



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 03:41 AM JST

PDB ID : 9XA7 / pdb_00009xa7
EMDB ID : EMD-66677
Title : Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 WT) from *Chaetomium thermophilum*, state A
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.20 Å (reported)
Based on initial model : 6RXU

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

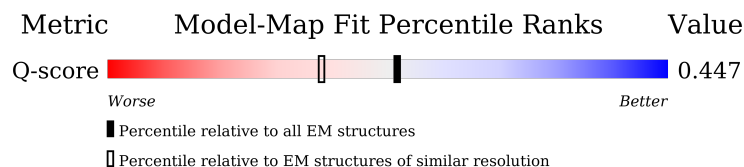
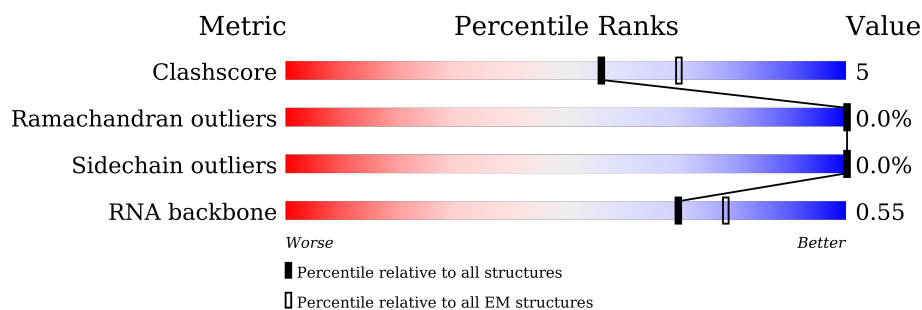
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



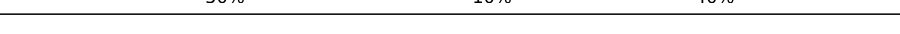
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	UA	904	
2	UB	907	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	177	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	

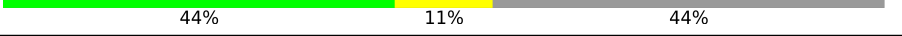
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	CK	297	
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cc	212	
36	Ce	203	
37	Cg	190	
38	Ch	151	
39	Ci	150	
40	Cj	143	
41	Cm	130	
42	Cn	145	
43	Co	136	
44	Cp	68	
45	CU	311	
46	C1	2311	
47	C2	274	
48	UH	930	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	UE	410	
49	UI	410	
50	US	549	
51	CI	156	
52	CX	480	
53	CY	381	
54	UP	364	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 179875 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UA	839	Total	C	N	O	P	S	
			6411	4118	1136	1132	1	24	
								0	0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	566	Total	C	N	O	S		
			4506	2845	858	790	13		
								0	0

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	79	Total	C	N	O		
			630	396	125	109		
							0	0

- Molecule 4 is a protein called UTP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	777	Total	C	N	O	S		
			6108	3872	1099	1113	24		
								0	0

- Molecule 5 is a protein called U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UF	331	Total	C	N	O	S		
			2599	1678	504	403	14		
								0	0

- Molecule 6 is a protein called U three protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UG	479	Total	C	N	O	S		
			3765	2391	700	662	12		
								0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	449	Total	C	N	O	S	0	0
			3412	2192	610	596	14		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1699	1068	351	275	5		

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	843	Total	C	N	O	S	0	0
			6545	4139	1151	1241	14		

- Molecule 11 is a protein called UTP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	177	Total	C	N	O	S	0	0
			1401	892	263	239	7		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	503	Total	C	N	O	S	0	0
			3811	2417	698	683	13		

- Molecule 13 is a protein called UTP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6012	3834	1038	1119	21		

- Molecule 14 is a protein called UTP18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	P	S	
			3498	2210	656	621	1	10	0
									0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	908	Total	C	N	O	S		
			6778	4361	1243	1148	26	0	0

- Molecule 16 is a protein called UTP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S		
			1480	938	286	246	10	0	0

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S		
			1815	1184	330	298	3	0	0

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CA	242	Total	C	N	O	S		
			1778	1149	327	293	9	0	0
18	CB	237	Total	C	N	O	S		
			1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CC	387	Total	C	N	O	S		
			2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CD	446	Total	C	N	O	S		
			3355	2150	594	600	11	0	0

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Ribosomal RNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	841	Total	C	N	O	S	0	0
			6666	4277	1246	1113	30		

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CM	445	Total	C	N	O	S	0	0
			3501	2195	672	619	15		

- Molecule 29 is a protein called Nucleolar essential protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CN	226	Total	C	N	O	S	0	0
			1762	1119	306	327	10		
29	CO	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CP	201	Total	C	N	O	S	0	0
			1625	1047	286	283	9		

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	180	Total	C	N	O	S	0	0
			1413	898	257	251	7		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	846	Total	C	N	O	S	0	0
			6677	4278	1137	1233	29		
32	CS	836	Total	C	N	O	S	0	0
			6591	4217	1118	1228	28		

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CT	131	Total	C	N	O	S	0	0
			1035	656	197	178	4		

- Molecule 34 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total	C	N	O	S	0	0
			1821	1160	341	315	5		

- Molecule 35 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cc	192	Total	C	N	O	S	0	0
			1464	926	278	253	7		

- Molecule 36 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ce	159	Total	C	N	O	S	0	0
			1279	810	237	232			

- Molecule 37 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Cg	159	Total	C	N	O	S	0	0
			1248	804	258	184	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ch	66	Total	C	N	O	S	0	0
			546	355	101	90			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cj	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 41 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Cm	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 42 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

- Molecule 43 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Co	92	Total	C	N	O	S	0	0
			741	474	139	126	2		

- Molecule 44 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Cp	61	Total	C	N	O	S	0	0
			458	286	97	74	1		

- Molecule 45 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 46 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C1	1189	Total	C	N	O	P	0	0
			25383	11319	4564	8311	1189		

- Molecule 47 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C2	229	Total	C	N	O	P	0	0
			4869	2172	851	1617	229		

- Molecule 48 is a protein called UTP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	UH	799	Total	C	N	O	S	0	0
			6198	3903	1105	1171	19		

- Molecule 49 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	UE	178	Total	C	N	O	S	0	0
			1362	851	251	254	6		
49	UI	128	Total	C	N	O	S	0	0
			996	622	187	181	6		

- Molecule 50 is a protein called CCAAT-binding factor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 51 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 52 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

- Molecule 53 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CY	123	Total	C	N	O	S	0	0
			979	592	195	189	3		

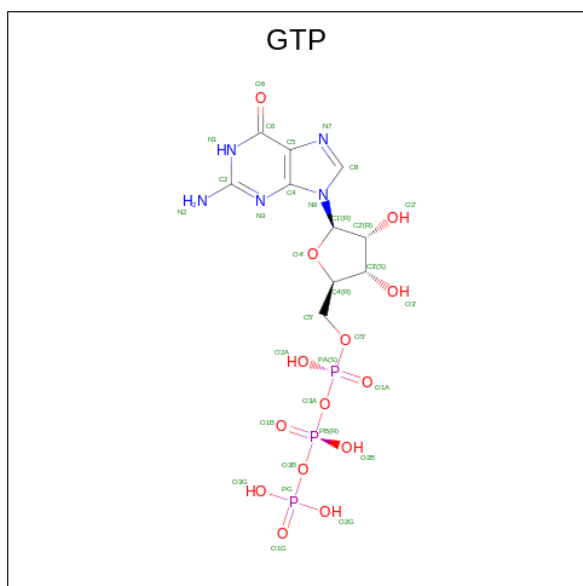
- Molecule 54 is a protein called UTP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UP	54	Total	C	N	O	0	0
			422	264	88	70		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	UX	1	Total	Zn	0
			1	1	

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

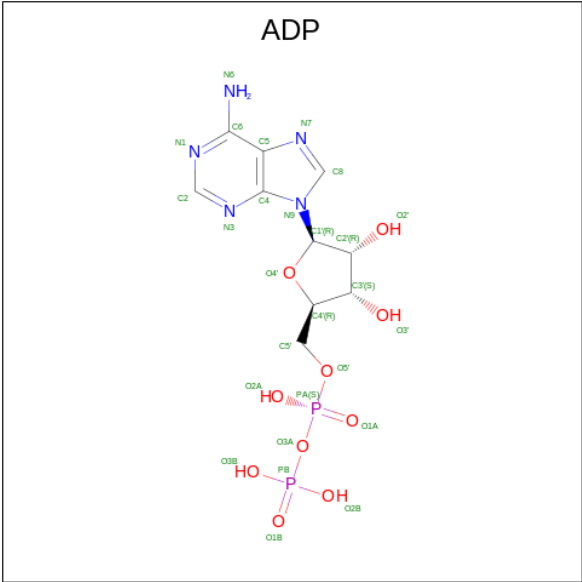


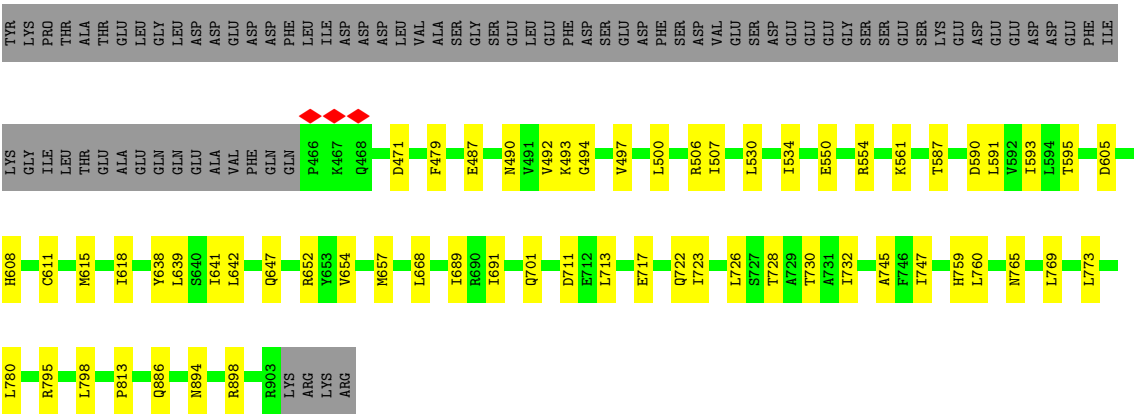
Mol	Chain	Residues	Atoms					AltConf
56	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	CI	1	Total	Mg	0
			1	1	

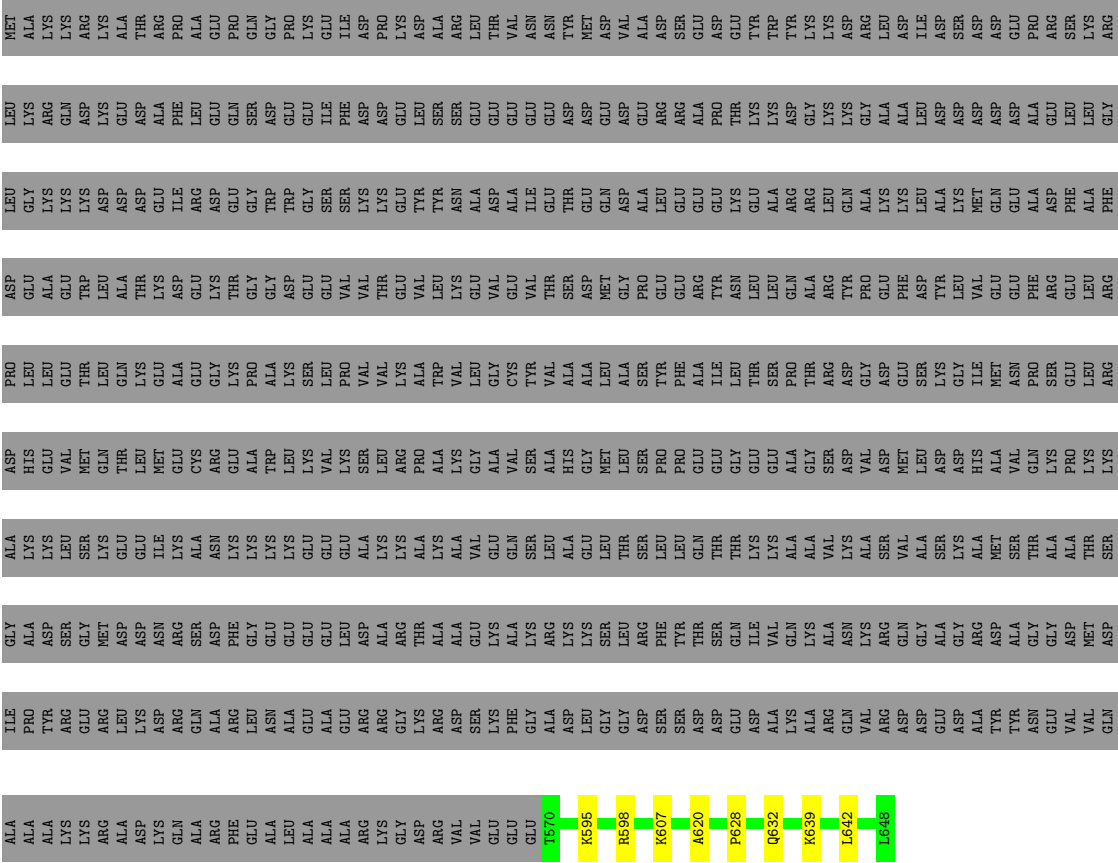
- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





• Molecule 3: Sas10 C-terminal domain-containing protein

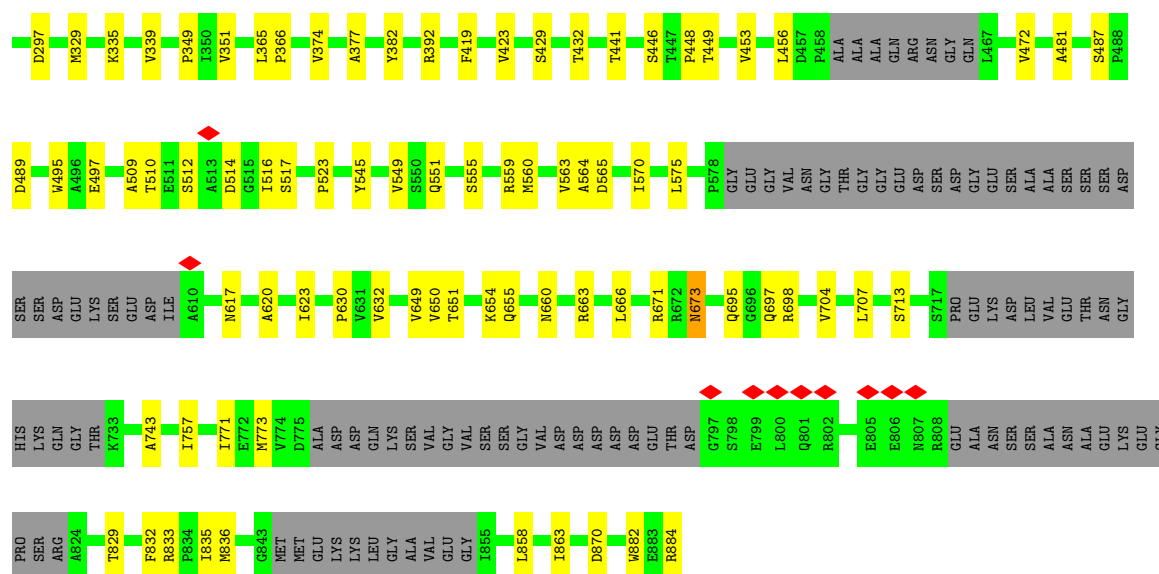
Chain UC: 11% 88%



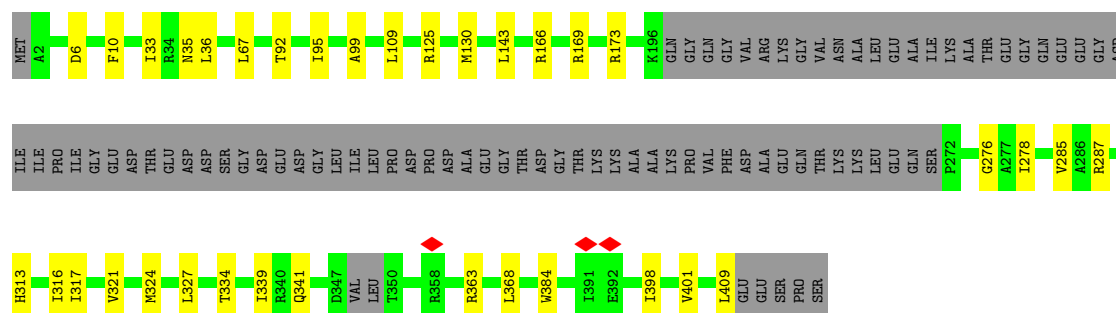
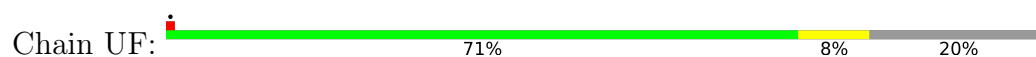
• Molecule 4: UTP4

Chain UD: 76% 12% 12%

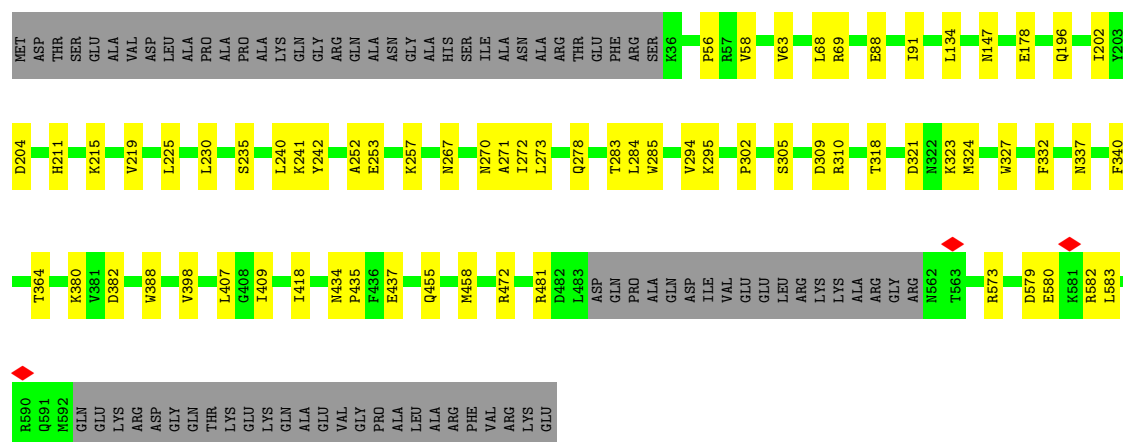
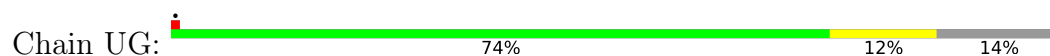




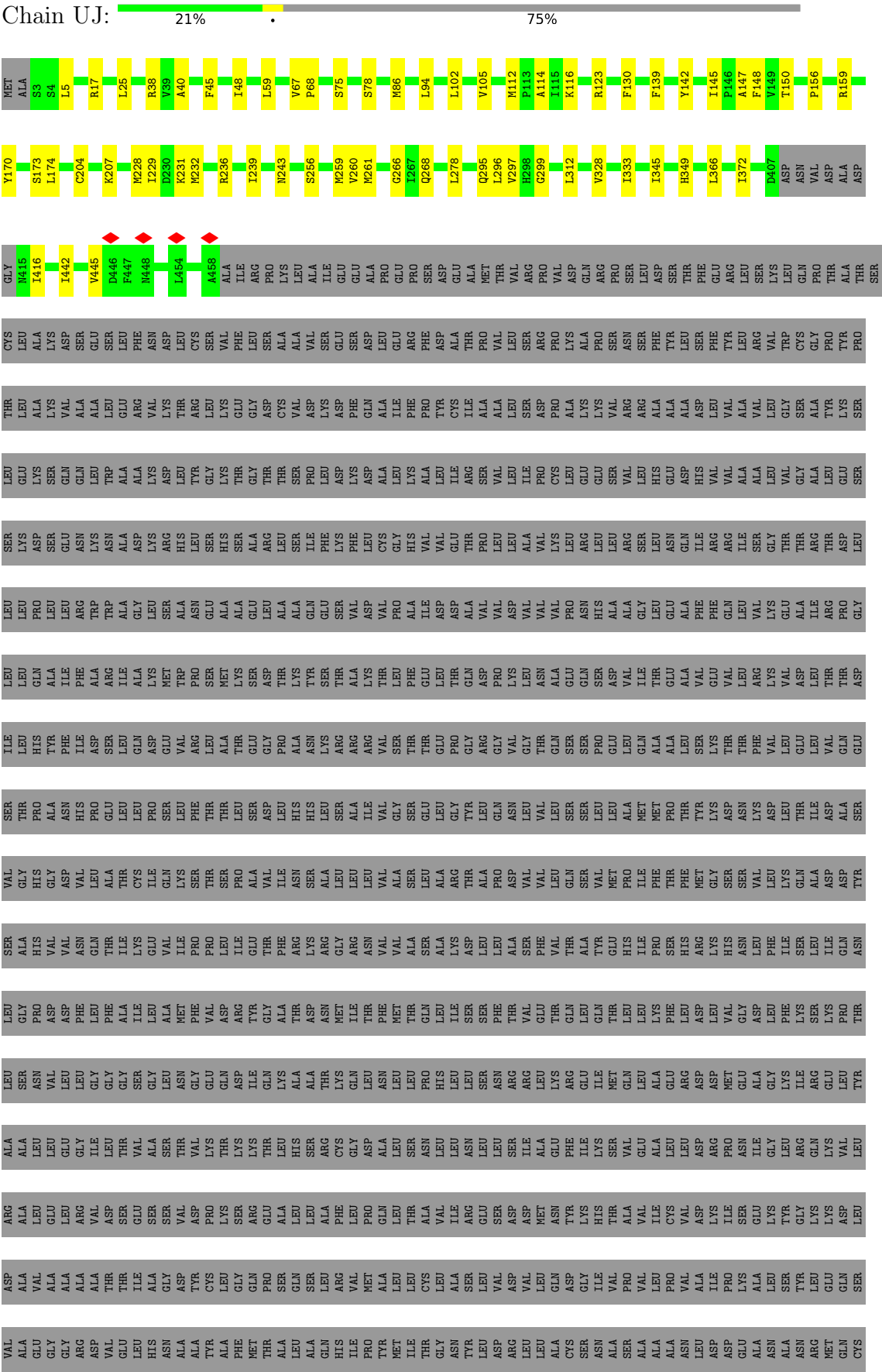
• Molecule 5: U3 snoRNP protein



• Molecule 6: U three protein 7



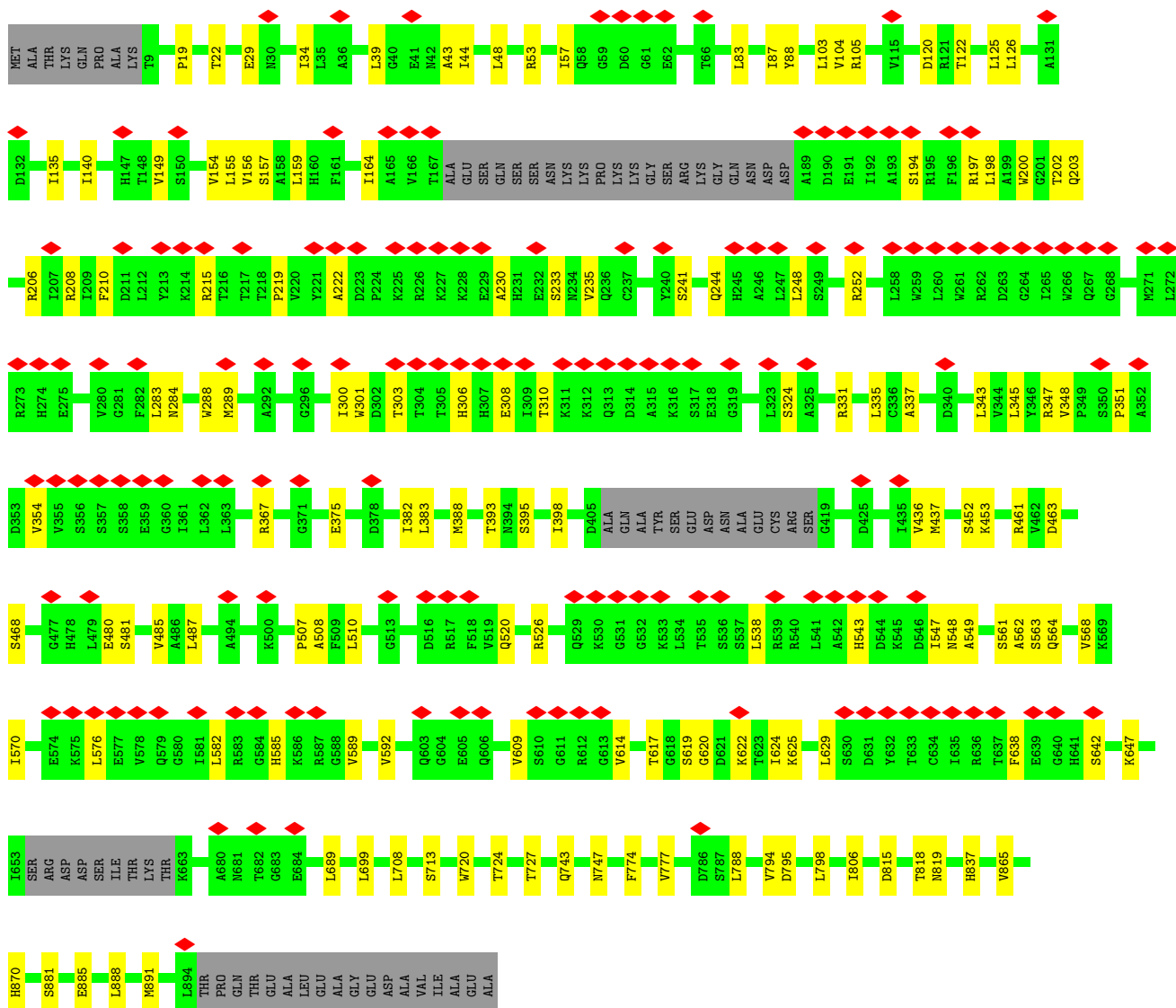
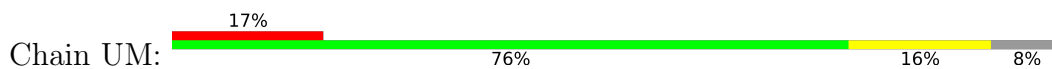
• Molecule 7: U3 small nucleolar RNA-associated protein 10



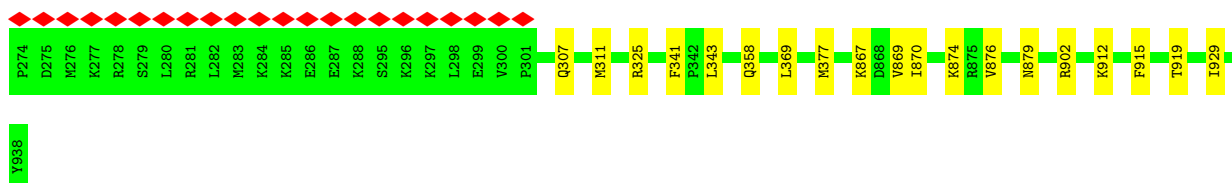
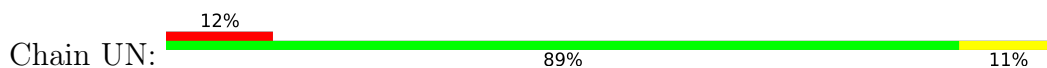


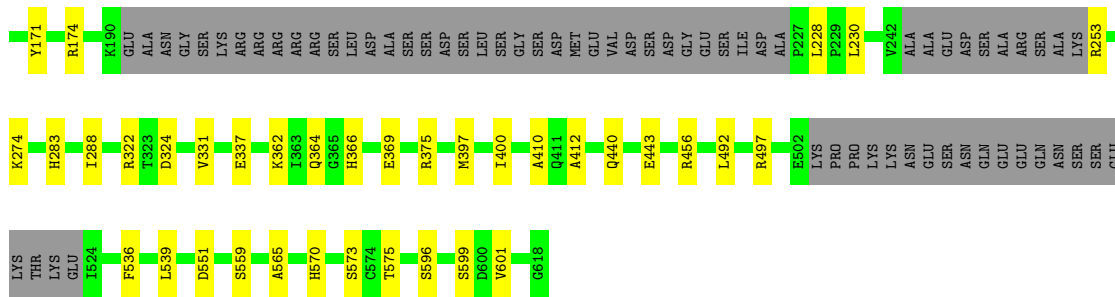


- Molecule 10: U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein



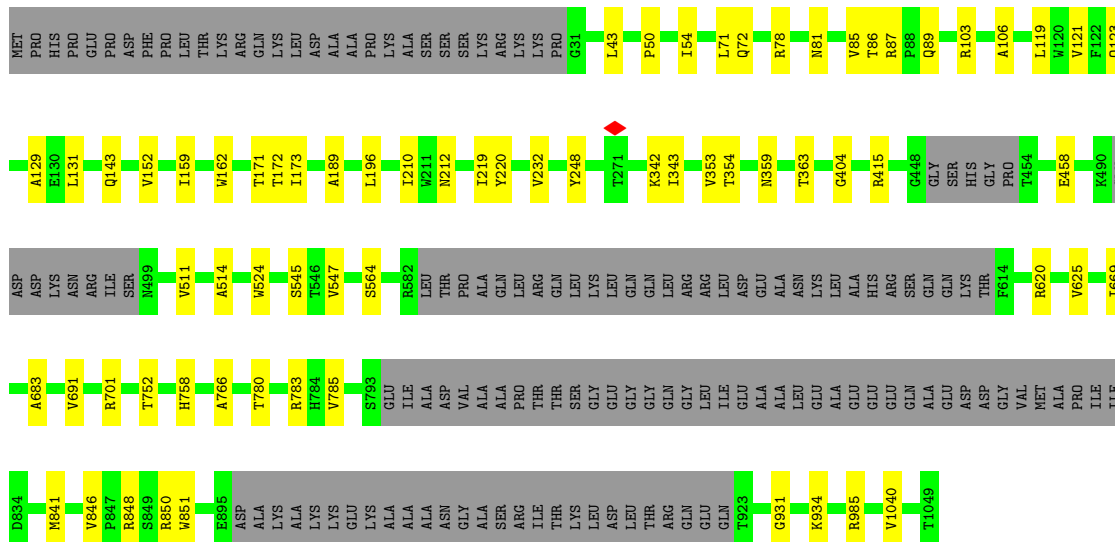
- Molecule 11: UTP14





• Molecule 15: Putative U3 snoRNP protein

Chain UU: 80% 7% 13%



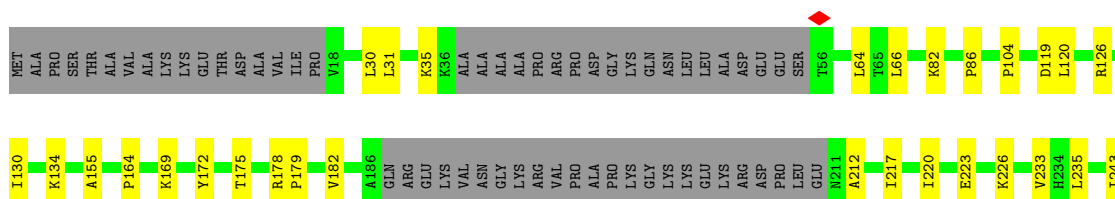
• Molecule 16: UTP24

Chain UX: 83% 16% .

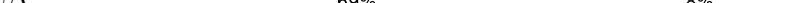


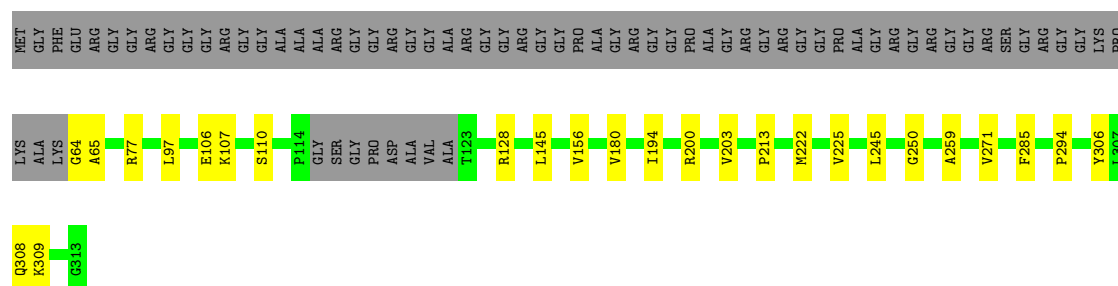
• Molecule 17: Ribosome biogenesis protein C8F11.04

Chain UZ: 50% 10% 40%

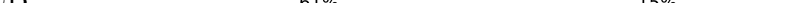


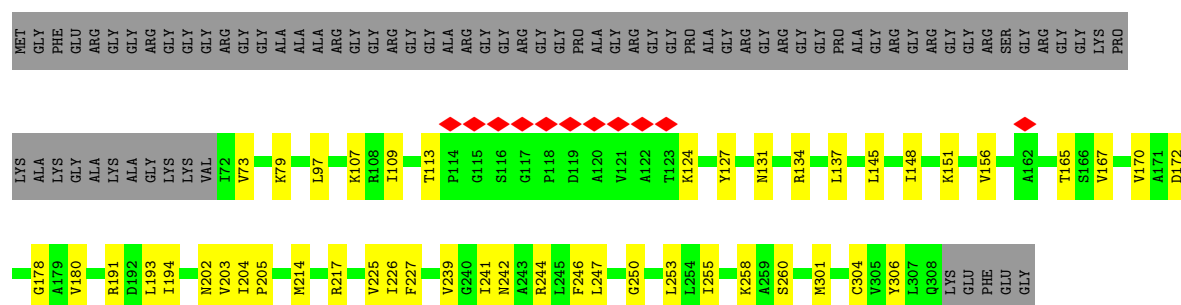
- Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CA: 

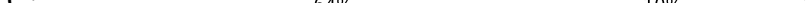


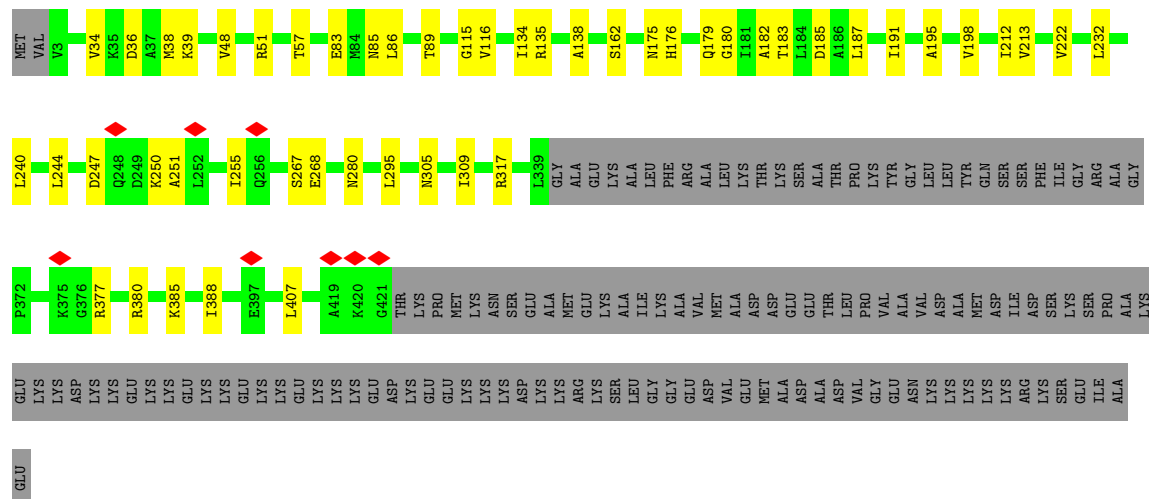
- Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CB: 

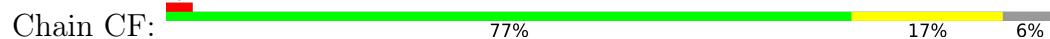
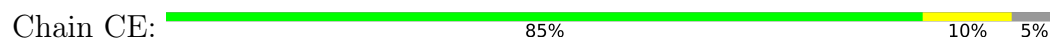


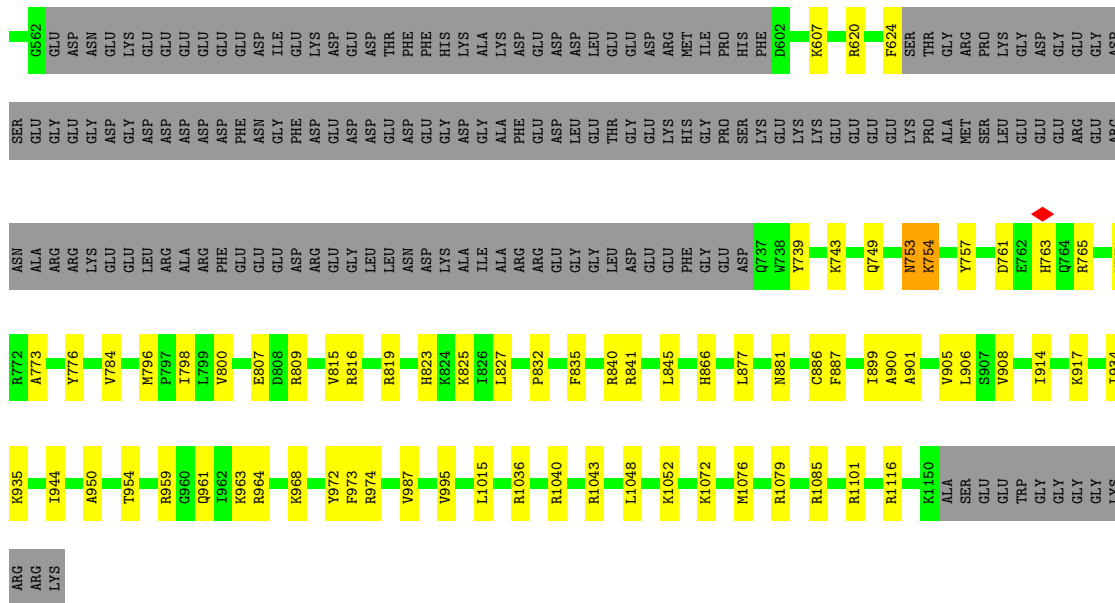
- Molecule 19: Nucleolar protein 56

Chain CC: 

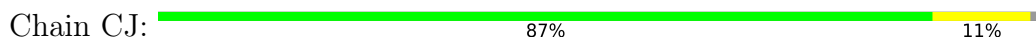


Chain CD:

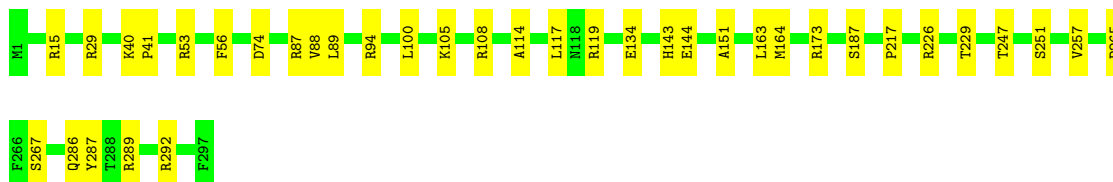




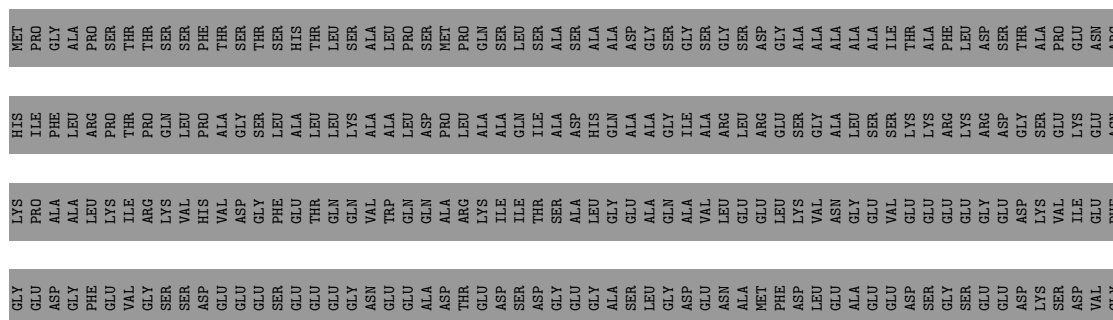
- Molecule 25: U3 small nucleolar ribonucleoprotein protein IMP3



- Molecule 26: U3 small nucleolar ribonucleoprotein protein IMP4

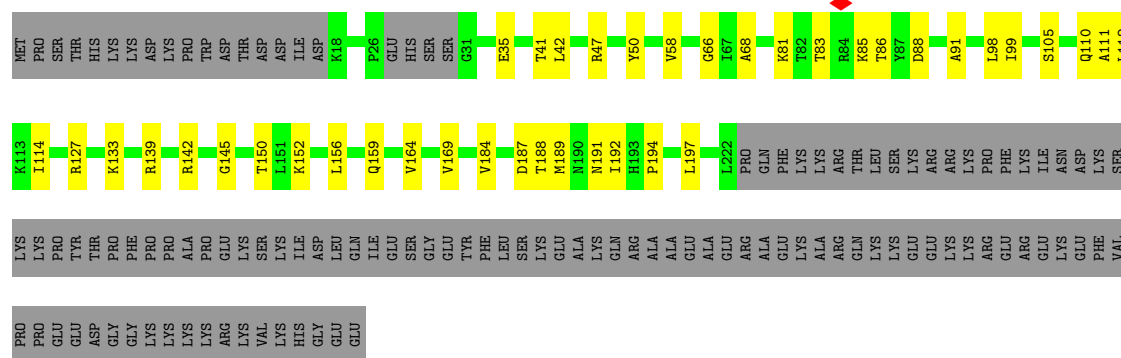


- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

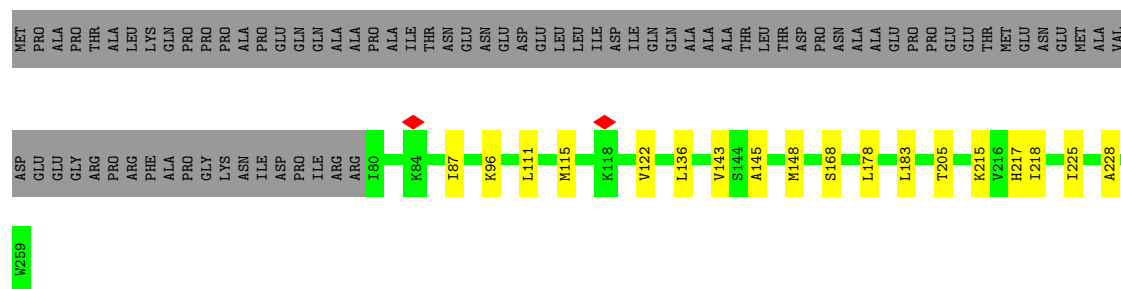




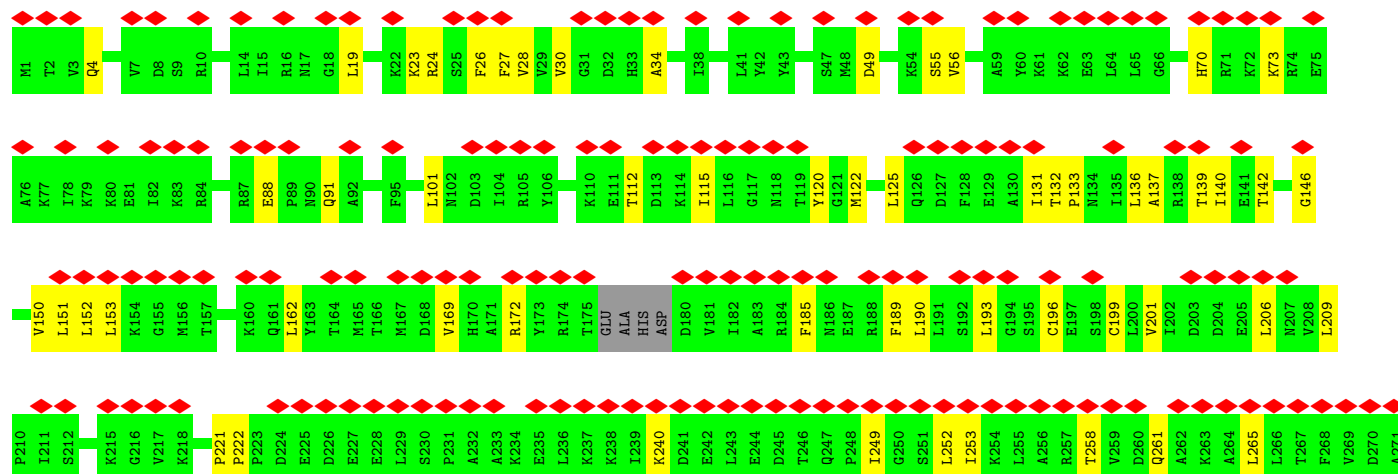
- Molecule 30: KRR1 small subunit processome component



- Molecule 31: Pre-rRNA-processing protein PNO1

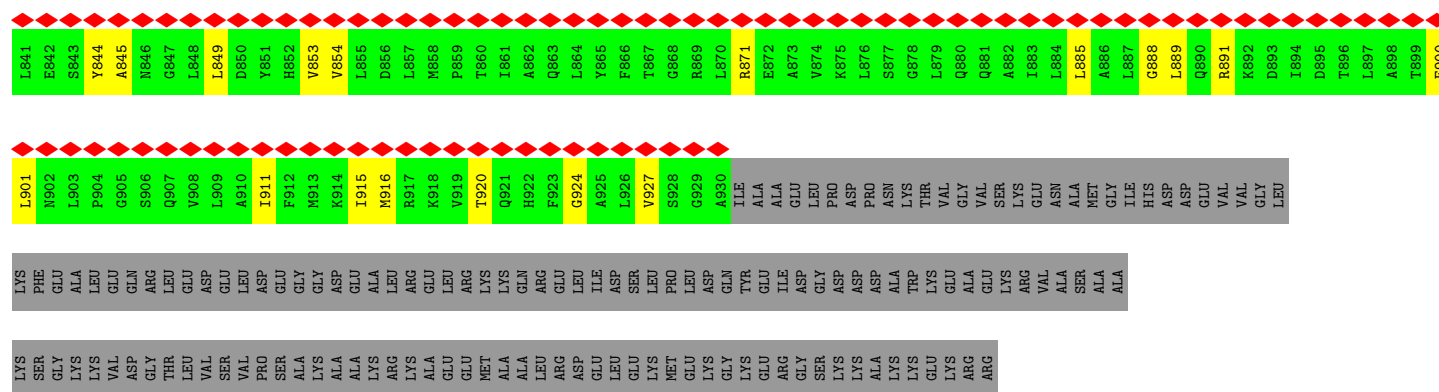


- Molecule 32: RNA cytidine acetyltransferase



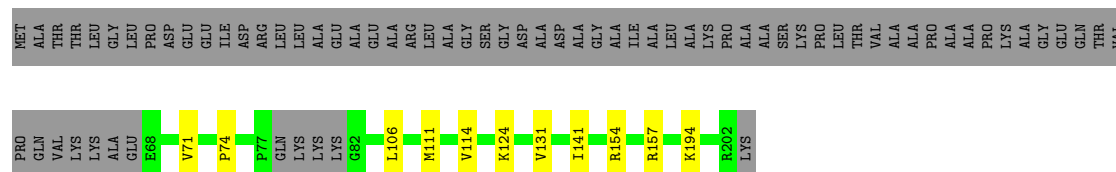


MET	THR	VAL	GLN	LYS	THR	VAL	D8	S9	R10	I11	P12	LYS	ARG	T13	L14	I15	R16	N17	G18	L19	Q20	T21	K22	K23	R24	S25	F26	F27	V28	V29	V30	G31	D32	H33	A34	K35	E36	A37	I38	V39	H40	L41	Y42	Y43	I44	M45	S46	S47	M48	D49	V50	H51	Q52	N53	K54	S55	V56	L57	M58	A59	Y60
K61	K62	GLU	LEU	LEU	GLY	PHE	THR	SER	HIS	ARG	LYS	LYS	ARG	GLU	ALA	LYS	LYS	LYS	GLU	ILE	LYS	ARG	GLY	ARG	GLU	PRO	ASN	GLN	A92	D93	F94	F95	E96	L97	F98	I99	S100	L101	N102	D103	I104	R105	L106	C107	Y108	Y109	K110	E111	T112	D113	K114	I115	L116	G117	N118	T119	Y120				
G121	M122	C123	I124	L125	Q126	D127	F128	E129	A130	I131	T132	P133	N134	I135	L136	A137	R138	T139	I140	E141	T142	V143	E144	G145	G146	G147	L148	V149	V150	L151	L152	L153	K154	G155	M156	T157	S158	L159	K160	Q161	L162	Y163	T164	M165	T166	M167	D168	V169	H170	A171	R172	Y173	R174	T175	E176	A177	H178	D179			
V181	I182	A183	R184	F185	M186	E187	R188	F189	L190	L191	S192	G193	G194	S195	C196	E197	S198	C199	L200	V201	I202	D203	D204	E205	L206	N207	V208	L209	P210	I211	S212	G213	G214	K215	G216	V217	K218	P219	L220	P221	P222	P223	D224	E225	D226	E227	E228	L229	S230	P231	A232	A233	K234	E235	L236	K237	K238	I239	K240		
D241	E242	L243	E244	D245	T246	Q247	P248	T249	G250	S251	L252	L253	K254	L255	A256	R257	T258	V259	D260	Q261	A262	K263	A264	L265	L266	T267	F268	V269	D270	A271	L272	A273	E274	K275	T276	L277	R278	N279	T280	V281	T282	L283	T284	A285	A286	R287	G288	K289	L290	K291	S292	A293	A294	M295	G296	V297	A298	I299	A300		
A301	A302	V303	A304	Y305	G306	Y307	S308	N309	I310	F311	I312	T313	S314	P315	S316	P317	E318	N319	L320	K321	T322	L323	F324	E325	F326	V327	F328	K329	G330	F331	D332	A333	L334	D335	Y336	K337	D338	H339	A340	D341	Y342	T343	G344	I345	Q346	S347	T348	N349	P350	E351	F352	N353	K354	A355	I356	V357	R358	V359	N360		
I361	H362	R363	N364	H365	K366	Q367	T368	I369	Q370	Y371	I372	R373	P374	Q375	D376	A377	H378	V379	L380	G381	Q382	A383	E384	L385	V386	V387	I388	D389	E390	A391	A392	A393	I394	P395	L396	P397	L398	V399	K400	R401	L402	M403	G404	P405	Y406	L407	V408	F409	M410	A411	S412	T413	I414	S415	G416	Y417	G418	G419	T420		
G421	R422	S423	L424	S425	L426	K427	L428	L429	K430	Q431	L432	R433	E434	Q435	S436	R437	ALA	GLY	ALA	ASN	PRO	ASN	GLY	GLY	ALA	VAL	GLU	VAL	ASP	ARG	SER	THR	LYS	ALA	LYS	LYS	GLU	THR	SER	VAL	GLY	R467	S468	L469	K470	E471	I472	L473	L474	S475	E476	P477	I478	R479	Y480						
A481	Q482	G483	D484	N485	V486	E487	K488	W489	A490	M491	T492	L493	L494	C495	L496	D497	ALA	THR	LEU	PRO	ARG	SER	LYS	ILE	SER	THR	G509	C510	P511	D512	P513	S514	C515	E517	L518	H520	V521	N522	R523	D524	T525	L526	F527	S528	F529	H530	P531	V532	S533	E534	K535	F536	L537	Q538	Q539	M540					
V541	A542	L543	Y544	V545	A546	S547	H548	Y549	K550	M551	S552	P553	N554	D555	L556	Q557	L558	M559	S560	D561	A562	P563	A564	H565	E566	L567	F568	V569	L570	T571	G572	P573	I574	Q575	E576	G577	R578	L579	P580	E581	P582	L583	C584	V585	I586	Q587	V588	Y589	P590	S591	G592	K593	I594	S595	K596	Q597	I599	L600			
K601	S602	L603	S604	R605	G606	Q607	Q608	P609	A610	G611	D612	L613	I614	P615	W616	L617	V618	S619	Q620	Q621	Q622	Q623	D624	D625	E626	F627	A628	S629	L630	S631	G632	A633	R634	I635	V636	R637	I638	A639	T640	N641	P642	D643	Y644	M645	S646	M647	G648	Y649	D650	S651	K652	A653	L654	Q655	L656	L657	D658	D659	Y660		
Y661	E662	G663	K664	F665	A666	ASP	LEU	SER	GLU	ASP	ALA	ALA	VAL	GLU	PRO	ARG	SER	ILE	PRO	THR	D685	A686	E687	L688	S689	K690	G691	S692	L693	F694	D695	D696	I697	K698	V699	R700	D701	M702	H703	E704	L705	P706	P707	L708	F709	S710	K711	L712	S713	E714	R715	R716	F717	E718	K719	L720					
D721	Y722	V723	G724	W725	S726	Y727	G728	L729	T730	Q731	Q732	L733	H734	K735	F736	W737	PRO	ARG	VAL	THR	D685	A686	E687	L688	S689	K690	G691	S692	L693	F694	D695	D696	I697	K698	V699	R700	D701	M702	H703	E704	L705	P706	P707	L708	F709	S710	K711	L712	S713	E714	R715	R716	F717	E718	K719	L720					
D781	F782	H783	K784	R785	F786	L787	G788	L789	L790	S791	Y792	K793	F794	R795	E796	F797	P798	S799	I800	L801	A802	L803	T804	I805	E806	E807	S808	A809	N810	A811	G812	N813	D814	L815	D816	P817	S818	N819	A820	P821	T822	E823	L824	T825	K826	A827	E828	L829	D830	Q831	L832	F833	T834	P835	F836	D837	H838	K839	R840		



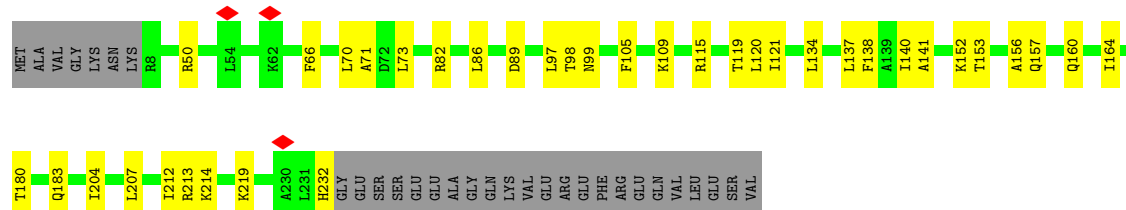
• Molecule 33: Fcf2 pre-rRNA processing C-terminal domain-containing protein

Chain CT: 59% 5% 35%



• Molecule 34: Small ribosomal subunit protein eS1

Chain Ca: 74% 15% 12%



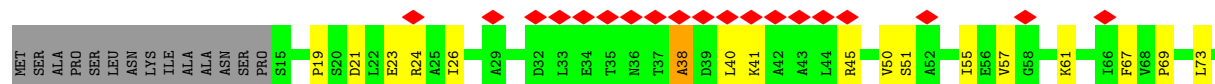
• Molecule 35: 40S ribosomal protein s5-like protein

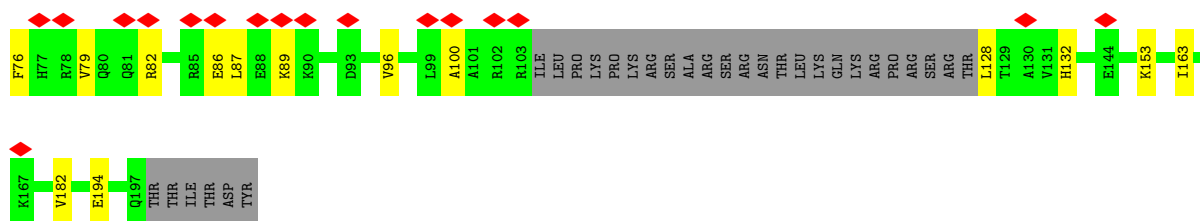
Chain Cc: 84% 6% 9%



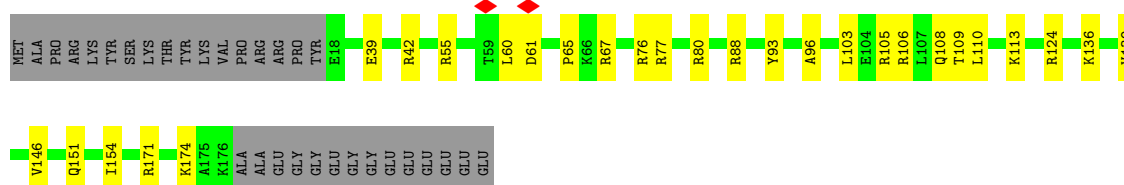
• Molecule 36: 40S ribosomal protein S7

Chain Ce: 18% 63% 15% 22%

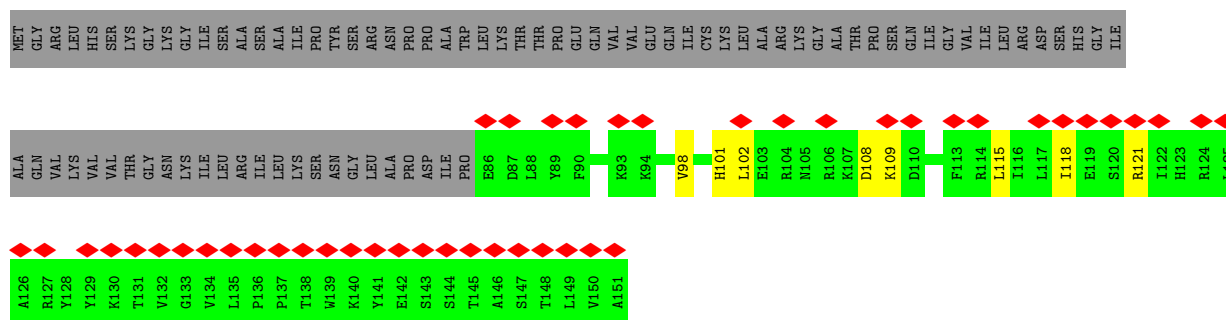
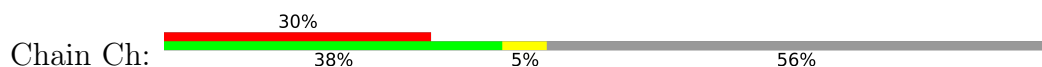




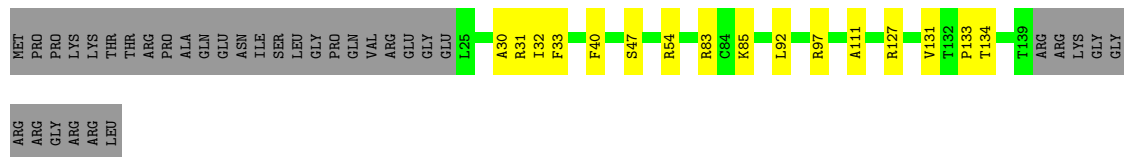
- Molecule 37: 40S ribosomal protein s9-like protein



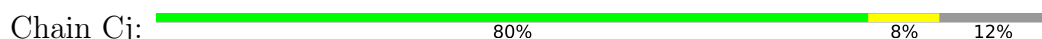
- Molecule 38: 40S ribosomal protein S13-like protein



- Molecule 39: 40S ribosomal protein S14-like protein

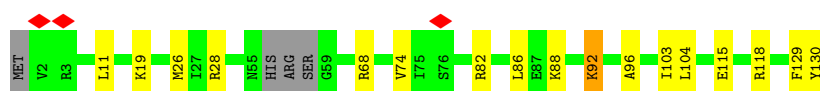


- Molecule 40: 40S ribosomal protein S16-like protein



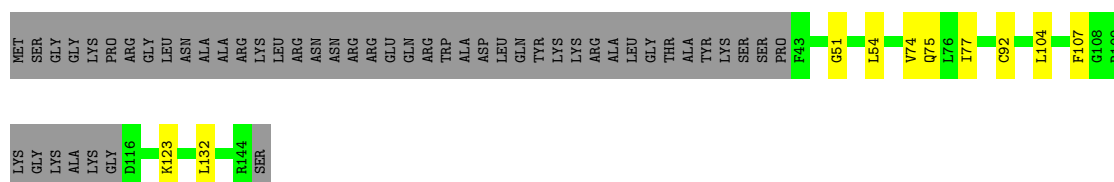
- Molecule 41: 40S ribosomal protein S22-like protein

Chain Cm:  84% 12%



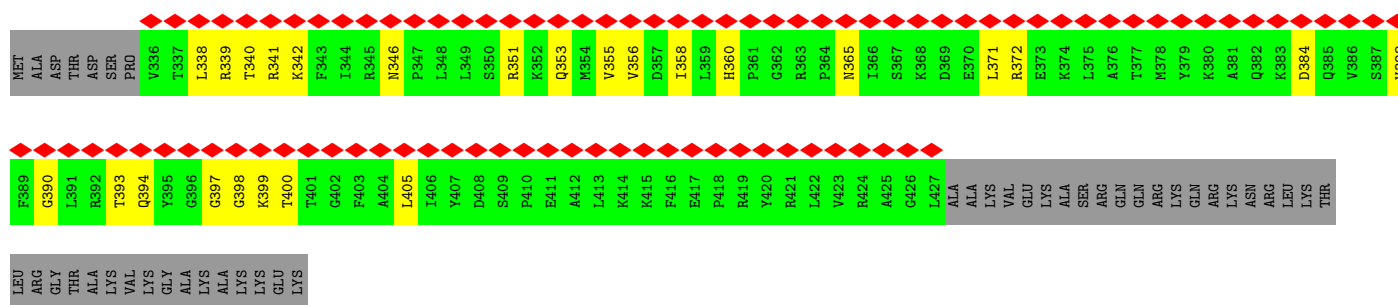
- Molecule 42: 40S ribosomal protein s23-like protein

Chain Cn:  59% 7% 34%



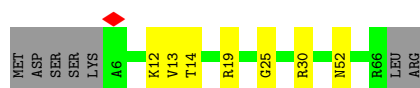
- Molecule 43: Small ribosomal subunit protein eS24

Chain Co:  49% 18% 32%



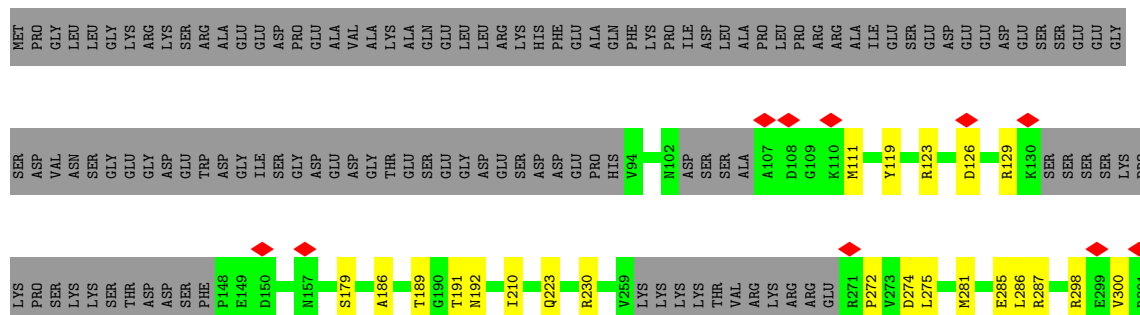
- Molecule 44: 40S ribosomal protein S28-like protein

Chain Cp:  79% 10% 10%



- Molecule 45: Faf1

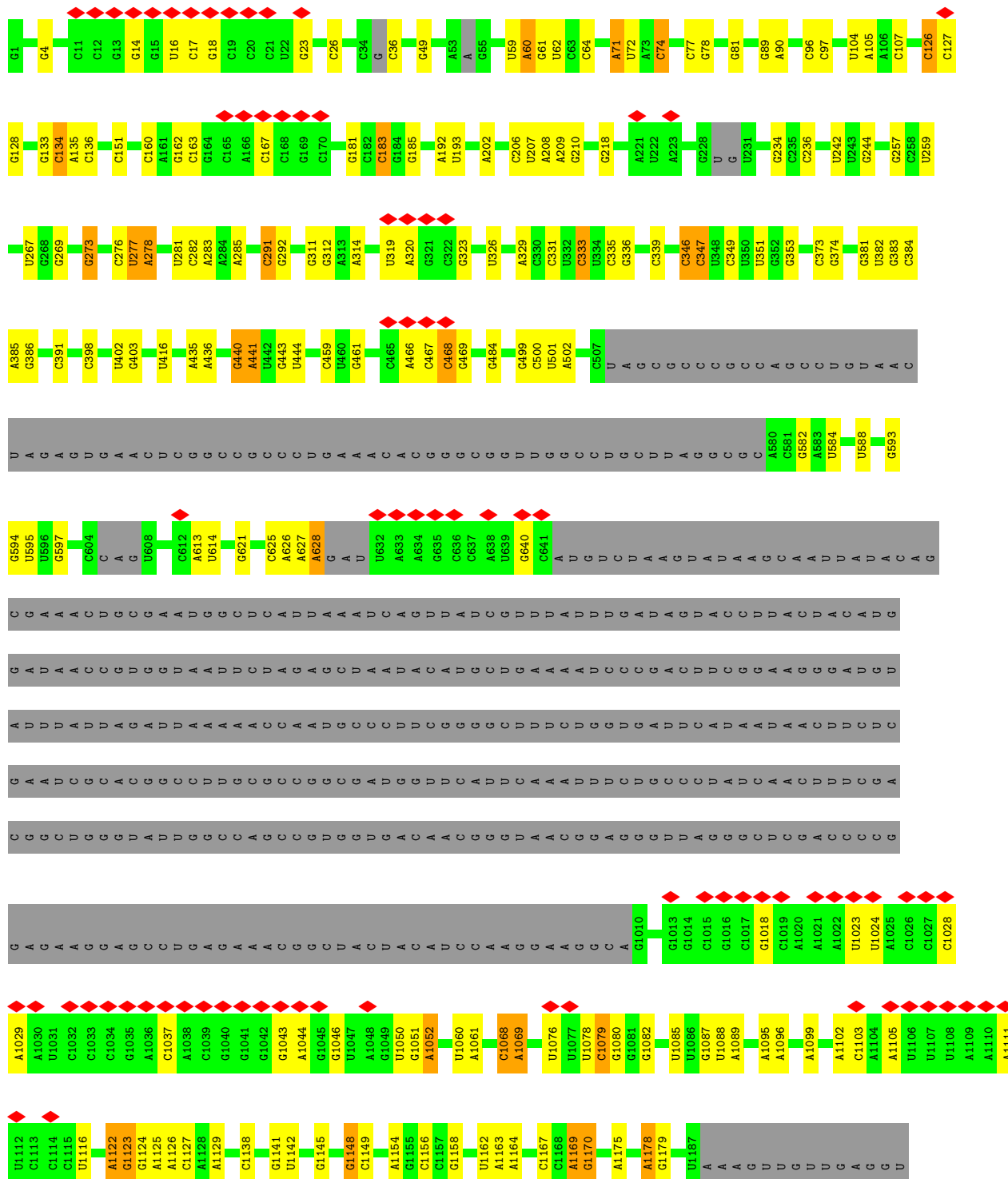
Chain CU:  50% 7% 43%

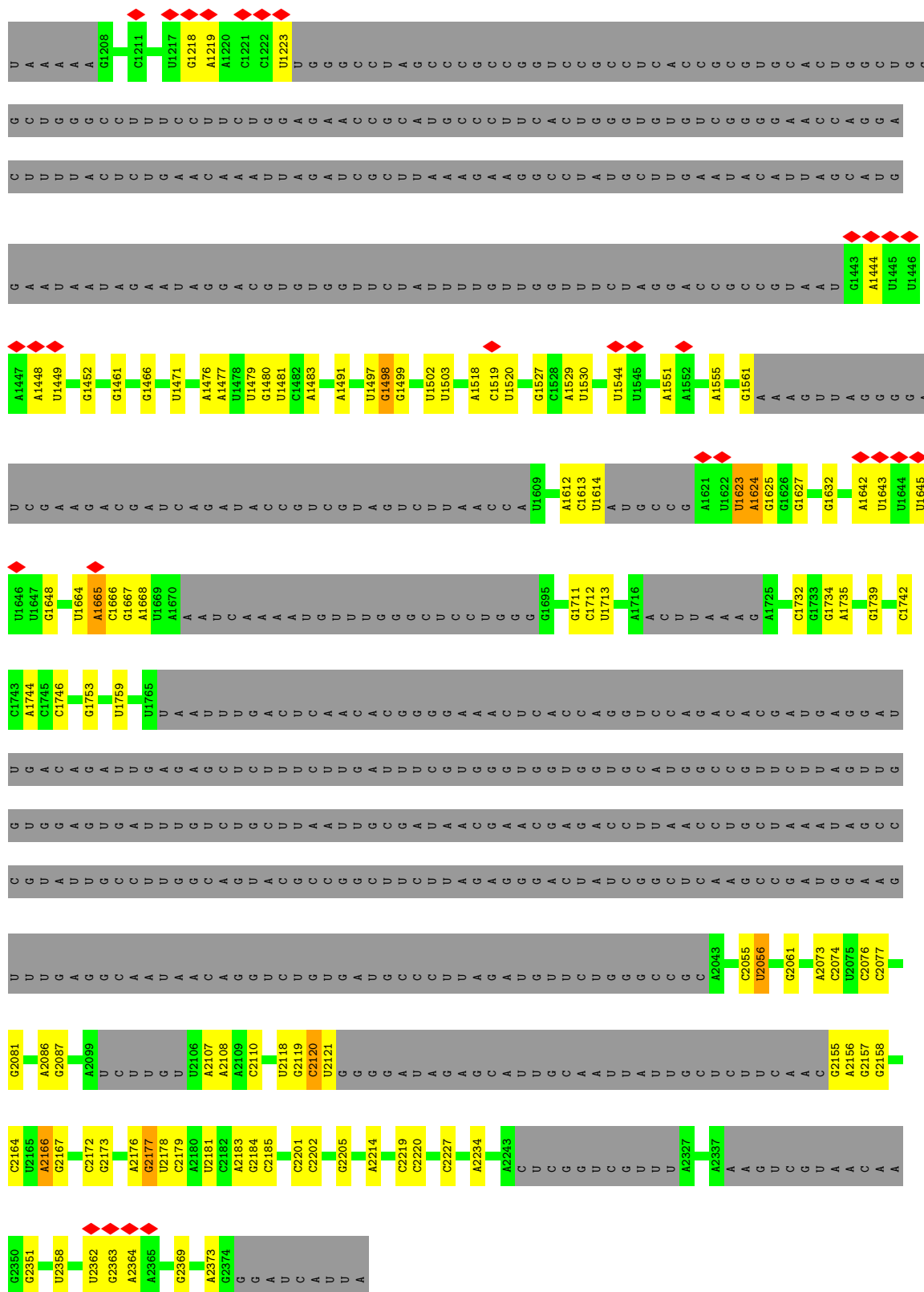


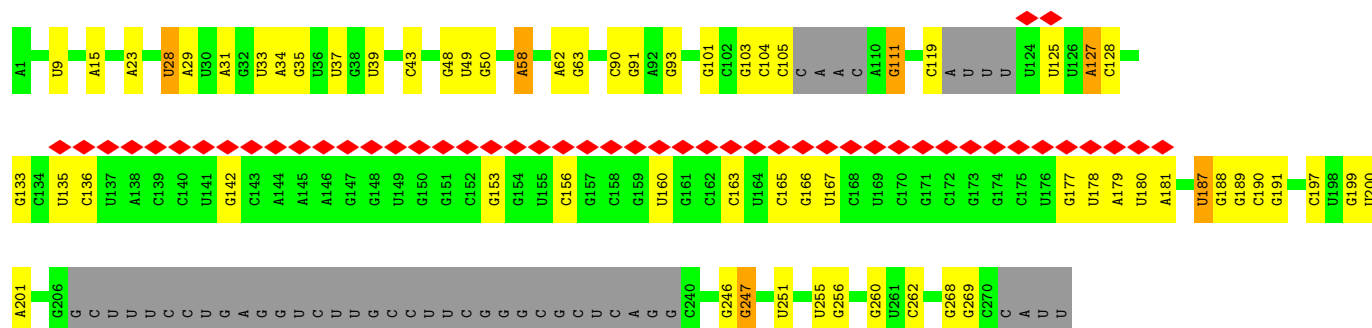
GLY
PRO
GLN
GLY
ARG
GLY
LVS
ARG
ARG
ARG

● Molecule 46: 35S rRNA

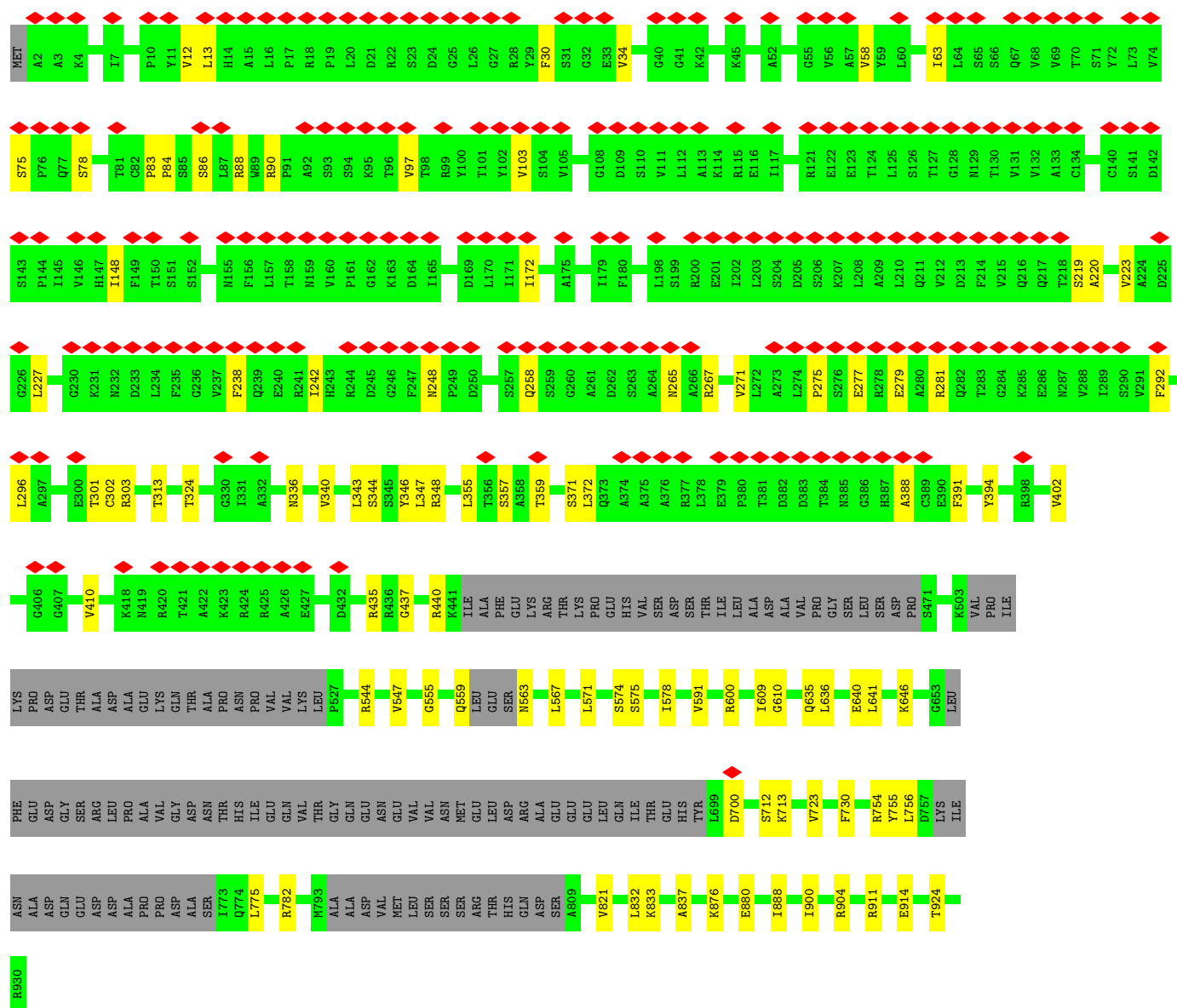
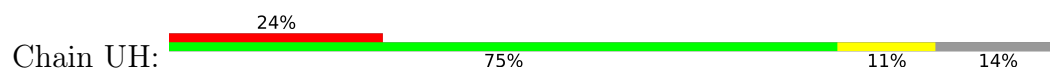
Chain C1: 5% 38% 11% 49%



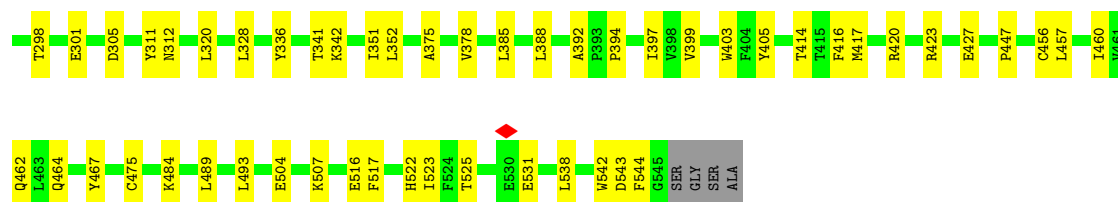




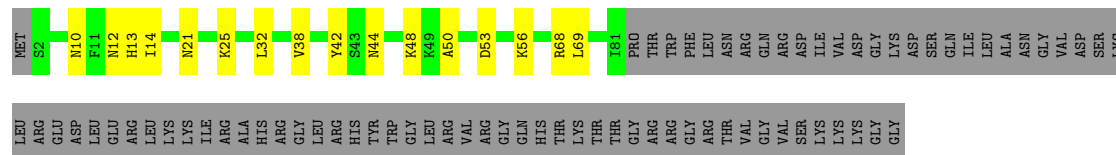
• Molecule 48: UTP8



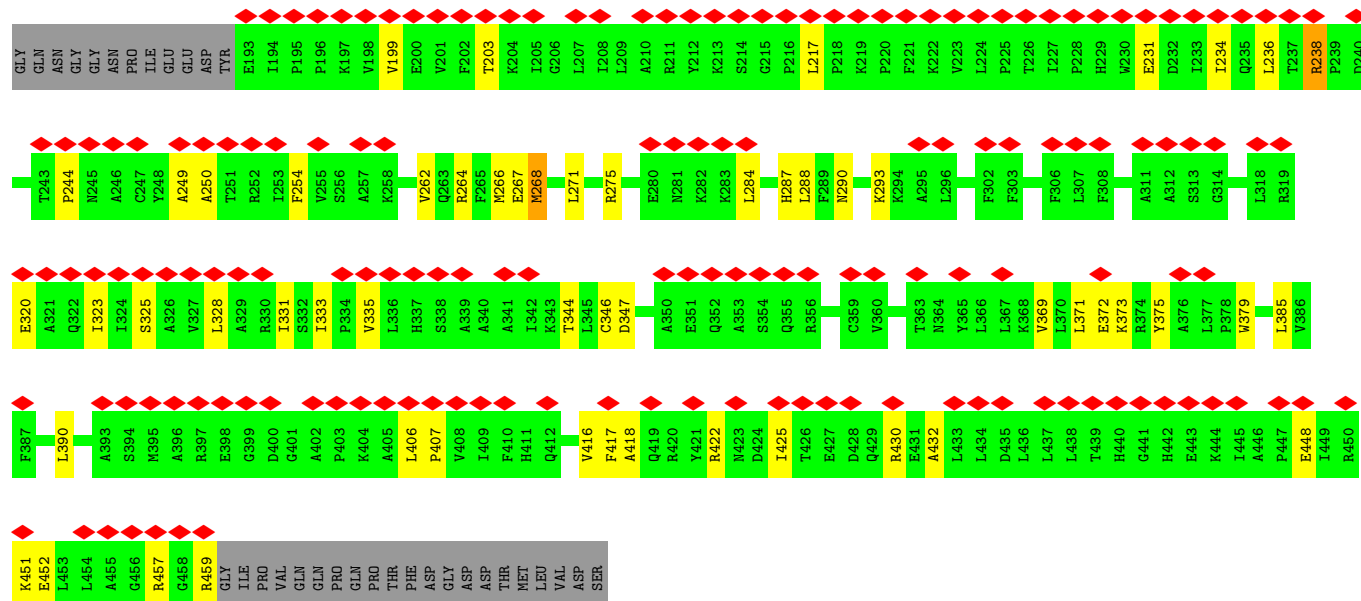
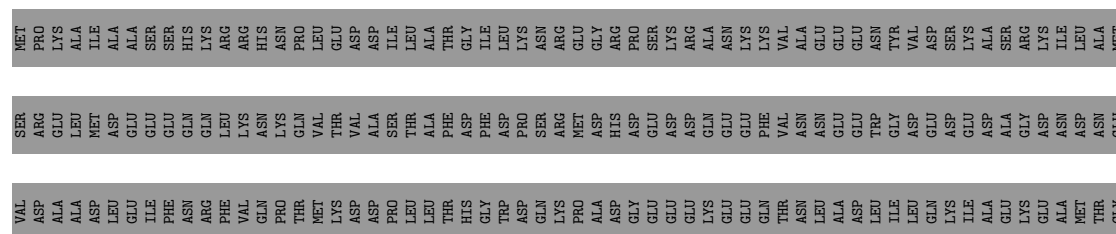
• Molecule 49: Small-subunit processome Utp12 domain-containing protein



• Molecule 51: Putative ribosomal protein



• Molecule 52: Bystin-like protein



• Molecule 53: U3 small nucleolar ribonucleoprotein protein lcp5-like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.579	Depositor
Minimum map value	-0.290	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	550.08, 550.08, 550.08	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, GTP, SEP, MG, 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	UA	0.16	0/6555	0.46	0/8909
2	UB	0.20	0/4592	0.49	0/6178
3	UC	0.16	0/638	0.46	0/845
4	UD	0.16	0/6250	0.44	0/8465
5	UF	0.19	0/2665	0.45	0/3606
6	UG	0.17	0/3838	0.44	0/5181
7	UJ	0.19	0/3471	0.46	0/4709
8	UK	0.16	0/1713	0.40	0/2266
9	UL	0.19	0/6299	0.50	0/8531
10	UM	0.18	0/6680	0.49	0/9090
11	UN	0.17	0/1425	0.40	0/1913
12	UO	0.18	0/3895	0.45	0/5302
13	UQ	0.15	0/6140	0.43	0/8352
14	UR	0.16	0/3560	0.43	0/4809
15	UU	0.17	0/6947	0.46	2/9452 (0.0%)
16	UX	0.16	0/1503	0.41	0/2022
17	UZ	0.19	0/1857	0.50	0/2526
18	CA	0.17	0/1814	0.42	0/2456
18	CB	0.20	0/1853	0.52	0/2511
19	CC	0.21	0/2911	0.49	0/3937
20	CD	0.19	0/3412	0.48	0/4617
21	CE	0.20	0/891	0.48	0/1214
21	CF	0.23	0/876	0.59	2/1195 (0.2%)
22	CG	0.17	0/3307	0.48	0/4462
23	CH	0.18	0/2939	0.48	0/3988
24	CI	0.18	0/6813	0.49	3/9182 (0.0%)
25	CJ	0.17	0/1462	0.42	0/1967
26	CK	0.16	0/2376	0.42	0/3214
27	CL	0.17	0/1812	0.43	0/2437
28	CM	0.17	0/3573	0.46	0/4829
29	CN	0.18	0/1797	0.48	0/2443
29	CO	0.21	0/1714	0.52	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.18	0/1655	0.47	0/2229
31	CQ	0.23	0/1436	0.51	0/1932
32	CR	0.21	0/6809	0.57	1/9215 (0.0%)
32	CS	0.21	0/6722	0.56	2/9099 (0.0%)
33	CT	0.14	0/1053	0.39	0/1413
34	Ca	0.20	0/1850	0.47	0/2486
35	Cc	0.16	0/1485	0.42	0/2008
36	Ce	0.22	0/1298	0.60	2/1750 (0.1%)
37	Cg	0.19	0/1265	0.49	0/1694
38	Ch	0.20	0/557	0.54	0/749
39	Ci	0.16	0/819	0.42	0/1107
40	Cj	0.19	0/958	0.43	0/1293
41	Cm	0.20	0/1001	0.56	1/1345 (0.1%)
42	Cn	0.14	0/712	0.41	0/954
43	Co	0.19	0/754	0.52	0/1011
44	Cp	0.17	0/461	0.42	0/620
45	CU	0.13	0/1350	0.35	0/1810
46	C1	0.09	0/28360	0.21	0/44174
47	C2	0.10	0/5434	0.21	0/8459
48	UH	0.17	0/6301	0.45	0/8526
49	UE	0.20	0/1374	0.46	0/1852
49	UI	0.23	0/1005	0.57	0/1352
50	US	0.21	0/3765	0.55	2/5100 (0.0%)
51	Cl	0.21	0/638	0.59	0/857
52	CX	0.24	0/2180	0.63	1/2956 (0.0%)
53	CY	0.23	0/986	0.59	1/1303 (0.1%)
54	UP	0.17	0/428	0.44	0/570
All	All	0.17	0/186234	0.44	17/258797 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	2
36	Ce	0	1
52	CX	0	1
All	All	0	4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	CF	67	HIS	CA-C-N	6.98	124.64	120.24
21	CF	67	HIS	C-N-CA	6.98	124.64	120.24
36	Ce	38	ALA	CA-C-N	6.81	133.96	121.70
36	Ce	38	ALA	C-N-CA	6.81	133.96	121.70
32	CS	798	PRO	N-CD-CG	-6.44	93.55	103.20
41	Cm	92	LYS	CA-CB-CG	6.26	126.62	114.10
53	CY	271	GLU	N-CA-CB	6.00	118.94	110.12
32	CS	798	PRO	CA-N-CD	-5.61	104.15	112.00
15	UU	171	THR	CA-C-N	5.58	129.88	121.40
15	UU	171	THR	C-N-CA	5.58	129.88	121.40
32	CR	807	GLU	N-CA-CB	5.53	119.41	110.40
24	CI	753	ASN	CA-C-N	5.34	131.74	121.54
24	CI	753	ASN	C-N-CA	5.34	131.74	121.54
50	US	245	ILE	CA-C-N	5.28	131.62	121.54
50	US	245	ILE	C-N-CA	5.28	131.62	121.54
24	CI	754	LYS	CA-CB-CG	5.17	124.43	114.10
52	CX	238	ARG	CA-CB-CG	5.14	124.39	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	CX	268	MET	Peptide
36	Ce	38	ALA	Peptide
1	UA	645	ALA	Mainchain
1	UA	646	SEP	Mainchain

5.2 Too-close contacts [i](#)

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	UA	6411	0	6305	54	0
2	UB	4506	0	4633	48	0
3	UC	630	0	687	9	0
4	UD	6108	0	6108	68	0
5	UF	2599	0	2650	23	0
6	UG	3765	0	3800	45	0
7	UJ	3412	0	3519	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	UK	1699	0	1832	15	0
9	UL	6175	0	6188	85	0
10	UM	6545	0	6547	95	0
11	UN	1401	0	1455	17	0
12	UO	3811	0	3861	34	0
13	UQ	6012	0	6044	75	0
14	UR	3498	0	3508	29	0
15	UU	6778	0	6782	40	0
16	UX	1480	0	1554	23	0
17	UZ	1815	0	1896	23	0
18	CA	1778	0	1830	19	0
18	CB	1816	0	1847	26	0
19	CC	2866	0	2960	36	0
20	CD	3355	0	3483	43	0
21	CE	879	0	918	7	0
21	CF	864	0	900	16	0
22	CG	3245	0	3262	41	0
23	CH	2888	0	2979	37	0
24	CI	6666	0	6826	98	0
25	CJ	1434	0	1482	15	0
26	CK	2329	0	2373	27	0
27	CL	1786	0	1826	17	0
28	CM	3501	0	3498	30	0
29	CN	1762	0	1807	18	0
29	CO	1683	0	1726	24	0
30	CP	1625	0	1718	25	0
31	CQ	1413	0	1479	11	0
32	CR	6677	0	6809	98	0
32	CS	6591	0	6674	122	0
33	CT	1035	0	1063	10	0
34	Ca	1821	0	1936	26	0
35	Cc	1464	0	1504	8	0
36	Ce	1279	0	1322	19	0
37	Cg	1248	0	1365	20	0
38	Ch	546	0	580	6	0
39	Ci	808	0	831	13	0
40	Cj	943	0	1002	10	0
41	Cm	985	0	1021	12	0
42	Cn	702	0	750	5	0
43	Co	741	0	785	18	0
44	Cp	458	0	489	7	0
45	CU	1337	0	1376	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	C1	25383	0	12859	93	0
47	C2	4869	0	2465	18	0
48	UH	6198	0	6272	66	0
49	UE	1362	0	1440	22	0
49	UI	996	0	1054	18	0
50	US	3672	0	3679	57	0
51	CI	633	0	676	9	0
52	CX	2130	0	2219	31	0
53	CY	979	0	995	22	0
54	UP	422	0	457	5	0
55	UX	1	0	0	0	0
56	CI	32	0	12	0	0
57	CI	1	0	0	0	0
58	CS	27	0	12	0	0
All	All	179875	0	167930	1692	0

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

All (1692) 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)
4:UD:441:THR:HA	4:UD:456:LEU:O	1.26	1.30
12:UO:333:HIS:HA	12:UO:346:ARG:O	1.43	1.17
12:UO:335:ALA:HA	12:UO:344:SER:O	1.44	1.15
15:UU:159:ILE:O	15:UU:172:THR:HA	1.46	1.12
48:UH:555:GLY:O	48:UH:567:LEU:HA	1.50	1.11
2:UB:587:THR:O	2:UB:591:LEU:HB2	1.66	0.93
14:UR:559:SER:O	14:UR:565:ALA:HB3	1.71	0.90
29:CO:121:LEU:HB3	29:CO:163:ILE:O	1.74	0.86
22:CG:110:LYS:HZ3	53:CY:328:LYS:HB3	1.42	0.83
24:CI:914:ILE:HB	24:CI:995:VAL:O	1.81	0.81
3:UC:628:PRO:HA	21:CF:47:ARG:HH22	1.48	0.79
49:UI:211:ALA:HB1	49:UI:214:LEU:HB2	1.64	0.77
23:CH:269:GLN:N	23:CH:269:GLN:HE21	1.83	0.77
48:UH:756:LEU:HD22	49:UI:174:GLN:HE21	1.50	0.75
1:UA:780:GLN:O	1:UA:784:SER:HB3	1.86	0.75
24:CI:129:MET:O	24:CI:133:ALA:HB2	1.87	0.75
32:CR:845:ALA:HA	32:CR:916:MET:HE1	1.69	0.74
43:Co:360:HIS:O	43:Co:398:GLY:HA2	1.88	0.73
32:CS:286:ALA:H	32:CS:289:ARG:HD3	1.52	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:441:THR:CA	4:UD:456:LEU:O	2.23	0.72
18:CA:180:VAL:HB	18:CA:203:VAL:HG12	1.71	0.72
32:CS:641:ASN:HB3	32:CS:644:TYR:HB2	1.72	0.71
13:UQ:401:ASN:HB2	13:UQ:414:HIS:HB3	1.73	0.71
32:CR:132:THR:HA	32:CR:557:GLN:HE21	1.56	0.71
19:CC:182:ALA:HB3	20:CD:185:ARG:HH22	1.56	0.69
32:CR:317:PRO:HA	32:CR:320:LEU:HB2	1.73	0.69
1:UA:408:ALA:HB3	1:UA:418:ARG:HB2	1.75	0.69
8:UK:64:TYR:HB2	8:UK:67:MET:HG3	1.74	0.69
24:CI:165:ASN:HD21	24:CI:229:MET:HG2	1.56	0.69
26:CK:117:LEU:HD11	40:Cj:126:PRO:HG2	1.74	0.69
32:CR:276:THR:HG22	32:CR:278:ARG:H	1.56	0.69
10:UM:345:LEU:HB2	10:UM:367:ARG:HB3	1.75	0.69
49:UE:185:ILE:HA	49:UE:188:MET:HG2	1.75	0.69
7:UJ:142:TYR:HB3	7:UJ:145:ILE:HD12	1.74	0.69
21:CE:35:LYS:HB2	21:CE:102:SER:HB3	1.74	0.69
52:CX:372:GLU:HG3	52:CX:416:VAL:HG21	1.75	0.69
48:UH:267:ARG:HB2	48:UH:296:LEU:O	1.93	0.69
29:CN:121:LEU:HB3	29:CN:163:ILE:O	1.92	0.68
20:CD:411:LYS:HZ2	47:C2:269:G:H5'	1.59	0.68
29:CO:171:LEU:HD21	29:CO:177:LYS:HD2	1.76	0.68
21:CF:33:GLN:HG3	21:CF:106:ASN:HD22	1.56	0.68
32:CR:570:LEU:HB3	32:CR:584:CYS:HB3	1.76	0.68
1:UA:316:ALA:O	1:UA:321:GLN:HB2	1.93	0.68
23:CH:215:VAL:HG11	23:CH:321:ILE:HD11	1.76	0.67
23:CH:215:VAL:HG12	23:CH:285:THR:HG22	1.76	0.67
31:CQ:205:THR:HG21	31:CQ:228:ALA:HB2	1.75	0.67
23:CH:218:ILE:HD11	23:CH:317:LEU:HD21	1.76	0.67
2:UB:561:LYS:NZ	50:US:516:GLU:O	2.28	0.67
17:UZ:169:LYS:O	17:UZ:172:TYR:C	2.38	0.67
4:UD:204:CYS:HB2	4:UD:208:THR:HB	1.77	0.67
32:CS:240:LYS:HG2	32:CS:253:ILE:HG22	1.75	0.67
9:UL:589:VAL:HB	9:UL:603:LEU:HB2	1.76	0.67
15:UU:78:ARG:O	15:UU:81:ASN:ND2	2.28	0.66
29:CN:112:ILE:HB	29:CN:124:VAL:HB	1.77	0.66
32:CR:252:LEU:HB3	32:CR:265:LEU:HD21	1.78	0.66
9:UL:375:ALA:HB3	9:UL:384:GLN:HB2	1.78	0.66
9:UL:478:LYS:HG3	9:UL:479:VAL:HG23	1.78	0.66
15:UU:159:ILE:O	15:UU:172:THR:CA	2.33	0.65
28:CM:224:LEU:HB2	28:CM:234:ILE:HG22	1.78	0.65
9:UL:816:PRO:HA	9:UL:819:VAL:HG22	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:637:ARG:NH1	32:CR:638:ILE:O	2.30	0.65
24:CI:944:ILE:HD13	24:CI:973:PHE:HB3	1.79	0.65
32:CR:851:TYR:HA	32:CR:854:VAL:HG12	1.78	0.65
48:UH:821:VAL:HG13	49:UI:210:ARG:HE	1.62	0.65
1:UA:364:ILE:HD11	1:UA:381:HIS:HD2	1.62	0.65
13:UQ:927:ALA:O	13:UQ:931:ASN:HB2	1.96	0.65
49:UE:156:VAL:HG21	50:US:301:GLU:HB3	1.76	0.65
41:Cm:88:LYS:HE3	45:CU:300:VAL:HG22	1.79	0.65
51:CI:38:VAL:HG13	51:CI:42:TYR:HD2	1.62	0.65
40:Cj:126:PRO:HB3	46:C1:2166:A:H5"	1.79	0.64
1:UA:21:LEU:HB2	1:UA:30:PHE:HB2	1.77	0.64
43:Co:365:ASN:ND2	46:C1:1105:A:N3	2.44	0.64
23:CH:251:HIS:HB3	45:CU:111:MET:HG2	1.78	0.64
24:CI:1101:ARG:HD2	33:CT:111:MET:HG2	1.78	0.64
32:CS:292:SER:HA	32:CS:295:MET:HE2	1.78	0.64
20:CD:122:ILE:O	20:CD:126:LEU:HB2	1.96	0.64
9:UL:917:MET:HE1	10:UM:870:HIS:HB2	1.80	0.64
34:Ca:164:ILE:HD11	34:Ca:207:LEU:HD21	1.80	0.64
48:UH:267:ARG:HH12	48:UH:302:CYS:HB2	1.62	0.64
28:CM:171:SER:HB3	28:CM:203:VAL:HB	1.80	0.64
8:UK:253:SER:HB3	8:UK:265:VAL:H	1.63	0.64
19:CC:180:GLY:HA3	19:CC:295:LEU:HD21	1.79	0.64
32:CS:246:THR:HG22	32:CS:248:PRO:HD2	1.80	0.64
14:UR:322:ARG:HH21	46:C1:133:G:H22	1.46	0.63
23:CH:253:ALA:HB2	45:CU:111:MET:HE2	1.80	0.63
32:CR:142:THR:HA	32:CR:479:ARG:HH12	1.63	0.63
4:UD:757:ILE:HB	4:UD:771:ILE:O	1.97	0.63
19:CC:212:ILE:HG23	19:CC:213:VAL:HG23	1.81	0.63
9:UL:380:VAL:HG22	9:UL:382:ASP:H	1.63	0.63
24:CI:754:LYS:HA	24:CI:757:TYR:HB2	1.81	0.63
9:UL:890:VAL:HA	10:UM:891:MET:HG2	1.81	0.63
32:CR:28:VAL:HG22	32:CR:151:LEU:HB3	1.79	0.63
32:CR:516:CYS:HB3	32:CR:570:LEU:HD11	1.79	0.63
32:CS:27:PHE:HB2	32:CS:150:VAL:HG12	1.80	0.63
3:UC:632:GLN:HB3	18:CA:64:GLY:HA3	1.81	0.63
9:UL:16:VAL:HA	9:UL:392:ASN:HD21	1.63	0.63
45:CU:285:GLU:OE2	45:CU:287:ARG:NH2	2.31	0.63
13:UQ:555:GLU:HG2	13:UQ:583:ILE:HG12	1.80	0.63
32:CR:201:VAL:HG13	32:CR:209:LEU:HB2	1.79	0.63
36:Ce:51:SER:HB2	36:Ce:67:PHE:HB2	1.80	0.63
20:CD:341:TYR:HB3	20:CD:345:TYR:HB2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:CK:53:ARG:HD3	45:CU:210:ILE:HG21	1.80	0.63
6:UG:202:ILE:HB	6:UG:211:HIS:HB2	1.81	0.62
32:CR:635:ILE:HB	32:CR:725:VAL:HG22	1.81	0.62
32:CS:418:GLU:HB2	32:CS:550:LYS:HE3	1.81	0.62
36:Ce:73:LEU:HD22	36:Ce:100:ALA:HB2	1.82	0.62
18:CA:222:MET:HG2	19:CC:135:ARG:HG2	1.81	0.62
21:CF:94:VAL:O	22:CG:591:TRP:NE1	2.30	0.62
10:UM:198:LEU:HB3	10:UM:210:PHE:HB3	1.81	0.62
13:UQ:421:MET:HE3	13:UQ:423:LEU:HD21	1.82	0.62
13:UQ:809:SER:HB3	13:UQ:830:VAL:HA	1.80	0.62
32:CS:592:GLY:HA3	32:CS:631:SER:HA	1.81	0.62
10:UM:398:ILE:HD11	10:UM:436:VAL:HG11	1.81	0.62
21:CF:106:ASN:HD21	21:CF:111:LEU:HD23	1.63	0.62
26:CK:143:HIS:HB2	26:CK:151:ALA:HB3	1.82	0.62
32:CR:19:LEU:HD13	32:CR:49:ASP:HB2	1.81	0.62
32:CR:112:THR:HA	32:CR:115:ILE:HG12	1.80	0.62
23:CH:170:ARG:HB2	23:CH:198:SER:HB3	1.81	0.62
24:CI:881:ASN:N	24:CI:905:VAL:O	2.32	0.62
46:C1:60:A:H62	48:UH:876:LYS:HA	1.63	0.62
2:UB:760:LEU:HD12	2:UB:769:LEU:HD11	1.82	0.62
49:UI:156:VAL:HG22	49:UI:168:LEU:HD21	1.81	0.62
28:CM:134:LEU:HB3	28:CM:148:ALA:HB3	1.81	0.62
37:Cg:105:ARG:HH21	37:Cg:110:LEU:HD11	1.65	0.62
12:UO:36:HIS:CE1	12:UO:91:PRO:HD3	2.35	0.61
29:CO:121:LEU:HD22	29:CO:163:ILE:HB	1.82	0.61
32:CS:806:GLU:OE2	32:CS:871:ARG:NH2	2.33	0.61
32:CS:24:ARG:NH1	32:CS:140:ILE:O	2.30	0.61
12:UO:104:CYS:O	12:UO:116:ALA:HA	2.01	0.61
12:UO:467:ARG:NH2	12:UO:507:ASP:OD2	2.33	0.61
13:UQ:383:GLN:NE2	14:UR:364:GLN:O	2.34	0.61
15:UU:159:ILE:HB	15:UU:173:ILE:HB	1.82	0.61
30:CP:191:ASN:OD1	46:C1:1612:A:N6	2.34	0.61
2:UB:747:ILE:HD12	2:UB:795:ARG:HE	1.65	0.61
4:UD:19:VAL:HG12	4:UD:46:ILE:HG12	1.82	0.61
13:UQ:218:ILE:HD12	13:UQ:235:HIS:HB3	1.82	0.61
18:CB:250:GLY:N	18:CB:306:TYR:O	2.33	0.61
20:CD:166:VAL:HG22	20:CD:303:ALA:HA	1.82	0.61
28:CM:251:GLU:OE1	28:CM:254:ASN:ND2	2.33	0.61
34:Ca:121:ILE:HB	34:Ca:141:ALA:HB3	1.82	0.61
46:C1:1623:U:H5''	46:C1:1624:A:H2'	1.83	0.61
49:UI:184:THR:O	49:UI:188:MET:HB2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:UF:321:VAL:HG11	5:UF:341:GLN:HE21	1.64	0.61
30:CP:42:LEU:HB3	34:Ca:115:ARG:HD3	1.83	0.61
2:UB:590:ASP:HA	2:UB:593:ILE:HG12	1.81	0.61
18:CB:178:GLY:O	18:CB:202:ASN:ND2	2.34	0.61
22:CG:107:TYR:HA	22:CG:110:LYS:HE3	1.83	0.61
32:CR:27:PHE:O	32:CR:150:VAL:HA	2.00	0.61
50:US:191:LYS:NZ	50:US:229:SER:O	2.33	0.61
48:UH:324:THR:HB	48:UH:336:ASN:HB2	1.81	0.61
7:UJ:112:MET:HE1	33:CT:71:VAL:HG23	1.81	0.61
12:UO:417:ARG:NH2	46:C1:78:G:O6	2.32	0.61
20:CD:361:ILE:HG13	20:CD:405:LEU:HD13	1.83	0.61
22:CG:175:SER:HG	22:CG:186:THR:HG1	1.46	0.61
32:CS:392:ALA:HA	32:CS:428:LEU:HD13	1.83	0.61
44:Cp:12:LYS:HZ2	44:Cp:14:THR:HG22	1.66	0.61
6:UG:305:SER:HG	6:UG:318:THR:HG1	1.45	0.61
13:UQ:88:ARG:HD3	13:UQ:441:VAL:HG21	1.83	0.61
13:UQ:466:LEU:HB3	13:UQ:833:SER:HB2	1.83	0.61
37:Cg:39:GLU:HA	37:Cg:42:ARG:HE	1.64	0.61
46:C1:1122:A:H5'	46:C1:1127:C:H41	1.66	0.61
24:CI:178:LYS:NZ	46:C1:1102:A:OP2	2.34	0.60
29:CO:84:ILE:HA	29:CO:87:ALA:HB3	1.83	0.60
31:CQ:122:VAL:HG21	31:CQ:143:VAL:HG21	1.82	0.60
10:UM:135:ILE:HB	10:UM:149:VAL:HB	1.84	0.60
13:UQ:165:ILE:HG12	13:UQ:190:MET:HE1	1.83	0.60
15:UU:511:VAL:HB	15:UU:524:TRP:HB2	1.82	0.60
29:CN:114:ILE:HB	29:CN:122:ILE:HB	1.83	0.60
12:UO:335:ALA:CA	12:UO:344:SER:O	2.36	0.60
4:UD:374:VAL:HG21	4:UD:863:ILE:HG13	1.83	0.60
8:UK:268:ARG:NH2	14:UR:539:LEU:O	2.34	0.60
9:UL:161:ILE:HB	9:UL:188:PHE:HB2	1.83	0.60
13:UQ:450:ALA:HB2	13:UQ:458:PRO:HB2	1.83	0.60
32:CR:133:PRO:HB2	32:CR:553:PRO:HB3	1.83	0.60
48:UH:313:THR:OG1	48:UH:348:ARG:NH1	2.33	0.60
50:US:218:ASP:O	50:US:222:ASN:ND2	2.35	0.60
13:UQ:813:ILE:HB	13:UQ:823:LEU:HB3	1.83	0.60
32:CR:240:LYS:HG2	32:CR:253:ILE:HG22	1.83	0.60
6:UG:204:ASP:OD2	16:UX:13:ARG:NH1	2.35	0.60
10:UM:155:LEU:HB3	10:UM:203:GLN:HB2	1.83	0.60
10:UM:289:MET:HE3	10:UM:301:TRP:HB2	1.83	0.60
32:CR:394:ILE:HG23	32:CR:398:LEU:HD23	1.83	0.60
17:UZ:169:LYS:O	17:UZ:172:TYR:O	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:US:388:LEU:O	50:US:392:ALA:HB2	2.02	0.60
51:CI:12:ASN:HB2	51:CI:25:LYS:HD3	1.83	0.60
51:CI:53:ASP:HB3	51:CI:56:LYS:HG3	1.84	0.60
18:CB:204:ILE:HD13	20:CD:143:LEU:HD12	1.82	0.59
33:CT:154:ARG:HA	33:CT:157:ARG:HD2	1.83	0.59
48:UH:258:GLN:O	48:UH:265:ASN:HA	2.02	0.59
5:UF:285:VAL:HG11	11:UN:369:LEU:HB2	1.84	0.59
36:Ce:23:GLU:HA	36:Ce:26:ILE:HG12	1.83	0.59
7:UJ:145:ILE:HG22	7:UJ:147:ALA:H	1.67	0.59
9:UL:48:LEU:HD22	9:UL:57:LEU:HD11	1.84	0.59
10:UM:104:VAL:HG12	10:UM:105:ARG:HG2	1.84	0.59
41:Cm:19:LYS:NZ	46:C1:1666:C:O2'	2.35	0.59
36:Ce:40:LEU:HD23	36:Ce:82:ARG:HD3	1.84	0.59
52:CX:371:LEU:HD21	52:CX:417:PHE:HB2	1.85	0.59
6:UG:472:ARG:NH1	46:C1:333:C:OP1	2.35	0.59
1:UA:316:ALA:O	1:UA:320:GLY:O	2.20	0.59
18:CA:106:GLU:OE2	18:CA:128:ARG:NH1	2.36	0.59
24:CI:620:ARG:HA	24:CI:624:PHE:HB2	1.84	0.59
32:CS:387:VAL:HG12	32:CS:409:PHE:HB2	1.84	0.59
2:UB:335:LEU:HD21	50:US:517:PHE:HB3	1.84	0.59
6:UG:407:LEU:HD23	6:UG:418:ILE:HD11	1.84	0.59
36:Ce:50:VAL:HG21	36:Ce:69:PRO:HD3	1.83	0.59
32:CS:614:ILE:HG13	32:CS:615:PRO:HD3	1.83	0.59
10:UM:547:ILE:HA	10:UM:563:SER:HA	1.84	0.59
32:CS:186:ASN:HA	32:CS:189:PHE:HB3	1.84	0.59
44:Cp:13:VAL:O	44:Cp:52:ASN:N	2.35	0.59
4:UD:115:ASP:HB2	4:UD:122:LYS:HB2	1.85	0.59
5:UF:10:PHE:HB2	11:UN:912:LYS:HD3	1.84	0.59
6:UG:455:GLN:H	6:UG:458:MET:HE3	1.68	0.59
53:CY:362:ARG:HH21	53:CY:363:TYR:HE1	1.50	0.59
8:UK:68:MET:HG3	47:C2:58:A:H4'	1.85	0.58
20:CD:49:ALA:HB1	20:CD:72:LYS:HE2	1.84	0.58
24:CI:917:LYS:NZ	46:C1:1142:U:OP1	2.35	0.58
32:CS:112:THR:HA	32:CS:115:ILE:HG12	1.85	0.58
32:CS:291:LYS:NZ	32:CS:412:SER:O	2.36	0.58
32:CS:700:ARG:HH21	32:CS:705:LEU:HD23	1.68	0.58
1:UA:363:LYS:HG2	1:UA:379:THR:HG22	1.85	0.58
9:UL:24:LEU:HD22	9:UL:41:VAL:HG12	1.84	0.58
20:CD:80:LEU:HD13	20:CD:86:VAL:HG11	1.85	0.58
15:UU:143:GLN:NE2	15:UU:189:ALA:O	2.37	0.58
52:CX:422:ARG:O	52:CX:430:ARG:NH2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:112:ILE:HB	29:CO:124:VAL:HB	1.84	0.58
37:Cg:146:VAL:HG11	37:Cg:154:ILE:HD11	1.84	0.58
50:US:127:SER:O	50:US:131:SER:HB3	2.03	0.58
2:UB:618:ILE:HG23	2:UB:639:LEU:HB3	1.85	0.58
10:UM:156:VAL:HA	10:UM:202:THR:HA	1.84	0.58
19:CC:179:GLN:HA	20:CD:185:ARG:HH21	1.68	0.58
19:CC:182:ALA:HB3	20:CD:185:ARG:NH2	2.18	0.58
20:CD:287:PRO:HB2	20:CD:391:ALA:HB2	1.85	0.58
30:CP:156:LEU:O	30:CP:159:GLN:NE2	2.36	0.58
32:CR:34:ALA:HB1	32:CR:152:LEU:HD22	1.85	0.58
10:UM:548:ASN:ND2	10:UM:564:GLN:OE1	2.35	0.58
18:CB:113:THR:HG23	18:CB:124:LYS:HB3	1.86	0.58
25:CJ:64:LEU:O	25:CJ:71:ARG:NH1	2.37	0.58
31:CQ:178:LEU:HG	31:CQ:183:LEU:HD22	1.85	0.58
6:UG:337:ASN:O	6:UG:380:LYS:NZ	2.37	0.58
24:CI:961:GLN:OE1	26:CK:286:GLN:NE2	2.37	0.58
2:UB:638:TYR:HD1	50:US:542:TRP:HZ3	1.51	0.58
5:UF:35:ASN:ND2	14:UR:60:LEU:O	2.37	0.58
9:UL:113:ILE:HD13	9:UL:129:SER:HB3	1.85	0.58
9:UL:372:VAL:HG12	9:UL:387:VAL:HG12	1.85	0.58
9:UL:814:ARG:NH1	9:UL:823:ASN:OD1	2.37	0.58
18:CB:180:VAL:HB	18:CB:203:VAL:HG12	1.85	0.58
48:UH:340:VAL:HB	48:UH:343:LEU:HB2	1.84	0.58
52:CX:284:LEU:HD11	52:CX:288:LEU:HD22	1.86	0.58
1:UA:445:ILE:HA	1:UA:470:PRO:HB3	1.85	0.58
4:UD:377:ALA:HB3	4:UD:382:TYR:HB2	1.86	0.58
10:UM:382:ILE:HG13	10:UM:383:LEU:HG	1.86	0.58
23:CH:114:LEU:O	23:CH:118:ALA:N	2.36	0.58
11:UN:874:LYS:NZ	46:C1:331:C:OP1	2.34	0.57
6:UG:332:PHE:HB3	11:UN:869:VAL:HG11	1.86	0.57
32:CR:24:ARG:NH1	32:CR:140:ILE:O	2.37	0.57
10:UM:547:ILE:HG22	10:UM:563:SER:HB2	1.87	0.57
24:CI:248:ASN:HB3	24:CI:271:SER:HB2	1.86	0.57
6:UG:398:VAL:HG12	6:UG:409:ILE:HG12	1.87	0.57
26:CK:289:ARG:NH2	46:C1:1145:G:OP2	2.37	0.57
1:UA:516:VAL:HG12	1:UA:527:ILE:HG12	1.86	0.57
13:UQ:564:GLU:OE1	13:UQ:573:GLN:NE2	2.35	0.57
37:Cg:77:ARG:NH1	53:CY:310:GLU:O	2.36	0.57
37:Cg:171:ARG:HH21	46:C1:1095:A:H5'	1.69	0.57
48:UH:301:THR:O	48:UH:303:ARG:NH1	2.38	0.57
13:UQ:499:LEU:HD22	13:UQ:513:LYS:HE2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:172:ARG:HH22	32:CS:609:PRO:HB2	1.69	0.57
9:UL:129:SER:OG	9:UL:131:ASP:OD1	2.23	0.57
10:UM:375:GLU:HA	10:UM:713:SER:HA	1.87	0.57
24:CI:807:GLU:O	24:CI:840:ARG:NH2	2.37	0.57
2:UB:759:HIS:O	2:UB:765:ASN:ND2	2.36	0.57
7:UJ:268:GLN:NE2	7:UJ:299:GLY:O	2.37	0.57
16:UX:63:ASN:HD21	16:UX:150:ASP:HB2	1.68	0.56
26:CK:100:LEU:HD13	26:CK:144:GLU:HB3	1.87	0.56
32:CS:416:GLY:O	32:CS:551:ASN:ND2	2.38	0.56
32:CS:798:PRO:HD2	32:CS:801:LEU:HB2	1.86	0.56
36:Ce:76:PHE:O	36:Ce:79:VAL:C	2.48	0.56
10:UM:324:SER:HB3	10:UM:337:ALA:HB3	1.87	0.56
15:UU:78:ARG:HB3	15:UU:81:ASN:HD22	1.69	0.56
27:CL:561:ARG:NH2	27:CL:567:ASN:O	2.38	0.56
5:UF:130:MET:HE1	5:UF:143:LEU:HD22	1.88	0.56
9:UL:862:ASN:OD1	9:UL:905:ASN:ND2	2.38	0.56
18:CB:226:ILE:HG12	18:CB:247:LEU:HD13	1.87	0.56
26:CK:40:LYS:NZ	26:CK:41:PRO:O	2.38	0.56
43:Co:339:ARG:HH12	43:Co:341:ARG:HD2	1.70	0.56
50:US:172:VAL:O	50:US:176:SER:HB3	2.05	0.56
24:CI:954:THR:HG22	24:CI:987:VAL:HG22	1.87	0.56
9:UL:130:LYS:HG2	9:UL:154:GLN:HG3	1.86	0.56
10:UM:508:ALA:HA	10:UM:526:ARG:HH22	1.69	0.56
14:UR:253:ARG:NH1	14:UR:599:SER:O	2.38	0.56
19:CC:377:ARG:NH2	47:C2:197:C:OP2	2.37	0.56
52:CX:390:LEU:HD11	52:CX:432:ALA:HB1	1.86	0.56
9:UL:25:VAL:HB	9:UL:40:ILE:HB	1.86	0.56
16:UX:13:ARG:HB3	25:CJ:19:ILE:HG13	1.87	0.56
16:UX:100:GLU:OE2	28:CM:349:ASN:ND2	2.37	0.56
17:UZ:82:LYS:O	17:UZ:269:ARG:NH2	2.37	0.56
34:Ca:86:LEU:HB3	34:Ca:98:THR:HB	1.88	0.56
50:US:312:ASN:OD1	50:US:336:TYR:OH	2.24	0.56
1:UA:306:ASN:ND2	1:UA:308:SER:OG	2.38	0.56
6:UG:573:ARG:HG3	6:UG:582:ARG:HH22	1.70	0.56
19:CC:247:ASP:O	19:CC:251:ALA:HB2	2.05	0.56
20:CD:143:LEU:CD1	20:CD:147:HIS:HE1	2.18	0.56
32:CR:291:LYS:HG2	32:CR:295:MET:HE1	1.87	0.56
32:CS:359:VAL:HB	32:CS:369:ILE:HG12	1.88	0.56
35:Cc:87:HIS:ND1	46:C1:2056:U:O4	2.38	0.56
48:UH:371:SER:HA	48:UH:437:GLY:HA2	1.88	0.56
49:UI:214:LEU:HA	49:UI:217:TRP:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CB:191:ARG:HA	18:CB:194:ILE:HG12	1.88	0.56
29:CN:166:PRO:HG2	29:CN:169:ASP:HB2	1.88	0.56
32:CS:132:THR:OG1	32:CS:134:ASN:OD1	2.24	0.56
4:UD:617:ASN:HB3	4:UD:620:ALA:HB2	1.87	0.56
6:UG:434:ASN:HB3	6:UG:437:GLU:HB3	1.88	0.56
12:UO:304:SER:OG	12:UO:306:ASN:OD1	2.23	0.56
15:UU:87:ARG:NH1	15:UU:89:GLN:OE1	2.39	0.56
1:UA:562:ASP:OD1	25:CJ:144:ARG:NH1	2.39	0.56
24:CI:58:LEU:HD13	46:C1:1018:G:H22	1.71	0.56
29:CO:171:LEU:HD12	29:CO:172:PRO:HD2	1.87	0.56
46:C1:628:A:H61	46:C1:1050:U:H3	1.53	0.56
9:UL:847:LEU:O	44:Cp:30:ARG:NH2	2.38	0.55
13:UQ:759:ASP:OD2	48:UH:435:ARG:NH1	2.38	0.55
24:CI:334:LEU:HD22	24:CI:341:ARG:HG3	1.87	0.55
32:CS:284:THR:HB	32:CS:473:THR:HG22	1.86	0.55
49:UI:184:THR:O	49:UI:188:MET:CB	2.54	0.55
6:UG:178:GLU:OE2	6:UG:196:GLN:NE2	2.39	0.55
13:UQ:731:LYS:HB2	13:UQ:749:ASP:HB2	1.88	0.55
13:UQ:920:VAL:HG21	14:UR:575:THR:HG21	1.87	0.55
38:Ch:102:LEU:HD21	38:Ch:115:LEU:HD13	1.88	0.55
15:UU:752:THR:N	15:UU:766:ALA:O	2.36	0.55
21:CF:90:ARG:NH1	22:CG:414:ASP:OD2	2.39	0.55
22:CG:438:LEU:HA	22:CG:463:PRO:HA	1.89	0.55
43:Co:394:GLN:NE2	43:Co:397:GLY:O	2.35	0.55
10:UM:135:ILE:HD11	10:UM:156:VAL:HG11	1.88	0.55
32:CR:24:ARG:HB2	32:CR:486:VAL:HG11	1.89	0.55
32:CR:547:SER:OG	32:CR:640:THR:O	2.24	0.55
34:Ca:157:GLN:HB2	34:Ca:160:GLN:HG3	1.88	0.55
37:Cg:139:VAL:HG13	53:CY:257:GLY:HA3	1.89	0.55
1:UA:223:LYS:HD2	1:UA:246:VAL:HG21	1.89	0.55
6:UG:241:LYS:HG2	6:UG:253:GLU:HG2	1.87	0.55
24:CI:268:ILE:HG12	24:CI:784:VAL:HG21	1.87	0.55
32:CR:88:GLU:HB2	32:CR:91:GLN:HB2	1.88	0.55
41:Cm:82:ARG:O	41:Cm:86:LEU:HB2	2.07	0.55
24:CI:1072:LYS:NZ	46:C1:218:G:O6	2.39	0.55
35:Cc:39:GLU:OE2	35:Cc:41:ARG:NH1	2.35	0.55
46:C1:1029:A:H61	46:C1:1046:G:H1'	1.72	0.55
7:UJ:372:ILE:HD11	7:UJ:416:ILE:HG12	1.88	0.55
9:UL:287:HIS:HE1	9:UL:376:LEU:HD11	1.71	0.55
28:CM:417:ARG:NH2	46:C1:1627:G:OP1	2.39	0.55
9:UL:626:SER:OG	9:UL:627:ALA:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:712:VAL:HG12	9:UL:722:VAL:HG22	1.88	0.55
24:CI:59:VAL:O	24:CI:239:ASN:ND2	2.39	0.55
32:CR:840:ARG:HH11	32:CS:623:GLN:HG2	1.71	0.55
48:UH:34:VAL:HG22	48:UH:86:SER:HB3	1.89	0.55
5:UF:169:ARG:NH2	19:CC:83:GLU:OE2	2.39	0.55
11:UN:343:LEU:HD11	28:CM:250:MET:HE1	1.89	0.55
13:UQ:540:LYS:HB2	13:UQ:553:ILE:HB	1.89	0.55
19:CC:222:VAL:HG11	19:CC:250:LYS:HE2	1.88	0.55
30:CP:187:ASP:HB3	30:CP:192:ILE:HB	1.88	0.55
36:Ce:55:ILE:HG13	36:Ce:182:VAL:HG23	1.89	0.55
37:Cg:60:LEU:HD23	37:Cg:67:ARG:HB2	1.89	0.55
4:UD:559:ARG:NH2	4:UD:575:LEU:O	2.40	0.55
10:UM:19:PRO:O	10:UM:53:ARG:NH2	2.39	0.55
10:UM:300:ILE:HG22	10:UM:310:THR:HG23	1.88	0.55
23:CH:269:GLN:N	23:CH:269:GLN:NE2	2.54	0.55
24:CI:555:GLN:HA	24:CI:558:ARG:HB3	1.89	0.55
52:CX:244:PRO:HB2	52:CX:287:HIS:HB2	1.89	0.55
2:UB:894:ASN:HB3	2:UB:898:ARG:HH12	1.71	0.54
4:UD:697:GLN:HG3	4:UD:713:SER:HB3	1.88	0.54
21:CF:94:VAL:HG12	21:CF:96:ARG:H	1.71	0.54
4:UD:564:ALA:HB1	4:UD:630:PRO:HG2	1.89	0.54
1:UA:683:THR:O	1:UA:775:ARG:NH2	2.40	0.54
2:UB:730:THR:HG23	2:UB:780:LEU:HD22	1.90	0.54
6:UG:278:GLN:HA	6:UG:302:PRO:HB3	1.88	0.54
9:UL:838:LYS:O	9:UL:842:LEU:N	2.39	0.54
13:UQ:747:LEU:HD21	13:UQ:778:THR:HG22	1.89	0.54
14:UR:253:ARG:NH2	14:UR:551:ASP:OD2	2.41	0.54
34:Ca:89:ASP:OD2	34:Ca:99:ASN:ND2	2.40	0.54
41:Cm:26:MET:HE1	41:Cm:28:ARG:HD2	1.89	0.54
1:UA:715:ILE:HG23	1:UA:736:MET:HG2	1.89	0.54
20:CD:354:SER:HA	20:CD:358:LYS:HE2	1.90	0.54
24:CI:963:LYS:NZ	46:C1:2181:U:OP2	2.39	0.54
26:CK:164:MET:HB2	26:CK:267:SER:HB3	1.89	0.54
29:CO:113:TYR:HD2	29:CO:121:LEU:HD21	1.73	0.54
48:UH:219:SER:HB2	48:UH:248:ASN:HD21	1.73	0.54
11:UN:325:ARG:NH1	28:CM:209:GLU:OE1	2.41	0.54
13:UQ:615:PHE:H	13:UQ:630:GLY:HA2	1.73	0.54
13:UQ:713:VAL:HG22	13:UQ:725:VAL:HG22	1.90	0.54
15:UU:669:ILE:N	15:UU:683:ALA:O	2.38	0.54
17:UZ:126:ARG:NH1	46:C1:2061:G:OP1	2.41	0.54
30:CP:83:THR:HG22	30:CP:85:LYS:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Cg:103:LEU:HD23	37:Cg:106:ARG:HD2	1.89	0.54
47:C2:101:G:H1	47:C2:251:U:H3	1.55	0.54
50:US:173:VAL:O	50:US:182:ARG:NH2	2.41	0.54
4:UD:660:ASN:OD1	4:UD:663:ARG:NH2	2.40	0.54
13:UQ:422:VAL:HB	13:UQ:432:MET:HB3	1.90	0.54
28:CM:332:THR:HG22	28:CM:343:THR:HG22	1.89	0.54
43:Co:358:ILE:HD11	43:Co:371:LEU:HD11	1.89	0.54
3:UC:642:LEU:HD21	46:C1:1082:G:H5''	1.90	0.54
6:UG:283:THR:OG1	6:UG:285:TRP:NE1	2.40	0.54
9:UL:222:ALA:HB3	9:UL:235:ALA:HB3	1.90	0.54
10:UM:562:ALA:HB2	10:UM:592:VAL:HG22	1.90	0.54
13:UQ:758:SER:OG	48:UH:440:ARG:NH1	2.40	0.54
26:CK:286:GLN:HE21	27:CL:526:VAL:HG12	1.72	0.54
46:C1:314:A:H61	46:C1:326:U:H3	1.54	0.54
48:UH:84:PRO:HB3	48:UH:103:VAL:HG12	1.90	0.54
9:UL:864:PHE:O	9:UL:868:GLU:HA	2.08	0.54
15:UU:50:PRO:HB2	15:UU:342:LYS:HD2	1.89	0.54
22:CG:106:ARG:NH2	53:CY:328:LYS:O	2.41	0.54
53:CY:287:SER:N	53:CY:290:GLU:OE2	2.40	0.54
1:UA:204:SER:OG	1:UA:206:ASP:O	2.27	0.54
2:UB:479:PHE:HB2	2:UB:507:ILE:HD13	1.88	0.54
2:UB:798:LEU:HD13	50:US:456:CYS:HB3	1.89	0.54
4:UD:54:GLU:HG2	4:UD:68:ILE:HG12	1.89	0.54
9:UL:19:SER:OG	9:UL:43:ALA:O	2.24	0.54
10:UM:43:ALA:HB3	10:UM:57:ILE:HB	1.90	0.54
17:UZ:31:LEU:HB2	17:UZ:35:LYS:HZ3	1.72	0.54
17:UZ:130:ILE:HG13	17:UZ:134:LYS:HE2	1.89	0.54
21:CF:18:VAL:HA	21:CF:21:LEU:HD12	1.90	0.54
9:UL:571:LEU:HD12	9:UL:580:LEU:HD11	1.89	0.53
12:UO:125:VAL:HB	12:UO:138:LYS:HB3	1.89	0.53
12:UO:424:TRP:HB3	12:UO:439:ASP:HB3	1.89	0.53
29:CO:239:SER:O	29:CO:243:HIS:ND1	2.40	0.53
30:CP:110:GLN:NE2	45:CU:179:SER:O	2.41	0.53
32:CR:885:LEU:HD12	32:CR:889:LEU:HD21	1.90	0.53
35:Cc:50:GLN:HE21	35:Cc:75:PRO:HA	1.72	0.53
47:C2:35:G:OP2	47:C2:35:G:N2	2.35	0.53
9:UL:803:ARG:NH2	9:UL:808:ASN:OD1	2.41	0.53
13:UQ:379:LEU:HD22	13:UQ:413:LEU:HD11	1.90	0.53
15:UU:343:ILE:HG22	15:UU:354:THR:HG22	1.90	0.53
15:UU:931:GLY:O	15:UU:934:LYS:C	2.51	0.53
21:CE:53:VAL:O	21:CE:79:TYR:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:364:GLN:NE2	53:CY:246:GLU:OE2	2.38	0.53
24:CI:517:VAL:HG12	32:CR:277:LEU:HD23	1.90	0.53
31:CQ:111:LEU:HD11	31:CQ:136:LEU:HA	1.91	0.53
32:CR:55:SER:HB3	32:CR:120:TYR:HD1	1.74	0.53
32:CR:829:LEU:O	32:CR:832:LEU:C	2.51	0.53
50:US:89:VAL:HG12	50:US:148:ALA:HB2	1.91	0.53
50:US:253:HIS:HD2	50:US:255:LEU:HB2	1.72	0.53
10:UM:647:LYS:HD2	10:UM:699:LEU:H	1.73	0.53
15:UU:212:ASN:HB2	15:UU:219:ILE:HD11	1.90	0.53
22:CG:398:MET:HA	22:CG:413:SER:HA	1.90	0.53
23:CH:375:TRP:O	24:CI:763:HIS:NE2	2.41	0.53
32:CS:125:LEU:HD12	32:CS:131:ILE:HD11	1.90	0.53
32:CS:289:ARG:HH21	32:CS:474:LEU:HB3	1.72	0.53
4:UD:481:ALA:HA	4:UD:497:GLU:HA	1.89	0.53
10:UM:308:GLU:OE2	10:UM:310:THR:OG1	2.20	0.53
18:CB:107:LYS:HE3	18:CB:109:ILE:HD11	1.90	0.53
23:CH:133:THR:HG22	23:CH:191:ILE:HG12	1.91	0.53
48:UH:220:ALA:HB1	48:UH:242:ILE:HD13	1.91	0.53
9:UL:394:LEU:HB2	9:UL:420:VAL:HB	1.91	0.53
13:UQ:88:ARG:NH2	13:UQ:416:ASP:O	2.42	0.53
17:UZ:235:LEU:HD11	17:UZ:270:PHE:HB3	1.90	0.53
24:CI:1085:ARG:NE	46:C1:391:C:OP1	2.39	0.53
28:CM:173:GLY:O	36:Ce:153:LYS:NZ	2.40	0.53
32:CS:540:MET:HE2	32:CS:567:LEU:HD23	1.91	0.53
34:Ca:97:LEU:HB3	34:Ca:232:HIS:CE1	2.44	0.53
2:UB:652:ARG:HD2	50:US:467:TYR:HA	1.90	0.53
2:UB:726:LEU:HD22	2:UB:773:LEU:HD21	1.91	0.53
7:UJ:174:LEU:HD13	33:CT:74:PRO:HB2	1.90	0.53
10:UM:87:ILE:HB	10:UM:105:ARG:HB2	1.90	0.53
10:UM:568:VAL:HB	10:UM:582:LEU:HB2	1.91	0.53
32:CS:402:LEU:O	32:CS:406:TYR:OH	2.20	0.53
2:UB:497:VAL:HA	2:UB:500:LEU:HD23	1.90	0.53
6:UG:318:THR:HG22	6:UG:324:MET:HG3	1.91	0.53
19:CC:183:THR:O	19:CC:187:LEU:HB2	2.08	0.53
32:CS:596:LYS:HA	32:CS:599:ILE:HD12	1.90	0.53
34:Ca:157:GLN:NE2	46:C1:1632:G:OP2	2.41	0.53
1:UA:149:GLN:HB2	1:UA:178:TRP:HH2	1.74	0.53
13:UQ:521:PRO:HG3	49:UE:26:THR:HG21	1.91	0.53
23:CH:80:GLY:O	24:CI:809:ARG:NH2	2.40	0.53
30:CP:35:GLU:OE2	39:CI:127:ARG:NH1	2.41	0.53
1:UA:544:GLN:OE1	40:Cj:114:ARG:NH1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:735:ARG:NH2	13:UQ:748:SER:O	2.41	0.53
15:UU:545:SER:OG	15:UU:625:VAL:O	2.26	0.53
19:CC:89:THR:HG23	19:CC:115:GLY:HA3	1.90	0.53
20:CD:217:ARG:NH2	20:CD:246:GLY:O	2.42	0.53
38:Ch:115:LEU:HA	38:Ch:118:ILE:HG22	1.91	0.53
51:Cl:10:ASN:HB3	51:Cl:13:HIS:HD2	1.73	0.53
2:UB:72:THR:OG1	29:CN:47:GLU:OE2	2.26	0.53
7:UJ:229:ILE:HD11	7:UJ:278:LEU:HD23	1.90	0.53
10:UM:29:GLU:HB2	10:UM:34:ILE:HB	1.90	0.53
21:CF:34:LEU:HD21	21:CF:101:VAL:HB	1.91	0.53
23:CH:215:VAL:HA	23:CH:285:THR:HA	1.89	0.53
32:CS:571:THR:HA	32:CS:583:LEU:HD13	1.91	0.53
2:UB:26:LYS:NZ	9:UL:110:LYS:O	2.42	0.52
6:UG:225:LEU:HD12	6:UG:230:LEU:HD23	1.90	0.52
9:UL:109:HIS:HD1	9:UL:129:SER:HG	1.53	0.52
24:CI:301:GLU:HG3	24:CI:771:TYR:HD1	1.73	0.52
29:CO:147:ARG:HH21	29:CO:150:ILE:HA	1.73	0.52
52:CX:267:GLU:HA	52:CX:271:LEU:HD23	1.90	0.52
13:UQ:632:ASP:OD2	13:UQ:636:ARG:NH2	2.42	0.52
23:CH:284:GLU:OE2	45:CU:119:TYR:OH	2.27	0.52
28:CM:67:GLN:OE1	41:Cm:68:ARG:NH2	2.42	0.52
29:CN:164:GLN:HB3	46:C1:2158:G:H5''	1.90	0.52
32:CR:310:ILE:HD12	32:CR:385:LEU:HD23	1.91	0.52
32:CS:278:ARG:HB3	32:CS:467:ARG:HG2	1.90	0.52
39:CI:134:THR:O	46:C1:1471:U:O2'	2.27	0.52
50:US:178:ILE:HG13	50:US:181:LEU:H	1.75	0.52
50:US:285:VAL:O	50:US:289:MET:HB2	2.09	0.52
10:UM:819:ASN:ND2	27:CL:699:ALA:O	2.42	0.52
13:UQ:383:GLN:OE1	13:UQ:386:THR:OG1	2.26	0.52
13:UQ:421:MET:HB3	13:UQ:433:TYR:HD1	1.75	0.52
32:CR:318:GLU:O	32:CR:321:LYS:NZ	2.36	0.52
4:UD:449:THR:HA	54:UP:330:ARG:HH21	1.74	0.52
8:UK:63:PHE:HB2	25:CJ:170:ILE:HD11	1.91	0.52
9:UL:422:LEU:O	9:UL:450:LYS:NZ	2.41	0.52
10:UM:194:SER:O	10:UM:197:ARG:NH2	2.42	0.52
13:UQ:257:ALA:HB3	13:UQ:260:ALA:HB3	1.92	0.52
34:Ca:71:ALA:HB3	39:CI:127:ARG:HH21	1.74	0.52
40:Cj:6:ALA:HA	40:Cj:22:CYS:O	2.09	0.52
7:UJ:256:SER:HB2	14:UR:230:LEU:HD23	1.92	0.52
8:UK:15:GLU:OE2	24:CI:1040:ARG:NH2	2.42	0.52
13:UQ:658:LEU:HD11	49:UE:32:ARG:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UB:554:ARG:HH21	50:US:523:ILE:HG22	1.75	0.52
13:UQ:81:VAL:HG22	13:UQ:855:ILE:HG12	1.92	0.52
24:CI:832:PRO:HG2	24:CI:1015:LEU:HD12	1.91	0.52
27:CL:719:ARG:NH2	27:CL:722:GLU:OE1	2.37	0.52
32:CS:112:THR:HB	32:CS:138:ARG:HD3	1.92	0.52
32:CS:310:ILE:HB	32:CS:369:ILE:HG22	1.91	0.52
43:Co:342:LYS:HB2	43:Co:355:VAL:HB	1.92	0.52
1:UA:356:VAL:HG22	1:UA:366:VAL:HG22	1.92	0.52
15:UU:119:LEU:HD22	15:UU:131:LEU:HD22	1.92	0.52
18:CA:250:GLY:HA2	18:CA:306:TYR:O	2.10	0.52
25:CJ:117:ARG:HG3	46:C1:353:G:H4'	1.92	0.52
38:Ch:109:LYS:NZ	46:C1:1561:G:OP1	2.41	0.52
1:UA:323:LEU:HD12	1:UA:335:LYS:HG3	1.91	0.52
5:UF:99:ALA:HB1	5:UF:109:LEU:HD21	1.91	0.52
6:UG:242:TYR:HB2	6:UG:252:ALA:HB3	1.92	0.52
8:UK:18:GLN:O	24:CI:1036:ARG:NH2	2.42	0.52
12:UO:36:HIS:HE1	12:UO:91:PRO:HD3	1.73	0.52
12:UO:121:GLY:HA2	12:UO:147:VAL:HG23	1.92	0.52
16:UX:152:ASP:OD1	16:UX:152:ASP:N	2.42	0.52
29:CN:96:LEU:HD21	29:CN:114:ILE:HD11	1.92	0.52
30:CP:66:GLY:O	30:CP:86:THR:OG1	2.24	0.52
6:UG:219:VAL:HA	6:UG:235:SER:HA	1.92	0.52
9:UL:441:LEU:HB2	9:UL:454:ILE:HD11	1.92	0.52
23:CH:203:PRO:HD2	23:CH:342:GLY:HA2	1.90	0.52
25:CJ:96:ALA:O	25:CJ:100:ASN:HB2	2.09	0.52
32:CR:559:MET:HB2	32:CR:567:LEU:HD21	1.92	0.52
10:UM:777:VAL:HG21	10:UM:794:VAL:HG21	1.92	0.52
12:UO:554:VAL:HG23	49:UE:230:VAL:HG13	1.93	0.52
24:CI:81:LYS:HA	24:CI:139:MET:HE1	1.91	0.52
38:Ch:101:HIS:NE2	38:Ch:108:ASP:OD2	2.43	0.52
49:UE:194:GLY:HA3	49:UE:235:LEU:HD22	1.91	0.52
53:CY:231:LEU:HD13	53:CY:321:ILE:HD12	1.92	0.52
4:UD:884:ARG:NH2	46:C1:71:A:O2'	2.39	0.51
7:UJ:204:CYS:HB3	7:UJ:261:MET:HE1	1.90	0.51
10:UM:233:SER:OG	34:Ca:50:ARG:NH2	2.43	0.51
18:CB:239:VAL:HG21	18:CB:255:ILE:HD12	1.92	0.51
19:CC:380:ARG:NH1	47:C2:111:G:O6	2.40	0.51
20:CD:214:LEU:O	20:CD:254:TYR:OH	2.27	0.51
47:C2:23:A:N6	47:C2:28:U:O2'	2.38	0.51
1:UA:23:SER:HB3	1:UA:28:HIS:HB2	1.91	0.51
10:UM:331:ARG:O	10:UM:347:ARG:NH1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:846:VAL:HG13	15:UU:850:ARG:HH21	1.74	0.51
20:CD:304:HIS:ND1	47:C2:93:G:OP2	2.44	0.51
32:CS:311:PHE:HB2	32:CS:386:VAL:HG22	1.91	0.51
37:Cg:88:ARG:HE	37:Cg:93:TYR:HD2	1.58	0.51
46:C1:81:G:H1	46:C1:126:C:H42	1.57	0.51
1:UA:183:GLU:HB2	1:UA:186:PHE:HB3	1.93	0.51
6:UG:63:VAL:O	6:UG:69:ARG:NH1	2.42	0.51
10:UM:351:PRO:HA	10:UM:354:VAL:HG12	1.90	0.51
22:CG:351:ASP:OD1	22:CG:351:ASP:N	2.43	0.51
37:Cg:136:LYS:H	53:CY:250:GLY:HA3	1.75	0.51
52:CX:325:SER:HB2	52:CX:369:VAL:HG11	1.92	0.51
2:UB:615:MET:HE2	2:UB:647:GLN:HE21	1.76	0.51
9:UL:12:LYS:HB3	9:UL:722:VAL:HB	1.92	0.51
20:CD:293:ILE:HG21	20:CD:369:ILE:HD11	1.93	0.51
22:CG:193:THR:HG23	22:CG:195:TRP:HE1	1.76	0.51
23:CH:218:ILE:O	23:CH:250:VAL:HA	2.11	0.51
24:CI:129:MET:O	24:CI:133:ALA:CB	2.56	0.51
32:CR:169:VAL:O	32:CR:172:ARG:NH1	2.30	0.51
32:CR:845:ALA:HB2	32:CR:920:THR:HG21	1.93	0.51
48:UH:347:LEU:HD21	48:UH:394:TYR:HB2	1.93	0.51
1:UA:221:GLU:HB3	1:UA:247:ASN:HB2	1.92	0.51
9:UL:431:SER:OG	9:UL:469:LEU:O	2.28	0.51
15:UU:210:ILE:HD12	15:UU:220:TYR:HB3	1.93	0.51
23:CH:7:GLU:HA	23:CH:32:HIS:HB2	1.93	0.51
32:CS:28:VAL:HB	32:CS:201:VAL:HG12	1.91	0.51
39:CI:30:ALA:HB2	39:CI:92:LEU:HD23	1.93	0.51
9:UL:899:LEU:HA	9:UL:902:VAL:HG12	1.93	0.51
24:CI:761:ASP:HA	24:CI:765:ARG:HB2	1.92	0.51
1:UA:559:ARG:NH1	1:UA:672:GLU:OE1	2.44	0.51
1:UA:627:SER:O	16:UX:-5:LYS:NZ	2.39	0.51
2:UB:769:LEU:HD22	2:UB:773:LEU:HD23	1.93	0.51
3:UC:595:LYS:HA	3:UC:598:ARG:HG2	1.93	0.51
4:UD:429:SER:HB3	4:UD:448:PRO:HD2	1.93	0.51
10:UM:155:LEU:O	10:UM:203:GLN:N	2.43	0.51
10:UM:480:GLU:OE2	46:C1:1498:G:N1	2.44	0.51
16:UX:178:LEU:HD23	16:UX:181:ALA:HB2	1.92	0.51
19:CC:175:ASN:OD1	19:CC:176:HIS:N	2.44	0.51
24:CI:886:CYS:HB2	24:CI:901:ALA:HB3	1.93	0.51
24:CI:1043:ARG:NH2	46:C1:2073:A:OP1	2.40	0.51
29:CN:80:MET:HG3	29:CN:82:ARG:HG3	1.91	0.51
30:CP:188:THR:HG23	30:CP:194:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:549:VAL:HG21	4:UD:563:VAL:HB	1.93	0.51
6:UG:58:VAL:HG23	11:UN:902:ARG:HH21	1.75	0.51
9:UL:903:ARG:HD3	10:UM:885:GLU:HG3	1.92	0.51
10:UM:743:GLN:NE2	10:UM:747:ASN:OD1	2.43	0.51
12:UO:463:ARG:NH1	13:UQ:524:VAL:O	2.43	0.51
20:CD:230:PRO:HG2	20:CD:233:ILE:HD12	1.93	0.51
32:CS:24:ARG:HH22	32:CS:140:ILE:HG23	1.75	0.51
50:US:394:PRO:HA	50:US:397:ILE:HD12	1.92	0.51
10:UM:288:TRP:HA	10:UM:301:TRP:O	2.10	0.51
12:UO:413:HIS:HB3	12:UO:417:ARG:H	1.76	0.51
18:CB:145:LEU:HD12	18:CB:148:ILE:HG22	1.93	0.51
19:CC:232:LEU:HD22	19:CC:255:ILE:HG23	1.93	0.51
22:CG:106:ARG:HH21	53:CY:328:LYS:HB2	1.76	0.51
30:CP:127:ARG:HH12	30:CP:133:LYS:HA	1.76	0.51
32:CR:514:SER:OG	32:CR:515:GLN:OE1	2.29	0.51
35:Cc:63:ARG:NH2	46:C1:2166:A:O2'	2.44	0.51
43:Co:358:ILE:O	43:Co:399:LYS:HA	2.11	0.51
46:C1:467:C:H4'	46:C1:468:C:H5'	1.93	0.51
48:UH:277:GLU:OE2	48:UH:281:ARG:NH2	2.44	0.51
2:UB:116:ILE:HG12	23:CH:66:ILE:HB	1.92	0.51
4:UD:651:THR:O	4:UD:654:LYS:N	2.44	0.51
4:UD:698:ARG:NH1	48:UH:914:GLU:OE2	2.34	0.51
7:UJ:86:MET:HE1	7:UJ:94:LEU:HD22	1.93	0.51
18:CA:259:ALA:HA	18:CA:271:VAL:HG11	1.92	0.51
22:CG:269:ARG:HG2	22:CG:285:THR:HG22	1.93	0.51
24:CI:835:PHE:O	24:CI:841:ARG:HA	2.11	0.51
32:CR:131:ILE:HD12	32:CR:136:LEU:HD11	1.92	0.51
32:CR:402:LEU:O	32:CR:406:TYR:OH	2.27	0.51
32:CS:397:PRO:HA	32:CS:400:LYS:HG2	1.93	0.51
42:Cn:51:GLY:HA2	42:Cn:77:ILE:HG13	1.93	0.51
46:C1:181:G:O2'	46:C1:183:C:N4	2.44	0.51
46:C1:2120:C:H1'	46:C1:2155:G:H22	1.76	0.51
9:UL:678:ILE:HB	9:UL:692:ILE:HB	1.93	0.50
9:UL:839:PRO:HB3	9:UL:876:ARG:HH12	1.76	0.50
10:UM:549:ALA:HB3	10:UM:562:ALA:HB3	1.92	0.50
15:UU:404:GLY:HA3	15:UU:758:HIS:HB2	1.93	0.50
16:UX:145:ILE:HG23	16:UX:164:PRO:HB2	1.92	0.50
18:CA:65:ALA:O	18:CA:107:LYS:NZ	2.40	0.50
18:CB:167:VAL:HA	18:CB:170:VAL:HG22	1.93	0.50
23:CH:83:THR:HA	23:CH:125:LYS:HB3	1.93	0.50
32:CR:285:ALA:HB3	32:CR:291:LYS:HD3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:571:THR:HG22	32:CR:582:PRO:HA	1.91	0.50
52:CX:284:LEU:HD13	52:CX:323:ILE:HD12	1.93	0.50
1:UA:773:LEU:HD23	1:UA:797:LEU:HD21	1.93	0.50
22:CG:257:ASP:OD2	22:CG:259:LYS:NZ	2.42	0.50
25:CJ:85:MET:HE1	27:CL:630:LEU:HD22	1.94	0.50
32:CS:605:ARG:NH1	32:CS:607:GLN:OE1	2.43	0.50
43:Co:346:ASN:ND2	43:Co:353:GLN:OE1	2.44	0.50
49:UE:185:ILE:HG21	49:UE:221:THR:HA	1.94	0.50
52:CX:335:VAL:HG23	52:CX:375:TYR:HB3	1.92	0.50
2:UB:471:ASP:OD2	2:UB:506:ARG:NH2	2.39	0.50
16:UX:41:PRO:HG2	16:UX:142:ARG:HE	1.77	0.50
20:CD:69:VAL:HG13	20:CD:73:LEU:HB3	1.92	0.50
23:CH:62:ASN:ND2	23:CH:89:MET:SD	2.84	0.50
32:CS:96:GLU:HA	32:CS:99:ILE:HG12	1.93	0.50
32:CS:239:ILE:HG23	32:CS:243:LEU:HD12	1.94	0.50
36:Ce:86:GLU:HA	36:Ce:89:LYS:HG2	1.94	0.50
42:Cn:74:VAL:HG21	42:Cn:104:LEU:HD11	1.94	0.50
45:CU:126:ASP:O	45:CU:129:ARG:NH1	2.40	0.50
13:UQ:915:ASP:OD1	13:UQ:915:ASP:N	2.44	0.50
17:UZ:30:LEU:HD22	17:UZ:283:VAL:HG12	1.93	0.50
22:CG:136:ARG:NH2	43:Co:346:ASN:OD1	2.45	0.50
24:CI:340:ASP:HB3	24:CI:345:LYS:HB2	1.94	0.50
32:CR:518:LEU:HD12	32:CR:570:LEU:HD13	1.94	0.50
32:CR:585:VAL:HB	32:CR:639:ALA:HB3	1.93	0.50
52:CX:275:ARG:NH1	52:CX:320:GLU:OE1	2.44	0.50
9:UL:599:LEU:HD21	9:UL:602:ASN:ND2	2.26	0.50
18:CB:137:LEU:HA	18:CB:301:MET:HE1	1.92	0.50
2:UB:886:GLN:OE1	47:C2:9:U:O2'	2.30	0.50
19:CC:240:LEU:HB3	19:CC:250:LYS:HB3	1.93	0.50
23:CH:232:ASN:O	23:CH:236:ILE:HG12	2.12	0.50
32:CS:24:ARG:HD2	32:CS:143:VAL:HG12	1.92	0.50
36:Ce:76:PHE:O	36:Ce:79:VAL:O	2.29	0.50
38:Ch:98:VAL:HG23	38:Ch:115:LEU:HD12	1.93	0.50
6:UG:134:LEU:HD21	7:UJ:5:LEU:HB2	1.94	0.50
13:UQ:815:ASN:HB2	13:UQ:822:LYS:HG3	1.93	0.50
24:CI:135:ILE:HG12	24:CI:165:ASN:HB2	1.94	0.50
43:Co:351:ARG:HD2	43:Co:405:LEU:HD23	1.94	0.50
48:UH:555:GLY:O	48:UH:567:LEU:CA	2.42	0.50
3:UC:620:ALA:HB1	18:CA:294:PRO:HG3	1.94	0.50
4:UD:487:SER:OG	4:UD:489:ASP:OD1	2.26	0.50
18:CA:250:GLY:CA	18:CA:306:TYR:O	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CF:95:SER:OG	47:C2:191:G:N1	2.43	0.50
24:CI:246:ILE:HG21	24:CI:270:LEU:HD22	1.93	0.50
32:CS:640:THR:OG1	32:CS:645:MET:SD	2.70	0.50
4:UD:253:ASP:OD1	4:UD:255:THR:OG1	2.28	0.50
4:UD:833:ARG:NH1	46:C1:62:U:O2'	2.45	0.50
7:UJ:236:ARG:HD2	7:UJ:239:ILE:HD12	1.94	0.50
10:UM:619:SER:OG	10:UM:620:GLY:N	2.44	0.50
32:CS:396:LEU:HA	32:CS:399:VAL:HG22	1.94	0.50
48:UH:911:ARG:HB3	48:UH:924:THR:HB	1.93	0.50
4:UD:510:THR:OG1	4:UD:517:SER:OG	2.30	0.49
10:UM:452:SER:OG	10:UM:453:LYS:N	2.45	0.49
10:UM:585:HIS:CE1	10:UM:625:LYS:HG3	2.47	0.49
21:CF:35:LYS:HB3	21:CF:40:GLU:HG2	1.93	0.49
24:CI:934:ILE:HD12	24:CI:987:VAL:HG21	1.94	0.49
28:CM:304:ASP:OD1	28:CM:306:THR:OG1	2.28	0.49
32:CR:133:PRO:HB3	32:CR:494:LEU:HD22	1.92	0.49
32:CR:361:ILE:HB	32:CR:367:GLN:HB2	1.94	0.49
50:US:218:ASP:OD1	50:US:222:ASN:ND2	2.44	0.49
50:US:236:SER:OG	50:US:238:ASP:OD1	2.28	0.49
1:UA:427:SER:O	1:UA:444:SER:OG	2.26	0.49
6:UG:267:ASN:O	6:UG:271:ALA:N	2.44	0.49
9:UL:899:LEU:HB3	10:UM:888:LEU:HD11	1.94	0.49
30:CP:47:ARG:HH12	30:CP:50:TYR:HD2	1.60	0.49
32:CR:70:HIS:HB3	32:CR:73:LYS:HB3	1.94	0.49
34:Ca:134:LEU:HB3	34:Ca:219:LYS:H	1.77	0.49
50:US:195:ASP:N	50:US:195:ASP:OD1	2.43	0.49
2:UB:668:LEU:HB3	2:UB:726:LEU:HD12	1.94	0.49
10:UM:222:ALA:HB2	10:UM:230:ALA:HA	1.94	0.49
11:UN:929:ILE:HD11	28:CM:79:LEU:HB2	1.93	0.49
19:CC:247:ASP:O	19:CC:251:ALA:CB	2.60	0.49
24:CI:959:ARG:NH1	26:CK:287:TYR:O	2.45	0.49
29:CN:103:PRO:HG3	29:CO:232:LEU:HD21	1.94	0.49
32:CR:125:LEU:HD22	32:CR:151:LEU:HG	1.93	0.49
50:US:176:SER:O	50:US:182:ARG:NH2	2.42	0.49
1:UA:724:LEU:HD22	1:UA:749:VAL:HG22	1.95	0.49
7:UJ:260:VAL:HG21	14:UR:228:LEU:HD21	1.94	0.49
10:UM:487:LEU:HD21	10:UM:507:PRO:HG2	1.92	0.49
17:UZ:64:LEU:HD11	17:UZ:281:PHE:HB3	1.94	0.49
18:CB:156:VAL:HG12	18:CB:225:VAL:HB	1.94	0.49
22:CG:164:THR:HG21	22:CG:222:LYS:HB3	1.94	0.49
23:CH:84:GLY:O	23:CH:90:ASN:ND2	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:34:THR:OG1	29:CO:36:ARG:NH1	2.46	0.49
36:Ce:21:ASP:OD1	36:Ce:21:ASP:N	2.43	0.49
1:UA:596:ILE:HD11	1:UA:675:VAL:HG21	1.95	0.49
4:UD:666:LEU:HB2	4:UD:671:ARG:HE	1.77	0.49
4:UD:833:ARG:NH2	46:C1:64:C:OP1	2.40	0.49
13:UQ:615:PHE:N	13:UQ:629:ILE:O	2.45	0.49
23:CH:219:ARG:HA	23:CH:251:HIS:O	2.12	0.49
25:CJ:168:GLN:HG2	25:CJ:172:LYS:HE3	1.94	0.49
28:CM:47:VAL:HB	28:CM:379:LEU:HD21	1.95	0.49
32:CR:567:LEU:HD13	32:CR:587:GLN:HB3	1.94	0.49
34:Ca:152:LYS:HG3	34:Ca:153:THR:HG23	1.94	0.49
36:Ce:57:VAL:HG23	36:Ce:61:LYS:HB2	1.95	0.49
49:UE:220:TRP:HA	49:UE:223:VAL:HG12	1.93	0.49
52:CX:199:VAL:HG22	52:CX:236:LEU:HD11	1.93	0.49
16:UX:1:ALA:HB1	25:CJ:37:MET:HE1	1.95	0.49
32:CS:586:ILE:HD11	32:CS:635:ILE:HD12	1.95	0.49
46:C1:381:G:H21	46:C1:385:A:H62	1.59	0.49
52:CX:418:ALA:O	52:CX:422:ARG:NH2	2.45	0.49
7:UJ:296:LEU:HD22	7:UJ:312:LEU:HD13	1.95	0.49
26:CK:173:ARG:NH1	26:CK:257:VAL:O	2.38	0.49
32:CS:32:ASP:O	32:CS:35:LYS:NZ	2.38	0.49
32:CS:844:TYR:CD2	32:CS:916:MET:HE2	2.48	0.49
46:C1:1753:G:N1	46:C1:2158:G:OP2	2.36	0.49
1:UA:798:ILE:HD12	15:UU:1040:VAL:HB	1.94	0.49
11:UN:341:PHE:HE1	28:CM:250:MET:HE2	1.78	0.49
17:UZ:86:PRO:HD3	17:UZ:261:THR:HG21	1.95	0.49
19:CC:195:ALA:HA	19:CC:198:VAL:HG12	1.95	0.49
20:CD:288:ASN:HB3	20:CD:372:SER:HB3	1.95	0.49
22:CG:270:LEU:HD11	22:CG:294:LEU:HD21	1.94	0.49
30:CP:58:VAL:HG13	30:CP:98:LEU:HD21	1.95	0.49
32:CR:23:LYS:O	32:CR:146:GLY:N	2.45	0.49
32:CR:725:VAL:O	32:CR:761:VAL:HA	2.13	0.49
32:CS:888:GLY:O	32:CS:891:ARG:NE	2.45	0.49
34:Ca:70:LEU:HA	34:Ca:73:LEU:HB2	1.95	0.49
48:UH:591:VAL:HG21	48:UH:609:ILE:HG21	1.95	0.49
2:UB:723:ILE:HG23	2:UB:773:LEU:HD22	1.95	0.49
10:UM:724:THR:HA	10:UM:727:THR:HG22	1.95	0.49
12:UO:299:VAL:HB	12:UO:309:ALA:HB3	1.95	0.49
16:UX:75:LEU:HD13	16:UX:118:TRP:HH2	1.78	0.49
20:CD:210:VAL:O	20:CD:214:LEU:HB3	2.13	0.49
22:CG:191:TYR:HE1	22:CG:231:LYS:HD3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:819:ARG:NH1	24:CI:823:HIS:O	2.46	0.49
5:UF:125:ARG:NH1	46:C1:444:U:OP1	2.43	0.49
10:UM:622:LYS:NZ	10:UM:642:SER:O	2.40	0.49
15:UU:691:VAL:HB	15:UU:701:ARG:HB2	1.93	0.49
18:CA:194:ILE:HD11	19:CC:162:SER:HB3	1.93	0.49
20:CD:201:LEU:HD21	20:CD:229:LEU:HD21	1.95	0.49
32:CR:139:THR:HA	32:CR:142:THR:HG22	1.94	0.49
32:CR:829:LEU:HD11	32:CR:923:PHE:HE1	1.78	0.49
32:CS:427:LYS:HD3	32:CS:430:LYS:HE3	1.95	0.49
49:UE:187:ARG:NH1	50:US:305:ASP:OD1	2.46	0.49
1:UA:577:THR:HG21	1:UA:677:GLY:HA2	1.95	0.48
4:UD:392:ARG:HB3	4:UD:419:PHE:HE1	1.78	0.48
6:UG:215:LYS:HG2	46:C1:291:C:C2	2.48	0.48
18:CB:253:LEU:HB3	18:CB:304:CYS:HB2	1.95	0.48
21:CE:34:LEU:HD11	21:CE:101:VAL:HG13	1.94	0.48
24:CI:950:ALA:O	24:CI:961:GLN:HA	2.12	0.48
25:CJ:64:LEU:HD11	27:CL:619:ILE:HG13	1.95	0.48
32:CS:849:LEU:HD12	32:CS:853:VAL:HG11	1.95	0.48
17:UZ:104:PRO:HG2	17:UZ:212:ALA:HB2	1.95	0.48
24:CI:302:LEU:HB2	24:CI:776:TYR:HB3	1.95	0.48
32:CR:776:GLY:HA3	32:CR:816:ASP:HB2	1.96	0.48
36:Ce:87:LEU:HB3	36:Ce:96:VAL:HG21	1.95	0.48
49:UE:158:ASN:HD21	49:UE:188:MET:HA	1.78	0.48
52:CX:425:ILE:O	52:CX:430:ARG:NH1	2.45	0.48
4:UD:132:ILE:HG12	4:UD:158:THR:HG22	1.95	0.48
6:UG:323:LYS:HE3	46:C1:278:A:H61	1.79	0.48
7:UJ:75:SER:N	7:UJ:78:SER:OG	2.44	0.48
23:CH:335:VAL:HG12	23:CH:339:MET:HE2	1.94	0.48
30:CP:139:ARG:NH1	30:CP:189:MET:O	2.45	0.48
32:CS:547:SER:OG	32:CS:637:ARG:NH2	2.46	0.48
32:CS:660:TYR:OH	32:CS:715:ARG:NH1	2.44	0.48
46:C1:461:G:N7	53:CY:377:ARG:NH2	2.62	0.48
4:UD:6:CYS:HB2	4:UD:863:ILE:HD13	1.95	0.48
18:CA:213:PRO:HB2	18:CA:245:LEU:HD22	1.94	0.48
22:CG:307:SER:OG	22:CG:308:LYS:N	2.45	0.48
32:CR:196:CYS:HB2	32:CR:489:TRP:CD1	2.48	0.48
32:CS:220:LEU:HD12	32:CS:221:PRO:HD2	1.95	0.48
3:UC:639:LYS:HB3	3:UC:642:LEU:HD13	1.95	0.48
4:UD:632:VAL:HB	4:UD:650:VAL:HB	1.96	0.48
6:UG:579:ASP:O	6:UG:582:ARG:N	2.46	0.48
10:UM:126:LEU:HB2	10:UM:140:ILE:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UO:216:VAL:HB	12:UO:227:MET:HB2	1.93	0.48
14:UR:331:VAL:HB	14:UR:337:GLU:HB2	1.96	0.48
16:UX:54:PRO:HB3	16:UX:85:ALA:HB1	1.94	0.48
29:CO:114:ILE:HB	29:CO:122:ILE:HB	1.94	0.48
48:UH:148:ILE:HG22	48:UH:172:ILE:HG12	1.95	0.48
5:UF:173:ARG:HD2	19:CC:57:THR:HB	1.94	0.48
10:UM:83:LEU:HD11	39:CI:85:LYS:HE3	1.95	0.48
14:UR:440:GLN:HG2	14:UR:456:ARG:HD2	1.94	0.48
15:UU:43:LEU:HA	15:UU:359:ASN:HD21	1.78	0.48
15:UU:232:VAL:HA	15:UU:248:TYR:HA	1.95	0.48
17:UZ:267:VAL:HG22	17:UZ:278:VAL:HG21	1.95	0.48
19:CC:185:ASP:OD1	19:CC:317:ARG:NH1	2.46	0.48
32:CS:27:PHE:O	32:CS:150:VAL:HA	2.14	0.48
50:US:522:HIS:NE2	50:US:531:GLU:OE1	2.47	0.48
4:UD:51:GLY:HA2	4:UD:77:VAL:HG23	1.95	0.48
5:UF:92:THR:HA	5:UF:95:ILE:HD12	1.96	0.48
6:UG:321:ASP:O	6:UG:323:LYS:N	2.46	0.48
9:UL:109:HIS:ND1	9:UL:129:SER:OG	2.42	0.48
9:UL:835:GLN:HE21	9:UL:870:ASN:HD22	1.62	0.48
9:UL:861:LEU:HD11	9:UL:877:ILE:HG22	1.95	0.48
13:UQ:109:THR:HG22	13:UQ:129:LEU:HG	1.96	0.48
22:CG:352:ARG:HB3	22:CG:398:MET:HE3	1.95	0.48
24:CI:113:ARG:HD3	24:CI:308:THR:HG23	1.95	0.48
24:CI:139:MET:HG2	24:CI:169:ILE:HB	1.96	0.48
25:CJ:79:LEU:HD12	25:CJ:91:LYS:HA	1.95	0.48
9:UL:41:VAL:HG11	9:UL:394:LEU:HD11	1.95	0.48
9:UL:517:HIS:HD2	9:UL:518:PRO:HD2	1.78	0.48
13:UQ:403:VAL:HB	13:UQ:412:ALA:HB3	1.96	0.48
20:CD:297:VAL:HG13	20:CD:343:ILE:HG22	1.96	0.48
50:US:154:THR:HG23	50:US:156:ARG:H	1.79	0.48
52:CX:422:ARG:NH1	52:CX:452:GLU:O	2.46	0.48
53:CY:235:ILE:HA	53:CY:239:VAL:HB	1.94	0.48
2:UB:21:PRO:HB3	46:C1:1732:C:H1'	1.94	0.48
3:UC:607:LYS:NZ	46:C1:1175:A:OP2	2.46	0.48
8:UK:2:SER:HA	8:UK:10:ARG:HH22	1.78	0.48
18:CB:97:LEU:HD13	18:CB:172:ASP:HA	1.96	0.48
22:CG:110:LYS:NZ	53:CY:328:LYS:HE3	2.28	0.48
24:CI:138:LEU:HD21	24:CI:150:THR:HG23	1.95	0.48
32:CS:885:LEU:HG	32:CS:889:LEU:HD12	1.95	0.48
37:Cg:65:PRO:HB2	53:CY:325:THR:HG21	1.95	0.48
5:UF:313:HIS:O	5:UF:317:ILE:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CB:79:LYS:HZ2	18:CB:151:LYS:HB2	1.79	0.48
24:CI:964:ARG:NH2	46:C1:1759:U:O3'	2.47	0.48
29:CO:99:LEU:HD21	29:CO:238:CYS:HB3	1.96	0.48
32:CR:265:LEU:HD13	32:CR:297:VAL:HG23	1.95	0.48
32:CS:29:VAL:HG23	32:CS:202:ILE:HG23	1.96	0.48
36:Ce:41:LYS:HD3	36:Ce:45:ARG:HD2	1.96	0.48
39:CI:97:ARG:HB3	39:CI:131:VAL:HG13	1.96	0.48
2:UB:595:THR:HA	2:UB:642:LEU:HD11	1.95	0.47
6:UG:147:ASN:HB2	6:UG:435:PRO:HA	1.95	0.47
14:UR:366:HIS:ND1	14:UR:369:GLU:OE2	2.38	0.47
18:CA:110:SER:HB3	33:CT:141:ILE:HD11	1.95	0.47
24:CI:73:ILE:HG22	24:CI:137:LEU:HB2	1.95	0.47
24:CI:246:ILE:HB	24:CI:798:ILE:HB	1.96	0.47
25:CJ:107:ALA:HA	25:CJ:110:ARG:HD3	1.96	0.47
26:CK:187:SER:O	26:CK:226:ARG:NH1	2.43	0.47
50:US:82:GLU:OE1	50:US:86:ARG:NH1	2.46	0.47
50:US:341:THR:HG22	50:US:447:PRO:HD2	1.95	0.47
4:UD:549:VAL:HA	4:UD:565:ASP:HA	1.96	0.47
6:UG:284:LEU:HB2	6:UG:294:VAL:HB	1.95	0.47
19:CC:86:LEU:HD13	19:CC:116:VAL:HG21	1.96	0.47
19:CC:385:LYS:HD3	19:CC:407:LEU:HD22	1.96	0.47
26:CK:247:THR:HG1	26:CK:251:SER:HG	1.60	0.47
32:CR:633:ALA:HB3	32:CR:723:VAL:HG22	1.95	0.47
39:CI:31:ARG:NH1	46:C1:1503:U:O2'	2.47	0.47
1:UA:11:LEU:HB2	1:UA:695:LEU:HB2	1.97	0.47
14:UR:400:ILE:HB	14:UR:410:ALA:HB3	1.95	0.47
36:Ce:57:VAL:O	36:Ce:61:LYS:HB2	2.14	0.47
45:CU:189:THR:HG23	45:CU:191:THR:H	1.79	0.47
50:US:423:ARG:N	50:US:427:GLU:OE2	2.48	0.47
1:UA:15:TYR:OH	1:UA:18:GLY:O	2.24	0.47
2:UB:320:THR:OG1	2:UB:321:GLU:N	2.47	0.47
22:CG:420:LEU:O	22:CG:429:LEU:N	2.46	0.47
32:CS:42:TYR:HA	32:CS:45:MET:HE2	1.96	0.47
32:CS:158:SER:HB2	32:CS:691:GLY:HA3	1.96	0.47
2:UB:728:THR:O	2:UB:732:ILE:HG13	2.14	0.47
4:UD:160:ASP:OD2	4:UD:162:ASN:ND2	2.47	0.47
9:UL:210:GLU:OE2	9:UL:212:HIS:NE2	2.45	0.47
23:CH:292:TYR:HE2	23:CH:324:GLY:HA3	1.80	0.47
26:CK:105:LYS:NZ	46:C1:2164:C:OP2	2.47	0.47
29:CO:37:LEU:O	29:CO:110:LEU:HA	2.14	0.47
31:CQ:218:ILE:HG22	31:CQ:225:ILE:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:UH:223:VAL:HG13	48:UH:227:LEU:HD12	1.95	0.47
9:UL:534:PHE:HB2	9:UL:560:ARG:HB2	1.96	0.47
10:UM:798:LEU:O	10:UM:837:HIS:NE2	2.45	0.47
15:UU:71:LEU:H	15:UU:86:THR:HB	1.79	0.47
15:UU:514:ALA:HB2	15:UU:547:VAL:HG13	1.97	0.47
28:CM:14:GLN:OE1	28:CM:21:GLN:NE2	2.47	0.47
32:CS:380:LEU:HD21	32:CS:402:LEU:HG	1.96	0.47
32:CS:742:PHE:HB3	32:CS:762:MET:HB3	1.95	0.47
45:CU:186:ALA:O	45:CU:192:ASN:ND2	2.38	0.47
3:UC:598:ARG:NH2	46:C1:1060:U:O2'	2.44	0.47
7:UJ:38:ARG:NH2	47:C2:43:C:OP1	2.48	0.47
7:UJ:442:ILE:HA	7:UJ:445:VAL:HG12	1.97	0.47
9:UL:425:HIS:CE1	9:UL:450:LYS:HG3	2.50	0.47
9:UL:509:HIS:HB3	9:UL:528:ALA:HB3	1.96	0.47
10:UM:248:LEU:HD22	10:UM:289:MET:HG2	1.97	0.47
12:UO:138:LYS:HD3	35:Cc:111:MET:HE1	1.96	0.47
13:UQ:248:ALA:HB3	13:UQ:309:LEU:HD12	1.97	0.47
15:UU:564:SER:HB3	15:UU:620:ARG:HH21	1.79	0.47
20:CD:403:ASN:OD1	20:CD:406:ARG:NH2	2.48	0.47
26:CK:89:LEU:HD11	26:CK:117:LEU:HB2	1.97	0.47
30:CP:58:VAL:HA	30:CP:112:LEU:HD21	1.97	0.47
32:CS:483:GLY:O	32:CS:488:LYS:NZ	2.47	0.47
32:CS:635:ILE:HB	32:CS:725:VAL:HG23	1.96	0.47
32:CS:845:ALA:HA	32:CS:916:MET:HE1	1.97	0.47
34:Ca:105:PHE:CD2	34:Ca:213:ARG:HA	2.50	0.47
34:Ca:214:LYS:NZ	46:C1:1471:U:OP1	2.46	0.47
42:Cn:92:CYS:HB3	42:Cn:132:LEU:HD21	1.96	0.47
43:Co:371:LEU:HB3	43:Co:388:VAL:HG21	1.96	0.47
46:C1:627:A:N6	46:C1:1051:G:O2'	2.48	0.47
48:UH:238:PHE:HE1	48:UH:275:PRO:HB3	1.80	0.47
51:Cl:50:ALA:O	51:Cl:68:ARG:NH1	2.47	0.47
53:CY:275:TYR:HA	53:CY:278:THR:HG22	1.97	0.47
4:UD:555:SER:HB2	4:UD:560:MET:HB3	1.97	0.47
4:UD:632:VAL:O	4:UD:649:VAL:HA	2.15	0.47
9:UL:396:LEU:HD23	9:UL:418:LEU:HD12	1.97	0.47
9:UL:702:LEU:HD11	9:UL:711:LEU:HD12	1.96	0.47
32:CR:547:SER:HB2	32:CR:637:ARG:HH22	1.79	0.47
32:CS:95:PHE:HA	32:CS:98:PHE:CE1	2.49	0.47
48:UH:372:LEU:HD13	48:UH:600:ARG:HH12	1.79	0.47
52:CX:430:ARG:NH2	52:CX:457:ARG:O	2.48	0.47
2:UB:654:VAL:HG12	2:UB:657:MET:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:112:MET:HG3	7:UJ:116:LYS:HE3	1.96	0.47
13:UQ:455:VAL:HA	48:UH:888:ILE:HD11	1.96	0.47
15:UU:415:ARG:NE	15:UU:458:GLU:O	2.46	0.47
16:UX:123:CYS:HB3	16:UX:125:HIS:NE2	2.29	0.47
21:CF:53:VAL:O	21:CF:79:TYR:HA	2.15	0.47
24:CI:974:ARG:NH1	46:C1:2183:A:OP2	2.48	0.47
32:CR:249:ILE:HA	32:CR:252:LEU:HD12	1.96	0.47
49:UE:229:LEU:HD23	49:UE:235:LEU:HD13	1.95	0.47
7:UJ:139:PHE:HB3	7:UJ:148:PHE:HD1	1.79	0.47
7:UJ:170:TYR:O	7:UJ:173:SER:O	2.33	0.47
9:UL:613:MET:HG2	9:UL:624:THR:HG22	1.97	0.47
13:UQ:637:PHE:O	13:UQ:664:SER:N	2.48	0.47
20:CD:119:PHE:HA	20:CD:122:ILE:HG12	1.97	0.47
28:CM:243:ASN:N	28:CM:258:ALA:O	2.42	0.47
34:Ca:204:ILE:O	46:C1:1648:G:O2'	2.33	0.47
48:UH:344:SER:OG	48:UH:357:SER:O	2.28	0.47
53:CY:230:THR:HG23	53:CY:231:LEU:HD12	1.96	0.47
1:UA:177:ILE:HB	1:UA:189:THR:HB	1.96	0.46
1:UA:730:TYR:HB3	1:UA:753:ILE:HG12	1.96	0.46
4:UD:339:VAL:HG13	4:UD:351:VAL:HG13	1.96	0.46
7:UJ:45:PHE:HA	7:UJ:48:ILE:HD12	1.96	0.46
10:UM:708:LEU:HB2	10:UM:720:TRP:HB2	1.98	0.46
26:CK:87:ARG:NH1	26:CK:134:GLU:O	2.47	0.46
32:CR:723:VAL:HG23	32:CR:766:LEU:HD11	1.97	0.46
32:CR:727:TYR:HE1	32:CR:762:MET:HB2	1.79	0.46
2:UB:116:ILE:HG13	23:CH:58:GLU:HG3	1.96	0.46
2:UB:492:VAL:HG22	2:UB:494:GLY:H	1.81	0.46
10:UM:283:LEU:HD23	10:UM:284:ASN:HB2	1.97	0.46
13:UQ:739:SER:O	13:UQ:784:HIS:NE2	2.48	0.46
24:CI:103:PRO:HG2	24:CI:247:ASP:HA	1.97	0.46
24:CI:122:GLU:HG3	24:CI:796:MET:HE1	1.96	0.46
24:CI:523:MET:HA	24:CI:526:ARG:HB2	1.97	0.46
27:CL:711:GLU:O	27:CL:715:ARG:HG3	2.14	0.46
39:CI:32:ILE:HG21	39:CI:111:ALA:HA	1.96	0.46
46:C1:1169:A:H4'	46:C1:1170:G:H5'	1.98	0.46
48:UH:575:SER:HA	48:UH:578:ILE:HG22	1.96	0.46
48:UH:646:LYS:HB2	48:UH:730:PHE:HE1	1.79	0.46
48:UH:700:ASP:OD1	48:UH:700:ASP:N	2.48	0.46
1:UA:576:ASN:HB2	1:UA:591:GLY:HA2	1.97	0.46
10:UM:22:THR:HG22	10:UM:39:LEU:HA	1.98	0.46
11:UN:915:PHE:O	11:UN:919:THR:OG1	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CB:258:LYS:HE2	18:CB:260:SER:HB3	1.96	0.46
22:CG:565:LEU:HG	22:CG:578:VAL:HG12	1.96	0.46
27:CL:704:ALA:HB3	27:CL:707:GLU:HG2	1.96	0.46
32:CR:828:GLU:O	32:CR:832:LEU:HB2	2.15	0.46
32:CS:93:ASP:OD1	32:CS:93:ASP:N	2.43	0.46
32:CS:141:GLU:O	32:CS:479:ARG:NH1	2.48	0.46
32:CS:154:LYS:HE3	32:CS:161:GLN:HG3	1.98	0.46
32:CS:162:LEU:HA	32:CS:165:MET:HG3	1.98	0.46
2:UB:689:ILE:O	2:UB:722:GLN:NE2	2.48	0.46
14:UR:570:HIS:ND1	14:UR:573:SER:OG	2.40	0.46
22:CG:126:GLU:OE1	22:CG:130:ARG:NH2	2.49	0.46
23:CH:172:GLU:OE1	45:CU:123:ARG:NH2	2.41	0.46
24:CI:274:LEU:HB2	24:CI:773:ALA:HA	1.97	0.46
31:CQ:96:LYS:HD3	31:CQ:96:LYS:HA	1.71	0.46
32:CR:725:VAL:HB	32:CR:762:MET:HB3	1.98	0.46
32:CS:143:VAL:HG21	32:CS:149:VAL:HG22	1.96	0.46
32:CS:571:THR:HG21	32:CS:580:PRO:HB2	1.98	0.46
34:Ca:119:THR:HG21	34:Ca:156:ALA:H	1.80	0.46
1:UA:3:THR:HG21	1:UA:607:LEU:HD13	1.97	0.46
24:CI:1116:ARG:NH2	46:C1:1079:C:OP2	2.49	0.46
25:CJ:102:THR:HG22	25:CJ:104:SER:H	1.81	0.46
29:CN:179:THR:HB	29:CN:221:VAL:HG11	1.97	0.46
36:Ce:82:ARG:HH12	36:Ce:86:GLU:HG2	1.81	0.46
12:UO:449:ASP:HB3	12:UO:452:ILE:HB	1.98	0.46
13:UQ:922:ALA:HB3	13:UQ:925:ARG:HG2	1.97	0.46
18:CB:131:ASN:HD22	18:CB:134:ARG:HD3	1.79	0.46
19:CC:267:SER:OG	19:CC:268:GLU:N	2.49	0.46
22:CG:231:LYS:NZ	47:C2:119:C:O2	2.39	0.46
24:CI:887:PHE:CE2	24:CI:899:ILE:HG22	2.51	0.46
32:CS:924:GLY:HA2	32:CS:927:VAL:HG12	1.97	0.46
47:C2:127:A:N7	47:C2:188:G:N2	2.64	0.46
49:UE:223:VAL:HG21	49:UI:268:ALA:HB3	1.98	0.46
49:UI:200:LEU:HD21	49:UI:214:LEU:HD22	1.97	0.46
49:UI:265:MET:HE2	49:UI:265:MET:HB3	1.85	0.46
1:UA:618:LEU:HD23	1:UA:673:VAL:HB	1.97	0.46
4:UD:563:VAL:O	4:UD:570:ILE:HA	2.15	0.46
5:UF:339:ILE:HG22	5:UF:363:ARG:HB3	1.98	0.46
7:UJ:48:ILE:HD13	7:UJ:123:ARG:HE	1.79	0.46
7:UJ:228:MET:HA	7:UJ:231:LYS:HG2	1.97	0.46
12:UO:169:VAL:HB	12:UO:183:PHE:HB2	1.98	0.46
14:UR:152:THR:HG21	46:C1:273:G:H21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:246:ILE:HD12	24:CI:270:LEU:HB3	1.98	0.46
32:CR:56:VAL:HA	32:CR:122:MET:HB3	1.98	0.46
32:CS:29:VAL:HA	32:CS:202:ILE:O	2.16	0.46
32:CS:723:VAL:HG23	32:CS:766:LEU:HD21	1.98	0.46
39:CI:54:ARG:NH1	46:C1:1502:U:O2	2.49	0.46
43:Co:371:LEU:HG	43:Co:388:VAL:HG11	1.97	0.46
2:UB:608:HIS:HB3	2:UB:611:CYS:HB3	1.96	0.46
7:UJ:67:VAL:HG23	7:UJ:68:PRO:HD3	1.98	0.46
13:UQ:645:ARG:NH1	13:UQ:646:ASP:OD2	2.48	0.46
17:UZ:66:LEU:HD13	17:UZ:281:PHE:CZ	2.50	0.46
18:CB:137:LEU:HD13	18:CB:227:PHE:HE2	1.81	0.46
24:CI:815:VAL:HG12	24:CI:905:VAL:HA	1.98	0.46
26:CK:217:PRO:HB3	27:CL:558:LEU:HD22	1.98	0.46
32:CS:58:TRP:HB2	32:CS:104:ILE:HD11	1.96	0.46
43:Co:353:GLN:HG3	43:Co:405:LEU:HG	1.97	0.46
4:UD:509:ALA:HB1	4:UD:516:ILE:HD11	1.98	0.46
9:UL:587:SER:HA	9:UL:609:PRO:HA	1.98	0.46
10:UM:520:GLN:HA	10:UM:538:LEU:O	2.15	0.46
13:UQ:929:ILE:HD12	13:UQ:951:LEU:HD22	1.98	0.46
21:CF:95:SER:HG	47:C2:191:G:H1	1.60	0.46
30:CP:184:VAL:HG13	30:CP:197:LEU:HD13	1.96	0.46
32:CR:544:TYR:HA	32:CR:637:ARG:HH21	1.80	0.46
34:Ca:120:LEU:HD11	34:Ca:140:ILE:HD11	1.97	0.46
47:C2:49:U:H2'	47:C2:50:G:H8	1.81	0.46
48:UH:88:ARG:O	48:UH:90:ARG:NH1	2.49	0.46
50:US:112:ASN:OD1	50:US:113:TRP:N	2.49	0.46
5:UF:339:ILE:HG13	5:UF:384:TRP:HZ3	1.81	0.46
9:UL:682:ASP:HB2	9:UL:689:ILE:HD11	1.98	0.46
14:UR:324:ASP:N	14:UR:324:ASP:OD1	2.47	0.46
23:CH:21:LEU:HD23	23:CH:31:ILE:HD11	1.98	0.46
24:CI:353:ILE:HD11	32:CR:206:LEU:HD12	1.96	0.46
28:CM:403:LYS:NZ	46:C1:1664:U:H4'	2.31	0.46
32:CR:874:VAL:HG13	32:CR:922:HIS:HD2	1.80	0.46
41:Cm:88:LYS:O	41:Cm:92:LYS:HB3	2.16	0.46
51:Cl:32:LEU:HD11	51:Cl:69:LEU:HD23	1.97	0.46
4:UD:283:SER:HB2	4:UD:329:MET:HG3	1.98	0.45
23:CH:22:VAL:HG13	23:CH:120:LEU:HD13	1.98	0.45
23:CH:139:THR:HB	23:CH:179:SER:H	1.82	0.45
26:CK:15:ARG:NH1	26:CK:74:ASP:OD2	2.46	0.45
28:CM:87:GLY:HA2	28:CM:112:ILE:HG23	1.98	0.45
36:Ce:163:ILE:HG22	36:Ce:194:GLU:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Cm:103:ILE:HD11	41:Cm:129:PHE:HE1	1.80	0.45
50:US:399:VAL:HG21	50:US:493:LEU:HD23	1.98	0.45
4:UD:695:GLN:HG3	4:UD:858:LEU:HD22	1.99	0.45
9:UL:384:GLN:HB3	9:UL:396:LEU:HD11	1.98	0.45
9:UL:468:ALA:HA	9:UL:484:THR:HG22	1.97	0.45
12:UO:46:HIS:NE2	12:UO:106:GLU:OE2	2.48	0.45
24:CI:379:LEU:HD23	32:CR:209:LEU:HD13	1.97	0.45
28:CM:201:THR:N	28:CM:216:VAL:O	2.49	0.45
32:CR:742:PHE:HB3	32:CR:762:MET:HG3	1.99	0.45
32:CS:659:ASP:HB2	32:CS:664:LYS:HG3	1.97	0.45
46:C1:1123:G:OP2	46:C1:1123:G:N2	2.47	0.45
48:UH:30:PHE:HB3	48:UH:83:PRO:HA	1.97	0.45
50:US:266:GLN:OE1	50:US:298:THR:OG1	2.35	0.45
14:UR:375:ARG:HH22	46:C1:134:C:H5	1.65	0.45
15:UU:353:VAL:HG22	15:UU:363:THR:HG22	1.99	0.45
24:CI:739:TYR:CZ	24:CI:743:LYS:HD2	2.51	0.45
32:CR:518:LEU:HD11	32:CR:653:ALA:HA	1.97	0.45
32:CS:26:PHE:O	32:CS:199:CYS:HA	2.16	0.45
32:CS:314:SER:OG	32:CS:316:SER:O	2.34	0.45
46:C1:1148:G:N2	46:C1:2179:C:OP2	2.49	0.45
50:US:264:GLN:HA	50:US:267:GLU:HG2	1.98	0.45
10:UM:393:THR:HG23	10:UM:395:SER:H	1.81	0.45
10:UM:570:ILE:HG12	10:UM:629:LEU:HD11	1.99	0.45
13:UQ:753:VAL:HB	13:UQ:763:ALA:HB3	1.98	0.45
17:UZ:155:ALA:O	17:UZ:182:VAL:N	2.50	0.45
22:CG:583:GLY:HA2	22:CG:599:CYS:HA	1.98	0.45
24:CI:71:VAL:HG22	24:CI:135:ILE:HB	1.99	0.45
24:CI:285:ARG:NH1	24:CI:295:THR:OG1	2.47	0.45
28:CM:86:SER:OG	28:CM:88:ASP:OD1	2.31	0.45
29:CO:122:ILE:HD12	29:CO:144:LEU:HD21	1.98	0.45
31:CQ:168:SER:OG	31:CQ:217:HIS:ND1	2.45	0.45
52:CX:264:ARG:HG2	52:CX:268:MET:HE1	1.99	0.45
8:UK:66:GLY:O	8:UK:70:ARG:HB2	2.17	0.45
9:UL:94:LEU:HD11	9:UL:139:LEU:HD22	1.99	0.45
9:UL:451:ILE:HB	9:UL:461:ARG:HB2	1.99	0.45
10:UM:283:LEU:HD21	10:UM:348:VAL:HG21	1.98	0.45
12:UO:547:VAL:HG11	49:UE:243:SER:HB3	1.99	0.45
18:CA:156:VAL:HG22	18:CA:225:VAL:HB	1.98	0.45
22:CG:339:LEU:HD23	22:CG:339:LEU:HA	1.83	0.45
32:CS:13:THR:O	32:CS:17:ASN:ND2	2.49	0.45
4:UD:297:ASP:OD1	4:UD:297:ASP:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:453:VAL:HB	4:UD:472:VAL:HB	1.98	0.45
4:UD:832:PHE:HB2	4:UD:835:ILE:HD11	1.98	0.45
6:UG:270:ASN:HB3	6:UG:272:ILE:HG12	1.98	0.45
10:UM:788:LEU:N	10:UM:795:ASP:OD2	2.42	0.45
23:CH:244:ASN:ND2	23:CH:247:VAL:O	2.48	0.45
24:CI:105:THR:HB	24:CI:335:TRP:HB3	1.98	0.45
27:CL:524:ASP:OD1	27:CL:525:HIS:N	2.49	0.45
30:CP:41:THR:HG22	30:CP:99:ILE:HG22	1.97	0.45
32:CR:795:ARG:NH1	32:CR:890:GLN:O	2.47	0.45
48:UH:544:ARG:HA	48:UH:547:VAL:HG12	1.99	0.45
2:UB:813:PRO:HA	29:CN:152:GLY:HA2	1.98	0.45
4:UD:120:ARG:HE	54:UP:330:ARG:HG2	1.81	0.45
5:UF:33:ILE:HG21	6:UG:91:ILE:HD11	1.99	0.45
5:UF:324:MET:HE1	5:UF:334:THR:HA	1.99	0.45
26:CK:163:LEU:HD11	26:CK:265:PRO:HB3	1.98	0.45
26:CK:292:ARG:NH1	27:CL:524:ASP:OD1	2.49	0.45
32:CS:188:ARG:NH1	32:CS:493:LEU:O	2.34	0.45
45:CU:223:GLN:O	45:CU:230:ARG:NH2	2.50	0.45
1:UA:777:VAL:O	1:UA:781:THR:OG1	2.29	0.45
2:UB:711:ASP:OD1	2:UB:711:ASP:N	2.45	0.45
4:UD:66:GLU:OE1	4:UD:545:TYR:OH	2.29	0.45
4:UD:836:MET:N	4:UD:863:ILE:O	2.50	0.45
5:UF:398:ILE:HA	5:UF:401:VAL:HG22	1.98	0.45
6:UG:580:GLU:HA	6:UG:583:LEU:HD13	1.98	0.45
8:UK:83:PHE:O	24:CI:1052:LYS:NZ	2.38	0.45
19:CC:187:LEU:O	19:CC:191:ILE:HD12	2.17	0.45
23:CH:284:GLU:OE1	45:CU:129:ARG:NH2	2.49	0.45
26:CK:134:GLU:HG3	40:Cj:128:LYS:HD3	1.98	0.45
49:UE:154:GLY:O	49:UE:158:ASN:ND2	2.35	0.45
1:UA:385:VAL:HA	1:UA:401:SER:HB2	1.97	0.45
9:UL:864:PHE:O	9:UL:867:ARG:O	2.35	0.45
12:UO:166:ASP:OD1	12:UO:168:THR:OG1	2.31	0.45
13:UQ:264:GLY:HA2	13:UQ:280:ARG:O	2.16	0.45
13:UQ:578:LYS:HD3	13:UQ:581:ARG:NE	2.31	0.45
32:CR:140:ILE:HD12	32:CR:490:LEU:HD13	1.99	0.45
32:CR:844:TYR:HA	32:CR:849:LEU:HB2	1.98	0.45
32:CS:56:VAL:HA	32:CS:122:MET:O	2.16	0.45
39:CI:83:ARG:HA	39:CI:83:ARG:HD2	1.74	0.45
41:Cm:115:GLU:HA	41:Cm:118:ARG:HD2	1.99	0.45
50:US:385:LEU:HD23	50:US:385:LEU:HA	1.83	0.45
2:UB:641:ILE:HG21	50:US:538:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:UG:327:TRP:HH2	11:UN:867:LYS:HA	1.82	0.45
11:UN:876:VAL:HG12	11:UN:879:ASN:H	1.82	0.45
13:UQ:241:PRO:HA	13:UQ:257:ALA:HA	1.98	0.45
19:CC:36:ASP:HA	19:CC:39:LYS:HG2	1.98	0.45
19:CC:179:GLN:HA	20:CD:185:ARG:NH2	2.29	0.45
22:CG:247:LYS:HA	22:CG:247:LYS:HD2	1.66	0.45
22:CG:298:ARG:HH22	22:CG:473:PRO:HG2	1.82	0.45
31:CQ:145:ALA:HA	31:CQ:148:MET:HE3	1.98	0.45
32:CR:162:LEU:HD13	32:CR:190:LEU:HD13	1.98	0.45
32:CS:361:ILE:HB	32:CS:367:GLN:HB2	1.98	0.45
32:CS:395:PRO:HG2	32:CS:398:LEU:HD23	1.99	0.45
48:UH:712:SER:HA	48:UH:775:LEU:HD11	1.99	0.45
1:UA:508:GLN:O	40:Cj:114:ARG:NH2	2.48	0.44
2:UB:605:ASP:OD1	2:UB:605:ASP:N	2.50	0.44
8:UK:64:TYR:HD1	8:UK:67:MET:HE3	1.82	0.44
13:UQ:359:HIS:HA	13:UQ:448:LYS:HD3	1.99	0.44
13:UQ:483:GLY:HA2	13:UQ:498:PRO:HD2	1.99	0.44
14:UR:171:TYR:HD2	15:UU:196:LEU:HD21	1.82	0.44
21:CF:21:LEU:HD23	21:CF:118:LEU:HD13	1.99	0.44
29:CN:77:MET:HA	29:CN:80:MET:HG2	1.99	0.44
37:Cg:174:LYS:NZ	46:C1:1095:A:OP2	2.42	0.44
41:Cm:86:LEU:HD11	41:Cm:104:LEU:HD11	1.99	0.44
50:US:88:PHE:HA	50:US:91:LEU:HG	1.99	0.44
6:UG:295:LYS:HB3	11:UN:870:ILE:HB	1.99	0.44
14:UR:492:LEU:HB3	14:UR:536:PHE:HB2	1.99	0.44
17:UZ:119:ASP:OD1	17:UZ:120:LEU:N	2.50	0.44
18:CB:242:ASN:O	18:CB:246:PHE:HB2	2.16	0.44
21:CF:55:LEU:HD21	21:CF:69:PRO:HD3	1.99	0.44
26:CK:292:ARG:NH1	27:CL:525:HIS:O	2.50	0.44
38:Ch:121:ARG:NH2	46:C1:1452:G:O3'	2.50	0.44
44:Cp:19:ARG:NH2	46:C1:1739:G:OP1	2.49	0.44
1:UA:780:GLN:O	1:UA:784:SER:CB	2.62	0.44
8:UK:48:LEU:HG	24:CI:1048:LEU:HD11	1.99	0.44
8:UK:79:ARG:HA	8:UK:79:ARG:HD3	1.72	0.44
9:UL:428:ASP:OD1	9:UL:428:ASP:N	2.49	0.44
22:CG:356:TYR:HB3	22:CG:365:LEU:HB2	1.99	0.44
32:CR:137:ALA:HA	32:CR:490:LEU:HD21	1.99	0.44
32:CS:256:ALA:HB2	32:CS:265:LEU:HD21	2.00	0.44
32:CS:727:TYR:HE1	32:CS:762:MET:HG2	1.83	0.44
50:US:146:LEU:HD12	50:US:162:PRO:HG2	1.99	0.44
50:US:328:LEU:HD23	50:US:328:LEU:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:UX:77:GLU:O	37:Cg:55:ARG:NH2	2.50	0.44
22:CG:504:ILE:HG22	22:CG:506:GLY:H	1.81	0.44
24:CI:91:ARG:HH21	24:CI:220:HIS:CE1	2.35	0.44
24:CI:816:ARG:HB2	24:CI:906:LEU:HD11	1.98	0.44
6:UG:340:PHE:HB3	46:C1:278:A:C6	2.53	0.44
10:UM:154:VAL:HG21	10:UM:206:ARG:HH22	1.83	0.44
12:UO:513:VAL:HG21	49:UE:266:LEU:HD11	2.00	0.44
18:CB:134:ARG:HH21	18:CB:165:THR:HG21	1.82	0.44
19:CC:34:VAL:O	19:CC:38:MET:HG2	2.18	0.44
20:CD:209:ARG:HB3	20:CD:228:ILE:HD13	2.00	0.44
24:CI:845:LEU:HD11	27:CL:490:LEU:HD13	1.99	0.44
30:CP:88:ASP:HB3	30:CP:91:ALA:HB2	1.99	0.44
32:CR:504:LYS:O	32:CR:508:THR:OG1	2.33	0.44
32:CS:586:ILE:HD13	32:CS:657:LEU:HD13	1.98	0.44
32:CS:685:ASP:OD1	32:CS:685:ASP:N	2.49	0.44
9:UL:233:ILE:HD11	9:UL:241:ILE:HD12	1.99	0.44
10:UM:303:THR:O	10:UM:306:HIS:ND1	2.51	0.44
10:UM:609:VAL:HG11	10:UM:614:VAL:HG13	2.00	0.44
10:UM:774:PHE:HA	10:UM:777:VAL:HG12	2.00	0.44
13:UQ:672:HIS:O	48:UH:635:GLN:NE2	2.42	0.44
13:UQ:747:LEU:HD22	13:UQ:780:LEU:HB2	2.00	0.44
22:CG:403:MET:HG2	22:CG:409:PHE:HB3	1.98	0.44
32:CS:522:ASN:HB3	32:CS:525:THR:HG22	1.98	0.44
50:US:163:ARG:HE	50:US:163:ARG:HB2	1.67	0.44
50:US:416:PHE:O	50:US:420:ARG:HB2	2.18	0.44
7:UJ:207:LYS:HD2	7:UJ:207:LYS:HA	1.76	0.44
7:UJ:366:LEU:HD23	7:UJ:366:LEU:HA	1.88	0.44
10:UM:252:ARG:HD3	34:Ca:50:ARG:HH12	1.82	0.44
15:UU:121:VAL:HB	15:UU:129:ALA:HB3	2.00	0.44
16:UX:91:ILE:HG21	16:UX:96:MET:HE2	2.00	0.44
22:CG:356:TYR:HD2	22:CG:365:LEU:HD12	1.83	0.44
22:CG:442:ILE:HD11	22:CG:459:PRO:HD2	2.00	0.44
32:CS:36:GLU:O	32:CS:40:HIS:ND1	2.46	0.44
32:CS:844:TYR:HB2	32:CS:849:LEU:HB2	2.00	0.44
46:C1:2358:U:H3	46:C1:2369:G:H1	1.66	0.44
48:UH:610:GLY:HA2	48:UH:640:GLU:HG3	2.00	0.44
50:US:414:THR:HB	50:US:417:MET:HE2	1.99	0.44
20:CD:31:GLU:O	20:CD:38:LYS:NZ	2.38	0.44
20:CD:219:ASN:O	20:CD:219:ASN:ND2	2.51	0.44
22:CG:365:LEU:HD22	53:CY:243:PRO:HB2	2.00	0.44
26:CK:108:ARG:NH1	26:CK:108:ARG:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CP:47:ARG:HE	30:CP:105:SER:HA	1.83	0.44
30:CP:152:LYS:HE2	30:CP:152:LYS:HB2	1.83	0.44
32:CR:312:ILE:HG23	32:CR:371:TYR:HA	1.99	0.44
32:CS:285:ALA:HB2	32:CS:474:LEU:HB2	2.00	0.44
48:UH:275:PRO:HB2	48:UH:279:GLU:HB2	1.99	0.44
7:UJ:25:LEU:HD22	28:CM:10:ILE:HG23	1.99	0.44
7:UJ:232:MET:HB3	7:UJ:243:ASN:HB3	2.00	0.44
9:UL:284:VAL:HG12	9:UL:295:VAL:HG23	2.00	0.44
9:UL:377:ASN:ND2	9:UL:384:GLN:OE1	2.33	0.44
13:UQ:172:SER:OG	13:UQ:174:GLU:OE1	2.36	0.44
13:UQ:847:ASP:OD1	13:UQ:847:ASP:N	2.46	0.44
16:UX:162:GLY:H	16:UX:177:ARG:HH12	1.66	0.44
24:CI:253:THR:HB	24:CI:267:THR:H	1.83	0.44
29:CN:88:ARG:NH2	29:CN:90:ASP:OD1	2.46	0.44
32:CR:28:VAL:HG21	32:CR:193:LEU:HD21	2.00	0.44
32:CR:568:PHE:HB2	32:CR:586:ILE:HB	1.99	0.44
32:CS:289:ARG:NH2	32:CS:476:GLU:O	2.51	0.44
32:CS:911:ILE:O	32:CS:915:ILE:HG12	2.18	0.44
33:CT:194:LYS:HB2	33:CT:194:LYS:HE3	1.82	0.44
34:Ca:138:PHE:O	34:Ca:213:ARG:N	2.51	0.44
43:Co:340:THR:HA	43:Co:356:VAL:HG12	1.99	0.44
48:UH:559:GLN:O	48:UH:563:ASN:HB2	2.18	0.44
48:UH:754:ARG:HA	49:UI:210:ARG:HB2	1.99	0.44
52:CX:203:THR:HA	52:CX:238:ARG:HH12	1.83	0.44
52:CX:250:ALA:O	52:CX:254:PHE:HB2	2.17	0.44
1:UA:420:PHE:HE1	1:UA:458:GLY:HA2	1.82	0.43
2:UB:745:ALA:HB3	50:US:462:GLN:HG3	2.00	0.43
9:UL:900:GLU:OE2	9:UL:903:ARG:NH2	2.51	0.43
10:UM:453:LYS:HA	10:UM:481:SER:HB2	1.99	0.43
13:UQ:751:LEU:HD22	13:UQ:791:LEU:HD22	2.00	0.43
14:UR:160:SER:HB2	14:UR:163:GLU:HG3	2.00	0.43
17:UZ:288:THR:O	46:C1:2081:G:O2'	2.36	0.43
20:CD:304:HIS:CD2	20:CD:322:LEU:HD22	2.53	0.43
29:CN:71:ASP:N	29:CN:71:ASP:OD1	2.51	0.43
30:CP:194:PRO:HA	30:CP:197:LEU:HD12	2.00	0.43
32:CR:392:ALA:HA	32:CR:424:LEU:HD22	1.99	0.43
42:Cn:54:LEU:HD11	42:Cn:75:GLN:HB2	1.99	0.43
49:UE:302:GLU:HA	49:UE:303:PRO:HD3	1.90	0.43
1:UA:155:ARG:N	1:UA:169:ALA:O	2.49	0.43
1:UA:532:GLY:HA3	1:UA:551:ARG:HG3	2.00	0.43
9:UL:513:ALA:HB3	9:UL:571:LEU:HD23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:591:VAL:HB	9:UL:601:LEU:HB2	2.00	0.43
10:UM:592:VAL:HG12	10:UM:617:THR:HG22	2.00	0.43
19:CC:51:ARG:NH1	19:CC:85:ASN:O	2.51	0.43
28:CM:423:ARG:NH1	28:CM:428:LYS:O	2.51	0.43
30:CP:145:GLY:HA3	30:CP:150:THR:HG22	1.99	0.43
50:US:311:TYR:O	50:US:342:LYS:NZ	2.42	0.43
51:CI:14:ILE:HD11	51:CI:21:ASN:HB3	2.00	0.43
4:UD:366:PRO:HG3	4:UD:704:VAL:HG21	1.99	0.43
9:UL:192:THR:OG1	9:UL:220:CYS:SG	2.67	0.43
22:CG:172:THR:HG23	22:CG:583:GLY:HA3	2.00	0.43
32:CR:536:PHE:HZ	32:CR:580:PRO:HD2	1.83	0.43
33:CT:106:LEU:HD13	33:CT:131:VAL:HA	2.00	0.43
36:Ce:128:LEU:O	36:Ce:132:HIS:ND1	2.40	0.43
46:C1:311:G:H21	46:C1:329:A:H62	1.66	0.43
50:US:522:HIS:ND1	50:US:525:THR:OG1	2.41	0.43
52:CX:328:LEU:HA	52:CX:331:ILE:HG22	1.99	0.43
1:UA:604:MET:HE3	1:UA:604:MET:HB3	1.86	0.43
4:UD:673:ASN:O	4:UD:673:ASN:ND2	2.51	0.43
6:UG:88:GLU:O	6:UG:91:ILE:HG22	2.19	0.43
10:UM:563:SER:OG	10:UM:564:GLN:N	2.51	0.43
18:CB:250:GLY:CA	18:CB:306:TYR:O	2.66	0.43
32:CS:384:GLU:O	32:CS:407:LEU:HD23	2.18	0.43
34:Ca:105:PHE:HD2	34:Ca:213:ARG:HA	1.82	0.43
37:Cg:61:ASP:OD1	37:Cg:61:ASP:N	2.51	0.43
50:US:351:ILE:HG23	50:US:352:LEU:HG	2.00	0.43
1:UA:21:LEU:HD13	1:UA:63:LEU:HB2	2.00	0.43
14:UR:274:LYS:HD3	14:UR:274:LYS:HA	1.76	0.43
16:UX:56:TYR:HB2	16:UX:87:VAL:HG12	2.01	0.43
22:CG:110:LYS:HZ3	53:CY:328:LYS:HE3	1.83	0.43
24:CI:146:PHE:HE2	24:CI:192:ARG:HB3	1.83	0.43
25:CJ:159:THR:OG1	25:CJ:160:TRP:N	2.51	0.43
32:CR:125:LEU:HD21	32:CR:131:ILE:HG21	2.01	0.43
32:CS:916:MET:O	32:CS:920:THR:OG1	2.33	0.43
48:UH:567:LEU:HD11	48:UH:609:ILE:HG23	1.99	0.43
49:UE:197:LEU:HD23	49:UE:200:LEU:HD12	2.00	0.43
50:US:403:TRP:HB2	50:US:489:LEU:HD11	2.00	0.43
52:CX:379:TRP:HD1	52:CX:459:ARG:HH11	1.67	0.43
1:UA:551:ARG:HG2	1:UA:573:LYS:HB3	1.99	0.43
4:UD:512:SER:OG	4:UD:514:ASP:OD1	2.30	0.43
13:UQ:159:ALA:HB1	13:UQ:187:LEU:HD21	2.00	0.43
17:UZ:262:VAL:O	17:UZ:266:LEU:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:39:VAL:HG23	29:CO:110:LEU:HD21	2.01	0.43
32:CR:26:PHE:O	32:CR:199:CYS:HA	2.18	0.43
34:Ca:180:THR:H	34:Ca:183:GLN:NE2	2.16	0.43
46:C1:2108:A:N3	46:C1:2172:C:O2'	2.49	0.43
48:UH:571:LEU:HB3	48:UH:574:SER:HB2	2.00	0.43
53:CY:300:ARG:NH1	53:CY:300:ARG:O	2.51	0.43
1:UA:196:GLN:HG3	1:UA:216:ASP:HB3	2.01	0.43
6:UG:240:LEU:HD21	6:UG:273:LEU:HD12	2.00	0.43
7:UJ:170:TYR:O	7:UJ:173:SER:C	2.61	0.43
13:UQ:606:HIS:HB3	13:UQ:632:ASP:HB2	2.01	0.43
17:UZ:217:ILE:HD13	17:UZ:220:ILE:HD12	2.00	0.43
19:CC:134:ILE:O	19:CC:138:ALA:HB2	2.19	0.43
24:CI:877:LEU:HD22	24:CI:908:VAL:HB	2.00	0.43
28:CM:242:CYS:HA	28:CM:259:SER:HA	2.01	0.43
40:Cj:94:ALA:HB2	40:Cj:102:LYS:HG3	2.00	0.43
48:UH:641:LEU:HD21	48:UH:713:LYS:HB2	2.00	0.43
4:UD:90:MET:HG3	4:UD:92:ASP:H	1.84	0.43
6:UG:309:ASP:OD1	6:UG:310:ARG:N	2.51	0.43
9:UL:907:ARG:HH22	10:UM:881:SER:HB2	1.83	0.43
10:UM:241:SER:OG	10:UM:244:GLN:OE1	2.36	0.43
18:CA:250:GLY:N	18:CA:306:TYR:O	2.52	0.43
20:CD:1:MET:N	20:CD:1:MET:SD	2.92	0.43
28:CM:258:ALA:HB2	28:CM:289:VAL:HB	2.01	0.43
29:CO:232:LEU:HD22	29:CO:236:VAL:HG11	2.00	0.43
31:CQ:87:ILE:HD11	31:CQ:122:VAL:HG22	2.01	0.43
32:CR:258:THR:HG23	32:CR:261:GLN:H	1.83	0.43
50:US:286:LEU:HB3	50:US:320:LEU:HB3	2.01	0.43
50:US:538:LEU:HG	50:US:544:PHE:HZ	1.83	0.43
52:CX:344:THR:O	52:CX:347:ASP:C	2.62	0.43
9:UL:200:LEU:HB3	9:UL:210:GLU:HB3	2.00	0.43
16:UX:44:MET:HE2	16:UX:44:MET:HB2	1.88	0.43
16:UX:72:LYS:NZ	45:CU:275:LEU:O	2.51	0.43
27:CL:536:GLU:HA	27:CL:539:GLU:HG2	2.01	0.43
32:CS:511:PRO:HG2	32:CS:583:LEU:HD21	2.01	0.43
35:Cc:195:SER:HB3	35:Cc:198:ILE:HB	2.01	0.43
52:CX:448:GLU:HA	52:CX:451:LYS:HG3	2.00	0.43
3:UC:639:LYS:NZ	33:CT:124:LYS:O	2.43	0.43
4:UD:432:THR:HG23	4:UD:448:PRO:HD3	2.00	0.43
10:UM:301:TRP:CZ3	10:UM:308:GLU:HB2	2.54	0.43
13:UQ:575:ASP:O	13:UQ:579:GLU:HG3	2.19	0.43
20:CD:143:LEU:HD12	20:CD:147:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CD:200:ILE:HG22	20:CD:201:LEU:HD12	2.01	0.43
24:CI:520:LYS:HB2	24:CI:523:MET:HE1	2.01	0.43
30:CP:68:ALA:HB3	30:CP:81:LYS:HG3	2.01	0.43
32:CR:903:LEU:HA	32:CR:904:PRO:HD3	1.89	0.43
32:CS:157:THR:OG1	32:CS:691:GLY:O	2.32	0.43
32:CS:277:LEU:HD12	32:CS:406:TYR:HA	2.00	0.43
52:CX:262:VAL:O	52:CX:266:MET:HG3	2.19	0.43
2:UB:550:GLU:O	2:UB:554:ARG:HG2	2.19	0.42
2:UB:713:LEU:HD13	2:UB:717:GLU:HG3	2.01	0.42
7:UJ:59:LEU:HD11	7:UJ:114:ALA:HA	2.01	0.42
13:UQ:113:VAL:HG22	13:UQ:123:ARG:HB3	2.01	0.42
13:UQ:674:ARG:HD3	48:UH:635:GLN:HG2	2.00	0.42
18:CB:193:LEU:HG	18:CB:205:PRO:HB3	2.00	0.42
21:CE:109:SER:HB3	21:CE:112:ASN:H	1.83	0.42
32:CS:245:ASP:OD1	32:CS:245:ASP:N	2.50	0.42
6:UG:481:ARG:NH2	46:C1:588:U:OP2	2.52	0.42
9:UL:839:PRO:HA	9:UL:842:LEU:HB3	1.99	0.42
9:UL:937:ARG:HD3	9:UL:937:ARG:HA	1.89	0.42
10:UM:48:LEU:HD12	10:UM:345:LEU:HD11	2.01	0.42
12:UO:206:VAL:HG21	12:UO:247:LEU:HD11	2.01	0.42
15:UU:841:MET:HA	15:UU:985:ARG:HB3	2.01	0.42
24:CI:68:PRO:O	24:CI:275:ARG:NH1	2.34	0.42
36:Ce:19:PRO:O	36:Ce:24:ARG:NH1	2.51	0.42
37:Cg:76:ARG:O	37:Cg:80:ARG:HG3	2.19	0.42
7:UJ:150:THR:HG22	33:CT:74:PRO:HD3	2.01	0.42
14:UR:157:LEU:HB3	14:UR:174:ARG:HB3	2.02	0.42
15:UU:131:LEU:HD23	15:UU:162:TRP:CD2	2.54	0.42
17:UZ:223:GLU:HA	17:UZ:226:LYS:HG2	2.00	0.42
19:CC:48:VAL:HG11	19:CC:134:ILE:HD11	2.00	0.42
24:CI:825:LYS:NZ	46:C1:1162:U:O3'	2.41	0.42
32:CR:30:VAL:HG22	32:CR:153:LEU:HD12	2.00	0.42
32:CS:791:SER:O	32:CS:795:ARG:NH2	2.52	0.42
44:Cp:13:VAL:O	44:Cp:52:ASN:CA	2.66	0.42
48:UH:357:SER:HB2	48:UH:391:PHE:CZ	2.54	0.42
7:UJ:17:ARG:HD3	7:UJ:130:PHE:CE2	2.54	0.42
7:UJ:297:VAL:HG11	7:UJ:328:VAL:HG23	2.00	0.42
7:UJ:345:ILE:O	7:UJ:349:HIS:HB2	2.19	0.42
8:UK:5:ARG:HH21	8:UK:10:ARG:HG2	1.84	0.42
8:UK:62:GLU:HG3	8:UK:67:MET:HE1	2.01	0.42
18:CA:180:VAL:O	18:CA:203:VAL:HA	2.19	0.42
24:CI:170:LEU:HG	24:CI:203:LEU:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:935:LYS:HB2	24:CI:972:TYR:CE1	2.54	0.42
27:CL:618:GLU:HG3	27:CL:622:MET:HE2	2.02	0.42
32:CS:283:LEU:HD11	32:CS:474:LEU:HG	2.01	0.42
37:Cg:105:ARG:NH2	37:Cg:151:GLN:OE1	2.51	0.42
4:UD:26:LEU:HD22	4:UD:335:LYS:HG3	2.00	0.42
10:UM:463:ASP:HB3	10:UM:468:SER:HB3	2.01	0.42
15:UU:848:ARG:HA	15:UU:851:TRP:NE1	2.34	0.42
20:CD:69:VAL:HG11	20:CD:102:LEU:HD11	2.01	0.42
24:CI:288:ILE:HG12	24:CI:800:VAL:HG22	2.02	0.42
24:CI:968:LYS:HA	24:CI:968:LYS:HD2	1.84	0.42
34:Ca:109:LYS:HA	34:Ca:109:LYS:HD2	1.80	0.42
45:CU:298:ARG:HA	45:CU:298:ARG:HD2	1.77	0.42
48:UH:12:VAL:HG22	48:UH:410:VAL:HG12	2.01	0.42
48:UH:13:LEU:HD11	48:UH:63:ILE:HG23	2.01	0.42
49:UE:306:VAL:O	49:UE:311:GLN:NE2	2.51	0.42
52:CX:290:ASN:HA	52:CX:293:LYS:HB2	2.01	0.42
2:UB:668:LEU:HD12	2:UB:691:ILE:HD11	2.01	0.42
5:UF:166:ARG:NH2	11:UN:358:GLN:O	2.53	0.42
9:UL:429:ILE:HA	9:UL:445:ALA:HB2	2.00	0.42
9:UL:571:LEU:HD13	9:UL:582:VAL:HG22	2.01	0.42
13:UQ:554:ASP:OD2	13:UQ:586:LYS:NZ	2.53	0.42
19:CC:305:ASN:O	19:CC:309:ILE:HG12	2.19	0.42
26:CK:88:VAL:O	26:CK:114:ALA:HA	2.19	0.42
32:CR:738:LYS:NZ	32:CR:804:THR:O	2.52	0.42
32:CS:183:ALA:HB1	32:CS:186:ASN:HD21	1.85	0.42
32:CS:310:ILE:HA	32:CS:385:LEU:O	2.20	0.42
32:CS:491:ASN:HD21	32:CS:497:ASP:HB3	1.84	0.42
52:CX:333:ILE:HG13	52:CX:375:TYR:HE2	1.85	0.42
2:UB:701:GLN:NE2	50:US:543:ASP:OD1	2.53	0.42
4:UD:221:ARG:NH1	4:UD:266:TYR:O	2.53	0.42
4:UD:551:GLN:HB2	4:UD:564:ALA:HB3	2.01	0.42
5:UF:276:GLY:HA3	5:UF:316:ILE:HD11	2.02	0.42
10:UM:208:ARG:HD3	10:UM:219:PRO:HA	2.02	0.42
13:UQ:562:ASP:OD1	13:UQ:562:ASP:N	2.50	0.42
15:UU:71:LEU:HD11	15:UU:106:ALA:HB2	2.01	0.42
17:UZ:233:VAL:HG22	17:UZ:243:ILE:HD12	2.01	0.42
29:CO:99:LEU:O	29:CO:105:ASN:ND2	2.53	0.42
29:CO:196:LEU:HD11	29:CO:202:ILE:HD12	2.01	0.42
32:CR:615:PRO:HA	32:CR:618:VAL:HG12	2.01	0.42
32:CS:12:PRO:HA	32:CS:15:ILE:HG22	2.01	0.42
32:CS:660:TYR:HB2	32:CS:712:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:751:ALA:HB1	32:CS:756:GLY:HA2	2.02	0.42
7:UJ:266:GLY:HA2	13:UQ:941:ILE:HG21	2.02	0.42
9:UL:851:PHE:HA	9:UL:854:ILE:HG12	2.02	0.42
10:UM:159:LEU:HD12	10:UM:198:LEU:HD11	2.01	0.42
20:CD:114:MET:HG2	20:CD:115:THR:HG23	2.02	0.42
21:CE:63:SER:HA	21:CE:66:LEU:HB2	2.01	0.42
23:CH:153:PHE:O	23:CH:157:VAL:HG22	2.20	0.42
24:CI:107:VAL:HG23	24:CI:308:THR:HG22	2.02	0.42
24:CI:254:HIS:HD1	24:CI:256:THR:HG22	1.85	0.42
32:CS:900:GLU:HG2	32:CS:901:LEU:HD12	2.01	0.42
50:US:504:GLU:HA	50:US:507:LYS:HG2	2.02	0.42
52:CX:217:LEU:HD11	52:CX:249:ALA:HB1	2.01	0.42
2:UB:490:ASN:HA	2:UB:493:LYS:HD3	2.02	0.42
4:UD:495:TRP:HH2	4:UD:523:PRO:HB3	1.85	0.42
10:UM:538:LEU:HD23	10:UM:576:LEU:HD13	2.02	0.42
12:UO:334:LEU:HB3	12:UO:346:ARG:HB2	2.00	0.42
15:UU:152:VAL:HG13	15:UU:159:ILE:HG23	2.01	0.42
24:CI:90:ARG:HH22	24:CI:96:THR:HG23	1.85	0.42
24:CI:254:HIS:ND1	24:CI:256:THR:HG22	2.35	0.42
24:CI:535:LYS:HE2	24:CI:538:ARG:HD2	2.00	0.42
29:CO:76:ILE:O	29:CO:80:MET:HG2	2.20	0.42
32:CS:579:LEU:HD12	32:CS:580:PRO:HD2	2.00	0.42
37:Cg:108:GLN:NE2	37:Cg:124:ARG:HB2	2.35	0.42
40:Cj:22:CYS:HB2	40:Cj:88:SER:OG	2.20	0.42
46:C1:1068:C:H2'	46:C1:1069:A:C8	2.55	0.42
48:UH:63:ILE:HD13	48:UH:402:VAL:HG21	2.02	0.42
48:UH:723:VAL:HG23	48:UH:782:ARG:HD3	2.01	0.42
1:UA:291:HIS:HE2	1:UA:325:TRP:HE1	1.68	0.42
7:UJ:156:PRO:HB2	7:UJ:159:ARG:HB2	2.02	0.42
10:UM:383:LEU:HD11	10:UM:388:MET:HE2	2.02	0.42
13:UQ:314:VAL:HG12	13:UQ:326:TYR:HB2	2.02	0.42
19:CC:244:LEU:HD23	19:CC:244:LEU:HA	1.89	0.42
20:CD:15:LEU:HD13	20:CD:76:LEU:HD21	2.02	0.42
21:CF:28:ALA:HB3	21:CF:34:LEU:HD12	2.02	0.42
22:CG:343:ARG:HD3	22:CG:358:LYS:HA	2.01	0.42
22:CG:352:ARG:HD3	22:CG:396:GLY:HA2	2.02	0.42
24:CI:353:ILE:O	32:CR:4:GLN:NE2	2.46	0.42
32:CS:406:TYR:CE1	32:CS:408:VAL:HG22	2.55	0.42
32:CS:790:LEU:HD23	32:CS:794:PHE:HB3	2.01	0.42
39:CI:33:PHE:HB3	39:CI:40:PHE:HB2	2.01	0.42
43:Co:372:ARG:HH21	43:Co:384:ASP:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Cp:13:VAL:O	44:Cp:52:ASN:HA	2.19	0.42
1:UA:226:ALA:HA	1:UA:241:MET:HG2	2.02	0.41
4:UD:495:TRP:CD1	4:UD:497:GLU:HB3	2.55	0.41
7:UJ:259:MET:HE3	7:UJ:295:GLN:HG2	2.02	0.41
7:UJ:333:ILE:HD12	7:UJ:333:ILE:HA	1.93	0.41
15:UU:780:THR:HG22	15:UU:785:VAL:HB	2.01	0.41
17:UZ:164:PRO:HB3	17:UZ:172:TYR:CZ	2.55	0.41
24:CI:935:LYS:NZ	46:C1:2077:C:OP1	2.53	0.41
28:CM:390:ARG:HA	28:CM:393:ARG:HG2	2.01	0.41
34:Ca:70:LEU:HD12	34:Ca:82:ARG:HB2	2.02	0.41
39:CI:97:ARG:HH21	39:CI:133:PRO:HG3	1.85	0.41
48:UH:636:LEU:HD12	48:UH:636:LEU:HA	1.90	0.41
49:UE:244:ARG:HE	49:UE:244:ARG:HB2	1.62	0.41
50:US:375:ALA:HA	50:US:378:VAL:HG12	2.02	0.41
50:US:457:LEU:HD12	50:US:460:ILE:HG12	2.02	0.41
2:UB:32:ALA:O	9:UL:691:ARG:NH1	2.53	0.41
2:UB:487:GLU:HA	2:UB:490:ASN:ND2	2.35	0.41
10:UM:88:TYR:HD1	10:UM:103:LEU:HA	1.85	0.41
18:CB:241:ILE:HA	18:CB:244:ARG:HG2	2.01	0.41
24:CI:333:LYS:HE2	24:CI:333:LYS:HB3	1.89	0.41
24:CI:607:LYS:HB3	24:CI:607:LYS:HE2	1.81	0.41
26:CK:229:THR:HG21	27:CL:545:ILE:HD11	2.01	0.41
46:C1:192:A:H1'	54:UP:349:ARG:HG2	2.02	0.41
48:UH:754:ARG:O	49:UI:210:ARG:N	2.45	0.41
48:UH:833:LYS:HB2	49:UI:246:LEU:HB3	2.02	0.41
50:US:224:PHE:HE2	50:US:281:GLN:HA	1.84	0.41
52:CX:373:LYS:HA	52:CX:373:LYS:HD2	1.80	0.41
4:UD:351:VAL:HG12	4:UD:743:ALA:HB2	2.01	0.41
6:UG:364:THR:HB	6:UG:388:TRP:HB3	2.02	0.41
7:UJ:102:LEU:HA	7:UJ:105:VAL:HG12	2.02	0.41
9:UL:640:ASP:OD1	9:UL:640:ASP:N	2.53	0.41
10:UM:157:SER:OG	10:UM:235:VAL:O	2.31	0.41
10:UM:562:ALA:HB1	10:UM:589:VAL:HG12	2.02	0.41
13:UQ:292:THR:HG23	13:UQ:361:VAL:HG12	2.02	0.41
14:UR:397:MET:HA	14:UR:412:ALA:O	2.20	0.41
18:CA:77:ARG:NH2	18:CA:145:LEU:O	2.47	0.41
29:CN:102:SER:HA	29:CO:236:VAL:HG21	2.02	0.41
32:CS:834:THR:HG23	32:CS:837:ASP:H	1.85	0.41
35:Cc:57:ILE:HD11	40:Cj:47:LYS:HG2	2.02	0.41
35:Cc:196:TYR:CZ	35:Cc:200:LYS:HE3	2.56	0.41
37:Cg:93:TYR:HA	37:Cg:96:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Co:338:LEU:HG	43:Co:358:ILE:HG12	2.03	0.41
46:C1:335:C:H2'	46:C1:336:G:C8	2.54	0.41
46:C1:373:C:H2'	46:C1:374:G:C8	2.55	0.41
52:CX:406:LEU:HA	52:CX:407:PRO:HD3	1.85	0.41
1:UA:132:GLU:O	15:UU:783:ARG:NH1	2.53	0.41
1:UA:316:ALA:O	1:UA:320:GLY:C	2.63	0.41
6:UG:63:VAL:HG13	6:UG:68:LEU:HD23	2.02	0.41
18:CB:214:MET:O	18:CB:217:ARG:NH1	2.52	0.41
21:CE:105:SER:OG	21:CE:112:ASN:OD1	2.38	0.41
23:CH:328:MET:HE2	23:CH:330:ALA:HB3	2.01	0.41
24:CI:866:HIS:O	46:C1:1156:C:N4	2.53	0.41
26:CK:94:ARG:HA	26:CK:119:ARG:HG2	2.03	0.41
29:CO:232:LEU:HD23	29:CO:232:LEU:HA	1.90	0.41
32:CS:255:LEU:HD11	32:CS:333:ALA:HB2	2.01	0.41
37:Cg:110:LEU:HD23	37:Cg:110:LEU:HA	1.92	0.41
49:UI:167:ASP:OD1	49:UI:167:ASP:N	2.53	0.41
4:UD:666:LEU:HB2	4:UD:671:ARG:NE	2.35	0.41
4:UD:773:MET:HG2	13:UQ:343:VAL:HG23	2.02	0.41
9:UL:119:ASP:CG	9:UL:124:ARG:H	2.28	0.41
9:UL:576:ASP:OD1	9:UL:576:ASP:N	2.49	0.41
13:UQ:770:THR:HG22	13:UQ:796:PRO:HB3	2.03	0.41
23:CH:357:SER:HB2	23:CH:360:LEU:HD13	2.01	0.41
23:CH:367:LEU:HD12	23:CH:375:TRP:HZ2	1.86	0.41
26:CK:29:ARG:HG3	26:CK:56:PHE:HD1	1.86	0.41
29:CN:69:ASN:O	29:CN:73:HIS:HB2	2.21	0.41
47:C2:246:G:H3'	47:C2:247:G:H5''	2.02	0.41
48:UH:832:LEU:HD23	49:UI:204:MET:HE1	2.02	0.41
50:US:464:GLN:NE2	50:US:475:CYS:O	2.37	0.41
53:CY:364:GLN:HA	53:CY:367:LEU:HG	2.02	0.41
9:UL:22:SER:OG	9:UL:23:ASN:N	2.53	0.41
10:UM:164:ILE:HD12	10:UM:197:ARG:HH11	1.86	0.41
13:UQ:711:LEU:HD12	13:UQ:725:VAL:HG13	2.02	0.41
15:UU:103:ARG:HG2	15:UU:123:GLN:HB2	2.02	0.41
18:CA:250:GLY:HA2	18:CA:308:GLN:HB2	2.03	0.41
20:CD:261:ALA:HA	20:CD:264:VAL:HG12	2.02	0.41
22:CG:598:ARG:NH2	47:C2:187:U:OP2	2.54	0.41
29:CO:205:PHE:HB3	29:CO:216:PHE:HE1	1.86	0.41
32:CS:59:ALA:HB3	32:CS:125:LEU:HD13	2.02	0.41
32:CS:134:ASN:OD1	32:CS:135:ILE:HD12	2.20	0.41
32:CS:267:THR:HG21	32:CS:472:ILE:HG21	2.02	0.41
4:UD:651:THR:HG22	4:UD:655:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:870:ASP:O	54:UP:356:ARG:NH1	2.53	0.41
5:UF:278:ILE:HD11	11:UN:377:MET:HE1	2.02	0.41
9:UL:673:SER:OG	9:UL:674:LYS:N	2.54	0.41
12:UO:40:ALA:HB2	51:CI:56:LYS:HE3	2.02	0.41
12:UO:392:LYS:HB3	12:UO:392:LYS:HE2	1.84	0.41
13:UQ:620:ASP:HA	13:UQ:621:PRO:HD3	1.94	0.41
17:UZ:178:ARG:HA	17:UZ:179:PRO:HD3	1.96	0.41
20:CD:411:LYS:NZ	47:C2:268:G:O2'	2.32	0.41
30:CP:164:VAL:HG22	30:CP:169:VAL:HG22	2.02	0.41
32:CR:774:TRP:CD1	32:CR:774:TRP:H	2.38	0.41
46:C1:1052:A:N1	46:C1:1178:A:O2'	2.44	0.41
46:C1:2176:A:N6	46:C1:2177:G:O6	2.54	0.41
48:UH:75:SER:HB3	48:UH:78:SER:HB3	2.03	0.41
50:US:126:LEU:HD11	50:US:168:GLU:HB3	2.02	0.41
52:CX:346:CYS:HB3	52:CX:385:LEU:HD23	2.02	0.41
6:UG:580:GLU:HA	6:UG:583:LEU:HB2	2.02	0.41
9:UL:861:LEU:HD22	9:UL:874:THR:HG23	2.03	0.41
12:UO:427:ALA:HB1	12:UO:432:ARG:HB2	2.02	0.41
13:UQ:616:ASP:OD1	13:UQ:617:LEU:N	2.53	0.41
15:UU:54:ILE:HD12	15:UU:54:ILE:HA	1.94	0.41
15:UU:72:GLN:HG2	15:UU:85:VAL:HG22	2.01	0.41
16:UX:112:ILE:HD11	41:Cm:96:ALA:HB2	2.01	0.41
19:CC:388:ILE:HD11	21:CF:64:ILE:HD12	2.03	0.41
28:CM:307:ILE:HD11	28:CM:326:MET:HE1	2.01	0.41
41:Cm:11:LEU:HD12	41:Cm:74:VAL:HB	2.03	0.41
4:UD:707:LEU:HB3	4:UD:829:THR:HG22	2.02	0.41
5:UF:287:ARG:HD2	5:UF:327:LEU:HD11	2.02	0.41
6:UG:134:LEU:HD11	7:UJ:5:LEU:HD13	2.01	0.41
6:UG:257:LYS:HB2	6:UG:257:LYS:HE3	1.78	0.41
10:UM:120:ASP:OD2	10:UM:122:THR:OG1	2.36	0.41
10:UM:335:LEU:HD11	10:UM:343:LEU:HB3	2.02	0.41
10:UM:689:LEU:HD23	10:UM:720:TRP:CD2	2.56	0.41
13:UQ:569:GLY:HA2	48:UH:837:ALA:HB1	2.03	0.41
14:UR:283:HIS:HB2	14:UR:288:ILE:HB	2.03	0.41
16:UX:13:ARG:HE	16:UX:13:ARG:HB2	1.70	0.41
17:UZ:175:THR:HA	17:UZ:178:ARG:HG3	2.01	0.41
19:CC:280:ASN:HD21	20:CD:267:ARG:NE	2.19	0.41
23:CH:181:ALA:HB1	23:CH:185:GLY:HA2	2.02	0.41
24:CI:177:LYS:HA	24:CI:177:LYS:HD3	1.82	0.41
28:CM:253:MET:HE3	28:CM:253:MET:HB3	1.96	0.41
32:CR:513:PRO:HB3	32:CR:652:LYS:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:240:LYS:O	32:CS:244:GLU:HB2	2.21	0.41
34:Ca:137:LEU:HB3	34:Ca:212:ILE:HD11	2.03	0.41
46:C1:625:C:H2'	46:C1:626:A:C8	2.55	0.41
46:C1:1665:A:N3	46:C1:1666:C:N4	2.69	0.41
48:UH:359:THR:HA	48:UH:388:ALA:HB2	2.02	0.41
48:UH:900:ILE:O	48:UH:904:ARG:HG2	2.21	0.41
50:US:126:LEU:HD12	50:US:126:LEU:HA	1.94	0.41
51:Cl:44:ASN:O	51:Cl:48:LYS:HG3	2.21	0.41
52:CX:231:GLU:HA	52:CX:234:ILE:HG22	2.03	0.41
53:CY:317:GLY:O	53:CY:321:ILE:HG12	2.21	0.41
1:UA:150:HIS:NE2	1:UA:168:SER:OG	2.39	0.41
2:UB:530:LEU:O	2:UB:534:ILE:HD12	2.21	0.41
4:UD:882:TRP:HZ3	54:UP:354:LYS:HG3	1.86	0.41
6:UG:382:ASP:HA	46:C1:277:U:H3'	2.03	0.41
10:UM:39:LEU:HD12	10:UM:44:ILE:HG13	2.01	0.41
10:UM:210:PHE:HE1	10:UM:215:ARG:HA	1.86	0.41
10:UM:437:MET:HE3	10:UM:437:MET:HB3	1.94	0.41
11:UN:307:GLN:O	11:UN:311:MET:HG3	2.22	0.41
12:UO:210:TYR:HA	12:UO:234:PRO:HB3	2.03	0.41
13:UQ:104:ILE:HG12	13:UQ:113:VAL:HG12	2.02	0.41
18:CA:285:PHE:CD2	18:CA:309:LYS:HD3	2.56	0.41
20:CD:317:SER:O	20:CD:321:ILE:HG12	2.21	0.41
24:CI:245:ILE:HG22	24:CI:275:ARG:HE	1.85	0.41
24:CI:1076:MET:HA	24:CI:1079:ARG:HG2	2.03	0.41
25:CJ:102:THR:HG22	25:CJ:104:SER:N	2.36	0.41
32:CS:198:SER:HB2	32:CS:485:ASN:HB2	2.03	0.41
37:Cg:109:THR:O	37:Cg:113:LYS:HG2	2.20	0.41
40:Cj:86:ALA:HB1	40:Cj:109:LEU:HD13	2.03	0.41
44:Cp:25:GLY:H	46:C1:1746:C:H4'	1.85	0.41
5:UF:36:LEU:HD21	5:UF:67:LEU:HD11	2.03	0.40
7:UJ:40:ALA:HB1	7:UJ:123:ARG:HH12	1.85	0.40
9:UL:452:TRP:HA	9:UL:459:CYS:HA	2.03	0.40
10:UM:120:ASP:CG	10:UM:125:LEU:H	2.30	0.40
10:UM:159:LEU:HD13	10:UM:200:TRP:HB3	2.03	0.40
10:UM:624:ILE:HB	10:UM:638:PHE:HB2	2.04	0.40
10:UM:806:ILE:HD11	10:UM:837:HIS:CE1	2.56	0.40
12:UO:171:LEU:HD13	12:UO:205:LEU:HD11	2.02	0.40
18:CB:73:VAL:HG11	18:CB:127:TYR:HE2	1.86	0.40
20:CD:80:LEU:HD23	20:CD:80:LEU:HA	1.93	0.40
24:CI:326:ARG:NH2	46:C1:640:G:O6	2.53	0.40
24:CI:333:LYS:HE3	32:CR:101:LEU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:35:LYS:HE2	29:CO:35:LYS:HB3	1.93	0.40
30:CP:142:ARG:HE	30:CP:142:ARG:HB2	1.66	0.40
32:CR:832:LEU:HB3	32:CR:833:PHE:H	1.65	0.40
32:CS:724:GLY:HA2	32:CS:763:ILE:HA	2.03	0.40
41:Cm:130:TYR:OH	45:CU:274:ASP:O	2.32	0.40
43:Co:393:THR:HA	43:Co:400:THR:HA	2.03	0.40
46:C1:440:G:H4'	46:C1:441:A:H5''	2.02	0.40
48:UH:755:TYR:HE2	49:UI:211:ALA:HB2	1.86	0.40
49:UE:197:LEU:HD23	49:UE:197:LEU:HA	1.90	0.40
4:UD:349:PRO:HB2	4:UD:365:LEU:HD12	2.03	0.40
4:UD:423:VAL:HG13	49:UE:307:TYR:HD2	1.85	0.40
4:UD:432:THR:N	4:UD:446:SER:O	2.47	0.40
4:UD:620:ALA:HA	4:UD:623:ILE:HD12	2.02	0.40
10:UM:461:ARG:HE	10:UM:463:ASP:HB2	1.86	0.40
10:UM:543:HIS:NE2	10:UM:561:SER:OG	2.51	0.40
12:UO:546:MET:HG2	49:UI:265:MET:HB2	2.03	0.40
18:CA:97:LEU:HD23	18:CA:200:ARG:HG2	2.03	0.40
19:CC:385:LYS:HA	19:CC:388:ILE:HG22	2.02	0.40
24:CI:827:LEU:HD21	24:CI:900:ALA:HB1	2.03	0.40
28:CM:422:GLU:O	28:CM:426:SER:OG	2.38	0.40
32:CS:564:ALA:HB1	32:CS:590:LEU:HB2	2.03	0.40
32:CS:844:TYR:CD2	32:CS:854:VAL:HG21	2.56	0.40
34:Ca:66:PHE:CZ	39:CI:47:SER:HB3	2.55	0.40
43:Co:390:GLY:HA2	53:CY:282:ARG:HD3	2.02	0.40
45:CU:272:PRO:HB2	45:CU:275:LEU:HG	2.03	0.40
46:C1:1476:A:H2'	46:C1:1477:A:H8	1.86	0.40
48:UH:271:VAL:HB	48:UH:292:PHE:HB3	2.03	0.40
48:UH:346:TYR:HA	48:UH:355:LEU:O	2.21	0.40
49:UE:189:ASP:CG	49:UE:190:SER:H	2.28	0.40
50:US:405:TYR:OH	50:US:484:LYS:O	2.38	0.40
12:UO:47:ILE:HG23	12:UO:75:VAL:HG22	2.03	0.40
12:UO:196:MET:HB2	12:UO:201:ASN:HB3	2.03	0.40
14:UR:443:GLU:OE1	14:UR:497:ARG:NH2	2.53	0.40
14:UR:596:SER:HB2	14:UR:601:VAL:HB	2.02	0.40
16:UX:114:ARG:NH2	28:CM:348:GLY:O	2.54	0.40
16:UX:123:CYS:HB3	16:UX:125:HIS:CD2	2.56	0.40
22:CG:578:VAL:HG22	22:CG:604:PHE:HB2	2.02	0.40
24:CI:1101:ARG:HB2	33:CT:114:VAL:HG21	2.03	0.40
29:CN:46:LEU:HD21	29:CN:92:THR:HG21	2.02	0.40
32:CR:185:PHE:O	32:CR:189:PHE:HB2	2.21	0.40
32:CR:221:PRO:HA	32:CR:222:PRO:HD3	1.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:310:ILE:HB	32:CR:369:ILE:HG12	2.02	0.40
32:CR:785:ARG:HH12	32:CS:853:VAL:HG13	1.86	0.40
32:CS:116:LEU:HD12	32:CS:138:ARG:HH21	1.85	0.40
46:C1:346:C:O2'	46:C1:347:C:O5'	2.36	0.40
46:C1:1479:U:H2'	46:C1:1480:G:C8	2.55	0.40
5:UF:6:ASP:OD2	11:UN:912:LYS:NZ	2.55	0.40
5:UF:368:LEU:HD21	5:UF:409:LEU:HD11	2.02	0.40
9:UL:492:TYR:CZ	9:UL:499:LEU:HD12	2.57	0.40
9:UL:612:SER:OG	9:UL:655:VAL:N	2.53	0.40
10:UM:485:VAL:HG13	10:UM:510:LEU:HD21	2.03	0.40
10:UM:815:ASP:O	10:UM:818:THR:OG1	2.31	0.40
10:UM:865:VAL:HG12	27:CL:679:PRO:HG3	2.03	0.40
13:UQ:453:ARG:NH1	48:UH:880:GLU:OE2	2.43	0.40
14:UR:362:LYS:HD3	46:C1:74:C:H1'	2.02	0.40
14:UR:456:ARG:HE	14:UR:456:ARG:HB3	1.56	0.40
20:CD:4:PHE:HD2	20:CD:86:VAL:HG13	1.86	0.40
21:CE:27:GLN:OE1	21:CE:114:LYS:NZ	2.54	0.40
24:CI:86:LYS:HA	24:CI:89:VAL:HG12	2.02	0.40
30:CP:111:ALA:O	30:CP:114:ILE:HG22	2.21	0.40
31:CQ:215:LYS:HD3	31:CQ:215:LYS:HA	1.97	0.40
32:CR:658:VAL:O	32:CR:662:GLU:HG2	2.20	0.40
32:CR:738:LYS:HE3	32:CR:738:LYS:HB2	1.93	0.40
32:CR:855:LEU:HD23	32:CR:855:LEU:HA	1.97	0.40
42:Cn:107:PHE:HD2	42:Cn:123:LYS:HB3	1.86	0.40
1:UA:787:MET:HG3	1:UA:826:MET:HE3	2.03	0.40
24:CI:749:GLN:O	24:CI:753:ASN:ND2	2.55	0.40
29:CN:45:SER:OG	29:CN:86:ASP:O	2.29	0.40
31:CQ:115:MET:HE3	31:CQ:115:MET:HB3	1.79	0.40
32:CS:384:GLU:O	32:CS:406:TYR:HB2	2.21	0.40
45:CU:281:MET:HE2	45:CU:286:LEU:HD13	2.04	0.40
48:UH:58:VAL:HG21	48:UH:103:VAL:HG11	2.03	0.40
48:UH:88:ARG:HE	48:UH:97:VAL:HG11	1.87	0.40
48:UH:755:TYR:HA	49:UI:207:ARG:HH22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	834/904 (92%)	805 (96%)	29 (4%)	0	100	100
2	UB	556/907 (61%)	538 (97%)	18 (3%)	0	100	100
3	UC	77/648 (12%)	74 (96%)	3 (4%)	0	100	100
4	UD	761/884 (86%)	731 (96%)	30 (4%)	0	100	100
5	UF	325/414 (78%)	316 (97%)	9 (3%)	0	100	100
6	UG	475/558 (85%)	456 (96%)	18 (4%)	1 (0%)	43	73
7	UJ	445/1802 (25%)	436 (98%)	9 (2%)	0	100	100
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	727 (95%)	40 (5%)	0	100	100
10	UM	835/912 (92%)	791 (95%)	44 (5%)	0	100	100
11	UN	171/177 (97%)	169 (99%)	2 (1%)	0	100	100
12	UO	497/557 (89%)	481 (97%)	15 (3%)	1 (0%)	43	73
13	UQ	775/960 (81%)	738 (95%)	36 (5%)	1 (0%)	48	79
14	UR	436/618 (71%)	427 (98%)	9 (2%)	0	100	100
15	UU	896/1049 (85%)	857 (96%)	39 (4%)	0	100	100
16	UX	188/193 (97%)	179 (95%)	9 (5%)	0	100	100
17	UZ	229/391 (59%)	221 (96%)	8 (4%)	0	100	100
18	CA	238/313 (76%)	230 (97%)	8 (3%)	0	100	100
18	CB	235/313 (75%)	222 (94%)	13 (6%)	0	100	100
19	CC	383/523 (73%)	368 (96%)	15 (4%)	0	100	100
20	CD	444/582 (76%)	431 (97%)	13 (3%)	0	100	100
21	CE	119/127 (94%)	115 (97%)	4 (3%)	0	100	100
21	CF	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
22	CG	402/630 (64%)	391 (97%)	11 (3%)	0	100	100
23	CH	383/411 (93%)	371 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	CI	829/1163 (71%)	798 (96%)	30 (4%)	1 (0%)	48	79
25	CJ	177/183 (97%)	176 (99%)	1 (1%)	0	100	100
26	CK	295/297 (99%)	282 (96%)	13 (4%)	0	100	100
27	CL	225/785 (29%)	218 (97%)	6 (3%)	1 (0%)	30	62
28	CM	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
29	CN	222/252 (88%)	209 (94%)	13 (6%)	0	100	100
29	CO	211/252 (84%)	205 (97%)	6 (3%)	0	100	100
30	CP	197/322 (61%)	195 (99%)	2 (1%)	0	100	100
31	CQ	178/259 (69%)	177 (99%)	1 (1%)	0	100	100
32	CR	836/1073 (78%)	807 (96%)	29 (4%)	0	100	100
32	CS	826/1073 (77%)	790 (96%)	36 (4%)	0	100	100
33	CT	127/203 (63%)	121 (95%)	6 (5%)	0	100	100
34	Ca	223/255 (88%)	213 (96%)	10 (4%)	0	100	100
35	Cc	188/212 (89%)	183 (97%)	4 (2%)	1 (0%)	24	59
36	Ce	155/203 (76%)	144 (93%)	11 (7%)	0	100	100
37	Cg	157/190 (83%)	156 (99%)	1 (1%)	0	100	100
38	Ch	64/151 (42%)	63 (98%)	1 (2%)	0	100	100
39	Ci	113/150 (75%)	111 (98%)	2 (2%)	0	100	100
40	Cj	124/143 (87%)	120 (97%)	4 (3%)	0	100	100
41	Cm	122/130 (94%)	119 (98%)	3 (2%)	0	100	100
42	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
43	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
44	Cp	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
45	CU	168/311 (54%)	161 (96%)	7 (4%)	0	100	100
48	UH	787/930 (85%)	769 (98%)	18 (2%)	0	100	100
49	UE	172/410 (42%)	158 (92%)	14 (8%)	0	100	100
49	UI	126/410 (31%)	121 (96%)	5 (4%)	0	100	100
50	US	443/549 (81%)	425 (96%)	16 (4%)	2 (0%)	24	59
51	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
52	CX	265/480 (55%)	248 (94%)	17 (6%)	0	100	100
53	CY	119/381 (31%)	118 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	UP	52/364 (14%)	49 (94%)	3 (6%)	0	100	100
All	All	18963/27314 (69%)	18259 (96%)	696 (4%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	Cc	88	GLY
50	US	246	GLU
12	UO	130	GLN
50	US	241	GLU
6	UG	56	PRO
24	CI	367	VAL
13	UQ	447	SER
27	CL	640	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	662/774 (86%)	662 (100%)	0	100	100
2	UB	474/788 (60%)	474 (100%)	0	100	100
3	UC	67/536 (12%)	67 (100%)	0	100	100
4	UD	657/738 (89%)	656 (100%)	1 (0%)	87	89
5	UF	250/341 (73%)	250 (100%)	0	100	100
6	UG	386/474 (81%)	386 (100%)	0	100	100
7	UJ	355/1526 (23%)	355 (100%)	0	100	100
8	UK	162/227 (71%)	162 (100%)	0	100	100
9	UL	667/821 (81%)	666 (100%)	1 (0%)	88	91
10	UM	712/770 (92%)	712 (100%)	0	100	100
11	UN	146/161 (91%)	146 (100%)	0	100	100
12	UO	403/456 (88%)	403 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	UQ	651/817 (80%)	651 (100%)	0	100	100
14	UR	360/523 (69%)	360 (100%)	0	100	100
15	UU	677/863 (78%)	677 (100%)	0	100	100
16	UX	152/167 (91%)	152 (100%)	0	100	100
17	UZ	186/329 (56%)	186 (100%)	0	100	100
18	CA	175/228 (77%)	175 (100%)	0	100	100
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	344/489 (70%)	344 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	331 (100%)	0	100	100
23	CH	303/320 (95%)	302 (100%)	1 (0%)	86	88
24	CI	681/1009 (68%)	681 (100%)	0	100	100
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	245 (100%)	0	100	100
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	364 (100%)	0	100	100
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	193 (100%)	0	100	100
30	CP	177/287 (62%)	177 (100%)	0	100	100
31	CQ	151/215 (70%)	151 (100%)	0	100	100
32	CR	731/916 (80%)	731 (100%)	0	100	100
32	CS	722/916 (79%)	722 (100%)	0	100	100
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cc	149/178 (84%)	149 (100%)	0	100	100
36	Ce	137/177 (77%)	137 (100%)	0	100	100
37	Cg	123/162 (76%)	123 (100%)	0	100	100
38	Ch	58/130 (45%)	58 (100%)	0	100	100
39	Ci	78/117 (67%)	78 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Cj	92/115 (80%)	92 (100%)	0	100	100
41	Cm	103/113 (91%)	103 (100%)	0	100	100
42	Cn	70/116 (60%)	70 (100%)	0	100	100
43	Co	79/115 (69%)	79 (100%)	0	100	100
44	Cp	47/61 (77%)	47 (100%)	0	100	100
45	CU	137/260 (53%)	137 (100%)	0	100	100
48	UH	674/788 (86%)	674 (100%)	0	100	100
49	UE	148/346 (43%)	148 (100%)	0	100	100
49	UI	108/346 (31%)	108 (100%)	0	100	100
50	US	404/493 (82%)	404 (100%)	0	100	100
51	Cl	71/135 (53%)	71 (100%)	0	100	100
52	CX	227/411 (55%)	227 (100%)	0	100	100
53	CY	100/322 (31%)	100 (100%)	0	100	100
54	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	15730/23090 (68%)	15727 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	UD	673	ASN
9	UL	602	ASN
23	CH	269	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	9	ASN
1	UA	110	HIS
1	UA	123	HIS
1	UA	156	HIS
1	UA	242	GLN
1	UA	353	GLN
1	UA	416	ASN
1	UA	459	GLN
1	UA	780	GLN
1	UA	846	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	UB	511	HIS
2	UB	528	GLN
2	UB	557	HIS
2	UB	645	GLN
2	UB	663	ASN
2	UB	789	GLN
4	UD	198	ASN
4	UD	402	GLN
4	UD	412	ASN
4	UD	655	GLN
4	UD	673	ASN
5	UF	338	HIS
5	UF	341	GLN
6	UG	74	ASN
6	UG	190	GLN
6	UG	267	ASN
6	UG	299	HIS
6	UG	331	ASN
6	UG	393	GLN
6	UG	464	ASN
7	UJ	11	GLN
7	UJ	158	GLN
7	UJ	184	GLN
7	UJ	317	GLN
8	UK	45	GLN
8	UK	213	GLN
9	UL	21	ASN
9	UL	602	ASN
9	UL	688	GLN
9	UL	843	HIS
9	UL	862	ASN
9	UL	870	ASN
9	UL	905	ASN
10	UM	455	ASN
10	UM	501	ASN
10	UM	505	HIS
10	UM	644	ASN
10	UM	681	ASN
11	UN	306	GLN
11	UN	320	ASN
11	UN	927	GLN
12	UO	24	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	UO	36	HIS
12	UO	271	ASN
12	UO	296	HIS
12	UO	512	HIS
14	UR	553	GLN
15	UU	72	GLN
15	UU	81	ASN
15	UU	575	HIS
15	UU	636	HIS
15	UU	894	GLN
17	UZ	33	HIS
17	UZ	90	ASN
17	UZ	110	ASN
18	CA	78	HIS
18	CA	277	GLN
18	CB	131	ASN
19	CC	88	GLN
19	CC	179	GLN
19	CC	205	HIS
19	CC	242	ASN
19	CC	246	GLN
20	CD	28	ASN
20	CD	91	HIS
20	CD	125	HIS
20	CD	147	HIS
20	CD	219	ASN
21	CE	106	ASN
21	CF	30	HIS
21	CF	106	ASN
23	CH	49	HIS
23	CH	62	ASN
24	CI	191	HIS
24	CI	239	ASN
24	CI	380	GLN
24	CI	888	GLN
24	CI	1134	GLN
25	CJ	45	HIS
25	CJ	100	ASN
26	CK	168	HIS
26	CK	232	ASN
26	CK	286	GLN
27	CL	637	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	CM	174	GLN
28	CM	230	ASN
28	CM	262	HIS
29	CN	23	GLN
29	CO	215	ASN
30	CP	147	ASN
31	CQ	137	GLN
32	CR	170	HIS
32	CR	339	HIS
32	CR	522	ASN
32	CR	557	GLN
32	CR	838	HIS
32	CR	881	GLN
32	CS	178	HIS
32	CS	261	GLN
32	CS	346	GLN
32	CS	353	ASN
32	CS	367	GLN
32	CS	734	HIS
32	CS	770	ASN
33	CT	92	ASN
34	Ca	58	ASN
34	Ca	74	GLN
34	Ca	160	GLN
34	Ca	211	HIS
35	Cc	50	GLN
35	Cc	59	HIS
35	Cc	103	HIS
36	Ce	197	GLN
40	Cj	5	GLN
41	Cm	64	GLN
42	Cn	94	ASN
43	Co	346	ASN
43	Co	353	GLN
45	CU	211	GLN
48	UH	6	GLN
48	UH	336	ASN
48	UH	740	ASN
49	UE	176	ASN
49	UE	311	GLN
50	US	152	HIS
50	US	253	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	US	264	GLN
50	US	353	HIS
50	US	468	HIS
50	US	488	ASN
52	CX	245	ASN
49	UI	174	GLN
49	UI	232	GLN
54	UP	309	ASN
54	UP	344	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	C1	1171/2311 (50%)	212 (18%)	13 (1%)
47	C2	225/274 (82%)	48 (21%)	1 (0%)
All	All	1396/2585 (54%)	260 (18%)	14 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	C1	4	G
46	C1	14	G
46	C1	16	U
46	C1	17	C
46	C1	18	G
46	C1	23	G
46	C1	26	C
46	C1	36	C
46	C1	49	G
46	C1	59	U
46	C1	60	A
46	C1	61	G
46	C1	71	A
46	C1	72	U
46	C1	74	C
46	C1	77	C
46	C1	90	A
46	C1	96	C
46	C1	97	C
46	C1	104	U
46	C1	105	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	107	C
46	C1	126	C
46	C1	127	C
46	C1	128	G
46	C1	134	C
46	C1	136	C
46	C1	151	C
46	C1	160	C
46	C1	162	G
46	C1	163	C
46	C1	167	C
46	C1	183	C
46	C1	185	G
46	C1	193	U
46	C1	202	A
46	C1	206	C
46	C1	207	U
46	C1	208	A
46	C1	209	A
46	C1	210	G
46	C1	234	G
46	C1	236	C
46	C1	242	U
46	C1	244	G
46	C1	257	G
46	C1	259	U
46	C1	267	U
46	C1	269	G
46	C1	273	G
46	C1	276	C
46	C1	277	U
46	C1	278	A
46	C1	281	U
46	C1	282	C
46	C1	283	A
46	C1	285	A
46	C1	291	C
46	C1	292	G
46	C1	312	G
46	C1	319	U
46	C1	320	A
46	C1	323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	333	C
46	C1	339	C
46	C1	346	C
46	C1	347	C
46	C1	349	C
46	C1	351	U
46	C1	382	U
46	C1	383	G
46	C1	384	C
46	C1	386	G
46	C1	398	C
46	C1	402	U
46	C1	403	G
46	C1	416	U
46	C1	435	A
46	C1	436	A
46	C1	440	G
46	C1	441	A
46	C1	443	G
46	C1	459	C
46	C1	466	A
46	C1	468	C
46	C1	469	G
46	C1	484	G
46	C1	499	G
46	C1	500	C
46	C1	501	U
46	C1	502	A
46	C1	582	G
46	C1	584	U
46	C1	594	G
46	C1	595	U
46	C1	597	G
46	C1	613	A
46	C1	614	U
46	C1	621	G
46	C1	628	A
46	C1	1023	U
46	C1	1024	U
46	C1	1028	C
46	C1	1037	C
46	C1	1043	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	1044	A
46	C1	1052	A
46	C1	1061	A
46	C1	1069	A
46	C1	1076	U
46	C1	1078	U
46	C1	1079	C
46	C1	1080	G
46	C1	1085	U
46	C1	1088	U
46	C1	1089	A
46	C1	1096	A
46	C1	1099	A
46	C1	1103	C
46	C1	1111	A
46	C1	1116	U
46	C1	1122	A
46	C1	1123	G
46	C1	1124	G
46	C1	1125	A
46	C1	1126	A
46	C1	1129	A
46	C1	1138	C
46	C1	1141	G
46	C1	1148	G
46	C1	1149	C
46	C1	1154	A
46	C1	1158	G
46	C1	1163	A
46	C1	1164	A
46	C1	1167	C
46	C1	1169	A
46	C1	1170	G
46	C1	1178	A
46	C1	1179	G
46	C1	1218	G
46	C1	1219	A
46	C1	1223	U
46	C1	1444	A
46	C1	1448	A
46	C1	1449	U
46	C1	1461	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	1466	G
46	C1	1481	U
46	C1	1483	A
46	C1	1491	A
46	C1	1497	U
46	C1	1498	G
46	C1	1499	G
46	C1	1518	A
46	C1	1519	C
46	C1	1520	U
46	C1	1527	G
46	C1	1529	A
46	C1	1530	U
46	C1	1544	U
46	C1	1551	A
46	C1	1555	A
46	C1	1613	C
46	C1	1614	U
46	C1	1623	U
46	C1	1624	A
46	C1	1625	G
46	C1	1642	A
46	C1	1643	U
46	C1	1645	U
46	C1	1665	A
46	C1	1667	G
46	C1	1668	A
46	C1	1711	G
46	C1	1712	C
46	C1	1713	U
46	C1	1735	A
46	C1	1742	C
46	C1	1744	A
46	C1	2055	C
46	C1	2056	U
46	C1	2074	C
46	C1	2076	C
46	C1	2086	A
46	C1	2087	G
46	C1	2107	A
46	C1	2110	C
46	C1	2118	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	2119	G
46	C1	2120	C
46	C1	2121	U
46	C1	2156	A
46	C1	2157	G
46	C1	2166	A
46	C1	2167	G
46	C1	2173	G
46	C1	2178	U
46	C1	2184	G
46	C1	2185	C
46	C1	2201	C
46	C1	2202	C
46	C1	2205	G
46	C1	2214	A
46	C1	2220	C
46	C1	2227	C
46	C1	2234	A
46	C1	2351	G
46	C1	2362	U
46	C1	2363	G
46	C1	2364	A
46	C1	2373	A
47	C2	15	A
47	C2	28	U
47	C2	29	A
47	C2	31	A
47	C2	33	U
47	C2	34	A
47	C2	37	U
47	C2	39	U
47	C2	48	G
47	C2	58	A
47	C2	62	A
47	C2	63	G
47	C2	90	C
47	C2	91	G
47	C2	103	G
47	C2	104	C
47	C2	105	C
47	C2	111	G
47	C2	125	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	C2	127	A
47	C2	128	C
47	C2	133	G
47	C2	135	U
47	C2	136	C
47	C2	142	G
47	C2	153	G
47	C2	156	C
47	C2	160	U
47	C2	163	C
47	C2	165	C
47	C2	166	G
47	C2	167	U
47	C2	177	G
47	C2	178	U
47	C2	179	A
47	C2	180	U
47	C2	181	A
47	C2	187	U
47	C2	189	G
47	C2	190	C
47	C2	199	G
47	C2	200	U
47	C2	201	A
47	C2	247	G
47	C2	255	U
47	C2	256	G
47	C2	260	G
47	C2	262	C

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	C1	89	G
46	C1	135	A
46	C1	209	A
46	C1	277	U
46	C1	281	U
46	C1	593	G
46	C1	1068	C
46	C1	1087	G
46	C1	1163	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	C1	1734	G
46	C1	2156	A
46	C1	2177	G
46	C1	2219	C
47	C2	255	U

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

2 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
1	SEP	UA	646	1	8,9,10	1.54	1 (12%)	8,12,14	1.65	2 (25%)
14	SEP	UR	139	14	8,9,10	1.54	1 (12%)	8,12,14	1.66	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	UA	646	1	-	0/5/8/10	-
14	SEP	UR	139	14	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	646	SEP	P-O1P	3.36	1.61	1.50
14	UR	139	SEP	P-O1P	3.35	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	UA	646	SEP	P-OG-CB	-3.15	109.63	118.30
14	UR	139	SEP	P-OG-CB	-3.08	109.82	118.30
14	UR	139	SEP	OG-CB-CA	3.00	111.07	108.14
1	UA	646	SEP	OG-CB-CA	2.93	110.99	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	UR	139	SEP	CB-OG-P-O3P
14	UR	139	SEP	CB-OG-P-O2P
14	UR	139	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	GTP	CI	1201	57	30,34,34	0.84	1 (3%)	46,54,54	1.70	12 (26%)
58	ADP	CS	1101	-	27,29,29	1.36	4 (14%)	42,45,45	1.96	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	CI	1201	57	-	4/22/38/38	0/3/3/3
58	ADP	CS	1101	-	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CS	1101	ADP	C5-C4	4.60	1.47	1.39
58	CS	1101	ADP	C5-C6	2.72	1.48	1.41
58	CS	1101	ADP	C8-N7	2.41	1.36	1.31
56	CI	1201	GTP	C2-N3	2.29	1.38	1.33
58	CS	1101	ADP	C5-N7	-2.07	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CS	1101	ADP	C5-C4-N3	-6.27	118.57	126.75
56	CI	1201	GTP	C5-C4-N3	-5.02	120.32	128.46
58	CS	1101	ADP	N3-C4-N9	4.89	135.14	127.08
56	CI	1201	GTP	C2-N3-C4	4.44	120.21	112.30
58	CS	1101	ADP	C2-N3-C4	3.90	120.97	111.75
58	CS	1101	ADP	C4-C5-N7	-3.31	106.59	110.62
56	CI	1201	GTP	N9-C4-N3	3.31	132.58	125.94
58	CS	1101	ADP	N3-C2-N1	-3.18	123.62	128.60
58	CS	1101	ADP	PA-O3A-PB	-3.13	122.08	132.83
56	CI	1201	GTP	PA-O3A-PB	-2.93	122.78	132.83
56	CI	1201	GTP	C2-N1-C6	-2.90	119.81	125.10
58	CS	1101	ADP	C5-N7-C8	2.77	107.44	103.51
56	CI	1201	GTP	N9-C8-N7	-2.55	108.60	113.39
58	CS	1101	ADP	C4-N9-C8	2.54	108.48	105.73
56	CI	1201	GTP	C5-C6-N1	2.51	119.56	113.19
56	CI	1201	GTP	C8-N7-C5	2.45	108.67	104.24
56	CI	1201	GTP	O3G-PG-O3B	2.43	112.77	104.64
56	CI	1201	GTP	O6-C6-C5	-2.42	120.18	126.60
58	CS	1101	ADP	C3'-C2'-C1'	2.36	105.90	101.43
56	CI	1201	GTP	PB-O3B-PG	-2.23	125.17	132.83
58	CS	1101	ADP	C6-C5-N7	2.19	136.09	132.02
56	CI	1201	GTP	C3'-C2'-C1'	2.15	105.52	101.43

There are no chirality outliers.

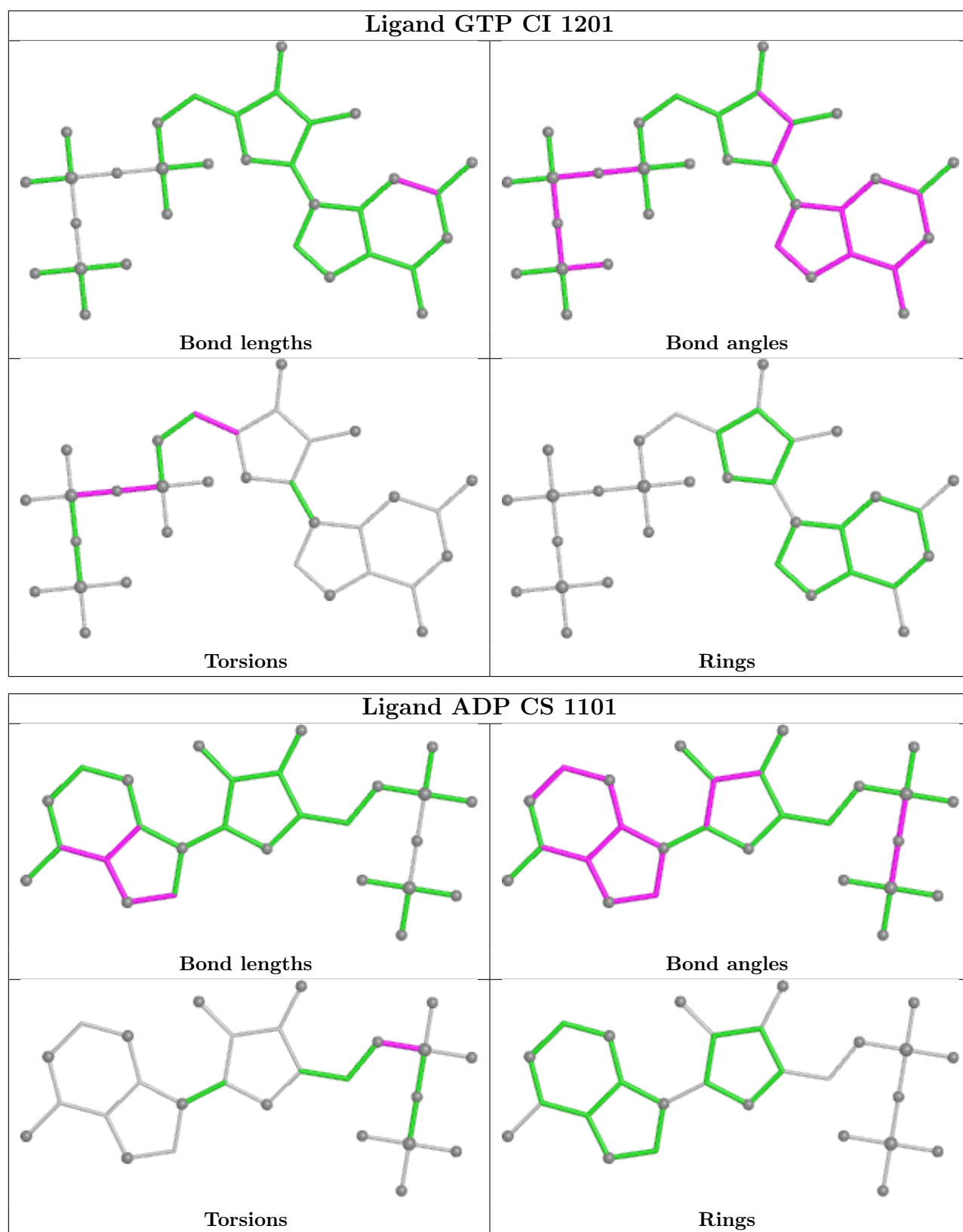
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	CS	1101	ADP	C5'-O5'-PA-O1A
58	CS	1101	ADP	C5'-O5'-PA-O2A
56	CI	1201	GTP	O4'-C4'-C5'-O5'
56	CI	1201	GTP	PB-O3A-PA-O5'
58	CS	1101	ADP	C5'-O5'-PA-O3A
56	CI	1201	GTP	C3'-C4'-C5'-O5'
56	CI	1201	GTP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	UN	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UN	380:SER	C	863:ASP	N	111.62
1	UN	288:LYS	C	295:SER	N	6.62

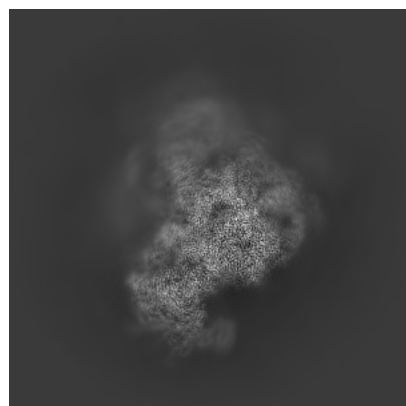
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66677. These allow visual inspection of the internal detail of the map and identification of artifacts.

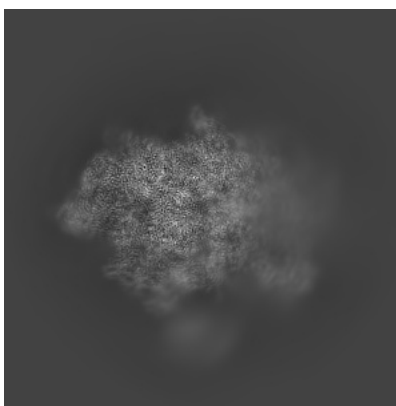
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

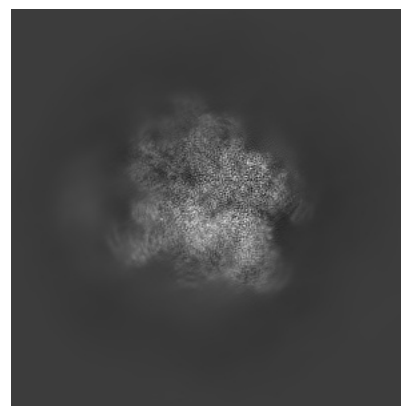
6.1.1 Primary map



X

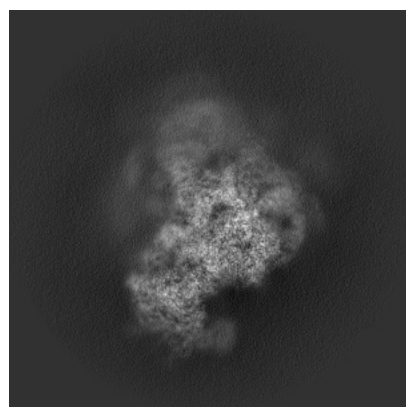


Y

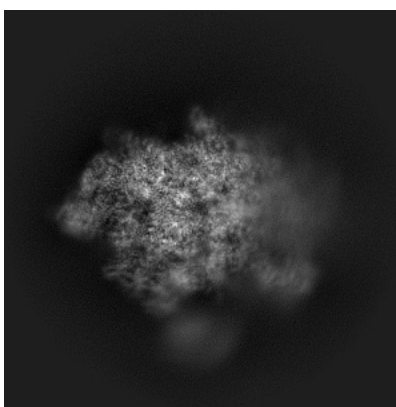


Z

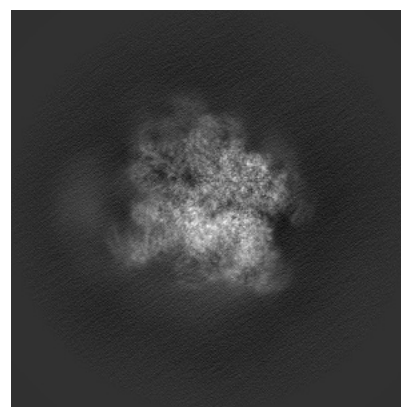
6.1.2 Raw map



X



Y

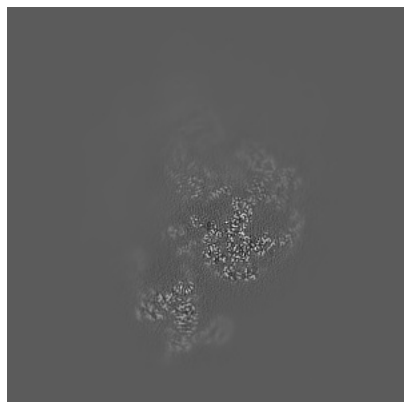


Z

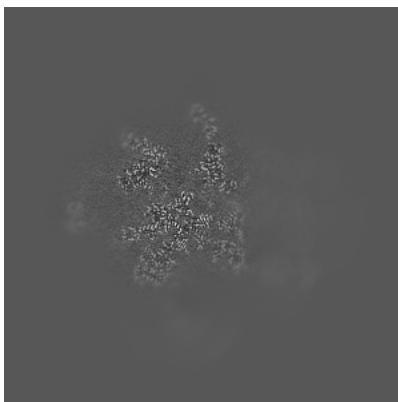
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

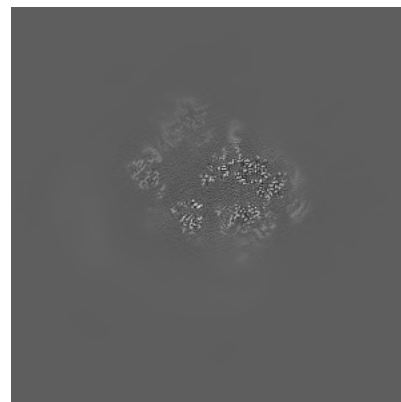
6.2.1 Primary map



X Index: 240

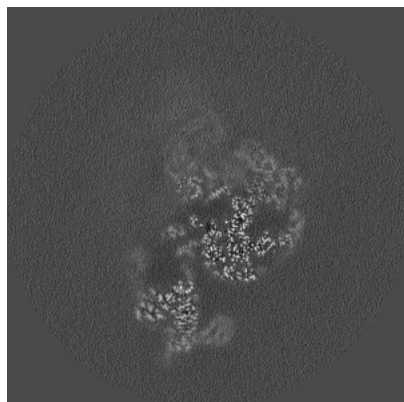


Y Index: 240

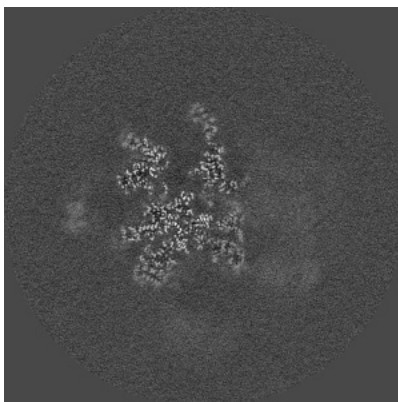


Z Index: 240

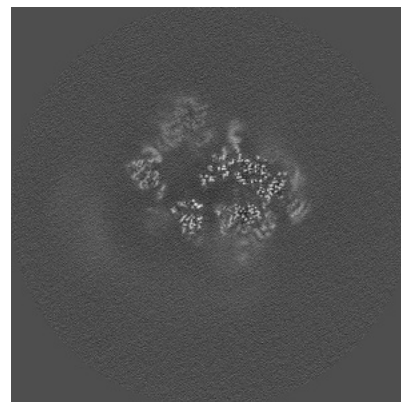
6.2.2 Raw map



X Index: 240



Y Index: 240

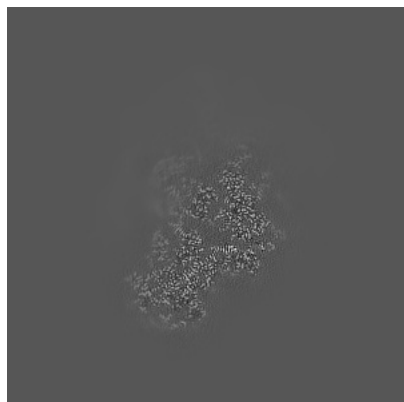


Z Index: 240

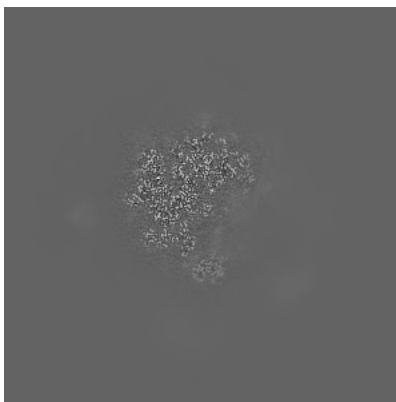
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 279

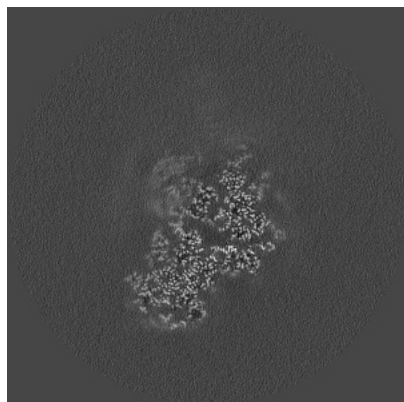


Y Index: 271

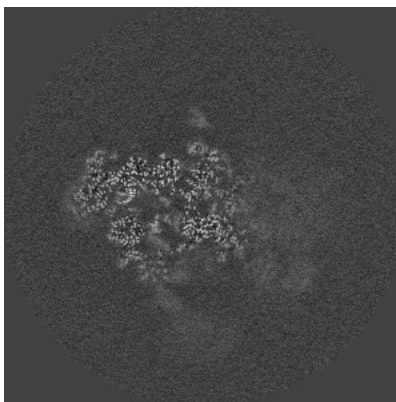


Z Index: 187

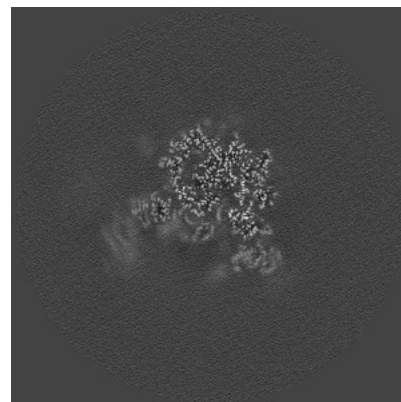
6.3.2 Raw map



X Index: 279



Y Index: 224

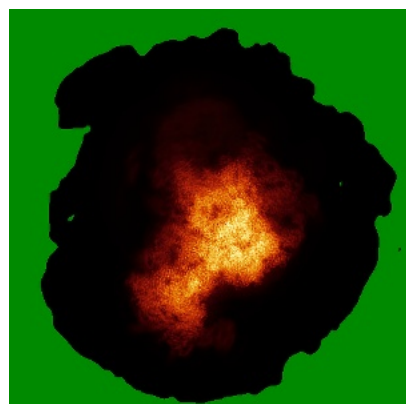


Z Index: 187

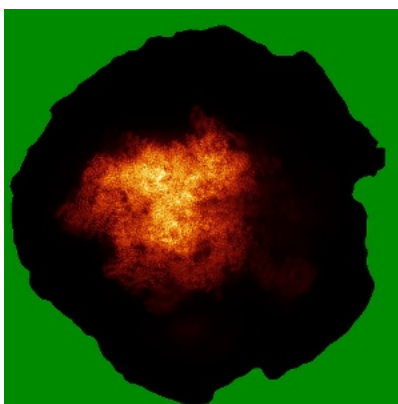
The images above show the largest variance slices of the map in three orthogonal directions.

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

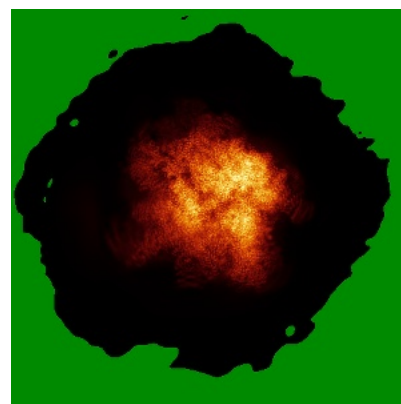
6.4.1 Primary map



X

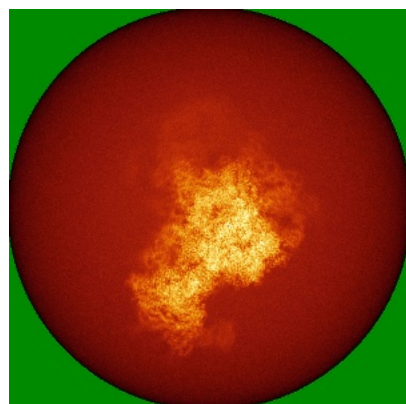


Y

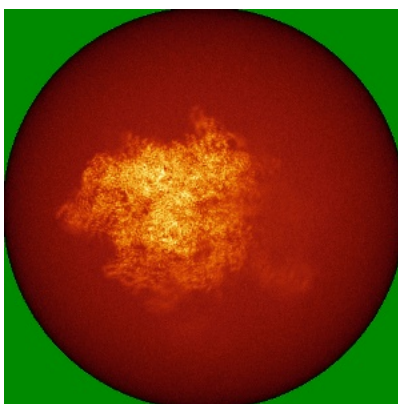


Z

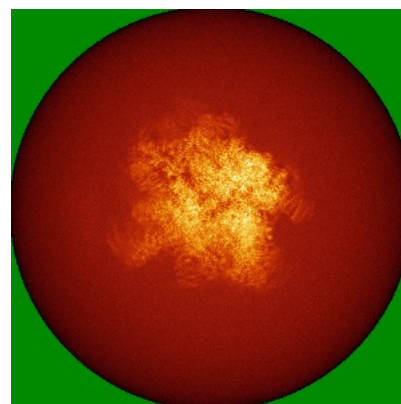
6.4.2 Raw map



X



Y



Z

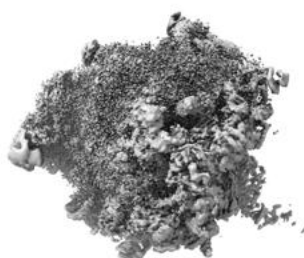
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



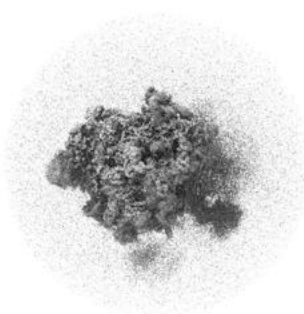
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

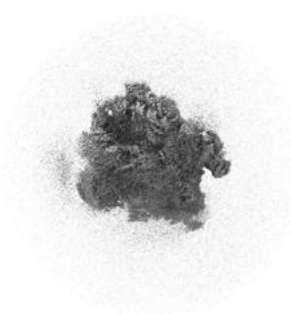
6.5.2 Raw map



X



Y



Z

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

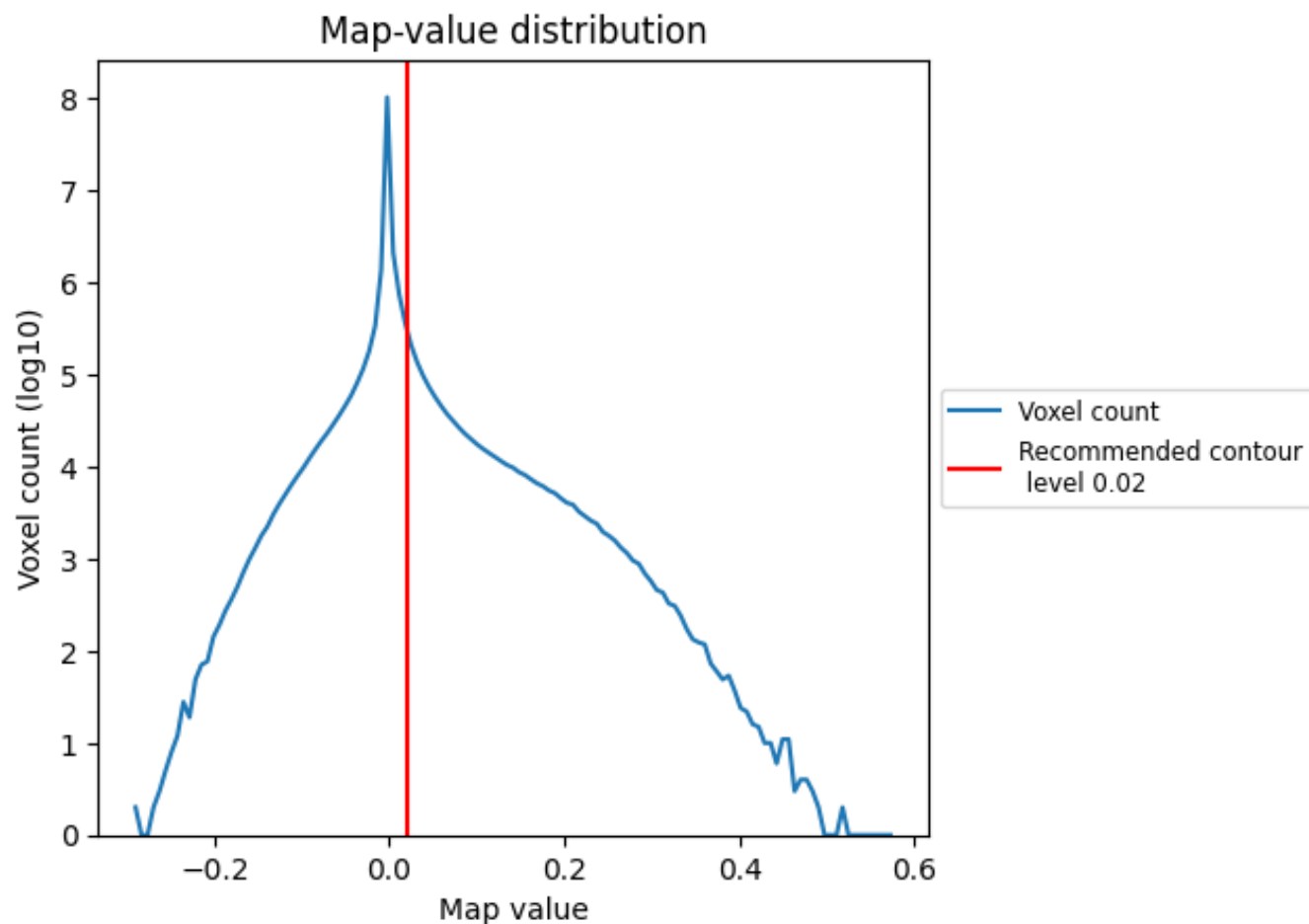
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

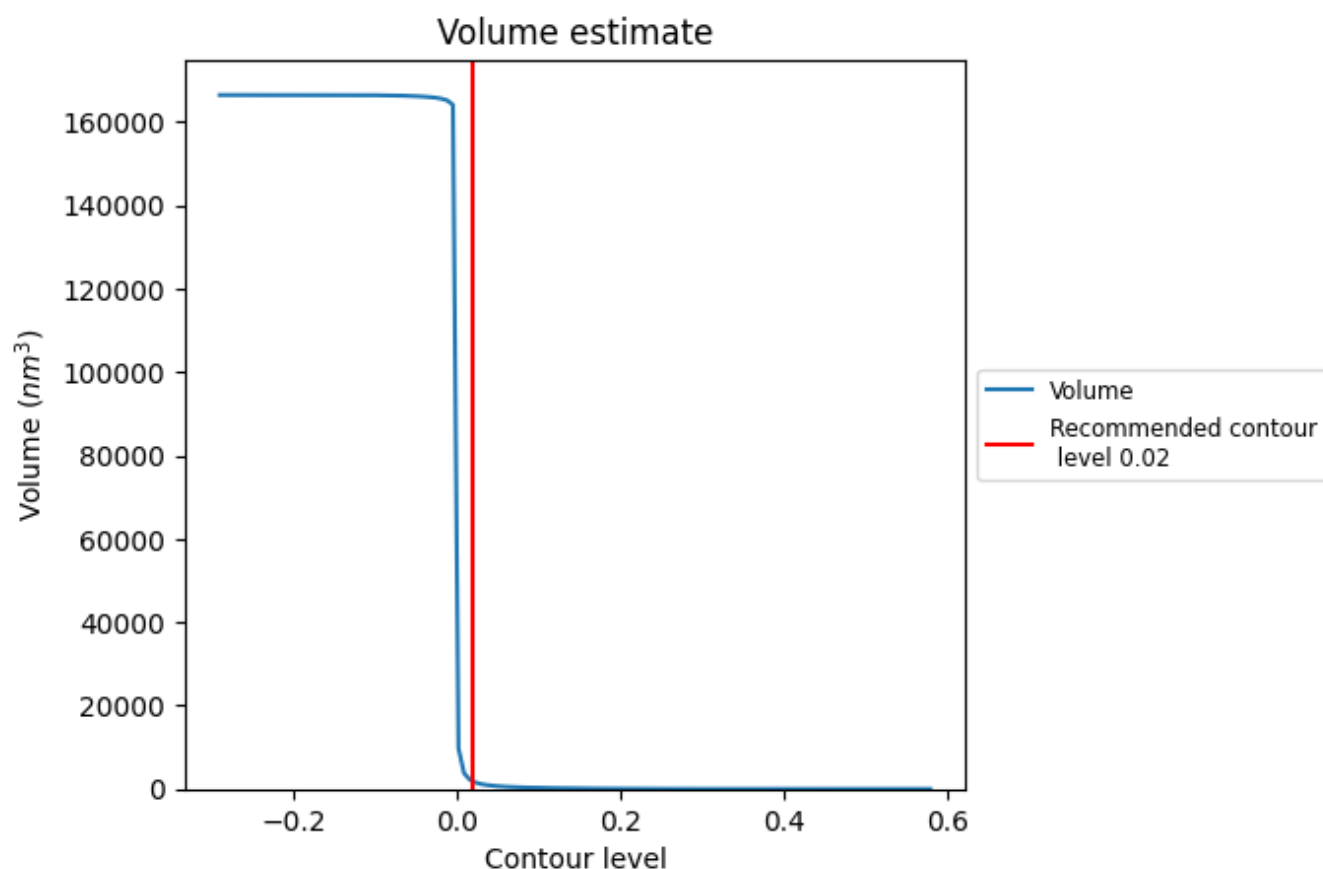
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

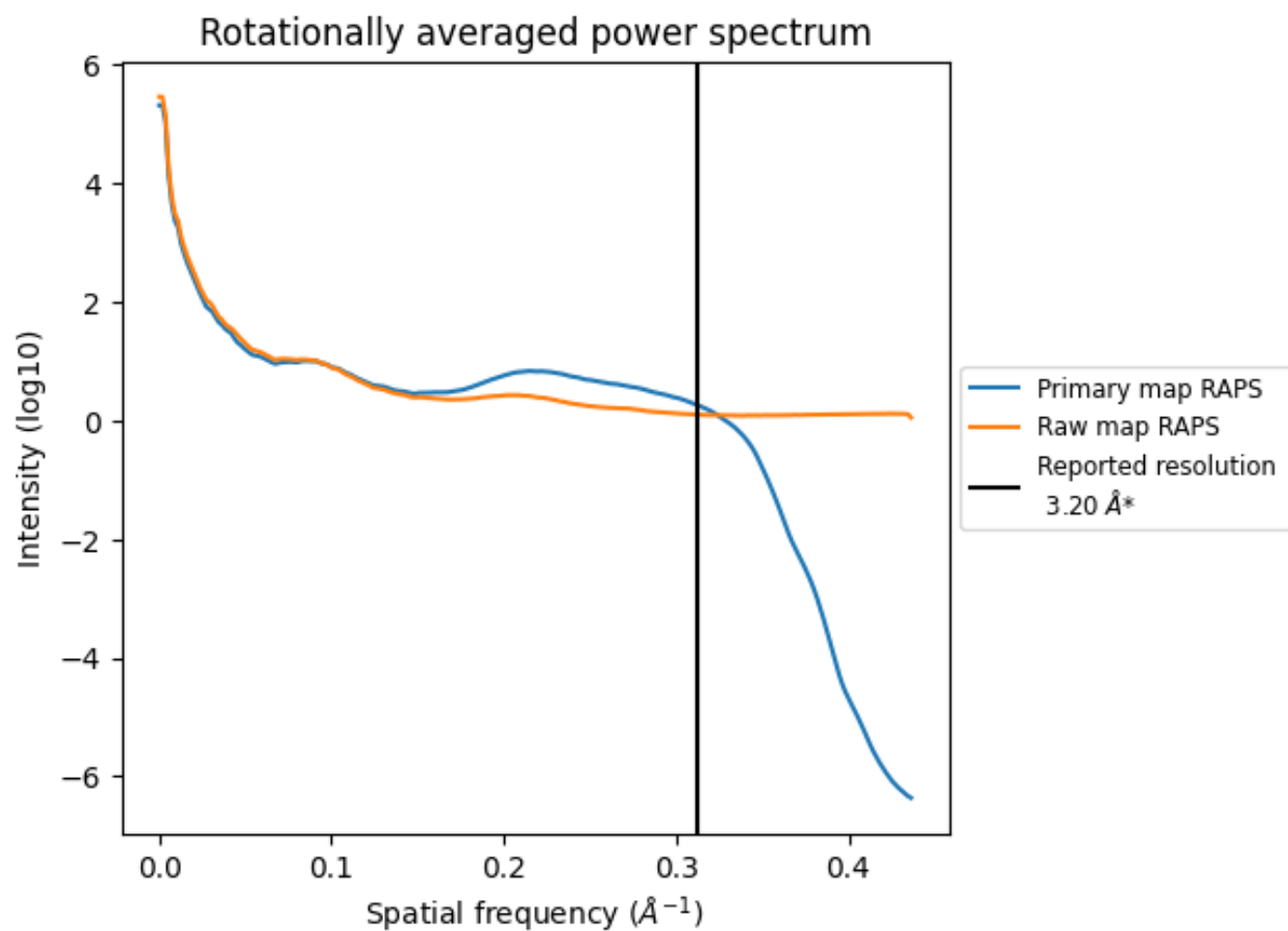
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1821 nm^3 ; this corresponds to an approximate mass of 1645 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

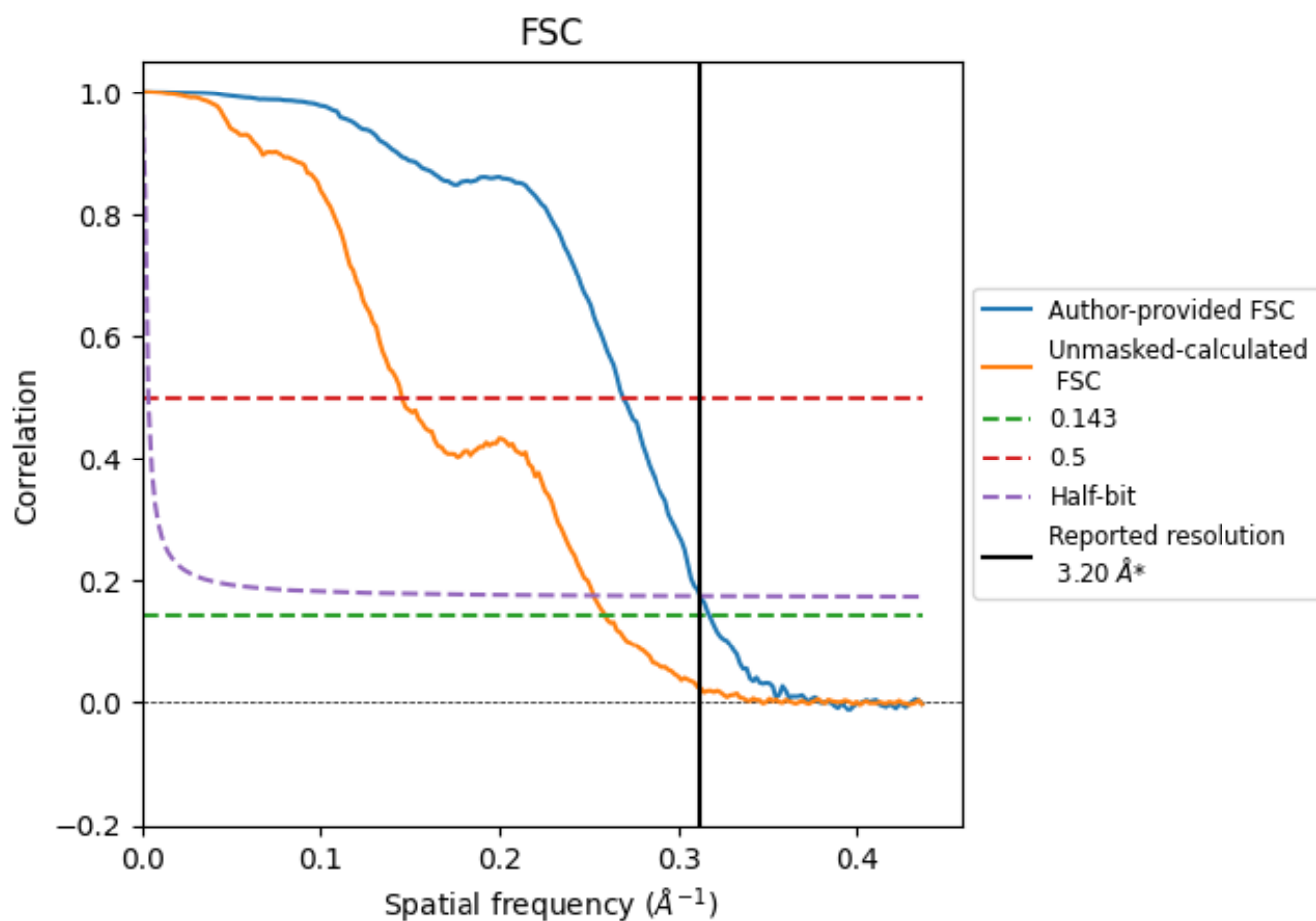


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

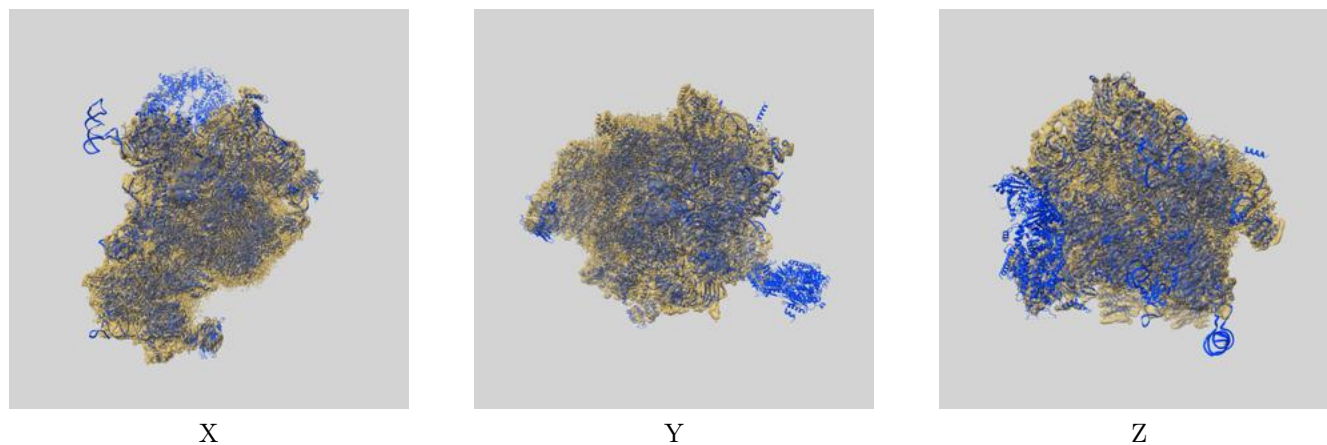
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.72	3.20
Unmasked-calculated*	3.86	6.89	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

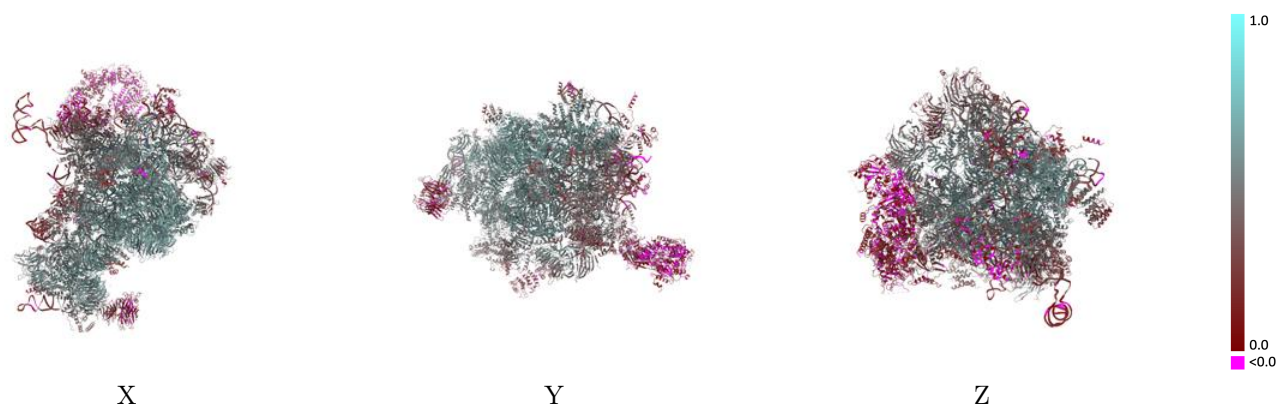
This section contains information regarding the fit between EMDB map EMD-66677 and PDB model 9XA7. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



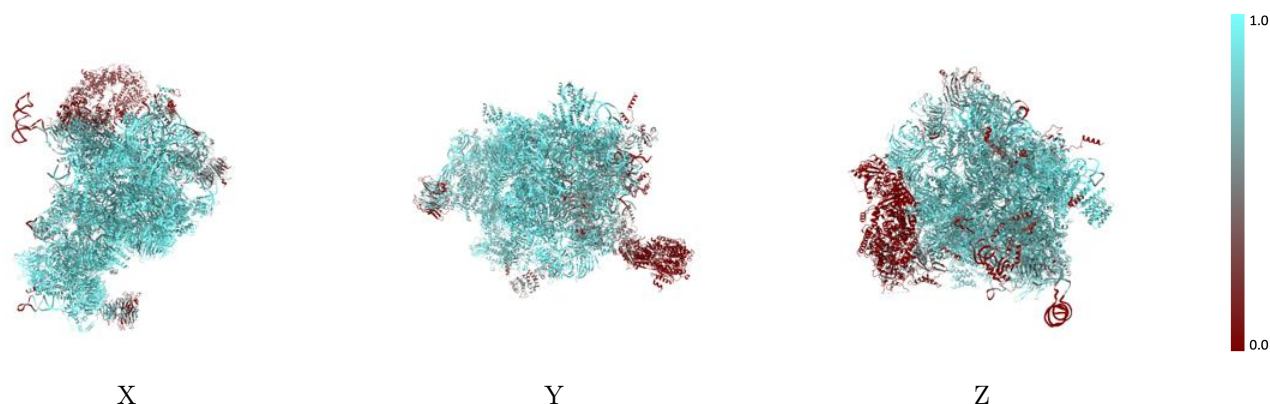
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



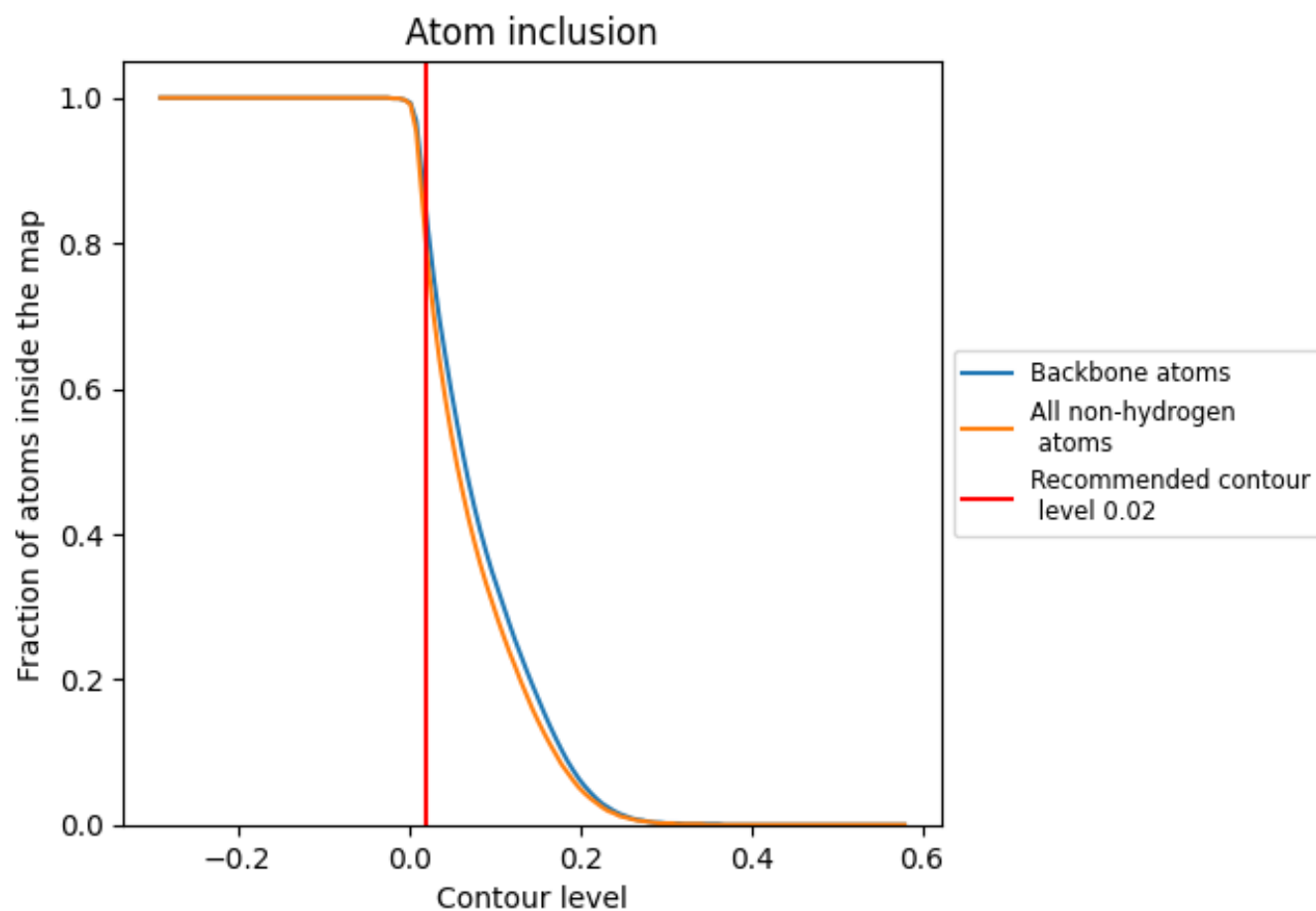
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4470
C1	 0.8650	 0.4430
C2	 0.7380	 0.4060
CA	 0.9750	 0.5870
CB	 0.8460	 0.4260
CC	 0.8920	 0.4620
CD	 0.8410	 0.4190
CE	 0.9640	 0.5780
CF	 0.8260	 0.4260
CG	 0.5990	 0.3160
CH	 0.8920	 0.4710
CI	 0.8300	 0.4590
CJ	 0.9890	 0.6310
CK	 0.9780	 0.6030
CL	 0.9490	 0.5640
CM	 0.9790	 0.5960
CN	 0.9320	 0.5130
CO	 0.8290	 0.4010
CP	 0.8440	 0.4760
CQ	 0.8960	 0.4330
CR	 0.1800	 0.1570
CS	 0.0010	 0.0540
CT	 0.9630	 0.5650
CU	 0.8310	 0.4660
CX	 0.3420	 0.1310
CY	 0.2950	 0.2700
Ca	 0.7470	 0.4100
Cc	 0.9660	 0.5780
Ce	 0.5920	 0.2880
Cg	 0.7850	 0.4620
Ch	 0.2680	 0.1790
Ci	 0.8680	 0.4580
Cj	 0.9840	 0.6100
Cl	 0.8340	 0.4020
Cm	 0.8870	 0.4870



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Cn	 0.9470	 0.5510
Co	 0.0380	 0.0380
Cp	 0.9680	 0.5700
UA	 0.9870	 0.6170
UB	 0.8650	 0.4240
UC	 0.9170	 0.5180
UD	 0.9490	 0.5380
UE	 0.9330	 0.5070
UF	 0.9120	 0.4680
UG	 0.9610	 0.5990
UH	 0.6320	 0.2930
UI	 0.8990	 0.4410
UJ	 0.9460	 0.5400
UK	 0.9540	 0.5620
UL	 0.9200	 0.4820
UM	 0.6510	 0.3710
UN	 0.8210	 0.5020
UO	 0.9780	 0.5720
UP	 0.9160	 0.4790
UQ	 0.9560	 0.5500
UR	 0.9840	 0.6100
US	 0.8840	 0.4270
UU	 0.9760	 0.5980
UX	 0.9520	 0.5550
UZ	 0.8850	 0.4400