



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:34 AM UTC

PDB ID : 8OIT / pdb\_00008oit  
EMDB ID : EMD-16899  
Title : 39S human mitochondrial large ribosomal subunit with mtRF1 and P-site tRNA  
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.  
Deposited on : 2023-03-23  
Resolution : 2.90 Å (reported)  
Based on initial models : ., 7QI4

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

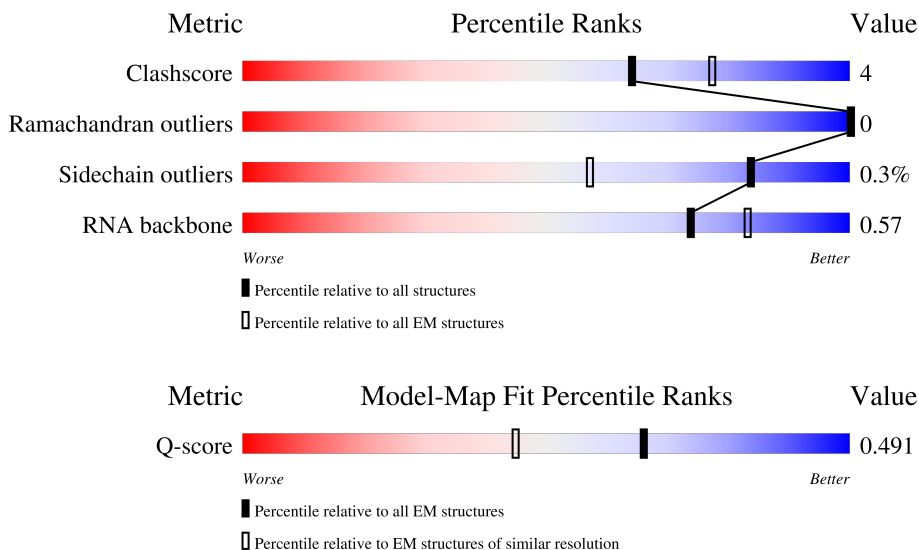
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 ( 2.40 - 3.40 )

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

Mol	Chain	Length	Quality of chain
1	B1	198	
1	B2	198	
1	B3	198	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B4	198	16% 13% 84%
1	B5	198	16% 15% 84%
1	B6	198	16% 13% 84%
2	B7	3	100% 67% 33%
3	B8	1561	7% 69% 28%
4	B9	72	39% 56% 40%
5	BA	206	73% 7% 19%
6	BB	153	20% 89% 10%
7	BC	216	27% 85% 10% 5%
8	BD	148	5% 73% 5% 22%
9	BE	256	7% 88% 7% 5%
10	BF	250	66% 6% 28%
11	BG	161	70% 6% 24%
12	BH	188	5% 55% 41%
13	BI	65	8% 74% 12% 14%
14	BJ	92	47% 50%
15	BK	188	44% 6% 49%
16	BL	305	70% 8% 22%
17	BM	348	78% 9% 12%
18	BN	311	67% 14% 19%
19	BO	267	48% 61% 15% 24%
20	BP	261	46% 75% 7% 19%
21	BQ	192	81% 83% 8% 9%
22	BR	178	88% 12%
23	BS	145	66% 13% 21%

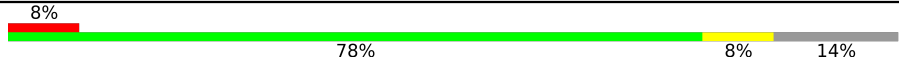
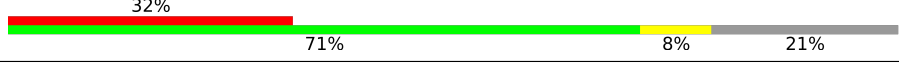
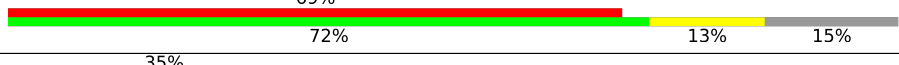


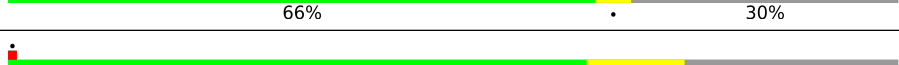



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	BT	296	90% 9% 6%
25	BU	251	79% 10% 12% 6%
26	BV	175	74% 14% 12% 6%
27	BW	180	73% 7% 20% 6%
28	BX	292	65% 12% 23% 6%
29	BY	149	84% 10% 6% 6%
30	BZ	205	72% 7% 21% 6%
31	Ba	123	72% 24% 10%
32	Bb	112	82% 8% 10% 32%
33	Bc	138	54% 5% 41% 40%
34	Bd	128	36% 16% 48% 29%
35	Be	102	75% 17% 8% 6%
36	Bf	206	64% 8% 29% 21%
37	Bg	222	67% 5% 27% 27%
38	Bh	196	77% 5% 17% 6%
39	Bi	439	78% 10% 12% 7%
40	Bj	325	35% 16% 50% 50%
41	Bl	103	36% 63% 6%
42	Bm	423	81% 12% 7% 6%
43	Bn	380	79% 14% 7% 14%
44	Bo	338	74% 13% 13% 19%
45	Bp	206	65% 7% 29% 49%
46	Bq	137	85% 5% 9% 14%
47	Br	142	64% 6% 30% 14%
48	Bs	215	57% 13% 30% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	212	
53	Bx	166	
54	By	158	
55	Bz	128	
56	AG	71	
57	Aa	484	

## 2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 113095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	B1	46	354	228	56	70	0	0
1	B2	32	257	168	40	49	0	0
1	B3	32	257	168	40	49	0	0
1	B4	31	245	159	39	47	0	0
1	B5	31	245	159	39	47	0	0
1	B6	31	245	159	39	47	0	0

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B7	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B8	1558	33070	14843	5963	10706	1558	0	0

- Molecule 4 is a RNA chain called CP Val-tRNA(Val).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B9	72	1524	685	269	498	72	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B9	70	C	G	conflict	GB NC_012920.1
B9	72	A	U	conflict	GB NC_012920.1

- Molecule 5 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BA	166	1369	875	254	233	7	0	0

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BB	152	1251	788	234	226	3	0	0

- Molecule 7 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BC	205	1676	1068	298	302	8	0	0

- Molecule 8 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BD	116	904	577	171	153	3	0	0

- Molecule 9 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BE	244	2044	1322	352	365	5	0	0

- Molecule 10 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BF	181	1556	995	298	259	4	0	0

- Molecule 11 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 12 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 13 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 14 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BK	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 16 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 17 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BM	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 18 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BN	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 19 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 20 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BP	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 21 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1455	936	259	253	7		

- Molecule 23 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BS	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BT	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 25 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BU	222	1786	1143	326	307	10	0	0

- Molecule 26 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BV	154	1259	792	241	219	7	0	0

- Molecule 27 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BW	144	1173	733	224	211	5	0	0

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BX	224	1866	1194	330	333	9	0	0

- Molecule 29 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BY	140	1154	732	231	187	4	0	0

- Molecule 30 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BZ	161	1293	835	227	227	4	0	0

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Ba	94	745	463	144	136	2	0	0

- Molecule 32 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Bb	101	774	479	148	142	5	0	0

- Molecule 33 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Bc	82	688	437	120	128	3	0	0

- Molecule 34 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bd	66	550	338	114	96	2	0	0

- Molecule 35 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Be	94	798	501	165	129	3	0	0

- Molecule 36 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Bf	147	1205	748	228	225	4	0	0

- Molecule 37 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Bg	161	1350	841	260	244	5	0	0

- Molecule 38 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bh	162	1322	839	252	223	8	0	0

- Molecule 39 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bj	164	Total	C	N	O	S	0	0
			1327	856	217	250	4		

- Molecule 41 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 42 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 43 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bn	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 44 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bo	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 45 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	147	Total	C	N	O	S	0	0
			1243	790	218	233	2		

- Molecule 46 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Bq	124	997	644	170	181	2	0	0

- Molecule 47 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Br	100	840	529	152	154	5	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Bs	151	1196	744	231	218	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP Q8N983

- Molecule 49 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Bt	286	2299	1470	397	423	9	0	0

- Molecule 50 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Bu	241	1985	1273	340	359	13	0	0

- Molecule 51 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Bv	238	1931	1222	339	364	6	0	0

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Bw	157	1252	799	207	242	4	0	0

- Molecule 53 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Bx	134	1113	719	193	199	2	0	0

- Molecule 54 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	By	110	895	568	156	168	3	0	0

- Molecule 55 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Bz	97	828	532	165	127	4	0	0

- Molecule 56 is a RNA chain called P-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	AG	71	1504	674	264	495	71	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB NC_012920.1
AG	70	C	-	insertion	GB NC_012920.1

- Molecule 57 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Aa	381	3114	1940	569	592	13	0	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	311	ALA	GLY	engineered mutation	UNP O75570
Aa	312	ALA	GLY	engineered mutation	UNP O75570
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	GLY	-	expression tag	UNP O75570
Aa	454	SER	-	expression tag	UNP O75570
Aa	455	GLY	-	expression tag	UNP O75570
Aa	456	GLY	-	expression tag	UNP O75570
Aa	457	SER	-	expression tag	UNP O75570
Aa	458	GLY	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	SER	-	expression tag	UNP O75570
Aa	461	GLY	-	expression tag	UNP O75570
Aa	462	GLY	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	TYR	-	expression tag	UNP O75570
Aa	465	LYS	-	expression tag	UNP O75570
Aa	466	ASP	-	expression tag	UNP O75570
Aa	467	HIS	-	expression tag	UNP O75570
Aa	468	ASP	-	expression tag	UNP O75570
Aa	469	GLY	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	TYR	-	expression tag	UNP O75570
Aa	472	LYS	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	HIS	-	expression tag	UNP O75570
Aa	475	ASP	-	expression tag	UNP O75570
Aa	476	ILE	-	expression tag	UNP O75570
Aa	477	ASP	-	expression tag	UNP O75570
Aa	478	TYR	-	expression tag	UNP O75570
Aa	479	LYS	-	expression tag	UNP O75570
Aa	480	ASP	-	expression tag	UNP O75570
Aa	481	ASP	-	expression tag	UNP O75570
Aa	482	ASP	-	expression tag	UNP O75570
Aa	483	ASP	-	expression tag	UNP O75570
Aa	484	LYS	-	expression tag	UNP O75570

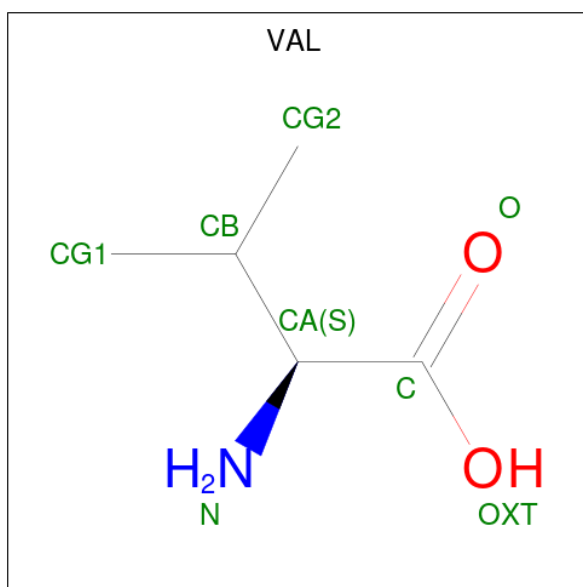
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
58	B8	30	Total K 30 30	0
58	BL	1	Total K 1 1	0
58	BT	1	Total K 1 1	0
58	Be	1	Total K 1 1	0
58	Bn	1	Total K 1 1	0

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
59	B8	216	Total Mg 216 216	0
59	BD	1	Total Mg 1 1	0
59	BL	3	Total Mg 3 3	0
59	BN	1	Total Mg 1 1	0
59	BO	1	Total Mg 1 1	0
59	BR	1	Total Mg 1 1	0
59	BT	1	Total Mg 1 1	0
59	BV	1	Total Mg 1 1	0
59	Bx	1	Total Mg 1 1	0
59	AG	1	Total Mg 1 1	0
59	Aa	1	Total Mg 1 1	0

- Molecule 60 is VALINE (CCD ID: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).

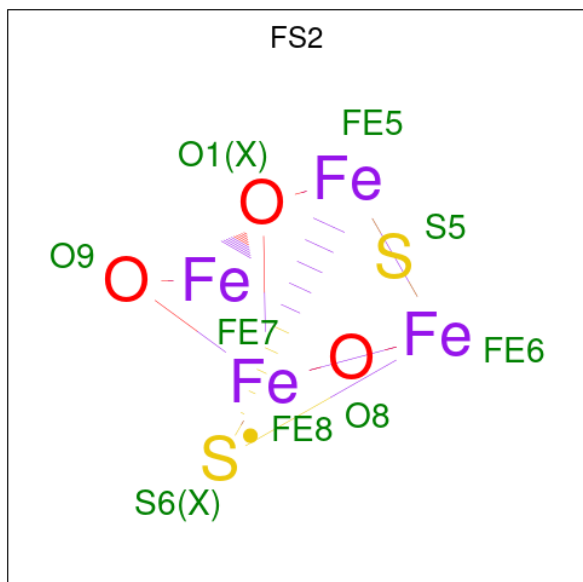


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	B9	1	7	5	1	1	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

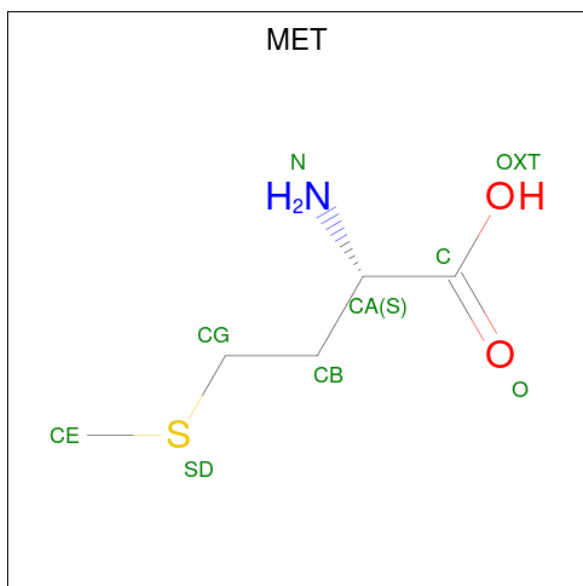
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	BH	1	1	1	0
61	Bl	1	1	1	0

- Molecule 62 is FE-S-O HYBRID CLUSTER (CCD ID: FS2) (formula: Fe<sub>4</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
62	Bh	1	Total	Fe	S	0
			4	2	2	

- Molecule 63 is METHIONINE (CCD ID: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



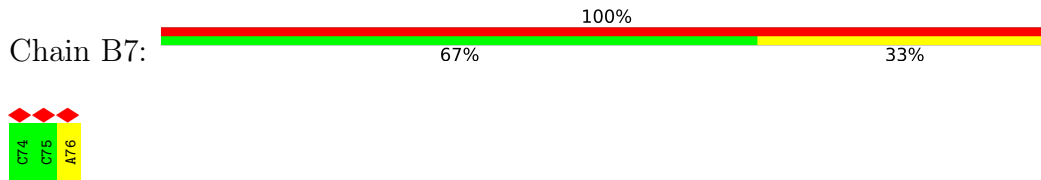
Mol	Chain	Residues	Atoms					AltConf
63	AG	1	Total	C	N	O	S	0
			8	5	1	1	1	



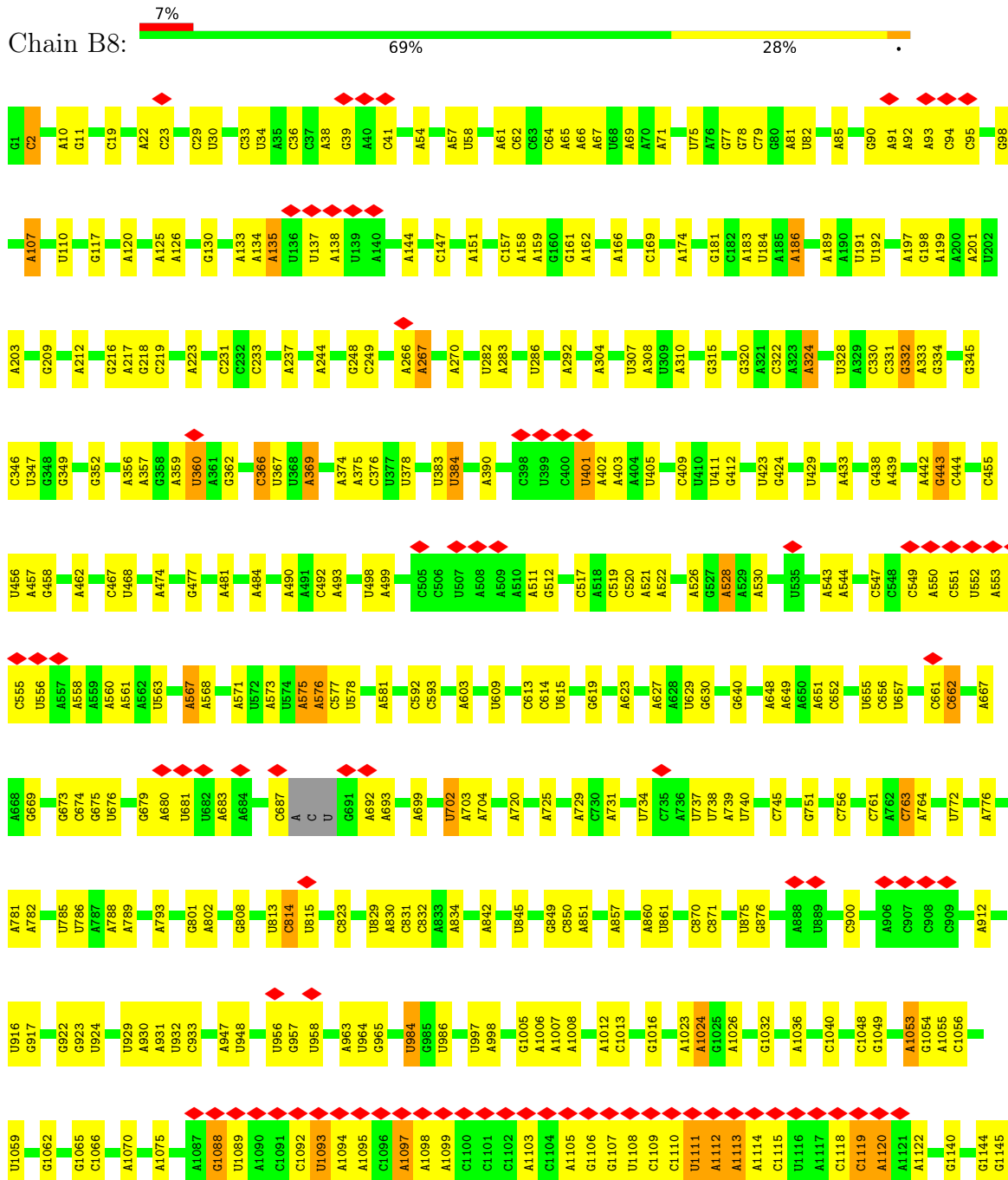


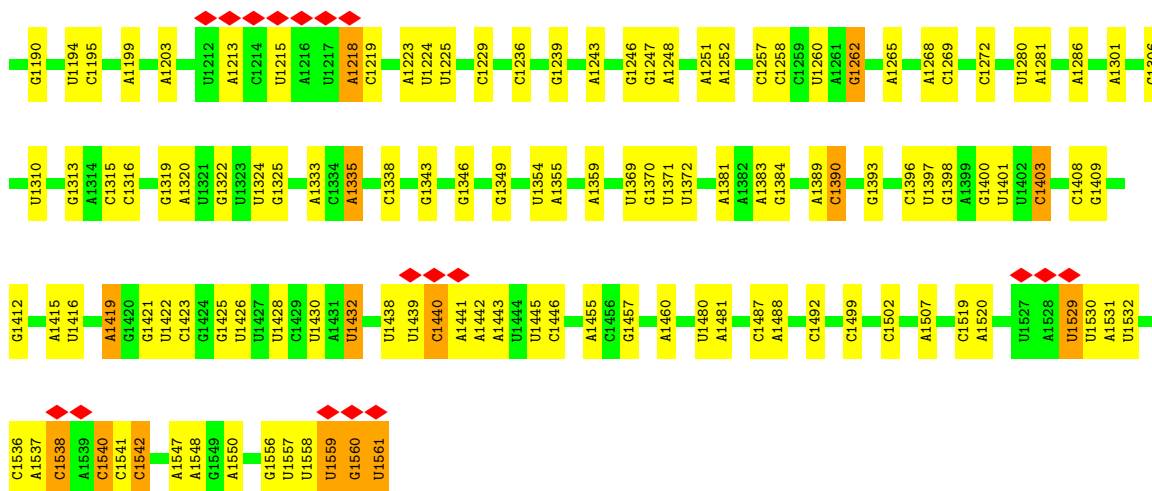
ALA	GLU
LYS	LYS
ILE	ALA
ALA	ALA
LEU	LEU
ALA	ALA
VAL	VAL
GLY	GLY
THR	THR
VAL	VAL
LEU	LEU
GLU	GLU

• Molecule 2: E-site tRNA

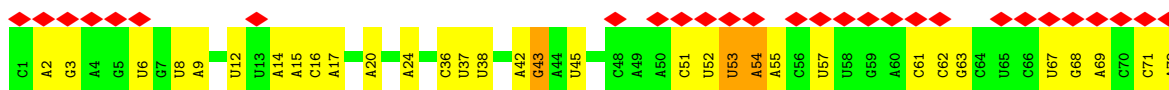
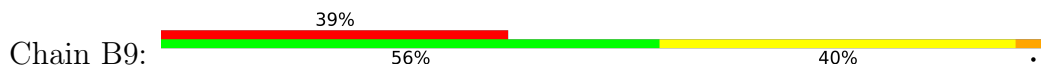


• Molecule 3: 16S rRNA

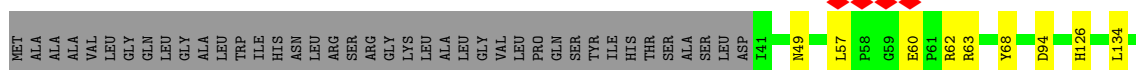
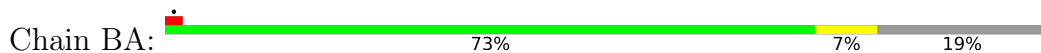




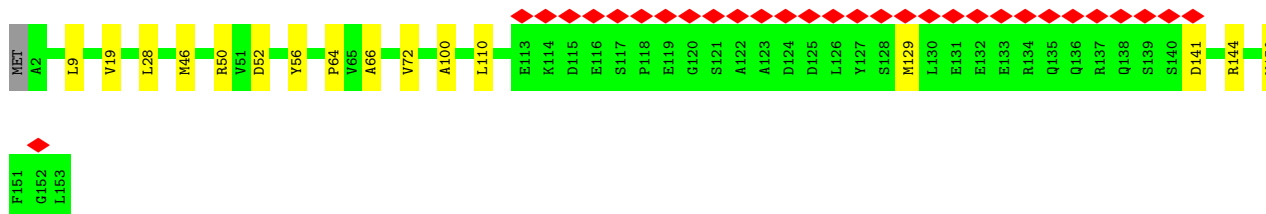
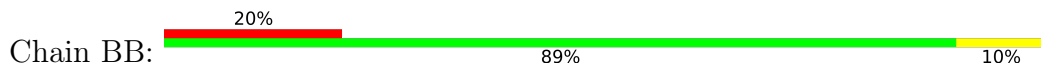
• Molecule 4: CP Val-tRNA(Val)



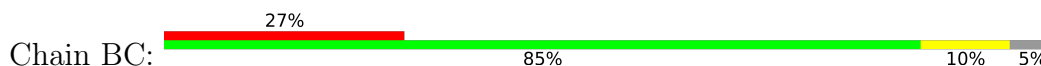
• Molecule 5: 39S ribosomal protein L22, mitochondrial

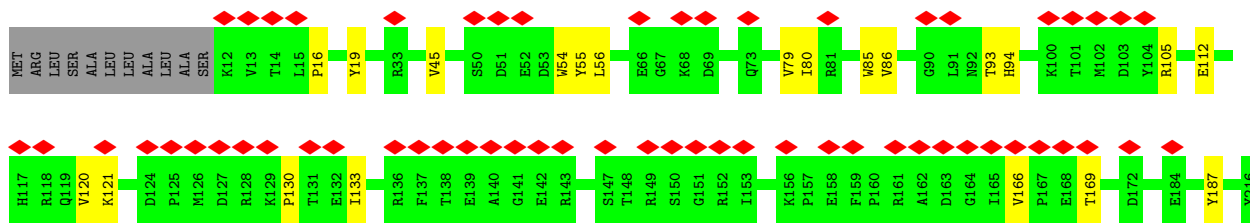


• Molecule 6: 39S ribosomal protein L23, mitochondrial

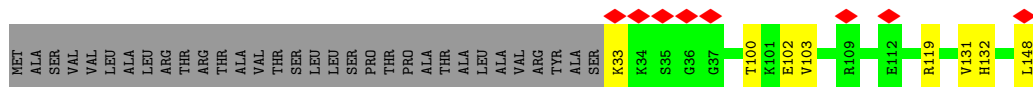
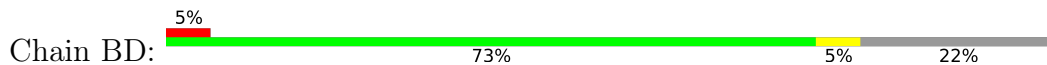


• Molecule 7: 39S ribosomal protein L24, mitochondrial

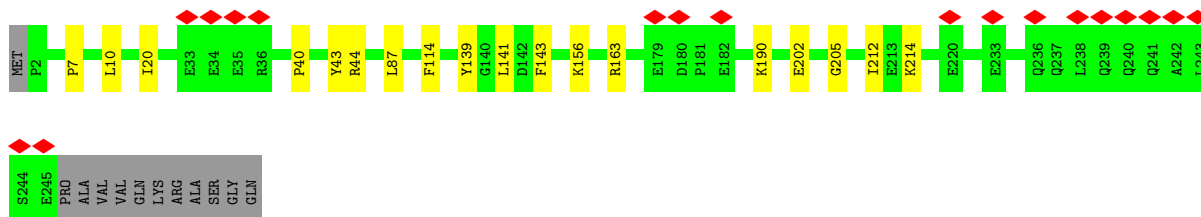
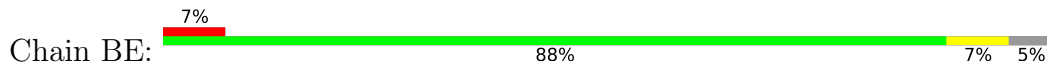




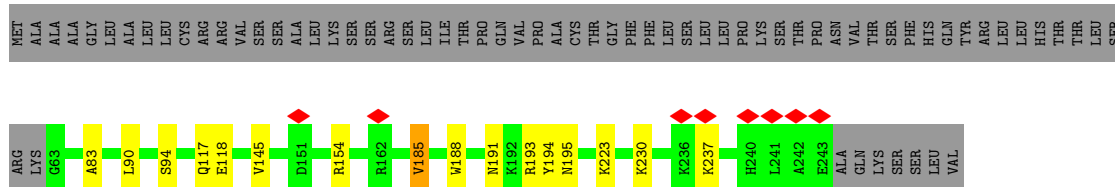
• Molecule 8: 39S ribosomal protein L27, mitochondrial



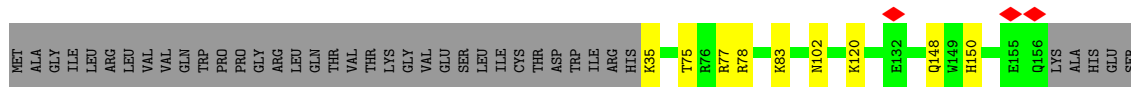
• Molecule 9: 39S ribosomal protein L28, mitochondrial



• Molecule 10: 39S ribosomal protein L47, mitochondrial



• Molecule 11: 39S ribosomal protein L30, mitochondrial

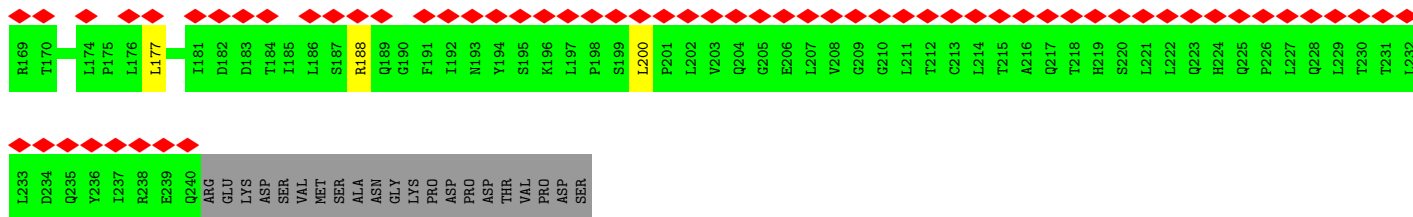


• Molecule 12: 39S ribosomal protein L32, mitochondrial

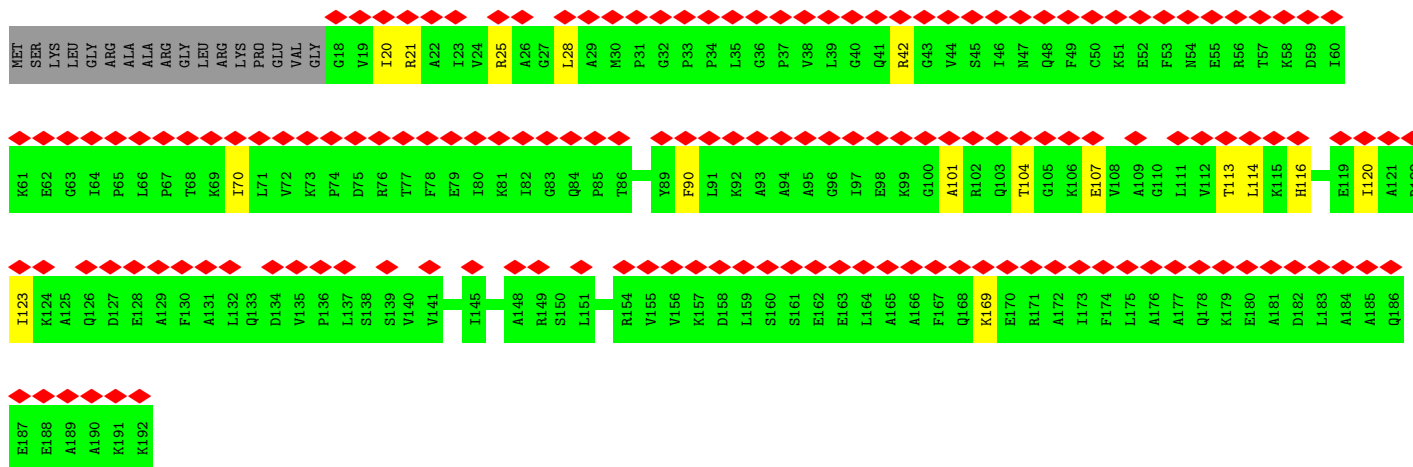
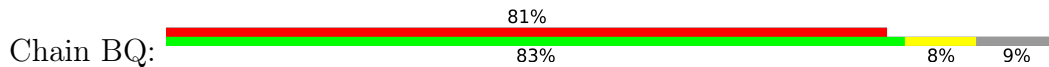




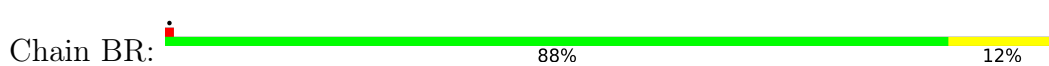




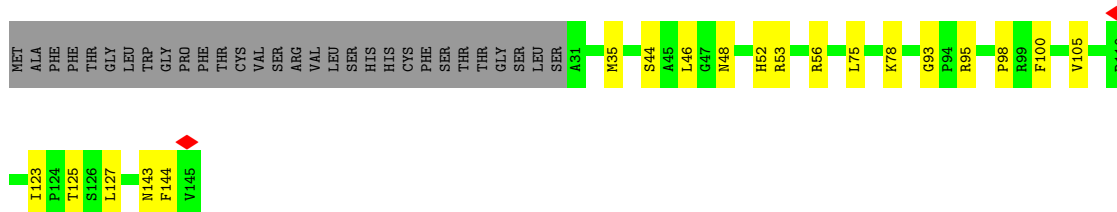
• Molecule 21: 39S ribosomal protein L11, mitochondrial



• Molecule 22: 39S ribosomal protein L13, mitochondrial

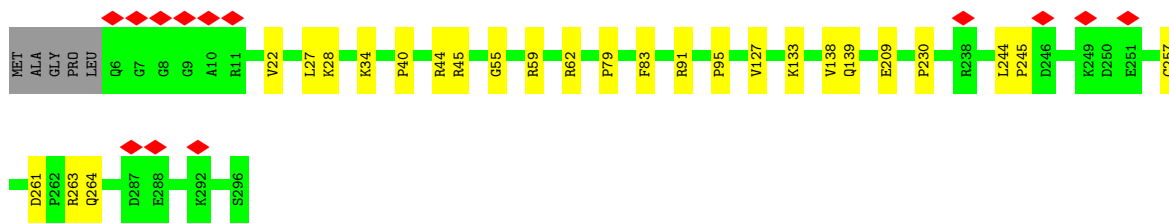


• Molecule 23: 39S ribosomal protein L14, mitochondrial

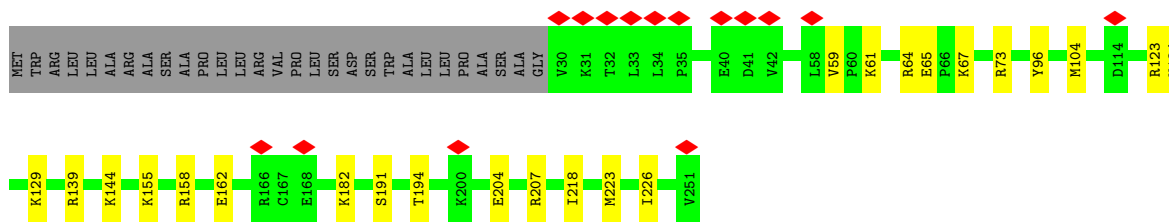
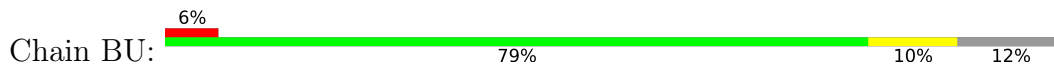


• Molecule 24: 39S ribosomal protein L15, mitochondrial

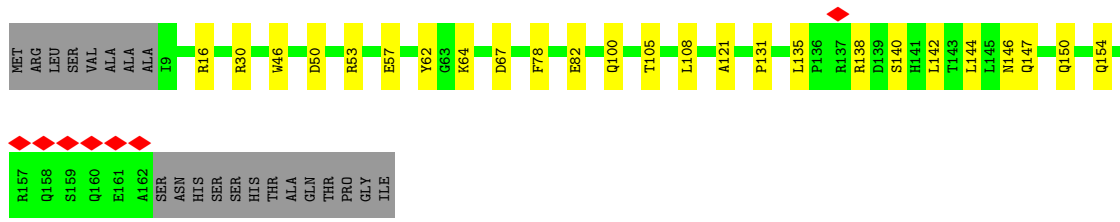
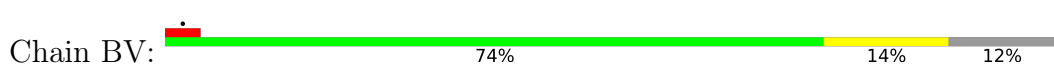




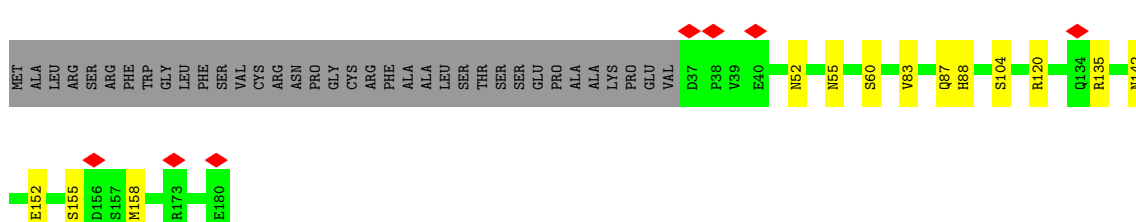
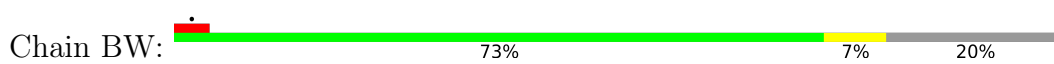
• Molecule 25: 39S ribosomal protein L16, mitochondrial



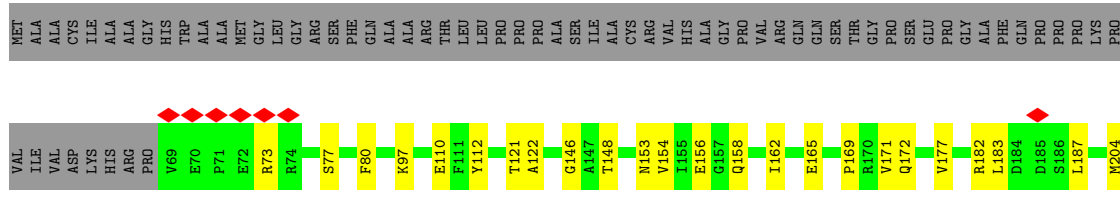
• Molecule 26: 39S ribosomal protein L17, mitochondrial



• Molecule 27: 39S ribosomal protein L18, mitochondrial

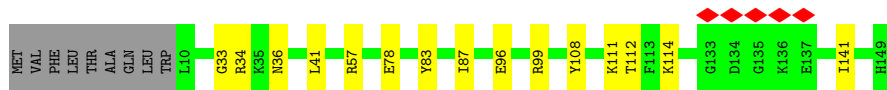
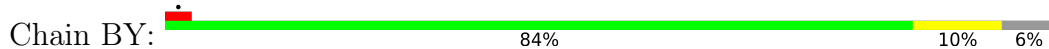


• Molecule 28: 39S ribosomal protein L19, mitochondrial

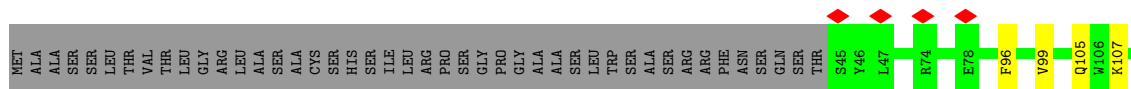




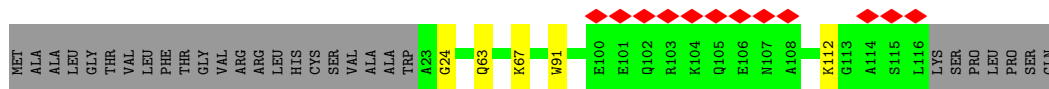
• Molecule 29: 39S ribosomal protein L20, mitochondrial



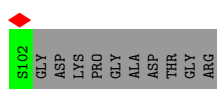
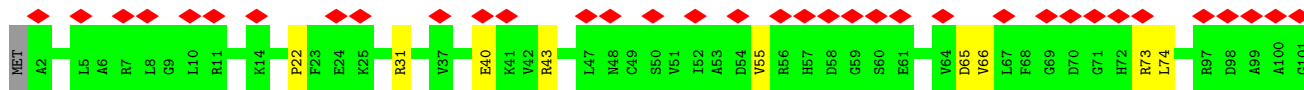
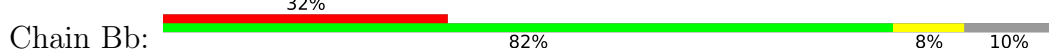
• Molecule 30: 39S ribosomal protein L21, mitochondrial



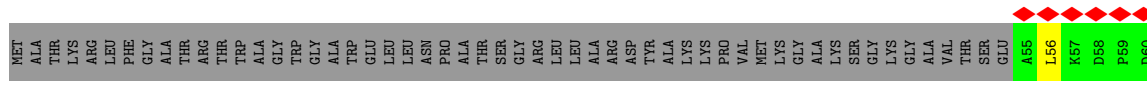
• Molecule 31: 39S ribosomal protein L52, mitochondrial

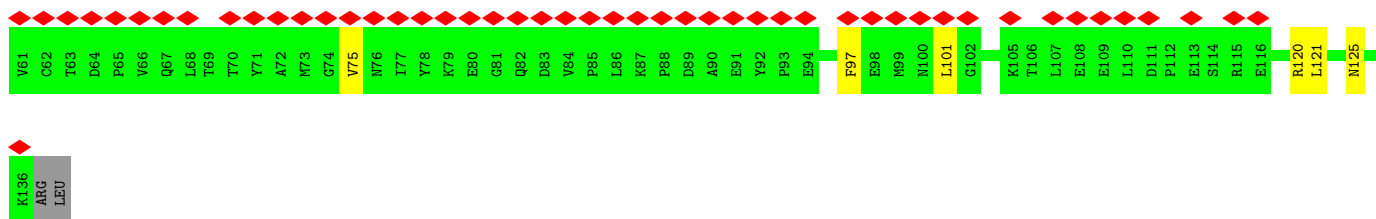


• Molecule 32: 39S ribosomal protein L53, mitochondrial

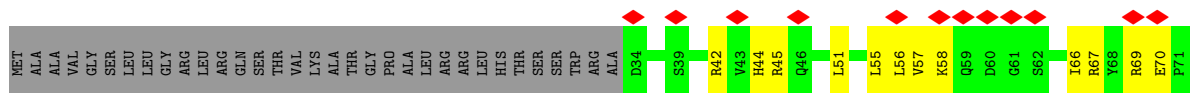
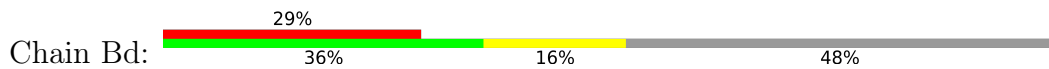


• Molecule 33: 39S ribosomal protein L54, mitochondrial

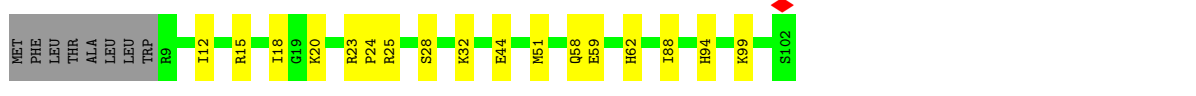
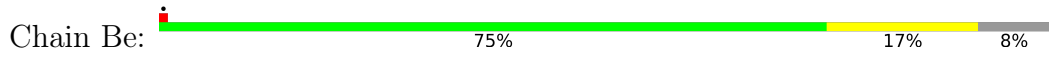




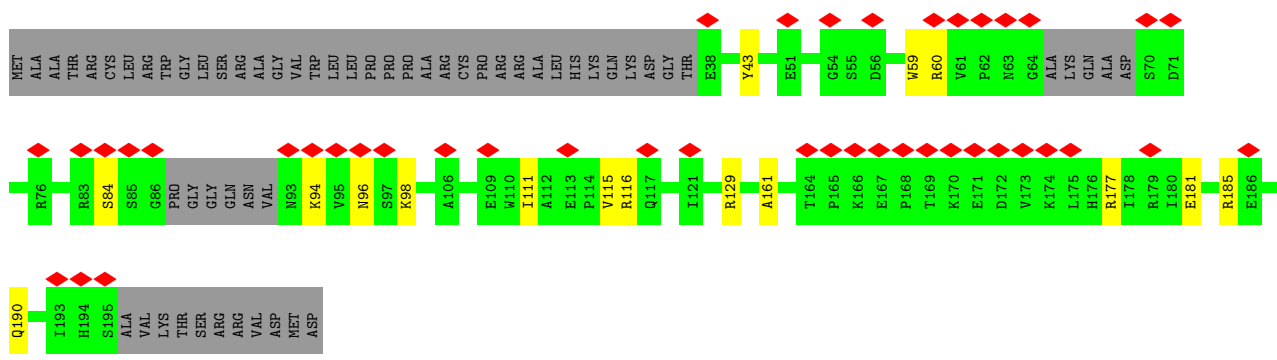
• Molecule 34: 39S ribosomal protein L55, mitochondrial



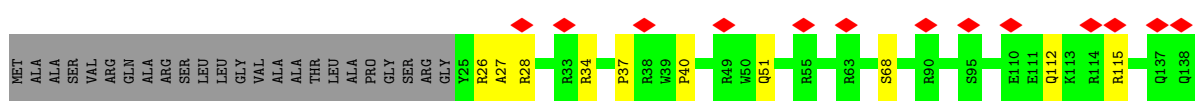
• Molecule 35: Ribosomal protein 63, mitochondrial



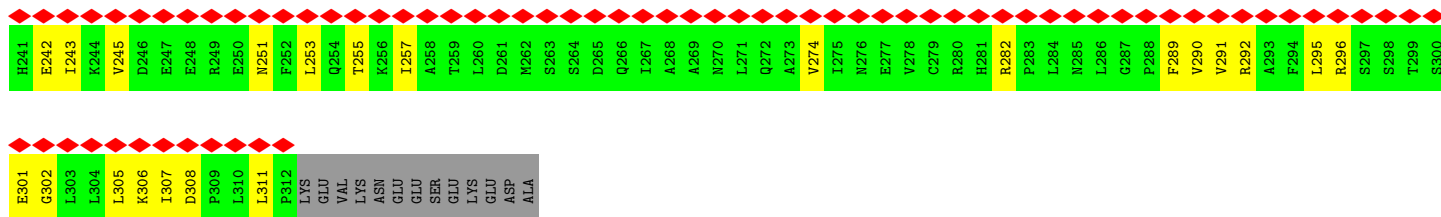
• Molecule 36: Peptidyl-tRNA hydrolase ICT1, mitochondrial



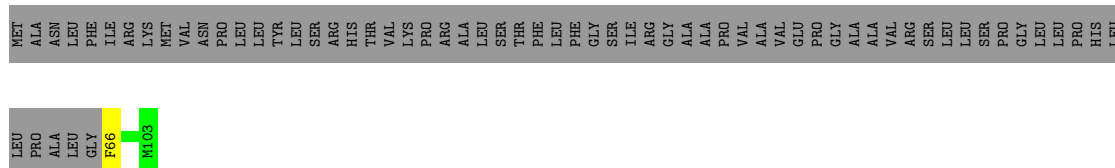
• Molecule 37: Growth arrest and DNA damage-inducible proteins-interacting protein 1



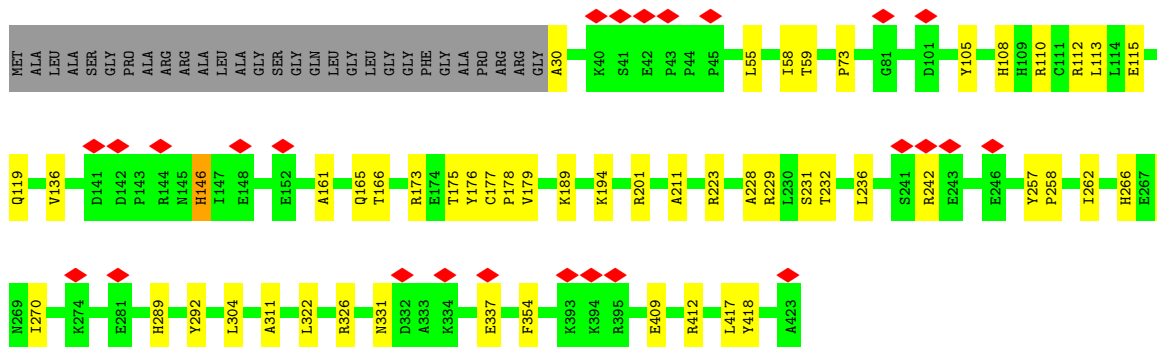
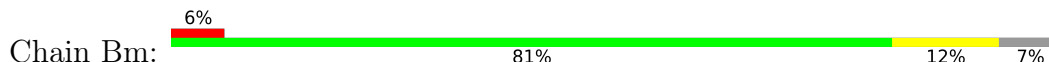




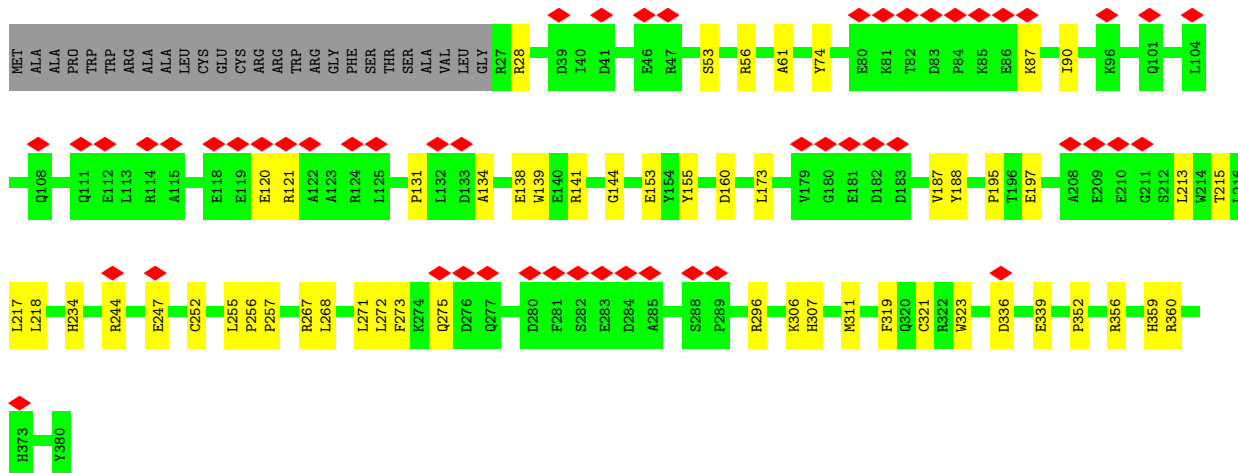
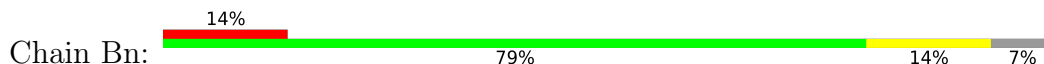
• Molecule 41: 39S ribosomal protein L36, mitochondrial



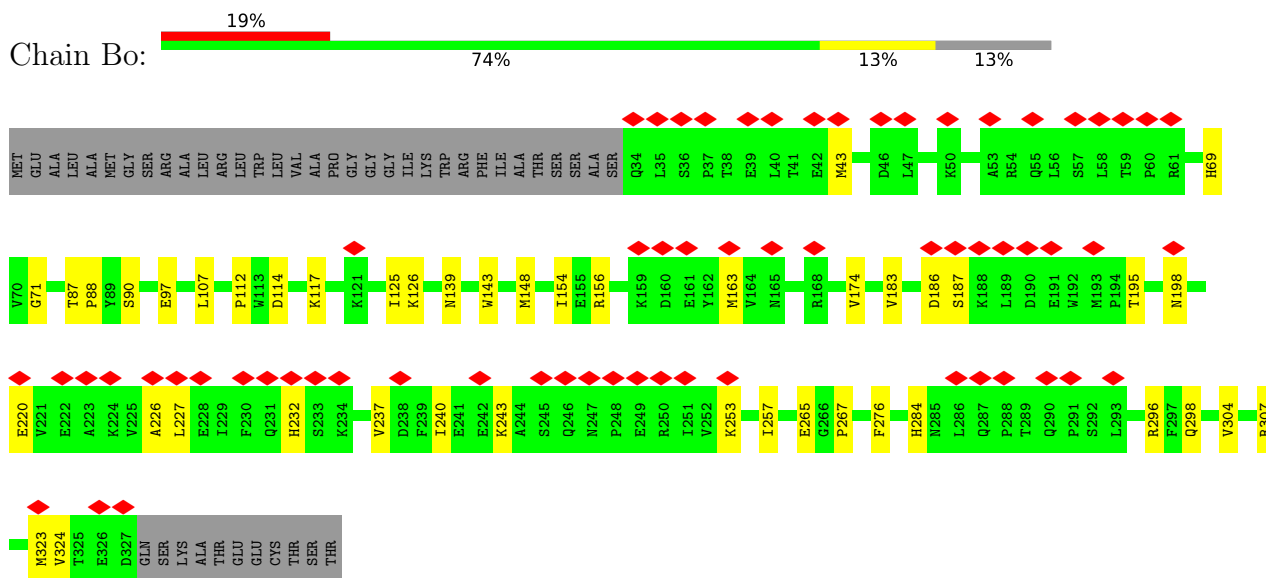
• Molecule 42: 39S ribosomal protein L37, mitochondrial



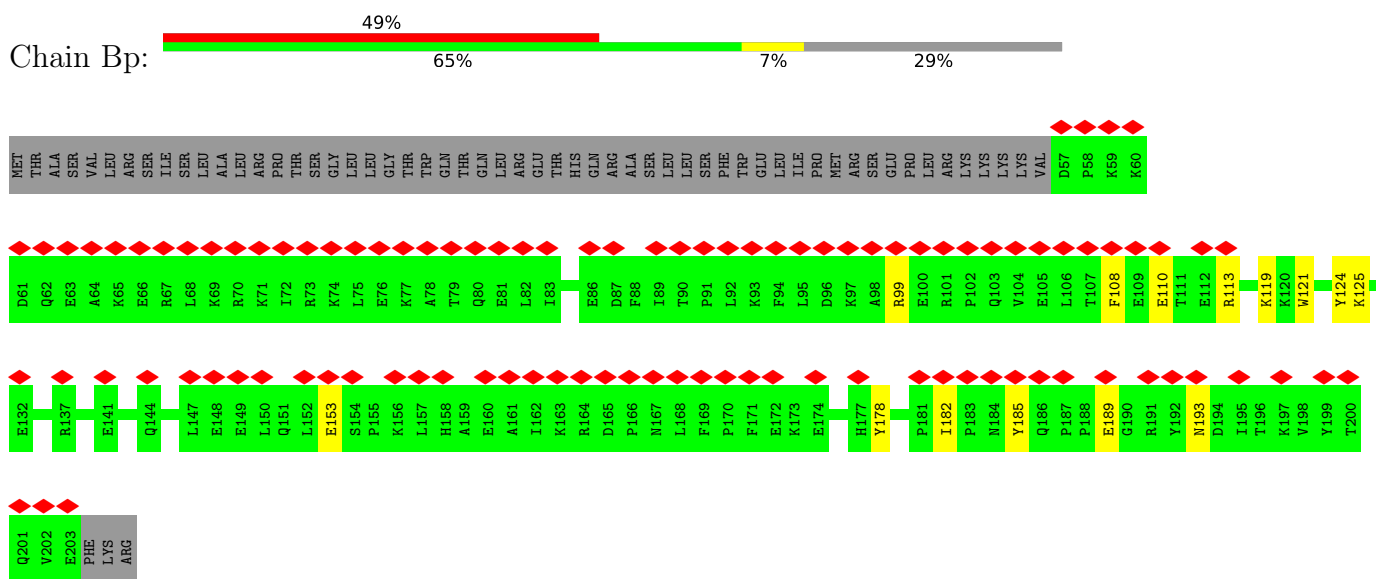
• Molecule 43: 39S ribosomal protein L38, mitochondrial



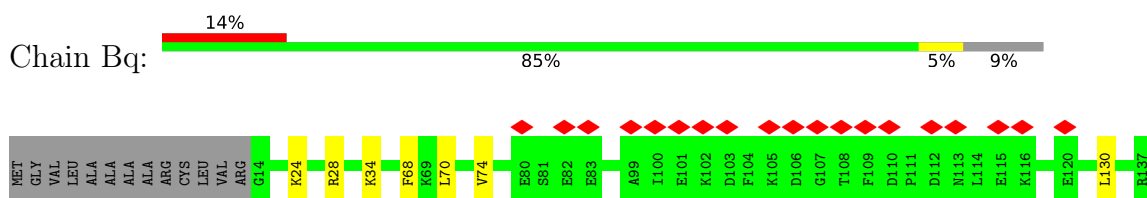
• Molecule 44: 39S ribosomal protein L39, mitochondrial



• Molecule 45: 39S ribosomal protein L40, mitochondrial



• Molecule 46: 39S ribosomal protein L41, mitochondrial

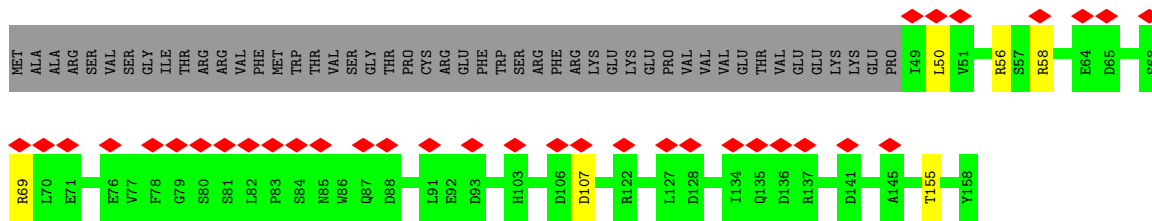


• Molecule 47: 39S ribosomal protein L42, mitochondrial

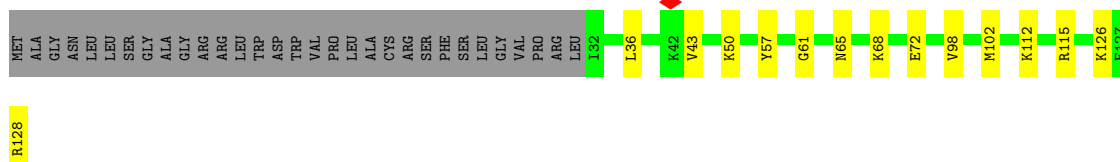




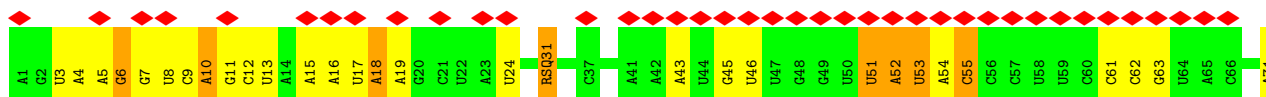




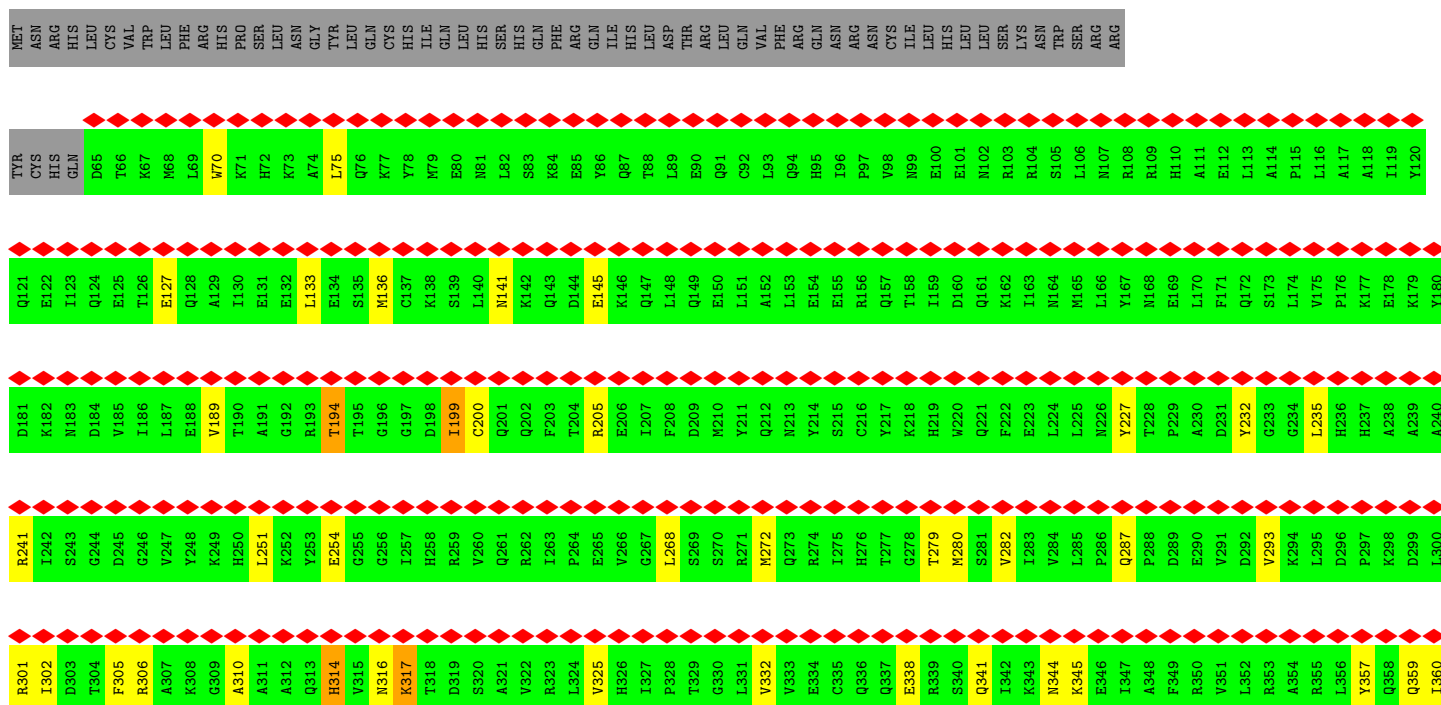
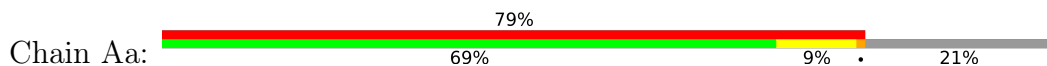
• Molecule 55: 39S ribosomal protein L51, mitochondrial



• Molecule 56: P-site Met-tRNA(Met)



• Molecule 57: Peptide chain release factor 1, mitochondrial



I361	E362	K363	D364	K365	R366	Q367	Q368	Q369	S370	A371	R372	K373	L374	Q375	V376	G377	T378	R379	A380	Q381	S382	E383	R384	I385	R386	T387	Y388	N389	F390	T391	Q392	D393	R394	V395	S396	D397	H398	R399	I400	A401	Y402	E403	V404	R405	D406	I407	K408	E409	F410	L411	C412	G413	G414	K415	G416	L417	D418	Q419	L420
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

I421	Q422	R423	L424	L425	Q426	S427	A428	D429	E430	E431	A432	I433	A434	E435	L436	L437	D438	E439	H440	L441	K442	S443	A444	K445	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	ASP	TYR	TYR	LYS	ASP	HIS	ASP	ASP	ASP	ASP	TYR	LYS	LYS	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	ASP	ASP	LYS
-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.267	Depositor
Minimum map value	-1.999	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.146	Depositor
Recommended contour level	0.75	Depositor
Map size ( $\text{\AA}$ )	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, PSU, 1MA, AYA, OMG, ACE, OMU, RSQ, 2MG, K, MG, FS2, ZN

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	B1	0.07	0/358	0.16	0/486
1	B2	0.08	0/259	0.18	0/350
1	B3	0.07	0/259	0.17	0/350
1	B4	0.05	0/246	0.14	0/331
1	B5	0.06	0/246	0.16	0/331
1	B6	0.06	0/246	0.16	0/331
2	B7	0.05	0/68	0.11	0/103
3	B8	0.09	0/36876	0.15	0/57402
4	B9	0.07	0/1627	0.13	0/2527
5	BA	0.09	0/1403	0.20	0/1886
6	BB	0.09	0/1274	0.20	0/1723
7	BC	0.08	0/1721	0.19	0/2333
8	BD	0.09	0/926	0.20	0/1244
9	BE	0.08	0/2099	0.18	0/2837
10	BF	0.08	0/1593	0.17	0/2136
11	BG	0.09	0/1021	0.21	0/1378
12	BH	0.08	0/913	0.18	0/1224
13	BI	0.08	0/469	0.20	0/621
14	BJ	0.09	0/383	0.20	0/507
15	BK	0.09	0/853	0.20	0/1136
16	BL	0.09	0/1896	0.20	0/2549
17	BM	0.09	0/2475	0.22	0/3355
18	BN	0.09	0/2090	0.21	0/2842
19	BO	0.08	0/1698	0.22	0/2292
20	BP	0.08	0/1731	0.20	0/2345
21	BQ	0.06	0/1348	0.17	0/1813
22	BR	0.09	0/1490	0.21	0/2021
23	BS	0.08	0/905	0.21	0/1218
24	BT	0.09	0/2381	0.21	0/3212
25	BU	0.08	0/1833	0.19	0/2468
26	BV	0.09	0/1283	0.20	0/1727
27	BW	0.08	0/1199	0.20	0/1623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
28	BX	0.08	0/1908	0.20	0/2569
29	BY	0.09	0/1175	0.18	0/1572
30	BZ	0.09	0/1320	0.23	0/1789
31	Ba	0.07	0/760	0.17	0/1023
32	Bb	0.07	0/777	0.17	0/1048
33	Bc	0.06	0/707	0.17	0/960
34	Bd	0.06	0/558	0.18	0/749
35	Be	0.09	0/819	0.20	0/1097
36	Bf	0.07	0/1223	0.17	0/1641
37	Bg	0.07	0/1384	0.17	0/1869
38	Bh	0.09	0/1362	0.22	0/1846
39	Bi	0.09	0/3239	0.20	0/4400
40	Bj	0.08	0/1354	0.22	0/1831
41	Bl	0.10	0/350	0.21	0/461
42	Bm	0.09	0/3305	0.20	0/4502
43	Bn	0.08	0/3043	0.20	0/4140
44	Bo	0.07	0/2447	0.19	0/3310
45	Bp	0.06	0/1269	0.16	0/1708
46	Bq	0.08	0/1025	0.20	0/1379
47	Br	0.09	0/866	0.23	0/1174
48	Bs	0.10	0/1219	0.22	0/1651
49	Bt	0.07	0/2347	0.19	0/3171
50	Bu	0.08	0/2039	0.20	0/2759
51	Bv	0.06	0/1970	0.17	0/2658
52	Bw	0.07	0/1273	0.17	0/1716
53	Bx	0.09	0/1151	0.21	0/1569
54	By	0.06	0/918	0.16	0/1249
55	Bz	0.10	0/850	0.21	0/1135
56	AG	0.09	0/1588	0.19	0/2466
57	Aa	0.12	0/3162	0.25	0/4253
All	All	0.09	0/118577	0.18	0/168396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	B1	354	0	377	3	0
1	B2	257	0	283	3	0
1	B3	257	0	283	1	0
1	B4	245	0	275	3	0
1	B5	245	0	275	1	0
1	B6	245	0	275	4	0
2	B7	62	0	34	0	0
3	B8	33070	0	16795	227	0
4	B9	1524	0	778	20	0
5	BA	1369	0	1410	11	0
6	BB	1251	0	1232	10	0
7	BC	1676	0	1687	14	0
8	BD	904	0	935	7	0
9	BE	2044	0	2060	13	0
10	BF	1556	0	1597	13	0
11	BG	996	0	1044	7	0
12	BH	898	0	916	5	0
13	BI	464	0	511	6	0
14	BJ	377	0	406	2	0
15	BK	832	0	883	12	0
16	BL	1859	0	1920	17	0
17	BM	2406	0	2415	21	0
18	BN	2031	0	2065	31	0
19	BO	1661	0	1734	32	0
20	BP	1695	0	1785	14	0
21	BQ	1330	0	1407	13	0
22	BR	1455	0	1452	14	0
23	BS	890	0	941	12	0
24	BT	2327	0	2395	20	0
25	BU	1786	0	1817	16	0
26	BV	1259	0	1294	18	0
27	BW	1173	0	1165	10	0
28	BX	1866	0	1900	22	0
29	BY	1154	0	1214	14	0
30	BZ	1293	0	1365	11	0
31	Ba	745	0	746	5	0
32	Bb	774	0	784	7	0
33	Bc	688	0	674	7	0
34	Bd	550	0	572	14	0
35	Be	798	0	804	14	0
36	Bf	1205	0	1223	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Bg	1350	0	1327	10	0
38	Bh	1322	0	1348	8	0
39	Bi	3155	0	3139	26	0
40	Bj	1327	0	1353	42	0
41	Bl	342	0	361	1	0
42	Bm	3210	0	3206	34	0
43	Bn	2948	0	2841	36	0
44	Bo	2390	0	2397	26	0
45	Bp	1243	0	1265	11	0
46	Bq	997	0	987	6	0
47	Br	840	0	810	7	0
48	Bs	1196	0	1195	21	0
49	Bt	2299	0	2320	18	0
50	Bu	1985	0	1976	16	0
51	Bv	1931	0	1916	24	0
52	Bw	1252	0	1269	14	0
53	Bx	1113	0	1097	7	0
54	By	895	0	881	6	0
55	Bz	828	0	857	11	0
56	AG	1504	0	764	20	0
57	Aa	3114	0	3115	35	0
58	B8	30	0	0	0	0
58	BL	1	0	0	0	0
58	BT	1	0	0	0	0
58	Be	1	0	0	0	0
58	Bn	1	0	0	0	0
59	AG	1	0	0	0	0
59	Aa	1	0	0	0	0
59	B8	216	0	0	0	0
59	BD	1	0	0	0	0
59	BL	3	0	0	0	0
59	BN	1	0	0	0	0
59	BO	1	0	0	0	0
59	BR	1	0	0	0	0
59	BT	1	0	0	0	0
59	BV	1	0	0	0	0
59	Bx	1	0	0	0	0
60	B9	7	0	8	0	0
61	BH	1	0	0	0	0
61	Bl	1	0	0	0	0
62	Bh	4	0	0	1	0
63	AG	8	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	113095	0	96168	812	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (812) 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)
3:B8:1401:U:H5''	57:Aa:310:ALA:HA	1.51	0.93
4:B9:6:U:H3	4:B9:63:G:H1	1.18	0.91
3:B8:1343:G:HO2'	41:Bl:66:PHE:N	1.72	0.85
3:B8:1107:G:N3	19:BO:179:ASN:ND2	2.30	0.79
3:B8:1111:U:O2	40:Bj:296:ARG:NH2	2.17	0.78
3:B8:829:U:OP2	3:B8:834:A:N6	2.16	0.78
3:B8:1109:C:H5'	40:Bj:116:SER:HB3	1.67	0.77
3:B8:107:A:N6	3:B8:110:U:OP2	2.18	0.76
3:B8:681:U:O4	3:B8:692:A:N6	2.19	0.75
20:BP:47:LEU:HD22	25:BU:226:ILE:HG12	1.70	0.73
19:BO:163:THR:HG21	40:Bj:87:TYR:HA	1.70	0.73
3:B8:1184:U:H4'	15:BK:138:PRO:HG2	1.72	0.72
3:B8:433:A:HO2'	11:BG:35:LYS:N	1.88	0.71
40:Bj:97:TYR:HB3	40:Bj:306:LYS:HB2	1.72	0.71
3:B8:1108:U:OP1	3:B8:1112:A:N6	2.23	0.71
57:Aa:70:TRP:HA	57:Aa:75:LEU:HD23	1.73	0.70
30:BZ:144:LEU:HB2	47:Br:58:ILE:HB	1.74	0.69
28:BX:182:ARG:HG3	28:BX:187:LEU:HD11	1.74	0.69
3:B8:320:G:OP1	16:BL:269:ARG:NH2	2.26	0.69
19:BO:53:THR:N	19:BO:86:THR:HG1	1.91	0.69
25:BU:124:VAL:HG12	25:BU:158:ARG:HE	1.58	0.69
1:B3:60:TYR:HB3	1:B3:65:GLN:HE21	1.56	0.68
3:B8:216:G:H1	55:Bz:61:GLY:HA3	1.58	0.68
47:Br:41:ASP:HB3	47:Br:46:ASN:HD22	1.58	0.67
18:BN:253:MET:HE3	18:BN:259:LEU:HD22	1.77	0.66
3:B8:438:G:N7	25:BU:67:LYS:NZ	2.42	0.66
39:Bi:177:LEU:HD23	39:Bi:238:ASN:HD22	1.59	0.66
9:BE:44:ARG:NH2	19:BO:84:GLU:OE1	2.29	0.66
44:Bo:112:PRO:HB2	44:Bo:267:PRO:HG2	1.78	0.65
44:Bo:298:GLN:HE22	44:Bo:323:MET:HA	1.60	0.65
49:Bt:215:ILE:HG23	49:Bt:219:LEU:HD12	1.78	0.65
42:Bm:115:GLU:HB2	42:Bm:119:GLN:HB2	1.79	0.65
7:BC:79:VAL:HG12	7:BC:86:VAL:HG12	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Aa:194:THR:OG1	57:Aa:279:THR:OG1	2.14	0.64
56:AG:51:PSU:H3'	56:AG:52:A:H8	1.62	0.64
4:B9:43:G:O6	27:BW:88:HIS:NE2	2.31	0.64
29:BY:33:GLY:O	29:BY:36:ASN:ND2	2.30	0.64
37:Bg:37:PRO:HG2	37:Bg:68:SER:HA	1.80	0.64
3:B8:1419:A:H62	57:Aa:314:HIS:CD2	2.16	0.64
7:BC:121:LYS:HD3	7:BC:130:PRO:HB2	1.80	0.64
9:BE:163:ARG:HE	42:Bm:55:LEU:HD11	1.63	0.64
40:Bj:245:VAL:HA	40:Bj:253:LEU:HD22	1.79	0.64
3:B8:1540:C:N4	3:B8:1557:U:O4	2.27	0.64
51:Bv:255:VAL:HB	51:Bv:259:GLU:HG3	1.78	0.64
3:B8:1012:A:OP1	29:BY:34:ARG:NH2	2.30	0.64
23:BS:46:LEU:HD12	23:BS:78:LYS:HD3	1.80	0.64
43:Bn:255:LEU:HD12	43:Bn:256:PRO:HD2	1.80	0.64
51:Bv:147:THR:HG21	51:Bv:248:ASN:HB3	1.81	0.63
17:BM:244:ALA:HB1	17:BM:248:ILE:HD11	1.80	0.63
43:Bn:155:TYR:O	43:Bn:267:ARG:NH1	2.31	0.63
34:Bd:81:LEU:HD11	45:Bp:189:GLU:HB3	1.81	0.63
16:BL:201:GLY:O	42:Bm:30:ALA:N	2.32	0.63
25:BU:124:VAL:HA	25:BU:158:ARG:HH21	1.61	0.63
37:Bg:112:GLN:OE1	37:Bg:115:ARG:NH2	2.31	0.63
16:BL:194:ASN:ND2	16:BL:245:GLY:O	2.32	0.62
3:B8:82:U:OP1	15:BK:94:LEU:N	2.32	0.62
25:BU:218:ILE:HG23	25:BU:223:MET:HB2	1.81	0.62
3:B8:135:A:OP2	7:BC:94:HIS:NE2	2.30	0.62
56:AG:9:C:O2'	56:AG:10:A:N7	2.28	0.62
42:Bm:229:ARG:NH1	42:Bm:231:SER:OG	2.33	0.62
54:By:69:ARG:NH2	54:By:107:ASP:OD2	2.31	0.61
3:B8:346:C:OP2	24:BT:59:ARG:NH1	2.34	0.61
19:BO:189:VAL:HG21	19:BO:208:LEU:HD21	1.82	0.61
3:B8:219:C:OP1	24:BT:133:LYS:NZ	2.33	0.61
39:Bi:49:ALA:O	39:Bi:61:ARG:NH1	2.34	0.61
39:Bi:287:LYS:NZ	42:Bm:166:THR:O	2.32	0.61
7:BC:54:TRP:NE1	7:BC:56:LEU:O	2.34	0.61
49:Bt:151:GLU:O	49:Bt:155:ASN:ND2	2.30	0.61
3:B8:117:G:N2	3:B8:120:A:OP2	2.32	0.61
36:Bf:190:GLN:NE2	43:Bn:188:TYR:OH	2.34	0.60
18:BN:114:THR:O	18:BN:156:ARG:NH1	2.34	0.60
53:Bx:118:TRP:NE1	53:Bx:142:GLU:OE2	2.28	0.60
36:Bf:111:ILE:O	36:Bf:116:ARG:NH1	2.34	0.60
39:Bi:204:CYS:SG	39:Bi:240:GLN:NE2	2.74	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Bp:182:ILE:HB	45:Bp:185:TYR:HB2	1.83	0.60
3:B8:64:C:OP1	19:BO:72:ARG:NE	2.34	0.60
3:B8:1146:G:O6	8:BD:33:LYS:NZ	2.34	0.60
3:B8:1561:U:H3	26:BV:53:ARG:HH22	1.50	0.60
18:BN:279:ARG:HH12	18:BN:282:PRO:HD3	1.66	0.60
49:Bt:161:THR:O	49:Bt:192:GLN:NE2	2.34	0.60
25:BU:123:ARG:NH1	25:BU:162:GLU:OE1	2.35	0.60
5:BA:57:LEU:HB2	5:BA:60:GLU:HG3	1.84	0.60
19:BO:98:LEU:HD23	19:BO:129:ALA:HB2	1.82	0.60
50:Bu:98:SER:OG	50:Bu:215:ARG:NH2	2.35	0.60
53:Bx:110:ILE:HD11	53:Bx:157:LEU:HD13	1.84	0.60
44:Bo:107:LEU:HB3	44:Bo:126:LYS:HB3	1.84	0.60
42:Bm:201:ARG:NH1	42:Bm:418:TYR:O	2.33	0.59
8:BD:100:THR:OG1	8:BD:132:HIS:NE2	2.29	0.59
6:BB:110:LEU:HD12	10:BF:118:GLU:HG2	1.85	0.59
3:B8:286:U:HO2'	3:B8:1428:U:HO2'	1.48	0.59
56:AG:18:A:H61	56:AG:43:A:H2'	1.67	0.59
3:B8:725:A:OP1	42:Bm:173:ARG:NH2	2.33	0.59
24:BT:44:ARG:HG3	24:BT:45:ARG:HG3	1.82	0.59
26:BV:16:ARG:NH2	26:BV:50:ASP:OD2	2.35	0.59
43:Bn:187:VAL:HG13	43:Bn:319:PHE:HB3	1.83	0.59
44:Bo:148:MET:HE2	44:Bo:257:ILE:HG12	1.85	0.59
3:B8:423:U:H4'	55:Bz:126:LYS:HE2	1.85	0.59
34:Bd:67:ARG:NH1	52:Bw:101:THR:OG1	2.35	0.59
51:Bv:164:LYS:HE2	51:Bv:167:ASP:HA	1.85	0.59
3:B8:283:A:O2'	3:B8:793:A:OP1	2.21	0.59
13:BI:47:ASP:HB3	13:BI:50:VAL:HG22	1.86	0.58
3:B8:674:C:H1'	3:B8:692:A:H4'	1.84	0.58
3:B8:1239:G:OP1	13:BI:63:ARG:NH1	2.31	0.58
17:BM:69:ASP:OD1	17:BM:154:ARG:NH1	2.36	0.58
33:Bc:121:LEU:O	33:Bc:125:ASN:ND2	2.34	0.58
36:Bf:84:SER:HB3	36:Bf:98:LYS:HB2	1.84	0.58
51:Bv:58:VAL:HB	51:Bv:153:LEU:HB3	1.84	0.58
4:B9:68:G:H2'	4:B9:69:A:H8	1.68	0.58
9:BE:7:PRO:HD2	9:BE:10:LEU:HD12	1.85	0.58
23:BS:93:GLY:O	23:BS:95:ARG:NH2	2.36	0.58
3:B8:75:U:O4	15:BK:108:LYS:NZ	2.37	0.58
18:BN:272:LYS:NZ	55:Bz:65:ASN:OD1	2.37	0.58
29:BY:96:GLU:O	30:BZ:105:GLN:NE2	2.31	0.58
6:BB:129:MET:HG3	50:Bu:82:ALA:HB2	1.84	0.58
37:Bg:163:LEU:HB2	37:Bg:171:ARG:HH12	1.67	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BM:50:ASP:O	26:BV:138:ARG:NH2	2.37	0.57
8:BD:148:LEU:OXT	43:Bn:339:GLU:N	2.37	0.57
43:Bn:215:THR:HB	43:Bn:273:PHE:HB2	1.85	0.57
3:B8:1113:A:H4'	40:Bj:302:GLY:H	1.68	0.57
43:Bn:217:LEU:HD11	43:Bn:271:LEU:HD12	1.86	0.57
3:B8:77:G:OP2	3:B8:79:C:N4	2.37	0.57
3:B8:578:U:OP1	29:BY:99:ARG:NH2	2.33	0.57
52:Bw:127:MET:HE3	52:Bw:128:PRO:HD2	1.86	0.57
3:B8:1398:G:N2	3:B8:1398:G:OP2	2.33	0.57
1:B1:76:LEU:H	1:B4:68:VAL:HG11	1.70	0.57
3:B8:1556:G:O2'	3:B8:1559:U:O4	2.22	0.57
17:BM:111:THR:OG1	17:BM:113:ASP:OD1	2.22	0.57
27:BW:52:ASN:HB3	27:BW:55:ASN:HB2	1.87	0.57
13:BI:13:SER:OG	13:BI:36:ARG:NH2	2.38	0.57
3:B8:788:A:O2'	17:BM:215:PHE:O	2.19	0.56
35:Be:88:ILE:HG13	53:Bx:142:GLU:HB3	1.86	0.56
43:Bn:244:ARG:NH1	43:Bn:247:GLU:OE1	2.38	0.56
3:B8:1257:C:O2	50:Bu:38:LYS:NZ	2.27	0.56
3:B8:1396:C:O2'	17:BM:233:GLN:OE1	2.20	0.56
19:BO:201:VAL:HG13	40:Bj:86:VAL:HG22	1.87	0.56
31:Ba:112:LYS:NZ	43:Bn:311:MET:O	2.38	0.56
3:B8:79:C:OP2	3:B8:1229:C:O2'	2.23	0.56
3:B8:1393:G:O2'	3:B8:1396:C:OP2	2.22	0.56
4:B9:42:A:H62	27:BW:120:ARG:HH12	1.53	0.56
7:BC:105:ARG:NH2	50:Bu:171:ASP:OD1	2.39	0.56
30:BZ:111:GLU:HG2	48:Bs:19:LEU:HD11	1.87	0.56
3:B8:861:U:O4	16:BL:246:ARG:NH2	2.39	0.56
57:Aa:293:VAL:HG22	57:Aa:360:ILE:HD12	1.88	0.56
3:B8:374:A:OP1	15:BK:153:THR:OG1	2.19	0.56
16:BL:194:ASN:OD1	16:BL:195:ASN:ND2	2.37	0.56
51:Bv:90:ARG:NH2	51:Bv:115:LEU:O	2.38	0.56
4:B9:24:A:N6	27:BW:87:GLN:OE1	2.37	0.56
11:BG:78:ARG:O	11:BG:83:LYS:NZ	2.39	0.56
39:Bi:66:TRP:O	39:Bi:69:THR:OG1	2.23	0.56
3:B8:183:A:OP2	30:BZ:177:ARG:NH1	2.33	0.56
3:B8:347:U:O2'	3:B8:1053:A:N1	2.37	0.56
7:BC:45:VAL:HG11	10:BF:237:LYS:HG3	1.88	0.56
18:BN:62:VAL:HG23	18:BN:82:LEU:HB2	1.88	0.56
37:Bg:40:PRO:HG2	37:Bg:51:GLN:HB3	1.88	0.56
52:Bw:106:TYR:OH	52:Bw:174:ILE:O	2.23	0.56
3:B8:310:A:OP1	14:BJ:56:SER:OG	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BN:211:ARG:HD3	54:By:58:ARG:HH21	1.71	0.56
56:AG:6:G:H1	56:AG:62:C:H42	1.53	0.56
3:B8:161:G:O6	48:Bs:4:ARG:NH2	2.36	0.56
6:BB:46:MET:HE1	6:BB:72:VAL:HG13	1.88	0.56
40:Bj:290:VAL:HG11	40:Bj:307:ILE:HD13	1.88	0.56
17:BM:45:SER:O	44:Bo:307:ARG:NH2	2.38	0.56
3:B8:845:U:OP1	16:BL:284:ARG:NH2	2.36	0.55
5:BA:63:ARG:NH1	50:Bu:228:PHE:O	2.39	0.55
44:Bo:296:ARG:NH1	44:Bo:324:VAL:O	2.39	0.55
3:B8:1306:G:O2'	3:B8:1335:A:N6	2.39	0.55
28:BX:73:ARG:NH1	28:BX:213:GLN:O	2.40	0.55
3:B8:1262:G:OP1	18:BN:137:ARG:NH1	2.34	0.55
24:BT:244:LEU:HD12	24:BT:245:PRO:HD2	1.88	0.55
3:B8:133:A:H4'	3:B8:134:A:H3'	1.88	0.55
19:BO:107:VAL:HG22	19:BO:108:ARG:H	1.71	0.55
44:Bo:156:ARG:O	47:Br:95:ARG:NH2	2.33	0.55
44:Bo:186:ASP:OD1	44:Bo:187:SER:N	2.40	0.55
5:BA:206:LEU:HD11	30:BZ:107:LYS:HD3	1.89	0.55
18:BN:243:ILE:HG22	37:Bg:27:ALA:HB2	1.89	0.55
24:BT:91:ARG:NH1	24:BT:209:GLU:OE2	2.39	0.55
15:BK:175:ASP:HB3	15:BK:178:GLN:HB2	1.90	0.54
35:Be:12:ILE:HG13	35:Be:23:ARG:HB2	1.88	0.54
6:BB:64:PRO:HB2	6:BB:100:ALA:HB3	1.89	0.54
40:Bj:128:ASP:N	40:Bj:289:PHE:O	2.41	0.54
40:Bj:295:LEU:HB2	40:Bj:305:LEU:HD11	1.90	0.54
21:BQ:114:LEU:HD21	33:Bc:101:LEU:HD21	1.89	0.54
34:Bd:82:ASP:O	34:Bd:89:ARG:NH2	2.41	0.54
48:Bs:136:LYS:O	49:Bt:259:ARG:NH2	2.34	0.54
57:Aa:293:VAL:HG21	57:Aa:357:TYR:HA	1.89	0.54
20:BP:45:GLN:NE2	35:Be:25:ARG:O	2.39	0.54
42:Bm:105:TYR:CZ	42:Bm:262:ILE:HD12	2.43	0.54
49:Bt:105:ARG:HG3	49:Bt:110:ILE:HB	1.90	0.54
1:B1:48:LEU:O	20:BP:142:ASN:ND2	2.41	0.53
3:B8:292:A:OP2	3:B8:831:C:N4	2.40	0.53
18:BN:184:GLN:HE22	24:BT:22:VAL:HG23	1.73	0.53
43:Bn:213:LEU:HB2	43:Bn:275:GLN:HB2	1.88	0.53
3:B8:93:A:H61	37:Bg:51:GLN:HE22	1.56	0.53
3:B8:655:U:O2'	26:BV:82:GLU:OE2	2.26	0.53
3:B8:916:U:O2'	56:AG:12:C:O2'	2.24	0.53
28:BX:177:VAL:HG11	28:BX:204:MET:HG3	1.90	0.53
31:Ba:112:LYS:HB2	43:Bn:90:ILE:HA	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:467:C:OP2	11:BG:77:ARG:NH1	2.42	0.53
3:B8:1542:C:H42	3:B8:1560:G:H1	1.53	0.53
7:BC:16:PRO:HG2	7:BC:19:TYR:HB2	1.90	0.53
44:Bo:243:LYS:NZ	44:Bo:265:GLU:OE1	2.33	0.53
45:Bp:178:TYR:O	51:Bv:136:ARG:NH1	2.40	0.53
51:Bv:185:ARG:NH1	51:Bv:207:ASN:OD1	2.37	0.53
15:BK:115:LEU:HB2	24:BT:83:PHE:HB3	1.91	0.53
42:Bm:165:GLN:NE2	42:Bm:175:THR:HG22	2.24	0.53
57:Aa:254:GLU:OE1	57:Aa:386:ARG:NH2	2.40	0.53
3:B8:1114:A:H5''	40:Bj:94:ARG:NH1	2.22	0.53
10:BF:154:ARG:HA	46:Bq:130:LEU:HD13	1.89	0.53
17:BM:76:LYS:HG3	17:BM:170:LEU:HD21	1.90	0.53
28:BX:153:ASN:OD1	28:BX:154:VAL:N	2.42	0.53
4:B9:12:U:O2'	4:B9:14:A:OP1	2.25	0.53
9:BE:156:LYS:NZ	9:BE:205:GLY:O	2.41	0.53
29:BY:111:LYS:NZ	30:BZ:139:ASP:O	2.41	0.53
3:B8:568:A:OP1	38:Bh:165:LYS:NZ	2.42	0.53
43:Bn:252:CYS:SG	43:Bn:296:ARG:NH1	2.82	0.53
49:Bt:259:ARG:HB2	49:Bt:271:PHE:HB2	1.90	0.53
3:B8:94:C:OP1	37:Bg:34:ARG:NH2	2.42	0.53
3:B8:1114:A:H2'	3:B8:1115:C:O4'	2.09	0.53
18:BN:70:ARG:HA	18:BN:196:PRO:HD3	1.90	0.52
35:Be:24:PRO:HG2	38:Bh:169:TRP:HB2	1.91	0.52
3:B8:169:C:H5''	22:BR:115:ASN:HB2	1.91	0.52
3:B8:676:U:OP1	39:Bi:223:ARG:NH2	2.42	0.52
40:Bj:95:GLN:HG3	40:Bj:96:ILE:HG13	1.91	0.52
50:Bu:81:THR:HG21	50:Bu:85:PHE:HE1	1.74	0.52
22:BR:32:ALA:HA	22:BR:108:ILE:HG12	1.91	0.52
47:Br:75:ILE:HD13	49:Bt:255:SER:HB2	1.90	0.52
20:BP:96:ILE:HA	20:BP:155:VAL:HG12	1.90	0.52
28:BX:250:THR:H	28:BX:253:GLN:HE21	1.58	0.52
3:B8:751:G:H5''	46:Bq:24:LYS:HG2	1.92	0.52
23:BS:100:PHE:HB3	28:BX:158:GLN:HE21	1.74	0.52
50:Bu:202:MET:HG2	50:Bu:203:MET:HG2	1.92	0.52
3:B8:521:A:N6	3:B8:528:A:OP2	2.40	0.52
3:B8:1268:A:H1'	56:AG:71:A:H2'	1.91	0.52
3:B8:1324:U:O3'	57:Aa:306:ARG:NH1	2.42	0.52
23:BS:52:HIS:CD2	23:BS:53:ARG:HG3	2.45	0.52
44:Bo:276:PHE:HB2	44:Bo:304:VAL:HG22	1.91	0.52
3:B8:699:A:OP1	10:BF:117:GLN:NE2	2.43	0.52
3:B8:1040:C:O2'	3:B8:1550:A:N1	2.41	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BW:104:SER:O	27:BW:135:ARG:NH1	2.43	0.52
5:BA:185:THR:HG23	5:BA:188:ALA:H	1.75	0.52
29:BY:112:THR:OG1	48:Bs:127:GLN:NE2	2.39	0.52
48:Bs:72:VAL:HG13	48:Bs:90:HIS:HB2	1.92	0.52
3:B8:1070:A:N3	3:B8:1251:A:O2'	2.38	0.52
7:BC:80:ILE:HD12	7:BC:85:TRP:HE3	1.74	0.52
44:Bo:114:ASP:HB2	44:Bo:117:LYS:HB2	1.92	0.52
49:Bt:168:HIS:O	49:Bt:172:ASN:ND2	2.33	0.52
3:B8:10:A:OP1	10:BF:230:LYS:NZ	2.43	0.51
3:B8:130:G:N1	3:B8:133:A:OP2	2.43	0.51
19:BO:244:LYS:HA	19:BO:247:ARG:HH21	1.75	0.51
44:Bo:284:HIS:HB3	44:Bo:323:MET:HE2	1.92	0.51
3:B8:1109:C:OP1	40:Bj:115:THR:OG1	2.28	0.51
6:BB:66:ALA:HB2	6:BB:100:ALA:HA	1.92	0.51
7:BC:93:THR:HG22	7:BC:112:GLU:HG3	1.92	0.51
43:Bn:173:LEU:HD13	43:Bn:272:LEU:HD22	1.90	0.51
17:BM:345:ILE:HG13	28:BX:169:PRO:HB2	1.92	0.51
40:Bj:133:LYS:HG2	40:Bj:134:LYS:H	1.74	0.51
4:B9:68:G:H2'	4:B9:69:A:C8	2.44	0.51
25:BU:204:GLU:HG3	25:BU:207:ARG:HH21	1.76	0.51
51:Bv:155:ARG:NH2	51:Bv:278:ASP:OD2	2.41	0.51
17:BM:99:LEU:HD22	17:BM:193:LEU:HB3	1.93	0.51
22:BR:78:SER:HB3	22:BR:89:GLN:HG2	1.92	0.51
26:BV:142:LEU:HA	26:BV:147:GLN:HE21	1.75	0.51
34:Bd:72:ARG:NH1	52:Bw:147:ASP:O	2.43	0.51
43:Bn:215:THR:OG1	43:Bn:275:GLN:OE1	2.28	0.51
3:B8:1310:U:H4'	57:Aa:341:GLN:HB3	1.92	0.51
14:BJ:51:ASN:O	14:BJ:54:GLN:NE2	2.44	0.51
21:BQ:20:ILE:HD11	21:BQ:42:ARG:HD3	1.93	0.51
50:Bu:152:LEU:HD22	50:Bu:176:ILE:HD11	1.91	0.51
56:AG:16:A:O2'	56:AG:54:A:O2'	2.21	0.51
3:B8:369:A:N7	3:B8:1059:U:O2'	2.42	0.51
3:B8:739:A:O2'	42:Bm:268:CYS:SG	2.64	0.51
3:B8:875:U:H5''	3:B8:876:G:H5'	1.92	0.51
4:B9:36:C:OP1	43:Bn:56:ARG:NH2	2.41	0.51
21:BQ:20:ILE:HB	21:BQ:70:ILE:HB	1.92	0.51
23:BS:125:THR:HG22	23:BS:144:PHE:HB3	1.93	0.51
40:Bj:110:GLN:HG2	40:Bj:115:THR:HG23	1.92	0.51
42:Bm:201:ARG:HB3	42:Bm:232:THR:HG22	1.93	0.51
4:B9:67:U:H2'	4:B9:68:G:C8	2.46	0.51
19:BO:201:VAL:HG22	40:Bj:86:VAL:HG13	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1541:C:H4'	3:B8:1542:C:H5	1.76	0.51
29:BY:111:LYS:HD3	48:Bs:127:GLN:HB3	1.91	0.51
3:B8:519:C:O2'	3:B8:528:A:OP1	2.27	0.51
42:Bm:354:PHE:HB3	42:Bm:417:LEU:HD11	1.92	0.51
3:B8:1106:G:N2	19:BO:179:ASN:OD1	2.44	0.50
32:Bb:65:ASP:OD2	32:Bb:73:ARG:NH2	2.43	0.50
34:Bd:51:LEU:HB3	34:Bd:67:ARG:HB3	1.92	0.50
3:B8:1390:C:H6	3:B8:1390:C:O5'	1.94	0.50
35:Be:59:GLU:O	35:Be:62:HIS:ND1	2.36	0.50
43:Bn:218:LEU:HD11	43:Bn:268:LEU:HB3	1.91	0.50
3:B8:401:U:O2'	43:Bn:28:ARG:NH2	2.44	0.50
3:B8:702:U:O4	39:Bi:270:LYS:NZ	2.44	0.50
3:B8:1338:C:O2'	3:B8:1381:A:N3	2.41	0.50
18:BN:103:GLN:O	18:BN:107:LYS:NZ	2.44	0.50
39:Bi:178:ASP:HA	39:Bi:239:ASN:HD21	1.77	0.50
39:Bi:271:LEU:HD23	39:Bi:273:LEU:HD13	1.93	0.50
48:Bs:49:ARG:HH21	48:Bs:94:VAL:HG11	1.77	0.50
48:Bs:89:ILE:HA	48:Bs:92:LYS:HD2	1.93	0.50
10:BF:83:ALA:N	46:Bq:74:VAL:O	2.43	0.50
57:Aa:395:VAL:HG23	57:Aa:407:ILE:HG12	1.94	0.50
3:B8:609:U:OP1	18:BN:255:LYS:NZ	2.40	0.50
7:BC:55:TYR:HB2	7:BC:133:ILE:HD11	1.92	0.50
8:BD:102:GLU:OE2	43:Bn:74:TYR:N	2.44	0.50
39:Bi:212:ARG:HD3	39:Bi:379:LEU:HB3	1.91	0.50
3:B8:1110:C:H5'	40:Bj:120:SER:HB2	1.92	0.50
3:B8:1408:C:H2'	3:B8:1409:G:C8	2.47	0.50
45:Bp:99:ARG:HG2	51:Bv:89:LEU:HD11	1.93	0.50
56:AG:13:U:H3	56:AG:19:A:H61	1.59	0.50
3:B8:244:A:N6	3:B8:334:G:O6	2.43	0.50
4:B9:38:U:H5''	27:BW:155:SER:HB3	1.93	0.50
3:B8:186:A:OP2	3:B8:1316:C:O2'	2.28	0.50
3:B8:457:A:H4'	3:B8:581:A:C5	2.47	0.50
3:B8:1301:A:O2'	25:BU:182:LYS:O	2.29	0.50
19:BO:53:THR:N	19:BO:86:THR:OG1	2.45	0.50
42:Bm:326:ARG:NH1	42:Bm:331:ASN:OD1	2.45	0.50
45:Bp:124:TYR:OH	51:Bv:67:GLN:NE2	2.45	0.50
50:Bu:164:VAL:HG12	50:Bu:261:MET:HB3	1.93	0.50
57:Aa:325:VAL:HG22	57:Aa:332:VAL:HG22	1.93	0.50
18:BN:49:ARG:NH1	18:BN:81:ASP:O	2.41	0.49
30:BZ:163:LYS:HB2	48:Bs:106:ASP:HB3	1.94	0.49
51:Bv:178:TRP:NE1	51:Bv:182:GLU:O	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:613:C:O2	49:Bt:43:LYS:NZ	2.36	0.49
10:BF:90:LEU:HB2	10:BF:145:VAL:HG21	1.94	0.49
43:Bn:87:LYS:NZ	43:Bn:153:GLU:OE2	2.43	0.49
49:Bt:245:LEU:HD12	49:Bt:253:PRO:HD3	1.94	0.49
22:BR:6:ARG:NH2	49:Bt:225:GLY:O	2.44	0.49
26:BV:67:ASP:OD1	26:BV:67:ASP:N	2.46	0.49
30:BZ:96:PHE:HB3	48:Bs:126:ILE:HD13	1.93	0.49
42:Bm:113:LEU:HD12	42:Bm:311:ALA:HB1	1.94	0.49
46:Bq:68:PHE:CE2	46:Bq:70:LEU:HB2	2.46	0.49
9:BE:202:GLU:HB3	9:BE:214:LYS:NZ	2.28	0.49
20:BP:101:ASN:HB3	20:BP:150:HIS:HB3	1.94	0.49
23:BS:75:LEU:HD11	23:BS:105:VAL:HG21	1.94	0.49
16:BL:111:ARG:NH2	16:BL:165:ASN:OD1	2.43	0.49
24:BT:263:ARG:HH21	36:Bf:43:TYR:HE2	1.60	0.49
39:Bi:332:LEU:HD13	39:Bi:372:TYR:HB2	1.94	0.49
51:Bv:200:MET:HA	51:Bv:241:GLY:HA3	1.93	0.49
3:B8:1108:U:O2'	40:Bj:116:SER:HB2	2.13	0.49
4:B9:61:C:H2'	4:B9:62:C:C6	2.47	0.49
47:Br:104:GLU:HB2	47:Br:107:PRO:HD2	1.95	0.49
3:B8:324:A:H61	3:B8:1066:C:H4'	1.77	0.49
16:BL:109:PHE:HB3	16:BL:204:ALA:HB3	1.95	0.49
22:BR:169:LEU:HD22	38:Bh:75:TRP:CD1	2.47	0.49
50:Bu:85:PHE:CZ	50:Bu:200:SER:HB3	2.47	0.49
52:Bw:94:HIS:ND1	52:Bw:154:GLU:OE2	2.32	0.49
52:Bw:127:MET:HB2	52:Bw:154:GLU:HB3	1.94	0.49
42:Bm:136:VAL:HG11	42:Bm:417:LEU:HD23	1.93	0.49
3:B8:1542:C:N4	3:B8:1560:G:H1	2.11	0.49
20:BP:76:ILE:HG22	20:BP:78:LEU:H	1.78	0.49
40:Bj:62:PRO:HG2	40:Bj:65:LYS:HD2	1.94	0.49
43:Bn:138:GLU:OE1	43:Bn:141:ARG:NH2	2.39	0.49
57:Aa:301:ARG:HH21	57:Aa:325:VAL:HG21	1.78	0.49
40:Bj:143:VAL:HG22	40:Bj:242:GLU:HA	1.95	0.48
44:Bo:220:GLU:HG2	44:Bo:253:LYS:HG2	1.95	0.48
26:BV:46:TRP:CD1	26:BV:121:ALA:HB2	2.48	0.48
40:Bj:130:ALA:O	40:Bj:282:ARG:NH1	2.41	0.48
3:B8:1412:G:N2	3:B8:1415:A:OP2	2.39	0.48
3:B8:1531:A:H2'	3:B8:1532:U:O4'	2.12	0.48
50:Bu:188:SER:HA	50:Bu:218:THR:HG22	1.95	0.48
3:B8:197:A:N1	3:B8:349:G:O2'	2.45	0.48
16:BL:257:ILE:O	16:BL:262:ARG:NH1	2.36	0.48
25:BU:73:ARG:O	25:BU:155:LYS:NZ	2.45	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BV:64:LYS:NZ	26:BV:100:GLN:O	2.46	0.48
31:Ba:91:TRP:CD2	35:Be:58:GLN:HG2	2.48	0.48
13:BI:34:ARG:HB3	13:BI:41:LEU:HD11	1.95	0.48
25:BU:64:ARG:NH1	25:BU:144:LYS:O	2.46	0.48
57:Aa:306:ARG:NH1	57:Aa:316:ASN:O	2.46	0.48
3:B8:517:C:O2'	21:BQ:104:THR:O	2.31	0.48
45:Bp:110:GLU:OE2	45:Bp:113:ARG:NH2	2.37	0.48
3:B8:67:A:H61	3:B8:90:G:H1'	1.79	0.48
3:B8:520:C:OP2	33:Be:120:ARG:NH1	2.33	0.48
11:BG:120:LYS:NZ	35:Be:44:GLU:OE2	2.45	0.48
22:BR:27:PRO:HG2	22:BR:30:LYS:HB2	1.94	0.48
3:B8:547:C:OP1	20:BP:128:ASN:N	2.43	0.48
3:B8:640:G:N2	3:B8:1006:A:OP2	2.43	0.48
5:BA:49:ASN:ND2	5:BA:68:TYR:O	2.35	0.48
20:BP:49:ALA:HB1	35:Be:32:LYS:HE2	1.95	0.48
3:B8:405:U:O2'	3:B8:1163:A:N7	2.42	0.48
4:B9:6:U:O2	4:B9:63:G:N2	2.38	0.48
17:BM:50:ASP:HA	17:BM:53:LEU:HG	1.95	0.48
18:BN:231:VAL:HG13	37:Bg:26:ARG:HD2	1.96	0.48
40:Bj:123:LEU:HB2	40:Bj:295:LEU:HD12	1.96	0.48
18:BN:220:ASP:O	18:BN:245:ALA:N	2.46	0.48
57:Aa:227:TYR:CZ	57:Aa:235:LEU:HD21	2.49	0.47
3:B8:33:C:OP1	46:Bq:34:LYS:NZ	2.46	0.47
3:B8:849:G:N7	16:BL:230:SER:OG	2.44	0.47
43:Bn:131:PRO:HG2	43:Bn:134:ALA:HB3	1.96	0.47
3:B8:332:G:N3	3:B8:1065:G:O2'	2.36	0.47
22:BR:140:ASN:HB2	49:Bt:262:GLY:HA2	1.96	0.47
23:BS:98:PRO:HA	28:BX:162:ILE:HG12	1.96	0.47
42:Bm:228:ALA:HB3	42:Bm:292:TYR:HB2	1.96	0.47
43:Bn:120:GLU:OE2	45:Bp:119:LYS:NZ	2.30	0.47
53:Bx:154:ASP:OD1	53:Bx:154:ASP:N	2.47	0.47
3:B8:703:A:OP1	6:BB:50:ARG:NH2	2.39	0.47
3:B8:1269:C:H5''	57:Aa:317:LYS:HD2	1.96	0.47
40:Bj:79:GLU:HG2	40:Bj:97:TYR:HE2	1.78	0.47
3:B8:98:G:OP1	55:Bz:50:LYS:NZ	2.46	0.47
5:BA:94:ASP:OD2	44:Bo:97:GLU:N	2.46	0.47
36:Bf:129:ARG:NH2	43:Bn:336:ASP:OD1	2.48	0.47
37:Bg:28:ARG:O	55:Bz:57:TYR:OH	2.27	0.47
39:Bi:239:ASN:HB2	39:Bi:299:PHE:HB2	1.97	0.47
48:Bs:27:GLN:NE2	49:Bt:177:GLN:OE1	2.47	0.47
3:B8:216:G:N7	18:BN:170:ARG:NH2	2.61	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1236:C:N3	13:BI:19:ARG:NH2	2.59	0.47
12:BH:108:ASP:OD1	12:BH:109:VAL:N	2.44	0.47
19:BO:156:GLN:OE1	19:BO:226:ASN:ND2	2.48	0.47
32:Bb:40:GLU:OE1	32:Bb:43:ARG:NH2	2.47	0.47
56:AG:51:PSU:H3'	56:AG:52:A:C8	2.44	0.47
23:BS:143:ASN:ND2	28:BX:156:GLU:HG3	2.30	0.47
36:Bf:185:ARG:NH1	43:Bn:197:GLU:OE2	2.47	0.47
42:Bm:211:ALA:HB1	42:Bm:322:LEU:HD23	1.97	0.47
43:Bn:359:HIS:CD2	43:Bn:360:ARG:HG3	2.50	0.47
39:Bi:191:HIS:O	39:Bi:428:ARG:NH2	2.47	0.47
3:B8:492:C:N4	3:B8:552:U:O2	2.48	0.47
38:Bh:71:PRO:HD2	38:Bh:107:LEU:HD23	1.96	0.47
44:Bo:195:THR:H	44:Bo:198:ASN:HD22	1.62	0.47
3:B8:575:A:H4'	3:B8:576:A:OP1	2.14	0.47
3:B8:1093:U:H4'	19:BO:247:ARG:HD2	1.97	0.47
3:B8:1457:G:N2	3:B8:1460:A:OP2	2.47	0.47
19:BO:193:PHE:O	19:BO:198:GLY:N	2.48	0.47
21:BQ:113:THR:OG1	21:BQ:116:HIS:ND1	2.35	0.47
24:BT:62:ARG:O	55:Bz:128:ARG:NH2	2.46	0.47
3:B8:739:A:O2'	42:Bm:270:ILE:O	2.33	0.46
19:BO:190:ALA:HA	19:BO:193:PHE:HD2	1.80	0.46
21:BQ:25:ARG:HD2	33:Bc:56:LEU:HB3	1.95	0.46
39:Bi:89:MET:HE3	39:Bi:275:LYS:HB3	1.97	0.46
40:Bj:257:ILE:HD12	40:Bj:274:VAL:HG21	1.97	0.46
42:Bm:161:ALA:HB1	42:Bm:176:TYR:HB2	1.97	0.46
3:B8:107:A:H4'	18:BN:115:LYS:NZ	2.30	0.46
3:B8:656:C:OP2	39:Bi:55:SER:OG	2.25	0.46
3:B8:1110:C:OP2	40:Bj:119:GLN:HA	2.16	0.46
3:B8:1114:A:H5''	40:Bj:94:ARG:HH12	1.79	0.46
3:B8:402:A:H2'	3:B8:403:A:C8	2.50	0.46
3:B8:1432:U:C2	12:BH:81:PRO:HA	2.50	0.46
19:BO:163:THR:HG22	40:Bj:88:LEU:HG	1.97	0.46
19:BO:242:LYS:HB2	19:BO:245:THR:HG23	1.96	0.46
44:Bo:163:MET:H	44:Bo:186:ASP:HB2	1.79	0.46
3:B8:1097:A:O2'	3:B8:1099:A:N7	2.49	0.46
5:BA:134:LEU:HD23	5:BA:174:GLU:HA	1.97	0.46
20:BP:102:VAL:HG23	20:BP:104:LEU:HG	1.97	0.46
22:BR:25:MET:O	22:BR:149:ARG:NH1	2.48	0.46
26:BV:150:GLN:HE21	26:BV:154:GLN:HE21	1.63	0.46
39:Bi:182:SER:O	42:Bm:189:LYS:NZ	2.46	0.46
3:B8:2:C:O2'	5:BA:143:ARG:O	2.27	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:411:U:H2'	3:B8:412:G:C8	2.50	0.46
3:B8:1354:U:H2'	3:B8:1355:A:H8	1.81	0.46
9:BE:87:LEU:O	19:BO:78:ARG:NH1	2.47	0.46
3:B8:181:G:H2'	3:B8:1023:A:N7	2.30	0.46
13:BI:34:ARG:HD3	13:BI:41:LEU:HG	1.98	0.46
3:B8:36:C:OP1	10:BF:193:ARG:NH2	2.44	0.46
3:B8:201:A:N3	15:BK:104:ARG:NH2	2.64	0.46
3:B8:499:A:OP1	21:BQ:21:ARG:NH2	2.49	0.46
3:B8:526:A:O2'	3:B8:543:A:N1	2.49	0.46
3:B8:813:U:H2'	3:B8:814:C:O4'	2.15	0.46
4:B9:62:C:H2'	4:B9:63:G:C8	2.51	0.46
42:Bm:112:ARG:HG2	42:Bm:304:LEU:HD22	1.98	0.46
44:Bo:139:ASN:HB3	44:Bo:174:VAL:HG21	1.98	0.46
48:Bs:76:VAL:HG22	48:Bs:86:GLU:HG3	1.98	0.46
3:B8:789:A:N6	3:B8:998:A:O2'	2.48	0.46
51:Bv:177:GLU:O	51:Bv:190:ARG:NH2	2.49	0.46
56:AG:61:C:H2'	56:AG:62:C:C6	2.50	0.46
57:Aa:232:TYR:CZ	57:Aa:268:LEU:HD22	2.51	0.46
3:B8:282:U:H2'	3:B8:283:A:C8	2.51	0.46
3:B8:1349:G:O2'	3:B8:1455:A:N1	2.49	0.46
16:BL:235:GLN:HB3	16:BL:294:SER:HA	1.98	0.46
56:AG:62:C:H2'	56:AG:63:G:C8	2.51	0.46
17:BM:345:ILE:O	28:BX:172:GLN:NE2	2.49	0.46
3:B8:198:G:H2'	24:BT:40:PRO:HG3	1.98	0.45
3:B8:1532:U:O2	17:BM:303:LYS:NZ	2.46	0.45
15:BK:188:VAL:O	43:Bn:356:ARG:NH2	2.49	0.45
16:BL:213:CYS:HB3	16:BL:246:ARG:HG2	1.98	0.45
28:BX:210:GLU:HB2	28:BX:213:GLN:HG3	1.97	0.45
44:Bo:195:THR:H	44:Bo:198:ASN:ND2	2.13	0.45
15:BK:96:TYR:OH	55:Bz:128:ARG:O	2.30	0.45
22:BR:5:SER:HB2	22:BR:8:PRO:HD2	1.98	0.45
28:BX:121:THR:HG22	28:BX:171:VAL:HA	1.98	0.45
49:Bt:72:ILE:HD13	49:Bt:178:LEU:HD13	1.97	0.45
3:B8:842:A:O2'	3:B8:871:C:OP1	2.25	0.45
27:BW:152:GLU:O	27:BW:155:SER:OG	2.27	0.45
28:BX:183:LEU:HD21	28:BX:219:GLU:HG2	1.97	0.45
38:Bh:70:CYS:HB3	62:Bh:201:FS2:S6	2.56	0.45
39:Bi:358:GLN:NE2	39:Bi:427:ASN:HD22	2.14	0.45
42:Bm:108:HIS:CE1	42:Bm:110:ARG:HB3	2.52	0.45
53:Bx:72:TRP:NE1	53:Bx:92:HIS:O	2.44	0.45
57:Aa:359:GLN:O	57:Aa:363:LYS:N	2.44	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BV:62:TYR:OH	28:BX:272:GLU:OE2	2.34	0.45
28:BX:122:ALA:HB2	28:BX:172:GLN:HE21	1.81	0.45
39:Bi:316:CYS:HB3	39:Bi:319:GLN:HB2	1.99	0.45
57:Aa:394:ARG:H	57:Aa:407:ILE:HD11	1.80	0.45
3:B8:93:A:N6	37:Bg:51:GLN:HE22	2.14	0.45
3:B8:1144:G:O2'	3:B8:1313:G:OP1	2.35	0.45
3:B8:1403:C:OP2	3:B8:1425:G:N2	2.45	0.45
42:Bm:409:GLU:HG2	42:Bm:412:ARG:HH21	1.81	0.45
3:B8:1119:C:H2'	3:B8:1120:A:H5''	1.97	0.45
26:BV:108:LEU:HD11	26:BV:135:LEU:HD23	1.99	0.45
34:Bd:55:LEU:HD12	51:Bv:128:PHE:HE1	1.82	0.45
3:B8:484:A:OP2	35:Be:28:SER:OG	2.28	0.45
3:B8:738:U:O2'	42:Bm:266:HIS:ND1	2.49	0.45
3:B8:1481:A:H4'	28:BX:146:GLY:O	2.17	0.45
4:B9:53:U:H5''	4:B9:54:A:C8	2.52	0.45
9:BE:114:PHE:HB3	9:BE:141:LEU:HD22	1.98	0.45
9:BE:139:TYR:HD1	19:BO:131:TYR:HB3	1.80	0.45
18:BN:223:HIS:HA	18:BN:226:MET:HE3	1.98	0.45
3:B8:740:U:P	42:Bm:223:ARG:HH12	2.40	0.45
7:BC:80:ILE:HB	7:BC:85:TRP:HB2	1.98	0.45
17:BM:334:ASP:HB3	17:BM:337:VAL:HG23	1.99	0.45
31:Ba:63:GLN:HE21	31:Ba:67:LYS:HE2	1.82	0.45
34:Bd:57:VAL:N	34:Bd:75:LEU:O	2.37	0.45
38:Bh:72:ILE:HD11	38:Bh:115:ILE:HD11	1.99	0.45
48:Bs:133:PHE:HE2	49:Bt:269:LEU:HD23	1.82	0.45
49:Bt:42:GLN:NE2	55:Bz:36:LEU:O	2.50	0.45
56:AG:31:RSQ:H2'	56:AG:31:RSQ:O2	2.17	0.45
1:B6:84:GLU:HG3	1:B6:88:LYS:HD2	1.97	0.45
3:B8:932:U:OP1	3:B8:1421:G:O2'	2.27	0.45
4:B9:71:C:N4	51:Bv:216:LYS:HB2	2.32	0.45
7:BC:86:VAL:HG21	7:BC:120:VAL:HG21	1.98	0.45
19:BO:177:LYS:HD2	40:Bj:114:PHE:O	2.17	0.45
32:Bb:66:VAL:HB	32:Bb:74:LEU:HB3	1.99	0.45
3:B8:383:U:HO2'	3:B8:384:U:H6	1.62	0.45
3:B8:801:G:O2'	3:B8:984:U:O4	2.30	0.45
3:B8:1269:C:H4'	57:Aa:317:LYS:HD2	1.98	0.45
21:BQ:28:LEU:HD13	33:Bc:56:LEU:HD22	1.99	0.45
42:Bm:146:HIS:O	42:Bm:194:LYS:NZ	2.49	0.45
57:Aa:205:ARG:HA	57:Aa:235:LEU:HD12	1.99	0.45
3:B8:1354:U:H2'	3:B8:1355:A:C8	2.51	0.44
3:B8:662:C:H41	3:B8:772:U:H3	1.64	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BC:187:TYR:HD1	10:BF:94:SER:HA	1.81	0.44
8:BD:33:LYS:HE3	25:BU:139:ARG:HD2	1.99	0.44
9:BE:20:ILE:HD13	9:BE:212:ILE:HG23	2.00	0.44
10:BF:191:ASN:HB3	10:BF:194:TYR:HB3	1.98	0.44
17:BM:150:LYS:HD2	17:BM:296:LEU:HD21	1.99	0.44
24:BT:28:LYS:HD3	35:Be:94:HIS:CD2	2.52	0.44
24:BT:127:VAL:HG21	24:BT:138:VAL:HG11	2.00	0.44
35:Be:15:ARG:HB3	35:Be:18:ILE:HG12	1.99	0.44
56:AG:5:A:H2	56:AG:63:G:H1	1.64	0.44
56:AG:15:A:H2	56:AG:18:A:H1'	1.82	0.44
21:BQ:90:PHE:HB3	21:BQ:120:ILE:HD13	2.00	0.44
22:BR:7:ALA:HB3	22:BR:8:PRO:HD3	1.99	0.44
27:BW:60:SER:HB3	36:Bf:177:ARG:HH11	1.81	0.44
34:Bd:56:LEU:HD22	34:Bd:66:ILE:HD13	1.99	0.44
36:Bf:115:VAL:HG13	36:Bf:161:ALA:HB3	1.99	0.44
56:AG:3:U:H2'	56:AG:4:A:C8	2.53	0.44
18:BN:211:ARG:HD3	54:By:58:ARG:HE	1.83	0.44
39:Bi:105:TRP:CG	39:Bi:271:LEU:HD13	2.52	0.44
45:Bp:193:ASN:O	52:Bw:133:GLU:N	2.43	0.44
51:Bv:60:SER:O	51:Bv:136:ARG:NH2	2.37	0.44
57:Aa:133:LEU:HA	57:Aa:136:MET:HE2	1.99	0.44
9:BE:40:PRO:HB3	9:BE:43:TYR:CZ	2.53	0.44
19:BO:154:LYS:HA	19:BO:228:LEU:HD13	1.98	0.44
40:Bj:139:PRO:HB3	40:Bj:245:VAL:HG21	2.00	0.44
44:Bo:87:THR:O	44:Bo:90:SER:OG	2.28	0.44
45:Bp:153:GLU:HG2	51:Bv:47:LEU:HD21	2.00	0.44
19:BO:159:ALA:O	19:BO:163:THR:HG23	2.18	0.44
27:BW:142:ASN:HD22	36:Bf:181:GLU:HG2	1.81	0.44
42:Bm:59:THR:HB	42:Bm:73:PRO:HG3	1.98	0.44
53:Bx:73:GLN:HB3	53:Bx:162:LEU:HD11	2.00	0.44
3:B8:144:A:N3	3:B8:192:U:O2'	2.45	0.44
3:B8:1199:A:OP1	15:BK:127:ALA:N	2.37	0.44
8:BD:119:ARG:HH12	52:Bw:63:ILE:HG23	1.82	0.44
18:BN:82:LEU:HB3	18:BN:87:PHE:CD1	2.53	0.44
19:BO:98:LEU:HD11	19:BO:105:VAL:HG12	2.00	0.44
26:BV:57:GLU:OE2	26:BV:105:THR:OG1	2.29	0.44
3:B8:561:A:N3	3:B8:1333:A:O2'	2.46	0.44
3:B8:648:A:H2'	3:B8:649:A:C8	2.53	0.44
3:B8:1118:C:H2'	3:B8:1119:C:C6	2.53	0.44
20:BP:188:ARG:HD2	32:Bb:55:VAL:HB	1.99	0.44
1:B4:75:THR:O	1:B4:79:ILE:HG13	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:189:A:OP1	3:B8:629:U:O2'	2.32	0.44
4:B9:2:A:H2'	4:B9:3:G:C8	2.52	0.44
18:BN:123:GLY:HA2	18:BN:141:ILE:HG12	1.99	0.44
36:Bf:94:LYS:HE2	36:Bf:96:ASN:HB2	2.00	0.44
39:Bi:91:TYR:HE2	39:Bi:229:LEU:HD22	1.82	0.44
40:Bj:77:TYR:HB2	40:Bj:97:TYR:OH	2.18	0.44
53:Bx:132:LEU:HD11	53:Bx:153:PHE:CZ	2.53	0.44
3:B8:474:A:OP1	29:BY:57:ARG:NH1	2.42	0.43
34:Bd:73:ARG:HH12	51:Bv:121:GLU:HB3	1.82	0.43
16:BL:110:LEU:HD22	42:Bm:30:ALA:HB2	2.00	0.43
20:BP:151:ASN:HD21	32:Bb:31:ARG:HH22	1.65	0.43
25:BU:67:LYS:HE3	25:BU:67:LYS:HB2	1.86	0.43
1:B5:64:ILE:HD13	1:B6:82:LEU:HD13	1.99	0.43
3:B8:360:U:H1'	3:B8:376:C:H1'	2.01	0.43
18:BN:67:GLU:HB2	18:BN:190:MET:SD	2.58	0.43
28:BX:227:LYS:HE3	28:BX:249:LEU:HD21	2.00	0.43
39:Bi:174:LEU:HB3	39:Bi:175:PRO:HD3	1.99	0.43
39:Bi:332:LEU:HD21	39:Bi:359:ALA:HB2	1.99	0.43
57:Aa:251:LEU:HA	57:Aa:254:GLU:HG2	2.00	0.43
3:B8:71:A:N1	3:B8:85:A:H5''	2.33	0.43
3:B8:640:G:O2'	3:B8:1005:G:O6	2.30	0.43
4:B9:53:U:H5''	4:B9:54:A:N7	2.32	0.43
17:BM:251:VAL:HG11	17:BM:257:MET:HE3	2.00	0.43
25:BU:191:SER:H	25:BU:194:THR:HG1	1.64	0.43
28:BX:233:TRP:HB3	28:BX:240:ILE:HD12	2.00	0.43
43:Bn:195:PRO:HG3	43:Bn:321:CYS:SG	2.58	0.43
3:B8:1529:U:H1'	22:BR:98:ARG:HA	2.00	0.43
16:BL:210:ALA:HB1	16:BL:249:ASN:HB2	2.01	0.43
39:Bi:246:GLN:NE2	39:Bi:354:PRO:O	2.52	0.43
42:Bm:236:LEU:HD21	42:Bm:289:HIS:CD2	2.54	0.43
44:Bo:154:ILE:HD13	44:Bo:183:VAL:HG21	1.99	0.43
49:Bt:79:LEU:HD13	49:Bt:214:PHE:HE1	1.83	0.43
52:Bw:189:HIS:HE1	52:Bw:194:PHE:HB2	1.83	0.43
55:Bz:112:LYS:HG2	55:Bz:115:ARG:HH21	1.83	0.43
3:B8:307:U:H2'	3:B8:308:A:H8	1.83	0.43
18:BN:211:ARG:NH2	54:By:56:ARG:O	2.38	0.43
29:BY:141:ILE:HG22	47:Br:51:LEU:HD12	1.99	0.43
43:Bn:323:TRP:NE1	43:Bn:339:GLU:OE2	2.48	0.43
48:Bs:49:ARG:HG3	48:Bs:50:GLU:HG2	1.99	0.43
57:Aa:385:ILE:HG22	57:Aa:399:ARG:HD3	2.00	0.43
3:B8:457:A:H2'	3:B8:458:G:H8	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BO:144:LYS:HA	19:BO:147:ARG:HE	1.84	0.43
19:BO:173:GLU:OE1	19:BO:246:LYS:NZ	2.52	0.43
21:BQ:101:ALA:HB1	21:BQ:107:GLU:HG3	2.00	0.43
26:BV:140:SER:O	26:BV:146:ASN:ND2	2.46	0.43
42:Bm:242:ARG:NH2	42:Bm:337:GLU:O	2.51	0.43
43:Bn:121:ARG:HD2	45:Bp:108:PHE:HZ	1.83	0.43
50:Bu:209:TYR:HE1	50:Bu:251:GLN:HG3	1.83	0.43
55:Bz:68:LYS:NZ	55:Bz:72:GLU:OE1	2.39	0.43
3:B8:357:A:O2'	3:B8:378:U:OP1	2.32	0.43
3:B8:1203:A:H3'	3:B8:1218:A:H62	1.83	0.43
24:BT:261:ASP:HB3	24:BT:264:GLN:HB2	2.00	0.43
34:Bd:69:ARG:HG3	34:Bd:70:GLU:HG3	2.00	0.43
40:Bj:115:THR:OG1	40:Bj:116:SER:N	2.52	0.43
43:Bn:139:TRP:O	43:Bn:144:GLY:N	2.52	0.43
48:Bs:33:VAL:HG12	48:Bs:43:ALA:HB1	2.00	0.43
3:B8:209:G:OP1	18:BN:92:ARG:NH1	2.41	0.43
3:B8:283:A:OP1	17:BM:232:GLY:HA2	2.19	0.43
3:B8:1024:A:N3	3:B8:1272:C:O2'	2.45	0.43
12:BH:96:ASN:ND2	12:BH:98:GLN:H	2.17	0.43
18:BN:72:PHE:HE2	54:By:50:LEU:HB3	1.83	0.43
23:BS:35:MET:O	23:BS:56:ARG:NH1	2.52	0.43
39:Bi:142:LEU:HD13	39:Bi:422:VAL:HG21	2.01	0.43
57:Aa:70:TRP:NE1	57:Aa:127:GLU:OE2	2.51	0.43
1:B4:84:GLU:HG3	1:B4:88:LYS:HD2	2.01	0.43
3:B8:375:A:N6	3:B8:424:G:O6	2.52	0.43
3:B8:1445:U:H2'	3:B8:1446:C:C6	2.54	0.43
44:Bo:88:PRO:HB3	44:Bo:125:ILE:HD11	2.01	0.43
3:B8:1012:A:H4'	29:BY:41:LEU:HD13	2.00	0.42
4:B9:15:A:HO2'	4:B9:17:A:H62	1.60	0.42
4:B9:36:C:H5''	43:Bn:53:SER:HB3	2.00	0.42
18:BN:212:TRP:O	18:BN:258:THR:OG1	2.20	0.42
18:BN:254:LEU:HD13	24:BT:27:LEU:HD11	2.01	0.42
21:BQ:114:LEU:HD13	33:Bc:97:PHE:HA	2.00	0.42
28:BX:77:SER:HB2	28:BX:80:PHE:HD1	1.84	0.42
56:AG:3:U:H2'	56:AG:4:A:H8	1.84	0.42
1:B2:60:TYR:HB2	1:B2:61:PRO:HD3	2.00	0.42
1:B6:70:ASP:O	1:B6:74:LEU:HG	2.19	0.42
3:B8:1325:G:H4'	3:B8:1372:U:H5'	2.01	0.42
44:Bo:227:LEU:HD22	44:Bo:237:VAL:HG13	2.01	0.42
55:Bz:98:VAL:O	55:Bz:102:MET:HG3	2.19	0.42
56:AG:52:A:H2'	56:AG:53:U:O4'	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Aa:280:MET:HE2	57:Aa:280:MET:HB2	1.96	0.42
3:B8:567:A:OP1	38:Bh:171:ARG:NH2	2.48	0.42
3:B8:603:A:N1	3:B8:623:A:O2'	2.49	0.42
11:BG:75:THR:HB	11:BG:83:LYS:HG2	2.01	0.42
16:BL:281:TRP:O	16:BL:285:LYS:NZ	2.53	0.42
17:BM:274:TRP:HE1	17:BM:286:ASN:HB2	1.85	0.42
17:BM:330:GLU:OE2	28:BX:97:LYS:NZ	2.53	0.42
23:BS:44:SER:O	23:BS:48:ASN:ND2	2.35	0.42
1:B6:74:LEU:HD22	1:B6:78:GLU:HG2	2.01	0.42
3:B8:669:G:N2	3:B8:756:C:O2'	2.53	0.42
3:B8:1440:C:O2'	3:B8:1442:A:OP2	2.26	0.42
5:BA:62:ARG:NE	50:Bu:230:ARG:HD2	2.34	0.42
28:BX:148:THR:HG22	28:BX:165:GLU:HG2	2.01	0.42
43:Bn:160:ASP:OD2	43:Bn:267:ARG:NH2	2.43	0.42
51:Bv:247:GLY:HA3	51:Bv:251:HIS:CE1	2.53	0.42
52:Bw:122:GLU:N	52:Bw:158:GLN:O	2.51	0.42
7:BC:166:VAL:HG12	7:BC:169:THR:H	1.83	0.42
9:BE:214:LYS:HB2	42:Bm:58:ILE:HD13	2.02	0.42
51:Bv:187:THR:HG23	51:Bv:190:ARG:HH21	1.84	0.42
52:Bw:135:LEU:HG	52:Bw:146:LEU:HA	2.00	0.42
3:B8:61:A:OP1	19:BO:74:HIS:NE2	2.52	0.42
39:Bi:207:HIS:ND1	39:Bi:234:ASP:OD1	2.41	0.42
51:Bv:58:VAL:N	51:Bv:153:LEU:O	2.52	0.42
3:B8:438:G:H2'	3:B8:439:A:H2'	2.02	0.42
25:BU:61:LYS:NZ	25:BU:65:GLU:OE2	2.40	0.42
50:Bu:122:ILE:HD13	50:Bu:134:ILE:HG13	2.00	0.42
57:Aa:302:ILE:HD13	57:Aa:345:LYS:HE3	2.02	0.42
3:B8:1032:G:H5'	22:BR:114:LYS:HE2	2.01	0.42
10:BF:188:TRP:O	10:BF:195:ASN:ND2	2.45	0.42
28:BX:110:GLU:OE2	28:BX:112:TYR:OH	2.28	0.42
34:Bd:45:ARG:NH2	52:Bw:104:GLU:OE2	2.51	0.42
40:Bj:243:ILE:HG23	40:Bj:255:THR:HG21	2.01	0.42
43:Bn:306:LYS:HG3	43:Bn:307:HIS:CD2	2.55	0.42
44:Bo:69:HIS:CD2	44:Bo:71:GLY:H	2.37	0.42
51:Bv:242:ASP:OD1	51:Bv:243:PHE:N	2.50	0.42
57:Aa:199:ILE:HG23	57:Aa:200:CYS:H	1.84	0.42
3:B8:1024:A:C6	3:B8:1315:C:H1'	2.55	0.42
3:B8:1190:G:H5''	43:Bn:352:PRO:HD3	2.02	0.42
3:B8:1390:C:O2	57:Aa:306:ARG:NH2	2.53	0.42
24:BT:230:PRO:HB3	36:Bf:60:ARG:O	2.19	0.42
42:Bm:165:GLN:NE2	42:Bm:179:VAL:HG21	2.35	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1324:U:H4'	57:Aa:316:ASN:O	2.20	0.42
24:BT:55:GLY:O	24:BT:59:ARG:HD2	2.20	0.42
24:BT:95:PRO:HA	24:BT:139:GLN:HG3	2.02	0.42
39:Bi:152:GLN:HE22	39:Bi:179:GLN:HE22	1.67	0.42
40:Bj:124:ASP:HB2	40:Bj:296:ARG:NH1	2.35	0.42
48:Bs:77:ALA:HB2	48:Bs:104:LEU:HD13	2.02	0.42
56:AG:18:A:H2'	56:AG:43:A:N6	2.35	0.42
3:B8:125:A:N6	3:B8:126:A:N1	2.68	0.41
3:B8:328:U:OP1	3:B8:331:C:N4	2.34	0.41
3:B8:366:C:N4	3:B8:1248:A:N7	2.68	0.41
3:B8:443:G:H22	3:B8:1023:A:P	2.42	0.41
3:B8:1224:U:H5''	3:B8:1225:U:O4'	2.20	0.41
38:Bh:136:PRO:HG2	38:Bh:139:VAL:HG21	2.02	0.41
57:Aa:360:ILE:HA	57:Aa:363:LYS:HB3	2.02	0.41
3:B8:577:C:OP1	31:Ba:24:GLY:N	2.53	0.41
57:Aa:241:ARG:HE	57:Aa:287:GLN:CD	2.27	0.41
3:B8:667:A:H5''	46:Bq:28:ARG:HD3	2.02	0.41
3:B8:1007:A:H2'	3:B8:1008:A:C8	2.55	0.41
3:B8:1113:A:H4'	40:Bj:301:GLU:HA	2.01	0.41
8:BD:103:VAL:HG11	43:Bn:61:ALA:HB1	2.01	0.41
25:BU:96:TYR:OH	25:BU:129:LYS:NZ	2.52	0.41
29:BY:108:TYR:HD1	48:Bs:125:SER:HB2	1.85	0.41
45:Bp:121:TRP:CZ2	45:Bp:125:LYS:HD3	2.55	0.41
57:Aa:338:GLU:O	57:Aa:344:ASN:ND2	2.46	0.41
1:B2:76:LEU:HD13	20:BP:200:LEU:HA	2.03	0.41
29:BY:83:TYR:CZ	29:BY:87:ILE:HG13	2.55	0.41
30:BZ:164:THR:OG1	30:BZ:165:GLU:N	2.53	0.41
44:Bo:43:MET:HE1	44:Bo:232:HIS:CD2	2.55	0.41
3:B8:657:U:H4'	26:BV:30:ARG:HH21	1.86	0.41
3:B8:673:G:H3'	3:B8:673:G:N3	2.35	0.41
3:B8:761:C:OP2	3:B8:763:C:N4	2.41	0.41
6:BB:141:ASP:HB3	6:BB:144:ARG:HG2	2.03	0.41
20:BP:151:ASN:ND2	32:Bb:31:ARG:HH22	2.17	0.41
25:BU:104:MET:HE3	25:BU:104:MET:HB3	1.94	0.41
27:BW:83:VAL:HG11	27:BW:158:MET:HE1	2.01	0.41
3:B8:191:U:H2'	3:B8:192:U:C6	2.56	0.41
3:B8:356:A:H2'	3:B8:357:A:C8	2.55	0.41
3:B8:1113:A:H2'	3:B8:1114:A:O4'	2.21	0.41
3:B8:1280:U:H2'	3:B8:1281:A:C8	2.55	0.41
11:BG:102:ASN:ND2	35:Be:51:MET:O	2.46	0.41
34:Bd:42:ARG:O	34:Bd:44:HIS:ND1	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Bj:72:ILE:HA	40:Bj:75:TYR:CE2	2.55	0.41
3:B8:69:A:O2'	3:B8:218:G:H1'	2.21	0.41
3:B8:91:A:H2'	3:B8:92:A:C8	2.56	0.41
3:B8:266:A:H4'	3:B8:267:A:C8	2.56	0.41
18:BN:187:LEU:HD13	18:BN:259:LEU:HD23	2.02	0.41
19:BO:185:ASN:OD1	19:BO:188:ILE:HG13	2.21	0.41
22:BR:37:ILE:HG23	22:BR:42:LEU:HB2	2.02	0.41
34:Bd:58:LYS:HG2	34:Bd:77:MET:HE2	2.02	0.41
43:Bn:234:HIS:CE1	43:Bn:257:PRO:HA	2.56	0.41
57:Aa:141:ASN:O	57:Aa:145:GLU:HG3	2.20	0.41
3:B8:237:A:N3	3:B8:1260:U:O2'	2.48	0.41
3:B8:860:A:H5''	16:BL:212:THR:HG21	2.02	0.41
5:BA:126:HIS:HD2	50:Bu:227:ARG:HH21	1.68	0.41
26:BV:144:LEU:HD12	44:Bo:174:VAL:HG11	2.03	0.41
42:Bm:177:CYS:HB3	42:Bm:178:PRO:HD3	2.02	0.41
52:Bw:104:GLU:HG2	52:Bw:155:ARG:HE	1.85	0.41
57:Aa:189:VAL:HG12	57:Aa:282:VAL:HG22	2.03	0.41
1:B1:85:LEU:HD23	1:B2:68:VAL:HG21	2.03	0.41
3:B8:249:C:O2'	3:B8:830:A:N1	2.50	0.41
3:B8:619:G:OP1	24:BT:34:LYS:NZ	2.50	0.41
3:B8:802:A:H5''	23:BS:35:MET:HE2	2.03	0.41
3:B8:964:U:OP1	16:BL:278:LYS:NZ	2.41	0.41
3:B8:997:U:H2'	3:B8:998:A:O4'	2.20	0.41
3:B8:1115:C:H4'	40:Bj:75:TYR:CE2	2.56	0.41
6:BB:52:ASP:O	6:BB:56:TYR:N	2.51	0.41
9:BE:44:ARG:HG3	19:BO:55:ILE:HG21	2.02	0.41
21:BQ:123:ILE:HG13	33:Bc:75:VAL:HG13	2.02	0.41
21:BQ:169:LYS:HE3	21:BQ:169:LYS:HB2	1.92	0.41
40:Bj:308:ASP:HA	40:Bj:311:LEU:HG	2.01	0.41
42:Bm:257:TYR:CD2	42:Bm:258:PRO:HA	2.56	0.41
48:Bs:131:HIS:HD2	48:Bs:133:PHE:H	1.67	0.41
51:Bv:109:GLU:HB2	51:Bv:112:GLN:NE2	2.36	0.41
3:B8:444:C:H4'	3:B8:1313:G:O2'	2.21	0.41
3:B8:1093:U:O2'	19:BO:247:ARG:HB3	2.21	0.41
3:B8:1422:U:H2'	3:B8:1423:C:C6	2.56	0.41
11:BG:148:GLN:HB3	11:BG:150:HIS:CE1	2.56	0.41
15:BK:104:ARG:NH1	15:BK:160:LYS:O	2.53	0.41
18:BN:94:ASP:OD1	18:BN:94:ASP:N	2.53	0.41
26:BV:30:ARG:HD2	26:BV:78:PHE:O	2.21	0.41
40:Bj:72:ILE:HA	40:Bj:75:TYR:CD2	2.56	0.41
56:AG:54:A:H2'	56:AG:55:C:H5''	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:468:U:O2'	3:B8:481:A:N3	2.52	0.40
3:B8:651:A:H5'	12:BH:135:ALA:HA	2.03	0.40
3:B8:916:U:H2'	3:B8:917:G:C8	2.56	0.40
3:B8:1372:U:H3	57:Aa:305:PHE:HB2	1.86	0.40
6:BB:150:TRP:CE2	50:Bu:172:MET:HG2	2.55	0.40
24:BT:257:CYS:SG	36:Bf:59:TRP:NE1	2.94	0.40
40:Bj:127:LEU:O	40:Bj:251:ASN:HB3	2.21	0.40
3:B8:785:U:H2'	3:B8:786:U:C6	2.56	0.40
3:B8:1088:G:H2'	3:B8:1089:U:C6	2.56	0.40
9:BE:143:PHE:HE2	9:BE:190:LYS:HE2	1.86	0.40
12:BH:137:ILE:HD12	26:BV:131:PRO:HD3	2.03	0.40
17:BM:311:GLY:HA2	17:BM:314:LEU:HD12	2.03	0.40
20:BP:177:LEU:HD22	32:Bb:22:PRO:HB3	2.03	0.40
23:BS:123:ILE:HD12	23:BS:127:LEU:HD12	2.03	0.40
49:Bt:148:MET:SD	49:Bt:149:PRO:HD2	2.61	0.40
56:AG:5:A:H2'	56:AG:6:G:C8	2.56	0.40
3:B8:1537:A:O2'	3:B8:1538:C:O4'	2.39	0.40
4:B9:72:A:H5'	51:Bv:170:VAL:HG21	2.02	0.40
5:BA:200:ARG:NH1	22:BR:52:ASP:O	2.49	0.40
15:BK:127:ALA:HA	24:BT:79:PRO:HD3	2.03	0.40
26:BV:46:TRP:HD1	26:BV:121:ALA:HB2	1.87	0.40
29:BY:114:LYS:HD2	47:Br:44:ASN:HB3	2.03	0.40
30:BZ:99:VAL:HG12	30:BZ:133:VAL:HG22	2.02	0.40
44:Bo:226:ALA:HB1	44:Bo:240:ILE:HD13	2.02	0.40
52:Bw:48:TYR:HB3	52:Bw:51:LYS:HG2	2.04	0.40
3:B8:66:A:H2	3:B8:91:A:N7	2.19	0.40
3:B8:442:A:H5''	35:Be:20:LYS:HB2	2.04	0.40
6:BB:9:LEU:HD21	10:BF:185:VAL:HG22	2.03	0.40
10:BF:223:LYS:HE2	10:BF:223:LYS:HB3	1.93	0.40
17:BM:96:ARG:HH21	17:BM:202:GLN:HE22	1.69	0.40
18:BN:218:LEU:HD23	18:BN:260:VAL:HB	2.04	0.40
19:BO:191:ARG:NH2	40:Bj:301:GLU:OE1	2.52	0.40
34:Bd:85:SER:O	34:Bd:89:ARG:HG3	2.22	0.40
40:Bj:123:LEU:HD21	40:Bj:125:LEU:HD21	2.03	0.40
40:Bj:291:VAL:HG12	40:Bj:292:ARG:HG3	2.04	0.40
3:B8:81:A:C5	3:B8:82:U:H1'	2.56	0.40
18:BN:61:PRO:HA	18:BN:84:PRO:HD3	2.02	0.40
29:BY:78:GLU:OE1	48:Bs:135:ASN:ND2	2.39	0.40
30:BZ:119:GLU:HG2	30:BZ:121:ASP:H	1.85	0.40
35:Be:99:LYS:O	48:Bs:44:ARG:NH2	2.54	0.40
48:Bs:66:ASN:ND2	54:By:155:THR:OG1	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	44/198 (22%)	44 (100%)	0	0	100	100
1	B2	30/198 (15%)	30 (100%)	0	0	100	100
1	B3	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
1	B4	29/198 (15%)	29 (100%)	0	0	100	100
1	B5	29/198 (15%)	29 (100%)	0	0	100	100
1	B6	29/198 (15%)	29 (100%)	0	0	100	100
5	BA	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
6	BB	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
7	BC	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
8	BD	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
10	BF	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
11	BG	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
12	BH	108/188 (57%)	108 (100%)	0	0	100	100
13	BI	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
14	BJ	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
17	BM	303/348 (87%)	300 (99%)	3 (1%)	0	100	100
18	BN	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
19	BO	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
20	BP	210/261 (80%)	205 (98%)	5 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	BQ	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
22	BR	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
23	BS	113/145 (78%)	113 (100%)	0	0	100	100
24	BT	289/296 (98%)	285 (99%)	4 (1%)	0	100	100
25	BU	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
26	BV	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
27	BW	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
28	BX	222/292 (76%)	220 (99%)	2 (1%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
31	Ba	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
32	Bb	99/112 (88%)	99 (100%)	0	0	100	100
33	Bc	80/138 (58%)	80 (100%)	0	0	100	100
34	Bd	64/128 (50%)	64 (100%)	0	0	100	100
35	Be	92/102 (90%)	92 (100%)	0	0	100	100
36	Bf	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
37	Bg	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
39	Bi	382/439 (87%)	377 (99%)	5 (1%)	0	100	100
40	Bj	160/325 (49%)	156 (98%)	4 (2%)	0	100	100
41	Bl	36/103 (35%)	36 (100%)	0	0	100	100
42	Bm	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
43	Bn	352/380 (93%)	343 (97%)	9 (3%)	0	100	100
44	Bo	292/338 (86%)	285 (98%)	7 (2%)	0	100	100
45	Bp	145/206 (70%)	145 (100%)	0	0	100	100
46	Bq	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
47	Br	96/142 (68%)	96 (100%)	0	0	100	100
48	Bs	149/215 (69%)	146 (98%)	3 (2%)	0	100	100
49	Bt	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
50	Bu	235/306 (77%)	233 (99%)	2 (1%)	0	100	100
51	Bv	236/279 (85%)	230 (98%)	6 (2%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Bw	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
53	Bx	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
54	By	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
55	Bz	95/128 (74%)	95 (100%)	0	0	100	100
57	Aa	379/484 (78%)	376 (99%)	3 (1%)	0	100	100
All	All	9277/12666 (73%)	9160 (99%)	117 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	40/158 (25%)	40 (100%)	0	100	100
1	B2	31/158 (20%)	31 (100%)	0	100	100
1	B3	31/158 (20%)	31 (100%)	0	100	100
1	B4	30/158 (19%)	30 (100%)	0	100	100
1	B5	30/158 (19%)	30 (100%)	0	100	100
1	B6	30/158 (19%)	30 (100%)	0	100	100
5	BA	146/176 (83%)	146 (100%)	0	100	100
6	BB	134/135 (99%)	132 (98%)	2 (2%)	57	84
7	BC	183/191 (96%)	183 (100%)	0	100	100
8	BD	94/119 (79%)	93 (99%)	1 (1%)	65	88
9	BE	220/229 (96%)	220 (100%)	0	100	100
10	BF	163/223 (73%)	162 (99%)	1 (1%)	78	93
11	BG	113/147 (77%)	113 (100%)	0	100	100
12	BH	99/164 (60%)	99 (100%)	0	100	100
13	BI	53/60 (88%)	53 (100%)	0	100	100
14	BJ	40/72 (56%)	40 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BK	88/166 (53%)	88 (100%)	0	100	100
16	BL	192/245 (78%)	191 (100%)	1 (0%)	81	93
17	BM	260/290 (90%)	259 (100%)	1 (0%)	84	94
18	BN	219/262 (84%)	219 (100%)	0	100	100
19	BO	182/228 (80%)	181 (100%)	1 (0%)	81	93
20	BP	194/232 (84%)	194 (100%)	0	100	100
21	BQ	138/150 (92%)	138 (100%)	0	100	100
22	BR	154/155 (99%)	154 (100%)	0	100	100
23	BS	98/124 (79%)	98 (100%)	0	100	100
24	BT	246/249 (99%)	246 (100%)	0	100	100
25	BU	189/211 (90%)	188 (100%)	1 (0%)	81	93
26	BV	134/150 (89%)	134 (100%)	0	100	100
27	BW	126/155 (81%)	126 (100%)	0	100	100
28	BX	206/256 (80%)	206 (100%)	0	100	100
29	BY	118/126 (94%)	118 (100%)	0	100	100
30	BZ	146/180 (81%)	146 (100%)	0	100	100
31	Ba	74/97 (76%)	74 (100%)	0	100	100
32	Bb	83/90 (92%)	83 (100%)	0	100	100
33	Bc	76/116 (66%)	76 (100%)	0	100	100
34	Bd	59/113 (52%)	59 (100%)	0	100	100
35	Be	80/87 (92%)	80 (100%)	0	100	100
36	Bf	135/181 (75%)	135 (100%)	0	100	100
37	Bg	138/178 (78%)	138 (100%)	0	100	100
38	Bh	147/169 (87%)	146 (99%)	1 (1%)	76	92
39	Bi	340/381 (89%)	339 (100%)	1 (0%)	86	96
40	Bj	150/287 (52%)	150 (100%)	0	100	100
41	Bl	37/89 (42%)	37 (100%)	0	100	100
42	Bm	353/368 (96%)	352 (100%)	1 (0%)	86	96
43	Bn	313/332 (94%)	313 (100%)	0	100	100
44	Bo	270/303 (89%)	269 (100%)	1 (0%)	84	94
45	Bp	136/190 (72%)	136 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Bq	104/112 (93%)	104 (100%)	0	100	100
47	Br	96/133 (72%)	96 (100%)	0	100	100
48	Bs	132/185 (71%)	130 (98%)	2 (2%)	57	84
49	Bt	251/288 (87%)	251 (100%)	0	100	100
50	Bu	223/274 (81%)	221 (99%)	2 (1%)	70	90
51	Bv	207/236 (88%)	207 (100%)	0	100	100
52	Bw	139/188 (74%)	139 (100%)	0	100	100
53	Bx	124/148 (84%)	124 (100%)	0	100	100
54	By	104/148 (70%)	104 (100%)	0	100	100
55	Bz	86/110 (78%)	85 (99%)	1 (1%)	63	86
57	Aa	338/427 (79%)	333 (98%)	5 (2%)	57	84
All	All	8322/10873 (76%)	8300 (100%)	22 (0%)	84	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BB	19	VAL
6	BB	28	LEU
8	BD	131	VAL
10	BF	185	VAL
16	BL	215	VAL
17	BM	151	THR
19	BO	102	VAL
25	BU	59	VAL
38	Bh	70	CYS
39	Bi	157	LEU
42	Bm	146	HIS
44	Bo	143	TRP
48	Bs	75	VAL
48	Bs	121	THR
50	Bu	81	THR
50	Bu	89	VAL
55	Bz	43	VAL
57	Aa	194	THR
57	Aa	199	ILE
57	Aa	272	MET
57	Aa	314	HIS
57	Aa	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	B1	69	GLN
1	B3	65	GLN
5	BA	126	HIS
5	BA	204	HIS
6	BB	27	GLN
6	BB	77	ASN
9	BE	172	GLN
10	BF	110	ASN
10	BF	179	HIS
11	BG	64	HIS
11	BG	150	HIS
12	BH	83	ASN
15	BK	170	ASN
17	BM	52	HIS
17	BM	63	GLN
17	BM	88	HIS
17	BM	125	GLN
17	BM	137	ASN
17	BM	280	HIS
18	BN	103	GLN
18	BN	208	HIS
19	BO	192	HIS
20	BP	93	ASN
20	BP	151	ASN
21	BQ	84	GLN
22	BR	9	GLN
22	BR	56	HIS
22	BR	94	GLN
23	BS	59	HIS
23	BS	143	ASN
24	BT	84	ASN
25	BU	237	HIS
26	BV	100	GLN
26	BV	147	GLN
26	BV	154	GLN
27	BW	142	ASN
28	BX	158	GLN
28	BX	172	GLN
28	BX	253	GLN
29	BY	149	HIS
30	BZ	84	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	BZ	118	ASN
30	BZ	140	ASN
33	Bc	82	GLN
33	Bc	135	ASN
34	Bd	65	HIS
35	Be	94	HIS
36	Bf	176	HIS
36	Bf	190	GLN
37	Bg	51	GLN
37	Bg	120	HIS
38	Bh	79	HIS
38	Bh	96	HIS
38	Bh	130	ASN
39	Bi	152	GLN
39	Bi	238	ASN
39	Bi	240	GLN
39	Bi	314	GLN
39	Bi	343	GLN
39	Bi	358	GLN
39	Bi	386	ASN
39	Bi	387	ASN
40	Bj	241	HIS
40	Bj	266	GLN
42	Bm	160	HIS
42	Bm	165	GLN
42	Bm	221	GLN
42	Bm	353	HIS
42	Bm	384	GLN
43	Bn	308	GLN
44	Bo	69	HIS
44	Bo	198	ASN
44	Bo	247	ASN
44	Bo	298	GLN
47	Br	46	ASN
47	Br	90	GLN
47	Br	111	GLN
48	Bs	66	ASN
48	Bs	129	GLN
48	Bs	131	HIS
49	Bt	73	GLN
49	Bt	80	GLN
49	Bt	118	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
49	Bt	168	HIS
49	Bt	193	GLN
49	Bt	204	GLN
50	Bu	167	HIS
51	Bv	67	GLN
51	Bv	75	GLN
51	Bv	212	HIS
51	Bv	251	HIS
51	Bv	252	HIS
52	Bw	61	HIS
52	Bw	92	ASN
52	Bw	189	HIS
53	Bx	93	ASN
53	Bx	141	ASN
54	By	135	GLN
57	Aa	107	ASN
57	Aa	124	GLN
57	Aa	314	HIS
57	Aa	341	GLN
57	Aa	368	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1556/1561 (99%)	236 (15%)	1 (0%)
4	B9	71/72 (98%)	11 (15%)	0
56	AG	70/71 (98%)	11 (15%)	0
All	All	1699/1707 (99%)	259 (15%)	1 (0%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	2	C
3	B8	11	G
3	B8	19	C
3	B8	22	A
3	B8	23	C
3	B8	29	C
3	B8	30	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	34	U
3	B8	38	A
3	B8	39	G
3	B8	41	C
3	B8	54	A
3	B8	57	A
3	B8	58	U
3	B8	62	C
3	B8	65	A
3	B8	78	G
3	B8	95	C
3	B8	107	A
3	B8	135	A
3	B8	137	U
3	B8	138	A
3	B8	147	C
3	B8	151	A
3	B8	157	C
3	B8	158	A
3	B8	159	A
3	B8	162	A
3	B8	166	A
3	B8	174	A
3	B8	184	U
3	B8	186	A
3	B8	199	A
3	B8	203	A
3	B8	212	A
3	B8	217	A
3	B8	223	A
3	B8	231	C
3	B8	233	C
3	B8	248	G
3	B8	267	A
3	B8	270	A
3	B8	304	A
3	B8	315	G
3	B8	322	C
3	B8	324	A
3	B8	330	C
3	B8	332	G
3	B8	333	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	345	G
3	B8	352	G
3	B8	359	A
3	B8	360	U
3	B8	362	G
3	B8	366	C
3	B8	367	U
3	B8	369	A
3	B8	384	U
3	B8	390	A
3	B8	401	U
3	B8	409	C
3	B8	429	U
3	B8	443	G
3	B8	455	C
3	B8	456	U
3	B8	462	A
3	B8	477	G
3	B8	490	A
3	B8	493	A
3	B8	498	U
3	B8	511	A
3	B8	512	G
3	B8	522	A
3	B8	528	A
3	B8	530	A
3	B8	544	A
3	B8	549	C
3	B8	550	A
3	B8	551	C
3	B8	553	A
3	B8	554	C
3	B8	555	C
3	B8	556	U
3	B8	558	A
3	B8	560	A
3	B8	563	U
3	B8	567	A
3	B8	571	A
3	B8	573	A
3	B8	575	A
3	B8	576	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	592	C
3	B8	593	C
3	B8	614	C
3	B8	615	U
3	B8	627	A
3	B8	630	G
3	B8	652	C
3	B8	661	C
3	B8	662	C
3	B8	675	G
3	B8	679	G
3	B8	680	A
3	B8	683	A
3	B8	687	C
3	B8	693	A
3	B8	702	U
3	B8	704	A
3	B8	720	A
3	B8	729	A
3	B8	731	A
3	B8	734	U
3	B8	737	U
3	B8	745	C
3	B8	763	C
3	B8	764	A
3	B8	776	A
3	B8	781	A
3	B8	782	A
3	B8	808	G
3	B8	814	C
3	B8	815	U
3	B8	823	C
3	B8	832	C
3	B8	850	C
3	B8	851	A
3	B8	857	A
3	B8	870	C
3	B8	900	C
3	B8	912	A
3	B8	922	G
3	B8	923	G
3	B8	924	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	929	U
3	B8	930	A
3	B8	931	A
3	B8	933	C
3	B8	948	U
3	B8	956	U
3	B8	957	G
3	B8	958	U
3	B8	963	A
3	B8	965	G
3	B8	984	U
3	B8	986	U
3	B8	1013	C
3	B8	1016	G
3	B8	1024	A
3	B8	1026	A
3	B8	1036	A
3	B8	1048	C
3	B8	1049	G
3	B8	1053	A
3	B8	1054	G
3	B8	1055	A
3	B8	1056	C
3	B8	1062	G
3	B8	1075	A
3	B8	1088	G
3	B8	1092	C
3	B8	1093	U
3	B8	1094	A
3	B8	1095	A
3	B8	1097	A
3	B8	1098	A
3	B8	1103	A
3	B8	1105	A
3	B8	1111	U
3	B8	1112	A
3	B8	1113	A
3	B8	1119	C
3	B8	1120	A
3	B8	1122	A
3	B8	1140	G
3	B8	1162	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	1163	A
3	B8	1177	C
3	B8	1194	U
3	B8	1195	C
3	B8	1213	A
3	B8	1215	U
3	B8	1218	A
3	B8	1219	C
3	B8	1223	A
3	B8	1243	A
3	B8	1246	G
3	B8	1247	G
3	B8	1252	A
3	B8	1258	C
3	B8	1262	G
3	B8	1265	A
3	B8	1286	A
3	B8	1319	G
3	B8	1320	A
3	B8	1322	G
3	B8	1335	A
3	B8	1346	G
3	B8	1359	A
3	B8	1371	U
3	B8	1383	A
3	B8	1384	G
3	B8	1389	A
3	B8	1390	C
3	B8	1400	G
3	B8	1403	C
3	B8	1416	U
3	B8	1419	A
3	B8	1426	U
3	B8	1430	U
3	B8	1432	U
3	B8	1438	U
3	B8	1439	U
3	B8	1440	C
3	B8	1441	A
3	B8	1443	A
3	B8	1480	U
3	B8	1487	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B8	1488	A
3	B8	1492	C
3	B8	1499	C
3	B8	1502	C
3	B8	1507	A
3	B8	1519	C
3	B8	1520	A
3	B8	1529	U
3	B8	1530	U
3	B8	1536	C
3	B8	1538	C
3	B8	1540	C
3	B8	1542	C
3	B8	1547	A
3	B8	1548	A
3	B8	1558	U
3	B8	1559	U
3	B8	1560	G
3	B8	1561	U
4	B9	8	U
4	B9	16	C
4	B9	20	A
4	B9	43	G
4	B9	45	U
4	B9	51	C
4	B9	52	U
4	B9	53	U
4	B9	54	A
4	B9	55	A
4	B9	57	U
56	AG	6	G
56	AG	7	G
56	AG	8	U
56	AG	10	A
56	AG	11	G
56	AG	17	U
56	AG	18	A
56	AG	45	G
56	AG	52	A
56	AG	53	U
56	AG	55	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B8	575	A

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMU	B8	1369	58,3	19,22,23	1.21	3 (15%)	25,31,34	1.78	5 (20%)
6	AYA	BB	2	6	6,7,8	0.81	0	6,8,10	0.63	0
56	PSU	AG	51	56	18,21,22	1.39	2 (11%)	21,30,33	1.94	3 (14%)
56	PSU	AG	24	56	18,21,22	1.34	2 (11%)	21,30,33	1.97	3 (14%)
3	OMG	B8	1145	56,58,3	23,26,27	1.17	3 (13%)	32,38,41	1.92	6 (18%)
3	PSU	B8	1397	3	18,21,22	1.40	2 (11%)	21,30,33	1.99	3 (14%)
32	AYA	Bb	2	32	6,7,8	0.69	0	6,8,10	0.70	0
56	PSU	AG	46	56	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
3	1MA	B8	947	3	21,25,26	0.42	0	30,37,40	0.73	1 (3%)
4	1MA	B9	9	4	21,25,26	0.48	0	30,37,40	0.77	1 (3%)
4	2MG	B9	10	4	23,26,27	0.45	0	33,38,41	0.52	0
22	SAC	BR	2	22	7,8,9	0.57	0	7,9,11	1.03	1 (14%)
3	OMG	B8	1370	3	23,26,27	1.18	3 (13%)	32,38,41	1.92	6 (18%)
4	PSU	B9	37	4	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
56	RSQ	AG	31	56	19,23,24	0.42	0	25,33,36	1.14	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	B8	1369	58,3	-	0/9/27/28	0/2/2/2
6	AYA	BB	2	6	-	1/5/6/8	-
56	PSU	AG	51	56	-	3/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	AG	24	56	-	0/7/25/26	0/2/2/2
3	OMG	B8	1145	56,58,3	-	0/9/27/28	0/3/3/3
3	PSU	B8	1397	3	-	0/7/25/26	0/2/2/2
32	AYA	Bb	2	32	-	3/5/6/8	-
56	PSU	AG	46	56	-	0/7/25/26	0/2/2/2
3	1MA	B8	947	3	-	0/7/25/26	0/3/3/3
4	1MA	B9	9	4	-	0/7/25/26	0/3/3/3
4	2MG	B9	10	4	-	0/9/27/28	0/3/3/3
22	SAC	BR	2	22	-	0/7/8/10	-
3	OMG	B8	1370	3	-	0/9/27/28	0/3/3/3
4	PSU	B9	37	4	-	0/7/25/26	0/2/2/2
56	RSQ	AG	31	56	-	2/9/27/28	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AG	46	PSU	C6-C5	3.54	1.39	1.35
56	AG	51	PSU	C6-C5	3.53	1.39	1.35
4	B9	37	PSU	C6-C5	3.37	1.39	1.35
56	AG	24	PSU	C6-C5	3.36	1.39	1.35
3	B8	1397	PSU	C6-C5	3.29	1.38	1.35
3	B8	1370	OMG	C5-C4	3.07	1.47	1.38
3	B8	1145	OMG	C5-C4	3.02	1.47	1.38
3	B8	1397	PSU	C4-N3	-2.74	1.33	1.38
3	B8	1369	OMU	C4-N3	-2.64	1.34	1.38
4	B9	37	PSU	C4-N3	-2.64	1.33	1.38
56	AG	46	PSU	C4-N3	-2.60	1.34	1.38
56	AG	24	PSU	C4-N3	-2.55	1.34	1.38
3	B8	1145	OMG	C6-N1	-2.49	1.34	1.38
56	AG	51	PSU	C4-N3	-2.48	1.34	1.38
3	B8	1370	OMG	C6-N1	-2.47	1.34	1.38
3	B8	1369	OMU	C2-N3	-2.21	1.34	1.38
3	B8	1145	OMG	C5-N7	-2.15	1.34	1.39
3	B8	1370	OMG	C5-N7	-2.12	1.34	1.39
3	B8	1369	OMU	C5-C4	-2.01	1.39	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1397	PSU	N1-C2-N3	6.32	121.84	115.17
56	AG	46	PSU	N1-C2-N3	6.18	121.68	115.17
4	B9	37	PSU	N1-C2-N3	6.14	121.64	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AG	24	PSU	N1-C2-N3	6.14	121.64	115.17
56	AG	51	PSU	N1-C2-N3	6.02	121.52	115.17
3	B8	1145	OMG	C5-C4-N3	-5.92	118.96	128.39
3	B8	1370	OMG	C5-C4-N3	-5.91	118.99	128.39
3	B8	1370	OMG	C2-N3-C4	4.85	120.66	112.30
3	B8	1145	OMG	C2-N3-C4	4.80	120.58	112.30
3	B8	1369	OMU	C4-N3-C2	-4.69	120.79	126.61
3	B8	1370	OMG	N9-C4-N3	4.45	134.86	125.95
3	B8	1145	OMG	N9-C4-N3	4.43	134.82	125.95
3	B8	1369	OMU	N3-C2-N1	4.19	120.35	114.89
4	B9	37	PSU	C4-N3-C2	-4.03	120.83	126.37
56	AG	46	PSU	C4-N3-C2	-3.96	120.92	126.37
56	AG	24	PSU	C4-N3-C2	-3.95	120.92	126.37
3	B8	1397	PSU	C4-N3-C2	-3.92	120.98	126.37
3	B8	1369	OMU	C5-C4-N3	3.80	120.12	114.80
56	AG	51	PSU	C4-N3-C2	-3.73	121.23	126.37
56	AG	24	PSU	O2-C2-N1	-3.53	119.15	122.79
3	B8	1397	PSU	O2-C2-N1	-3.52	119.16	122.79
56	AG	51	PSU	O2-C2-N1	-3.47	119.21	122.79
4	B9	37	PSU	O2-C2-N1	-3.41	119.27	122.79
56	AG	46	PSU	O2-C2-N1	-3.36	119.32	122.79
3	B8	1370	OMG	C6-C5-N7	3.11	135.95	130.29
3	B8	1145	OMG	C6-C5-N7	3.02	135.79	130.29
3	B8	1369	OMU	O4-C4-C5	-2.97	120.04	125.16
56	AG	31	RSQ	C1'-N1-C6	-2.92	116.33	121.15
56	AG	31	RSQ	C1'-N1-C2	2.87	124.79	118.44
22	BR	2	SAC	O-C-CA	-2.59	118.12	124.77
3	B8	1370	OMG	C4-C5-N7	-2.45	106.78	110.67
3	B8	1145	OMG	C4-C5-N7	-2.41	106.85	110.67
3	B8	1369	OMU	O2-C2-N1	-2.27	119.84	122.80
4	B9	9	1MA	N1-C6-N6	2.22	125.29	119.71
3	B8	947	1MA	N1-C6-N6	2.18	125.18	119.71
3	B8	1370	OMG	O6-C6-C5	-2.14	120.89	126.53
3	B8	1145	OMG	O6-C6-C5	-2.13	120.91	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	AG	51	PSU	O4'-C1'-C5-C4
56	AG	51	PSU	O4'-C1'-C5-C6
32	Bb	2	AYA	OT-CT-N-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	Bb	2	AYA	CM-CT-N-CA
56	AG	31	RSQ	C2'-C1'-N1-C2
6	BB	2	AYA	C-CA-N-CT
32	Bb	2	AYA	C-CA-N-CT
56	AG	31	RSQ	C2'-C1'-N1-C6
56	AG	51	PSU	C2'-C1'-C5-C6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AG	51	PSU	2	0
56	AG	31	RSQ	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 267 ligands modelled in this entry, 264 are monoatomic - leaving 3 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	$\# Z  > 2$
62	FS2	Bh	201	38,20	0,5,14	-	-	-		
63	MET	AG	101	56	6,7,8	0.47	0	2,7,9	0.14	0
60	VAL	B9	101	4	4,6,7	0.55	0	6,7,9	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	FS2	Bh	201	38,20	-	-	0/2/2/6
63	MET	AG	101	56	-	1/5/6/8	-
60	VAL	B9	101	4	-	3/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	B9	101	VAL	N-CA-CB-CG2
60	B9	101	VAL	C-CA-CB-CG1
60	B9	101	VAL	C-CA-CB-CG2
63	AG	101	MET	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	Bh	201	FS2	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

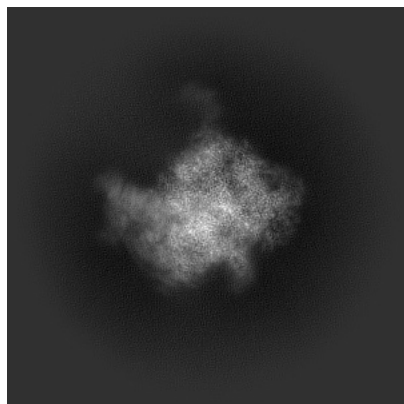
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16899. These allow visual inspection of the internal detail of the map and identification of artifacts.

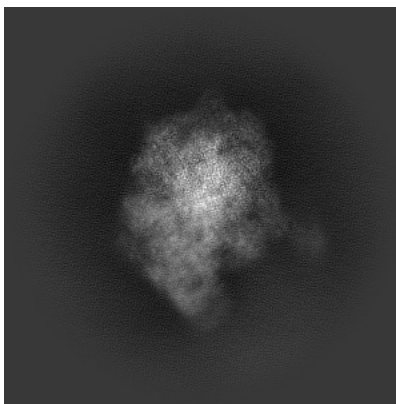
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

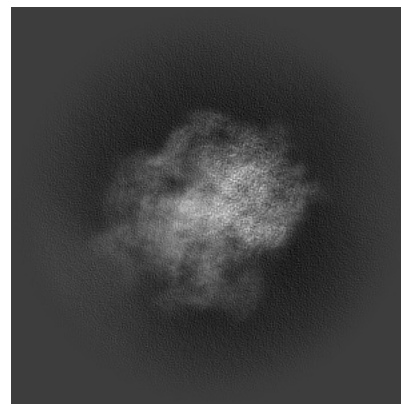
#### 6.1.1 Primary map



X

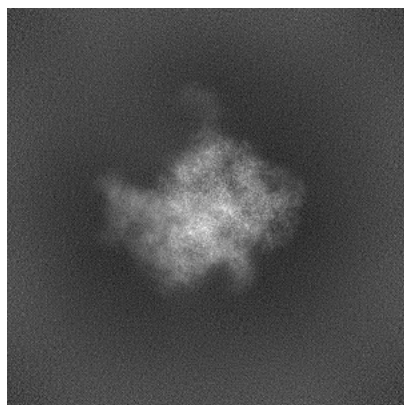


Y

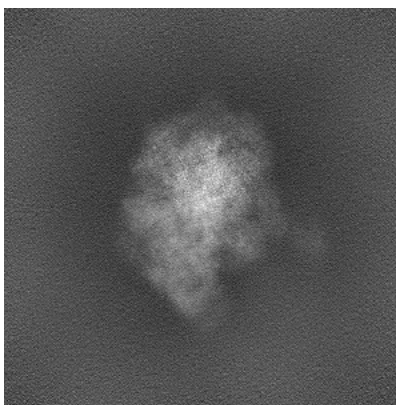


Z

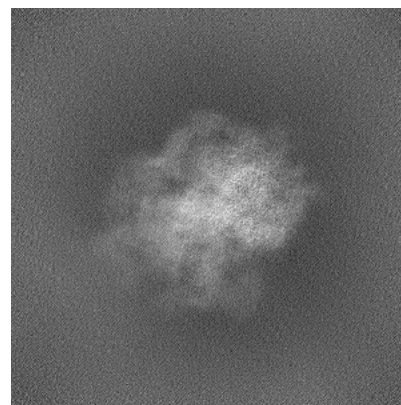
#### 6.1.2 Raw map



X



Y

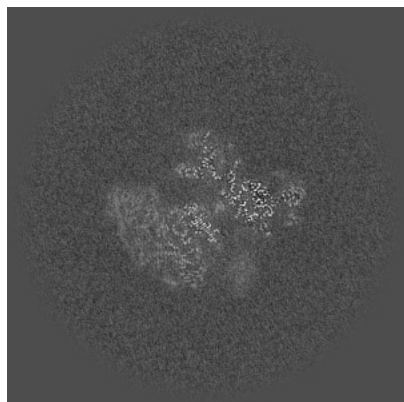


Z

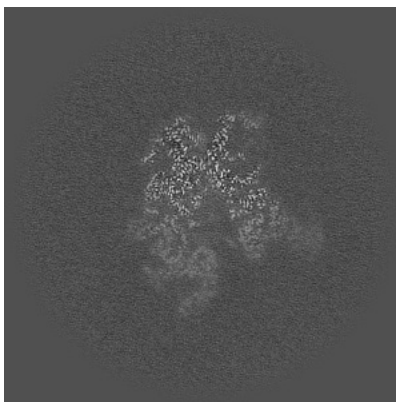
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

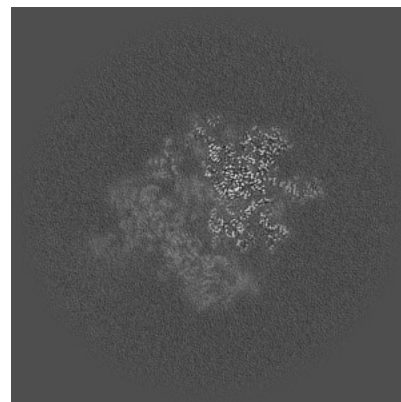
### 6.2.1 Primary map



X Index: 256

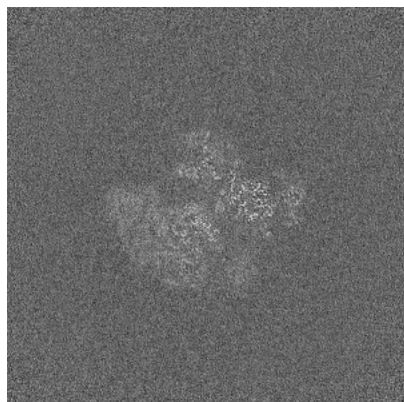


Y Index: 256

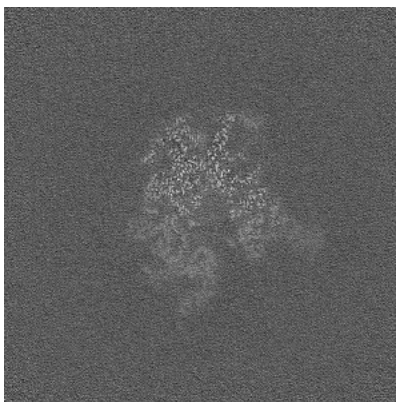


Z Index: 256

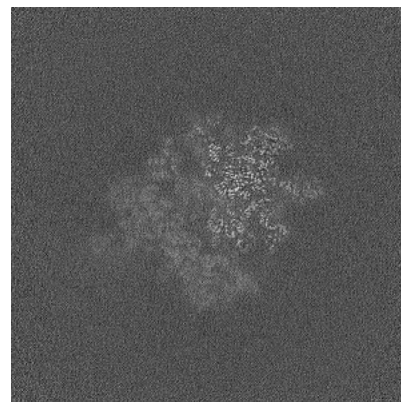
### 6.2.2 Raw map



X Index: 256



Y Index: 256

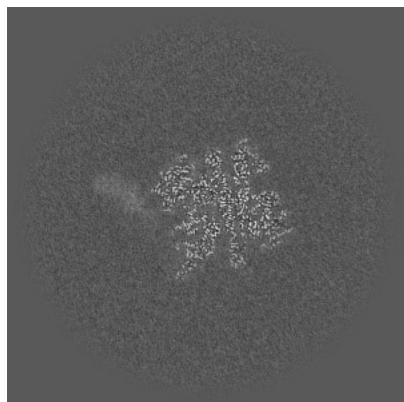


Z Index: 256

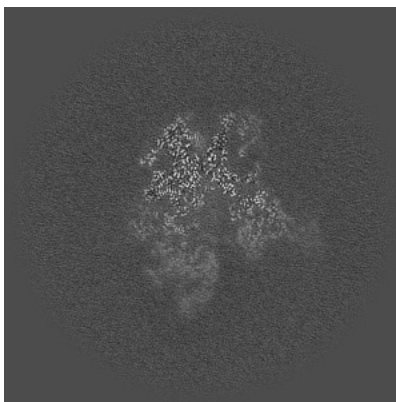
The images above show central slices of the map in three orthogonal directions.

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

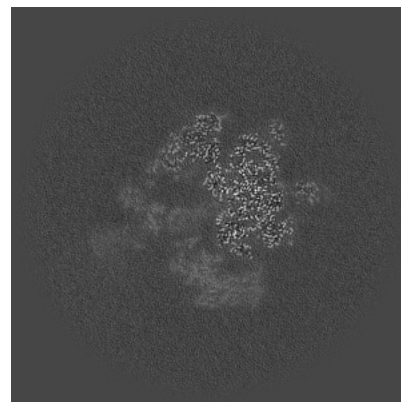
### 6.3.1 Primary map



X Index: 297

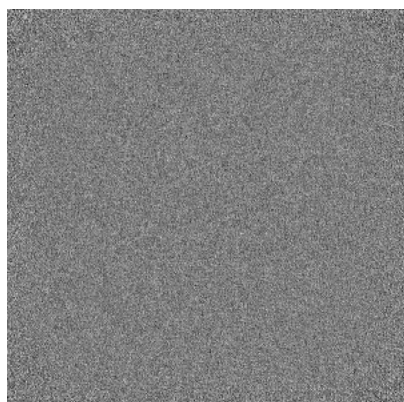


Y Index: 254

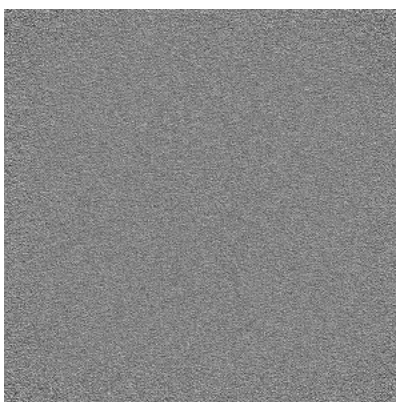


Z Index: 269

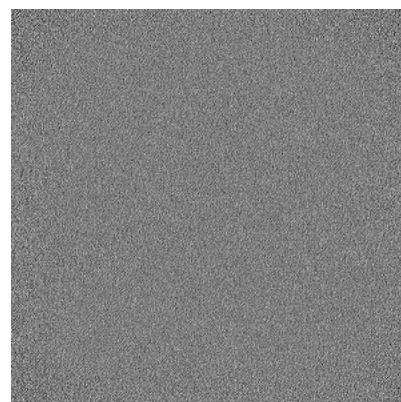
### 6.3.2 Raw map



X Index: 0



Y Index: 0

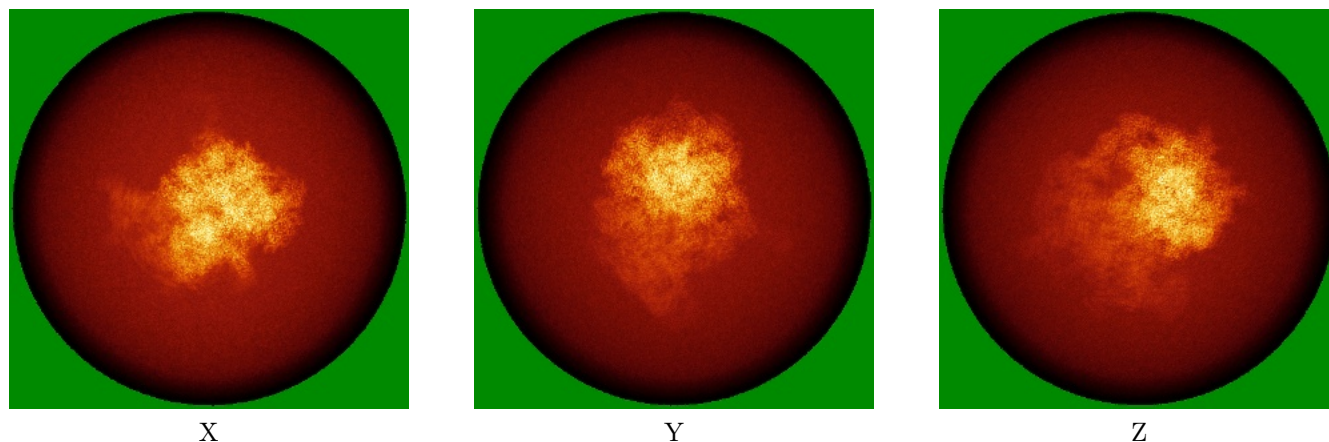


Z Index: 0

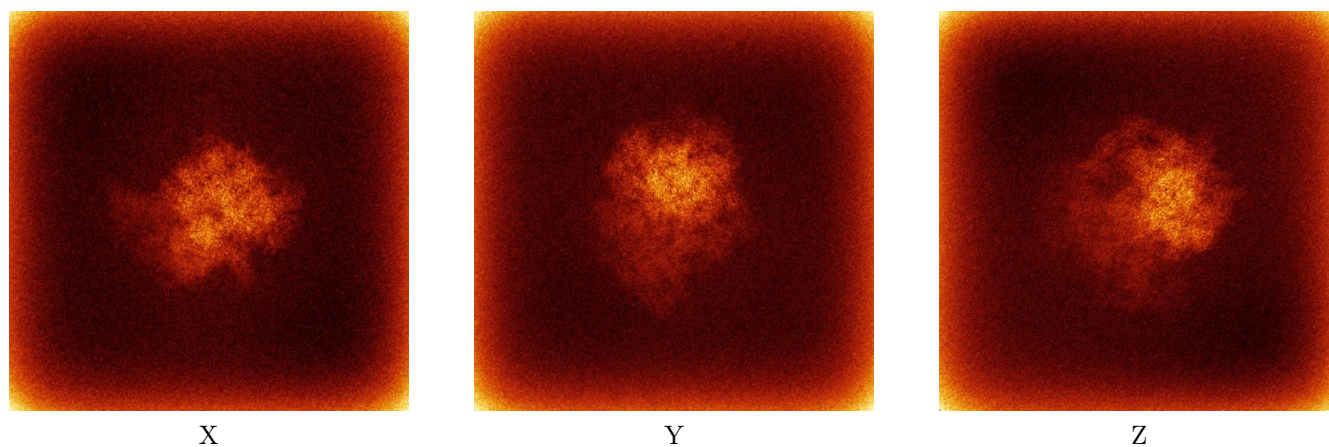
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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.

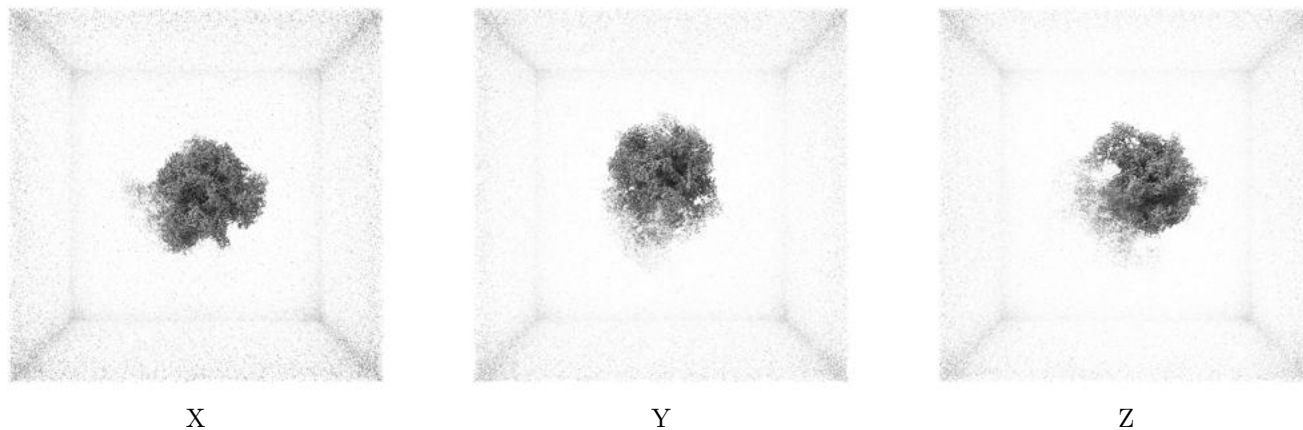
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

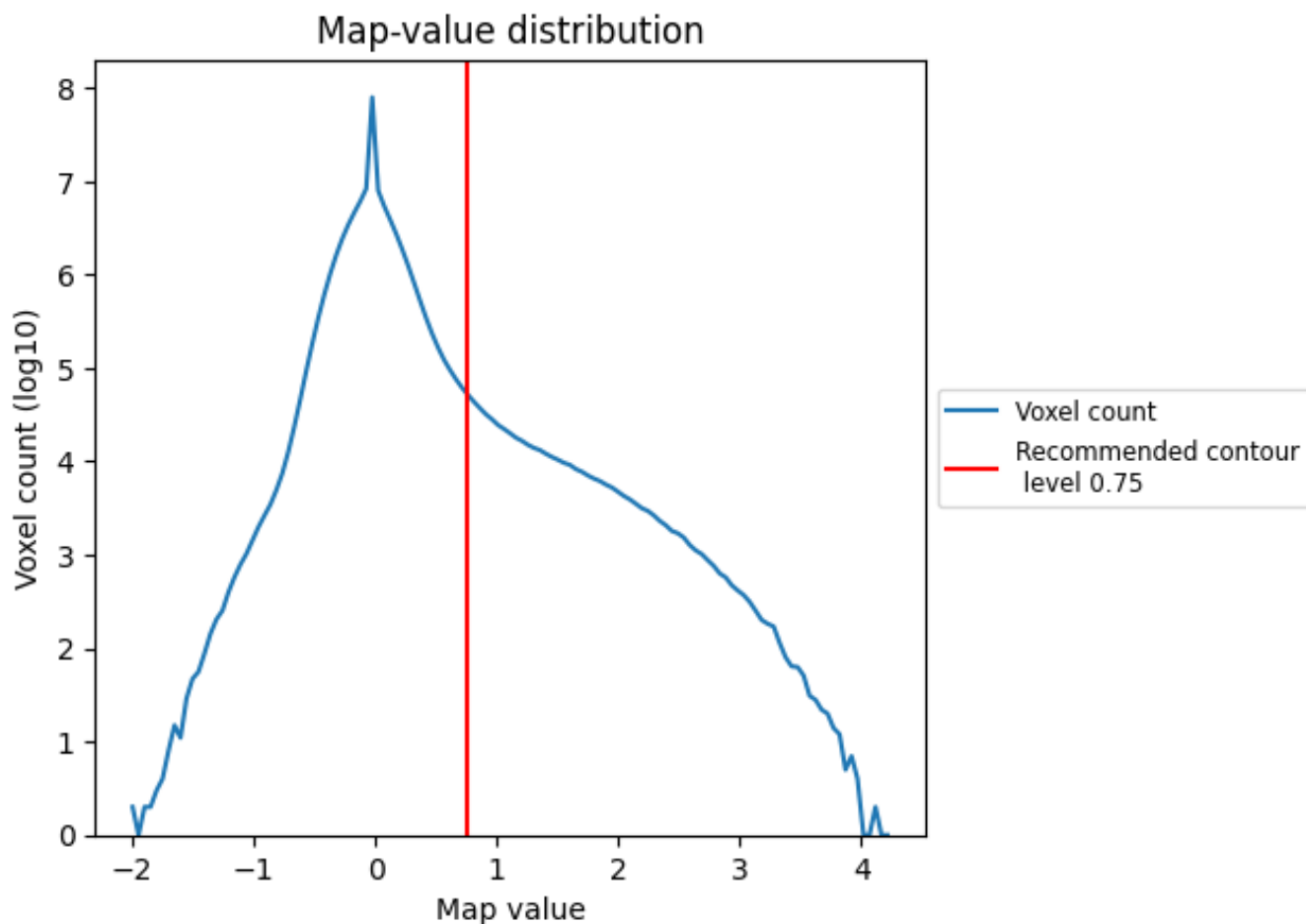
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

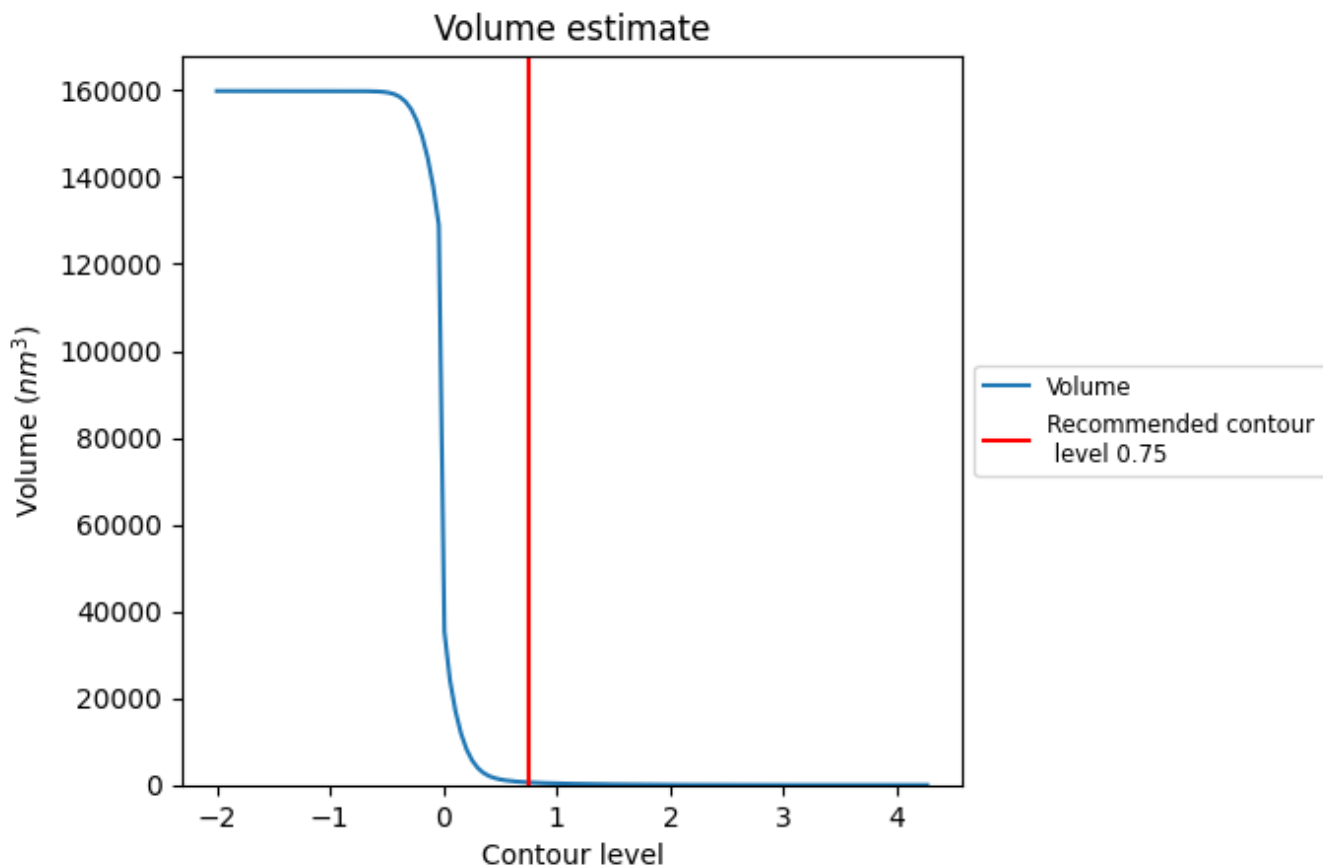
This section contains the results of statistical analysis of the map.

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



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

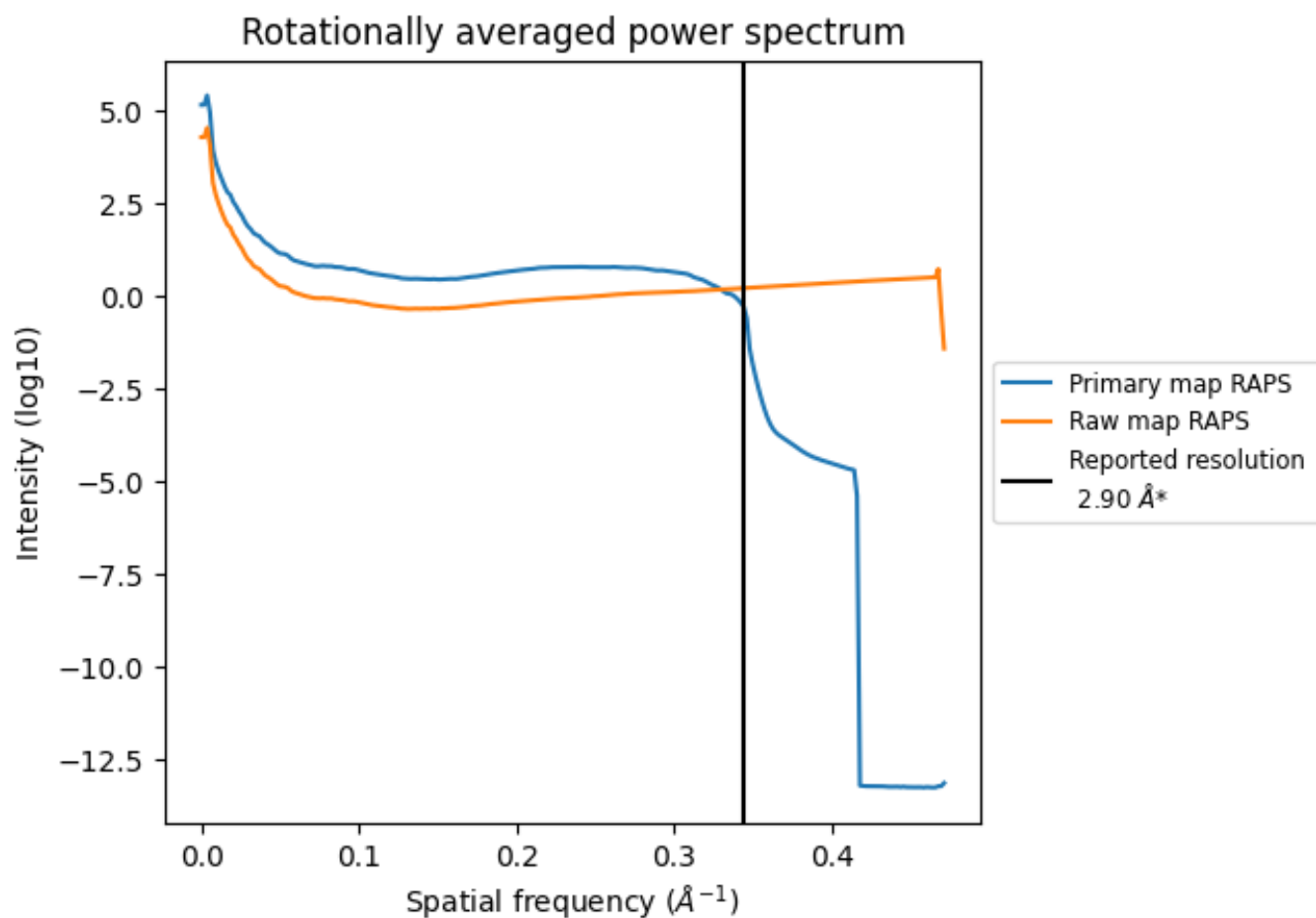
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 590 nm<sup>3</sup>; this corresponds to an approximate mass of 533 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 i

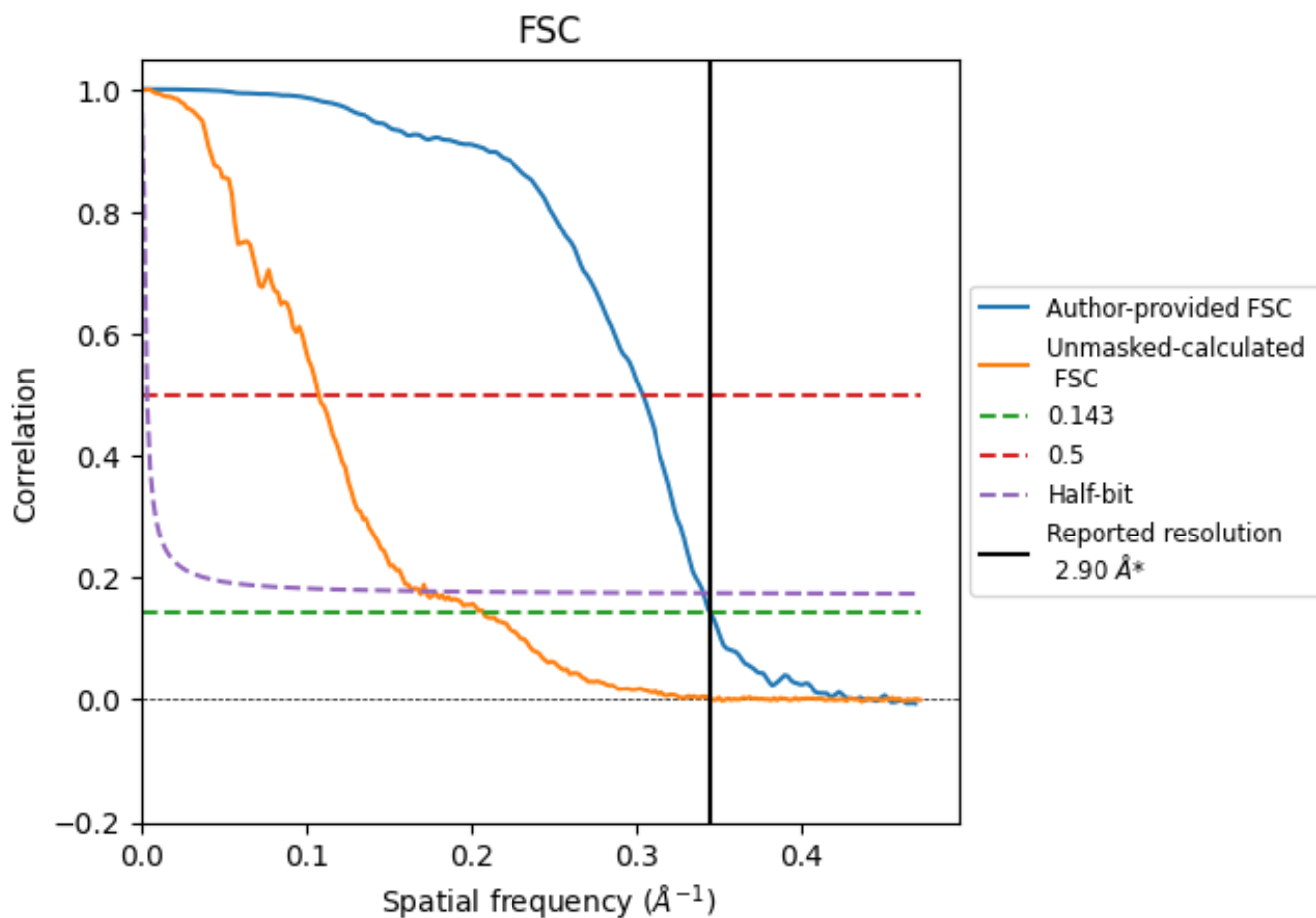


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

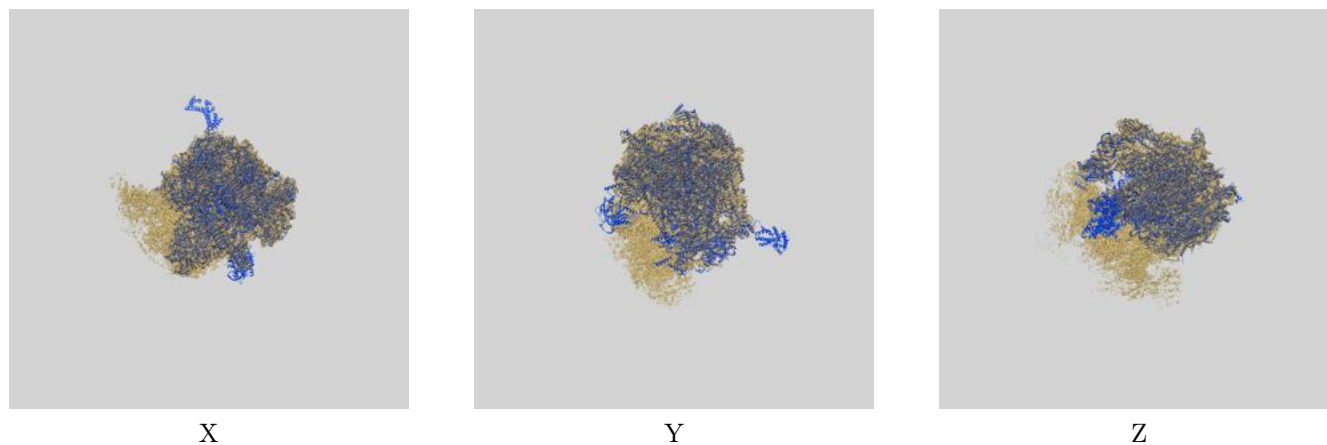
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.29	2.94
Unmasked-calculated*	4.83	9.30	5.93

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.83 differs from the reported value 2.9 by more than 10 %

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

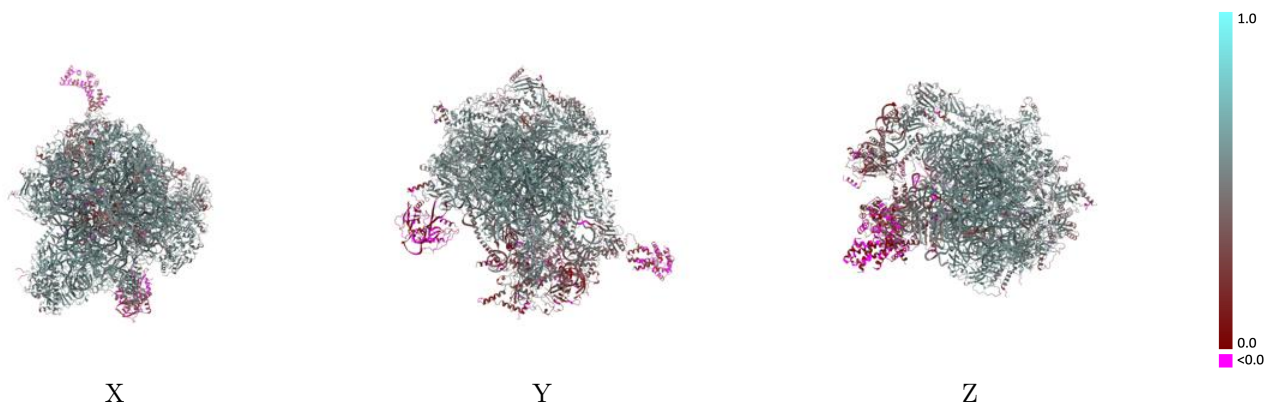
This section contains information regarding the fit between EMDB map EMD-16899 and PDB model 8OIT. Per-residue inclusion information can be found in section 3 on page 19.

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



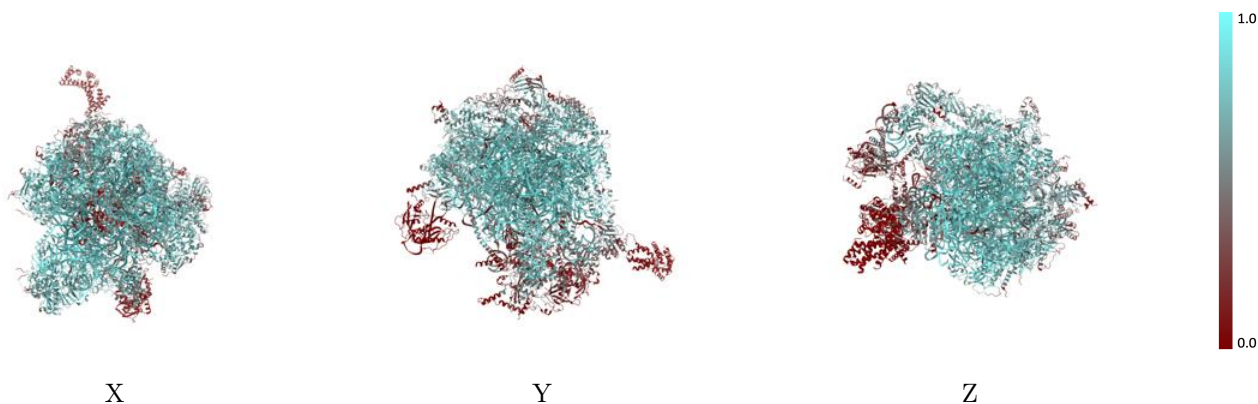
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



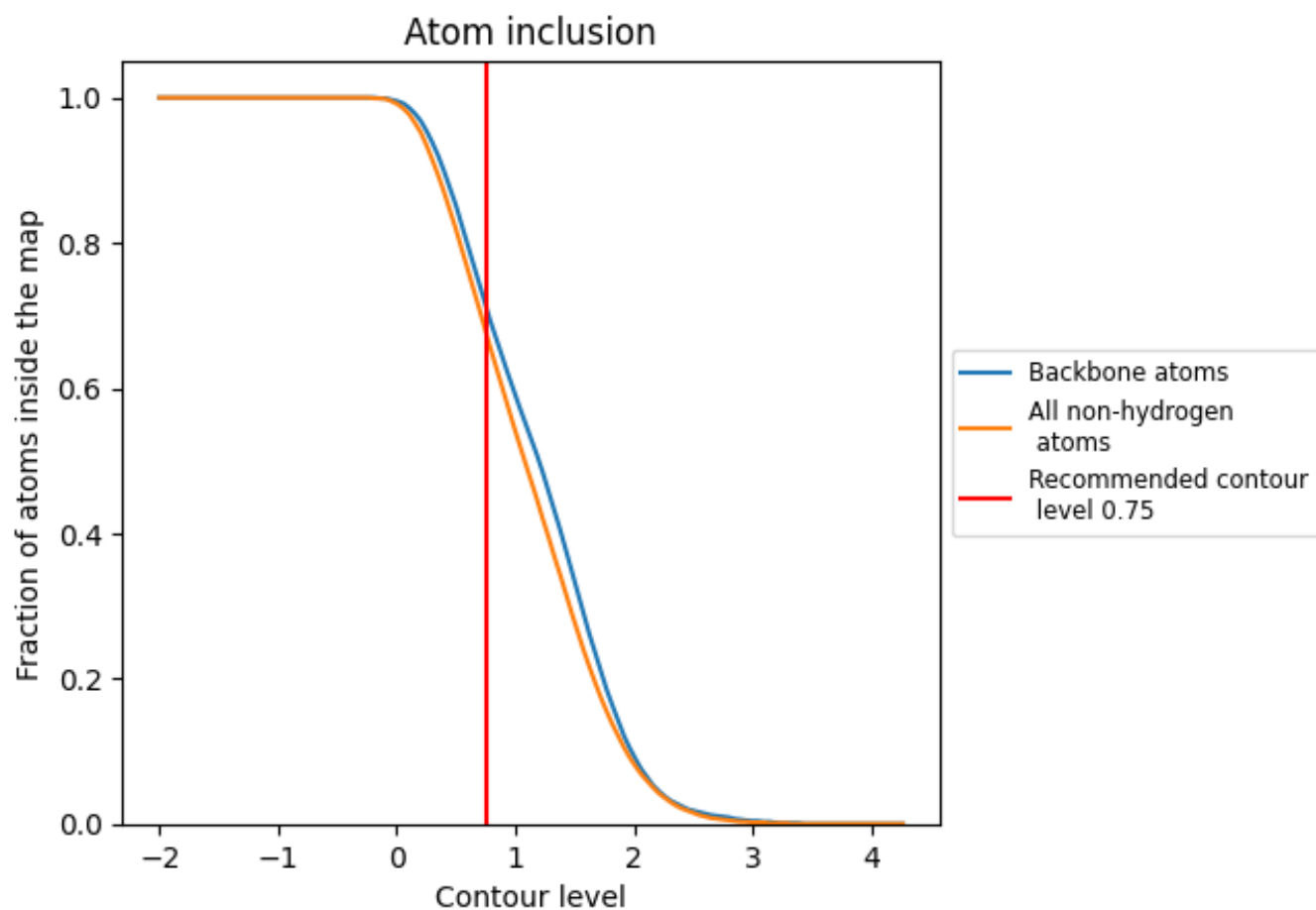
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 68% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.4910
AG	 0.3600	 0.3100
Aa	 0.0150	 0.1020
B1	 0.0230	 0.1990
B2	 0.0080	 0.0960
B3	 0.0000	 0.0740
B4	 0.0000	 0.0850
B5	 0.0000	 -0.0030
B6	 0.0000	 0.0050
B7	 0.1290	 0.4350
B8	 0.8620	 0.5550
B9	 0.5550	 0.3740
BA	 0.7920	 0.5740
BB	 0.6950	 0.5180
BC	 0.5170	 0.4850
BD	 0.8150	 0.5780
BE	 0.7160	 0.5340
BF	 0.7450	 0.5540
BG	 0.8010	 0.5690
BH	 0.7130	 0.5520
BI	 0.6900	 0.5230
BJ	 0.8750	 0.6110
BK	 0.8690	 0.6040
BL	 0.8090	 0.5720
BM	 0.8030	 0.5620
BN	 0.7970	 0.5710
BO	 0.2840	 0.2670
BP	 0.3740	 0.3490
BQ	 0.1620	 0.2570
BR	 0.8370	 0.5830
BS	 0.8100	 0.5700
BT	 0.7910	 0.5700
BU	 0.7720	 0.5530
BV	 0.7930	 0.5660
BW	 0.7570	 0.5470



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion	Q-score
BX	 0.7470	 0.5400
BY	 0.8150	 0.5830
BZ	 0.7850	 0.5660
Ba	 0.6760	 0.5070
Bb	 0.4720	 0.4420
Bc	 0.3020	 0.3210
Bd	 0.3530	 0.3110
Be	 0.8460	 0.5870
Bf	 0.5220	 0.4570
Bg	 0.4640	 0.3870
Bh	 0.7760	 0.5420
Bi	 0.7540	 0.5470
Bj	 0.0030	 0.0410
Bl	 0.8530	 0.5780
Bm	 0.7440	 0.5420
Bn	 0.6680	 0.4950
Bo	 0.5930	 0.4880
Bp	 0.2910	 0.3170
Bq	 0.6800	 0.5170
Br	 0.6560	 0.5020
Bs	 0.7970	 0.5730
Bt	 0.6830	 0.5290
Bu	 0.4640	 0.4540
Bv	 0.2030	 0.2770
Bw	 0.4040	 0.3890
Bx	 0.7410	 0.5500
By	 0.5190	 0.4880
Bz	 0.8530	 0.5910