LM	31	ILE
81	LN	378	ILE
81	LN	383	ILE
81	LN	384	ARG
82	LO	123	ILE
85	La	32	VAL
85	La	175	ILE
85	La	208	GLU
86	Lb	3	HIS
86	Lb	344	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
2	Lc	43	ASN
2	Lc	48	ASN
2	Lc	50	GLN
2	Lc	60	HIS
2	Lc	112	HIS
2	Lc	310	HIS
2	Lc	317	ASN
2	Lc	347	HIS
2	Lc	362	GLN
3	Ld	122	GLN
3	Ld	198	HIS
3	Ld	225	GLN
5	Lf	42	ASN
5	Lf	167	HIS
5	Lf	180	GLN
5	Lf	184	ASN
6	Lg	34	GLN
6	Lg	75	GLN
7	Lh	44	ASN
10	Lk	127	GLN
11	Ll	27	HIS
11	Ll	50	ASN
11	Ll	94	ASN
12	Lm	77	HIS
12	Lm	101	ASN
13	Ln	45	ASN
13	Ln	96	GLN
13	Ln	120	GLN
14	Lo	107	HIS
15	Lp	14	ASN
15	Lp	56	GLN
17	Lr	40	HIS
17	Lr	60	HIS
18	Ls	12	GLN
18	Ls	50	ASN
23	Lx	28	ASN
25	Lz	26	HIS
26	Na	208	ASN
27	Nb	15	GLN
27	Nb	17	GLN
28	Nd	87	GLN
28	Nd	178	HIS
29	Nm	90	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	Nm	218	ASN
29	Nm	233	ASN
29	Nm	258	GLN
29	Nm	294	HIS
29	Nm	322	HIS
29	Nm	356	GLN
33	SA	52	ASN
33	SA	88	ASN
33	SA	165	GLN
34	SB	124	HIS
35	SC	79	HIS
35	SC	101	HIS
35	SC	110	GLN
35	SC	203	ASN
36	SD	18	GLN
36	SD	65	ASN
36	SD	100	ASN
36	SD	141	ASN
37	SE	61	GLN
38	SF	90	HIS
38	SF	138	ASN
39	SG	32	HIS
39	SG	103	ASN
41	Sa	103	ASN
42	Sb	31	ASN
43	Sc	48	GLN
43	Sc	77	HIS
43	Sc	80	GLN
43	Sc	86	GLN
44	Sd	11	HIS
44	Sd	105	ASN
45	Se	2	GLN
46	Sf	24	GLN
46	Sf	70	ASN
47	Sg	31	HIS
50	Si	126	GLN
50	Si	145	HIS
51	Sj	8	ASN
51	Sj	25	ASN
52	Sk	49	HIS
52	Sk	84	HIS
53	Sl	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	Sm	106	GLN
55	Sn	113	ASN
55	Sn	118	ASN
59	Sr	111	ASN
60	Ss	26	GLN
60	Ss	62	HIS
60	Ss	76	GLN
60	Ss	226	HIS
60	Ss	311	GLN
61	St	110	ASN
61	St	113	GLN
62	Su	75	GLN
62	Su	159	GLN
62	Su	208	HIS
63	Sv	115	GLN
63	Sv	178	HIS
63	Sv	277	HIS
64	Sw	67	GLN
64	Sw	138	HIS
64	Sw	161	GLN
65	Sx	159	HIS
65	Sx	165	ASN
66	Sy	177	GLN
66	Sy	187	HIS
66	Sy	225	GLN
67	Sz	25	GLN
67	Sz	97	GLN
67	Sz	112	ASN
69	LA	30	GLN
71	LC	19	GLN
71	LC	33	ASN
71	LC	38	ASN
73	LE	51	GLN
73	LE	76	ASN
74	LF	33	GLN
74	LF	34	HIS
74	LF	92	GLN
75	LG	41	ASN
76	LH	8	GLN
76	LH	37	HIS
76	LH	156	HIS
77	LI	39	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
77	LI	116	GLN
78	LJ	85	GLN
79	LK	42	ASN
79	LK	98	HIS
80	LM	112	GLN
81	LN	402	GLN
83	LP	175	ASN
83	LP	205	GLN
84	LQ	34	ASN
84	LQ	70	GLN
84	LQ	125	ASN
85	La	50	HIS
85	La	83	HIS
85	La	97	ASN
85	La	205	ASN
86	Lb	213	GLN
86	Lb	289	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3376/5070 (66%)	462 (13%)	5 (0%)
30	S1	1765/1869 (94%)	255 (14%)	0
31	S2	6/1824 (0%)	0	0
32	S3	72/76 (94%)	9 (12%)	0
48	L2	117/121 (96%)	9 (7%)	0
68	L3	145/157 (92%)	16 (11%)	0
All	All	5481/9117 (60%)	751 (13%)	5 (0%)

All (751) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	13	U
1	L1	25	A
1	L1	30	C
1	L1	39	A
1	L1	42	A
1	L1	48	G
1	L1	58	G
1	L1	59	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	64	A
1	L1	65	A
1	L1	73	A
1	L1	85	G
1	L1	91	G
1	L1	95	G
1	L1	98	A
1	L1	104	G
1	L1	119	G
1	L1	120	A
1	L1	132	G
1	L1	135	G
1	L1	136	C
1	L1	138	G
1	L1	139	G
1	L1	143	C
1	L1	159	C
1	L1	172	C
1	L1	189	G
1	L1	200	U
1	L1	209	U
1	L1	210	C
1	L1	216	C
1	L1	218	A
1	L1	220	C
1	L1	232	G
1	L1	233	U
1	L1	234	G
1	L1	241	G
1	L1	266	C
1	L1	297	U
1	L1	316	U
1	L1	326	C
1	L1	340	C
1	L1	387	G
1	L1	403	G
1	L1	410	A
1	L1	412	G
1	L1	414	C
1	L1	415	G
1	L1	449	C
1	L1	450	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	452	A
1	L1	453	G
1	L1	454	U
1	L1	457	G
1	L1	468	U
1	L1	487	G
1	L1	493	G
1	L1	502	C
1	L1	503	C
1	L1	504	G
1	L1	509	A
1	L1	666	G
1	L1	667	A
1	L1	688	U
1	L1	695	G
1	L1	697	G
1	L1	704	C
1	L1	708	G
1	L1	730	G
1	L1	731	G
1	L1	738	C
1	L1	739	G
1	L1	741	C
1	L1	915	A
1	L1	916	C
1	L1	917	A
1	L1	918	G
1	L1	932	A
1	L1	933	G
1	L1	934	C
1	L1	935	A
1	L1	936	C
1	L1	943	A
1	L1	944	A
1	L1	945	U
1	L1	956	A
1	L1	960	A
1	L1	961	G
1	L1	962	C
1	L1	964	A
1	L1	965	G
1	L1	966	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	967	C
1	L1	971	U
1	L1	982	U
1	L1	1071	C
1	L1	1073	G
1	L1	1084	C
1	L1	1182	C
1	L1	1183	C
1	L1	1185	G
1	L1	1198	G
1	L1	1199	G
1	L1	1200	G
1	L1	1210	C
1	L1	1211	G
1	L1	1214	C
1	L1	1215	C
1	L1	1216	C
1	L1	1261	G
1	L1	1266	G
1	L1	1269	G
1	L1	1271	G
1	L1	1272	C
1	L1	1273	G
1	L1	1280	C
1	L1	1281	G
1	L1	1284	G
1	L1	1285	U
1	L1	1287	G
1	L1	1293	G
1	L1	1294	A
1	L1	1295	C
1	L1	1301	C
1	L1	1314	C
1	L1	1326	A2M
1	L1	1337	A
1	L1	1354	A
1	L1	1359	G
1	L1	1365	C
1	L1	1366	G
1	L1	1377	G
1	L1	1379	C
1	L1	1387	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1397	A
1	L1	1404	G
1	L1	1420	A
1	L1	1435	G
1	L1	1436	C
1	L1	1439	C
1	L1	1444	G
1	L1	1457	G
1	L1	1476	C
1	L1	1483	C
1	L1	1497	A
1	L1	1498	G
1	L1	1501	C
1	L1	1502	G
1	L1	1516	G
1	L1	1518	A
1	L1	1525	A
1	L1	1534	A2M
1	L1	1547	A
1	L1	1562	G
1	L1	1566	C
1	L1	1578	U
1	L1	1591	U
1	L1	1596	U
1	L1	1597	G
1	L1	1613	A
1	L1	1624	G
1	L1	1625	OMG
1	L1	1631	A
1	L1	1633	G
1	L1	1634	A
1	L1	1641	G
1	L1	1654	G
1	L1	1661	C
1	L1	1676	C
1	L1	1677	PSU
1	L1	1678	C
1	L1	1699	A
1	L1	1700	G
1	L1	1701	A
1	L1	1705	G
1	L1	1707	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	1722	C
1	L1	1735	U
1	L1	1787	A
1	L1	1789	C
1	L1	1794	A
1	L1	1804	A
1	L1	1806	G
1	L1	1818	G
1	L1	1821	G
1	L1	1822	U
1	L1	1834	U
1	L1	1836	G
1	L1	1837	A
1	L1	1842	G
1	L1	1855	G
1	L1	1869	G
1	L1	1881	OMC
1	L1	1897	A
1	L1	1910	G
1	L1	1918	U
1	L1	1921	C
1	L1	1922	G
1	L1	1925	G
1	L1	1931	C
1	L1	1932	A
1	L1	1940	G
1	L1	1948	G
1	L1	1955	G
1	L1	2043	A
1	L1	2046	G
1	L1	2048	U
1	L1	2055	G
1	L1	2056	G
1	L1	2069	A
1	L1	2084	C
1	L1	2091	C
1	L1	2092	G
1	L1	2093	A
1	L1	2094	G
1	L1	2095	A
1	L1	2097	U
1	L1	2098	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	2258	C
1	L1	2259	G
1	L1	2269	C
1	L1	2289	C
1	L1	2300	A
1	L1	2301	G
1	L1	2306	G
1	L1	2313	A
1	L1	2316	G
1	L1	2322	G
1	L1	2339	G
1	L1	2347	A
1	L1	2348	G
1	L1	2351	OMC
1	L1	2360	A
1	L1	2364	OMG
1	L1	2397	G
1	L1	2402	G
1	L1	2417	A
1	L1	2421	G
1	L1	2425	U
1	L1	2450	G
1	L1	2463	G
1	L1	2474	G
1	L1	2475	G
1	L1	2479	G
1	L1	2493	G
1	L1	2504	C
1	L1	2505	C
1	L1	2513	A
1	L1	2519	U
1	L1	2529	A
1	L1	2549	G
1	L1	2554	U
1	L1	2573	A
1	L1	2577	C
1	L1	2586	G
1	L1	2587	A
1	L1	2600	A
1	L1	2601	A
1	L1	2627	C
1	L1	2638	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	2653	C
1	L1	2661	U
1	L1	2662	G
1	L1	2663	G
1	L1	2669	C
1	L1	2675	G
1	L1	2681	G
1	L1	2687	U
1	L1	2694	G
1	L1	2695	A
1	L1	2696	A
1	L1	2711	G
1	L1	2712	G
1	L1	2725	A
1	L1	2726	G
1	L1	2743	A
1	L1	2760	G
1	L1	2762	G
1	L1	2764	A
1	L1	2788	U
1	L1	2790	U
1	L1	2814	C
1	L1	2826	U
1	L1	2827	G
1	L1	2828	U
1	L1	2830	G
1	L1	2838	G
1	L1	2841	G
1	L1	2855	G
1	L1	2892	C
1	L1	3606	U
1	L1	3615	G
1	L1	3616	U
1	L1	3626	G
1	L1	3635	A
1	L1	3646	A
1	L1	3648	A
1	L1	3653	A
1	L1	3662	A
1	L1	3664	G
1	L1	3673	C
1	L1	3692	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	3696	C
1	L1	3701	OMC
1	L1	3709	U
1	L1	3710	G
1	L1	3711	A
1	L1	3712	A
1	L1	3713	U
1	L1	3714	G
1	L1	3729	U
1	L1	3734	PSU
1	L1	3735	G
1	L1	3750	G
1	L1	3753	G
1	L1	3759	A
1	L1	3760	A
1	L1	3761	C
1	L1	3766	A
1	L1	3776	G
1	L1	3777	G
1	L1	3780	G
1	L1	3784	A
1	L1	3811	G
1	L1	3814	U
1	L1	3817	A
1	L1	3819	G
1	L1	3838	U
1	L1	3840	U
1	L1	3877	A
1	L1	3878	C
1	L1	3879	G
1	L1	3892	U
1	L1	3897	G
1	L1	3901	A
1	L1	3905	A
1	L1	3906	A
1	L1	3907	G
1	L1	3908	A
1	L1	3915	U
1	L1	3926	C
1	L1	3938	G
1	L1	3939	G
1	L1	4076	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4077	A
1	L1	4084	G
1	L1	4092	G
1	L1	4093	G
1	L1	4119	C
1	L1	4122	G
1	L1	4127	A
1	L1	4162	C
1	L1	4163	U
1	L1	4168	G
1	L1	4170	A
1	L1	4183	G
1	L1	4184	G
1	L1	4191	G
1	L1	4212	A
1	L1	4225	G
1	L1	4229	U
1	L1	4233	A
1	L1	4234	A
1	L1	4251	A
1	L1	4254	G
1	L1	4255	A
1	L1	4266	G
1	L1	4268	A
1	L1	4273	A
1	L1	4281	A
1	L1	4291	G
1	L1	4304	A
1	L1	4305	G
1	L1	4306	OMU
1	L1	4329	G
1	L1	4330	G
1	L1	4332	C
1	L1	4339	A
1	L1	4373	G
1	L1	4377	G
1	L1	4378	A
1	L1	4380	A
1	L1	4382	G
1	L1	4386	C
1	L1	4387	C
1	L1	4394	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4415	A
1	L1	4416	G
1	L1	4422	A
1	L1	4430	G
1	L1	4440	G
1	L1	4448	G
1	L1	4464	A
1	L1	4466	C
1	L1	4495	G
1	L1	4512	U
1	L1	4513	A
1	L1	4518	A
1	L1	4524	G
1	L1	4548	A
1	L1	4560	C
1	L1	4567	G
1	L1	4575	G
1	L1	4581	G
1	L1	4584	A
1	L1	4590	A2M
1	L1	4608	G
1	L1	4636	U
1	L1	4637	OMG
1	L1	4652	G
1	L1	4670	C
1	L1	4672	A
1	L1	4691	A
1	L1	4694	G
1	L1	4707	A
1	L1	4708	A
1	L1	4709	U
1	L1	4722	G
1	L1	4730	C
1	L1	4731	G
1	L1	4732	G
1	L1	4733	C
1	L1	4735	G
1	L1	4741	C
1	L1	4742	G
1	L1	4754	G
1	L1	4757	C
1	L1	4759	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L1	4761	G
1	L1	4765	G
1	L1	4870	G
1	L1	4871	C
1	L1	4877	G
1	L1	4882	U
1	L1	4883	C
1	L1	4889	G
1	L1	4895	C
1	L1	4900	C
1	L1	4901	G
1	L1	4910	A
1	L1	4912	G
1	L1	4913	G
1	L1	4914	C
1	L1	4926	C
1	L1	4940	C
1	L1	4944	C
1	L1	4947	U
1	L1	4951	G
1	L1	4976	U
1	L1	4987	C
1	L1	4988	U
1	L1	5013	C
1	L1	5014	A
1	L1	5017	G
1	L1	5034	A
1	L1	5041	G
1	L1	5050	C
1	L1	5054	C
1	L1	5055	G
1	L1	5062	G
1	L1	5069	U
30	S1	4	C
30	S1	17	C
30	S1	26	U
30	S1	33	G
30	S1	41	G
30	S1	44	U
30	S1	46	A
30	S1	56	G
30	S1	64	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	65	C
30	S1	67	C
30	S1	68	A
30	S1	70	G
30	S1	74	G
30	S1	76	U
30	S1	77	A
30	S1	79	A
30	S1	100	U
30	S1	103	A
30	S1	110	U
30	S1	113	G
30	S1	115	U
30	S1	126	G
30	S1	130	G
30	S1	143	U
30	S1	159	A2M
30	S1	160	U
30	S1	163	U
30	S1	168	C
30	S1	175	A
30	S1	182	C
30	S1	184	G
30	S1	190	G
30	S1	192	C
30	S1	194	C
30	S1	226	A
30	S1	228	C
30	S1	281	C
30	S1	287	U
30	S1	294	U
30	S1	295	C
30	S1	307	G
30	S1	309	G
30	S1	312	G
30	S1	319	C
30	S1	326	C
30	S1	327	G
30	S1	328	U
30	S1	329	G
30	S1	330	G
30	S1	333	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	335	G
30	S1	362	C
30	S1	364	A
30	S1	368	U
30	S1	369	C
30	S1	385	G
30	S1	386	C
30	S1	400	C
30	S1	409	C
30	S1	421	G
30	S1	448	A
30	S1	449	A
30	S1	450	C
30	S1	470	G
30	S1	472	C
30	S1	474	G
30	S1	482	G
30	S1	487	U
30	S1	492	C
30	S1	501	C
30	S1	508	A
30	S1	525	A
30	S1	541	U
30	S1	542	U
30	S1	544	G
30	S1	547	G
30	S1	548	C
30	S1	555	A
30	S1	559	G
30	S1	563	G
30	S1	588	G
30	S1	589	G
30	S1	591	U
30	S1	593	C
30	S1	607	U
30	S1	608	C
30	S1	614	C
30	S1	628	A
30	S1	629	A
30	S1	631	U
30	S1	643	A
30	S1	644	OMG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	655	A
30	S1	660	C
30	S1	668	A2M
30	S1	669	A
30	S1	671	A
30	S1	672	A
30	S1	673	G
30	S1	684	G
30	S1	690	G
30	S1	697	G
30	S1	746	C
30	S1	748	C
30	S1	749	U
30	S1	790	C
30	S1	798	G
30	S1	799	OMU
30	S1	811	A
30	S1	821	G
30	S1	822	PSU
30	S1	830	A
30	S1	831	G
30	S1	836	G
30	S1	837	A
30	S1	838	G
30	S1	839	C
30	S1	841	G
30	S1	847	A
30	S1	869	A
30	S1	870	A
30	S1	874	G
30	S1	878	G
30	S1	881	G
30	S1	891	G
30	S1	894	G
30	S1	913	A
30	S1	914	U
30	S1	920	A
30	S1	922	A
30	S1	933	G
30	S1	943	U
30	S1	955	A
30	S1	963	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	970	G
30	S1	985	G
30	S1	990	A
30	S1	992	A
30	S1	1017	U
30	S1	1023	A
30	S1	1027	A
30	S1	1061	U
30	S1	1062	A
30	S1	1083	A
30	S1	1085	C
30	S1	1115	U
30	S1	1121	G
30	S1	1130	G
30	S1	1133	A
30	S1	1144	A
30	S1	1148	A
30	S1	1153	C
30	S1	1154	U
30	S1	1157	G
30	S1	1166	G
30	S1	1171	G
30	S1	1195	A
30	S1	1207	G
30	S1	1215	C
30	S1	1224	G
30	S1	1242	U
30	S1	1248	B8N
30	S1	1251	A
30	S1	1253	A
30	S1	1256	G
30	S1	1257	G
30	S1	1259	A
30	S1	1274	G
30	S1	1275	G
30	S1	1286	G
30	S1	1293	A
30	S1	1302	G
30	S1	1303	C
30	S1	1309	C
30	S1	1330	G
30	S1	1342	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	1343	U
30	S1	1348	G
30	S1	1358	U
30	S1	1364	U
30	S1	1371	U
30	S1	1372	U
30	S1	1375	G
30	S1	1378	A
30	S1	1397	U
30	S1	1404	U
30	S1	1405	A
30	S1	1418	C
30	S1	1419	C
30	S1	1420	G
30	S1	1421	A
30	S1	1423	C
30	S1	1433	C
30	S1	1435	C
30	S1	1437	C
30	S1	1438	A
30	S1	1439	A
30	S1	1447	OMG
30	S1	1454	A
30	S1	1463	U
30	S1	1464	C
30	S1	1466	G
30	S1	1489	A
30	S1	1490	OMG
30	S1	1494	U
30	S1	1495	G
30	S1	1497	G
30	S1	1508	A
30	S1	1509	U
30	S1	1521	C
30	S1	1533	A
30	S1	1553	C
30	S1	1570	G
30	S1	1579	A
30	S1	1580	A
30	S1	1585	U
30	S1	1588	A
30	S1	1596	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	S1	1599	U
30	S1	1601	A
30	S1	1618	C
30	S1	1621	U
30	S1	1623	A
30	S1	1624	U
30	S1	1637	A
30	S1	1654	G
30	S1	1665	G
30	S1	1680	G
30	S1	1685	U
30	S1	1695	A
30	S1	1699	A
30	S1	1721	U
30	S1	1722	G
30	S1	1742	C
30	S1	1744	G
30	S1	1757	G
30	S1	1765	C
30	S1	1766	C
30	S1	1776	G
30	S1	1783	C
30	S1	1824	A
30	S1	1825	A
30	S1	1826	G
30	S1	1829	G
30	S1	1835	A
30	S1	1836	G
30	S1	1838	U
30	S1	1849	G
30	S1	1851	MA6
30	S1	1861	G
30	S1	1862	G
30	S1	1863	A
30	S1	1865	C
30	S1	1869	A
32	S3	2	C
32	S3	10	G
32	S3	19	G
32	S3	21	A
32	S3	42	G
32	S3	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	S3	48	C
32	S3	62	U
32	S3	76	A
48	L2	7	G
48	L2	38	U
48	L2	53	U
48	L2	54	A
48	L2	63	C
48	L2	64	G
48	L2	91	C
48	L2	110	G
48	L2	119	U
68	L3	34	U
68	L3	35	C
68	L3	39	G
68	L3	59	A
68	L3	62	A
68	L3	63	U
68	L3	82	A
68	L3	87	G
68	L3	94	G
68	L3	103	A
68	L3	105	C
68	L3	110	U
68	L3	111	U
68	L3	114	G
68	L3	150	C
68	L3	151	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	486	C
1	L1	964	A
1	L1	1365	C
1	L1	1633	G
1	L1	2091	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

212 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	$\# Z > 2$
30	6MZ	S1	1832	30	18,25,26	0.88	1 (5%)	16,36,39	1.76	4 (25%)
30	4AC	S1	1337	30	21,24,25	1.11	2 (9%)	29,34,37	1.05	2 (6%)
1	PSU	L1	4403	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	L1	2632	1	18,21,22	1.36	3 (16%)	22,30,33	1.87	3 (13%)
30	PSU	S1	1045	30	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	OMG	L1	1625	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
30	OMU	S1	1804	30	19,22,23	1.24	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	L1	1860	1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
1	5MC	L1	3782	1	18,22,23	0.96	2 (11%)	26,32,35	1.22	3 (11%)
30	PSU	S1	801	30	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
1	OMU	L1	2415	1	19,22,23	1.24	3 (15%)	26,31,34	1.68	5 (19%)
30	PSU	S1	1056	30	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
30	PSU	S1	822	30	18,21,22	1.39	2 (11%)	22,30,33	1.91	3 (13%)
30	PSU	S1	1367	30	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
30	G7M	S1	1639	30,32	20,26,27	2.94	7 (35%)	17,39,42	0.99	1 (5%)
30	OMU	S1	1288	30	19,22,23	1.22	2 (10%)	26,31,34	1.70	4 (15%)
30	PSU	S1	1046	30	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	L1	1536	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	L1	2787	1	18,25,26	0.93	1 (5%)	18,36,39	1.25	2 (11%)
30	A2M	S1	159	30	18,25,26	0.99	1 (5%)	18,36,39	1.40	2 (11%)
30	PSU	S1	686	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
30	PSU	S1	1347	30	18,21,22	1.36	3 (16%)	22,30,33	1.93	4 (18%)
30	A2M	S1	576	30	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
30	OMG	S1	1490	30	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	PSU	L1	3851	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
30	A2M	S1	484	30	18,25,26	0.98	1 (5%)	18,36,39	1.25	2 (11%)
1	OMC	L1	2351	1	19,22,23	0.83	0	26,31,34	0.97	2 (7%)
1	OMC	L1	2861	1	19,22,23	0.82	0	26,31,34	0.82	0
1	OMC	L1	2824	1	19,22,23	0.82	0	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	S1	1244	30	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
30	OMU	S1	1442	30	19,22,23	1.25	3 (15%)	26,31,34	1.73	4 (15%)
1	PSU	L1	4576	1	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
30	A2M	S1	468	30	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
30	PSU	S1	1643	30	18,21,22	1.37	3 (16%)	22,30,33	1.88	3 (13%)
1	A2M	L1	3724	1	18,25,26	1.00	1 (5%)	18,36,39	1.18	2 (11%)
30	OMC	S1	462	30	19,22,23	0.81	0	26,31,34	0.78	0
30	OMG	S1	683	30	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	L1	3785	1	18,25,26	0.91	1 (5%)	18,36,39	1.32	2 (11%)
30	A2M	S1	668	30	18,25,26	0.97	1 (5%)	18,36,39	1.35	2 (11%)
30	PSU	S1	1625	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
30	PSU	S1	649	30	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
30	PSU	S1	1081	30	18,21,22	1.43	4 (22%)	22,30,33	1.86	4 (18%)
30	PSU	S1	1174	30	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
30	PSU	S1	109	30	18,21,22	1.39	3 (16%)	22,30,33	1.89	3 (13%)
1	PSU	L1	4500	1	18,21,22	1.34	2 (11%)	22,30,33	1.95	5 (22%)
30	PSU	S1	1238	30	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
1	OMG	L1	1522	1	18,26,27	0.97	1 (5%)	19,38,41	1.08	2 (10%)
1	OMC	L1	2365	1	19,22,23	0.82	0	26,31,34	0.74	0
1	PSU	L1	4299	1	18,21,22	1.37	3 (16%)	22,30,33	1.87	3 (13%)
1	PSU	L1	4579	1	18,21,22	1.36	3 (16%)	22,30,33	1.93	4 (18%)
1	OMG	L1	4392	1	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	L1	5010	1	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
1	A2M	L1	4571	1	18,25,26	0.97	1 (5%)	18,36,39	1.20	2 (11%)
30	PSU	S1	1232	30	18,21,22	1.35	3 (16%)	22,30,33	1.91	4 (18%)
30	A2M	S1	1383	30	18,25,26	1.06	2 (11%)	18,36,39	1.40	2 (11%)
1	PSU	L1	4493	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
1	OMG	L1	2424	1	18,26,27	0.93	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	L1	4423	1	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
1	OMG	L1	3792	1	18,26,27	0.96	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	L1	1323	1	18,25,26	0.97	1 (5%)	18,36,39	1.19	2 (11%)
1	A2M	L1	2363	1	18,25,26	0.96	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	L1	4673	1	18,21,22	1.39	3 (16%)	22,30,33	1.90	3 (13%)
1	PSU	L1	3637	1	18,21,22	1.38	3 (16%)	22,30,33	1.94	3 (13%)
30	A2M	S1	27	30	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	4521	1	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
1	PSU	L1	4628	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
30	PSU	S1	105	30	18,21,22	1.40	2 (11%)	22,30,33	1.89	3 (13%)
30	OMU	S1	428	30	19,22,23	1.22	2 (10%)	26,31,34	1.67	4 (15%)
30	A2M	S1	512	30	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
30	PSU	S1	1445	30	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
30	OMU	S1	627	30	19,22,23	1.22	3 (15%)	26,31,34	1.62	4 (15%)
30	OMU	S1	116	30	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
68	OMG	L3	75	68	18,26,27	0.97	1 (5%)	19,38,41	1.07	2 (10%)
1	OMG	L1	3744	1	18,26,27	0.96	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	L1	3730	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
30	OMC	S1	1391	30	19,22,23	0.81	0	26,31,34	0.82	0
1	OMC	L1	2804	1	19,22,23	0.83	0	26,31,34	0.80	0
1	PSU	L1	4689	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	L1	3853	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	3 (13%)
30	PSU	S1	93	30	18,21,22	1.38	3 (16%)	22,30,33	1.86	3 (13%)
68	PSU	L3	69	68	18,21,22	1.38	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	L1	3920	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L1	4471	1	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	L1	4532	1	18,21,22	1.40	3 (16%)	22,30,33	1.88	3 (13%)
1	A2M	L1	1326	1	18,25,26	0.90	1 (5%)	18,36,39	1.26	2 (11%)
30	PSU	S1	296	30	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
30	PSU	S1	1177	30	18,21,22	1.37	3 (16%)	22,30,33	1.89	3 (13%)
1	OMC	L1	2422	1	19,22,23	0.83	0	26,31,34	0.86	1 (3%)
1	OMG	L1	3627	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	L1	4442	1	18,21,22	1.38	3 (16%)	22,30,33	1.95	5 (22%)
30	A2M	S1	99	30	18,25,26	1.01	1 (5%)	18,36,39	1.19	2 (11%)
30	PSU	S1	1136	30	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	L1	4457	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
30	PSU	S1	34	30	18,21,22	1.39	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	L1	4494	1	18,26,27	0.96	1 (5%)	19,38,41	1.07	2 (10%)
50	NMM	Si	67	50	9,11,12	0.59	0	6,12,14	0.47	0
30	OMC	S1	174	30	19,22,23	0.81	0	26,31,34	0.78	0
1	PSU	L1	5001	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	L1	3715	1	18,21,22	1.40	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L1	3899	1	18,26,27	0.96	1 (5%)	19,38,41	1.11	2 (10%)
30	PSU	S1	1004	30	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	L1	1677	1	18,21,22	1.38	2 (11%)	22,30,33	1.88	4 (18%)
30	OMG	S1	601	30	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	PSU	L1	1782	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
30	PSU	S1	815	30	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
30	OMC	S1	797	30	19,22,23	0.82	0	26,31,34	0.83	0
1	A2M	L1	2401	1	18,25,26	0.97	1 (5%)	18,36,39	1.18	2 (11%)
30	PSU	S1	866	30	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	L1	4370	1	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	L1	3695	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	L1	1881	1	19,22,23	0.86	0	26,31,34	1.30	1 (3%)
1	PSU	L1	3770	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	L1	4523	1	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	L1	4552	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
30	PSU	S1	681	30	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
30	PSU	S1	814	30	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
30	PSU	S1	966	30	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
30	MA6	S1	1850	30	18,26,27	1.12	2 (11%)	19,38,41	1.96	3 (15%)
1	A2M	L1	398	1	18,25,26	0.96	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	L1	2508	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
1	OMU	L1	4227	1	19,22,23	1.26	2 (10%)	26,31,34	1.73	4 (15%)
30	B8N	S1	1248	30	24,29,30	1.31	3 (12%)	29,42,45	1.31	4 (13%)
47	HY3	Sg	62	47	6,8,9	0.82	0	5,10,12	1.30	1 (20%)
1	OMG	L1	4196	32,1	18,26,27	0.96	1 (5%)	19,38,41	1.05	2 (10%)
30	OMC	S1	517	30	19,22,23	0.81	0	26,31,34	0.80	0
1	OMG	L1	1316	1	18,26,27	0.97	1 (5%)	19,38,41	1.12	2 (10%)
1	A2M	L1	1534	1	18,25,26	0.93	1 (5%)	18,36,39	1.32	2 (11%)
39	IAS	SG	138	39	6,7,8	0.97	0	6,8,10	1.31	1 (16%)
30	OMG	S1	644	30	18,26,27	0.95	1 (5%)	19,38,41	1.05	2 (10%)
1	OMG	L1	4499	1	18,26,27	0.95	1 (5%)	19,38,41	1.04	2 (10%)
1	A2M	L1	3867	1	18,25,26	0.97	1 (5%)	18,36,39	1.26	2 (11%)
1	A2M	L1	3825	1	18,25,26	1.00	1 (5%)	18,36,39	1.26	2 (11%)
1	OMC	L1	3841	1	19,22,23	0.83	0	26,31,34	0.85	1 (3%)
1	PSU	L1	2839	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	S1	609	30	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	L1	4293	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L1	1744	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
30	A2M	S1	166	30	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
30	PSU	S1	863	30	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
1	A2M	L1	3718	1	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	L1	4623	1	18,26,27	0.96	1 (5%)	19,38,41	1.11	2 (10%)
1	5MC	L1	4447	1	18,22,23	1.00	2 (11%)	26,32,35	1.18	2 (7%)
30	OMC	S1	1272	30	19,22,23	0.82	0	26,31,34	0.82	0
1	OMC	L1	3808	1	19,22,23	0.83	0	26,31,34	0.81	0
30	PSU	S1	1692	30	18,21,22	1.38	2 (11%)	22,30,33	1.96	4 (18%)
30	MA6	S1	1851	30	18,26,27	1.13	2 (11%)	19,38,41	1.93	3 (15%)
1	OMU	L1	3925	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	5 (19%)
1	OMU	L1	4498	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
30	A2M	S1	1031	30	18,25,26	1.00	1 (5%)	18,36,39	1.23	2 (11%)
1	OMC	L1	3887	1	19,22,23	0.81	0	26,31,34	0.79	0
30	A2M	S1	590	30	18,25,26	1.00	1 (5%)	18,36,39	1.19	2 (11%)
30	OMG	S1	1447	30	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	6MZ	L1	4220	1	18,25,26	0.85	1 (5%)	16,36,39	2.14	4 (25%)
1	PSU	L1	1781	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	OMU	L1	2837	1	19,22,23	1.23	3 (15%)	26,31,34	1.76	5 (19%)
1	UR3	L1	4530	1	19,22,23	0.94	0	26,32,35	1.36	1 (3%)
30	PSU	S1	406	30	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
30	A2M	S1	1678	30	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
30	PSU	S1	119	30	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
30	OMU	S1	172	30	19,22,23	1.21	3 (15%)	26,31,34	1.71	4 (15%)
1	PSU	L1	1683	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
30	4AC	S1	1842	30	21,24,25	1.12	2 (9%)	29,34,37	1.16	3 (10%)
1	PSU	L1	1792	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
30	OMU	S1	799	30	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMU	L1	4620	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	5 (19%)
30	OMG	S1	1328	30	18,26,27	0.96	1 (5%)	19,38,41	1.06	2 (10%)
1	OMG	L1	2364	1	18,26,27	0.92	1 (5%)	19,38,41	1.05	2 (10%)
1	OMG	L1	4618	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	OMC	L1	4536	1	19,22,23	0.83	0	26,31,34	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	S1	354	30	19,22,23	1.25	3 (15%)	26,31,34	1.76	5 (19%)
30	OMG	S1	436	30	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	L1	4420	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	L1	1871	1	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
1	A2M	L1	1524	1	18,25,26	0.96	1 (5%)	18,36,39	1.24	2 (11%)
1	1MA	L1	1322	1	16,25,26	1.46	2 (12%)	18,37,40	1.05	3 (16%)
1	PSU	L1	4361	1	18,21,22	1.39	3 (16%)	22,30,33	1.90	3 (13%)
1	PSU	L1	1582	1	18,21,22	1.36	3 (16%)	22,30,33	1.96	4 (18%)
1	A2M	L1	4590	1	18,25,26	1.01	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	L1	3734	1	18,21,22	1.35	3 (16%)	22,30,33	1.92	4 (18%)
1	OMU	L1	4306	1	19,22,23	1.25	3 (15%)	26,31,34	1.70	4 (15%)
30	OMG	S1	509	30	18,26,27	0.95	1 (5%)	19,38,41	1.05	2 (10%)
1	A2M	L1	400	1	18,25,26	0.99	1 (5%)	18,36,39	1.18	2 (11%)
1	PSU	L1	4312	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	L1	3830	1	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	L1	4353	1	18,21,22	1.37	3 (16%)	22,30,33	1.91	4 (18%)
1	OMC	L1	3701	1	19,22,23	0.80	0	26,31,34	0.75	0
1	PSU	L1	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	L1	4296	1	18,21,22	1.36	3 (16%)	22,30,33	1.92	4 (18%)
1	PSU	L1	3639	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
1	OMG	L1	3944	1	18,26,27	0.95	1 (5%)	19,38,41	1.07	1 (5%)
1	PSU	L1	4972	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	L1	4456	1	19,22,23	0.83	0	26,31,34	0.78	0
1	PSU	L1	1862	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	L3	55	68	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
30	OMU	S1	1326	30	19,22,23	1.20	3 (15%)	26,31,34	1.71	5 (19%)
30	PSU	S1	210	30	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	L1	4228	1	18,26,27	0.93	1 (5%)	19,38,41	1.13	2 (10%)
1	OMG	L1	4637	1	18,26,27	0.95	1 (5%)	19,38,41	1.14	2 (10%)
30	OMC	S1	1703	30	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	PSU	L1	3844	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	L1	2876	1	18,26,27	0.96	1 (5%)	19,38,41	1.08	2 (10%)
30	PSU	S1	572	30	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
30	PSU	S1	218	30	18,21,22	1.36	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	L1	3884	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L1	2815	1	18,25,26	0.99	1 (5%)	18,36,39	1.18	2 (11%)
1	OMC	L1	3869	1	19,22,23	0.82	0	26,31,34	0.78	0
1	PSU	L1	4431	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
30	OMU	S1	121	30	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
1	OMC	L1	1340	1	19,22,23	0.82	0	26,31,34	0.79	0
1	UY1	L1	3818	1	19,22,23	0.91	1 (5%)	22,31,34	1.71	3 (13%)
30	PSU	S1	651	30	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
30	PSU	S1	36	30	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)

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
30	6MZ	S1	1832	30	-	0/5/27/28	0/3/3/3
30	4AC	S1	1337	30	-	2/11/29/30	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	2632	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	1045	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	1625	1	-	0/5/27/28	0/3/3/3
30	OMU	S1	1804	30	-	1/9/27/28	0/2/2/2
1	PSU	L1	1860	1	-	0/7/25/26	0/2/2/2
1	5MC	L1	3782	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	801	30	-	0/7/25/26	0/2/2/2
1	OMU	L1	2415	1	-	0/9/27/28	0/2/2/2
30	PSU	S1	1056	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	822	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1367	30	-	0/7/25/26	0/2/2/2
30	G7M	S1	1639	30,32	-	0/3/25/26	0/3/3/3
30	OMU	S1	1288	30	-	0/9/27/28	0/2/2/2
30	PSU	S1	1046	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	1536	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	2787	1	-	0/5/27/28	0/3/3/3
30	A2M	S1	159	30	-	1/5/27/28	0/3/3/3
30	PSU	S1	686	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1347	30	-	0/7/25/26	0/2/2/2
30	A2M	S1	576	30	-	2/5/27/28	0/3/3/3
30	OMG	S1	1490	30	-	1/5/27/28	0/3/3/3
1	PSU	L1	3851	1	-	3/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A2M	S1	484	30	-	2/5/27/28	0/3/3/3
1	OMC	L1	2351	1	-	2/9/27/28	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	2824	1	-	1/9/27/28	0/2/2/2
30	PSU	S1	1244	30	-	0/7/25/26	0/2/2/2
30	OMU	S1	1442	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	4576	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	468	30	-	0/5/27/28	0/3/3/3
30	PSU	S1	1643	30	-	0/7/25/26	0/2/2/2
1	A2M	L1	3724	1	-	0/5/27/28	0/3/3/3
30	OMC	S1	462	30	-	0/9/27/28	0/2/2/2
30	OMG	S1	683	30	-	0/5/27/28	0/3/3/3
1	A2M	L1	3785	1	-	2/5/27/28	0/3/3/3
30	A2M	S1	668	30	-	3/5/27/28	0/3/3/3
30	PSU	S1	1625	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	649	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1081	30	-	3/7/25/26	0/2/2/2
30	PSU	S1	1174	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	109	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4500	1	-	1/7/25/26	0/2/2/2
30	PSU	S1	1238	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	1522	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	2365	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4579	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	4392	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	5010	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4571	1	-	0/5/27/28	0/3/3/3
30	PSU	S1	1232	30	-	0/7/25/26	0/2/2/2
30	A2M	S1	1383	30	-	0/5/27/28	0/3/3/3
1	PSU	L1	4493	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	2424	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4423	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3792	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	1323	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	2363	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4673	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3637	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	27	30	-	0/5/27/28	0/3/3/3
1	PSU	L1	4521	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4628	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
30	PSU	S1	105	30	-	0/7/25/26	0/2/2/2
30	OMU	S1	428	30	-	4/9/27/28	0/2/2/2
30	A2M	S1	512	30	-	0/5/27/28	0/3/3/3
30	PSU	S1	1445	30	-	0/7/25/26	0/2/2/2
30	OMU	S1	627	30	-	1/9/27/28	0/2/2/2
30	OMU	S1	116	30	-	0/9/27/28	0/2/2/2
68	OMG	L3	75	68	-	0/5/27/28	0/3/3/3
1	OMG	L1	3744	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	3730	1	-	0/7/25/26	0/2/2/2
30	OMC	S1	1391	30	-	0/9/27/28	0/2/2/2
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3853	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	93	30	-	0/7/25/26	0/2/2/2
68	PSU	L3	69	68	-	0/7/25/26	0/2/2/2
1	PSU	L1	3920	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4471	1	-	2/7/25/26	0/2/2/2
1	PSU	L1	4532	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1326	1	-	1/5/27/28	0/3/3/3
30	PSU	S1	296	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	1177	30	-	0/7/25/26	0/2/2/2
1	OMC	L1	2422	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	3627	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	99	30	-	1/5/27/28	0/3/3/3
30	PSU	S1	1136	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4457	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	34	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	4494	1	-	0/5/27/28	0/3/3/3
50	NMM	Si	67	50	-	0/9/11/13	-
30	OMC	S1	174	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	5001	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3899	1	-	0/5/27/28	0/3/3/3
30	PSU	S1	1004	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	1677	1	-	3/7/25/26	0/2/2/2
30	OMG	S1	601	30	-	0/5/27/28	0/3/3/3
1	PSU	L1	1782	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	815	30	-	0/7/25/26	0/2/2/2
30	OMC	S1	797	30	-	0/9/27/28	0/2/2/2
1	A2M	L1	2401	1	-	0/5/27/28	0/3/3/3
30	PSU	S1	866	30	-	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	OMG	L1	4370	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	3695	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1881	1	-	4/9/27/28	0/2/2/2
1	PSU	L1	3770	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4523	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	4552	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	681	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	814	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	966	30	-	0/7/25/26	0/2/2/2
30	MA6	S1	1850	30	-	0/7/29/30	0/3/3/3
1	A2M	L1	398	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	4227	1	-	1/9/27/28	0/2/2/2
30	B8N	S1	1248	30	-	4/16/34/35	0/2/2/2
47	HY3	Sg	62	47	-	1/1/12/14	0/1/1/1
1	OMG	L1	4196	32,1	-	0/5/27/28	0/3/3/3
30	OMC	S1	517	30	-	0/9/27/28	0/2/2/2
1	OMG	L1	1316	1	-	2/5/27/28	0/3/3/3
1	A2M	L1	1534	1	-	2/5/27/28	0/3/3/3
39	IAS	SG	138	39	-	1/7/7/8	-
30	OMG	S1	644	30	-	4/5/27/28	0/3/3/3
1	OMG	L1	4499	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	3867	1	-	1/5/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	2839	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	609	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1744	1	-	0/7/25/26	0/2/2/2
30	A2M	S1	166	30	-	0/5/27/28	0/3/3/3
30	PSU	S1	863	30	-	0/7/25/26	0/2/2/2
1	A2M	L1	3718	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4623	1	-	1/5/27/28	0/3/3/3
1	5MC	L1	4447	1	-	4/7/25/26	0/2/2/2
30	OMC	S1	1272	30	-	0/9/27/28	0/2/2/2
1	OMC	L1	3808	1	-	1/9/27/28	0/2/2/2
30	PSU	S1	1692	30	-	0/7/25/26	0/2/2/2
30	MA6	S1	1851	30	-	2/7/29/30	0/3/3/3
1	OMU	L1	3925	1	-	0/9/27/28	0/2/2/2
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
30	A2M	S1	1031	30	-	1/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	L1	3887	1	-	2/9/27/28	0/2/2/2
30	A2M	S1	590	30	-	0/5/27/28	0/3/3/3
30	OMG	S1	1447	30	-	2/5/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1781	1	-	2/7/25/26	0/2/2/2
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
30	PSU	S1	406	30	-	0/7/25/26	0/2/2/2
30	A2M	S1	1678	30	-	0/5/27/28	0/3/3/3
30	PSU	S1	119	30	-	0/7/25/26	0/2/2/2
30	OMU	S1	172	30	-	0/9/27/28	0/2/2/2
1	PSU	L1	1683	1	-	0/7/25/26	0/2/2/2
30	4AC	S1	1842	30	-	4/11/29/30	0/2/2/2
1	PSU	L1	1792	1	-	0/7/25/26	0/2/2/2
30	OMU	S1	799	30	-	2/9/27/28	0/2/2/2
1	OMU	L1	4620	1	-	0/9/27/28	0/2/2/2
30	OMG	S1	1328	30	-	0/5/27/28	0/3/3/3
1	OMG	L1	2364	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	4618	1	-	1/5/27/28	0/3/3/3
1	OMC	L1	4536	1	-	1/9/27/28	0/2/2/2
30	OMU	S1	354	30	-	0/9/27/28	0/2/2/2
30	OMG	S1	436	30	-	0/5/27/28	0/3/3/3
1	PSU	L1	4420	1	-	3/7/25/26	0/2/2/2
1	A2M	L1	1871	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	1524	1	-	0/5/27/28	0/3/3/3
1	1MA	L1	1322	1	-	0/3/25/26	0/3/3/3
1	PSU	L1	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	1582	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	4590	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	3734	1	-	4/7/25/26	0/2/2/2
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
30	OMG	S1	509	30	-	1/5/27/28	0/3/3/3
1	A2M	L1	400	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4312	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	3830	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4353	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	3701	1	-	6/9/27/28	0/2/2/2
1	PSU	L1	3768	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	3639	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	OMG	L1	3944	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4972	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	1862	1	-	0/7/25/26	0/2/2/2
68	PSU	L3	55	68	-	0/7/25/26	0/2/2/2
30	OMU	S1	1326	30	-	0/9/27/28	0/2/2/2
30	PSU	S1	210	30	-	0/7/25/26	0/2/2/2
1	OMG	L1	4228	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	4637	1	-	2/5/27/28	0/3/3/3
30	OMC	S1	1703	30	-	1/9/27/28	0/2/2/2
1	PSU	L1	3844	1	-	1/7/25/26	0/2/2/2
1	OMG	L1	2876	1	-	1/5/27/28	0/3/3/3
30	PSU	S1	572	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	218	30	-	0/7/25/26	0/2/2/2
1	PSU	L1	3884	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	2815	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	3869	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4431	1	-	0/7/25/26	0/2/2/2
30	OMU	S1	121	30	-	1/9/27/28	0/2/2/2
1	OMC	L1	1340	1	-	1/9/27/28	0/2/2/2
1	UY1	L1	3818	1	-	3/9/27/28	0/2/2/2
30	PSU	S1	651	30	-	0/7/25/26	0/2/2/2
30	PSU	S1	36	30	-	0/7/25/26	0/2/2/2

All (354) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S1	1639	G7M	C5-C4	7.28	1.53	1.39
30	S1	1639	G7M	O6-C6	7.22	1.38	1.23
30	S1	1639	G7M	C2-N2	4.46	1.44	1.34
1	L1	1322	1MA	C2-N3	4.29	1.34	1.29
30	S1	1639	G7M	C2-N1	3.77	1.47	1.37
30	S1	1248	B8N	C4-N3	-3.33	1.34	1.40
30	S1	1639	G7M	C8-N9	3.30	1.39	1.33
30	S1	1639	G7M	C2-N3	3.28	1.41	1.33
30	S1	1851	MA6	C5-N7	3.26	1.51	1.39
30	S1	1850	MA6	C5-N7	3.24	1.51	1.39
30	S1	34	PSU	C6-C5	3.22	1.39	1.35
1	L1	4420	PSU	C6-C5	3.21	1.39	1.35
30	S1	1445	PSU	C6-C5	3.21	1.39	1.35
1	L1	4423	PSU	C6-C5	3.18	1.39	1.35
1	L1	3734	PSU	C6-C5	3.16	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1322	1MA	C6-N6	3.14	1.35	1.27
30	S1	210	PSU	C6-C5	3.11	1.38	1.35
30	S1	1625	PSU	C6-C5	3.10	1.38	1.35
30	S1	218	PSU	C6-C5	3.09	1.38	1.35
1	L1	3715	PSU	C6-C5	3.09	1.38	1.35
30	S1	1639	G7M	C6-N1	3.09	1.42	1.37
30	S1	105	PSU	C6-C5	3.09	1.38	1.35
1	L1	3770	PSU	C6-C5	3.08	1.38	1.35
30	S1	609	PSU	C6-C5	3.07	1.38	1.35
30	S1	1842	4AC	C4-N4	-3.06	1.35	1.39
1	L1	1744	PSU	C6-C5	3.03	1.38	1.35
30	S1	651	PSU	C6-C5	3.03	1.38	1.35
30	S1	866	PSU	C6-C5	3.03	1.38	1.35
1	L1	5010	PSU	C6-C5	3.02	1.38	1.35
30	S1	1174	PSU	C6-C5	3.02	1.38	1.35
30	S1	572	PSU	C6-C5	3.02	1.38	1.35
30	S1	406	PSU	C6-C5	3.02	1.38	1.35
30	S1	801	PSU	C6-C5	3.01	1.38	1.35
1	L1	1677	PSU	C6-C5	3.01	1.38	1.35
30	S1	1136	PSU	C6-C5	3.01	1.38	1.35
30	S1	1081	PSU	C6-C5	2.99	1.38	1.35
30	S1	814	PSU	C6-C5	2.99	1.38	1.35
30	S1	822	PSU	C6-C5	2.98	1.38	1.35
30	S1	1337	4AC	C4-N4	-2.98	1.35	1.39
1	L1	4532	PSU	C6-C5	2.98	1.38	1.35
1	L1	4312	PSU	C6-C5	2.98	1.38	1.35
1	L1	1860	PSU	C6-C5	2.98	1.38	1.35
1	L1	4552	PSU	C6-C5	2.97	1.38	1.35
68	L3	69	PSU	C6-C5	2.97	1.38	1.35
30	S1	1244	PSU	C6-C5	2.97	1.38	1.35
1	L1	2632	PSU	C6-C5	2.96	1.38	1.35
30	S1	863	PSU	C6-C5	2.96	1.38	1.35
30	S1	1692	PSU	C6-C5	2.96	1.38	1.35
1	L1	3768	PSU	C6-C5	2.96	1.38	1.35
30	S1	1177	PSU	C6-C5	2.96	1.38	1.35
1	L1	3730	PSU	C6-C5	2.96	1.38	1.35
30	S1	1004	PSU	C6-C5	2.95	1.38	1.35
30	S1	36	PSU	C6-C5	2.95	1.38	1.35
1	L1	4353	PSU	C6-C5	2.95	1.38	1.35
1	L1	4361	PSU	C6-C5	2.95	1.38	1.35
30	S1	109	PSU	C6-C5	2.95	1.38	1.35
30	S1	1056	PSU	C6-C5	2.94	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1792	PSU	C6-C5	2.94	1.38	1.35
30	S1	93	PSU	C6-C5	2.94	1.38	1.35
1	L1	4972	PSU	C6-C5	2.93	1.38	1.35
1	L1	4471	PSU	C6-C5	2.93	1.38	1.35
30	S1	686	PSU	C6-C5	2.92	1.38	1.35
30	S1	966	PSU	C6-C5	2.92	1.38	1.35
30	S1	1238	PSU	C6-C5	2.92	1.38	1.35
1	L1	4576	PSU	C6-C5	2.91	1.38	1.35
30	S1	119	PSU	C6-C5	2.91	1.38	1.35
68	L3	55	PSU	C6-C5	2.91	1.38	1.35
1	L1	3695	PSU	C6-C5	2.91	1.38	1.35
1	L1	4403	PSU	C6-C5	2.91	1.38	1.35
30	S1	1367	PSU	C6-C5	2.90	1.38	1.35
1	L1	4353	PSU	C4-N3	-2.90	1.33	1.38
30	S1	1347	PSU	C6-C5	2.90	1.38	1.35
30	S1	109	PSU	C4-N3	-2.90	1.33	1.38
1	L1	5001	PSU	C6-C5	2.89	1.38	1.35
1	L1	3851	PSU	C6-C5	2.88	1.38	1.35
1	L1	4457	PSU	C6-C5	2.88	1.38	1.35
1	L1	2839	PSU	C4-N3	-2.88	1.33	1.38
1	L1	1536	PSU	C4-N3	-2.88	1.33	1.38
1	L1	3920	PSU	C6-C5	2.88	1.38	1.35
1	L1	3637	PSU	C4-N3	-2.87	1.33	1.38
1	L1	4293	PSU	C6-C5	2.87	1.38	1.35
1	L1	4579	PSU	C4-N3	-2.87	1.33	1.38
30	S1	649	PSU	C6-C5	2.87	1.38	1.35
1	L1	1683	PSU	C4-N3	-2.86	1.33	1.38
1	L1	3695	PSU	C4-N3	-2.86	1.33	1.38
1	L1	4431	PSU	C6-C5	2.86	1.38	1.35
1	L1	4442	PSU	C4-N3	-2.86	1.33	1.38
1	L1	1582	PSU	C4-N3	-2.86	1.33	1.38
1	L1	4552	PSU	C4-N3	-2.86	1.33	1.38
30	S1	1692	PSU	C4-N3	-2.86	1.33	1.38
1	L1	1683	PSU	C6-C5	2.86	1.38	1.35
30	S1	815	PSU	C6-C5	2.85	1.38	1.35
30	S1	814	PSU	C4-N3	-2.85	1.33	1.38
1	L1	1862	PSU	C4-N3	-2.85	1.33	1.38
30	S1	649	PSU	C4-N3	-2.85	1.33	1.38
30	S1	815	PSU	C4-N3	-2.85	1.33	1.38
1	L1	4628	PSU	C4-N3	-2.85	1.33	1.38
30	S1	93	PSU	C4-N3	-2.85	1.33	1.38
30	S1	681	PSU	C4-N3	-2.84	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4579	PSU	C6-C5	2.84	1.38	1.35
1	L1	4493	PSU	C4-N3	-2.84	1.33	1.38
1	L1	4299	PSU	C6-C5	2.84	1.38	1.35
1	L1	4532	PSU	C4-N3	-2.83	1.33	1.38
1	L1	4361	PSU	C4-N3	-2.83	1.33	1.38
1	L1	4457	PSU	C4-N3	-2.83	1.33	1.38
1	L1	4296	PSU	C4-N3	-2.83	1.33	1.38
1	L1	2508	PSU	C6-C5	2.83	1.38	1.35
30	S1	1045	PSU	C4-N3	-2.82	1.33	1.38
30	S1	1643	PSU	C4-N3	-2.82	1.33	1.38
30	S1	1248	B8N	C6-C5	2.82	1.38	1.34
30	S1	1643	PSU	C6-C5	2.82	1.38	1.35
30	S1	1248	B8N	C2-N3	-2.82	1.33	1.38
1	L1	1782	PSU	C6-C5	2.82	1.38	1.35
1	L1	2508	PSU	C4-N3	-2.82	1.33	1.38
1	L1	4689	PSU	C4-N3	-2.82	1.33	1.38
1	L1	3639	PSU	C4-N3	-2.82	1.33	1.38
1	L1	1860	PSU	C4-N3	-2.82	1.33	1.38
68	L3	69	PSU	C4-N3	-2.82	1.33	1.38
1	L1	4673	PSU	C4-N3	-2.82	1.33	1.38
30	S1	1046	PSU	C6-C5	2.82	1.38	1.35
1	L1	4972	PSU	C4-N3	-2.82	1.33	1.38
30	S1	1232	PSU	C4-N3	-2.81	1.33	1.38
30	S1	651	PSU	C4-N3	-2.81	1.33	1.38
1	L1	3639	PSU	C6-C5	2.81	1.38	1.35
1	L1	4500	PSU	C6-C5	2.81	1.38	1.35
1	L1	5010	PSU	C4-N3	-2.81	1.33	1.38
1	L1	4431	PSU	C4-N3	-2.81	1.33	1.38
1	L1	3844	PSU	C4-N3	-2.81	1.33	1.38
1	L1	3844	PSU	C6-C5	2.81	1.38	1.35
30	S1	801	PSU	C4-N3	-2.81	1.33	1.38
1	L1	3884	PSU	C6-C5	2.80	1.38	1.35
30	S1	1238	PSU	C4-N3	-2.80	1.33	1.38
1	L1	3920	PSU	C4-N3	-2.80	1.33	1.38
1	L1	1677	PSU	C4-N3	-2.80	1.33	1.38
1	L1	1792	PSU	C4-N3	-2.80	1.33	1.38
30	S1	863	PSU	C4-N3	-2.80	1.33	1.38
1	L1	1782	PSU	C4-N3	-2.80	1.33	1.38
1	L1	3768	PSU	C4-N3	-2.80	1.33	1.38
30	S1	681	PSU	C6-C5	2.80	1.38	1.35
1	L1	5001	PSU	C4-N3	-2.80	1.33	1.38
1	L1	1781	PSU	C6-C5	2.80	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4493	PSU	C6-C5	2.79	1.38	1.35
1	L1	4471	PSU	C4-N3	-2.79	1.33	1.38
1	L1	1862	PSU	C6-C5	2.79	1.38	1.35
1	L1	4521	PSU	C4-N3	-2.79	1.33	1.38
1	L1	4673	PSU	C6-C5	2.79	1.38	1.35
68	L3	75	OMG	C6-N1	-2.79	1.33	1.37
30	S1	105	PSU	C4-N3	-2.79	1.33	1.38
1	L1	3853	PSU	C6-C5	2.79	1.38	1.35
30	S1	1136	PSU	C4-N3	-2.79	1.33	1.38
1	L1	1582	PSU	C6-C5	2.79	1.38	1.35
1	L1	2839	PSU	C6-C5	2.78	1.38	1.35
1	L1	4299	PSU	C4-N3	-2.78	1.33	1.38
30	S1	572	PSU	C4-N3	-2.78	1.33	1.38
1	L1	4689	PSU	C6-C5	2.78	1.38	1.35
1	L1	3884	PSU	C4-N3	-2.78	1.33	1.38
1	L1	2876	OMG	C6-N1	-2.78	1.33	1.37
1	L1	4442	PSU	C6-C5	2.77	1.38	1.35
1	L1	1781	PSU	C4-N3	-2.77	1.33	1.38
30	S1	296	PSU	C6-C5	2.77	1.38	1.35
30	S1	119	PSU	C4-N3	-2.77	1.33	1.38
1	L1	1522	OMG	C6-N1	-2.77	1.33	1.37
30	S1	1367	PSU	C4-N3	-2.77	1.33	1.38
30	S1	1347	PSU	C4-N3	-2.77	1.33	1.38
30	S1	1177	PSU	C4-N3	-2.76	1.33	1.38
1	L1	3851	PSU	C4-N3	-2.76	1.33	1.38
30	S1	1056	PSU	C4-N3	-2.76	1.33	1.38
1	L1	4628	PSU	C6-C5	2.76	1.38	1.35
68	L3	55	PSU	C4-N3	-2.76	1.33	1.38
1	L1	4403	PSU	C4-N3	-2.76	1.33	1.38
1	L1	4296	PSU	C6-C5	2.76	1.38	1.35
1	L1	4312	PSU	C4-N3	-2.75	1.33	1.38
30	S1	1174	PSU	C4-N3	-2.75	1.33	1.38
30	S1	822	PSU	C4-N3	-2.75	1.33	1.38
1	L1	3853	PSU	C4-N3	-2.75	1.33	1.38
1	L1	4293	PSU	C4-N3	-2.75	1.33	1.38
30	S1	609	PSU	C4-N3	-2.75	1.33	1.38
30	S1	1232	PSU	C6-C5	2.75	1.38	1.35
1	L1	3715	PSU	C4-N3	-2.75	1.33	1.38
1	L1	4196	OMG	C6-N1	-2.75	1.33	1.37
30	S1	1081	PSU	C4-N3	-2.74	1.33	1.38
30	S1	1625	PSU	C4-N3	-2.74	1.33	1.38
1	L1	1536	PSU	C6-C5	2.74	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	4227	OMU	C4-N3	-2.74	1.33	1.38
1	L1	4306	OMU	C4-N3	-2.74	1.33	1.38
30	S1	1004	PSU	C4-N3	-2.74	1.33	1.38
1	L1	4620	OMU	C4-N3	-2.73	1.33	1.38
1	L1	3770	PSU	C4-N3	-2.73	1.33	1.38
1	L1	3730	PSU	C4-N3	-2.73	1.33	1.38
30	S1	296	PSU	C4-N3	-2.73	1.33	1.38
1	L1	2632	PSU	C4-N3	-2.72	1.33	1.38
1	L1	4500	PSU	C4-N3	-2.72	1.33	1.38
1	L1	4623	OMG	C6-N1	-2.72	1.33	1.37
1	L1	3744	OMG	C6-N1	-2.72	1.33	1.37
30	S1	1244	PSU	C4-N3	-2.72	1.33	1.38
30	S1	686	PSU	C4-N3	-2.71	1.33	1.38
1	L1	4447	5MC	C6-C5	2.71	1.39	1.34
30	S1	34	PSU	C4-N3	-2.71	1.33	1.38
1	L1	1744	PSU	C4-N3	-2.71	1.33	1.38
30	S1	1045	PSU	C6-C5	2.71	1.38	1.35
1	L1	3925	OMU	C4-N3	-2.71	1.33	1.38
1	L1	4576	PSU	C4-N3	-2.71	1.33	1.38
1	L1	4499	OMG	C6-N1	-2.70	1.33	1.37
30	S1	1046	PSU	C4-N3	-2.70	1.33	1.38
30	S1	218	PSU	C4-N3	-2.70	1.33	1.38
1	L1	4494	OMG	C6-N1	-2.70	1.33	1.37
30	S1	121	OMU	C4-N3	-2.69	1.33	1.38
30	S1	509	OMG	C6-N1	-2.69	1.33	1.37
1	L1	1625	OMG	C6-N1	-2.69	1.33	1.37
1	L1	4637	OMG	C6-N1	-2.69	1.33	1.37
1	L1	3899	OMG	C6-N1	-2.69	1.33	1.37
1	L1	1316	OMG	C6-N1	-2.69	1.33	1.37
1	L1	4392	OMG	C6-N1	-2.69	1.33	1.37
30	S1	36	PSU	C4-N3	-2.68	1.33	1.38
1	L1	3627	OMG	C6-N1	-2.68	1.33	1.37
1	L1	3734	PSU	C4-N3	-2.68	1.33	1.38
1	L1	3792	OMG	C6-N1	-2.67	1.33	1.37
30	S1	966	PSU	C4-N3	-2.66	1.33	1.38
1	L1	4521	PSU	C6-C5	2.66	1.38	1.35
1	L1	4370	OMG	C6-N1	-2.66	1.33	1.37
30	S1	866	PSU	C4-N3	-2.66	1.33	1.38
30	S1	1442	OMU	C4-N3	-2.65	1.33	1.38
1	L1	4498	OMU	C4-N3	-2.65	1.33	1.38
30	S1	1447	OMG	C6-N1	-2.64	1.33	1.37
30	S1	1328	OMG	C6-N1	-2.64	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2424	OMG	C6-N1	-2.64	1.33	1.37
1	L1	2837	OMU	C4-N3	-2.64	1.33	1.38
1	L1	4228	OMG	C6-N1	-2.63	1.33	1.37
30	S1	601	OMG	C6-N1	-2.63	1.33	1.37
30	S1	644	OMG	C6-N1	-2.63	1.33	1.37
30	S1	354	OMU	C4-N3	-2.63	1.33	1.38
30	S1	428	OMU	C4-N3	-2.63	1.33	1.38
30	S1	436	OMG	C6-N1	-2.63	1.34	1.37
1	L1	2415	OMU	C4-N3	-2.62	1.33	1.38
1	L1	4423	PSU	C4-N3	-2.62	1.34	1.38
30	S1	406	PSU	C4-N3	-2.62	1.34	1.38
30	S1	210	PSU	C4-N3	-2.60	1.34	1.38
1	L1	3637	PSU	C6-C5	2.60	1.38	1.35
30	S1	683	OMG	C6-N1	-2.59	1.34	1.37
1	L1	4618	OMG	C6-N1	-2.59	1.34	1.37
30	S1	1490	OMG	C6-N1	-2.58	1.34	1.37
30	S1	116	OMU	C4-N3	-2.58	1.33	1.38
30	S1	1445	PSU	C4-N3	-2.58	1.34	1.38
1	L1	3782	5MC	C6-N1	-2.57	1.33	1.38
30	S1	172	OMU	C4-N3	-2.57	1.34	1.38
1	L1	2364	OMG	C6-N1	-2.56	1.34	1.37
30	S1	1804	OMU	C4-N3	-2.54	1.34	1.38
30	S1	1326	OMU	C4-N3	-2.53	1.34	1.38
30	S1	799	OMU	C4-N3	-2.53	1.34	1.38
30	S1	1288	OMU	C4-N3	-2.52	1.34	1.38
1	L1	3782	5MC	C6-C5	2.47	1.38	1.34
1	L1	3944	OMG	C6-N1	-2.47	1.34	1.37
30	S1	1850	MA6	C4-N3	-2.45	1.32	1.35
30	S1	1851	MA6	C4-N3	-2.44	1.32	1.35
30	S1	627	OMU	C4-N3	-2.44	1.34	1.38
30	S1	354	OMU	C2-N3	-2.43	1.33	1.38
1	L1	4420	PSU	C4-N3	-2.43	1.34	1.38
30	S1	576	A2M	C5-C4	2.43	1.47	1.40
1	L1	4447	5MC	C6-N1	-2.42	1.33	1.38
30	S1	590	A2M	C5-C4	2.42	1.47	1.40
1	L1	3925	OMU	C2-N3	-2.39	1.33	1.38
30	S1	99	A2M	C5-C4	2.39	1.47	1.40
30	S1	166	A2M	C5-C4	2.38	1.47	1.40
30	S1	121	OMU	C2-N3	-2.37	1.33	1.38
1	L1	4306	OMU	C2-N3	-2.36	1.33	1.38
1	L1	3867	A2M	C5-C4	2.35	1.47	1.40
30	S1	159	A2M	C5-C4	2.35	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	2401	A2M	C5-C4	2.35	1.47	1.40
30	S1	1678	A2M	C5-C4	2.33	1.47	1.40
1	L1	1323	A2M	C5-C4	2.33	1.47	1.40
1	L1	400	A2M	C5-C4	2.33	1.47	1.40
1	L1	3724	A2M	C5-C4	2.33	1.47	1.40
30	S1	468	A2M	C5-C4	2.32	1.47	1.40
30	S1	1383	A2M	C5-C4	2.32	1.47	1.40
30	S1	27	A2M	C5-C4	2.32	1.47	1.40
1	L1	4620	OMU	C2-N3	-2.32	1.33	1.38
1	L1	2837	OMU	C2-N3	-2.31	1.33	1.38
30	S1	512	A2M	C5-C4	2.31	1.47	1.40
30	S1	484	A2M	C5-C4	2.31	1.47	1.40
1	L1	4590	A2M	C5-C4	2.30	1.47	1.40
1	L1	3830	A2M	C5-C4	2.30	1.47	1.40
1	L1	3718	A2M	C5-C4	2.30	1.47	1.40
30	S1	116	OMU	C2-N3	-2.30	1.33	1.38
30	S1	668	A2M	C5-C4	2.30	1.47	1.40
30	S1	1832	6MZ	C5-C4	2.30	1.47	1.40
1	L1	398	A2M	C5-C4	2.29	1.47	1.40
1	L1	1871	A2M	C5-C4	2.29	1.47	1.40
1	L1	2815	A2M	C5-C4	2.28	1.47	1.40
30	S1	1442	OMU	C2-N3	-2.28	1.33	1.38
1	L1	2363	A2M	C5-C4	2.28	1.47	1.40
1	L1	3825	A2M	C5-C4	2.27	1.46	1.40
1	L1	4571	A2M	C5-C4	2.26	1.46	1.40
1	L1	4498	OMU	C2-N3	-2.26	1.33	1.38
1	L1	4227	OMU	C2-N3	-2.26	1.33	1.38
1	L1	4523	A2M	C5-C4	2.26	1.46	1.40
30	S1	172	OMU	C2-N3	-2.25	1.34	1.38
1	L1	1326	A2M	C5-C4	2.25	1.46	1.40
1	L1	2787	A2M	C5-C4	2.25	1.46	1.40
30	S1	1031	A2M	C5-C4	2.25	1.46	1.40
30	S1	1326	OMU	C2-N3	-2.24	1.34	1.38
1	L1	4220	6MZ	C5-C4	2.24	1.46	1.40
1	L1	1524	A2M	C5-C4	2.24	1.46	1.40
30	S1	1081	PSU	C2-N3	-2.21	1.33	1.37
30	S1	428	OMU	C2-N3	-2.21	1.34	1.38
30	S1	1288	OMU	C2-N3	-2.20	1.34	1.38
1	L1	2415	OMU	C2-N3	-2.19	1.34	1.38
1	L1	3785	A2M	C5-C4	2.19	1.46	1.40
30	S1	1383	A2M	O4'-C1'	2.19	1.44	1.41
1	L1	1534	A2M	C5-C4	2.19	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S1	1804	OMU	C2-N3	-2.17	1.34	1.38
30	S1	1337	4AC	C7-N4	-2.15	1.33	1.37
1	L1	3639	PSU	C2-N3	-2.14	1.33	1.37
30	S1	1842	4AC	C7-N4	-2.13	1.33	1.37
1	L1	3818	UY1	C4-N3	-2.13	1.34	1.38
1	L1	4457	PSU	C2-N3	-2.13	1.33	1.37
30	S1	121	OMU	C5-C4	-2.11	1.39	1.43
1	L1	2837	OMU	C5-C4	-2.11	1.39	1.43
1	L1	3925	OMU	C5-C4	-2.11	1.39	1.43
30	S1	116	OMU	C5-C4	-2.11	1.39	1.43
1	L1	4498	OMU	C5-C4	-2.10	1.39	1.43
30	S1	799	OMU	C2-N3	-2.10	1.34	1.38
30	S1	627	OMU	C2-N1	2.09	1.41	1.38
30	S1	1081	PSU	C2-N1	-2.08	1.33	1.36
30	S1	354	OMU	C5-C4	-2.08	1.39	1.43
1	L1	4361	PSU	C2-N3	-2.07	1.34	1.37
30	S1	627	OMU	C2-N3	-2.07	1.34	1.38
30	S1	1347	PSU	C2-N3	-2.07	1.34	1.37
1	L1	2415	OMU	C5-C4	-2.06	1.39	1.43
1	L1	4299	PSU	C2-N3	-2.06	1.34	1.37
30	S1	1643	PSU	C2-N3	-2.06	1.34	1.37
1	L1	3853	PSU	C2-N3	-2.06	1.34	1.37
1	L1	4306	OMU	C5-C4	-2.05	1.39	1.43
1	L1	4442	PSU	C2-N3	-2.05	1.34	1.37
1	L1	4620	OMU	C5-C4	-2.04	1.39	1.43
30	S1	1177	PSU	C2-N3	-2.04	1.34	1.37
30	S1	109	PSU	C2-N3	-2.04	1.34	1.37
1	L1	2632	PSU	C2-N3	-2.04	1.34	1.37
30	S1	1804	OMU	C2-N1	2.04	1.41	1.38
1	L1	4532	PSU	C2-N3	-2.04	1.34	1.37
1	L1	4521	PSU	C2-N3	-2.03	1.34	1.37
30	S1	1442	OMU	C5-C4	-2.02	1.39	1.43
1	L1	3734	PSU	C2-N3	-2.02	1.34	1.37
1	L1	4673	PSU	C2-N3	-2.02	1.34	1.37
1	L1	4579	PSU	C2-N3	-2.01	1.34	1.37
30	S1	799	OMU	C2-N1	2.01	1.41	1.38
1	L1	3637	PSU	C2-N1	-2.01	1.34	1.36
1	L1	4296	PSU	C2-N3	-2.01	1.34	1.37
30	S1	1232	PSU	C2-N3	-2.01	1.34	1.37
30	S1	93	PSU	C2-N3	-2.00	1.34	1.37
30	S1	1326	OMU	C5-C4	-2.00	1.39	1.43
30	S1	172	OMU	C5-C4	-2.00	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	5010	PSU	C2-N3	-2.00	1.34	1.37
1	L1	1582	PSU	C2-N3	-2.00	1.34	1.37
1	L1	4353	PSU	C2-N3	-2.00	1.34	1.37

All (560) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	S1	1692	PSU	N1-C2-N3	6.24	122.19	115.13
1	L1	1582	PSU	N1-C2-N3	6.23	122.19	115.13
1	L1	5010	PSU	N1-C2-N3	6.19	122.14	115.13
68	L3	69	PSU	N1-C2-N3	6.17	122.12	115.13
30	S1	801	PSU	N1-C2-N3	6.16	122.11	115.13
30	S1	651	PSU	N1-C2-N3	6.15	122.09	115.13
30	S1	863	PSU	N1-C2-N3	6.14	122.09	115.13
1	L1	4500	PSU	N1-C2-N3	6.13	122.07	115.13
30	S1	649	PSU	N1-C2-N3	6.13	122.07	115.13
30	S1	681	PSU	N1-C2-N3	6.13	122.07	115.13
30	S1	815	PSU	N1-C2-N3	6.12	122.07	115.13
1	L1	4442	PSU	N1-C2-N3	6.12	122.06	115.13
30	S1	1238	PSU	N1-C2-N3	6.12	122.06	115.13
1	L1	3637	PSU	N1-C2-N3	6.10	122.04	115.13
30	S1	105	PSU	N1-C2-N3	6.10	122.04	115.13
1	L1	3730	PSU	N1-C2-N3	6.10	122.04	115.13
30	S1	1004	PSU	N1-C2-N3	6.10	122.04	115.13
30	S1	572	PSU	N1-C2-N3	6.10	122.04	115.13
30	S1	1347	PSU	N1-C2-N3	6.09	122.03	115.13
1	L1	4296	PSU	N1-C2-N3	6.09	122.03	115.13
1	L1	3853	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	2508	PSU	N1-C2-N3	6.08	122.02	115.13
30	S1	109	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	3715	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	1683	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	4972	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	4361	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	4579	PSU	N1-C2-N3	6.08	122.02	115.13
1	L1	4532	PSU	N1-C2-N3	6.07	122.01	115.13
30	S1	822	PSU	N1-C2-N3	6.07	122.01	115.13
1	L1	2839	PSU	N1-C2-N3	6.06	122.00	115.13
1	L1	4293	PSU	N1-C2-N3	6.06	122.00	115.13
1	L1	1677	PSU	N1-C2-N3	6.06	121.99	115.13
1	L1	4628	PSU	N1-C2-N3	6.06	121.99	115.13
30	S1	1232	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(°)
1	L1	4673	PSU	N1-C2-N3	6.05	121.99	115.13
1	L1	3768	PSU	N1-C2-N3	6.05	121.98	115.13
1	L1	1792	PSU	N1-C2-N3	6.04	121.98	115.13
1	L1	3884	PSU	N1-C2-N3	6.04	121.97	115.13
1	L1	4353	PSU	N1-C2-N3	6.04	121.97	115.13
1	L1	3920	PSU	N1-C2-N3	6.03	121.96	115.13
1	L1	1781	PSU	N1-C2-N3	6.02	121.95	115.13
30	S1	1625	PSU	N1-C2-N3	6.02	121.95	115.13
1	L1	4471	PSU	N1-C2-N3	6.01	121.94	115.13
1	L1	4493	PSU	N1-C2-N3	6.01	121.94	115.13
1	L1	1860	PSU	N1-C2-N3	6.01	121.94	115.13
30	S1	1177	PSU	N1-C2-N3	6.01	121.94	115.13
30	S1	1136	PSU	N1-C2-N3	6.01	121.94	115.13
30	S1	866	PSU	N1-C2-N3	6.01	121.94	115.13
30	S1	1056	PSU	N1-C2-N3	6.00	121.93	115.13
1	L1	4431	PSU	N1-C2-N3	6.00	121.93	115.13
30	S1	686	PSU	N1-C2-N3	5.99	121.92	115.13
1	L1	4689	PSU	N1-C2-N3	5.99	121.92	115.13
30	S1	609	PSU	N1-C2-N3	5.99	121.92	115.13
1	L1	3695	PSU	N1-C2-N3	5.99	121.92	115.13
30	S1	34	PSU	N1-C2-N3	5.99	121.92	115.13
30	S1	296	PSU	N1-C2-N3	5.99	121.92	115.13
30	S1	1367	PSU	N1-C2-N3	5.98	121.91	115.13
1	L1	3844	PSU	N1-C2-N3	5.98	121.91	115.13
1	L1	4220	6MZ	C2-N1-C6	5.98	121.72	116.59
30	S1	1643	PSU	N1-C2-N3	5.97	121.89	115.13
30	S1	36	PSU	N1-C2-N3	5.96	121.89	115.13
1	L1	1744	PSU	N1-C2-N3	5.96	121.89	115.13
30	S1	119	PSU	N1-C2-N3	5.96	121.88	115.13
1	L1	1536	PSU	N1-C2-N3	5.95	121.87	115.13
30	S1	814	PSU	N1-C2-N3	5.95	121.87	115.13
1	L1	1862	PSU	N1-C2-N3	5.95	121.87	115.13
30	S1	1045	PSU	N1-C2-N3	5.95	121.87	115.13
30	S1	1244	PSU	N1-C2-N3	5.94	121.86	115.13
1	L1	5001	PSU	N1-C2-N3	5.94	121.86	115.13
1	L1	4312	PSU	N1-C2-N3	5.93	121.85	115.13
68	L3	55	PSU	N1-C2-N3	5.93	121.85	115.13
1	L1	4552	PSU	N1-C2-N3	5.93	121.85	115.13
30	S1	1174	PSU	N1-C2-N3	5.93	121.85	115.13
30	S1	93	PSU	N1-C2-N3	5.93	121.84	115.13
1	L1	4299	PSU	N1-C2-N3	5.92	121.84	115.13
1	L1	4521	PSU	N1-C2-N3	5.92	121.83	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3639	PSU	N1-C2-N3	5.90	121.81	115.13
1	L1	3851	PSU	N1-C2-N3	5.89	121.80	115.13
1	L1	2632	PSU	N1-C2-N3	5.89	121.80	115.13
30	S1	406	PSU	N1-C2-N3	5.88	121.80	115.13
30	S1	1445	PSU	N1-C2-N3	5.88	121.79	115.13
1	L1	1782	PSU	N1-C2-N3	5.88	121.79	115.13
30	S1	210	PSU	N1-C2-N3	5.88	121.79	115.13
1	L1	4403	PSU	N1-C2-N3	5.87	121.78	115.13
1	L1	3770	PSU	N1-C2-N3	5.87	121.78	115.13
30	S1	966	PSU	N1-C2-N3	5.85	121.76	115.13
30	S1	1046	PSU	N1-C2-N3	5.85	121.76	115.13
30	S1	218	PSU	N1-C2-N3	5.85	121.75	115.13
1	L1	4457	PSU	N1-C2-N3	5.82	121.73	115.13
30	S1	1850	MA6	C4-C5-N7	-5.81	103.35	109.40
1	L1	4420	PSU	N1-C2-N3	5.79	121.69	115.13
1	L1	4423	PSU	N1-C2-N3	5.78	121.68	115.13
30	S1	1081	PSU	N1-C2-N3	5.76	121.66	115.13
1	L1	4530	UR3	C4-N3-C2	-5.65	119.24	124.56
1	L1	4576	PSU	N1-C2-N3	5.63	121.51	115.13
30	S1	1851	MA6	C4-C5-N7	-5.60	103.56	109.40
1	L1	3734	PSU	N1-C2-N3	5.55	121.42	115.13
30	S1	1832	6MZ	C2-N1-C6	5.39	121.21	116.59
1	L1	3818	UY1	N1-C2-N3	4.83	120.60	115.13
30	S1	354	OMU	C4-N3-C2	-4.65	120.45	126.58
30	S1	121	OMU	C4-N3-C2	-4.60	120.51	126.58
30	S1	1288	OMU	C4-N3-C2	-4.58	120.53	126.58
1	L1	4227	OMU	C4-N3-C2	-4.58	120.54	126.58
30	S1	1326	OMU	C4-N3-C2	-4.57	120.55	126.58
1	L1	4620	OMU	C4-N3-C2	-4.56	120.56	126.58
1	L1	2837	OMU	C4-N3-C2	-4.54	120.59	126.58
1	L1	3925	OMU	C4-N3-C2	-4.54	120.60	126.58
30	S1	799	OMU	C4-N3-C2	-4.50	120.64	126.58
30	S1	172	OMU	C4-N3-C2	-4.49	120.66	126.58
30	S1	1442	OMU	C4-N3-C2	-4.48	120.67	126.58
1	L1	4498	OMU	C4-N3-C2	-4.47	120.68	126.58
1	L1	4306	OMU	C4-N3-C2	-4.45	120.72	126.58
30	S1	116	OMU	C4-N3-C2	-4.41	120.76	126.58
30	S1	1804	OMU	C4-N3-C2	-4.40	120.77	126.58
30	S1	428	OMU	C4-N3-C2	-4.39	120.80	126.58
1	L1	2415	OMU	C4-N3-C2	-4.34	120.86	126.58
30	S1	627	OMU	C4-N3-C2	-4.27	120.94	126.58
1	L1	4220	6MZ	C9-N6-C6	-4.26	119.20	122.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4227	OMU	N3-C2-N1	4.24	120.51	114.89
30	S1	1850	MA6	N3-C2-N1	-4.22	122.08	128.68
1	L1	2837	OMU	N3-C2-N1	4.20	120.47	114.89
1	L1	3925	OMU	N3-C2-N1	4.20	120.47	114.89
30	S1	1442	OMU	N3-C2-N1	4.20	120.46	114.89
30	S1	1692	PSU	C4-N3-C2	-4.20	120.29	126.34
1	L1	4498	OMU	N3-C2-N1	4.20	120.46	114.89
1	L1	4620	OMU	N3-C2-N1	4.19	120.45	114.89
30	S1	1842	4AC	N4-C4-N3	4.19	120.88	113.85
30	S1	121	OMU	N3-C2-N1	4.18	120.44	114.89
30	S1	354	OMU	N3-C2-N1	4.17	120.43	114.89
30	S1	649	PSU	C4-N3-C2	-4.17	120.33	126.34
30	S1	1851	MA6	C1'-N9-C4	-4.17	119.32	126.64
30	S1	1850	MA6	C1'-N9-C4	-4.14	119.36	126.64
30	S1	1288	OMU	N3-C2-N1	4.14	120.39	114.89
1	L1	1582	PSU	C4-N3-C2	-4.14	120.37	126.34
30	S1	428	OMU	N3-C2-N1	4.13	120.37	114.89
30	S1	572	PSU	C4-N3-C2	-4.13	120.39	126.34
1	L1	1781	PSU	C4-N3-C2	-4.12	120.40	126.34
30	S1	1238	PSU	C4-N3-C2	-4.11	120.41	126.34
30	S1	863	PSU	C4-N3-C2	-4.10	120.43	126.34
30	S1	1851	MA6	N3-C2-N1	-4.10	122.27	128.68
30	S1	1232	PSU	C4-N3-C2	-4.10	120.44	126.34
1	L1	4442	PSU	C4-N3-C2	-4.08	120.45	126.34
1	L1	4500	PSU	C4-N3-C2	-4.08	120.45	126.34
1	L1	3818	UY1	C4-N3-C2	-4.08	120.46	126.34
30	S1	1045	PSU	C4-N3-C2	-4.08	120.46	126.34
1	L1	4493	PSU	C4-N3-C2	-4.08	120.46	126.34
1	L1	4579	PSU	C4-N3-C2	-4.07	120.47	126.34
1	L1	2508	PSU	C4-N3-C2	-4.07	120.47	126.34
1	L1	4353	PSU	C4-N3-C2	-4.07	120.47	126.34
30	S1	1347	PSU	C4-N3-C2	-4.07	120.48	126.34
1	L1	4306	OMU	N3-C2-N1	4.07	120.29	114.89
1	L1	3730	PSU	C4-N3-C2	-4.06	120.49	126.34
1	L1	1782	PSU	C4-N3-C2	-4.06	120.49	126.34
1	L1	4447	5MC	C5-C6-N1	-4.05	119.17	123.34
30	S1	172	OMU	N3-C2-N1	4.05	120.27	114.89
1	L1	4296	PSU	C4-N3-C2	-4.05	120.50	126.34
1	L1	4521	PSU	C4-N3-C2	-4.04	120.51	126.34
30	S1	799	OMU	N3-C2-N1	4.04	120.25	114.89
30	S1	1804	OMU	N3-C2-N1	4.04	120.25	114.89
1	L1	1677	PSU	C4-N3-C2	-4.04	120.52	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	5010	PSU	C4-N3-C2	-4.03	120.54	126.34
30	S1	801	PSU	C4-N3-C2	-4.03	120.54	126.34
30	S1	815	PSU	C4-N3-C2	-4.03	120.54	126.34
1	L1	2839	PSU	C4-N3-C2	-4.02	120.54	126.34
1	L1	4628	PSU	C4-N3-C2	-4.02	120.55	126.34
1	L1	4420	PSU	O2-C2-N1	-4.01	118.37	122.79
68	L3	69	PSU	C4-N3-C2	-4.01	120.56	126.34
30	S1	681	PSU	C4-N3-C2	-4.01	120.56	126.34
30	S1	1056	PSU	C4-N3-C2	-4.01	120.56	126.34
1	L1	4972	PSU	C4-N3-C2	-4.00	120.57	126.34
1	L1	3637	PSU	C4-N3-C2	-4.00	120.57	126.34
30	S1	651	PSU	C4-N3-C2	-4.00	120.58	126.34
30	S1	1136	PSU	C4-N3-C2	-4.00	120.58	126.34
1	L1	4431	PSU	C4-N3-C2	-3.99	120.59	126.34
1	L1	3884	PSU	C4-N3-C2	-3.99	120.59	126.34
30	S1	866	PSU	C4-N3-C2	-3.98	120.60	126.34
1	L1	1792	PSU	C4-N3-C2	-3.98	120.61	126.34
30	S1	36	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L1	3770	PSU	C4-N3-C2	-3.97	120.61	126.34
1	L1	1683	PSU	C4-N3-C2	-3.97	120.62	126.34
1	L1	4293	PSU	C4-N3-C2	-3.96	120.63	126.34
1	L1	3768	PSU	C4-N3-C2	-3.96	120.63	126.34
1	L1	5001	PSU	C4-N3-C2	-3.96	120.63	126.34
1	L1	4673	PSU	C4-N3-C2	-3.96	120.64	126.34
1	L1	4361	PSU	C4-N3-C2	-3.95	120.64	126.34
1	L1	4299	PSU	C4-N3-C2	-3.95	120.65	126.34
30	S1	1004	PSU	C4-N3-C2	-3.95	120.65	126.34
30	S1	93	PSU	C4-N3-C2	-3.94	120.66	126.34
30	S1	116	OMU	N3-C2-N1	3.94	120.12	114.89
1	L1	1862	PSU	C4-N3-C2	-3.94	120.66	126.34
1	L1	3853	PSU	C4-N3-C2	-3.94	120.66	126.34
30	S1	1174	PSU	C4-N3-C2	-3.94	120.67	126.34
68	L3	55	PSU	C4-N3-C2	-3.94	120.67	126.34
30	S1	1625	PSU	C4-N3-C2	-3.94	120.67	126.34
1	L1	2415	OMU	N3-C2-N1	3.93	120.11	114.89
1	L1	3695	PSU	C4-N3-C2	-3.93	120.68	126.34
30	S1	109	PSU	C4-N3-C2	-3.93	120.68	126.34
1	L1	3844	PSU	C4-N3-C2	-3.92	120.68	126.34
1	L1	3637	PSU	O2-C2-N1	-3.92	118.48	122.79
30	S1	1244	PSU	C4-N3-C2	-3.92	120.70	126.34
30	S1	1326	OMU	N3-C2-N1	3.91	120.08	114.89
1	L1	4403	PSU	C4-N3-C2	-3.91	120.70	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	2632	PSU	C4-N3-C2	-3.91	120.71	126.34
30	S1	1177	PSU	C4-N3-C2	-3.91	120.71	126.34
30	S1	686	PSU	C4-N3-C2	-3.91	120.71	126.34
30	S1	119	PSU	C4-N3-C2	-3.91	120.71	126.34
30	S1	218	PSU	C4-N3-C2	-3.91	120.71	126.34
1	L1	1536	PSU	C4-N3-C2	-3.91	120.71	126.34
1	L1	4312	PSU	C4-N3-C2	-3.90	120.71	126.34
1	L1	4552	PSU	C4-N3-C2	-3.89	120.73	126.34
30	S1	1046	PSU	C4-N3-C2	-3.89	120.74	126.34
1	L1	1860	PSU	C4-N3-C2	-3.89	120.74	126.34
1	L1	1744	PSU	C4-N3-C2	-3.89	120.74	126.34
30	S1	1643	PSU	C4-N3-C2	-3.89	120.74	126.34
30	S1	1367	PSU	C4-N3-C2	-3.89	120.74	126.34
30	S1	814	PSU	C4-N3-C2	-3.88	120.74	126.34
1	L1	3851	PSU	C4-N3-C2	-3.88	120.75	126.34
1	L1	3920	PSU	C4-N3-C2	-3.86	120.77	126.34
30	S1	966	PSU	C4-N3-C2	-3.86	120.77	126.34
30	S1	296	PSU	C4-N3-C2	-3.85	120.79	126.34
1	L1	4457	PSU	C4-N3-C2	-3.85	120.79	126.34
1	L1	4532	PSU	C4-N3-C2	-3.84	120.80	126.34
30	S1	406	PSU	C4-N3-C2	-3.84	120.80	126.34
30	S1	609	PSU	C4-N3-C2	-3.84	120.80	126.34
1	L1	3639	PSU	C4-N3-C2	-3.84	120.81	126.34
1	L1	4471	PSU	C4-N3-C2	-3.82	120.84	126.34
1	L1	4576	PSU	C4-N3-C2	-3.81	120.84	126.34
30	S1	105	PSU	C4-N3-C2	-3.81	120.86	126.34
30	S1	34	PSU	C4-N3-C2	-3.79	120.87	126.34
1	L1	4689	PSU	C4-N3-C2	-3.78	120.89	126.34
30	S1	627	OMU	N3-C2-N1	3.78	119.91	114.89
1	L1	3782	5MC	C5-C6-N1	-3.77	119.46	123.34
1	L1	3715	PSU	C4-N3-C2	-3.76	120.91	126.34
1	L1	4423	PSU	C4-N3-C2	-3.76	120.92	126.34
30	S1	210	PSU	C4-N3-C2	-3.76	120.92	126.34
30	S1	354	OMU	C5-C4-N3	3.75	120.46	114.84
30	S1	822	PSU	O2-C2-N1	-3.75	118.67	122.79
30	S1	822	PSU	C4-N3-C2	-3.73	120.96	126.34
30	S1	121	OMU	C5-C4-N3	3.73	120.41	114.84
30	S1	1326	OMU	C5-C4-N3	3.71	120.39	114.84
30	S1	1445	PSU	C4-N3-C2	-3.70	121.00	126.34
1	L1	1744	PSU	O2-C2-N1	-3.68	118.74	122.79
1	L1	1536	PSU	O2-C2-N1	-3.67	118.75	122.79
1	L1	3734	PSU	C3'-C2'-C1'	3.63	105.87	101.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	S1	116	OMU	C5-C4-N3	3.63	120.27	114.84
30	S1	1442	OMU	C5-C4-N3	3.62	120.25	114.84
1	L1	4306	OMU	C5-C4-N3	3.61	120.25	114.84
1	L1	4620	OMU	C5-C4-N3	3.61	120.25	114.84
1	L1	4227	OMU	C5-C4-N3	3.61	120.24	114.84
30	S1	1288	OMU	C5-C4-N3	3.61	120.23	114.84
30	S1	406	PSU	O2-C2-N1	-3.60	118.83	122.79
30	S1	1004	PSU	O2-C2-N1	-3.60	118.83	122.79
30	S1	172	OMU	C5-C4-N3	3.60	120.22	114.84
30	S1	296	PSU	O2-C2-N1	-3.59	118.84	122.79
30	S1	799	OMU	C5-C4-N3	3.58	120.20	114.84
1	L1	3734	PSU	C4-N3-C2	-3.58	121.19	126.34
1	L1	3925	OMU	C5-C4-N3	3.58	120.19	114.84
30	S1	627	OMU	C5-C4-N3	3.57	120.18	114.84
30	S1	681	PSU	O2-C2-N1	-3.56	118.87	122.79
1	L1	2415	OMU	C5-C4-N3	3.56	120.17	114.84
1	L1	2837	OMU	C5-C4-N3	3.56	120.17	114.84
30	S1	36	PSU	O2-C2-N1	-3.56	118.87	122.79
30	S1	428	OMU	C5-C4-N3	3.56	120.16	114.84
30	S1	815	PSU	O2-C2-N1	-3.56	118.88	122.79
1	L1	4420	PSU	C4-N3-C2	-3.55	121.23	126.34
30	S1	686	PSU	O2-C2-N1	-3.52	118.91	122.79
1	L1	3884	PSU	O2-C2-N1	-3.51	118.92	122.79
30	S1	1174	PSU	O2-C2-N1	-3.51	118.93	122.79
1	L1	4628	PSU	O2-C2-N1	-3.50	118.94	122.79
30	S1	1248	B8N	C4-N3-C2	-3.49	121.04	125.46
1	L1	2508	PSU	O2-C2-N1	-3.49	118.95	122.79
30	S1	1804	OMU	C5-C4-N3	3.49	120.06	114.84
1	L1	3920	PSU	O2-C2-N1	-3.48	118.96	122.79
1	L1	3715	PSU	O2-C2-N1	-3.48	118.96	122.79
30	S1	1046	PSU	O2-C2-N1	-3.47	118.97	122.79
1	L1	4442	PSU	O2-C2-N1	-3.47	118.97	122.79
1	L1	3844	PSU	O2-C2-N1	-3.46	118.98	122.79
1	L1	4498	OMU	C5-C4-N3	3.46	120.02	114.84
1	L1	3853	PSU	O2-C2-N1	-3.45	118.99	122.79
30	S1	1081	PSU	C4-N3-C2	-3.45	121.37	126.34
30	S1	863	PSU	O2-C2-N1	-3.45	118.99	122.79
1	L1	4500	PSU	O2-C2-N1	-3.45	119.00	122.79
1	L1	4673	PSU	O2-C2-N1	-3.44	119.01	122.79
1	L1	4431	PSU	O2-C2-N1	-3.43	119.01	122.79
1	L1	4552	PSU	O2-C2-N1	-3.43	119.01	122.79
30	S1	105	PSU	O2-C2-N1	-3.43	119.01	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4493	PSU	O2-C2-N1	-3.43	119.01	122.79
30	S1	801	PSU	O2-C2-N1	-3.42	119.02	122.79
1	L1	1792	PSU	O2-C2-N1	-3.42	119.03	122.79
30	S1	814	PSU	O2-C2-N1	-3.41	119.03	122.79
1	L1	3770	PSU	O2-C2-N1	-3.40	119.05	122.79
1	L1	4689	PSU	O2-C2-N1	-3.39	119.06	122.79
1	L1	5001	PSU	O2-C2-N1	-3.39	119.06	122.79
1	L1	5010	PSU	O2-C2-N1	-3.39	119.06	122.79
1	L1	1862	PSU	O2-C2-N1	-3.39	119.06	122.79
1	L1	1683	PSU	O2-C2-N1	-3.39	119.06	122.79
30	S1	1445	PSU	O2-C2-N1	-3.38	119.06	122.79
1	L1	3695	PSU	O2-C2-N1	-3.38	119.07	122.79
1	L1	4471	PSU	O2-C2-N1	-3.38	119.07	122.79
30	S1	609	PSU	O2-C2-N1	-3.37	119.08	122.79
30	S1	1367	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L1	4296	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L1	1781	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L1	3730	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L1	1582	PSU	O2-C2-N1	-3.36	119.09	122.79
1	L1	4972	PSU	O2-C2-N1	-3.36	119.09	122.79
30	S1	1056	PSU	O2-C2-N1	-3.36	119.09	122.79
30	S1	966	PSU	O2-C2-N1	-3.36	119.10	122.79
68	L3	55	PSU	O2-C2-N1	-3.35	119.10	122.79
30	S1	1347	PSU	O2-C2-N1	-3.35	119.10	122.79
30	S1	1177	PSU	O2-C2-N1	-3.35	119.11	122.79
30	S1	1244	PSU	O2-C2-N1	-3.34	119.11	122.79
68	L3	69	PSU	O2-C2-N1	-3.34	119.11	122.79
30	S1	210	PSU	O2-C2-N1	-3.34	119.12	122.79
1	L1	3851	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L1	4576	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L1	4521	PSU	O2-C2-N1	-3.33	119.13	122.79
1	L1	4579	PSU	O2-C2-N1	-3.32	119.13	122.79
1	L1	4293	PSU	O2-C2-N1	-3.32	119.14	122.79
30	S1	866	PSU	O2-C2-N1	-3.31	119.14	122.79
30	S1	119	PSU	O2-C2-N1	-3.31	119.14	122.79
1	L1	4403	PSU	O2-C2-N1	-3.31	119.15	122.79
30	S1	27	A2M	N3-C2-N1	-3.30	123.52	128.68
1	L1	4532	PSU	O2-C2-N1	-3.30	119.16	122.79
1	L1	4312	PSU	O2-C2-N1	-3.29	119.16	122.79
1	L1	1881	OMC	O4'-C1'-N1	3.29	115.89	108.36
30	S1	1643	PSU	O2-C2-N1	-3.29	119.17	122.79
1	L1	398	A2M	N3-C2-N1	-3.29	123.54	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1677	PSU	O2-C2-N1	-3.28	119.18	122.79
30	S1	1625	PSU	O2-C2-N1	-3.28	119.18	122.79
1	L1	1860	PSU	O2-C2-N1	-3.27	119.19	122.79
30	S1	651	PSU	O2-C2-N1	-3.27	119.19	122.79
30	S1	572	PSU	O2-C2-N1	-3.26	119.20	122.79
30	S1	1081	PSU	O2-C2-N1	-3.26	119.20	122.79
30	S1	484	A2M	N3-C2-N1	-3.25	123.59	128.68
1	L1	3768	PSU	O2-C2-N1	-3.25	119.21	122.79
30	S1	1337	4AC	N4-C4-N3	3.25	119.31	113.85
30	S1	1238	PSU	O2-C2-N1	-3.25	119.21	122.79
30	S1	1692	PSU	O2-C2-N1	-3.25	119.22	122.79
1	L1	1782	PSU	O2-C2-N1	-3.24	119.22	122.79
1	L1	4299	PSU	O2-C2-N1	-3.24	119.22	122.79
1	L1	4361	PSU	O2-C2-N1	-3.23	119.23	122.79
1	L1	1524	A2M	N3-C2-N1	-3.23	123.62	128.68
1	L1	2815	A2M	N3-C2-N1	-3.23	123.62	128.68
1	L1	3718	A2M	N3-C2-N1	-3.23	123.63	128.68
1	L1	4220	6MZ	N3-C2-N1	-3.22	123.64	128.68
30	S1	34	PSU	O2-C2-N1	-3.22	119.24	122.79
30	S1	649	PSU	O2-C2-N1	-3.22	119.25	122.79
1	L1	1534	A2M	N3-C2-N1	-3.21	123.65	128.68
30	S1	512	A2M	N3-C2-N1	-3.21	123.66	128.68
30	S1	1045	PSU	O2-C2-N1	-3.21	119.26	122.79
1	L1	3785	A2M	N3-C2-N1	-3.20	123.67	128.68
1	L1	4423	PSU	O2-C2-N1	-3.20	119.27	122.79
1	L1	4523	A2M	N3-C2-N1	-3.19	123.69	128.68
1	L1	4353	PSU	O2-C2-N1	-3.19	119.28	122.79
1	L1	1871	A2M	N3-C2-N1	-3.18	123.71	128.68
1	L1	4457	PSU	O2-C2-N1	-3.18	119.29	122.79
1	L1	4590	A2M	N3-C2-N1	-3.17	123.72	128.68
1	L1	2787	A2M	N3-C2-N1	-3.17	123.72	128.68
1	L1	3639	PSU	O2-C2-N1	-3.17	119.31	122.79
30	S1	166	A2M	N3-C2-N1	-3.17	123.73	128.68
30	S1	1031	A2M	N3-C2-N1	-3.16	123.74	128.68
1	L1	3734	PSU	O2-C2-N1	-3.16	119.31	122.79
30	S1	1136	PSU	O2-C2-N1	-3.16	119.32	122.79
30	S1	218	PSU	O2-C2-N1	-3.15	119.32	122.79
30	S1	576	A2M	N3-C2-N1	-3.15	123.76	128.68
30	S1	1383	A2M	N3-C2-N1	-3.14	123.77	128.68
1	L1	2632	PSU	O2-C2-N1	-3.14	119.33	122.79
30	S1	109	PSU	O2-C2-N1	-3.14	119.34	122.79
30	S1	468	A2M	N3-C2-N1	-3.13	123.78	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	3867	A2M	N3-C2-N1	-3.13	123.79	128.68
30	S1	1232	PSU	O2-C2-N1	-3.12	119.36	122.79
1	L1	400	A2M	N3-C2-N1	-3.11	123.81	128.68
1	L1	2839	PSU	O2-C2-N1	-3.11	119.36	122.79
30	S1	668	A2M	N3-C2-N1	-3.10	123.83	128.68
30	S1	116	OMU	O4-C4-C5	-3.10	119.71	125.16
30	S1	1678	A2M	N3-C2-N1	-3.10	123.84	128.68
30	S1	1326	OMU	O4-C4-C5	-3.09	119.72	125.16
1	L1	3825	A2M	N3-C2-N1	-3.09	123.86	128.68
30	S1	1248	B8N	N3-C2-N1	3.08	121.11	116.76
1	L1	2837	OMU	O4-C4-C5	-3.07	119.76	125.16
30	S1	93	PSU	O2-C2-N1	-3.07	119.41	122.79
1	L1	3724	A2M	N3-C2-N1	-3.07	123.88	128.68
1	L1	3830	A2M	N3-C2-N1	-3.06	123.89	128.68
1	L1	1326	A2M	N3-C2-N1	-3.06	123.89	128.68
1	L1	4571	A2M	N3-C2-N1	-3.06	123.89	128.68
1	L1	2401	A2M	N3-C2-N1	-3.06	123.90	128.68
30	S1	159	A2M	N3-C2-N1	-3.06	123.90	128.68
1	L1	2415	OMU	O4-C4-C5	-3.05	119.79	125.16
30	S1	1639	G7M	C2-N1-C6	-3.05	119.48	125.10
30	S1	590	A2M	N3-C2-N1	-3.04	123.93	128.68
30	S1	99	A2M	N3-C2-N1	-3.03	123.94	128.68
30	S1	799	OMU	O4-C4-C5	-3.02	119.85	125.16
30	S1	121	OMU	O4-C4-C5	-3.02	119.85	125.16
1	L1	3925	OMU	O4-C4-C5	-2.98	119.92	125.16
30	S1	172	OMU	O4-C4-C5	-2.98	119.92	125.16
1	L1	2363	A2M	N3-C2-N1	-2.97	124.03	128.68
30	S1	354	OMU	O4-C4-C5	-2.97	119.94	125.16
30	S1	159	A2M	C4-C5-N7	-2.94	106.33	109.40
30	S1	1832	6MZ	N3-C2-N1	-2.93	124.10	128.68
30	S1	627	OMU	O4-C4-C5	-2.93	120.01	125.16
1	L1	4498	OMU	O4-C4-C5	-2.92	120.03	125.16
30	S1	1804	OMU	O4-C4-C5	-2.92	120.03	125.16
1	L1	4227	OMU	O4-C4-C5	-2.88	120.09	125.16
1	L1	4620	OMU	O4-C4-C5	-2.87	120.11	125.16
1	L1	4306	OMU	O4-C4-C5	-2.87	120.12	125.16
30	S1	1442	OMU	O4-C4-C5	-2.85	120.14	125.16
30	S1	428	OMU	O4-C4-C5	-2.85	120.15	125.16
30	S1	1288	OMU	O4-C4-C5	-2.84	120.17	125.16
1	L1	1323	A2M	N3-C2-N1	-2.83	124.25	128.68
30	S1	668	A2M	C4-C5-N7	-2.83	106.45	109.40
30	S1	468	A2M	C4-C5-N7	-2.77	106.52	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4523	A2M	C4-C5-N7	-2.76	106.52	109.40
1	L1	1534	A2M	C4-C5-N7	-2.75	106.53	109.40
1	L1	1871	A2M	C4-C5-N7	-2.75	106.53	109.40
30	S1	1383	A2M	C4-C5-N7	-2.73	106.56	109.40
1	L1	1323	A2M	C4-C5-N7	-2.70	106.59	109.40
1	L1	4590	A2M	C4-C5-N7	-2.70	106.59	109.40
1	L1	3825	A2M	C4-C5-N7	-2.69	106.59	109.40
30	S1	1031	A2M	C4-C5-N7	-2.69	106.60	109.40
1	L1	1326	A2M	C4-C5-N7	-2.68	106.60	109.40
30	S1	576	A2M	C4-C5-N7	-2.68	106.61	109.40
1	L1	2401	A2M	C4-C5-N7	-2.67	106.61	109.40
1	L1	2363	A2M	C4-C5-N7	-2.67	106.61	109.40
1	L1	398	A2M	C4-C5-N7	-2.67	106.62	109.40
1	L1	4571	A2M	C4-C5-N7	-2.66	106.62	109.40
1	L1	2815	A2M	C4-C5-N7	-2.66	106.63	109.40
1	L1	3818	UY1	O2-C2-N1	-2.65	119.87	122.79
30	S1	27	A2M	C4-C5-N7	-2.64	106.65	109.40
30	S1	1337	4AC	C6-C5-C4	2.63	120.18	116.96
1	L1	3724	A2M	C4-C5-N7	-2.63	106.66	109.40
30	S1	99	A2M	C4-C5-N7	-2.63	106.66	109.40
30	S1	484	A2M	C4-C5-N7	-2.62	106.67	109.40
30	S1	512	A2M	C4-C5-N7	-2.61	106.68	109.40
1	L1	3718	A2M	C4-C5-N7	-2.61	106.68	109.40
1	L1	3830	A2M	C4-C5-N7	-2.60	106.69	109.40
30	S1	1678	A2M	C4-C5-N7	-2.60	106.69	109.40
1	L1	4220	6MZ	C4-C5-N7	-2.57	106.72	109.40
30	S1	1081	PSU	C6-C5-C4	-2.55	116.41	118.20
39	SG	138	IAS	OD1-CG-CB	-2.54	118.02	125.43
1	L1	3785	A2M	C4-C5-N7	-2.53	106.77	109.40
1	L1	4447	5MC	C5-C4-N3	-2.53	118.95	121.67
1	L1	1524	A2M	C4-C5-N7	-2.51	106.78	109.40
1	L1	3867	A2M	C4-C5-N7	-2.49	106.80	109.40
30	S1	166	A2M	C4-C5-N7	-2.49	106.80	109.40
1	L1	400	A2M	C4-C5-N7	-2.47	106.82	109.40
1	L1	4637	OMG	C8-N7-C5	2.47	107.70	102.99
1	L1	2787	A2M	C4-C5-N7	-2.45	106.84	109.40
1	L1	2351	OMC	O2-C2-N3	-2.44	118.37	122.33
68	L3	75	OMG	C5-C6-N1	2.41	118.21	113.95
1	L1	3782	5MC	C5-C4-N3	-2.41	119.08	121.67
1	L1	2424	OMG	C5-C6-N1	2.39	118.18	113.95
30	S1	601	OMG	C8-N7-C5	2.39	107.55	102.99
1	L1	4228	OMG	C8-N7-C5	2.39	107.53	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4499	OMG	C8-N7-C5	2.38	107.53	102.99
1	L1	4494	OMG	C8-N7-C5	2.38	107.53	102.99
1	L1	4623	OMG	C8-N7-C5	2.37	107.51	102.99
30	S1	1328	OMG	C8-N7-C5	2.37	107.50	102.99
1	L1	4370	OMG	C8-N7-C5	2.36	107.49	102.99
30	S1	1842	4AC	C6-C5-C4	2.36	119.85	116.96
1	L1	4392	OMG	C8-N7-C5	2.35	107.47	102.99
1	L1	3792	OMG	C8-N7-C5	2.35	107.46	102.99
1	L1	3627	OMG	C8-N7-C5	2.34	107.45	102.99
1	L1	1522	OMG	C5-C6-N1	2.34	118.08	113.95
30	S1	1447	OMG	C8-N7-C5	2.34	107.44	102.99
1	L1	1316	OMG	C5-C6-N1	2.34	118.08	113.95
30	S1	683	OMG	C8-N7-C5	2.33	107.44	102.99
1	L1	1316	OMG	C8-N7-C5	2.33	107.43	102.99
1	L1	4637	OMG	C5-C6-N1	2.33	118.06	113.95
1	L1	3782	5MC	O2-C2-N3	-2.32	118.56	122.33
30	S1	590	A2M	C4-C5-N7	-2.32	106.98	109.40
30	S1	436	OMG	C8-N7-C5	2.32	107.41	102.99
1	L1	3899	OMG	C5-C6-N1	2.32	118.05	113.95
1	L1	4370	OMG	C5-C6-N1	2.32	118.05	113.95
30	S1	601	OMG	C5-C6-N1	2.30	118.02	113.95
1	L1	2876	OMG	C5-C6-N1	2.30	118.01	113.95
30	S1	1832	6MZ	C9-N6-C6	-2.30	120.89	122.87
68	L3	75	OMG	C8-N7-C5	2.30	107.37	102.99
1	L1	4618	OMG	C5-C6-N1	2.30	118.01	113.95
1	L1	1522	OMG	C8-N7-C5	2.30	107.36	102.99
30	S1	1490	OMG	C5-C6-N1	2.29	118.00	113.95
1	L1	2424	OMG	C8-N7-C5	2.29	107.36	102.99
1	L1	4392	OMG	C5-C6-N1	2.29	118.00	113.95
1	L1	1625	OMG	C5-C6-N1	2.29	118.00	113.95
1	L1	3944	OMG	C8-N7-C5	2.28	107.34	102.99
1	L1	4498	OMU	O2-C2-N1	-2.28	119.75	122.79
1	L1	2364	OMG	C5-C6-N1	2.28	117.98	113.95
1	L1	4499	OMG	C5-C6-N1	2.28	117.98	113.95
30	S1	1490	OMG	C8-N7-C5	2.28	107.33	102.99
1	L1	4494	OMG	C5-C6-N1	2.28	117.97	113.95
1	L1	4623	OMG	C5-C6-N1	2.27	117.96	113.95
30	S1	1447	OMG	C5-C6-N1	2.27	117.96	113.95
30	S1	509	OMG	C8-N7-C5	2.27	107.31	102.99
1	L1	3744	OMG	C5-C6-N1	2.26	117.95	113.95
1	L1	4196	OMG	C5-C6-N1	2.26	117.95	113.95
30	S1	1248	B8N	C5-C4-N3	2.26	120.36	116.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	S1	644	OMG	C5-C6-N1	2.26	117.94	113.95
1	L1	3744	OMG	C8-N7-C5	2.26	107.29	102.99
1	L1	4618	OMG	C8-N7-C5	2.25	107.28	102.99
1	L1	4228	OMG	C5-C6-N1	2.24	117.91	113.95
30	S1	644	OMG	C8-N7-C5	2.24	107.26	102.99
30	S1	1328	OMG	C5-C6-N1	2.23	117.90	113.95
30	S1	509	OMG	C5-C6-N1	2.23	117.89	113.95
30	S1	683	OMG	C5-C6-N1	2.23	117.89	113.95
1	L1	1582	PSU	C5-C6-N1	-2.22	118.77	122.11
30	S1	1248	B8N	O2-C2-N3	-2.22	118.90	121.99
1	L1	2364	OMG	C8-N7-C5	2.22	107.22	102.99
1	L1	1625	OMG	C8-N7-C5	2.22	107.22	102.99
47	Sg	62	HY3	C5-C4-C3	2.22	107.13	103.74
30	S1	1232	PSU	C5-C6-N1	-2.22	118.78	122.11
1	L1	2876	OMG	C8-N7-C5	2.22	107.21	102.99
1	L1	3792	OMG	C5-C6-N1	2.21	117.86	113.95
30	S1	436	OMG	C5-C6-N1	2.21	117.85	113.95
1	L1	4493	PSU	C5-C6-N1	-2.21	118.80	122.11
1	L1	3730	PSU	C5-C6-N1	-2.21	118.80	122.11
1	L1	3925	OMU	O2-C2-N1	-2.20	119.86	122.79
30	S1	1703	OMC	O2-C2-N3	-2.20	118.75	122.33
30	S1	649	PSU	C5-C6-N1	-2.20	118.81	122.11
1	L1	1781	PSU	C5-C6-N1	-2.17	118.85	122.11
30	S1	1832	6MZ	C4-C5-N7	-2.17	107.14	109.40
1	L1	1322	1MA	C8-N7-C5	2.17	107.11	102.99
1	L1	4196	OMG	C8-N7-C5	2.16	107.10	102.99
1	L1	3627	OMG	C5-C6-N1	2.16	117.76	113.95
30	S1	1842	4AC	C5-C4-N4	-2.14	119.20	122.92
30	S1	1238	PSU	C5-C6-N1	-2.14	118.90	122.11
1	L1	4500	PSU	C5-C6-N1	-2.13	118.92	122.11
30	S1	1045	PSU	C5-C6-N1	-2.12	118.93	122.11
1	L1	1782	PSU	C5-C6-N1	-2.11	118.94	122.11
1	L1	4442	PSU	C5-C6-N1	-2.11	118.94	122.11
1	L1	4521	PSU	C5-C6-N1	-2.11	118.94	122.11
1	L1	2422	OMC	O2-C2-N3	-2.11	118.90	122.33
1	L1	2837	OMU	O2-C2-N1	-2.11	119.98	122.79
30	S1	1326	OMU	O2-C2-N1	-2.10	119.99	122.79
1	L1	4353	PSU	C5-C6-N1	-2.10	118.96	122.11
1	L1	3841	OMC	O2-C2-N3	-2.10	118.92	122.33
30	S1	354	OMU	O2-C2-N1	-2.10	120.00	122.79
1	L1	2415	OMU	C1'-N1-C2	2.09	121.36	117.57
1	L1	4296	PSU	C5-C6-N1	-2.09	118.97	122.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	4442	PSU	O4'-C1'-C2'	2.09	108.09	105.14
1	L1	4620	OMU	O2-C2-N1	-2.08	120.02	122.79
1	L1	2508	PSU	C5-C6-N1	-2.08	118.98	122.11
1	L1	3899	OMG	C8-N7-C5	2.08	106.96	102.99
1	L1	2351	OMC	C1'-N1-C2	2.08	123.07	118.42
30	S1	1136	PSU	C5-C6-N1	-2.08	118.99	122.11
30	S1	1347	PSU	C5-C6-N1	-2.08	118.99	122.11
30	S1	1692	PSU	C5-C6-N1	-2.07	119.01	122.11
1	L1	1322	1MA	N1-C2-N3	-2.07	123.61	126.02
1	L1	2839	PSU	C5-C6-N1	-2.06	119.02	122.11
1	L1	4521	PSU	O4'-C1'-C2'	2.06	108.05	105.14
30	S1	572	PSU	C5-C6-N1	-2.06	119.02	122.11
30	S1	121	OMU	O2-C2-N1	-2.05	120.06	122.79
1	L1	1677	PSU	C5-C6-N1	-2.04	119.06	122.11
1	L1	4579	PSU	C5-C6-N1	-2.03	119.07	122.11
68	L3	69	PSU	C5-C6-N1	-2.03	119.07	122.11
1	L1	4431	PSU	C5-C6-N1	-2.02	119.07	122.11
1	L1	5010	PSU	C5-C6-N1	-2.02	119.07	122.11
1	L1	1322	1MA	C5-C6-N1	2.02	116.91	113.90
1	L1	4500	PSU	O4'-C1'-C2'	2.01	107.98	105.14
30	S1	218	PSU	C5-C6-N1	-2.01	119.10	122.11

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	Sg	62	HY3	O-C-CA-C3
1	L1	1326	A2M	C1'-C2'-O2'-CM'
1	L1	1677	PSU	C2'-C1'-C5-C4
1	L1	1881	OMC	O4'-C1'-N1-C2
1	L1	1881	OMC	O4'-C1'-N1-C6
1	L1	1881	OMC	C3'-C4'-C5'-O5'
1	L1	1881	OMC	O4'-C4'-C5'-O5'
1	L1	2364	OMG	O4'-C4'-C5'-O5'
1	L1	2364	OMG	C3'-C4'-C5'-O5'
1	L1	3734	PSU	O4'-C1'-C5-C4
1	L1	3734	PSU	O4'-C1'-C5-C6
1	L1	3785	A2M	O4'-C4'-C5'-O5'
1	L1	3818	UY1	O4'-C1'-C5-C4
1	L1	3818	UY1	O4'-C1'-C5-C6
1	L1	3867	A2M	C1'-C2'-O2'-CM'
1	L1	4420	PSU	C2'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	L1	4447	5MC	C2'-C1'-N1-C2
1	L1	4447	5MC	C2'-C1'-N1-C6
1	L1	4471	PSU	C3'-C4'-C5'-O5'
1	L1	4590	A2M	C4'-C5'-O5'-P
30	S1	428	OMU	C2'-C1'-N1-C2
30	S1	428	OMU	C2'-C1'-N1-C6
30	S1	644	OMG	O4'-C4'-C5'-O5'
30	S1	644	OMG	C3'-C4'-C5'-O5'
30	S1	668	A2M	O4'-C4'-C5'-O5'
30	S1	668	A2M	C1'-C2'-O2'-CM'
30	S1	799	OMU	C4'-C5'-O5'-P
30	S1	1081	PSU	C2'-C1'-C5-C4
30	S1	1081	PSU	C2'-C1'-C5-C6
30	S1	1248	B8N	N34-C33-C34-O35
30	S1	1337	4AC	O7-C7-N4-C4
30	S1	1337	4AC	CM7-C7-N4-C4
30	S1	1447	OMG	C3'-C4'-C5'-O5'
30	S1	1842	4AC	N3-C4-N4-C7
30	S1	1842	4AC	C5-C4-N4-C7
30	S1	1842	4AC	CM7-C7-N4-C4
1	L1	3701	OMC	C2'-C1'-N1-C6
1	L1	1781	PSU	O4'-C4'-C5'-O5'
1	L1	3701	OMC	O4'-C4'-C5'-O5'
1	L1	3734	PSU	O4'-C4'-C5'-O5'
1	L1	4471	PSU	O4'-C4'-C5'-O5'
1	L1	4637	OMG	O4'-C4'-C5'-O5'
1	L1	1781	PSU	C3'-C4'-C5'-O5'
1	L1	3701	OMC	C3'-C4'-C5'-O5'
1	L1	3734	PSU	C3'-C4'-C5'-O5'
1	L1	3785	A2M	C3'-C4'-C5'-O5'
1	L1	3851	PSU	C3'-C4'-C5'-O5'
1	L1	3851	PSU	O4'-C4'-C5'-O5'
1	L1	4637	OMG	C3'-C4'-C5'-O5'
30	S1	484	A2M	O4'-C4'-C5'-O5'
30	S1	668	A2M	C3'-C4'-C5'-O5'
30	S1	1248	B8N	N34-C33-C34-O36
1	L1	3701	OMC	C2'-C1'-N1-C2
30	S1	576	A2M	C3'-C4'-C5'-O5'
1	L1	4420	PSU	C3'-C4'-C5'-O5'
1	L1	4420	PSU	O4'-C4'-C5'-O5'
30	S1	576	A2M	O4'-C4'-C5'-O5'
30	S1	1447	OMG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	S1	1851	MA6	C5-C6-N6-C9
30	S1	644	OMG	C4'-C5'-O5'-P
1	L1	1534	A2M	O4'-C4'-C5'-O5'
30	S1	1842	4AC	O7-C7-N4-C4
1	L1	4500	PSU	C4'-C5'-O5'-P
30	S1	428	OMU	O4'-C1'-N1-C6
30	S1	1248	B8N	C32-C33-C34-O36
30	S1	428	OMU	O4'-C1'-N1-C2
1	L1	3701	OMC	O4'-C1'-N1-C6
30	S1	1851	MA6	C4'-C5'-O5'-P
1	L1	1340	OMC	O4'-C4'-C5'-O5'
1	L1	3887	OMC	C3'-C2'-O2'-CM2
1	L1	4623	OMG	C3'-C2'-O2'-CM2
30	S1	121	OMU	C3'-C2'-O2'-CM2
1	L1	3844	PSU	C4'-C5'-O5'-P
30	S1	484	A2M	C3'-C4'-C5'-O5'
30	S1	1248	B8N	C32-C33-C34-O35
1	L1	4447	5MC	O4'-C1'-N1-C6
1	L1	3701	OMC	O4'-C1'-N1-C2
1	L1	398	A2M	O4'-C4'-C5'-O5'
1	L1	3818	UY1	C4'-C5'-O5'-P
1	L1	3851	PSU	C4'-C5'-O5'-P
1	L1	3887	OMC	C4'-C5'-O5'-P
1	L1	2876	OMG	C3'-C2'-O2'-CM2
30	S1	1703	OMC	C3'-C2'-O2'-CM2
1	L1	4447	5MC	O4'-C1'-N1-C2
39	SG	138	IAS	CA-CB-CG-OD1
1	L1	2351	OMC	O4'-C4'-C5'-O5'
30	S1	509	OMG	C3'-C4'-C5'-O5'
1	L1	3808	OMC	C3'-C2'-O2'-CM2
30	S1	644	OMG	C3'-C2'-O2'-CM2
30	S1	1031	A2M	C3'-C2'-O2'-CM'
1	L1	2824	OMC	O4'-C4'-C5'-O5'
1	L1	4618	OMG	O4'-C4'-C5'-O5'
30	S1	99	A2M	O4'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C4'-C5'-O5'
30	S1	159	A2M	O4'-C4'-C5'-O5'
1	L1	1316	OMG	C1'-C2'-O2'-CM2
1	L1	4227	OMU	C3'-C2'-O2'-CM2
1	L1	1534	A2M	C3'-C4'-C5'-O5'
1	L1	4523	A2M	O4'-C4'-C5'-O5'
30	S1	799	OMU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	S1	1804	OMU	O4'-C4'-C5'-O5'
1	L1	1677	PSU	O4'-C1'-C5-C6
1	L1	2351	OMC	C2'-C1'-N1-C2
30	S1	1081	PSU	C4'-C5'-O5'-P
1	L1	1316	OMG	C3'-C2'-O2'-CM2
1	L1	4536	OMC	C3'-C2'-O2'-CM2
30	S1	1490	OMG	C3'-C2'-O2'-CM2
30	S1	627	OMU	C4'-C5'-O5'-P

There are no ring outliers.

70 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	S1	1832	6MZ	1	0
30	S1	1337	4AC	1	0
1	L1	1625	OMG	1	0
1	L1	3782	5MC	1	0
1	L1	2415	OMU	2	0
30	S1	1639	G7M	1	0
30	S1	159	A2M	2	0
30	S1	576	A2M	1	0
30	S1	1490	OMG	2	0
30	S1	484	A2M	1	0
1	L1	2351	OMC	1	0
1	L1	2861	OMC	1	0
30	S1	1442	OMU	1	0
1	L1	3724	A2M	2	0
30	S1	462	OMC	1	0
1	L1	3785	A2M	1	0
30	S1	668	A2M	2	0
1	L1	4571	A2M	2	0
30	S1	1232	PSU	2	0
30	S1	512	A2M	1	0
30	S1	116	OMU	3	0
68	L3	75	OMG	1	0
1	L1	3744	OMG	1	0
30	S1	1391	OMC	1	0
1	L1	2804	OMC	1	0
1	L1	1326	A2M	2	0
30	S1	296	PSU	1	0
30	S1	99	A2M	1	0
1	L1	4457	PSU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	3899	OMG	1	0
30	S1	601	OMG	1	0
30	S1	797	OMC	2	0
1	L1	4523	A2M	1	0
30	S1	681	PSU	1	0
30	S1	1850	MA6	1	0
1	L1	398	A2M	1	0
1	L1	1316	OMG	1	0
1	L1	1534	A2M	1	0
1	L1	3825	A2M	2	0
1	L1	4293	PSU	1	0
30	S1	166	A2M	2	0
30	S1	863	PSU	1	0
1	L1	3718	A2M	1	0
1	L1	4447	5MC	1	0
30	S1	1272	OMC	1	0
1	L1	3808	OMC	1	0
30	S1	1031	A2M	2	0
1	L1	3887	OMC	1	0
30	S1	1447	OMG	1	0
30	S1	1678	A2M	3	0
30	S1	1842	4AC	2	0
30	S1	799	OMU	2	0
1	L1	4620	OMU	3	0
30	S1	1328	OMG	1	0
1	L1	4536	OMC	1	0
30	S1	354	OMU	1	0
30	S1	436	OMG	2	0
1	L1	4420	PSU	1	0
1	L1	1871	A2M	1	0
1	L1	4590	A2M	1	0
1	L1	4306	OMU	1	0
30	S1	509	OMG	2	0
1	L1	3830	A2M	1	0
1	L1	4456	OMC	1	0
30	S1	210	PSU	2	0
30	S1	1703	OMC	1	0
1	L1	2815	A2M	2	0
30	S1	121	OMU	2	0
1	L1	1340	OMC	1	0
1	L1	3818	UY1	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	COA	Nd	301	-	41,50,50	3.85	15 (36%)	52,75,75	2.99	6 (11%)
89	GTP	L2	201	48	26,34,34	0.95	2 (7%)	32,54,54	0.76	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	COA	Nd	301	-	-	13/44/64/64	0/3/3/3
89	GTP	L2	201	48	-	2/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	Nd	301	COA	O4B-C1B	13.69	1.60	1.41
88	Nd	301	COA	C2B-C1B	-13.27	1.33	1.53
88	Nd	301	COA	C5P-N4P	6.92	1.49	1.33
88	Nd	301	COA	C3B-C4B	-5.89	1.37	1.52
88	Nd	301	COA	C9P-N8P	5.50	1.45	1.33
88	Nd	301	COA	P3B-O3B	4.90	1.68	1.59
88	Nd	301	COA	C2B-C3B	4.35	1.62	1.52
88	Nd	301	COA	C6A-N6A	4.13	1.49	1.34
88	Nd	301	COA	O4B-C4B	3.75	1.53	1.45
88	Nd	301	COA	C5A-C4A	-2.93	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	Nd	301	COA	P2A-O6A	2.68	1.70	1.59
89	L2	201	GTP	C5-C6	-2.63	1.42	1.47
88	Nd	301	COA	C3P-N4P	2.52	1.51	1.46
88	Nd	301	COA	C2A-N3A	2.49	1.36	1.32
88	Nd	301	COA	O5P-C5P	-2.11	1.19	1.23
88	Nd	301	COA	P1A-O5B	2.07	1.67	1.59
89	L2	201	GTP	C8-N7	-2.06	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	Nd	301	COA	C5A-C6A-N6A	15.22	143.47	120.35
88	Nd	301	COA	N6A-C6A-N1A	-10.99	95.75	118.57
88	Nd	301	COA	C1B-N9A-C4A	6.25	137.62	126.64
88	Nd	301	COA	N3A-C2A-N1A	-5.60	119.93	128.68
88	Nd	301	COA	C3B-C2B-C1B	2.83	106.15	99.89
88	Nd	301	COA	P2A-O3A-P1A	-2.67	123.67	132.83
89	L2	201	GTP	O6-C6-C5	2.03	128.34	124.37

There are no chirality outliers.

All (15) torsion outliers are listed below:

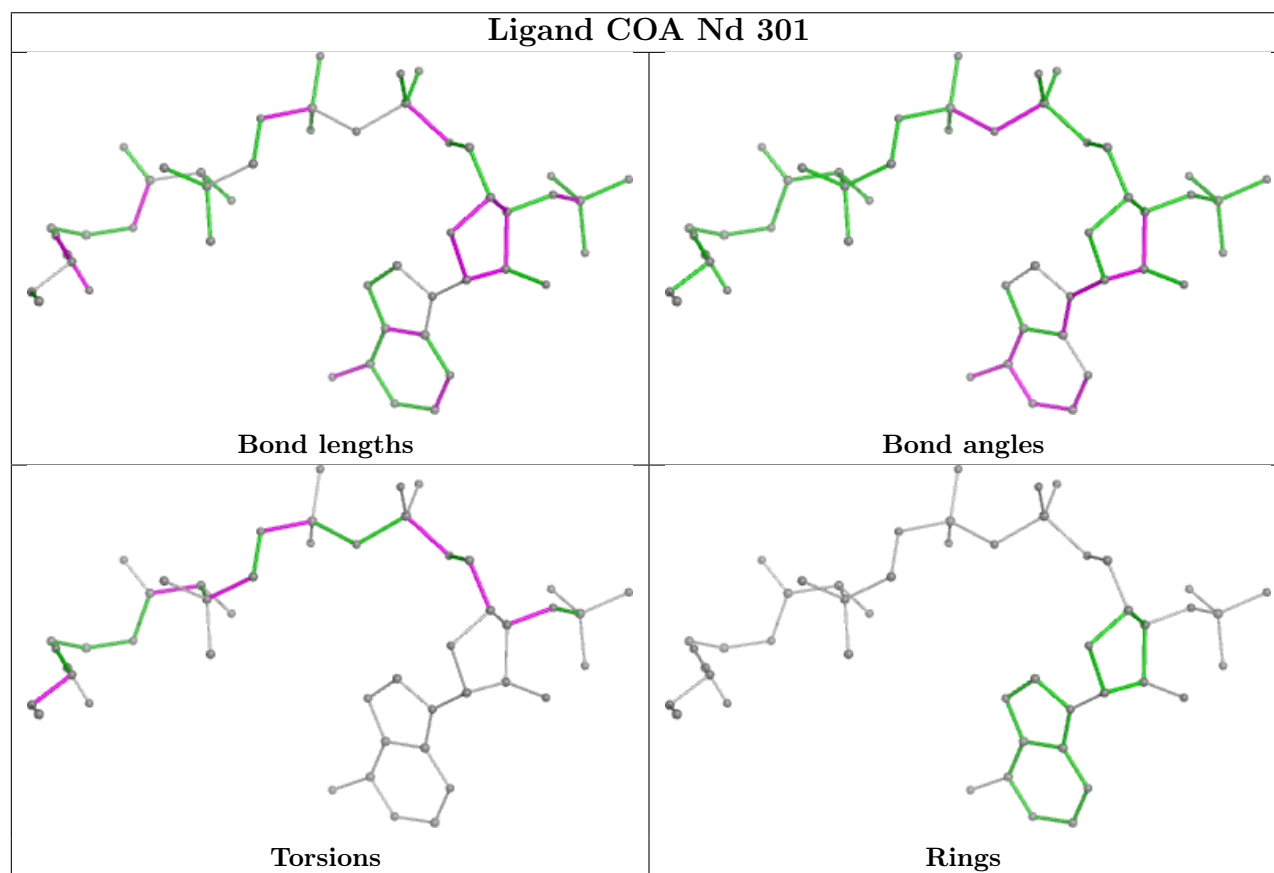
Mol	Chain	Res	Type	Atoms
88	Nd	301	COA	C5B-O5B-P1A-O1A
88	Nd	301	COA	C5B-O5B-P1A-O2A
88	Nd	301	COA	CAP-CBP-CCP-O6A
88	Nd	301	COA	N8P-C9P-CAP-OAP
89	L2	201	GTP	O4'-C4'-C5'-O5'
89	L2	201	GTP	C3'-C4'-C5'-O5'
88	Nd	301	COA	C2B-C3B-O3B-P3B
88	Nd	301	COA	O9P-C9P-CAP-OAP
88	Nd	301	COA	CEP-CBP-CCP-O6A
88	Nd	301	COA	C4B-C3B-O3B-P3B
88	Nd	301	COA	S1P-C2P-C3P-N4P
88	Nd	301	COA	CDP-CBP-CCP-O6A
88	Nd	301	COA	CCP-O6A-P2A-O3A
88	Nd	301	COA	C5B-O5B-P1A-O3A
88	Nd	301	COA	C3B-C4B-C5B-O5B

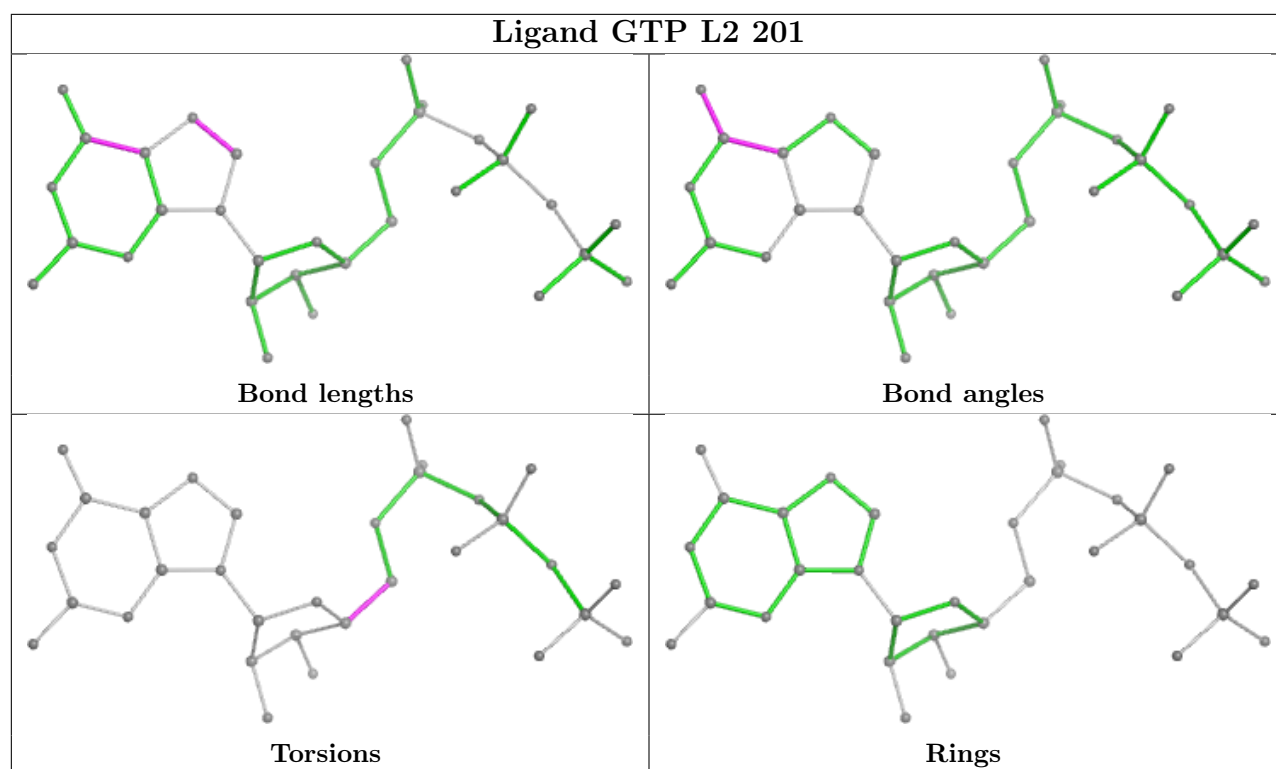
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	Nd	301	COA	5	0
89	L2	201	GTP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

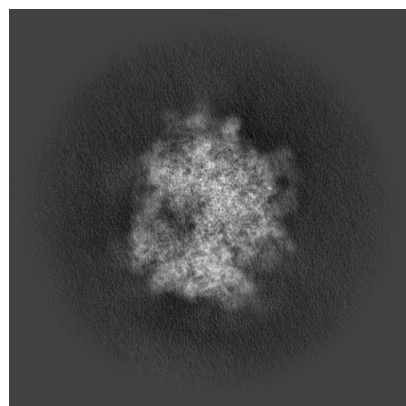
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55351. These allow visual inspection of the internal detail of the map and identification of artifacts.

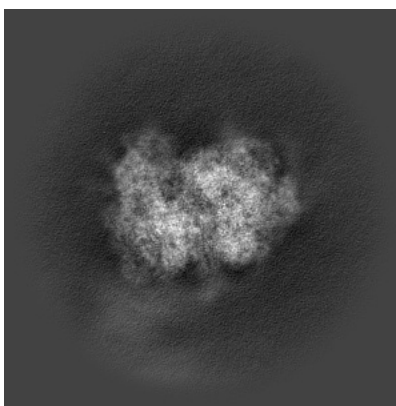
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

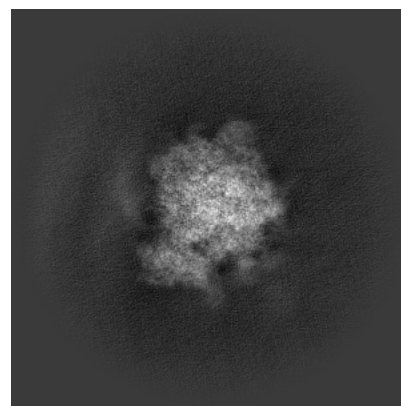
6.1.1 Primary map



X

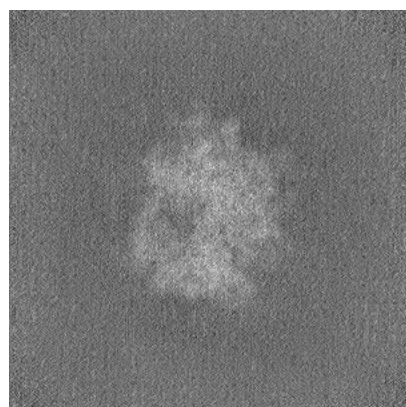


Y

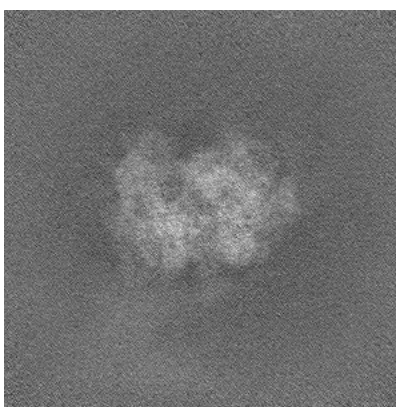


Z

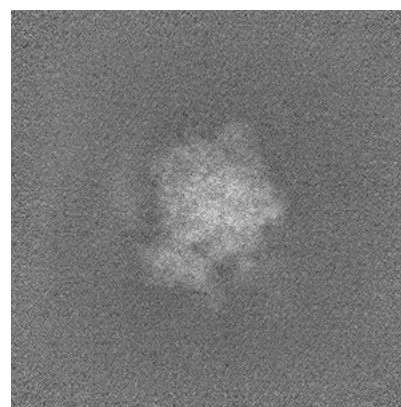
6.1.2 Raw map



X



Y

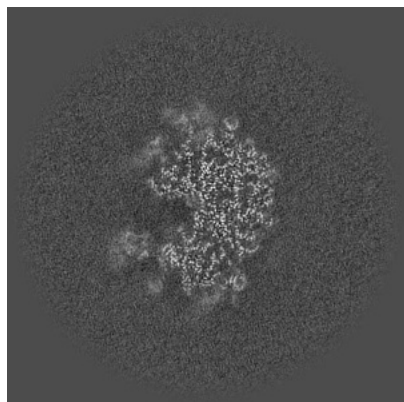


Z

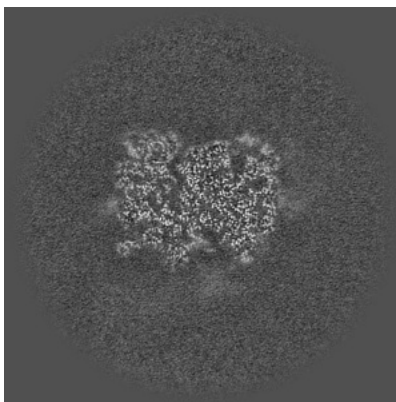
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

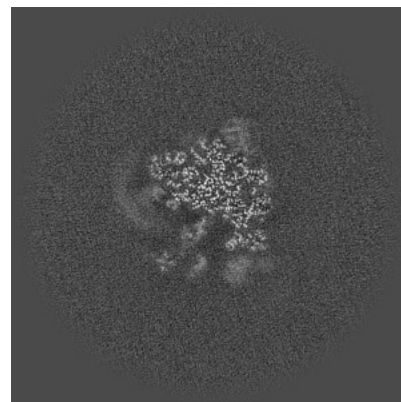
6.2.1 Primary map



X Index: 280

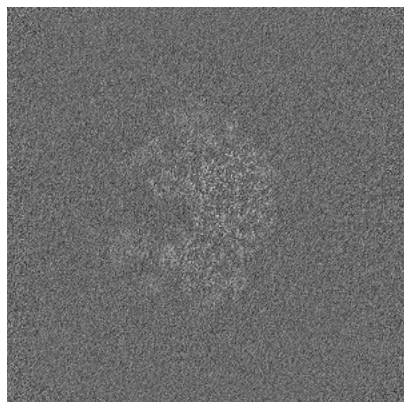


Y Index: 280

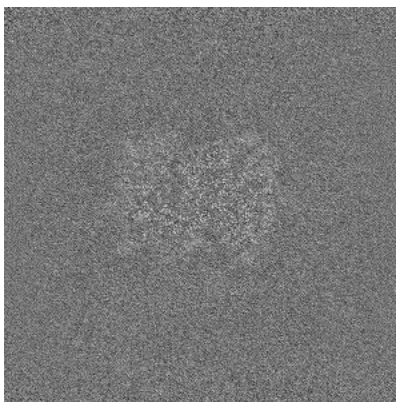


Z Index: 280

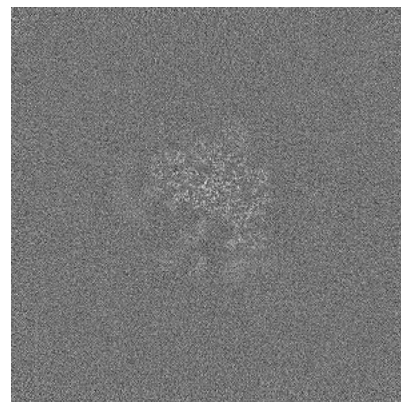
6.2.2 Raw map



X Index: 280



Y Index: 280

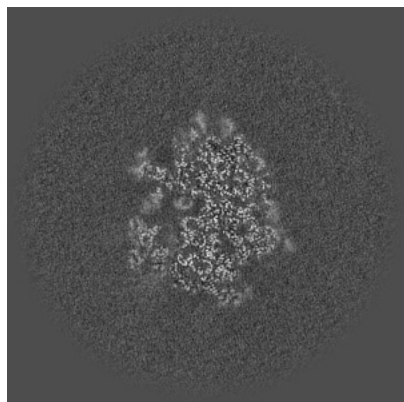


Z Index: 280

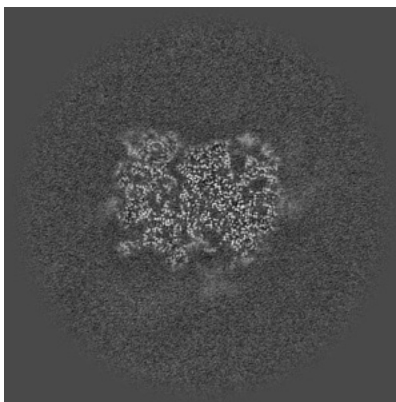
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

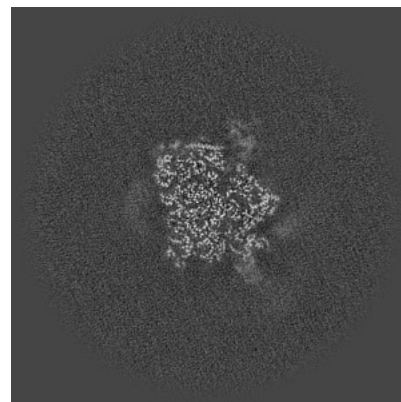
6.3.1 Primary map



X Index: 263

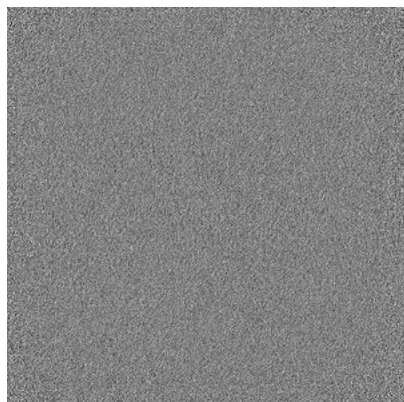


Y Index: 281

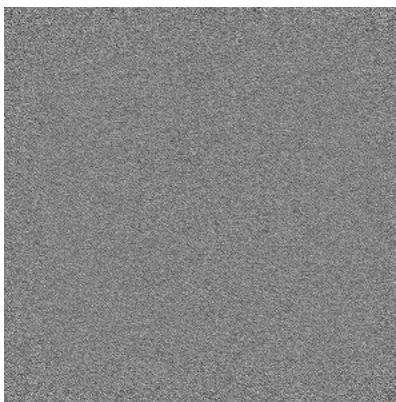


Z Index: 309

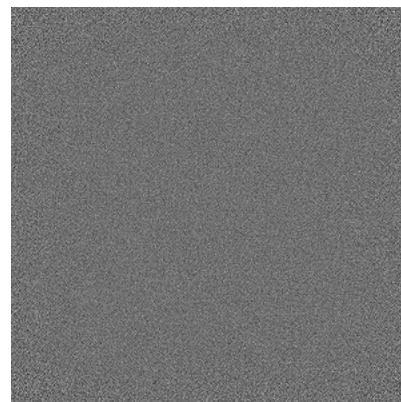
6.3.2 Raw map



X Index: 0



Y Index: 0

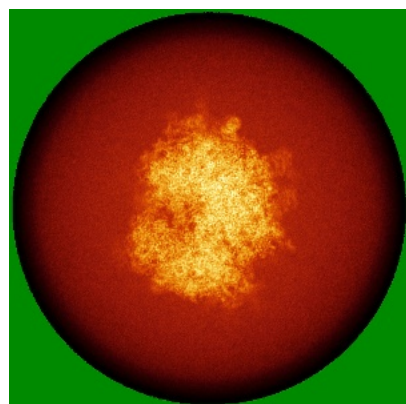


Z Index: 0

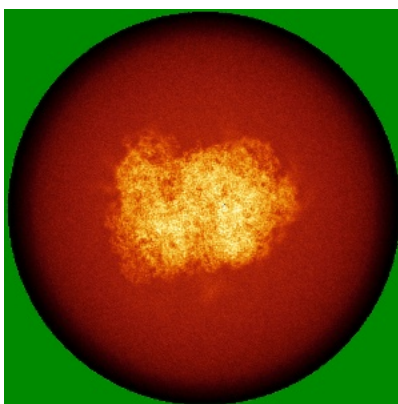
The images above show the largest variance slices of the map in three orthogonal directions.

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

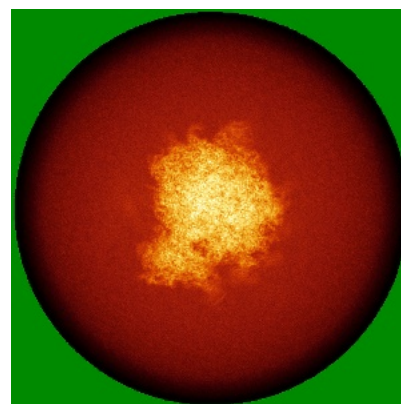
6.4.1 Primary map



X

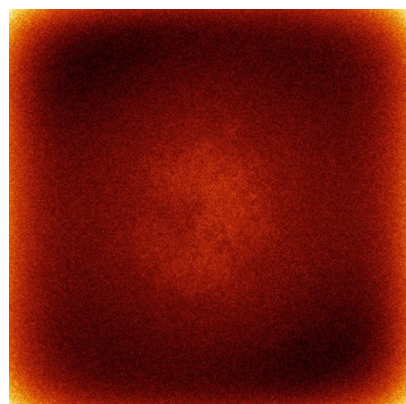


Y

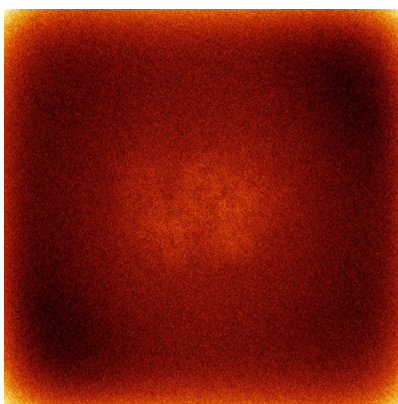


Z

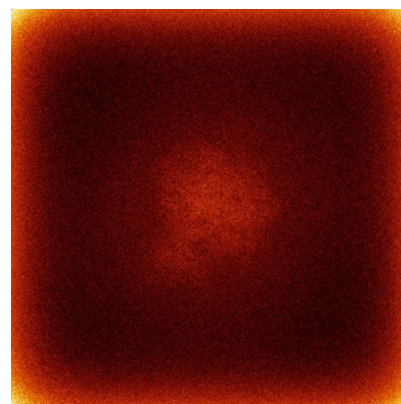
6.4.2 Raw map



X



Y

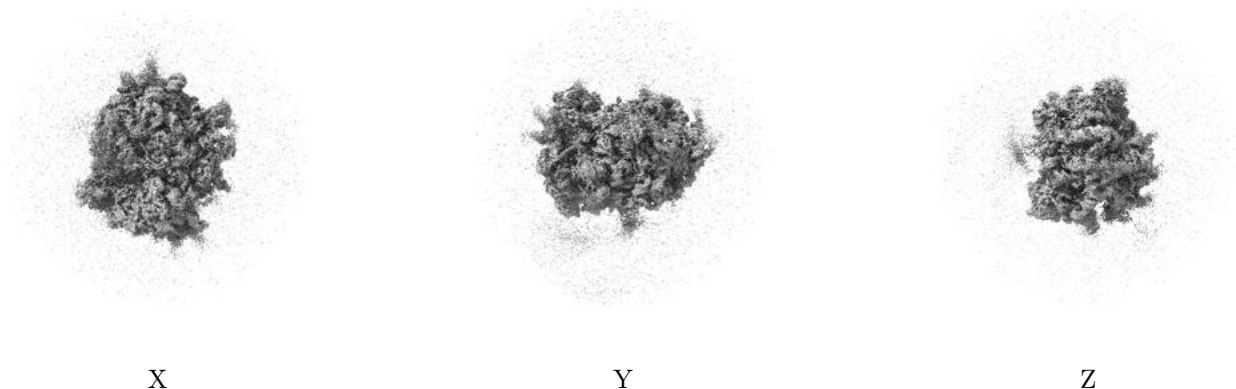


Z

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

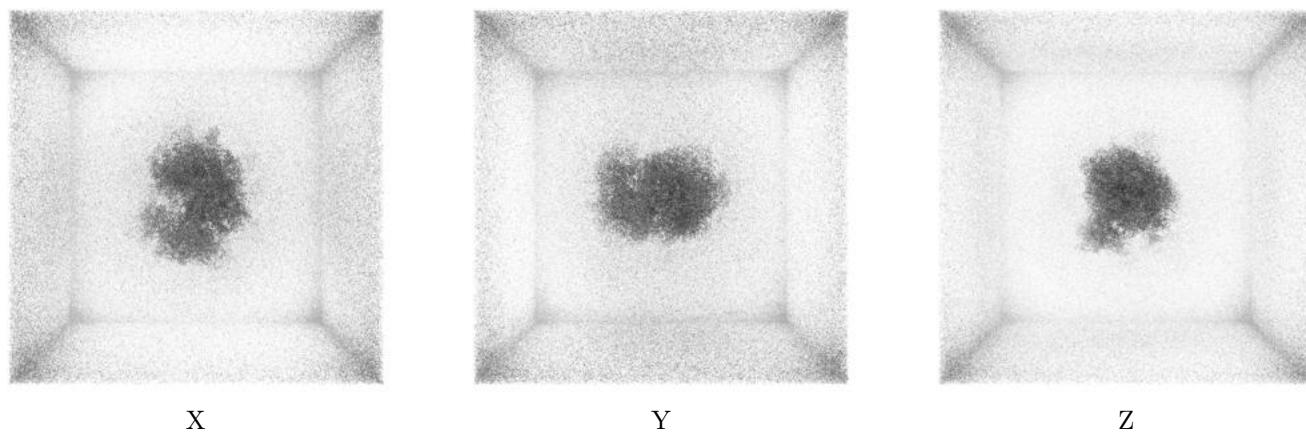
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

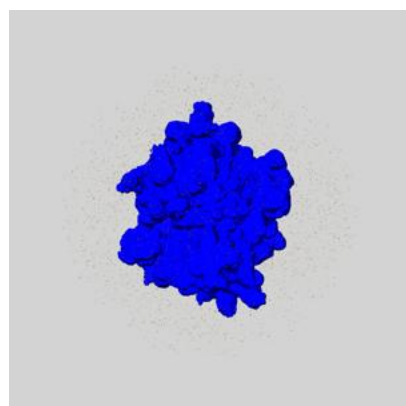
6.6 Mask visualisation [i](#)

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

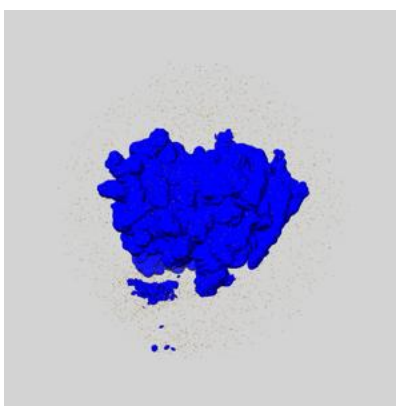
A mask typically either:

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

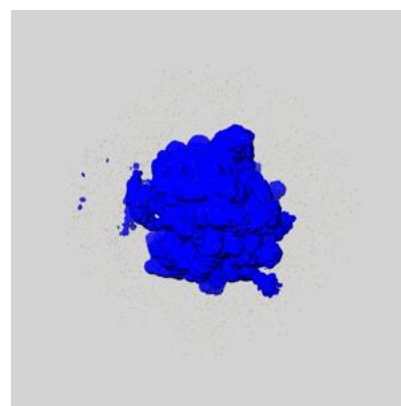
6.6.1 emd_55351_msk_1.map [i](#)



X



Y

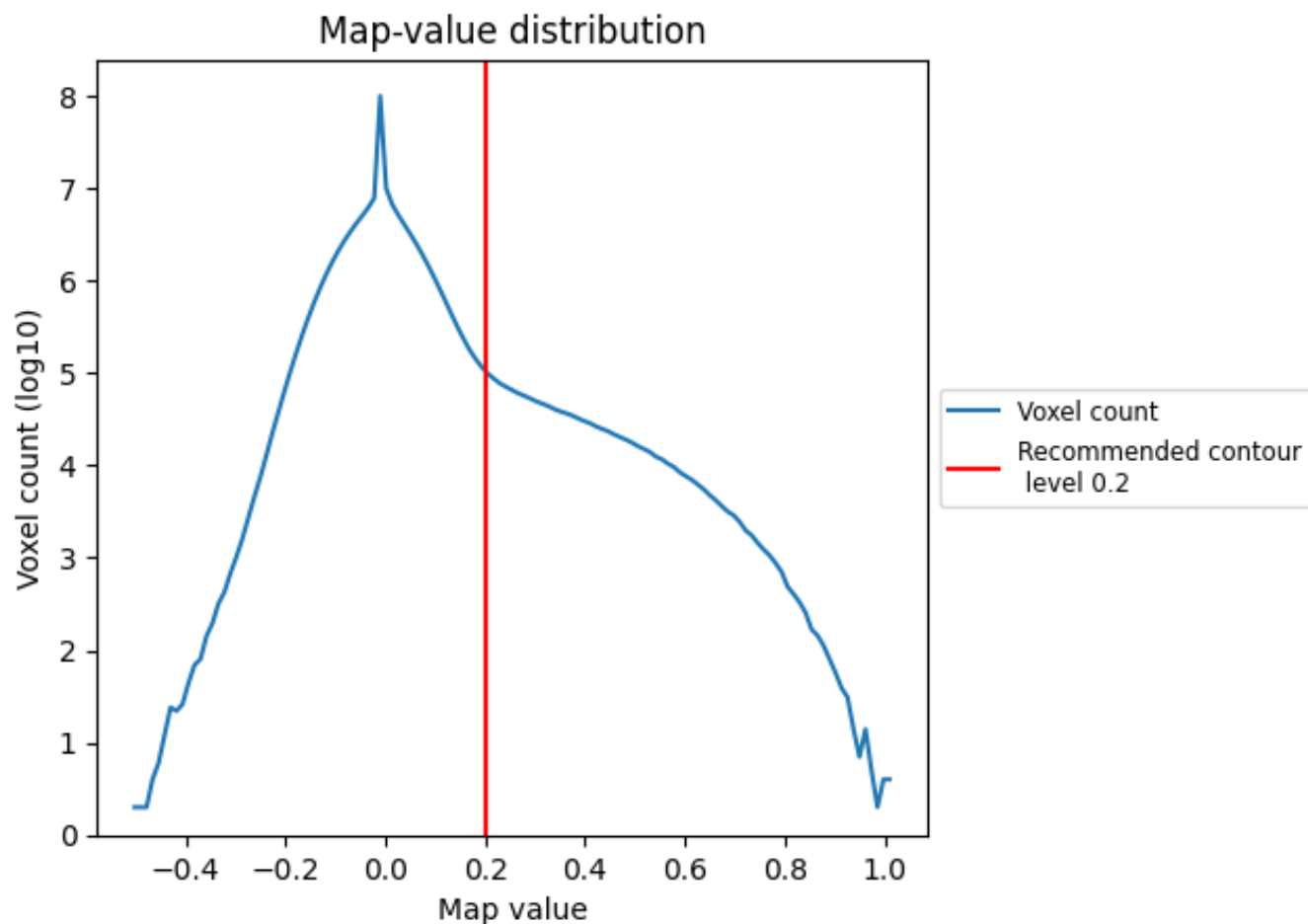


Z

7 Map analysis [i](#)

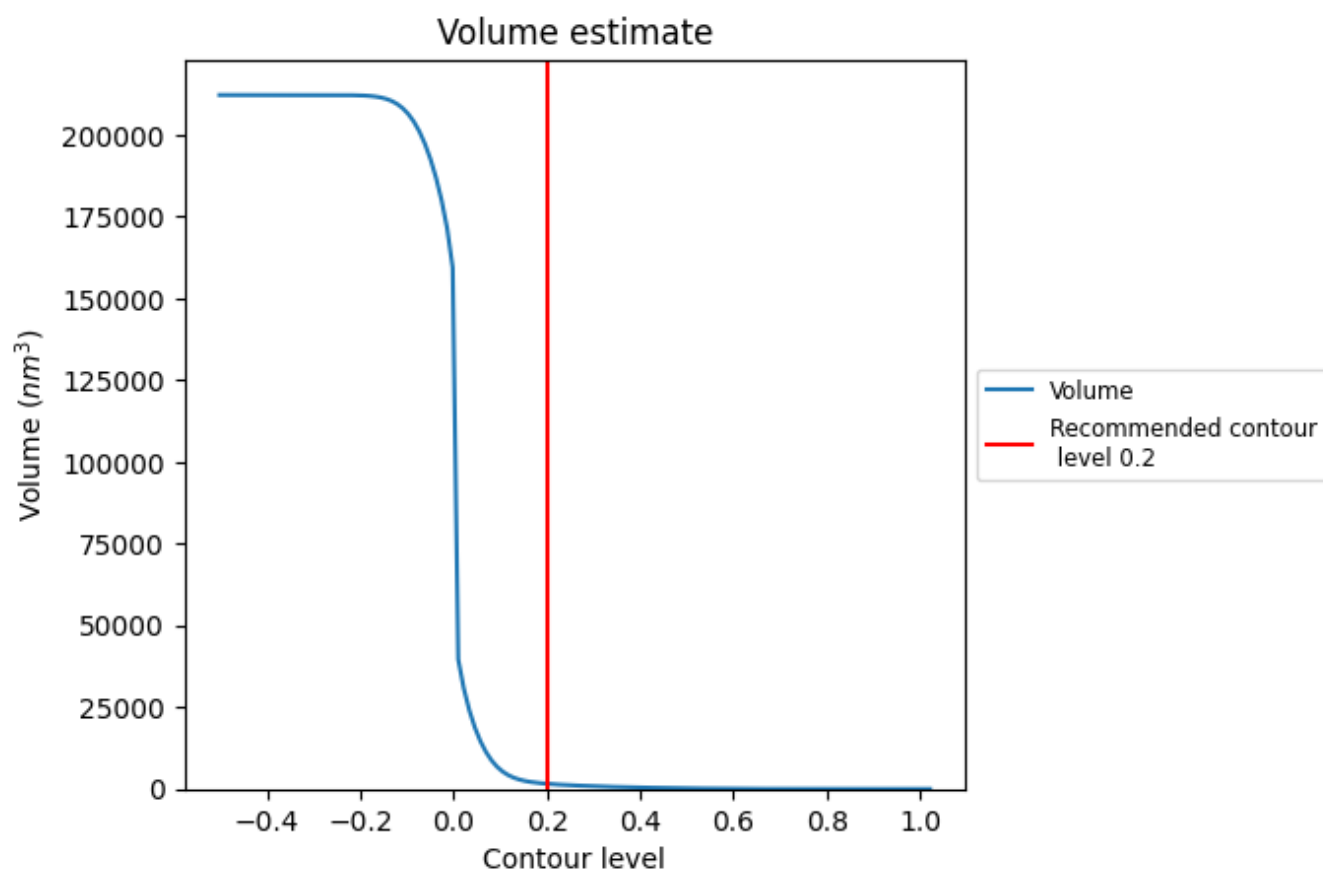
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

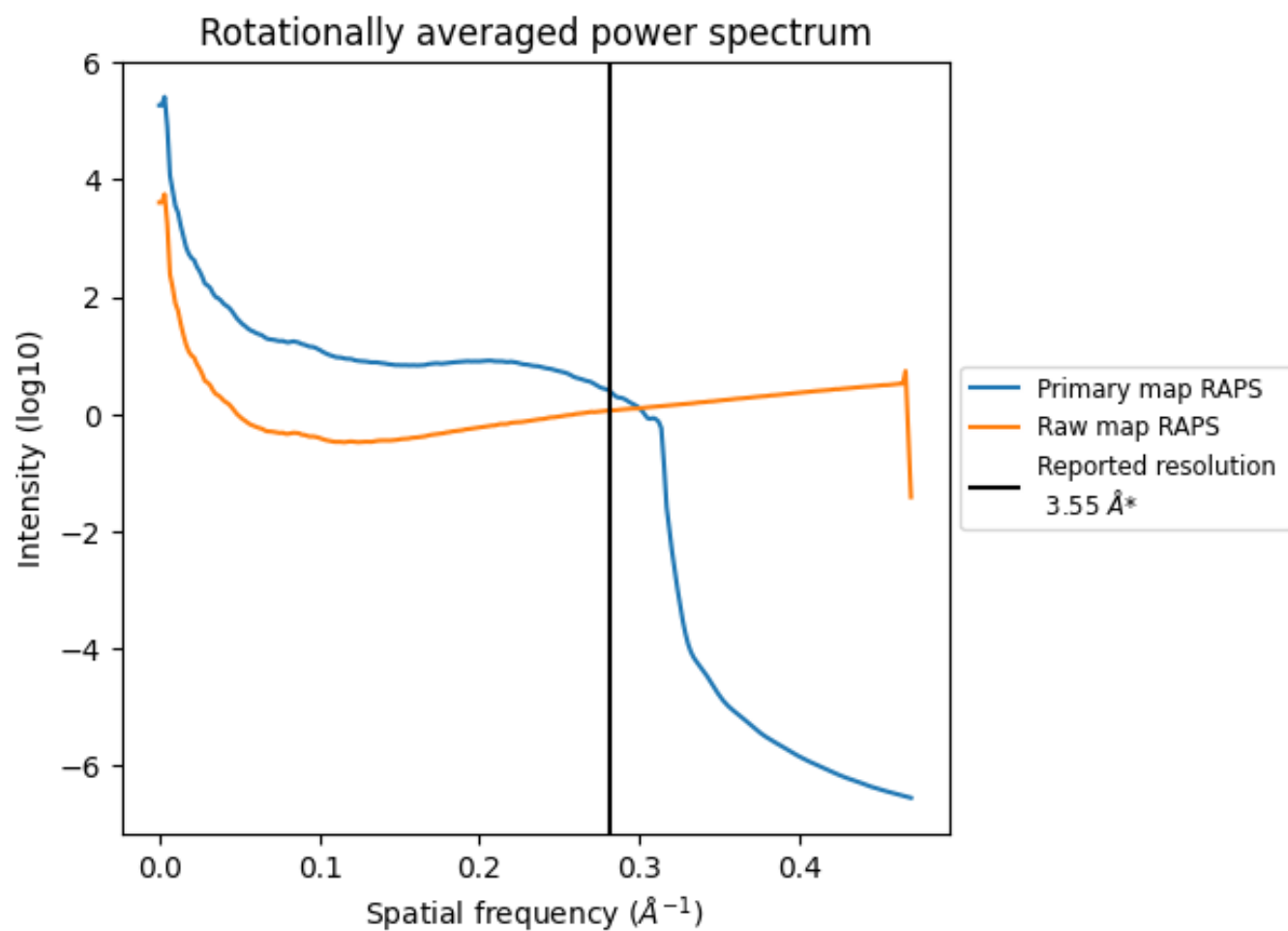
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm³; this corresponds to an approximate mass of 1430 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 ⓘ

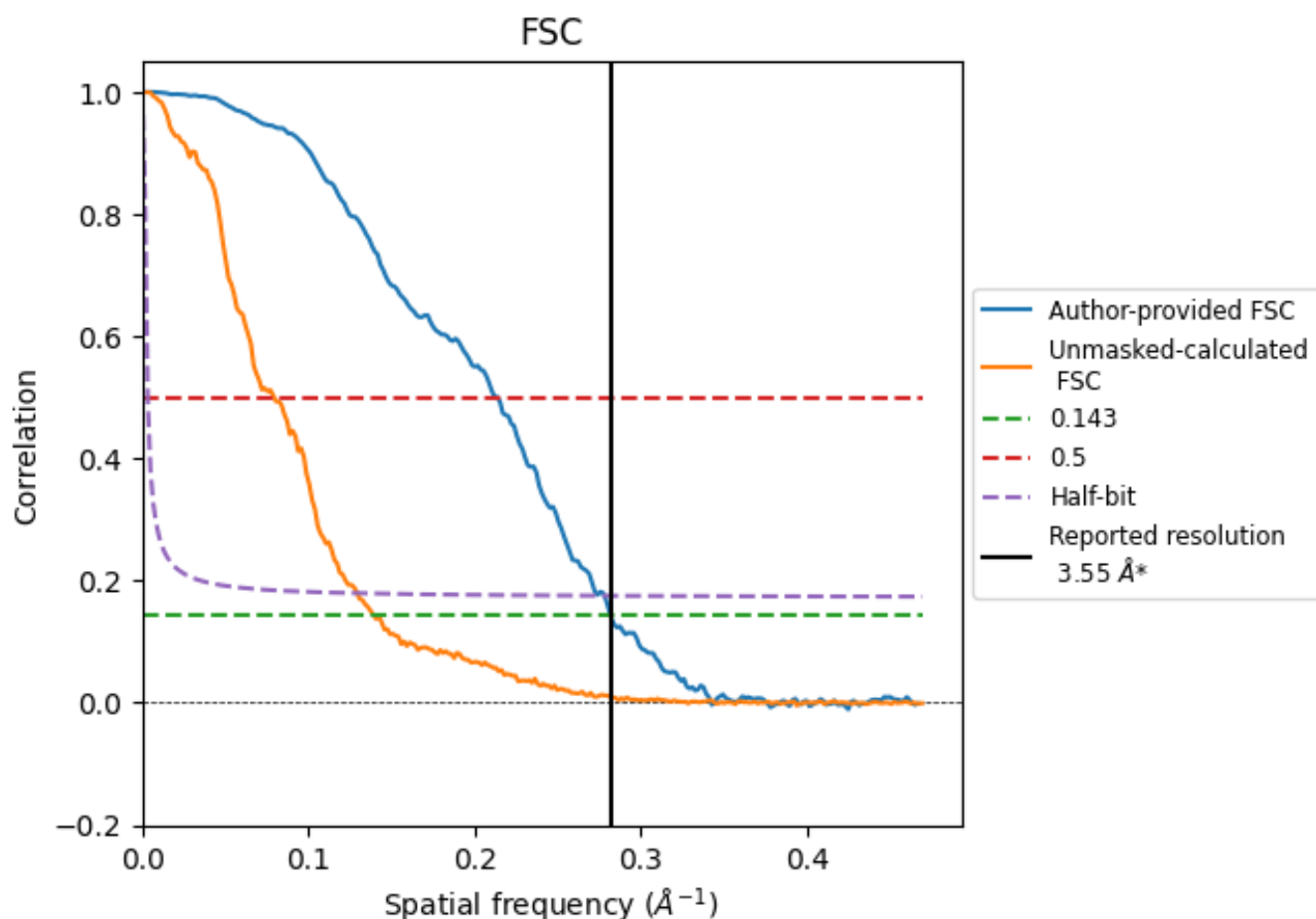


*Reported resolution corresponds to spatial frequency of 0.282 \AA^{-1}

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 0.282 \AA^{-1}

8.2 Resolution estimates [i](#)

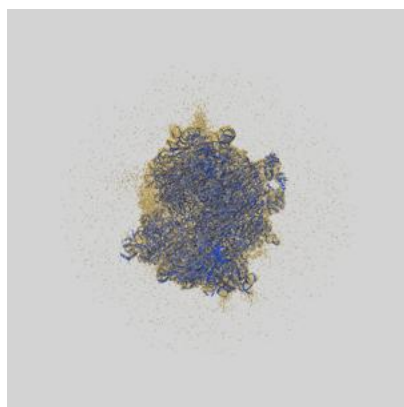
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.55	4.68	3.60
Unmasked-calculated*	7.17	12.59	7.72

*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 7.17 differs from the reported value 3.55 by more than 10 %

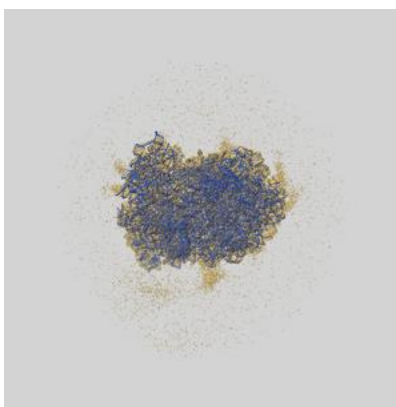
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55351 and PDB model 9SYR. Per-residue inclusion information can be found in section 3 on page 24.

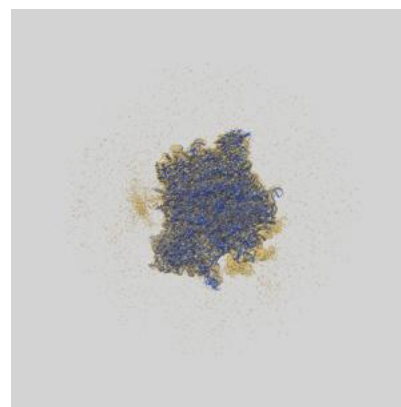
9.1 Map-model overlay [i](#)



X



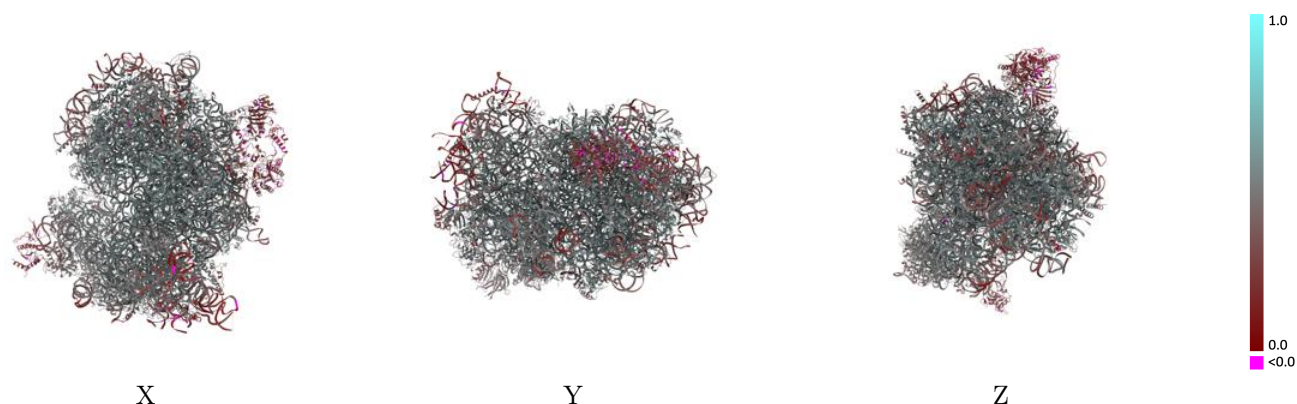
Y



Z

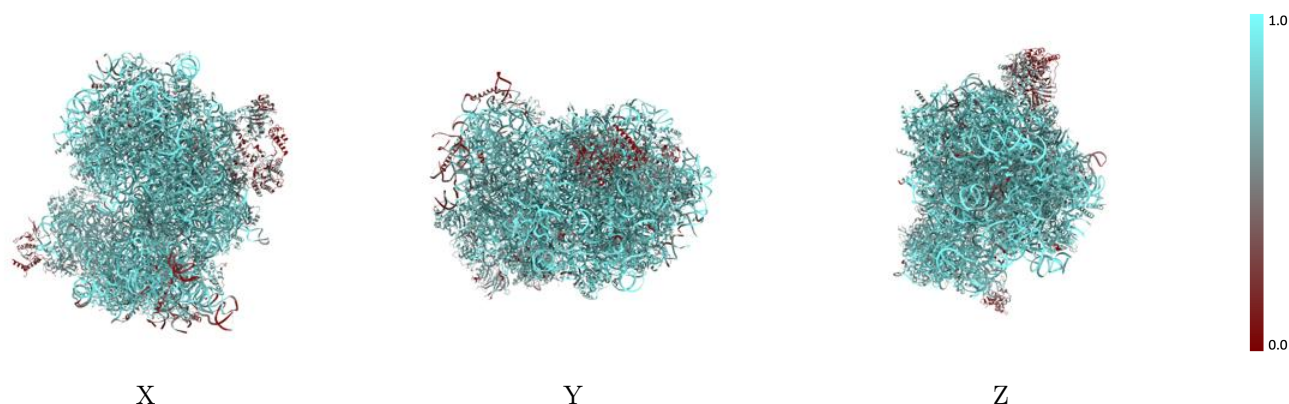
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



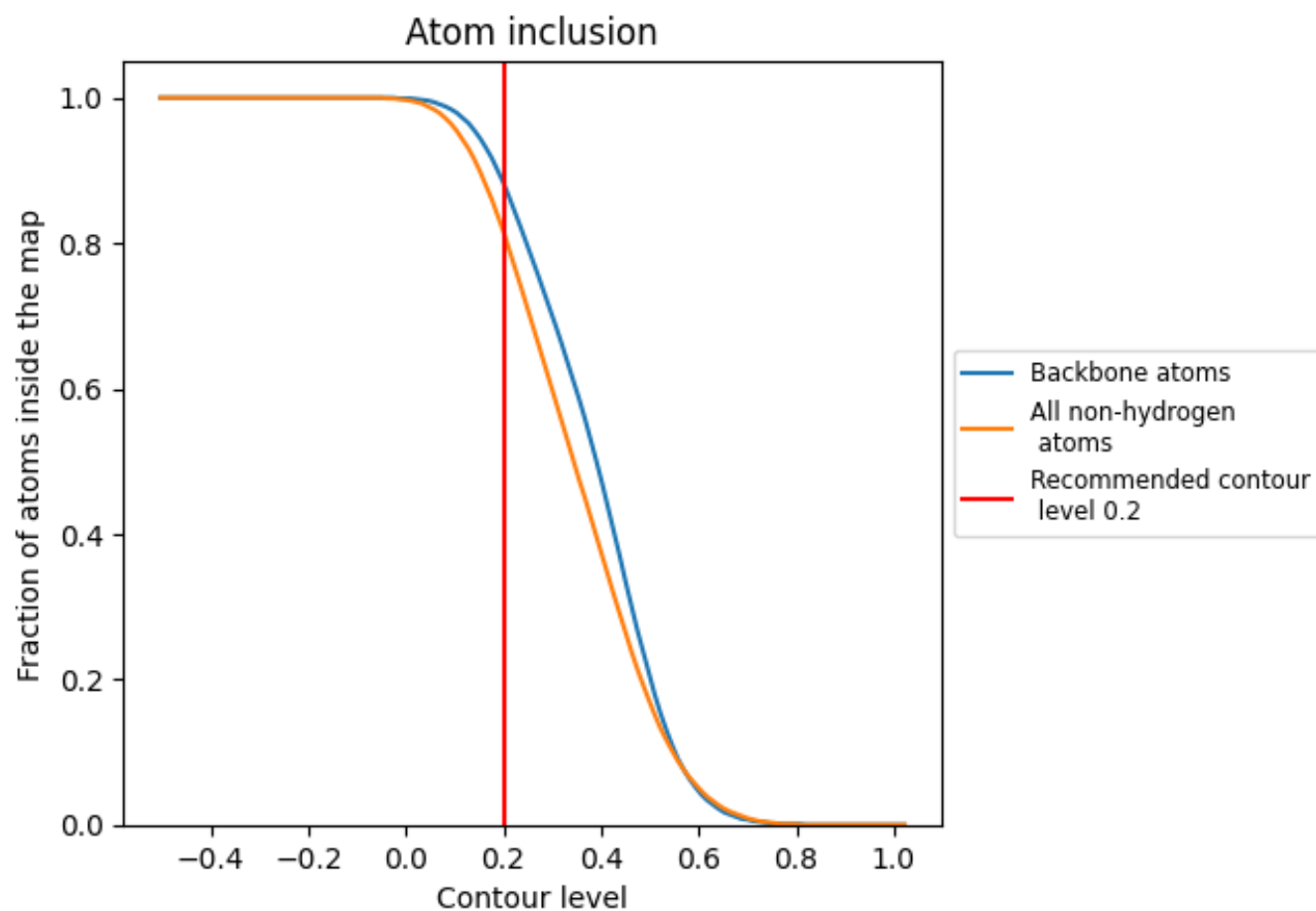
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.4720
L1	 0.9060	 0.4830
L2	 0.9670	 0.5050
L3	 0.9360	 0.5010
LA	 0.8500	 0.5430
LB	 0.6910	 0.4550
LC	 0.7940	 0.5330
LD	 0.7430	 0.5020
LE	 0.7850	 0.5190
LF	 0.7660	 0.5290
LG	 0.8310	 0.5190
LH	 0.8310	 0.5440
LI	 0.7960	 0.5150
LJ	 0.7770	 0.4900
LK	 0.7810	 0.4970
LM	 0.7720	 0.5060
LN	 0.5020	 0.4660
LO	 0.7750	 0.4880
LP	 0.7820	 0.5020
LQ	 0.7940	 0.4970
La	 0.8120	 0.5470
Lb	 0.8190	 0.5300
Lc	 0.8090	 0.5200
Ld	 0.8180	 0.4890
Le	 0.7870	 0.4910
Lf	 0.7960	 0.5190
Lg	 0.8090	 0.5370
Lh	 0.8030	 0.5340
Li	 0.7860	 0.5010
Lj	 0.8200	 0.5230
Lk	 0.7930	 0.5210
Ll	 0.7770	 0.4660
Lm	 0.7870	 0.5330
Ln	 0.5520	 0.4130
Lo	 0.7430	 0.5010























Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lp	 0.7810	 0.4970
Lq	 0.8190	 0.5060
Lr	 0.8320	 0.5330
Ls	 0.7280	 0.4590
Lt	 0.7750	 0.5050
Lu	 0.8040	 0.5150
Lv	 0.8230	 0.5360
Lw	 0.8430	 0.5450
Lx	 0.7780	 0.5070
Ly	 0.7610	 0.4870
Lz	 0.7420	 0.4850
Na	 0.3420	 0.2330
Nb	 0.4100	 0.3030
Nd	 0.5310	 0.2690
Nm	 0.2760	 0.2020
S1	 0.8600	 0.4510
S2	 0.7970	 0.4790
S3	 0.8440	 0.4410
SA	 0.7440	 0.4820
SB	 0.7920	 0.4890
SC	 0.6920	 0.4730
SD	 0.7330	 0.4960
SE	 0.6510	 0.4190
SF	 0.7620	 0.5000
SG	 0.7250	 0.4980
SH	 0.1900	 0.2180
Sa	 0.7070	 0.4560
Sb	 0.6960	 0.4570
Sc	 0.7120	 0.4790
Sd	 0.7570	 0.4630
Se	 0.7550	 0.5010
Sf	 0.7880	 0.5250
Sg	 0.7970	 0.5230
Sh	 0.7520	 0.4540
Si	 0.7230	 0.4580
Sj	 0.7670	 0.5020
Sk	 0.6940	 0.4560
Sl	 0.6730	 0.4370
Sm	 0.6380	 0.4370
Sn	 0.6330	 0.4490
So	 0.6670	 0.4770
Sp	 0.7260	 0.4670

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sq	 0.6420	 0.5000
Sr	 0.0660	 0.2120
Ss	 0.6010	 0.3930
St	 0.7550	 0.4800
Su	 0.7020	 0.4870
Sv	 0.7560	 0.5060
Sw	 0.7570	 0.4950
Sx	 0.6520	 0.4520
Sy	 0.6760	 0.4170
Sz	 0.6610	 0.4250