



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:51 AM UTC

PDB ID : 9CN3 / pdb_00009cn3
EMDB ID : EMD-45757
Title : Human 39S mitoribosome in complex with antibiotic Linezolid
Authors : Raskar, T.; Bibel, B.; Galonic Fujimori, D.; Fraser, J.
Deposited on : 2024-07-15
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

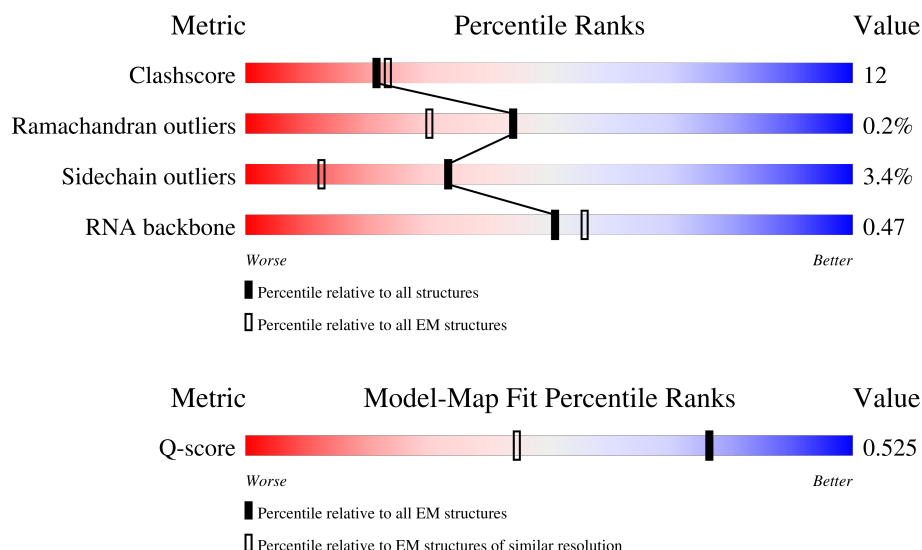
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.62 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.



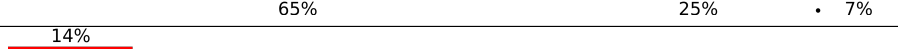
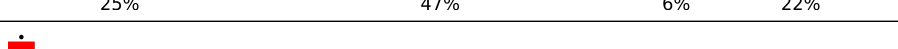
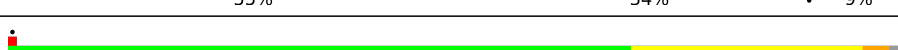
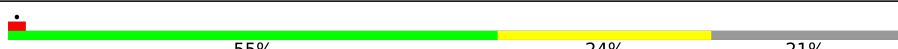
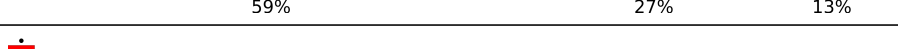
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8810 (2.12 - 3.12)

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	0	188	
2	1	65	
3	2	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1559	
12	B	72	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	179	
25	Q	292	
26	R	149	
27	S	205	
28	T	212	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	U	153	
30	V	216	
31	W	148	
32	X	256	
33	Y	250	
34	Z	161	
35	a	142	
36	b	155	
37	c	332	
38	d	306	
39	e	279	
40	f	194	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	u	710	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	TA	198	23%17%6%77%
54	TB	198	14%10%86%
54	TC	198	36%36%64%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 107417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	393	Total	C	N	O	S	0	0
			3205	2070	559	565	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	297	Total	C	N	O	S	0	0
			2410	1540	409	443	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1527	Total	C	N	O	P	0	0
			32395	14536	5844	10488	1527		

- Molecule 12 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	239	Total	C	N	O	S	0	0
			1866	1162	377	318	9		

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	306	Total	C	N	O	S	0	0
			2410	1547	419	433	11		

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	98	Total	C	N	O		0	0
			806	510	156	140			

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	179	Total	C	N	O	S	0	0
			1435	925	258	242	10		

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 24 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	143	Total	C	N	O	S	0	0
			1165	729	223	208	5		

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	220	Total	C	N	O	S	0	0
			1834	1174	326	325	9		

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	152	Total	C	N	O	S	0	0
			1222	773	233	213	3		

- Molecule 30 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	206	Total	C	N	O	S	0	0
			1682	1071	299	304	8		

- Molecule 31 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 32 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 33 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 34 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	108	Total	C	N	O	S	0	0
			896	560	162	169	5		

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	289	Total	C	N	O	S	0	0
			2322	1483	400	430	9		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	257	Total	C	N	O	S	0	0
			2075	1326	363	372	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	146	Total	C	N	O	S	0	0
			1126	714	186	222	4		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	132	Total	C	N	O	S	0	0
			1096	709	191	194	2		

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	110	Total	C	N	O	S	0	0
			894	568	156	167	3		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	93	Total	C	N	O	S	0	0
			740	460	143	135	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	72	Total	C	N	O	S	0	0
			619	394	112	111	2		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	152	Total	C	N	O	S	0	0
			1227	762	232	229	4		

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	168	Total	C	N	O	S	0	0
			1294	801	255	233	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	393	Total	C	N	O	S	0	0
			3178	2036	565	563	14		

- Molecule 53 is a protein called P-site finger.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	u	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 54 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	TA	45	Total	C	N	O	0	0
			345	222	54	69		
54	TB	27	Total	C	N	O	0	0
			213	137	33	43		
54	TC	71	Total	C	N	O	0	0
			352	210	71	71		

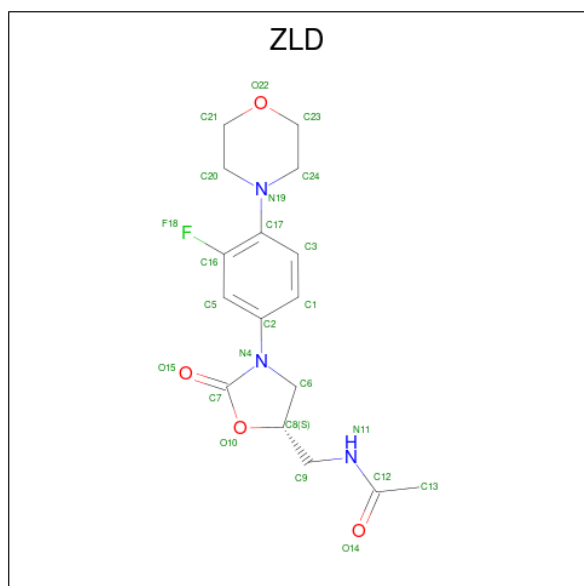
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	r	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	100	Total	Mg	0
			100	100	
56	D	1	Total	Mg	0
			1	1	
56	g	1	Total	Mg	0
			1	1	

- Molecule 57 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					AltConf
57	A	1	Total	C	F	N	O	0
			24	16	1	3	4	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	0	16	Total 16	O 16	0
58	1	8	Total 8	O 8	0
58	2	10	Total 10	O 10	0
58	3	15	Total 15	O 15	0
58	4	7	Total 7	O 7	0
58	5	63	Total 63	O 63	0
58	6	99	Total 99	O 99	0
58	7	96	Total 96	O 96	0
58	8	44	Total 44	O 44	0
58	9	23	Total 23	O 23	0
58	A	1975	Total 1975	O 1975	0
58	B	99	Total 99	O 99	0
58	D	31	Total 31	O 31	0
58	E	51	Total 51	O 51	0
58	F	24	Total 24	O 24	0
58	H	29	Total 29	O 29	0
58	I	62	Total 62	O 62	0
58	J	107	Total 107	O 107	0
58	K	28	Total 28	O 28	0
58	L	14	Total 14	O 14	0
58	M	39	Total 39	O 39	0
58	N	49	Total 49	O 49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	O	26	Total 26	O 26	0
58	P	34	Total 34	O 34	0
58	Q	50	Total 50	O 50	0
58	R	20	Total 20	O 20	0
58	S	27	Total 27	O 27	0
58	T	29	Total 29	O 29	0
58	U	35	Total 35	O 35	0
58	V	37	Total 37	O 37	0
58	W	19	Total 19	O 19	0
58	X	30	Total 30	O 30	0
58	Y	22	Total 22	O 22	0
58	Z	27	Total 27	O 27	0
58	a	18	Total 18	O 18	0
58	b	34	Total 34	O 34	0
58	c	21	Total 21	O 21	0
58	d	10	Total 10	O 10	0
58	e	196	Total 196	O 196	0
58	f	59	Total 59	O 59	0
58	g	27	Total 27	O 27	0
58	h	36	Total 36	O 36	0
58	i	28	Total 28	O 28	0

Continued on next page...

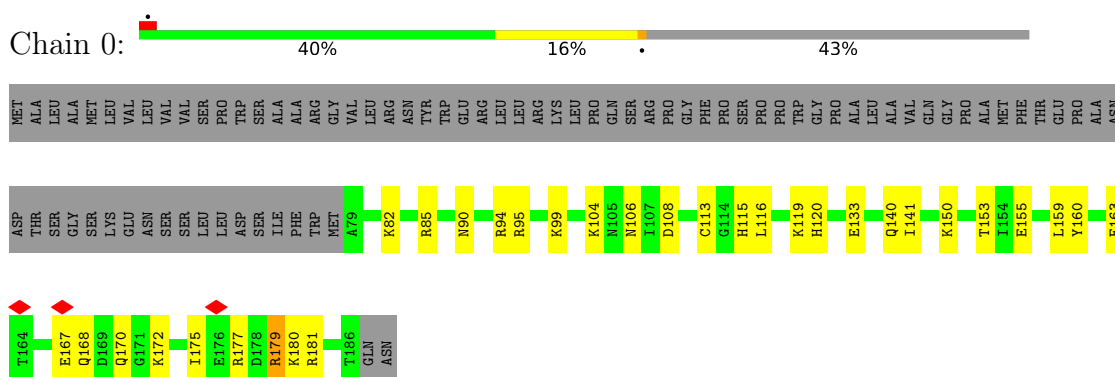
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	j	24	Total 24	O 24	0
58	k	32	Total 32	O 32	0
58	l	50	Total 50	O 50	0
58	m	33	Total 33	O 33	0
58	o	18	Total 18	O 18	0
58	p	57	Total 57	O 57	0
58	q	6	Total 6	O 6	0
58	r	44	Total 44	O 44	0
58	s	57	Total 57	O 57	0
58	u	32	Total 32	O 32	0
58	TA	43	Total 43	O 43	0
58	TB	22	Total 22	O 22	0
58	TC	37	Total 37	O 37	0

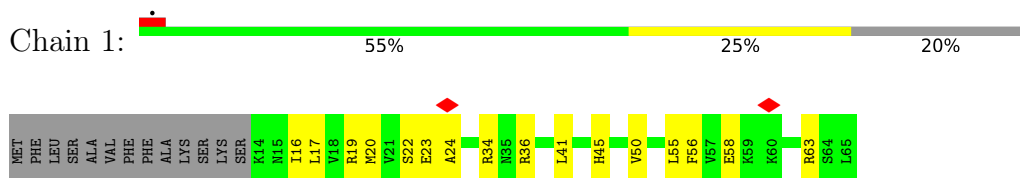
3 Residue-property plots

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

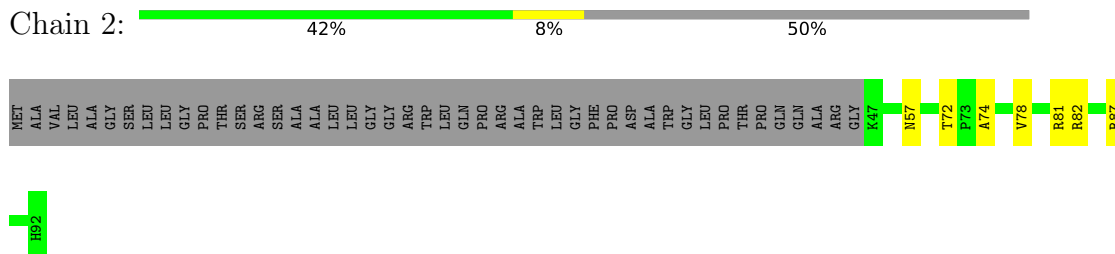
- Molecule 1: 39S ribosomal protein L32, mitochondrial



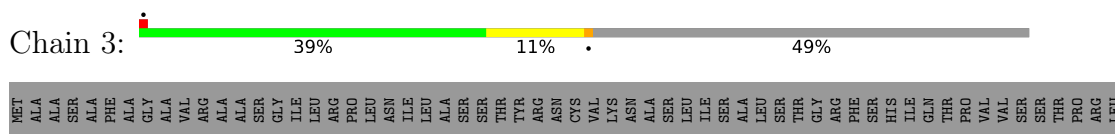
- Molecule 2: 39S ribosomal protein L33, mitochondrial

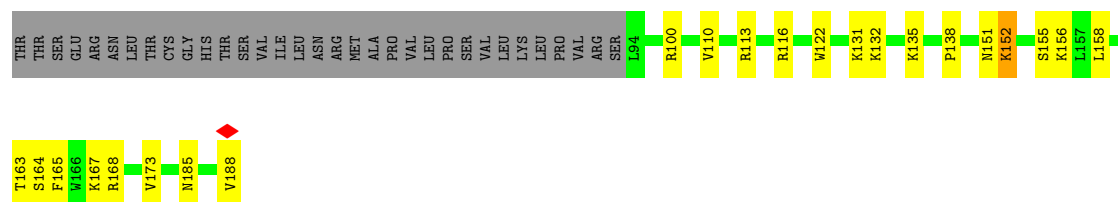


- Molecule 3: 39S ribosomal protein L34, mitochondrial



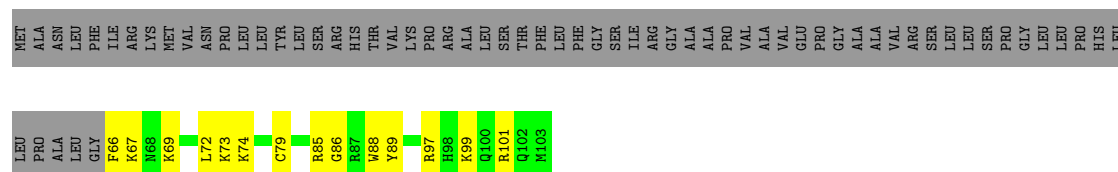
- Molecule 4: 39S ribosomal protein L35, mitochondrial





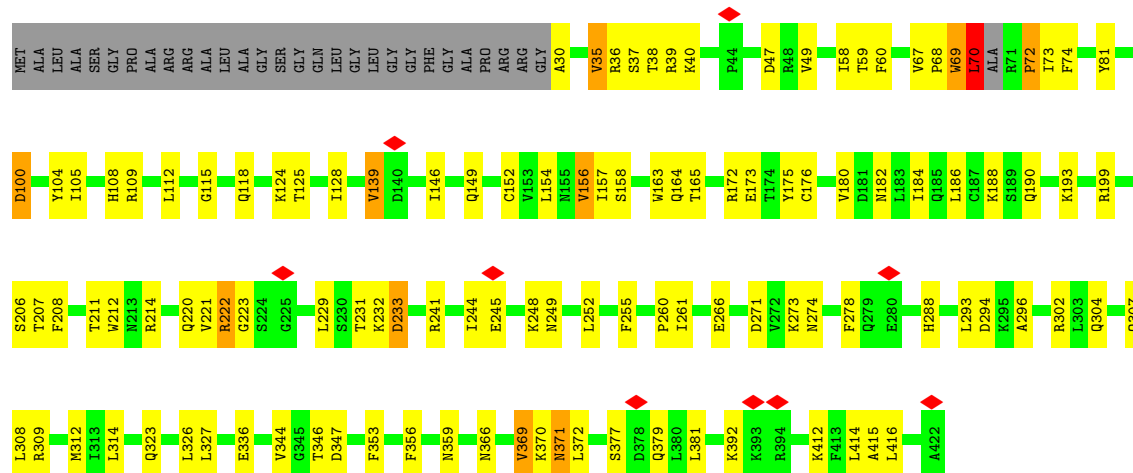
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4: 23% 14% 63%



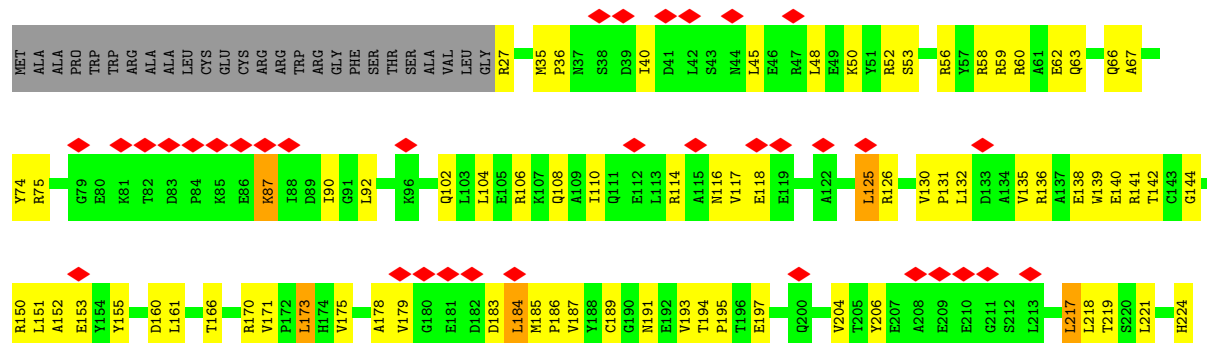
- Molecule 6: 39S ribosomal protein L37, mitochondrial

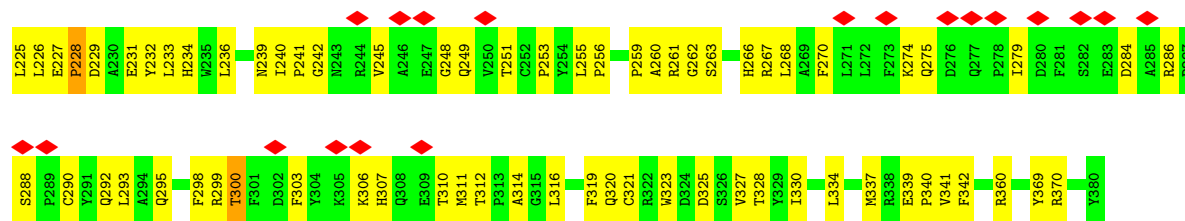
Chain 5: 65% 25% 7%



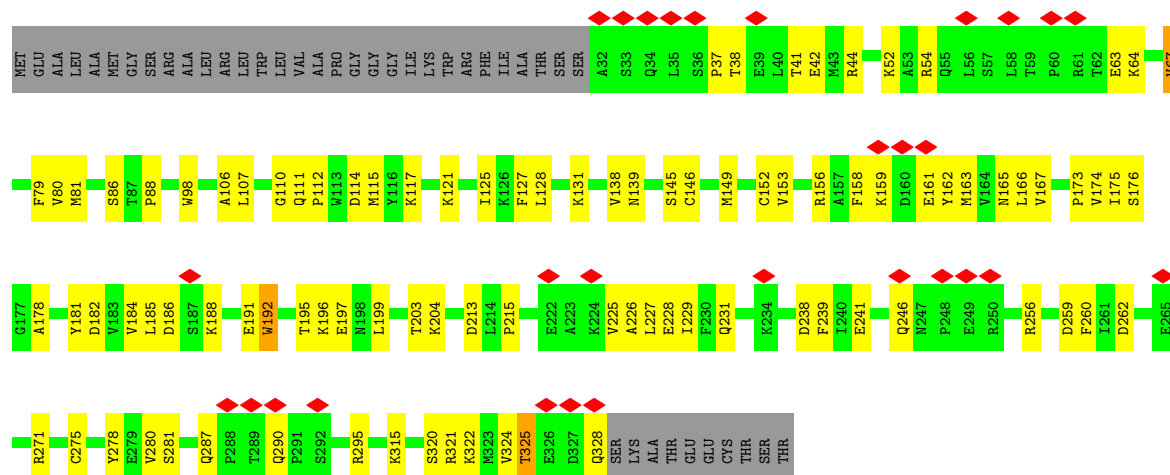
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 14% 55% 36% 7%

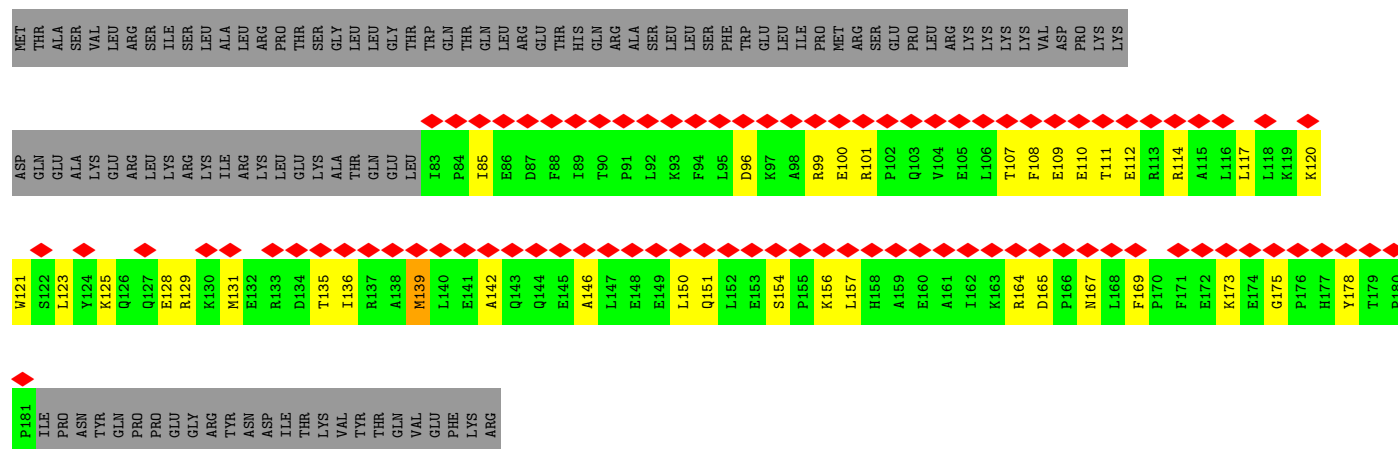
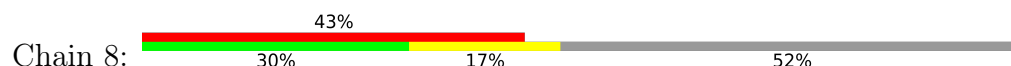




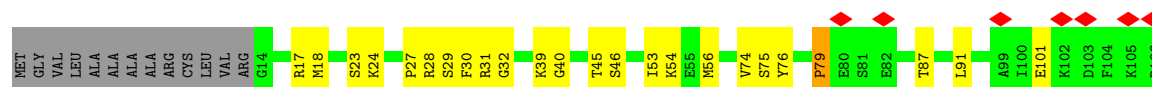
• Molecule 8: 39S ribosomal protein L39, mitochondrial

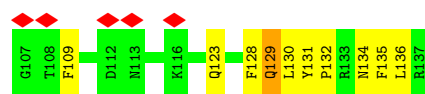


• Molecule 9: 39S ribosomal protein L40, mitochondrial

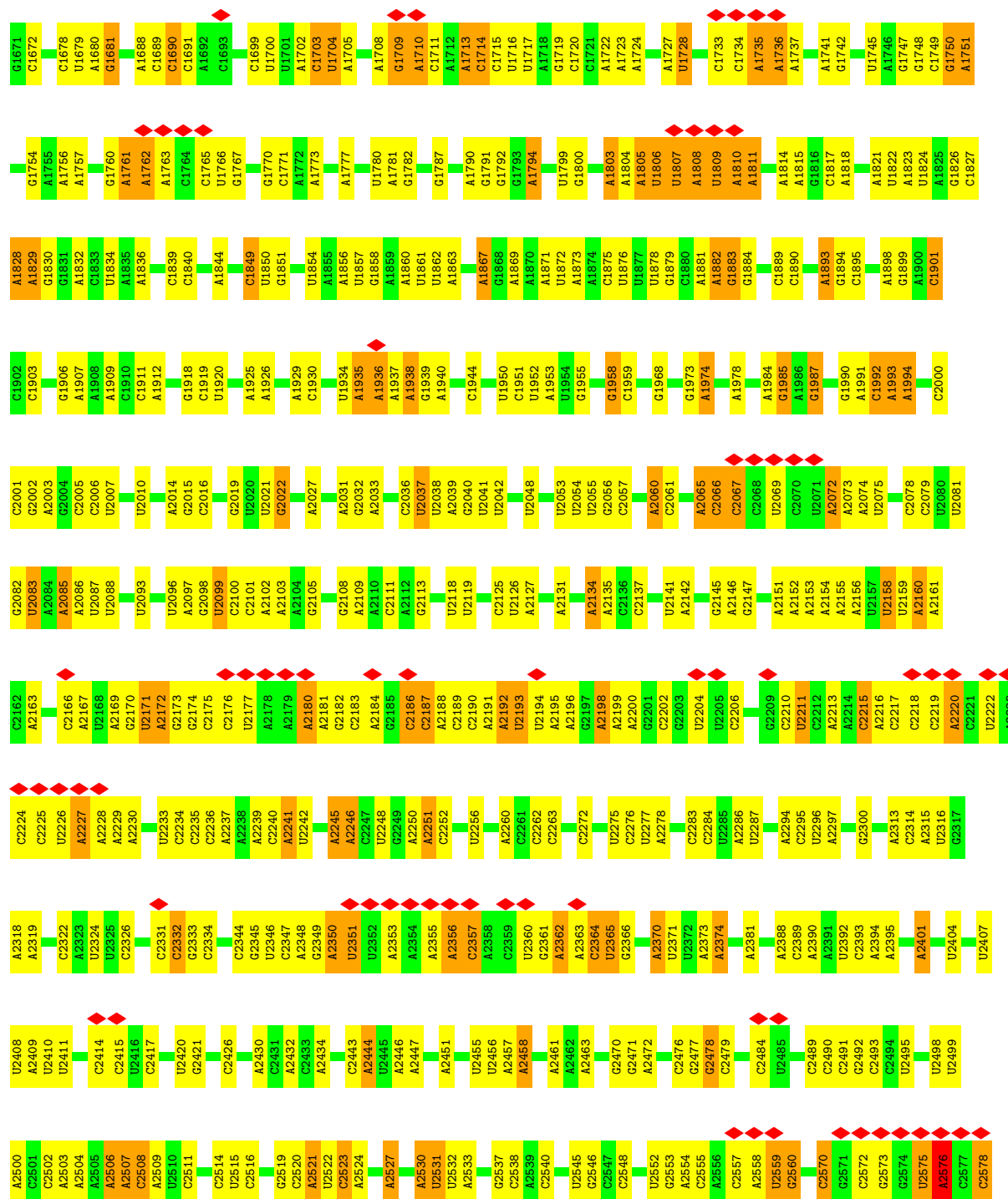


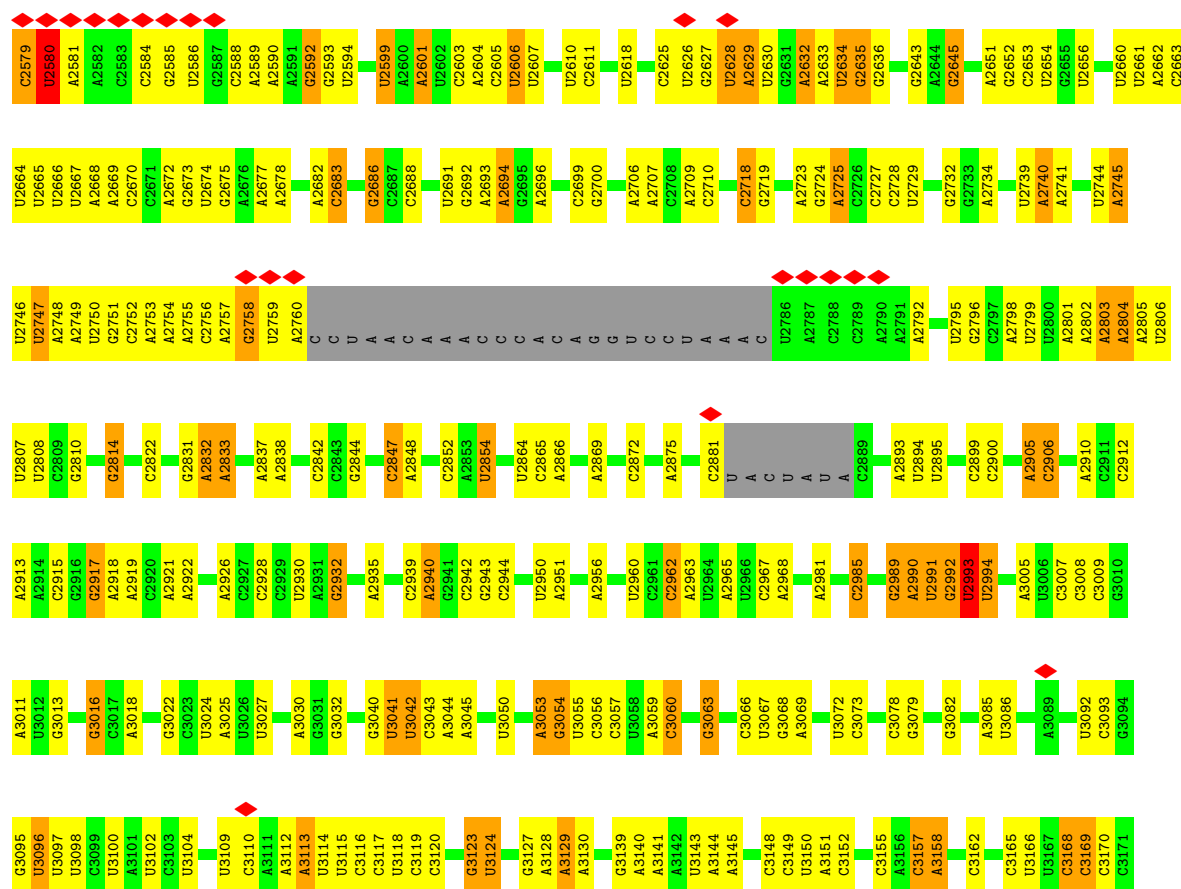
• Molecule 10: 39S ribosomal protein L41, mitochondrial



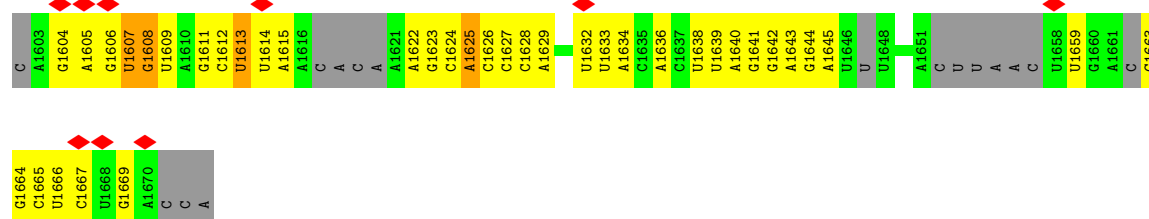


• Molecule 11: 16S rRNA

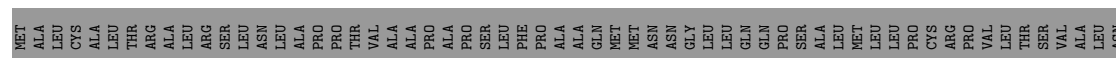


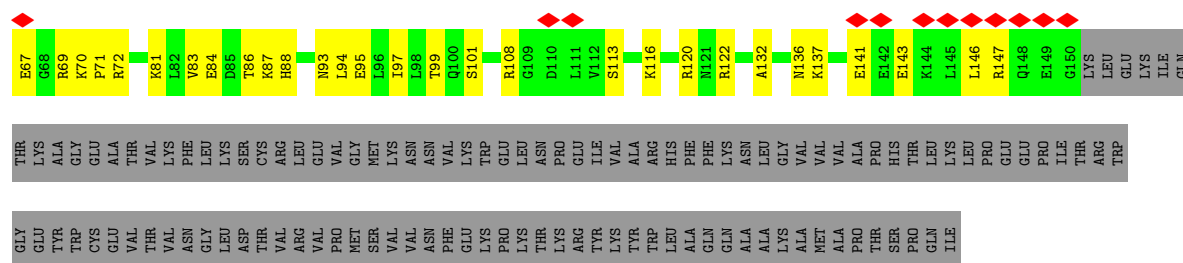


• Molecule 12: tRNA

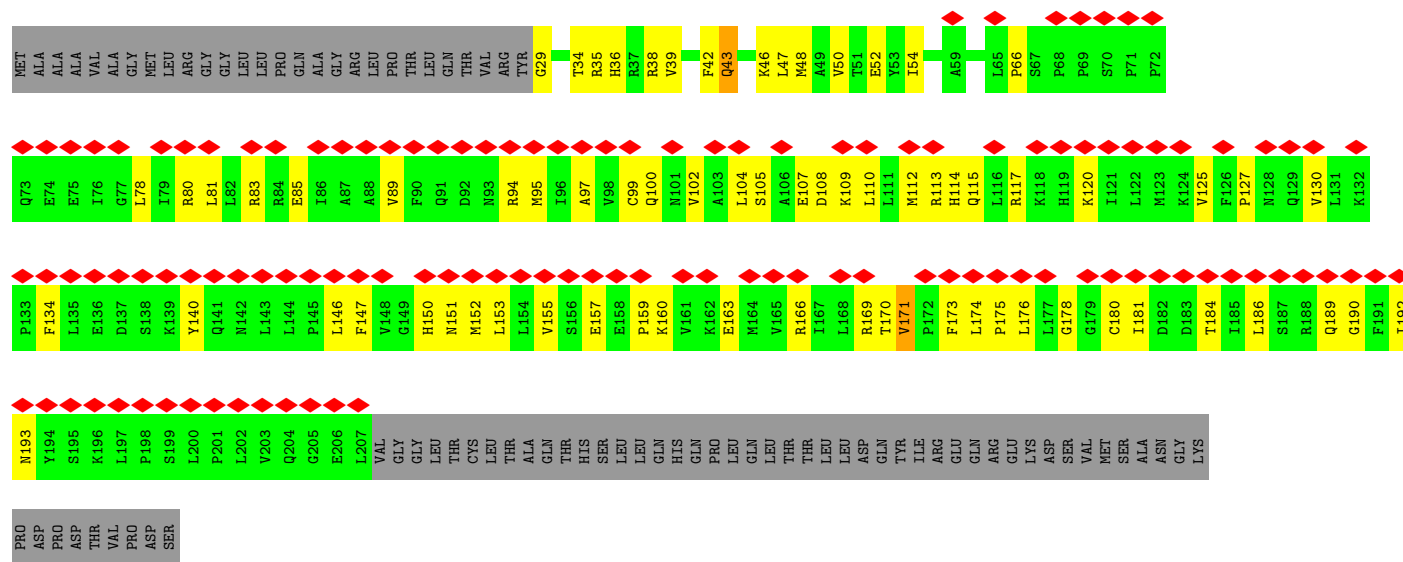


• Molecule 13: 39S ribosomal protein L2, mitochondrial

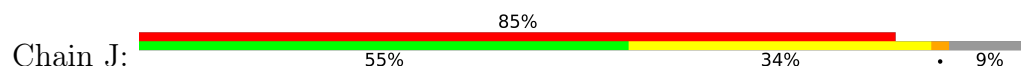




• Molecule 17: 39S ribosomal protein L10, mitochondrial

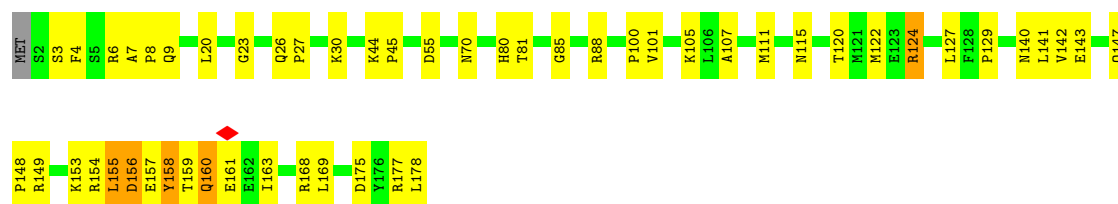


• Molecule 18: 39S ribosomal protein L11, mitochondrial



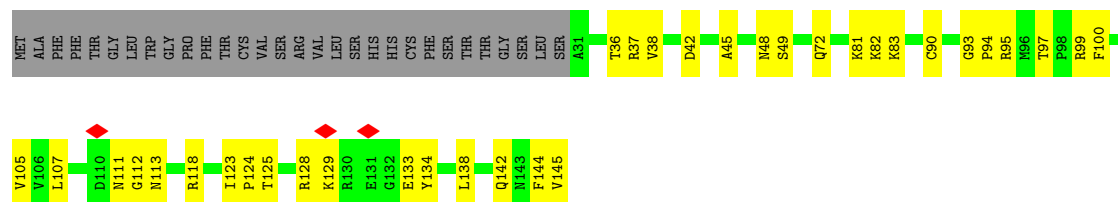
• Molecule 19: 39S ribosomal protein L13, mitochondrial

Chain K: 



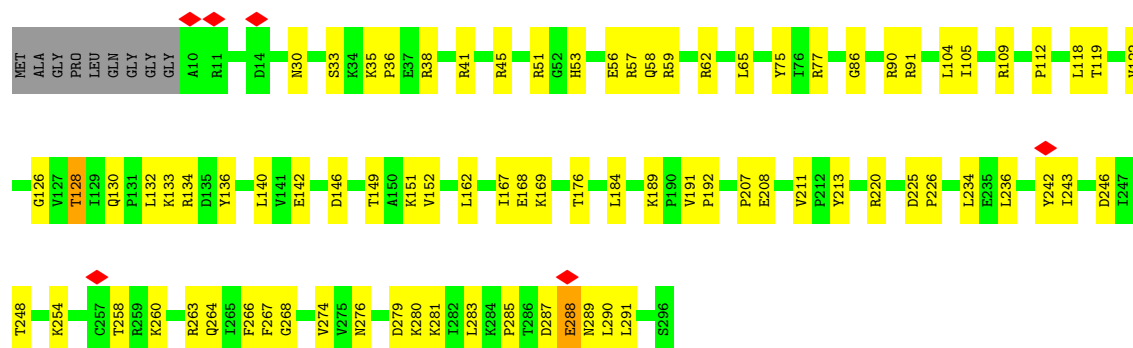
- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L: 



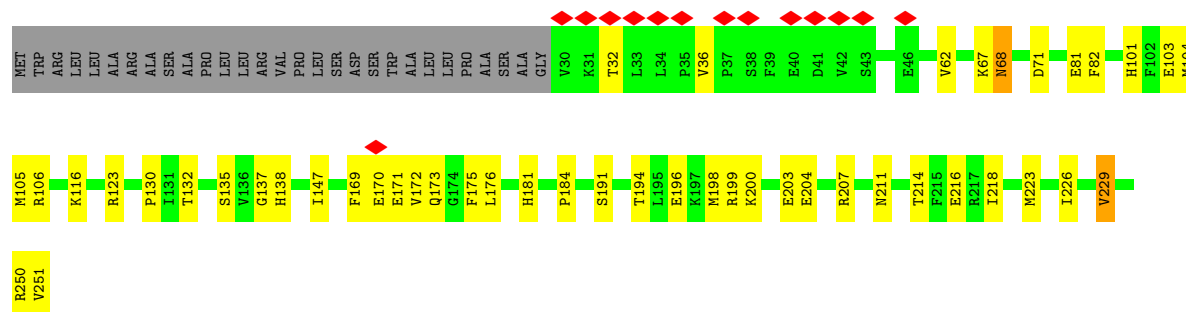
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M: 



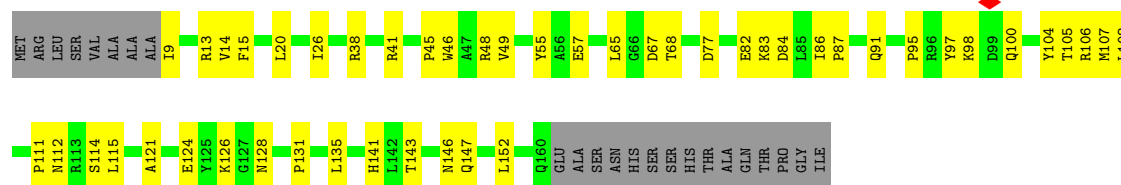
- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N: 

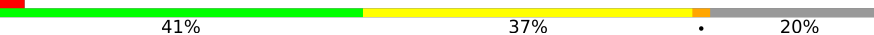


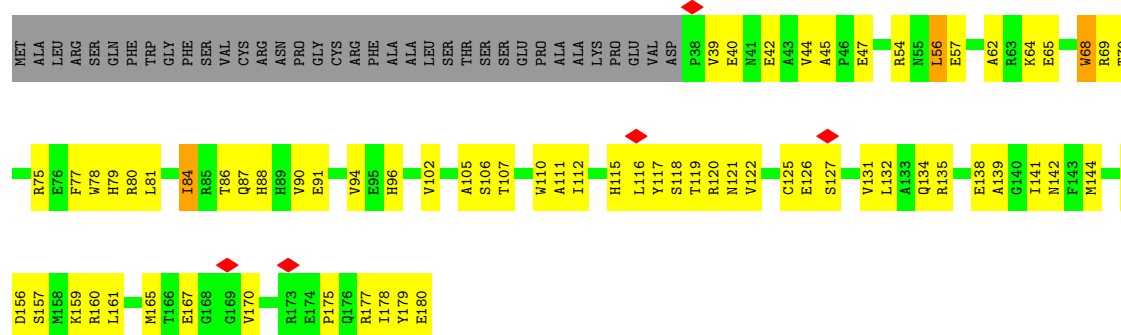
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O: 



- Molecule 24: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain P: 



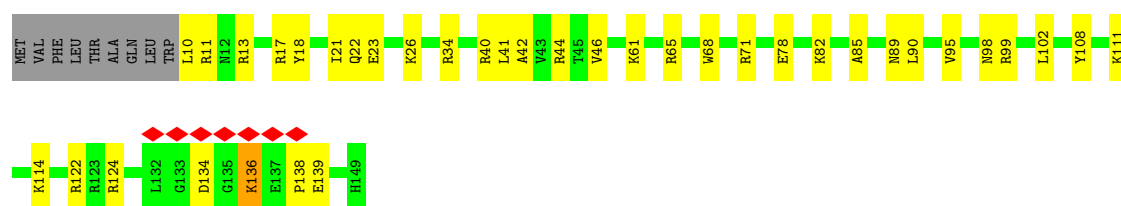
- Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q: 



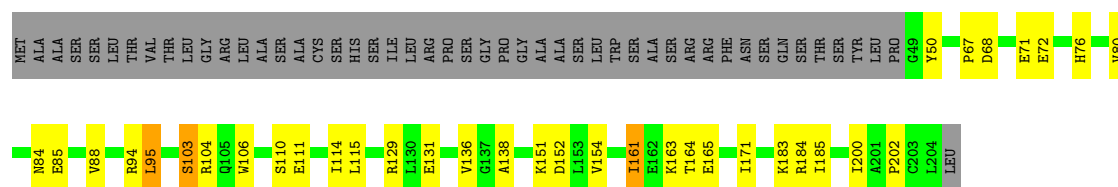
- Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R: 



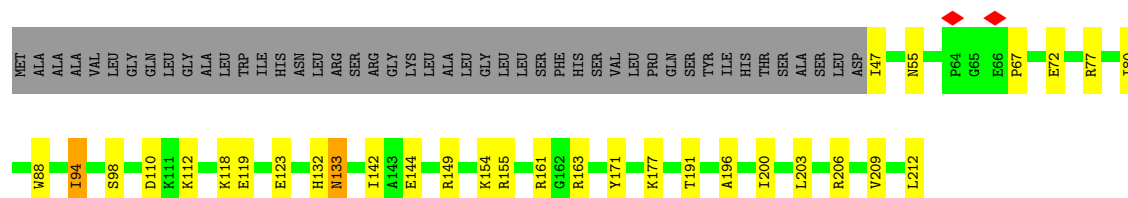
- Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S: 



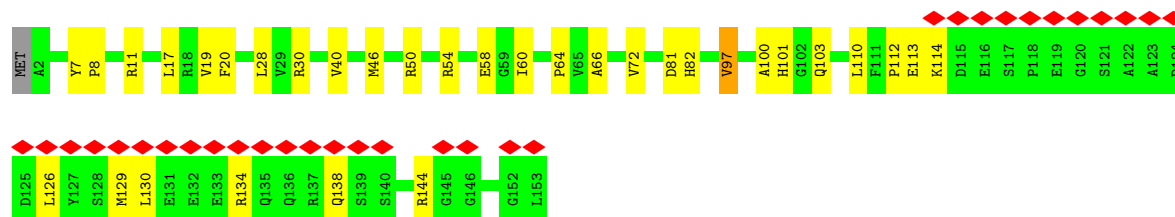
- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T: 



- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U: 



- Molecule 30: 39S ribosomal protein L24, mitochondrial

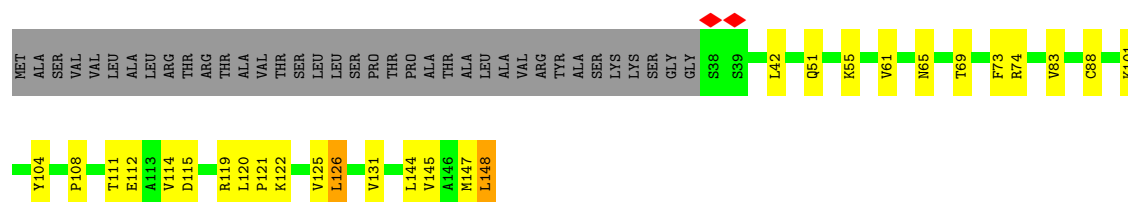
Chain V: 



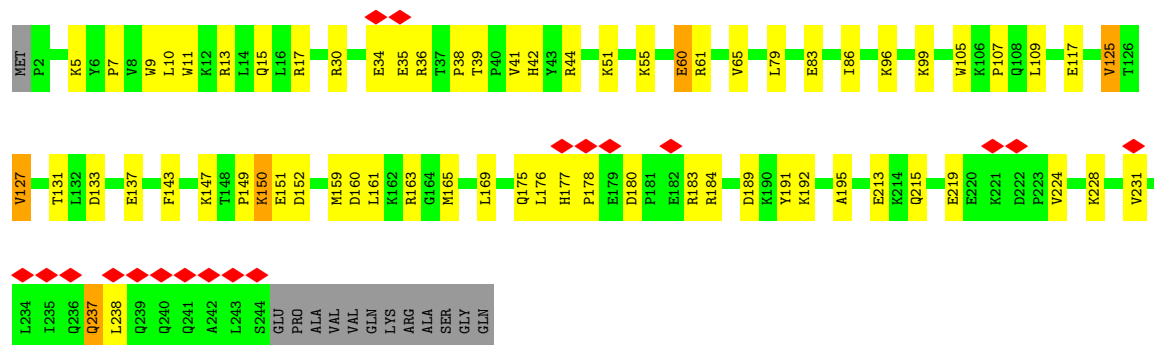
- Molecule 31: 39S ribosomal protein L27, mitochondrial

Chain W: 

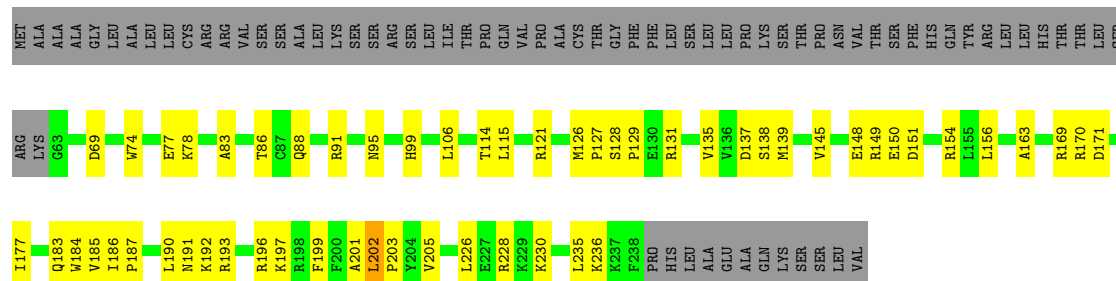




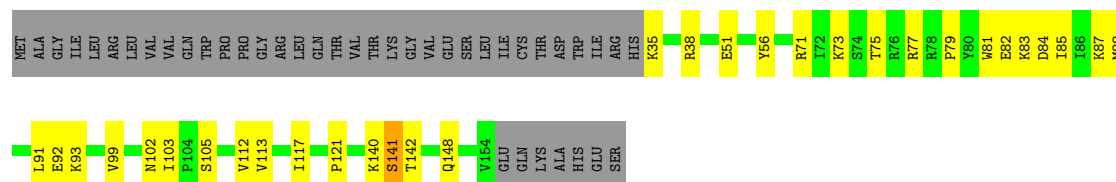
- Molecule 32: 39S ribosomal protein L28, mitochondrial



- Molecule 33: 39S ribosomal protein L47, mitochondrial

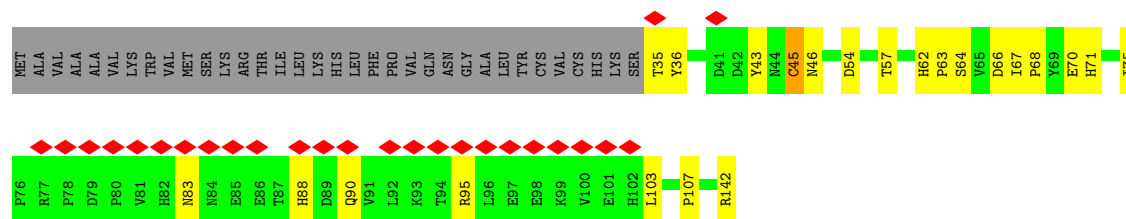


- Molecule 34: 39S ribosomal protein L30, mitochondrial



- Molecule 35: 39S ribosomal protein L42, mitochondrial





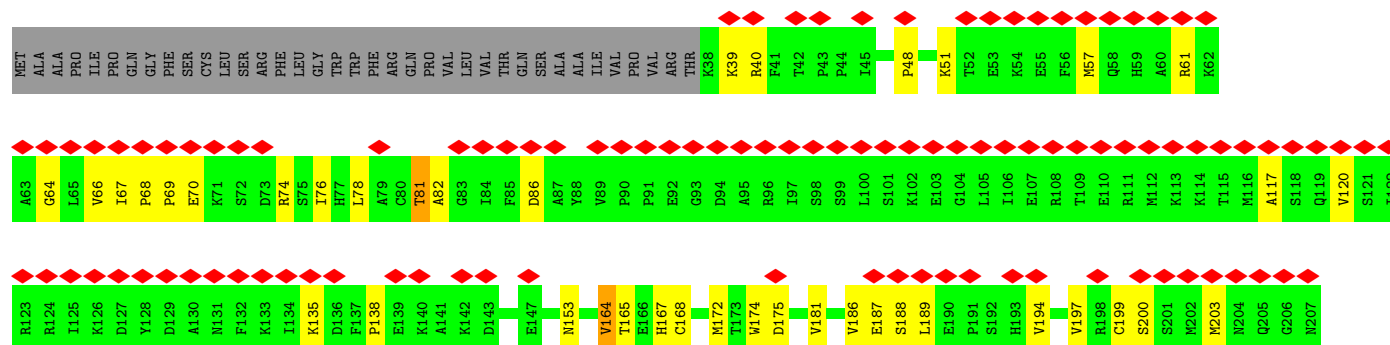
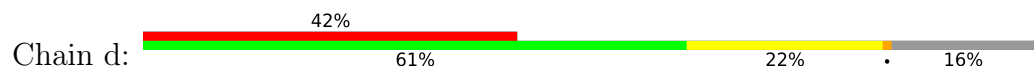
- Molecule 36: 39S ribosomal protein L43, mitochondrial

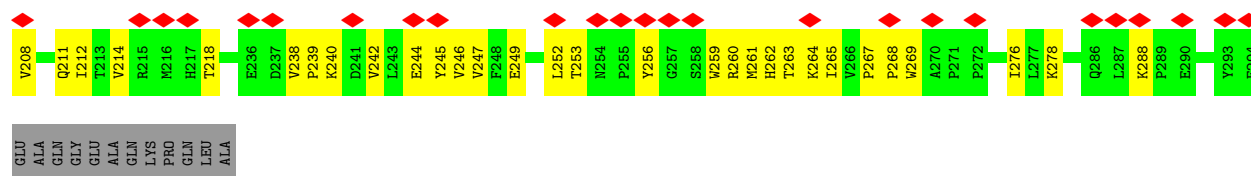


- Molecule 37: 39S ribosomal protein L44, mitochondrial



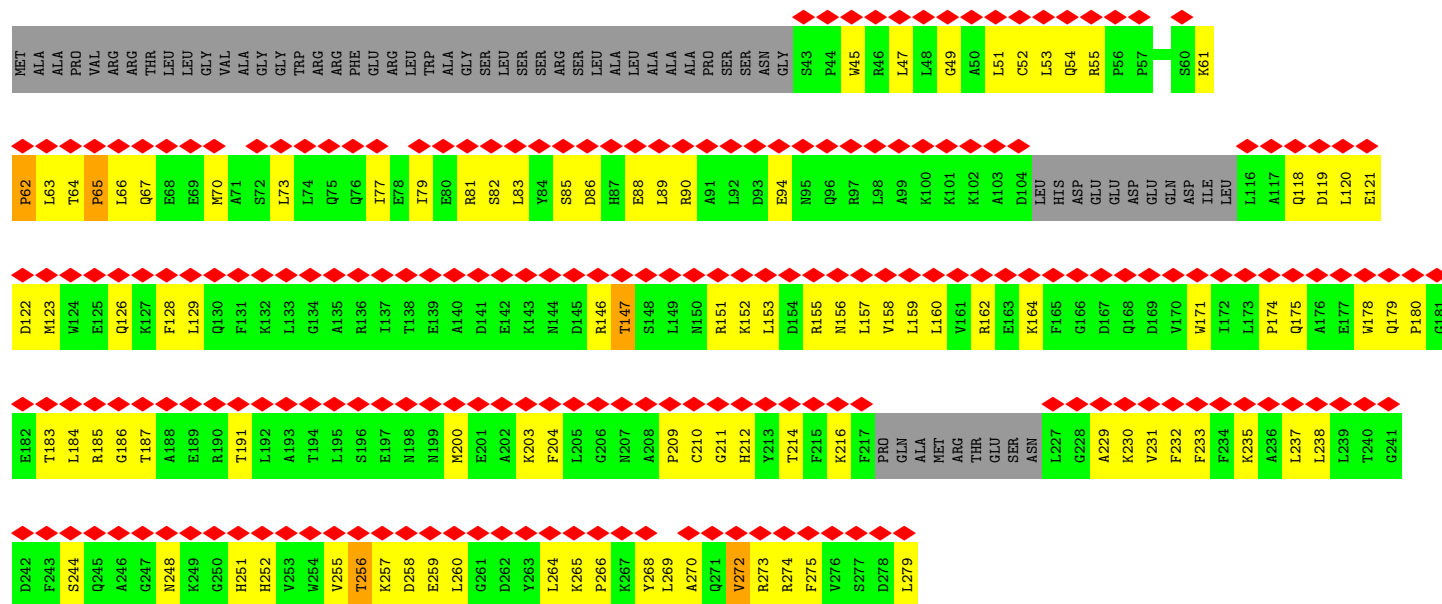
- Molecule 38: 39S ribosomal protein L45, mitochondrial





• Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:



• Molecule 40: 39S ribosomal protein L48, mitochondrial

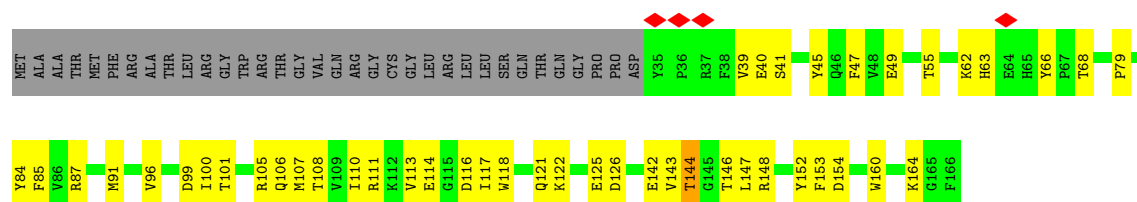
Chain f:



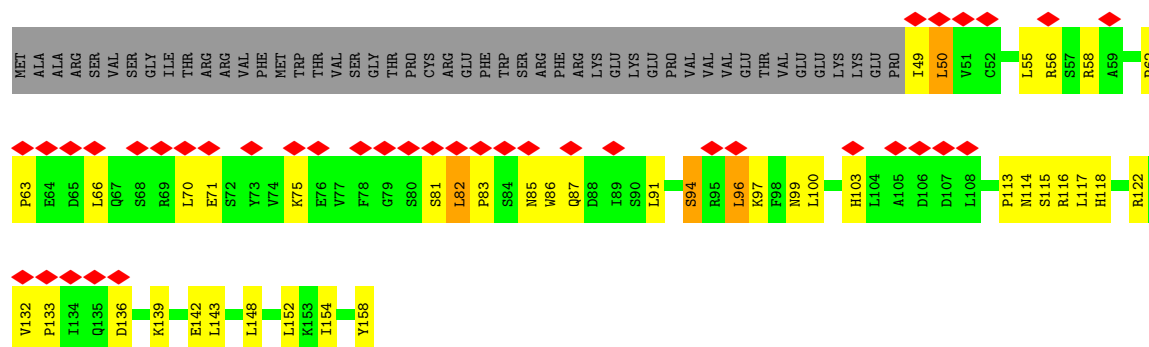
• Molecule 41: 39S ribosomal protein L49, mitochondrial

Chain g:

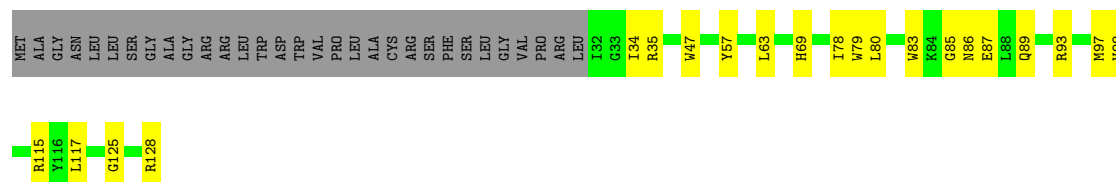




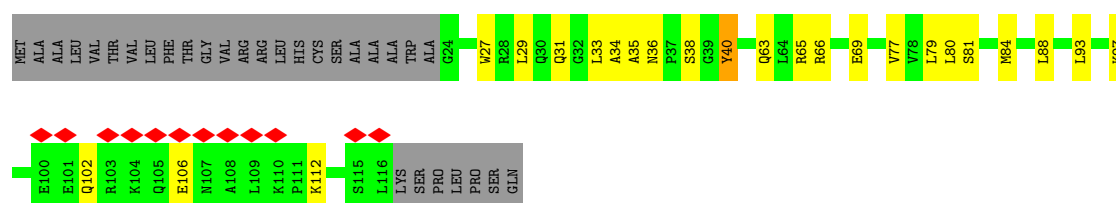
- Molecule 42: 39S ribosomal protein L50, mitochondrial



- Molecule 43: 39S ribosomal protein L51, mitochondrial

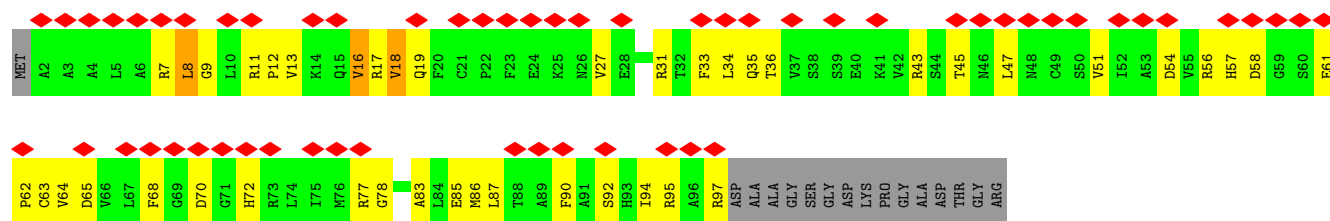


- Molecule 44: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

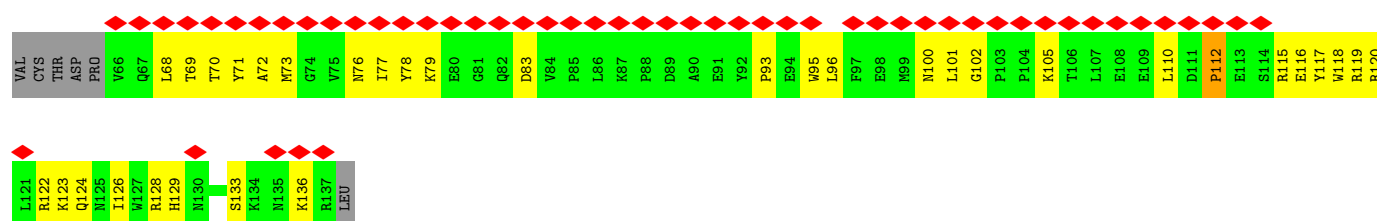
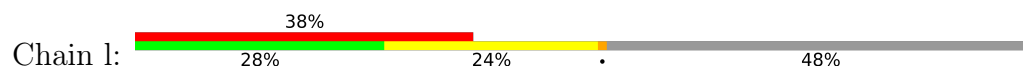


- Molecule 45: 39S ribosomal protein L53, mitochondrial

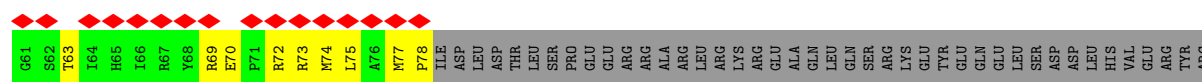
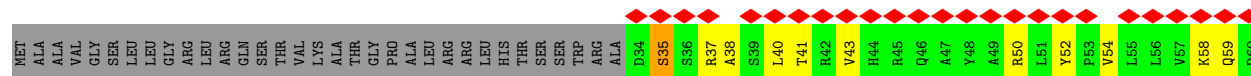




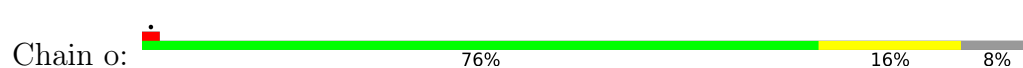
• Molecule 46: 39S ribosomal protein L54, mitochondrial



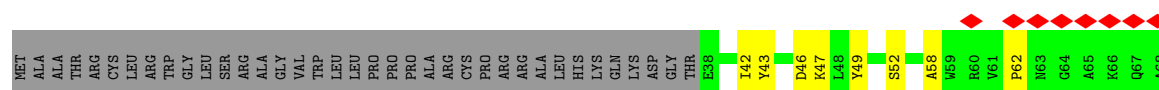
• Molecule 47: 39S ribosomal protein L55, mitochondrial



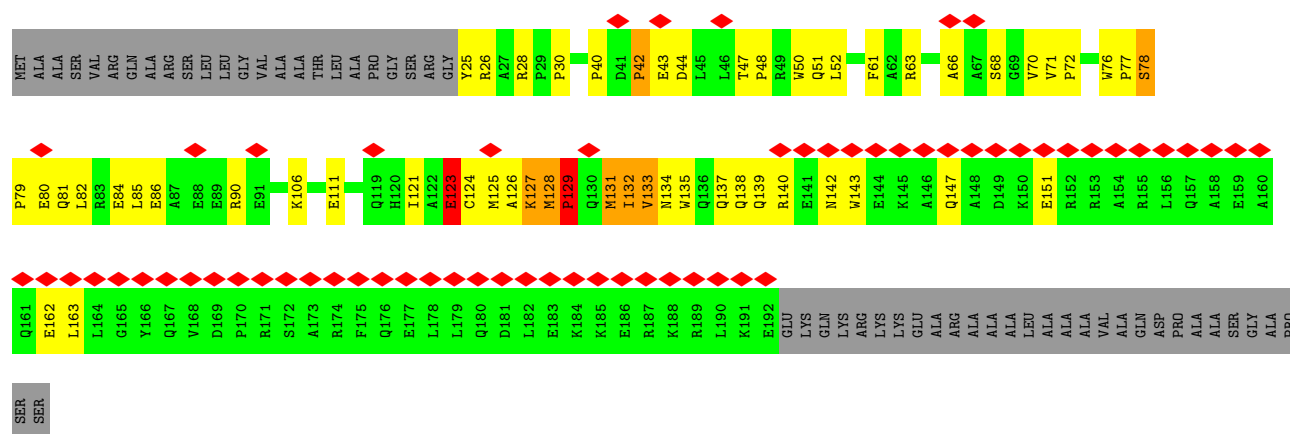
• Molecule 48: Ribosomal protein 63, mitochondrial



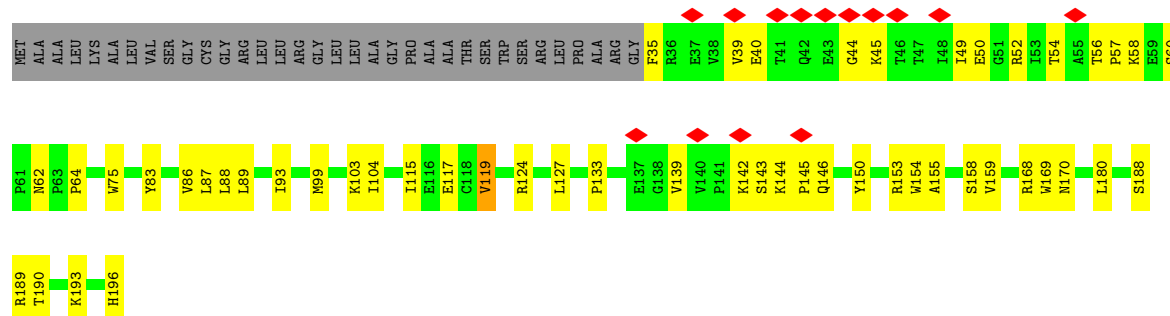
• Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial



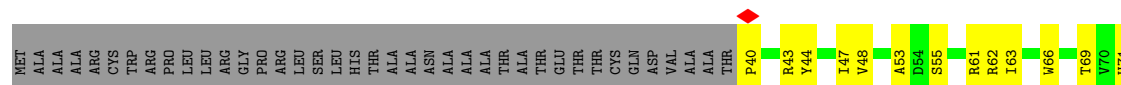
- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

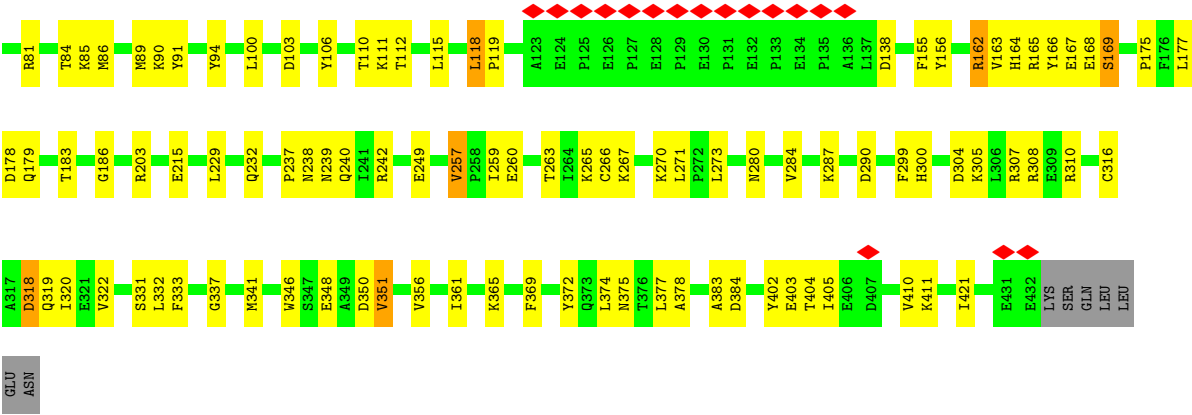


- Molecule 51: 39S ribosomal protein S18a, mitochondrial

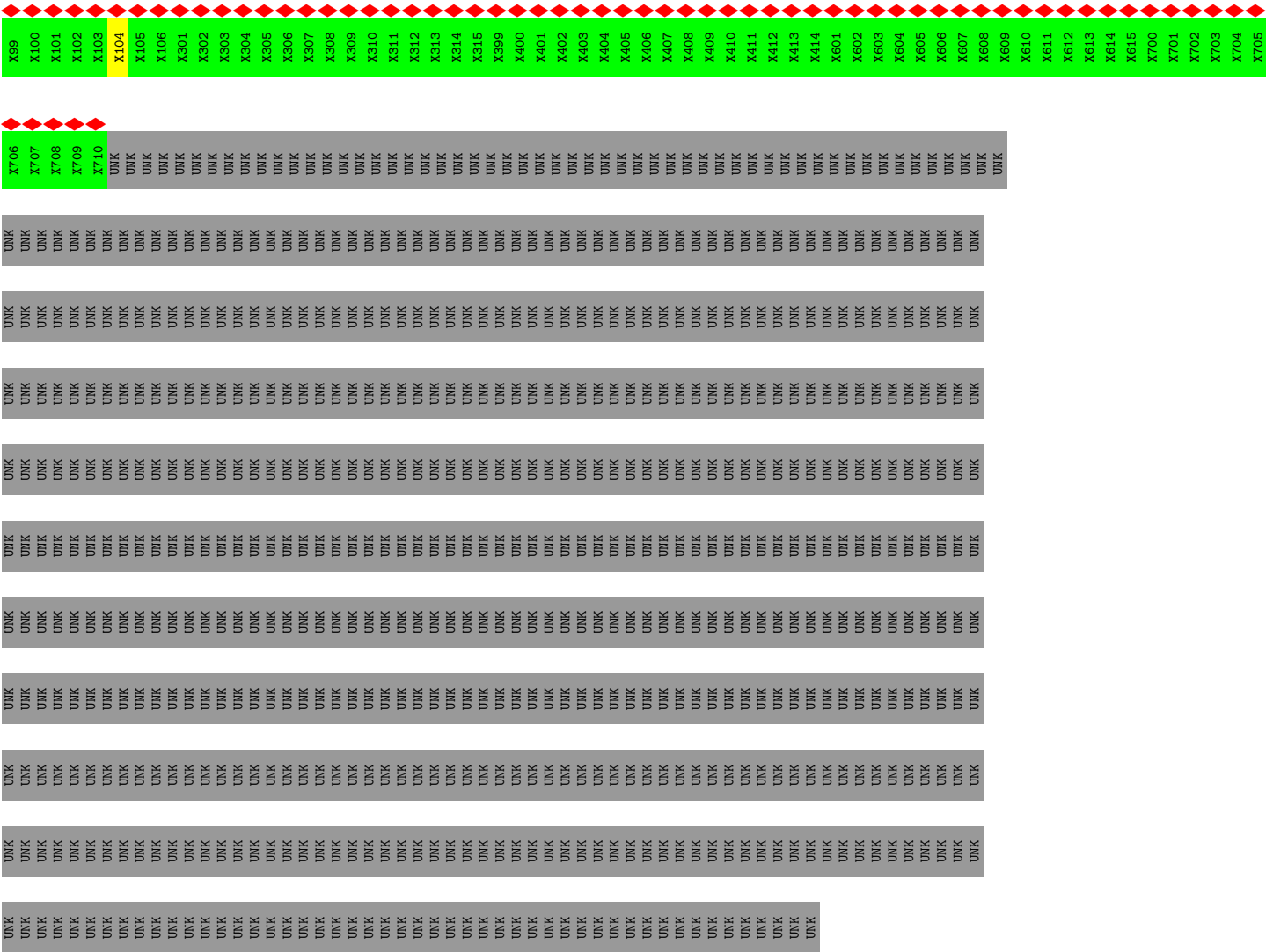


- Molecule 52: 39S ribosomal protein S30, mitochondrial





• Molecule 53: P-site finger



• Molecule 54: 39S ribosomal protein L12, mitochondrial

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	347872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.661	Depositor
Minimum map value	-2.742	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.38	Depositor
Map size ($\text{\AA}$)	484.4, 484.4, 484.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.865, 0.865, 0.865	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZLD, 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	0	0.19	0/895	0.41	0/1201
2	1	0.16	0/438	0.42	0/583
3	2	0.18	0/382	0.29	0/507
4	3	0.18	0/852	0.32	0/1136
5	4	0.14	0/350	0.36	0/461
6	5	0.21	0/3300	0.40	0/4495
7	6	0.20	0/3043	0.51	3/4140 (0.1%)
8	7	0.14	0/2467	0.36	0/3337
9	8	0.15	0/855	0.36	0/1152
10	9	0.19	0/1025	0.42	1/1379 (0.1%)
11	A	0.33	9/36246 (0.0%)	0.33	4/56422 (0.0%)
12	B	0.10	0/1328	0.25	0/2056
13	D	0.16	0/1904	0.37	0/2561
14	E	0.15	0/2479	0.37	0/3360
15	F	0.18	0/2071	0.42	0/2817
16	H	0.17	0/820	0.46	0/1102
17	I	0.48	2/1467 (0.1%)	0.78	4/1984 (0.2%)
18	J	0.87	6/1348 (0.4%)	1.35	11/1813 (0.6%)
19	K	0.19	0/1495	0.41	0/2029
20	L	0.17	0/904	0.45	2/1218 (0.2%)
21	M	0.19	0/2359	0.44	0/3185
22	N	0.17	0/1833	0.39	0/2468
23	O	0.18	0/1269	0.38	0/1708
24	P	0.19	0/1191	0.47	0/1611
25	Q	0.15	0/1875	0.34	0/2523
26	R	0.21	0/1174	0.43	0/1572
27	S	0.19	0/1276	0.39	0/1729
28	T	0.20	0/1402	0.39	1/1886 (0.1%)
29	U	0.18	0/1252	0.38	0/1697
30	V	0.14	0/1727	0.40	0/2341
31	W	0.18	0/893	0.40	0/1204
32	X	0.21	0/2090	0.41	0/2825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.16	0/1552	0.34	0/2079
34	Z	0.18	0/1003	0.37	0/1354
35	a	0.16	0/923	0.34	0/1254
36	b	0.17	0/1202	0.36	0/1626
37	c	0.16	0/2371	0.32	0/3205
38	d	0.72	3/2132 (0.1%)	0.78	5/2887 (0.2%)
39	e	0.59	3/1797 (0.2%)	0.95	6/2422 (0.2%)
40	f	0.19	0/1144	0.54	2/1551 (0.1%)
41	g	0.18	0/1132	0.43	0/1543
42	h	0.16	0/917	0.43	0/1249
43	i	0.21	0/849	0.41	0/1135
44	j	0.16	0/755	0.38	0/1016
45	k	0.44	2/754 (0.3%)	0.88	4/1017 (0.4%)
46	l	0.68	1/636 (0.2%)	1.04	4/860 (0.5%)
47	m	0.15	0/379	0.40	0/510
48	o	0.17	0/818	0.43	0/1097
49	p	0.18	0/1246	0.49	1/1675 (0.1%)
50	q	0.35	1/1325 (0.1%)	0.55	1/1799 (0.1%)
51	r	0.17	0/1362	0.39	0/1846
52	s	0.17	0/3262	0.39	2/4435 (0.0%)
54	TA	1.34	3/349 (0.9%)	2.02	5/475 (1.1%)
54	TB	0.12	0/212	0.36	0/286
54	TC	0.09	0/351	0.24	0/488
All	All	0.31	30/108481 (0.0%)	0.46	56/154311 (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
13	D	0	1
14	E	0	1
19	K	0	1
24	P	0	1
33	Y	0	1
34	Z	0	1
42	h	0	2
49	p	0	1
50	q	0	1
All	All	0	10

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	268	PRO	CG-CD	-30.05	0.48	1.50
11	A	2576	A	C6-N1	23.35	1.82	1.35
18	J	136	PRO	CG-CD	-22.68	0.73	1.50
11	A	2576	A	N1-C2	22.25	1.78	1.34
54	TA	52	PRO	CG-CD	-21.99	0.76	1.50
11	A	2576	A	N3-C4	21.68	1.78	1.34
11	A	2576	A	C2-N3	21.07	1.75	1.33
39	e	62	PRO	CG-CD	-19.83	0.83	1.50
11	A	2576	A	C5-C6	18.27	1.77	1.41
11	A	2576	A	C5-C4	16.41	1.71	1.38
46	l	112	PRO	CG-CD	-15.26	0.98	1.50
17	I	66	PRO	CG-CD	-15.07	0.99	1.50
18	J	136	PRO	CB-CG	12.60	2.12	1.49
11	A	2992	G	O3'-P	-11.70	1.43	1.61
39	e	62	PRO	CB-CG	9.92	1.99	1.49
38	d	268	PRO	CB-CG	9.90	1.99	1.49
18	J	74	PRO	CB-CG	-9.53	1.02	1.49
45	k	62	PRO	CG-CD	-9.13	1.19	1.50
18	J	74	PRO	CG-CD	-8.44	1.22	1.50
39	e	62	PRO	CA-CB	-8.01	1.43	1.53
54	TA	52	PRO	CB-CG	7.97	1.89	1.49
18	J	136	PRO	CA-CB	-7.40	1.43	1.53
17	I	66	PRO	N-CD	6.64	1.57	1.47
54	TA	52	PRO	CA-CB	-6.27	1.44	1.53
45	k	62	PRO	CB-CG	-5.98	1.19	1.49
50	q	123	GLU	C-O	5.90	1.31	1.24
38	d	268	PRO	N-CD	5.67	1.55	1.47
11	A	2993	U	O3'-P	-5.66	1.52	1.61
11	A	2991	U	O3'-P	-5.49	1.52	1.61
18	J	74	PRO	N-CA	5.21	1.54	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	TA	52	PRO	N-CD-CG	-32.86	53.91	103.20
38	d	268	PRO	N-CD-CG	-28.97	59.74	103.20
39	e	62	PRO	N-CD-CG	-28.41	60.59	103.20
18	J	136	PRO	N-CD-CG	-25.46	65.00	103.20
39	e	62	PRO	CA-CB-CG	-21.30	64.02	104.50
54	TA	52	PRO	CA-CB-CG	-21.14	64.34	104.50
18	J	74	PRO	CB-CG-CD	20.41	171.43	106.10
46	l	112	PRO	N-CD-CG	-19.63	73.76	103.20
18	J	136	PRO	CA-CB-CG	-19.50	67.44	104.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	I	66	PRO	N-CD-CG	-19.29	74.26	103.20
18	J	74	PRO	N-CD-CG	-18.81	74.98	103.20
18	J	74	PRO	CA-CB-CG	-17.47	71.30	104.50
45	k	62	PRO	N-CD-CG	-16.89	77.86	103.20
39	e	62	PRO	N-CA-CB	-16.27	89.66	103.32
18	J	136	PRO	N-CA-CB	-15.77	86.69	103.25
46	l	112	PRO	CB-CG-CD	13.78	150.18	106.10
54	TA	52	PRO	N-CA-CB	-13.49	89.09	103.25
18	J	136	PRO	CB-CG-CD	-13.45	63.08	106.10
18	J	31	PRO	CA-N-CD	-13.01	93.78	112.00
38	d	268	PRO	CB-CG-CD	-12.97	64.58	106.10
46	l	112	PRO	CA-CB-CG	-12.83	80.13	104.50
17	I	66	PRO	CA-CB-CG	-12.46	80.82	104.50
38	d	268	PRO	CA-CB-CG	-12.01	81.67	104.50
45	k	62	PRO	CA-CB-CG	-11.88	81.94	104.50
45	k	62	PRO	CA-N-CD	-10.98	96.62	112.00
17	I	66	PRO	CB-CG-CD	10.97	141.21	106.10
7	6	241	PRO	CA-N-CD	-10.84	96.83	112.00
38	d	268	PRO	N-CA-CB	-10.68	92.80	103.48
40	f	179	PRO	CA-N-CD	-10.41	97.43	112.00
18	J	136	PRO	CA-N-CD	-9.89	98.16	112.00
17	I	66	PRO	CA-N-CD	-9.67	98.46	112.00
7	6	228	PRO	CA-N-CD	-9.24	99.06	112.00
11	A	2576	A	N1-C2-N3	-8.41	104.06	129.30
39	e	62	PRO	CB-CG-CD	-8.14	80.06	106.10
38	d	268	PRO	CA-N-CD	-7.94	100.88	112.00
39	e	62	PRO	CA-N-CD	-7.92	100.91	112.00
11	A	2579	C	P-O3'-C3'	-7.87	108.40	120.20
18	J	74	PRO	CA-N-CD	-7.58	101.38	112.00
11	A	2580	U	P-O3'-C3'	-7.56	108.85	120.20
28	T	67	PRO	CA-N-CD	-7.39	101.65	112.00
18	J	31	PRO	N-CD-CG	-7.20	92.40	103.20
46	l	112	PRO	CA-N-CD	-7.10	102.06	112.00
20	L	112	GLY	CA-C-N	6.92	134.15	121.70
20	L	112	GLY	C-N-CA	6.92	134.15	121.70
39	e	65	PRO	CA-N-CD	-6.84	102.42	112.00
54	TA	52	PRO	CA-N-CD	-6.78	102.51	112.00
11	A	2576	A	C2-N3-C4	6.68	130.63	110.60
50	q	129	PRO	CA-N-CD	-6.48	102.92	112.00
10	9	79	PRO	CA-N-CD	-6.09	103.47	112.00
52	s	162	ARG	CA-C-N	6.02	132.53	121.70
52	s	162	ARG	C-N-CA	6.02	132.53	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	62	PRO	CB-CG-CD	5.99	125.28	106.10
49	p	191	LYS	CA-CB-CG	5.65	125.40	114.10
40	f	127	MET	CB-CG-SD	5.34	128.72	112.70
7	6	184	LEU	CA-CB-CG	5.32	134.90	116.30
54	TA	52	PRO	CB-CA-C	5.13	120.03	111.56

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	206	TYR	Peptide
14	E	316	PHE	Peptide
19	K	3	SER	Peptide
24	P	68	TRP	Peptide
33	Y	202	LEU	Peptide
34	Z	141	SER	Peptide
42	h	132	VAL	Peptide
42	h	82	LEU	Peptide
49	p	83	ARG	Peptide
50	q	78	SER	Peptide

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	0	880	0	902	27	0
2	1	433	0	475	17	0
3	2	376	0	406	5	0
4	3	831	0	883	16	0
5	4	342	0	361	12	0
6	5	3205	0	3201	81	0
7	6	2948	0	2841	122	0
8	7	2410	0	2415	63	0
9	8	836	0	844	37	0
10	9	997	0	987	34	0
11	A	32395	0	16450	495	0
12	B	1191	0	607	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	1866	0	1927	60	0
14	E	2410	0	2418	47	0
15	F	2013	0	2044	57	0
16	H	806	0	849	27	0
17	I	1435	0	1521	58	0
18	J	1330	0	1407	62	0
19	K	1451	0	1448	40	0
20	L	889	0	941	23	0
21	M	2305	0	2378	67	0
22	N	1786	0	1817	41	0
23	O	1245	0	1283	35	0
24	P	1165	0	1162	54	0
25	Q	1834	0	1872	34	0
26	R	1153	0	1214	30	0
27	S	1251	0	1322	28	0
28	T	1368	0	1410	19	0
29	U	1222	0	1187	31	0
30	V	1682	0	1692	61	0
31	W	871	0	898	21	0
32	X	2035	0	2054	43	0
33	Y	1517	0	1561	42	0
34	Z	978	0	1030	24	0
35	a	896	0	847	19	0
36	b	1178	0	1180	35	0
37	c	2322	0	2338	55	0
38	d	2075	0	2037	49	0
39	e	1762	0	1767	94	0
40	f	1126	0	1106	51	0
41	g	1096	0	1081	35	0
42	h	894	0	881	34	0
43	i	827	0	857	18	0
44	j	740	0	741	20	0
45	k	743	0	758	33	0
46	l	619	0	611	29	0
47	m	372	0	387	31	0
48	o	797	0	804	15	0
49	p	1227	0	1239	51	0
50	q	1294	0	1178	58	0
51	r	1322	0	1349	45	0
52	s	3178	0	3124	73	0
53	u	325	0	77	1	0
54	TA	345	0	364	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	TB	213	0	234	8	0
54	TC	352	0	169	0	0
55	0	1	0	0	0	0
55	4	1	0	0	0	0
55	r	1	0	0	0	0
56	A	100	0	0	0	0
56	D	1	0	0	0	0
56	g	1	0	0	0	0
57	A	24	0	20	3	0
58	0	16	0	0	1	0
58	1	8	0	0	0	0
58	2	10	0	0	0	0
58	3	15	0	0	1	0
58	4	7	0	0	0	0
58	5	63	0	0	1	0
58	6	99	0	0	2	0
58	7	96	0	0	7	0
58	8	44	0	0	3	0
58	9	23	0	0	0	0
58	A	1975	0	0	11	0
58	B	99	0	0	3	0
58	D	31	0	0	1	0
58	E	51	0	0	0	0
58	F	24	0	0	2	0
58	H	29	0	0	1	0
58	I	62	0	0	6	0
58	J	107	0	0	5	0
58	K	28	0	0	0	0
58	L	14	0	0	1	0
58	M	39	0	0	0	0
58	N	49	0	0	0	0
58	O	26	0	0	0	0
58	P	34	0	0	2	0
58	Q	50	0	0	1	0
58	R	20	0	0	3	0
58	S	27	0	0	0	0
58	T	29	0	0	0	0
58	TA	43	0	0	0	0
58	TB	22	0	0	3	0
58	TC	37	0	0	0	0
58	U	35	0	0	1	0
58	V	37	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	W	19	0	0	0	0
58	X	30	0	0	2	0
58	Y	22	0	0	1	0
58	Z	27	0	0	2	0
58	a	18	0	0	1	0
58	b	34	0	0	1	0
58	c	21	0	0	0	0
58	d	10	0	0	0	0
58	e	196	0	0	11	0
58	f	59	0	0	4	0
58	g	27	0	0	1	0
58	h	36	0	0	2	0
58	i	28	0	0	0	0
58	j	24	0	0	1	0
58	k	32	0	0	2	0
58	l	50	0	0	2	0
58	m	33	0	0	3	0
58	o	18	0	0	0	0
58	p	57	0	0	2	0
58	q	6	0	0	0	0
58	r	44	0	0	1	0
58	s	57	0	0	1	0
58	u	32	0	0	0	0
All	All	107417	0	86956	2218	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 12.

All (2218) 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)
11:A:2576:A:C5	11:A:2576:A:C6	1.77	1.65
11:A:2576:A:C4	11:A:2576:A:N3	1.78	1.52
11:A:2576:A:N3	11:A:2576:A:C2	1.75	1.51
11:A:2576:A:C2	11:A:2576:A:N1	1.78	1.48
11:A:2576:A:C6	11:A:2576:A:N1	1.82	1.47
11:A:3110:C:H42	11:A:3203:A:N6	1.43	1.16
11:A:3110:C:N4	11:A:3203:A:H61	1.44	1.15
51:r:144:LYS:HD3	51:r:145:PRO:HD2	1.44	1.00
40:f:127:MET:HE3	40:f:128:PRO:HD2	1.43	0.98
7:6:194:THR:HG23	49:p:185:ARG:HH12	1.31	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:68:ASN:ND2	22:N:68:ASN:O	1.99	0.96
12:B:1607:U:H3	12:B:1664:G:H1	1.15	0.95
6:5:59:THR:HA	6:5:70:LEU:HG	1.50	0.91
50:q:125:MET:O	50:q:129:PRO:HD2	1.68	0.91
7:6:184:LEU:HD12	49:p:190:GLN:H	1.37	0.90
24:P:81:LEU:HB2	24:P:144:MET:HE3	1.54	0.89
11:A:1873:A:H61	11:A:1901:C:H42	1.21	0.88
11:A:3110:C:N3	11:A:3203:A:N1	2.23	0.86
24:P:84:ILE:HG12	24:P:91:GLU:HG2	1.57	0.86
9:8:85:ILE:HB	40:f:128:PRO:HG3	1.58	0.85
5:4:66:PHE:N	11:A:3013:G:HO2'	1.74	0.83
49:p:128:ASN:OD1	49:p:129:ARG:N	2.11	0.83
40:f:101:THR:HG1	47:m:41:THR:HG1	1.25	0.81
11:A:1849:C:OP2	21:M:53:HIS:NE2	2.12	0.81
25:Q:76:LEU:HD21	25:Q:282:ILE:HD11	1.62	0.81
24:P:112:ILE:HG13	24:P:116:LEU:HD23	1.61	0.80
50:q:128:MET:HB3	50:q:129:PRO:HD2	1.63	0.80
7:6:175:VAL:HG12	7:6:204:VAL:HG22	1.64	0.80
11:A:3011:A:O2'	11:A:3173:G:N2	2.15	0.80
29:U:66:ALA:HB2	29:U:100:ALA:HA	1.61	0.80
12:B:1627:C:N3	58:B:1701:HOH:O	2.14	0.79
51:r:35:PHE:N	51:r:56:THR:HG1	1.80	0.79
11:A:3110:C:H42	11:A:3203:A:H61	0.80	0.79
45:k:57:HIS:HB3	54:TA:53:LEU:HD13	1.64	0.79
15:F:282:PRO:O	15:F:290:TYR:OH	2.02	0.78
11:A:1994:A:O2'	11:A:2002:G:N7	2.14	0.78
11:A:2108:G:N7	22:N:67:LYS:NZ	2.31	0.78
39:e:65:PRO:HD2	39:e:66:LEU:H	1.49	0.78
7:6:126:ARG:HB3	24:P:160:ARG:HH22	1.47	0.78
12:B:1641:G:N1	58:B:1701:HOH:O	2.16	0.77
18:J:111:LEU:HD23	18:J:154:ARG:HH22	1.51	0.76
19:K:158:TYR:HB3	19:K:163:ILE:HD11	1.67	0.76
33:Y:151:ASP:OD1	33:Y:154:ARG:NH2	2.17	0.76
28:T:144:GLU:HG3	28:T:177:LYS:HD3	1.68	0.76
11:A:2073:A:H62	11:A:2832:A:H2	1.31	0.76
11:A:2643:G:O2'	11:A:2645:G:OP2	2.01	0.76
18:J:42:ARG:O	18:J:76:ARG:NH2	2.19	0.75
30:V:126:MET:HE3	30:V:152:ARG:HD3	1.66	0.75
34:Z:71:ARG:NH2	34:Z:92:GLU:O	2.19	0.75
11:A:2171:U:H4'	11:A:2172:A:H3'	1.68	0.75
23:O:111:PRO:O	23:O:112:ASN:ND2	2.19	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:128:ILE:HD11	6:5:372:LEU:HD12	1.69	0.74
42:h:71:GLU:OE1	42:h:75:LYS:NZ	2.20	0.74
2:1:50:VAL:HG11	50:q:125:MET:HE1	1.69	0.74
7:6:155:TYR:O	7:6:267:ARG:NH1	2.20	0.74
54:TB:74:LEU:HD21	54:TB:82:LEU:HD13	1.68	0.74
11:A:1879:G:OP1	15:F:92:ARG:NH2	2.21	0.73
23:O:106:ARG:HD2	23:O:135:LEU:HD21	1.69	0.73
39:e:255:VAL:HG13	39:e:259:GLU:HB2	1.68	0.73
22:N:218:ILE:HG23	22:N:223:MET:HB2	1.69	0.73
1:0:119:LYS:O	1:0:120:HIS:ND1	2.22	0.73
29:U:81:ASP:OD1	29:U:82:HIS:N	2.21	0.73
39:e:185:ARG:HH21	39:e:204:PHE:HB3	1.52	0.73
2:1:24:ALA:HB1	50:q:125:MET:CE	2.19	0.73
8:7:197:GLU:OE1	8:7:197:GLU:N	2.18	0.73
38:d:197:VAL:HG13	38:d:212:ILE:HG12	1.70	0.73
51:r:142:LYS:NZ	51:r:143:SER:O	2.22	0.73
11:A:2661:U:OP2	14:E:238:ARG:NH2	2.21	0.72
45:k:11:ARG:HD2	45:k:12:PRO:HD3	1.72	0.72
47:m:37:ARG:NH2	58:m:201:HOH:O	2.22	0.72
21:M:104:LEU:HD11	21:M:126:GLY:HA3	1.72	0.72
24:P:68:TRP:O	24:P:70:THR:N	2.20	0.72
25:Q:120:THR:HB	25:Q:132:GLN:HG3	1.72	0.72
39:e:162:ARG:HB2	39:e:251:HIS:HB2	1.72	0.72
39:e:268:TYR:HD1	39:e:269:LEU:HD22	1.53	0.72
7:6:279:ILE:HD12	7:6:310:THR:HG21	1.70	0.72
11:A:2373:A:OP1	29:U:50:ARG:NH2	2.22	0.71
40:f:135:LEU:HB2	40:f:145:LEU:HD21	1.72	0.71
11:A:2599:U:OP2	11:A:2625:C:N4	2.24	0.71
19:K:168:ARG:HD3	51:r:57:PRO:HB2	1.72	0.71
42:h:122:ARG:HE	42:h:124:ARG:HH22	1.38	0.71
9:8:100:GLU:HG2	9:8:101:ARG:HE	1.53	0.71
37:c:203:LEU:HA	37:c:211:THR:HG21	1.72	0.71
39:e:61:LYS:HZ2	47:m:35:SER:HB2	1.54	0.71
44:j:102:GLN:NE2	44:j:106:GLU:OE2	2.23	0.71
46:l:110:LEU:HD23	46:l:117:TYR:HA	1.73	0.71
49:p:113:GLU:OE1	49:p:116:ARG:NH1	2.23	0.71
6:5:296:ALA:HB3	6:5:302:ARG:HG3	1.73	0.70
1:0:140:GLN:HG3	1:0:177:ARG:HB3	1.72	0.70
11:A:1747:G:N2	11:A:1750:G:O2'	2.24	0.70
11:A:1867:A:H62	11:A:2295:C:H5	1.38	0.70
17:I:85:GLU:OE2	46:l:115:ARG:NH2	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1709:G:OP1	33:Y:192:LYS:NZ	2.24	0.70
11:A:2499:U:OP2	11:A:2504:A:N6	2.20	0.70
45:k:18:VAL:HG12	45:k:64:VAL:HG22	1.71	0.70
11:A:1756:A:H2'	11:A:1757:A:H8	1.56	0.70
37:c:155:ASN:HD22	37:c:232:TRP:HD1	1.39	0.70
39:e:81:ARG:NH2	47:m:43:VAL:O	2.24	0.70
11:A:2994:U:H5''	11:A:3060:C:N4	2.07	0.70
16:H:69:ARG:HH12	16:H:70:LYS:HE3	1.57	0.70
45:k:56:ARG:HH12	45:k:61:GLU:H	1.39	0.70
46:l:77:ILE:HG23	46:l:78:TYR:HD1	1.56	0.70
6:5:81:TYR:CE1	30:V:211:LYS:HD3	2.27	0.70
17:I:100:GLN:NE2	45:k:35:GLN:OE1	2.25	0.70
1:0:177:ARG:HH12	1:0:179:ARG:HD3	1.56	0.70
13:D:121:PRO:HB3	13:D:166:SER:HA	1.72	0.70
11:A:1736:A:N6	11:A:1761:A:O2'	2.25	0.70
11:A:2578:C:H2'	11:A:2579:C:C6	2.27	0.70
18:J:84:GLN:HB2	18:J:127:ASP:HB3	1.74	0.70
11:A:2530:A:H4'	11:A:2531:U:H5''	1.73	0.69
27:S:88:VAL:HG12	27:S:202:PRO:HB3	1.74	0.69
11:A:1777:A:N6	11:A:1780:U:OP2	2.25	0.69
11:A:2932:G:OP1	15:F:137:ARG:NH1	2.25	0.69
17:I:157:GLU:OE1	17:I:157:GLU:N	2.22	0.69
11:A:1936:A:OP1	11:A:1938:A:N6	2.25	0.69
7:6:337:MET:O	49:p:129:ARG:NH2	2.26	0.69
11:A:2016:C:OP2	21:M:59:ARG:NH1	2.26	0.69
25:Q:95:GLU:O	25:Q:99:MET:HG3	1.92	0.69
30:V:132:GLU:OE1	30:V:132:GLU:N	2.25	0.69
7:6:183:ASP:HB2	49:p:189:ARG:HB3	1.74	0.69
38:d:67:ILE:HA	38:d:70:GLU:HG3	1.72	0.69
7:6:306:LYS:HG3	7:6:307:HIS:CD2	2.27	0.69
11:A:2677:A:H2'	11:A:2678:A:C8	2.28	0.69
17:I:186:LEU:HD12	17:I:190:GLY:HA3	1.75	0.68
18:J:21:ARG:HG3	18:J:69:LYS:HE3	1.74	0.68
13:D:136:SER:O	13:D:249:ASN:ND2	2.26	0.68
15:F:113:LYS:HG3	15:F:157:GLY:H	1.58	0.68
11:A:2248:U:OP1	26:R:99:ARG:NH2	2.27	0.68
39:e:85:SER:HB3	39:e:88:GLU:HB2	1.75	0.68
39:e:274:ARG:NH1	39:e:275:PHE:HB3	2.08	0.68
52:s:118:LEU:HD13	52:s:119:PRO:HD2	1.76	0.68
7:6:184:LEU:HD12	49:p:190:GLN:N	2.08	0.68
19:K:27:PRO:HG2	19:K:30:LYS:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:169:LYS:HD2	21:M:242:TYR:HB3	1.76	0.68
22:N:81:GLU:O	22:N:123:ARG:NH2	2.26	0.68
30:V:105:ARG:HH22	38:d:174:TRP:HZ3	1.41	0.68
37:c:202:LEU:HG	37:c:211:THR:HG22	1.75	0.68
11:A:2430:A:N6	28:T:161:ARG:O	2.27	0.68
11:A:2725:A:N6	11:A:2990:A:H62	1.92	0.68
36:b:37:GLY:O	36:b:44:ARG:NH2	2.27	0.68
7:6:185:MET:HE3	7:6:193:VAL:HG22	1.74	0.68
21:M:112:PRO:HB3	21:M:152:VAL:HG12	1.74	0.68
21:M:208:GLU:OE1	50:q:106:LYS:NZ	2.27	0.68
15:F:175:LYS:HG3	15:F:273:LEU:HD13	1.75	0.67
6:5:100:ASP:OD1	6:5:100:ASP:N	2.23	0.67
2:1:23:GLU:OE1	2:1:23:GLU:N	2.27	0.67
11:A:2055:U:H2'	11:A:2056:G:H8	1.58	0.67
11:A:2103:A:HO2'	34:Z:35:LYS:N	1.92	0.67
54:TB:74:LEU:HG	54:TB:78:GLU:HB3	1.76	0.67
7:6:194:THR:HG23	49:p:185:ARG:NH1	2.06	0.67
51:r:117:GLU:HG3	51:r:180:LEU:HD12	1.75	0.67
39:e:54:GLN:HE22	39:e:235:LYS:HB2	1.60	0.67
8:7:159:LYS:HB2	35:a:88:HIS:HA	1.74	0.67
29:U:46:MET:HE1	29:U:72:VAL:HG13	1.76	0.67
52:s:242:ARG:NH1	52:s:290:ASP:OD2	2.27	0.67
14:E:210:THR:OG1	14:E:262:GLY:O	2.13	0.67
19:K:160:GLN:HA	19:K:163:ILE:HG12	1.77	0.67
11:A:1794:A:OP1	15:F:142:ARG:NH2	2.26	0.66
16:H:97:ILE:HD11	16:H:137:LYS:HD3	1.76	0.66
30:V:55:TYR:O	30:V:145:ARG:NH1	2.28	0.66
41:g:113:VAL:HG11	41:g:117:ILE:HG13	1.77	0.66
11:A:2190:C:OP2	46:l:120:ARG:NH1	2.20	0.66
11:A:2740:A:H2'	11:A:2741:A:C8	2.30	0.66
37:c:213:LEU:HD22	37:c:216:ARG:HH21	1.60	0.66
44:j:36:ASN:OD1	44:j:38:SER:OG	2.11	0.66
50:q:131:MET:O	50:q:134:ASN:HB2	1.94	0.66
58:8:301:HOH:O	39:e:203:LYS:NZ	2.29	0.66
14:E:133:THR:OG1	14:E:144:THR:OG1	2.14	0.66
36:b:66:ASN:OD1	36:b:68:ARG:NH1	2.28	0.66
37:c:85:LEU:O	37:c:89:LYS:HG2	1.95	0.66
10:9:24:LYS:HG2	11:A:2421:G:H5''	1.76	0.66
22:N:250:ARG:NH1	22:N:250:ARG:O	2.29	0.66
42:h:122:ARG:HH21	42:h:124:ARG:HH12	1.44	0.66
44:j:34:ALA:HB2	44:j:40:TYR:CD2	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:113:ARG:NH2	11:A:1750:G:OP2	2.29	0.66
51:r:40:GLU:HG2	51:r:49:ILE:HG12	1.76	0.66
10:9:32:GLY:HA2	11:A:2420:U:H1'	1.75	0.66
15:F:116:THR:HG23	15:F:118:ALA:H	1.61	0.66
21:M:288:GLU:HA	21:M:291:LEU:HD23	1.76	0.66
45:k:19:GLN:HG3	45:k:54:ASP:HB2	1.77	0.66
2:1:17:LEU:HB3	2:1:63:ARG:HB3	1.78	0.66
24:P:165:MET:HE3	24:P:170:VAL:HG11	1.78	0.66
25:Q:227:LYS:NZ	25:Q:234:GLU:OE2	2.29	0.66
44:j:34:ALA:HB2	44:j:40:TYR:HD2	1.61	0.66
11:A:3068:G:OP2	11:A:3068:G:N2	2.24	0.66
32:X:189:ASP:HB3	32:X:192:LYS:HZ3	1.61	0.66
8:7:159:LYS:HE3	8:7:161:GLU:HB2	1.78	0.65
9:8:167:ASN:ND2	58:8:301:HOH:O	2.27	0.65
27:S:131:GLU:HG2	27:S:151:LYS:HE3	1.78	0.65
30:V:56:LEU:HB3	30:V:122:LEU:HD11	1.79	0.65
32:X:7:PRO:HD2	32:X:10:LEU:HD12	1.78	0.65
51:r:35:PHE:N	51:r:56:THR:OG1	2.27	0.65
5:4:101:ARG:NH1	11:A:3174:U:OP1	2.30	0.65
11:A:1803:A:OP1	30:V:34:LYS:NZ	2.29	0.65
13:D:220:VAL:HG12	13:D:221:ASN:H	1.62	0.65
28:T:119:GLU:O	28:T:123:GLU:HG3	1.97	0.65
11:A:2111:C:OP1	17:I:35:ARG:NH1	2.29	0.65
13:D:207:ILE:HD12	13:D:207:ILE:H	1.60	0.65
15:F:140:SER:OG	15:F:141:ILE:O	2.11	0.65
23:O:124:GLU:OE1	23:O:128:ASN:ND2	2.29	0.65
26:R:134:ASP:O	26:R:136:LYS:NZ	2.30	0.65
36:b:80:LEU:HD11	37:c:78:ARG:HD3	1.78	0.65
15:F:83:HIS:HD2	15:F:85:ASP:H	1.42	0.65
21:M:142:GLU:HG3	21:M:162:LEU:HD23	1.79	0.65
39:e:85:SER:HB2	47:m:50:ARG:HG3	1.79	0.65
50:q:42:PRO:O	50:q:44:ASP:N	2.29	0.65
20:L:133:GLU:OE1	20:L:133:GLU:N	2.30	0.65
8:7:38:THR:O	8:7:42:GLU:HG2	1.97	0.64
11:A:2580:U:H2'	11:A:2581:A:O4'	1.97	0.64
14:E:76:LYS:HG3	14:E:170:LEU:HD21	1.80	0.64
15:F:116:THR:HG22	15:F:119:GLU:HG3	1.79	0.64
21:M:264:GLN:NE2	21:M:266:PHE:O	2.24	0.64
27:S:136:VAL:HG21	27:S:200:ILE:HD11	1.79	0.64
39:e:83:LEU:O	58:e:302:HOH:O	2.15	0.64
11:A:2545:U:H5''	11:A:2546:G:H5'	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:308:ARG:HG3	52:s:320:ILE:HD12	1.80	0.64
20:L:45:ALA:O	20:L:49:SER:HB3	1.97	0.64
19:K:26:GLN:HE21	19:K:148:PRO:HD2	1.63	0.64
25:Q:256:GLU:HA	25:Q:259:LYS:HD3	1.79	0.64
9:8:173:LYS:HD2	39:e:237:LEU:HD11	1.78	0.64
33:Y:91:ARG:NH1	33:Y:148:GLU:OE1	2.30	0.64
11:A:1741:A:OP2	21:M:134:ARG:NH2	2.30	0.64
22:N:181:HIS:ND1	22:N:181:HIS:O	2.31	0.64
11:A:1935:A:H3'	11:A:1936:A:H5''	1.79	0.64
7:6:184:LEU:HA	49:p:191:LYS:HZ2	1.63	0.64
16:H:58:ARG:HH21	32:X:65:VAL:HG23	1.63	0.64
17:I:114:HIS:HA	17:I:117:ARG:HG3	1.80	0.64
11:A:2326:C:OP2	52:s:55:SER:OG	2.15	0.63
17:I:105:SER:OG	17:I:108:ASP:OD2	2.16	0.63
39:e:159:LEU:O	58:e:301:HOH:O	2.15	0.63
6:5:308:LEU:O	6:5:312:MET:HG2	1.98	0.63
41:g:99:ASP:OD2	41:g:148:ARG:NH2	2.31	0.63
8:7:145:SER:O	8:7:149:MET:HG3	1.98	0.63
11:A:1873:A:H61	11:A:1901:C:N4	1.96	0.63
11:A:2096:U:O4	21:M:57:ARG:NH2	2.31	0.63
36:b:35:ARG:HD3	48:o:101:TRP:CD1	2.33	0.63
39:e:119:ASP:OD1	39:e:120:LEU:N	2.31	0.63
52:s:203:ARG:NH1	52:s:238:ASN:OD1	2.31	0.63
54:TB:82:LEU:HA	58:TB:216:HOH:O	1.98	0.63
8:7:166:LEU:HB3	8:7:181:TYR:HE1	1.63	0.63
11:A:2580:U:H3'	11:A:2581:A:H8	1.63	0.63
11:A:3082:G:N2	11:A:3085:A:OP2	2.27	0.63
20:L:93:GLY:O	20:L:95:ARG:NH2	2.31	0.63
37:c:57:PRO:HB2	37:c:184:PHE:HE2	1.63	0.63
44:j:63:GLN:OE1	44:j:66:ARG:NH1	2.31	0.63
49:p:98:LYS:NZ	49:p:136:THR:OG1	2.31	0.63
11:A:1805:A:OP2	30:V:94:HIS:NE2	2.30	0.63
11:A:1985:G:OP1	11:A:1987:G:O2'	2.16	0.63
11:A:2075:U:O2'	11:A:2833:A:N7	2.28	0.63
24:P:161:LEU:O	24:P:165:MET:HG2	1.99	0.63
38:d:247:VAL:HG23	38:d:262:HIS:HB3	1.80	0.63
39:e:55:ARG:O	39:e:156:ASN:ND2	2.30	0.63
46:l:110:LEU:HD21	46:l:116:GLU:HG3	1.79	0.63
11:A:2245:A:H5''	51:r:189:ARG:HH12	1.63	0.63
15:F:63:GLN:O	58:F:401:HOH:O	2.16	0.63
31:W:104:TYR:HD2	31:W:126:LEU:HD12	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h:75:LYS:HZ2	42:h:82:LEU:HD11	1.64	0.63
11:A:2060:A:O2'	11:A:2061:C:O2	2.13	0.63
18:J:149:ARG:NH1	46:l:101:LEU:O	2.31	0.63
16:H:87:LYS:HG3	16:H:88:HIS:HD1	1.64	0.63
35:a:103:LEU:HD22	35:a:107:PRO:HB2	1.80	0.63
41:g:108:THR:HG21	41:g:153:PHE:H	1.64	0.63
8:7:158:PHE:O	35:a:90:GLN:NE2	2.32	0.62
26:R:114:LYS:HD3	35:a:45:CYS:HB2	1.81	0.62
9:8:164:ARG:HH22	40:f:167:ALA:HB3	1.63	0.62
11:A:2137:C:OP2	34:Z:77:ARG:NH1	2.31	0.62
49:p:81:TYR:CE1	49:p:143:GLN:HB2	2.34	0.62
6:5:139:VAL:HB	6:5:415:ALA:HB2	1.81	0.62
6:5:164:GLN:HG3	6:5:165:THR:HG23	1.81	0.62
11:A:2175:C:O2	18:J:102:ARG:NH1	2.31	0.62
6:5:104:TYR:CE1	6:5:266:GLU:HB3	2.34	0.62
21:M:287:ASP:O	21:M:289:ASN:N	2.32	0.62
30:V:79:VAL:HG22	30:V:86:VAL:HG12	1.80	0.62
4:3:168:ARG:NH1	11:A:1890:C:OP2	2.33	0.62
16:H:65:ALA:HB3	16:H:71:PRO:HA	1.80	0.62
40:f:171:LEU:O	40:f:175:GLN:HG2	1.99	0.62
7:6:114:ARG:NH2	12:B:1643:A:OP1	2.31	0.62
17:I:173:PHE:HB3	45:k:51:VAL:HG23	1.82	0.62
18:J:25:ARG:HA	18:J:65:PRO:HA	1.82	0.62
20:L:72:GLN:OE1	20:L:83:LYS:NZ	2.32	0.62
30:V:59:GLY:O	30:V:75:LYS:NZ	2.32	0.62
7:6:67:ALA:O	7:6:75:ARG:NH2	2.33	0.62
11:A:2040:G:O2'	21:M:56:GLU:OE1	2.16	0.62
15:F:49:ARG:NH1	15:F:81:ASP:O	2.32	0.62
50:q:125:MET:O	50:q:129:PRO:CD	2.44	0.62
9:8:139:MET:HE3	40:f:169:ILE:HD12	1.82	0.62
8:7:156:ARG:NH1	8:7:259:ASP:OD1	2.23	0.61
15:F:71:GLY:HA3	15:F:74:GLN:HG3	1.81	0.61
19:K:80:HIS:ND1	19:K:81:THR:O	2.29	0.61
23:O:45:PRO:HG2	23:O:48:ARG:HD2	1.82	0.61
24:P:78:TRP:O	24:P:96:HIS:ND1	2.33	0.61
26:R:18:TYR:HB3	43:i:34:ILE:HD11	1.80	0.61
4:3:152:LYS:O	4:3:156:LYS:HG2	2.00	0.61
15:F:142:ARG:HA	15:F:149:GLY:HA2	1.80	0.61
8:7:173:PRO:O	8:7:176:SER:OG	2.16	0.61
17:I:117:ARG:NH2	18:J:131:ALA:O	2.33	0.61
40:f:48:TYR:N	58:f:203:HOH:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:96:ASP:O	9:8:99:ARG:NH1	2.33	0.61
11:A:1672:C:O2'	28:T:149:ARG:O	2.18	0.61
34:Z:112:VAL:HG12	34:Z:113:VAL:HG13	1.83	0.61
41:g:39:VAL:HG21	50:q:72:PRO:HB2	1.81	0.61
52:s:81:ARG:O	52:s:85:LYS:HB3	2.01	0.61
6:5:124:LYS:HA	6:5:252:LEU:HD21	1.81	0.61
11:A:2580:U:H3'	11:A:2581:A:C8	2.36	0.61
21:M:290:LEU:HD21	50:q:77:PRO:HD2	1.82	0.61
39:e:155:ARG:HD2	39:e:279:LEU:HD12	1.81	0.61
4:3:163:THR:HG21	11:A:1742:G:H5'	1.82	0.61
11:A:1771:C:OP1	37:c:33:LYS:NZ	2.34	0.61
11:A:2194:U:O4	17:I:109:LYS:NZ	2.34	0.61
17:I:125:VAL:HG12	17:I:152:MET:HB2	1.82	0.61
21:M:30:ASN:O	21:M:33:SER:OG	2.18	0.61
39:e:178:TRP:HD1	39:e:187:THR:HG21	1.65	0.61
11:A:2362:A:N6	11:A:2432:A:O4'	2.34	0.61
11:A:2553:G:N2	13:D:280:GLY:O	2.30	0.61
17:I:34:THR:HG23	17:I:36:HIS:H	1.65	0.61
30:V:203:GLY:O	30:V:205:LYS:NZ	2.34	0.61
54:TA:86:LEU:HD11	54:TB:71:ILE:HG13	1.81	0.61
10:9:53:ILE:HG22	10:9:56:MET:H	1.66	0.60
11:A:2199:A:N6	58:A:3610:HOH:O	2.34	0.60
30:V:101:THR:OG1	30:V:104:TYR:O	2.18	0.60
39:e:88:GLU:OE2	47:m:50:ARG:NH1	2.34	0.60
17:I:152:MET:N	58:I:301:HOH:O	2.34	0.60
36:b:35:ARG:HD3	48:o:101:TRP:HD1	1.64	0.60
47:m:69:ARG:HG2	47:m:70:GLU:H	1.65	0.60
11:A:2086:A:H2'	11:A:2087:U:C6	2.36	0.60
11:A:2374:A:OP1	52:s:305:LYS:NZ	2.34	0.60
22:N:204:GLU:OE2	22:N:207:ARG:NH1	2.34	0.60
50:q:48:PRO:HG2	50:q:51:GLN:HG3	1.81	0.60
33:Y:115:LEU:HD21	33:Y:127:PRO:HG2	1.82	0.60
40:f:122:GLU:OE1	40:f:122:GLU:N	2.28	0.60
49:p:99:ALA:HB2	49:p:146:ASN:HB3	1.84	0.60
5:4:85:ARG:N	11:A:3189:C:OP1	2.32	0.60
6:5:68:PRO:HG2	6:5:69:TRP:NE1	2.16	0.60
7:6:45:LEU:HD11	40:f:64:LYS:HG2	1.84	0.60
11:A:1800:G:N2	11:A:1803:A:OP2	2.32	0.60
15:F:48:LEU:HD13	42:h:94:SER:HB2	1.83	0.60
27:S:85:GLU:HA	27:S:88:VAL:HG22	1.82	0.60
40:f:134:VAL:HG21	47:m:75:LEU:HD11	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:203:THR:HG22	8:7:280:VAL:H	1.66	0.60
10:9:101:GLU:HG3	32:X:238:LEU:HD21	1.83	0.60
17:I:104:LEU:HD21	17:I:108:ASP:HB2	1.84	0.60
20:L:111:ASN:OD1	20:L:113:ASN:ND2	2.35	0.60
11:A:2103:A:OP2	17:I:38:ARG:NH2	2.35	0.60
11:A:2537:G:O2'	11:A:2634:U:OP2	2.19	0.60
11:A:3096:U:O4	38:d:39:LYS:NZ	2.34	0.60
58:A:3559:HOH:O	13:D:262:ARG:NH1	2.34	0.60
30:V:100:LYS:HB3	38:d:64:GLY:H	1.67	0.60
32:X:161:LEU:O	32:X:165:MET:HG3	2.02	0.60
33:Y:69:ASP:N	33:Y:69:ASP:OD1	2.33	0.60
33:Y:126:MET:HB3	33:Y:129:PRO:HG3	1.84	0.60
40:f:174:ILE:HD12	40:f:184:LEU:HD11	1.82	0.60
18:J:159:LEU:HB3	18:J:163:GLU:HB2	1.84	0.60
40:f:111:HIS:HE1	40:f:157:VAL:HB	1.67	0.60
46:l:119:ARG:HA	46:l:122:ARG:HD2	1.83	0.60
3:2:72:THR:HG22	3:2:74:ALA:H	1.67	0.59
13:D:126:VAL:HA	13:D:142:VAL:HG22	1.83	0.59
38:d:76:ILE:HD12	38:d:76:ILE:H	1.67	0.59
39:e:248:ASN:OD1	58:e:303:HOH:O	2.16	0.59
39:e:264:LEU:HD13	39:e:270:ALA:HA	1.82	0.59
6:5:38:THR:HG21	13:D:68:SER:HB3	1.84	0.59
12:B:1626:C:N4	24:P:87:GLN:OE1	2.34	0.59
23:O:68:THR:HB	52:s:40:PRO:HG2	1.83	0.59
8:7:226:ALA:HA	8:7:229:ILE:HD12	1.83	0.59
11:A:1747:G:OP2	11:A:1749:C:N4	2.34	0.59
12:B:1663:C:H2'	12:B:1664:G:H8	1.66	0.59
13:D:199:GLU:OE1	13:D:199:GLU:N	2.35	0.59
37:c:89:LYS:O	37:c:93:VAL:HG23	2.02	0.59
50:q:138:GLN:O	50:q:142:ASN:ND2	2.35	0.59
7:6:195:PRO:HG2	7:6:327:VAL:HG22	1.85	0.59
7:6:229:ASP:O	58:6:401:HOH:O	2.17	0.59
11:A:2155:A:N6	51:r:169:TRP:O	2.35	0.59
11:A:2515:U:O2'	13:D:282:ALA:O	2.20	0.59
35:a:68:PRO:HG2	35:a:71:HIS:CD2	2.37	0.59
9:8:146:ALA:HA	39:e:212:HIS:CE1	2.37	0.59
14:E:236:THR:HG23	14:E:239:ARG:HG3	1.85	0.59
7:6:136:ARG:O	7:6:140:GLU:HG3	2.03	0.59
16:H:120:ARG:NH1	58:H:302:HOH:O	2.36	0.59
30:V:178:SER:OG	30:V:181:ASP:OD1	2.16	0.59
37:c:47:ARG:HH11	37:c:47:ARG:HG2	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:76:ASN:H	46:l:79:LYS:HB2	1.68	0.59
9:8:151:GLN:NE2	58:8:306:HOH:O	2.34	0.59
11:A:2065:A:OP1	40:f:48:TYR:N	2.36	0.59
9:8:101:ARG:NH1	39:e:82:SER:OG	2.36	0.59
13:D:177:ARG:HG3	13:D:180:ASP:OD2	2.02	0.59
18:J:49:PHE:CE1	18:J:80:ILE:HG12	2.38	0.59
19:K:26:GLN:NE2	19:K:149:ARG:H	2.00	0.59
24:P:120:ARG:NH1	58:P:203:HOH:O	2.36	0.59
35:a:142:ARG:NH1	58:a:203:HOH:O	2.36	0.59
32:X:177:HIS:ND1	32:X:178:PRO:O	2.28	0.59
39:e:67:GLN:HE22	47:m:40:LEU:HD23	1.68	0.59
41:g:160:TRP:O	41:g:164:LYS:HG3	2.03	0.59
11:A:3115:U:H2'	11:A:3116:C:C6	2.38	0.58
14:E:69:ASP:OD1	14:E:171:PRO:HB3	2.02	0.58
11:A:2234:C:O2'	11:A:2688:C:O2'	2.21	0.58
30:V:53:ASP:N	30:V:53:ASP:OD1	2.35	0.58
15:F:196:PRO:HD2	15:F:202:TYR:HE2	1.69	0.58
18:J:187:GLU:HB3	18:J:191:LYS:NZ	2.19	0.58
23:O:141:HIS:O	23:O:147:GLN:NE2	2.35	0.58
39:e:260:LEU:O	39:e:264:LEU:HG	2.04	0.58
11:A:1953:A:O2'	11:A:2463:A:OP1	2.22	0.58
19:K:6:ARG:NH1	37:c:230:GLU:OE2	2.37	0.58
19:K:140:ASN:HD21	37:c:265:THR:HG23	1.69	0.58
7:6:240:ILE:HD13	7:6:248:GLY:HA3	1.85	0.58
11:A:2917:G:O6	21:M:77:ARG:NH1	2.36	0.58
14:E:129:VAL:HG12	14:E:189:PRO:HA	1.84	0.58
45:k:58:ASP:HB3	54:TA:53:LEU:HD21	1.86	0.58
5:4:69:LYS:HB2	5:4:72:LEU:HD23	1.84	0.58
7:6:253:PRO:HD2	7:6:290:CYS:SG	2.44	0.58
16:H:97:ILE:HG13	16:H:132:ALA:HB2	1.86	0.58
52:s:177:LEU:HD23	52:s:238:ASN:HD22	1.68	0.58
6:5:36:ARG:HH11	6:5:36:ARG:HG3	1.69	0.58
18:J:56:ARG:HH12	18:J:80:ILE:HD13	1.67	0.58
29:U:20:PHE:O	33:Y:99:HIS:NE2	2.35	0.58
39:e:128:PHE:HB2	47:m:73:ARG:HD3	1.85	0.58
2:1:24:ALA:HA	50:q:124:CYS:HB3	1.86	0.58
8:7:191:GLU:OE1	8:7:191:GLU:N	2.37	0.58
10:9:131:TYR:HA	33:Y:154:ARG:HD2	1.86	0.58
11:A:2408:U:H2'	11:A:2409:A:H8	1.67	0.58
11:A:3181:U:OP2	11:A:3182:A:O2'	2.19	0.58
16:H:132:ALA:HA	16:H:136:ASN:HD21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:132:ILE:O	50:q:135:TRP:N	2.36	0.58
2:l:55:LEU:HG	50:q:132:ILE:HD13	1.86	0.58
6:5:58:ILE:HD11	32:X:213:GLU:HG3	1.86	0.58
9:8:131:MET:O	9:8:135:THR:HG23	2.03	0.58
11:A:2101:C:H2'	11:A:2102:A:H8	1.69	0.58
33:Y:135:VAL:O	33:Y:139:MET:HG3	2.03	0.58
54:TB:64:ILE:N	58:TB:202:HOH:O	2.37	0.58
11:A:2740:A:H2'	11:A:2741:A:H8	1.69	0.58
11:A:3168:C:N3	14:E:303:LYS:NZ	2.48	0.58
24:P:142:ASN:HA	24:P:170:VAL:HG23	1.86	0.58
37:c:84:SER:HB2	37:c:87:LEU:HB2	1.86	0.58
38:d:82:ALA:O	38:d:167:HIS:NE2	2.36	0.58
6:5:105:ILE:HD13	6:5:220:GLN:HB3	1.86	0.57
7:6:286:ARG:NH1	7:6:295:GLN:O	2.37	0.57
11:A:2198:A:OP1	46:l:123:LYS:NZ	2.31	0.57
14:E:91:GLU:O	14:E:94:SER:OG	2.20	0.57
34:Z:75:THR:HB	34:Z:83:LYS:HG2	1.85	0.57
35:a:70:GLU:N	35:a:70:GLU:OE2	2.37	0.57
40:f:179:PRO:HB3	47:m:38:ALA:HB3	1.86	0.57
50:q:128:MET:HB3	50:q:129:PRO:CD	2.31	0.57
39:e:64:THR:HG22	39:e:67:GLN:H	1.68	0.57
42:h:96:LEU:HA	42:h:99:ASN:HD22	1.69	0.57
47:m:75:LEU:N	58:m:202:HOH:O	2.26	0.57
11:A:1955:G:HO2'	11:A:1958:G:HO2'	1.52	0.57
11:A:3200:U:H4'	11:A:3201:A:H5''	1.87	0.57
12:B:1608:G:N2	58:B:1707:HOH:O	2.36	0.57
17:I:166:ARG:HH11	17:I:169:ARG:HH11	1.52	0.57
39:e:70:MET:HE2	47:m:40:LEU:HD11	1.86	0.57
11:A:1810:A:H2'	11:A:1811:A:C8	2.39	0.57
12:B:1663:C:H2'	12:B:1664:G:C8	2.38	0.57
15:F:63:GLN:OE1	42:h:97:LYS:NZ	2.37	0.57
38:d:187:GLU:O	38:d:218:THR:OG1	2.22	0.57
51:r:99:MET:HE1	51:r:115:ILE:HG22	1.86	0.57
7:6:184:LEU:HD22	7:6:186:PRO:HG3	1.86	0.57
9:8:164:ARG:NH2	40:f:163:SER:O	2.36	0.57
19:K:45:PRO:O	26:R:71:ARG:HG2	2.04	0.57
21:M:243:ILE:HG23	49:p:74:LEU:HD12	1.85	0.57
30:V:40:ARG:NH2	58:V:306:HOH:O	2.37	0.57
30:V:112:GLU:OE1	38:d:74:ARG:NH2	2.38	0.57
37:c:155:ASN:HD22	37:c:232:TRP:CD1	2.22	0.57
8:7:231:GLN:NE2	58:7:408:HOH:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:117:LEU:HA	9:8:120:LYS:HD2	1.85	0.57
10:9:45:THR:HG22	10:9:46:SER:H	1.69	0.57
12:B:1628:C:H2'	12:B:1629:A:H8	1.68	0.57
32:X:13:ARG:O	32:X:17:ARG:HG2	2.05	0.57
47:m:69:ARG:NH2	47:m:70:GLU:OE2	2.36	0.57
10:9:128:PHE:CD1	10:9:135:PHE:HB3	2.40	0.57
16:H:67:GLU:OE2	32:X:61:ARG:NH1	2.29	0.57
22:N:101:HIS:O	22:N:105:MET:HG2	2.05	0.57
31:W:55:LYS:HE2	31:W:61:VAL:HG22	1.86	0.57
11:A:2192:A:H2'	11:A:2193:U:C6	2.40	0.57
18:J:122:ARG:NH1	58:J:214:HOH:O	2.38	0.57
19:K:163:ILE:HD12	51:r:87:LEU:HD21	1.86	0.57
23:O:91:GLN:NE2	52:s:44:TYR:OH	2.37	0.57
32:X:183:ARG:NH2	58:X:304:HOH:O	2.38	0.57
8:7:322:LYS:NZ	58:7:406:HOH:O	2.35	0.57
9:8:150:LEU:HD12	39:e:209:PRO:HG3	1.86	0.57
37:c:98:ILE:HG12	37:c:119:LEU:HD23	1.86	0.57
8:7:107:LEU:HD13	8:7:128:LEU:HD11	1.87	0.56
11:A:2127:A:H4'	11:A:2251:A:C5	2.40	0.56
11:A:2388:A:H5'	13:D:74:ILE:HG22	1.87	0.56
11:A:2727:C:H2'	11:A:2728:C:H6	1.70	0.56
11:A:3018:A:H61	11:A:3130:A:H61	1.52	0.56
37:c:105:ARG:HD2	37:c:112:LYS:HD3	1.87	0.56
50:q:123:GLU:CD	50:q:127:LYS:HD2	2.30	0.56
2:1:45:HIS:ND1	11:A:2852:C:O2'	2.19	0.56
13:D:194:ASN:HD22	13:D:247:VAL:HG22	1.70	0.56
18:J:53:PHE:O	18:J:57:THR:HG23	2.05	0.56
19:K:4:PHE:HB3	19:K:9:GLN:HB2	1.87	0.56
19:K:156:ASP:OD2	19:K:156:ASP:N	2.32	0.56
6:5:326:LEU:HG	6:5:327:LEU:HD23	1.87	0.56
11:A:1808:A:N3	11:A:1809:U:O2'	2.38	0.56
13:D:79:MET:HE3	13:D:104:TYR:HB2	1.86	0.56
13:D:112:PHE:CZ	13:D:167:ASN:HB2	2.40	0.56
15:F:234:THR:HG21	15:F:242:LEU:HB2	1.87	0.56
18:J:78:PHE:CD2	18:J:80:ILE:HD11	2.40	0.56
18:J:122:ARG:HD2	18:J:122:ARG:C	2.30	0.56
22:N:196:GLU:O	22:N:200:LYS:HG2	2.05	0.56
46:l:100:ASN:HB3	46:l:105:LYS:HE2	1.87	0.56
50:q:70:VAL:HG22	50:q:71:VAL:H	1.69	0.56
51:r:60:SER:HB2	51:r:75:TRP:HH2	1.70	0.56
6:5:30:ALA:N	13:D:201:GLY:O	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.87	0.56
11:A:1860:A:O2'	26:R:34:ARG:NH2	2.38	0.56
18:J:184:ALA:HA	18:J:187:GLU:OE2	2.06	0.56
52:s:215:GLU:HG2	52:s:229:LEU:HD21	1.87	0.56
52:s:260:GLU:OE1	52:s:260:GLU:N	2.36	0.56
11:A:1889:C:OP1	21:M:133:LYS:NZ	2.35	0.56
11:A:2109:A:H61	11:A:2981:A:H2	1.52	0.56
42:h:86:TRP:CE2	42:h:87:GLN:HG3	2.41	0.56
1:0:141:ILE:HG12	1:0:175:ILE:HD13	1.87	0.56
11:A:2507:A:O2'	11:A:2508:C:OP1	2.23	0.56
12:B:1639:U:H5''	24:P:155:SER:OG	2.06	0.56
13:D:184:LEU:HD13	13:D:226:ILE:HD11	1.88	0.56
6:5:229:LEU:HB3	6:5:288:HIS:HB3	1.87	0.56
7:6:126:ARG:NH1	12:B:1641:G:OP1	2.38	0.56
11:A:1873:A:N6	11:A:1901:C:H42	1.99	0.56
11:A:2331:C:H5'	11:A:2444:A:H62	1.71	0.56
24:P:116:LEU:HD11	24:P:119:THR:HA	1.87	0.56
30:V:136:ARG:HG3	30:V:146:VAL:HB	1.86	0.56
7:6:62:GLU:O	7:6:66:GLN:NE2	2.39	0.56
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.88	0.56
8:7:256:ARG:NH2	58:7:407:HOH:O	2.38	0.56
11:A:1919:C:O2'	11:A:2500:A:N1	2.38	0.56
11:A:2196:A:O2'	11:A:2213:A:N1	2.35	0.56
11:A:2575:U:H3'	11:A:2581:A:H61	1.71	0.56
29:U:11:ARG:HB3	30:V:211:LYS:NZ	2.21	0.56
42:h:113:PRO:O	42:h:117:LEU:HB2	2.06	0.56
45:k:33:PHE:HA	45:k:36:THR:HG22	1.87	0.56
11:A:2514:C:H2'	11:A:2515:U:H6	1.69	0.56
26:R:10:LEU:HB3	26:R:13:ARG:HD2	1.88	0.56
7:6:35:MET:HG3	7:6:36:PRO:HD2	1.88	0.56
11:A:2350:A:N3	11:A:2353:A:N6	2.54	0.56
11:A:2632:A:O2'	11:A:2635:G:N3	2.37	0.56
18:J:56:ARG:HH22	18:J:80:ILE:HB	1.71	0.56
11:A:2159:U:OP2	51:r:153:ARG:NH2	2.38	0.55
11:A:2740:A:N3	11:A:2921:A:O2'	2.35	0.55
7:6:50:LYS:O	31:W:122:LYS:NZ	2.39	0.55
11:A:3115:U:H2'	11:A:3116:C:H6	1.70	0.55
44:j:27:TRP:O	44:j:31:GLN:HG2	2.06	0.55
11:A:1826:G:H4'	11:A:1828:A:C2	2.40	0.55
36:b:56:ARG:NH1	58:b:205:HOH:O	2.38	0.55
47:m:72:ARG:NH1	58:m:203:HOH:O	2.30	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:48:PRO:HD2	38:d:51:LYS:HE3	1.88	0.55
39:e:200:MET:HA	39:e:200:MET:HE2	1.89	0.55
8:7:199:LEU:O	8:7:203:THR:HG23	2.07	0.55
9:8:129:ARG:HG2	12:B:1627:C:H5'	1.89	0.55
11:A:2727:C:H2'	11:A:2728:C:C6	2.41	0.55
18:J:140:VAL:O	18:J:144:ILE:HG12	2.06	0.55
30:V:121:LYS:NZ	58:V:308:HOH:O	2.40	0.55
39:e:79:ILE:HG12	47:m:50:ARG:HH21	1.70	0.55
40:f:188:GLU:HG3	40:f:189:HIS:H	1.71	0.55
7:6:104:LEU:O	7:6:108:GLN:HG2	2.06	0.55
8:7:281:SER:HB3	8:7:321:ARG:HG2	1.86	0.55
30:V:65:LEU:HD21	30:V:121:LYS:HD3	1.89	0.55
38:d:208:VAL:HG23	38:d:252:LEU:HB2	1.88	0.55
39:e:119:ASP:O	39:e:123:MET:HG2	2.07	0.55
48:o:54:MET:HE3	48:o:59:GLU:HB3	1.88	0.55
52:s:266:CYS:SG	52:s:267:LYS:N	2.79	0.55
6:5:353:PHE:HB3	6:5:416:LEU:HD11	1.88	0.55
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.89	0.55
11:A:1990:G:OP1	13:D:269:ARG:NH2	2.40	0.55
11:A:3173:G:H2'	11:A:3174:U:O4'	2.06	0.55
36:b:131:HIS:O	36:b:134:THR:OG1	2.24	0.55
39:e:90:ARG:NH2	39:e:94:GLU:OE1	2.34	0.55
45:k:68:PHE:HE1	45:k:72:HIS:HB2	1.72	0.55
10:9:23:SER:OG	11:A:2420:U:O2'	2.24	0.55
11:A:2240:C:N4	51:r:196:HIS:HB2	2.22	0.55
14:E:74:ALA:HA	14:E:77:LEU:HD23	1.89	0.55
22:N:68:ASN:HD22	22:N:68:ASN:C	2.05	0.55
39:e:65:PRO:HD2	39:e:66:LEU:N	2.21	0.55
39:e:258:ASP:N	39:e:258:ASP:OD1	2.38	0.55
11:A:1906:G:H2'	11:A:2014:A:H61	1.72	0.55
11:A:2710:C:O2'	11:A:3220:A:N1	2.38	0.55
25:Q:152:ARG:HH21	25:Q:191:ARG:HA	1.72	0.55
39:e:73:LEU:O	39:e:77:ILE:HD12	2.06	0.55
39:e:210:CYS:N	39:e:233:PHE:O	2.39	0.55
45:k:95:ARG:NH2	58:k:206:HOH:O	2.39	0.55
51:r:50:GLU:HB2	51:r:52:ARG:NH2	2.22	0.55
7:6:239:ASN:OD1	7:6:249:GLN:NE2	2.37	0.55
11:A:2294:A:OP2	21:M:41:ARG:NE	2.31	0.55
15:F:221:LEU:HD12	15:F:264:PRO:HB2	1.89	0.55
21:M:234:LEU:HD22	49:p:62:PRO:HG2	1.89	0.55
23:O:55:TYR:OH	25:Q:268:ASP:OD1	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:109:ILE:HD12	38:d:76:ILE:HG21	1.89	0.55
39:e:164:LYS:NZ	58:e:320:HOH:O	2.39	0.55
7:6:240:ILE:HD12	7:6:245:VAL:HA	1.89	0.54
11:A:2227:A:N6	58:A:3502:HOH:O	2.39	0.54
11:A:2653:C:HO2'	11:A:2654:U:H6	1.54	0.54
14:E:57:ASN:OD1	23:O:141:HIS:NE2	2.39	0.54
17:I:83:ARG:NE	17:I:83:ARG:HA	2.22	0.54
24:P:56:LEU:HB3	24:P:62:ALA:HB2	1.87	0.54
24:P:155:SER:O	24:P:159:LYS:HG3	2.07	0.54
31:W:119:ARG:HH11	40:f:65:ALA:HB3	1.72	0.54
36:b:45:GLU:O	36:b:49:ARG:HG3	2.07	0.54
6:5:69:TRP:HD1	11:A:1713:A:N1	2.05	0.54
11:A:1762:A:H62	50:q:63:ARG:HH21	1.54	0.54
11:A:2275:U:H2'	11:A:2276:C:C6	2.42	0.54
11:A:2521:A:N6	13:D:202:ARG:O	2.40	0.54
32:X:189:ASP:HB3	32:X:192:LYS:NZ	2.22	0.54
39:e:86:ASP:O	39:e:89:LEU:HD23	2.07	0.54
40:f:106:TYR:O	40:f:110:VAL:HG12	2.06	0.54
40:f:133:GLU:O	58:f:201:HOH:O	2.18	0.54
42:h:56:ARG:NH1	58:h:203:HOH:O	2.38	0.54
50:q:82:LEU:O	50:q:86:GLU:HG2	2.08	0.54
11:A:1807:U:O2'	11:A:1808:A:O4'	2.26	0.54
11:A:2410:U:H2'	11:A:2411:U:H6	1.71	0.54
21:M:246:ASP:OD2	21:M:248:THR:OG1	2.24	0.54
42:h:63:PRO:HD2	42:h:66:LEU:HD13	1.89	0.54
50:q:78:SER:O	50:q:80:GLU:N	2.40	0.54
6:5:105:ILE:HD12	6:5:222:ARG:HD3	1.89	0.54
7:6:260:ALA:HB3	7:6:263:SER:HB2	1.87	0.54
14:E:80:LEU:HD12	14:E:322:ASP:HB2	1.87	0.54
32:X:127:VAL:HG22	32:X:131:THR:HG23	1.90	0.54
39:e:179:GLN:HG2	39:e:180:PRO:HD2	1.88	0.54
39:e:264:LEU:HD22	39:e:269:LEU:HB3	1.90	0.54
52:s:265:LYS:H	52:s:265:LYS:HD2	1.72	0.54
52:s:318:ASP:OD1	52:s:318:ASP:N	2.28	0.54
1:0:163:GLU:OE2	1:0:181:ARG:NH1	2.41	0.54
5:4:88:TRP:CZ2	11:A:2160:A:H5'	2.42	0.54
7:6:239:ASN:HD22	7:6:275:GLN:HE21	1.56	0.54
11:A:1867:A:N1	11:A:2019:G:O2'	2.32	0.54
11:A:3078:C:H2'	11:A:3079:G:C8	2.43	0.54
22:N:101:HIS:CE1	22:N:184:PRO:HG3	2.43	0.54
35:a:35:THR:OG1	35:a:36:TYR:N	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:r:168:ARG:NH2	58:r:311:HOH:O	2.39	0.54
7:6:175:VAL:HG23	7:6:187:VAL:HB	1.88	0.54
11:A:1709:G:H4'	11:A:1710:A:OP1	2.07	0.54
11:A:1756:A:H2'	11:A:1757:A:C8	2.41	0.54
11:A:2065:A:C8	31:W:74:ARG:HA	2.42	0.54
11:A:2527:A:H5''	13:D:66:TRP:HZ2	1.72	0.54
36:b:64:TYR:OH	37:c:71:GLU:OE2	2.26	0.54
7:6:330:ILE:HG23	7:6:334:LEU:HD12	1.89	0.54
10:9:23:SER:O	10:9:31:ARG:HG3	2.08	0.54
17:I:114:HIS:NE2	17:I:115:GLN:OE1	2.41	0.54
22:N:203:GLU:O	22:N:207:ARG:HG2	2.07	0.54
39:e:183:THR:HG23	39:e:186:GLY:H	1.72	0.54
39:e:266:PRO:HD2	39:e:269:LEU:HB2	1.90	0.54
40:f:163:SER:HB3	40:f:166:PHE:HB2	1.90	0.54
9:8:164:ARG:NH2	40:f:167:ALA:HB3	2.22	0.54
12:B:1642:G:H2'	12:B:1643:A:C8	2.42	0.54
33:Y:128:SER:HB2	33:Y:131:ARG:HH11	1.73	0.54
49:p:109:GLU:OE2	49:p:109:GLU:N	2.35	0.54
52:s:166:TYR:O	52:s:167:GLU:HG2	2.08	0.54
52:s:351:VAL:HG21	52:s:375:ASN:O	2.08	0.54
4:3:131:LYS:NZ	58:3:201:HOH:O	2.31	0.54
7:6:141:ARG:HG3	7:6:141:ARG:HH11	1.73	0.54
11:A:2746:U:H2'	11:A:2747:U:C6	2.42	0.54
13:D:139:ILE:HD12	13:D:150:TRP:CE3	2.42	0.54
18:J:102:ARG:NE	18:J:102:ARG:O	2.40	0.54
22:N:194:THR:O	22:N:198:MET:HG3	2.07	0.54
50:q:128:MET:O	50:q:132:ILE:HG12	2.07	0.54
7:6:306:LYS:HG3	7:6:307:HIS:HD2	1.70	0.54
8:7:131:LYS:NZ	58:7:409:HOH:O	2.39	0.54
11:A:1826:G:H4'	11:A:1828:A:H2	1.73	0.54
11:A:2939:C:H2'	11:A:2940:A:C8	2.43	0.54
25:Q:246:ASP:OD2	25:Q:246:ASP:N	2.41	0.54
32:X:160:ASP:OD1	32:X:163:ARG:NH2	2.41	0.54
36:b:72:VAL:HG13	36:b:90:HIS:HB2	1.90	0.54
39:e:157:LEU:HG	39:e:256:THR:HG23	1.89	0.54
48:o:56:ARG:HA	48:o:59:GLU:HG2	1.90	0.54
4:3:185:ASN:ND2	7:6:369:TYR:O	2.37	0.53
6:5:35:VAL:HG13	11:A:2523:C:OP2	2.08	0.53
7:6:197:GLU:OE2	49:p:189:ARG:NH2	2.41	0.53
11:A:1984:A:H8	11:A:1987:G:N2	2.05	0.53
13:D:154:THR:HG22	13:D:157:MET:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:216:TYR:OH	33:Y:191:ASN:ND2	2.36	0.53
36:b:103:LYS:O	36:b:107:GLN:HG3	2.08	0.53
3:2:87:ARG:NH2	11:A:1792:G:N7	2.45	0.53
8:7:88:PRO:HB3	8:7:125:ILE:HD11	1.90	0.53
9:8:146:ALA:HB1	39:e:209:PRO:HG2	1.89	0.53
15:F:133:THR:OG1	15:F:134:GLY:N	2.41	0.53
42:h:139:LYS:O	42:h:142:GLU:HG3	2.08	0.53
1:0:180:LYS:NZ	1:0:181:ARG:O	2.36	0.53
9:8:107:THR:HG22	9:8:109:GLU:H	1.74	0.53
11:A:2939:C:O2'	11:A:2940:A:O5'	2.22	0.53
14:E:68:GLU:OE1	14:E:154:ARG:NH2	2.42	0.53
30:V:117:HIS:CE1	30:V:118:ARG:HD3	2.43	0.53
39:e:162:ARG:HD3	39:e:171:TRP:CG	2.43	0.53
46:l:76:ASN:ND2	58:l:205:HOH:O	2.39	0.53
49:p:46:ASP:OD1	49:p:47:LYS:N	2.41	0.53
50:q:47:THR:HG21	50:q:52:LEU:HD21	1.90	0.53
7:6:132:LEU:HA	7:6:135:VAL:HG12	1.89	0.53
11:A:2409:A:H2'	11:A:2410:U:C6	2.43	0.53
27:S:183:LYS:HE2	27:S:185:ILE:HD11	1.90	0.53
29:U:11:ARG:HB3	30:V:211:LYS:HZ2	1.73	0.53
32:X:215:GLN:HG3	32:X:219:GLU:OE2	2.08	0.53
45:k:83:ALA:O	45:k:87:LEU:HB2	2.07	0.53
11:A:2753:A:H2'	11:A:2754:A:H8	1.74	0.53
11:A:3188:U:O2'	11:A:3192:C:N4	2.41	0.53
48:o:88:ILE:HG22	48:o:92:LEU:HG	1.90	0.53
50:q:123:GLU:O	50:q:127:LYS:HG3	2.09	0.53
11:A:2318:A:H2'	11:A:2319:A:C8	2.43	0.53
15:F:196:PRO:HD2	15:F:202:TYR:CE2	2.44	0.53
27:S:163:LYS:HB2	36:b:106:ASP:HB3	1.91	0.53
35:a:46:ASN:O	35:a:63:PRO:HD2	2.09	0.53
47:m:59:GLN:NE2	47:m:78:PRO:O	2.39	0.53
49:p:102:ARG:HB3	49:p:134:ILE:HD13	1.91	0.53
11:A:2082:G:H2'	11:A:2083:U:O4'	2.08	0.53
11:A:2191:A:N6	11:A:2198:A:OP2	2.41	0.53
17:I:190:GLY:HA2	17:I:193:ASN:ND2	2.24	0.53
24:P:105:ALA:HB2	24:P:132:LEU:HB3	1.89	0.53
37:c:229:PHE:HZ	37:c:301:LEU:HB3	1.74	0.53
47:m:70:GLU:O	47:m:72:ARG:N	2.41	0.53
52:s:85:LYS:HE3	52:s:86:MET:HE2	1.90	0.53
52:s:100:LEU:O	52:s:319:GLN:NE2	2.35	0.53
2:1:24:ALA:HB1	50:q:125:MET:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:114:ARG:HE	24:P:117:TYR:HE1	1.55	0.53
10:9:128:PHE:HD1	10:9:135:PHE:HB3	1.73	0.53
11:A:2686:G:H5'	11:A:3104:U:H4'	1.91	0.53
13:D:86:ASP:OD1	13:D:88:THR:OG1	2.19	0.53
15:F:77:VAL:HG23	15:F:77:VAL:O	2.08	0.53
30:V:97:TYR:HB2	30:V:105:ARG:HD2	1.91	0.53
35:a:67:ILE:HD11	37:c:259:ARG:HE	1.74	0.53
11:A:1883:G:H5''	41:g:91:MET:HE2	1.91	0.53
13:D:169:ILE:HD11	13:D:185:GLY:HA3	1.89	0.53
20:L:142:GLN:OE1	20:L:142:GLN:N	2.41	0.53
46:l:69:THR:HB	46:l:71:TYR:HE1	1.73	0.53
49:p:76:ARG:HH12	49:p:109:GLU:CD	2.17	0.53
5:4:97:ARG:NH1	11:A:3016:G:N7	2.46	0.53
7:6:114:ARG:HH22	12:B:1643:A:P	2.31	0.53
11:A:1839:C:H5''	19:K:115:ASN:HB2	1.90	0.53
11:A:3024:U:H2'	11:A:3025:A:H8	1.74	0.53
17:I:29:GLY:N	58:I:306:HOH:O	2.41	0.53
29:U:101:HIS:HB2	29:U:103:GLN:NE2	2.24	0.53
37:c:245:LEU:HB3	37:c:250:VAL:HB	1.89	0.53
11:A:2673:G:H5''	28:T:112:LYS:HB2	1.91	0.52
11:A:3054:G:H2'	11:A:3055:U:C6	2.44	0.52
15:F:51:VAL:HG23	15:F:81:ASP:OD1	2.09	0.52
34:Z:102:ASN:H	44:j:84:MET:HE1	1.74	0.52
54:TA:63:LYS:NZ	54:TB:78:GLU:OE2	2.35	0.52
6:5:180:VAL:O	6:5:184:ILE:HD13	2.08	0.52
11:A:2078:C:N4	58:A:3672:HOH:O	2.39	0.52
35:a:62:HIS:ND1	35:a:62:HIS:O	2.42	0.52
41:g:144:THR:O	41:g:146:THR:N	2.43	0.52
52:s:48:VAL:HG22	52:s:61:ARG:HD2	1.91	0.52
7:6:27:ARG:N	11:A:2072:A:OP2	2.42	0.52
7:6:184:LEU:HA	49:p:191:LYS:NZ	2.24	0.52
11:A:2145:G:N3	27:S:104:ARG:NH2	2.45	0.52
11:A:2286:A:H2'	11:A:2287:U:C6	2.44	0.52
11:A:3158:A:H8	23:O:13:ARG:HH22	1.58	0.52
18:J:52:GLU:O	18:J:56:ARG:HD3	2.08	0.52
39:e:160:LEU:O	39:e:252:HIS:HA	2.09	0.52
40:f:187:LYS:HG2	40:f:188:GLU:H	1.74	0.52
44:j:29:LEU:HG	44:j:35:ALA:HB2	1.92	0.52
45:k:97:ARG:NH2	58:k:208:HOH:O	2.41	0.52
51:r:50:GLU:HB2	51:r:52:ARG:HH21	1.73	0.52
6:5:359:ASN:H	6:5:371:ASN:HD22	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2747:U:H2'	11:A:2748:A:H8	1.75	0.52
18:J:154:ARG:NE	18:J:156:VAL:HG13	2.24	0.52
22:N:103:GLU:OE2	22:N:106:ARG:NH1	2.42	0.52
27:S:50:TYR:HD2	51:r:64:PRO:HG3	1.74	0.52
38:d:66:VAL:O	38:d:69:PRO:HD2	2.10	0.52
6:5:69:TRP:O	6:5:70:LEU:HD13	2.10	0.52
7:6:106:ARG:O	7:6:110:ILE:HG22	2.10	0.52
7:6:292:GLN:HB2	7:6:295:GLN:HE21	1.73	0.52
11:A:1787:G:N2	11:A:1790:A:OP2	2.35	0.52
11:A:2653:C:O2'	11:A:2654:U:H5''	2.09	0.52
58:A:3654:HOH:O	14:E:300:LYS:NZ	2.43	0.52
21:M:35:LYS:HG2	21:M:36:PRO:HD2	1.92	0.52
24:P:39:VAL:HB	24:P:42:GLU:HG3	1.90	0.52
25:Q:240:ILE:HG21	25:Q:243:ILE:HD12	1.92	0.52
38:d:57:MET:HA	38:d:57:MET:HE2	1.91	0.52
6:5:271:ASP:N	6:5:271:ASP:OD1	2.39	0.52
8:7:227:LEU:HD21	8:7:241:GLU:OE2	2.09	0.52
11:A:1728:U:O2'	32:X:96:LYS:O	2.17	0.52
15:F:94:ASP:OD1	21:M:30:ASN:ND2	2.42	0.52
6:5:125:THR:HG22	6:5:371:ASN:HB2	1.91	0.52
11:A:3113:A:H2'	11:A:3114:U:C6	2.45	0.52
17:I:80:ARG:NH2	58:I:307:HOH:O	2.42	0.52
21:M:281:LYS:HD3	41:g:41:SER:HB2	1.92	0.52
26:R:17:ARG:O	26:R:21:ILE:HG12	2.09	0.52
37:c:57:PRO:HB2	37:c:184:PHE:CE2	2.43	0.52
51:r:60:SER:HB2	51:r:75:TRP:CH2	2.45	0.52
4:3:110:VAL:HG13	4:3:158:LEU:HD22	1.92	0.52
6:5:233:ASP:OD1	6:5:233:ASP:N	2.39	0.52
8:7:54:ARG:NH1	58:7:410:HOH:O	2.42	0.52
11:A:2401:A:OP2	13:D:255:ARG:NH2	2.42	0.52
11:A:2570:C:O5'	11:A:2592:G:O2'	2.28	0.52
15:F:241:ASN:OD1	15:F:256:HIS:NE2	2.37	0.52
29:U:7:TYR:O	33:Y:183:GLN:NE2	2.35	0.52
38:d:211:GLN:NE2	38:d:249:GLU:OE1	2.42	0.52
39:e:53:LEU:HD13	39:e:159:LEU:HB3	1.91	0.52
42:h:122:ARG:NH2	42:h:124:ARG:HH12	2.08	0.52
52:s:239:ASN:HB2	52:s:299:PHE:HB2	1.91	0.52
7:6:161:LEU:HB3	7:6:300:THR:HG21	1.92	0.52
7:6:187:VAL:HG11	7:6:270:PHE:HE2	1.75	0.52
11:A:2081:U:H2'	11:A:2082:G:C8	2.45	0.52
11:A:2363:A:H3'	11:A:2364:C:H5''	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2822:C:O2'	11:A:2915:C:OP2	2.27	0.52
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.91	0.52
17:I:94:ARG:NE	17:I:159:PRO:HG3	2.24	0.52
18:J:113:THR:HG22	18:J:116:HIS:ND1	2.24	0.52
22:N:81:GLU:OE2	22:N:82:PHE:N	2.43	0.52
41:g:142:GLU:HG3	48:o:86:ARG:O	2.10	0.52
7:6:341:VAL:HG23	31:W:145:VAL:HG23	1.91	0.52
10:9:74:VAL:O	33:Y:83:ALA:HB3	2.09	0.52
11:A:2651:A:H2'	11:A:2652:G:O4'	2.10	0.52
15:F:283:LEU:HD21	21:M:122:VAL:HG12	1.92	0.52
18:J:156:VAL:HA	46:l:101:LEU:HD13	1.92	0.52
19:K:26:GLN:HE22	19:K:149:ARG:H	1.55	0.52
29:U:129:MET:HE1	38:d:81:THR:C	2.35	0.52
31:W:104:TYR:HB3	31:W:126:LEU:HB2	1.91	0.52
32:X:11:TRP:O	32:X:15:GLN:HG2	2.10	0.52
2:1:34:ARG:HG3	2:1:41:LEU:HD21	1.92	0.51
8:7:325:THR:O	8:7:325:THR:OG1	2.27	0.51
11:A:1703:C:O2'	11:A:1704:U:OP2	2.28	0.51
11:A:2837:A:H2'	11:A:2838:A:C8	2.45	0.51
26:R:78:GLU:OE2	58:R:201:HOH:O	2.19	0.51
34:Z:93:LYS:NZ	58:Z:204:HOH:O	2.37	0.51
35:a:75:ILE:HG23	37:c:289:VAL:HG11	1.92	0.51
52:s:90:LYS:HD2	52:s:232:GLN:HB2	1.92	0.51
1:0:155:GLU:HB2	1:0:172:LYS:HG2	1.91	0.51
4:3:132:LYS:HD2	4:3:135:LYS:HD2	1.92	0.51
5:4:74:LYS:HB3	5:4:79:CYS:HB2	1.92	0.51
6:5:40:LYS:HE3	11:A:1709:G:C8	2.45	0.51
11:A:1765:C:O2	50:q:28:ARG:NH2	2.43	0.51
17:I:43:GLN:HB2	22:N:229:VAL:HG21	1.93	0.51
37:c:244:GLU:OE1	37:c:248:ARG:NH1	2.43	0.51
49:p:79:ILE:HG12	49:p:101:VAL:HG12	1.92	0.51
6:5:172:ARG:NH1	6:5:347:ASP:OD1	2.43	0.51
8:7:37:PRO:O	8:7:41:THR:HG23	2.10	0.51
11:A:1737:A:H61	11:A:1760:G:H1'	1.75	0.51
12:B:1607:U:O2'	12:B:1608:G:OP1	2.24	0.51
15:F:220:ASP:O	15:F:245:ALA:N	2.43	0.51
21:M:279:ASP:O	21:M:281:LYS:HG2	2.09	0.51
37:c:149:PRO:HD3	37:c:305:TYR:CE1	2.45	0.51
39:e:51:LEU:HD12	39:e:52:CYS:N	2.25	0.51
6:5:199:ARG:HB3	6:5:232:LYS:HG3	1.92	0.51
11:A:1850:U:O2'	11:A:2134:A:N1	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2347:C:H2'	11:A:2348:A:C8	2.45	0.51
18:J:52:GLU:O	18:J:55:GLU:HG3	2.10	0.51
21:M:118:LEU:O	21:M:122:VAL:HG23	2.10	0.51
38:d:276:ILE:HG22	38:d:278:LYS:H	1.74	0.51
41:g:101:THR:HG23	41:g:107:MET:HE1	1.92	0.51
52:s:66:TRP:O	52:s:69:THR:HG22	2.10	0.51
52:s:162:ARG:H	52:s:163:VAL:HA	1.74	0.51
1:O:106:ASN:ND2	11:A:3212:C:O2'	2.43	0.51
2:1:50:VAL:HG11	50:q:125:MET:CE	2.37	0.51
11:A:1714:C:N4	58:A:3657:HOH:O	2.38	0.51
11:A:1881:A:OP2	41:g:111:ARG:NH2	2.43	0.51
13:D:185:GLY:HA2	13:D:219:LYS:HD3	1.92	0.51
19:K:70:ASN:ND2	51:r:154:TRP:HB2	2.26	0.51
54:TA:62:PRO:O	54:TA:66:GLN:HG2	2.10	0.51
11:A:1907:A:N3	11:A:2930:U:O2'	2.41	0.51
11:A:2215:C:H3'	11:A:2216:A:H8	1.75	0.51
21:M:285:PRO:HB3	50:q:76:TRP:CE2	2.45	0.51
27:S:152:ASP:OD1	27:S:152:ASP:N	2.44	0.51
28:T:154:LYS:O	28:T:155:ARG:NH1	2.43	0.51
44:j:79:LEU:HD23	44:j:80:LEU:HD23	1.91	0.51
6:5:37:SER:HB3	11:A:2523:C:H5'	1.93	0.51
6:5:112:LEU:HB2	6:5:115:GLY:HA2	1.93	0.51
10:9:76:TYR:CD1	33:Y:83:ALA:HB2	2.45	0.51
11:A:2145:G:N2	27:S:103:SER:OG	2.44	0.51
11:A:2795:U:H2'	11:A:2796:G:H8	1.76	0.51
14:E:96:ARG:HB3	14:E:316:PHE:CE1	2.46	0.51
24:P:167:GLU:N	24:P:167:GLU:OE1	2.44	0.51
38:d:86:ASP:OD1	38:d:86:ASP:N	2.41	0.51
38:d:165:THR:HG23	38:d:260:ARG:HB2	1.93	0.51
54:TB:75:THR:O	54:TB:79:ILE:HG13	2.11	0.51
11:A:2245:A:H4'	11:A:2246:A:OP1	2.11	0.51
13:D:196:VAL:HG22	13:D:206:TYR:HB2	1.93	0.51
21:M:243:ILE:HD12	21:M:243:ILE:O	2.11	0.51
34:Z:51:GLU:OE1	34:Z:51:GLU:N	2.41	0.51
49:p:71:ASP:N	49:p:71:ASP:OD1	2.43	0.51
52:s:103:ASP:OD1	52:s:103:ASP:N	2.44	0.51
11:A:2101:C:H2'	11:A:2102:A:C8	2.46	0.51
11:A:2560:G:H8	11:A:2560:G:OP2	1.93	0.51
11:A:2572:C:H2'	11:A:2573:G:C8	2.46	0.51
11:A:3199:U:H5''	11:A:3201:A:N7	2.25	0.51
13:D:64:VAL:O	13:D:80: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:F:231:VAL:HG22	50:q:26:ARG:HE	1.75	0.51
17:I:52:GLU:O	22:N:211:ASN:ND2	2.44	0.51
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.93	0.51
11:A:1826:G:N2	11:A:2686:G:N7	2.59	0.51
11:A:1830:G:OP1	36:b:2:THR:HG21	2.10	0.51
11:A:2333:G:H2'	11:A:2334:C:C6	2.45	0.51
11:A:3127:G:H2'	11:A:3128:A:H2'	1.93	0.51
43:i:57:TYR:OH	50:q:28:ARG:O	2.21	0.51
11:A:2240:C:C4	51:r:196:HIS:HB2	2.45	0.50
11:A:2991:U:C4	57:A:3400:ZLD:H8	2.46	0.50
11:A:3169:C:H2'	11:A:3170:C:O2	2.11	0.50
20:L:45:ALA:O	20:L:49:SER:CB	2.59	0.50
51:r:39:VAL:HB	51:r:52:ARG:CZ	2.41	0.50
6:5:214:ARG:NH2	6:5:366:ASN:OD1	2.40	0.50
7:6:114:ARG:NE	24:P:117:TYR:HE1	2.09	0.50
7:6:261:ARG:HG2	7:6:323:TRP:CE2	2.46	0.50
8:7:81:MET:HB3	8:7:86:SER:OG	2.11	0.50
10:9:123:GLN:NE2	10:9:130:LEU:HB2	2.26	0.50
11:A:2099:U:H2'	11:A:2100:C:C6	2.46	0.50
13:D:118:LYS:NZ	13:D:120:GLY:O	2.45	0.50
15:F:61:PRO:HA	15:F:84:PRO:HD3	1.92	0.50
16:H:64:LEU:HD11	32:X:61:ARG:HD3	1.93	0.50
18:J:170:GLU:HA	18:J:173:ILE:HG12	1.93	0.50
20:L:90:CYS:O	20:L:99:ARG:NH1	2.44	0.50
21:M:260:LYS:HB2	21:M:267:PHE:CE1	2.46	0.50
23:O:57:GLU:OE1	23:O:105:THR:OG1	2.27	0.50
30:V:97:TYR:CB	30:V:105:ARG:HD2	2.41	0.50
32:X:34:GLU:HG2	32:X:36:ARG:HG3	1.93	0.50
37:c:251:SER:OG	37:c:277:ASP:OD1	2.27	0.50
9:8:164:ARG:NH2	40:f:164:ALA:HA	2.26	0.50
11:A:2194:U:O4	11:A:2195:A:N6	2.43	0.50
11:A:2256:U:OP1	44:j:66:ARG:NH2	2.44	0.50
11:A:3114:U:H2'	11:A:3115:U:C6	2.46	0.50
13:D:154:THR:OG1	13:D:246:ARG:O	2.15	0.50
15:F:85:ASP:OD1	41:g:87:ARG:NH2	2.43	0.50
20:L:128:ARG:HD3	20:L:138:LEU:HD22	1.94	0.50
42:h:96:LEU:HA	42:h:99:ASN:ND2	2.26	0.50
5:4:99:LYS:NZ	11:A:3175:A:OP1	2.45	0.50
11:A:1806:U:H1'	11:A:1807:U:OP2	2.11	0.50
23:O:77:ASP:O	23:O:83:LYS:NZ	2.45	0.50
27:S:94:ARG:NH2	27:S:111:GLU:OE1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:129:ARG:HD3	27:S:131:GLU:HG3	1.94	0.50
34:Z:141:SER:O	34:Z:142:THR:HG23	2.11	0.50
41:g:144:THR:O	41:g:144:THR:OG1	2.29	0.50
44:j:93:LEU:HD13	44:j:97:LYS:HG2	1.92	0.50
51:r:124:ARG:NH1	51:r:153:ARG:O	2.44	0.50
51:r:169:TRP:CD1	51:r:170:ASN:HD22	2.29	0.50
7:6:340:PRO:HB3	31:W:147:MET:HE1	1.94	0.50
10:9:136:LEU:HD22	29:U:17:LEU:HD11	1.92	0.50
11:A:2355:A:H3'	11:A:2356:A:H4'	1.92	0.50
11:A:2585:G:N2	58:A:3746:HOH:O	2.45	0.50
11:A:3189:C:O2'	51:r:155:ALA:N	2.39	0.50
30:V:23:MET:HE2	30:V:114:PRO:HD3	1.93	0.50
33:Y:128:SER:HB2	33:Y:131:ARG:HD3	1.93	0.50
38:d:288:LYS:HD3	38:d:288:LYS:H	1.76	0.50
41:g:40:GLU:OE2	41:g:40:GLU:N	2.44	0.50
49:p:111:ILE:HG22	49:p:115:VAL:HG13	1.94	0.50
5:4:86:GLY:H	11:A:3189:C:H5''	1.74	0.50
7:6:160:ASP:HB3	7:6:221:LEU:HD22	1.92	0.50
11:A:1690:C:H2'	11:A:1691:C:C6	2.47	0.50
11:A:1861:U:H2'	11:A:1862:U:C6	2.47	0.50
11:A:1993:A:N3	11:A:1994:A:H5''	2.27	0.50
11:A:2458:A:OP1	23:O:9:ILE:N	2.45	0.50
11:A:2548:C:O2'	11:A:2590:A:H1'	2.12	0.50
25:Q:99:MET:O	25:Q:103:ARG:HG3	2.12	0.50
28:T:133:ASN:O	28:T:133:ASN:ND2	2.40	0.50
29:U:30:ARG:O	33:Y:121:ARG:NH1	2.44	0.50
40:f:111:HIS:CE1	40:f:157:VAL:HB	2.46	0.50
44:j:65:ARG:O	44:j:69:GLU:HG3	2.12	0.50
7:6:56:ARG:O	7:6:59:ARG:HG3	2.12	0.50
8:7:238:ASP:OD1	8:7:239:PHE:N	2.44	0.50
11:A:2506:A:H1'	11:A:2601:A:N6	2.26	0.50
18:J:119:GLU:HA	18:J:122:ARG:HG3	1.94	0.50
18:J:191:LYS:NZ	58:J:213:HOH:O	2.37	0.50
21:M:149:THR:O	21:M:149:THR:OG1	2.28	0.50
37:c:105:ARG:NE	37:c:105:ARG:HA	2.27	0.50
41:g:106:GLN:HG2	41:g:152:TYR:CE2	2.47	0.50
43:i:86:ASN:H	43:i:89:GLN:HB2	1.76	0.50
49:p:102:ARG:HG2	49:p:102:ARG:HH11	1.76	0.50
52:s:115:LEU:HD21	52:s:257:VAL:HG11	1.92	0.50
7:6:102:GLN:OE1	7:6:106:ARG:NH1	2.44	0.50
7:6:116:ASN:OD1	7:6:117:VAL:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:64:LYS:HD2	8:7:80:VAL:HG12	1.94	0.50
11:A:2944:C:OP1	48:o:21:HIS:ND1	2.41	0.50
35:a:43:TYR:HD2	36:b:135:ASN:HA	1.77	0.50
46:l:112:PRO:HA	46:l:117:TYR:CD2	2.47	0.50
8:7:185:LEU:HD12	8:7:295:ARG:HH12	1.76	0.50
8:7:328:GLN:NE2	58:7:414:HOH:O	2.45	0.50
11:A:2538:C:H5''	11:A:2635:G:OP2	2.12	0.50
11:A:2744:U:O2	11:A:2745:A:N6	2.45	0.50
21:M:226:PRO:HB2	49:p:58:ALA:HB2	1.93	0.50
49:p:187:ARG:NH1	58:p:312:HOH:O	2.45	0.50
51:r:93:ILE:HG21	51:r:119:VAL:HG21	1.94	0.50
7:6:266:HIS:O	7:6:320:GLN:HA	2.12	0.49
11:A:2315:A:O2'	11:A:2316:U:H6	1.95	0.49
11:A:3009:C:H5	11:A:3030:A:H61	1.60	0.49
14:E:227:GLN:HB2	14:E:236:THR:O	2.11	0.49
37:c:184:PHE:O	37:c:186:VAL:HG23	2.12	0.49
38:d:81:THR:HG22	38:d:82:ALA:H	1.77	0.49
40:f:93:ILE:HB	40:f:157:VAL:HG13	1.92	0.49
40:f:127:MET:HE3	40:f:128:PRO:CD	2.31	0.49
6:5:244:ILE:HG23	6:5:369:VAL:HG21	1.94	0.49
11:A:1974:A:H5'	13:D:261:GLY:HA2	1.94	0.49
11:A:2691:U:H2'	11:A:2692:G:C8	2.46	0.49
11:A:3078:C:H2'	11:A:3079:G:H8	1.76	0.49
11:A:3143:U:H2'	11:A:3144:A:H8	1.77	0.49
19:K:23:GLY:O	19:K:26:GLN:HG2	2.12	0.49
24:P:77:PHE:CZ	24:P:80:ARG:HD2	2.47	0.49
26:R:18:TYR:O	26:R:22:GLN:HG2	2.12	0.49
30:V:33:ARG:HH11	30:V:33:ARG:HG3	1.76	0.49
40:f:178:LEU:HD23	40:f:179:PRO:CD	2.41	0.49
6:5:125:THR:HG21	6:5:356:PHE:HE1	1.77	0.49
6:5:146:ILE:HB	6:5:149:GLN:HB2	1.94	0.49
6:5:190:GLN:NE2	6:5:193:LYS:HE3	2.26	0.49
7:6:125:LEU:C	7:6:126:ARG:HG2	2.38	0.49
7:6:303:PHE:HA	7:6:306:LYS:HE3	1.92	0.49
11:A:1882:A:H4'	11:A:1883:G:H5'	1.95	0.49
11:A:1952:U:H2'	11:A:1953:A:C8	2.47	0.49
21:M:51:ARG:HB3	21:M:58:GLN:HA	1.94	0.49
45:k:11:ARG:HD2	45:k:12:PRO:CD	2.41	0.49
10:9:39:LYS:HD2	29:U:7:TYR:CD2	2.47	0.49
34:Z:140:LYS:HG2	44:j:40:TYR:CE1	2.46	0.49
44:j:63:GLN:NE2	58:j:203:HOH:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:126:ALA:O	50:q:127:LYS:C	2.56	0.49
7:6:58:ARG:O	7:6:62:GLU:HG3	2.12	0.49
7:6:126:ARG:HH22	24:P:122:VAL:HG21	1.77	0.49
15:F:79:LEU:HD12	42:h:94:SER:HB3	1.95	0.49
19:K:159:THR:O	19:K:161:GLU:N	2.45	0.49
21:M:276:ASN:O	21:M:280:LYS:HA	2.12	0.49
25:Q:102:ARG:HH21	25:Q:106:LEU:HD22	1.77	0.49
30:V:194:LEU:O	30:V:198:VAL:HG22	2.12	0.49
42:h:81:SER:C	42:h:83:PRO:HD3	2.37	0.49
43:i:83:TRP:CH2	43:i:85:GLY:HA3	2.47	0.49
50:q:139:GLN:HA	50:q:142:ASN:HD21	1.77	0.49
6:5:152:CYS:HB3	6:5:186:LEU:HD11	1.94	0.49
11:A:1857:U:H2'	11:A:1858:G:C8	2.48	0.49
50:q:124:CYS:HA	50:q:127:LYS:HD3	1.95	0.49
7:6:131:PRO:HD2	24:P:115:HIS:NE2	2.27	0.49
7:6:224:HIS:CE1	7:6:227:GLU:HB3	2.48	0.49
8:7:195:THR:OG1	8:7:196:LYS:N	2.46	0.49
11:A:1722:A:H2'	11:A:1723:A:O4'	2.13	0.49
23:O:38:ARG:NE	23:O:82:GLU:OE1	2.42	0.49
26:R:82:LYS:NZ	58:R:204:HOH:O	2.45	0.49
34:Z:51:GLU:CD	34:Z:51:GLU:H	2.20	0.49
50:q:121:ILE:HG23	50:q:125:MET:HE3	1.95	0.49
1:0:85:ARG:NH2	58:O:303:HOH:O	2.45	0.49
8:7:173:PRO:HB2	8:7:175:ILE:HG22	1.94	0.49
11:A:1984:A:H8	11:A:1987:G:H21	1.59	0.49
11:A:2559:U:H4'	11:A:2560:G:O5'	2.11	0.49
11:A:3123:G:O2'	11:A:3124:U:O5'	2.31	0.49
16:H:59:TRP:CE3	16:H:81:LYS:HE2	2.47	0.49
19:K:169:LEU:HD11	51:r:88:LEU:HG	1.94	0.49
20:L:118:ARG:HG3	20:L:142:GLN:HE22	1.78	0.49
20:L:129:LYS:HD3	25:Q:125:TYR:HE2	1.78	0.49
21:M:285:PRO:HB3	50:q:76:TRP:NE1	2.27	0.49
27:S:76:HIS:O	27:S:80:VAL:HG23	2.12	0.49
41:g:118:TRP:NE1	41:g:142:GLU:OE2	2.44	0.49
51:r:193:LYS:HG2	51:r:196:HIS:HB3	1.95	0.49
52:s:53:ALA:O	52:s:62:ARG:NH2	2.45	0.49
1:0:82:LYS:NZ	11:A:2718:C:OP1	2.25	0.49
11:A:2527:A:OP2	13:D:67:LYS:NZ	2.46	0.49
15:F:249:ASN:O	15:F:253:MET:HG3	2.13	0.49
25:Q:268:ASP:O	25:Q:270:MET:N	2.46	0.49
36:b:144:ARG:HG2	36:b:147:GLU:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:174:TRP:HD1	38:d:175:ASP:OD1	1.96	0.49
39:e:86:ASP:HB2	47:m:69:ARG:HE	1.78	0.49
10:9:91:LEU:HD23	33:Y:156:LEU:HD12	1.94	0.49
11:A:2158:U:O2'	51:r:153:ARG:NH2	2.45	0.49
11:A:2663:C:H2'	11:A:2664:U:H6	1.78	0.49
17:I:95:MET:HB2	17:I:180:CYS:O	2.12	0.49
22:N:214:THR:HG22	22:N:216:GLU:H	1.78	0.49
32:X:143:PHE:CD1	32:X:147:LYS:HE3	2.48	0.49
41:g:144:THR:O	41:g:146:THR:HG22	2.13	0.49
47:m:58:LYS:HG2	47:m:59:GLN:H	1.78	0.49
5:4:89:TYR:CE2	5:4:101:ARG:HG3	2.48	0.48
11:A:2180:A:O2'	11:A:2206:C:O3'	2.31	0.48
17:I:54:ILE:HD12	22:N:211:ASN:HB3	1.94	0.48
18:J:187:GLU:HB3	18:J:191:LYS:HZ1	1.77	0.48
20:L:72:GLN:NE2	58:L:203:HOH:O	2.45	0.48
20:L:145:VAL:HG21	25:Q:160:VAL:HG11	1.95	0.48
49:p:99:ALA:O	49:p:136:THR:HA	2.13	0.48
3:2:82:ARG:HD3	11:A:1791:G:OP2	2.13	0.48
8:7:186:ASP:OD1	8:7:188:LYS:HB3	2.13	0.48
11:A:1680:A:H5'	11:A:1681:G:OP2	2.13	0.48
11:A:2275:U:H2'	11:A:2276:C:H6	1.76	0.48
15:F:83:HIS:CD2	15:F:85:ASP:HB2	2.48	0.48
18:J:65:PRO:HD2	18:J:89:TYR:CE2	2.48	0.48
19:K:26:GLN:NE2	19:K:147:GLN:HB3	2.28	0.48
21:M:225:ASP:OD1	21:M:225:ASP:N	2.44	0.48
22:N:116:LYS:HB2	22:N:116:LYS:HE3	1.62	0.48
25:Q:84:ARG:NH2	25:Q:272:GLU:O	2.44	0.48
29:U:134:ARG:O	29:U:138:GLN:HG3	2.13	0.48
37:c:170:ALA:HB1	37:c:175:VAL:HG22	1.94	0.48
39:e:178:TRP:CD1	39:e:187:THR:HG21	2.47	0.48
39:e:257:LYS:HE2	39:e:273:ARG:HB2	1.93	0.48
6:5:304:GLN:HB2	6:5:307:GLN:HG3	1.94	0.48
7:6:184:LEU:O	49:p:189:ARG:HG2	2.13	0.48
8:7:121:LYS:HD3	8:7:121:LYS:H	1.79	0.48
13:D:74:ILE:HD11	13:D:149:ARG:HA	1.94	0.48
13:D:138:ASP:OD2	13:D:249:ASN:HB2	2.13	0.48
17:I:140:TYR:OH	17:I:180:CYS:SG	2.65	0.48
1:0:168:GLN:OE1	1:0:168:GLN:N	2.41	0.48
6:5:231:THR:HG23	6:5:288:HIS:HB2	1.95	0.48
11:A:3143:U:H2'	11:A:3144:A:C8	2.48	0.48
14:E:227:GLN:NE2	14:E:236:THR:O	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:169:PHE:O	22:N:173:GLN:HB3	2.13	0.48
24:P:125:CYS:SG	24:P:157:SER:OG	2.59	0.48
32:X:42:HIS:NE2	32:X:83:GLU:HB2	2.29	0.48
32:X:150:LYS:HE3	32:X:150:LYS:HB2	1.57	0.48
37:c:159:PHE:CD2	37:c:231:MET:HG2	2.48	0.48
39:e:244:SER:O	58:e:303:HOH:O	2.20	0.48
51:r:58:LYS:HD3	51:r:58:LYS:N	2.29	0.48
6:5:60:PHE:CZ	6:5:72:PRO:HD3	2.48	0.48
21:M:136:TYR:HA	21:M:184:LEU:HD11	1.96	0.48
45:k:63:CYS:HA	45:k:77:ARG:HA	1.93	0.48
1:0:90:ASN:O	1:0:94:ARG:HG2	2.12	0.48
11:A:1809:U:H3	11:A:1810:A:HO2'	1.61	0.48
11:A:2579:C:H2'	11:A:2580:U:N1	2.28	0.48
17:I:99:CYS:O	58:I:301:HOH:O	2.20	0.48
21:M:38:ARG:HD2	21:M:45:ARG:NE	2.28	0.48
21:M:287:ASP:O	21:M:287:ASP:OD2	2.32	0.48
30:V:72:LYS:HD3	30:V:91:LEU:HD22	1.95	0.48
52:s:249:GLU:HA	52:s:356:VAL:HG11	1.95	0.48
6:5:278:PHE:HA	52:s:156:TYR:OH	2.12	0.48
7:6:195:PRO:HD3	7:6:321:CYS:SG	2.54	0.48
16:H:146:LEU:HD12	16:H:147:ARG:N	2.28	0.48
28:T:161:ARG:C	28:T:163:ARG:H	2.21	0.48
45:k:68:PHE:CZ	45:k:70:ASP:HB2	2.49	0.48
52:s:263:THR:HG23	52:s:265:LYS:NZ	2.28	0.48
2:1:22:SER:HB3	2:1:56:PHE:CZ	2.48	0.48
11:A:1807:U:O2'	11:A:1808:A:O5'	2.27	0.48
11:A:2683:C:OP2	26:R:34:ARG:NH1	2.47	0.48
11:A:2758:G:H2'	11:A:2759:U:O4'	2.14	0.48
12:B:1628:C:H42	12:B:1640:A:H61	1.61	0.48
18:J:78:PHE:HD2	18:J:80:ILE:HD11	1.78	0.48
50:q:131:MET:O	50:q:132:ILE:C	2.57	0.48
6:5:118:GLN:NE2	6:5:260:PRO:O	2.47	0.48
8:7:287:GLN:NE2	8:7:290:GLN:O	2.47	0.48
11:A:1834:U:C4	28:T:206:ARG:HA	2.49	0.48
11:A:2347:C:H2'	11:A:2348:A:H8	1.79	0.48
17:I:189:GLN:O	17:I:192:ILE:HG22	2.14	0.48
32:X:169:LEU:HB3	32:X:195:ALA:HB2	1.95	0.48
7:6:136:ARG:NE	7:6:140:GLU:OE2	2.45	0.48
10:9:79:PRO:O	10:9:79:PRO:HD2	2.14	0.48
11:A:2195:A:H2'	11:A:2196:A:C2	2.49	0.48
18:J:114:LEU:HD21	46:l:96:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:65:ARG:HA	26:R:68:TRP:CE3	2.48	0.48
2:1:45:HIS:HB3	2:1:56:PHE:CD1	2.49	0.47
10:9:39:LYS:HD3	11:A:1705:A:C8	2.49	0.47
11:A:2516:C:H5''	13:D:285:LYS:HG2	1.95	0.47
11:A:2604:A:N6	58:A:3765:HOH:O	2.47	0.47
14:E:266:ARG:HE	14:E:266:ARG:HB3	1.51	0.47
17:I:110:LEU:HA	17:I:113:ARG:HB2	1.95	0.47
23:O:55:TYR:HE1	25:Q:268:ASP:O	1.97	0.47
34:Z:56:TYR:HB2	48:o:47:TYR:CE2	2.49	0.47
42:h:75:LYS:HD2	42:h:82:LEU:HD11	1.96	0.47
45:k:11:ARG:NH1	45:k:12:PRO:HG3	2.29	0.47
7:6:193:VAL:HB	7:6:319:PHE:CD2	2.50	0.47
11:A:1822:U:O2	11:A:2707:A:O2'	2.31	0.47
11:A:2470:G:O2'	20:L:36:THR:HG22	2.14	0.47
11:A:3063:G:O2'	11:A:3066:C:OP2	2.24	0.47
17:I:81:LEU:O	17:I:85:GLU:HG2	2.14	0.47
41:g:100:ILE:HA	41:g:105:ARG:O	2.14	0.47
52:s:111:LYS:NZ	52:s:384:ASP:OD1	2.38	0.47
6:5:36:ARG:HA	6:5:39:ARG:HG3	1.96	0.47
6:5:60:PHE:HB3	6:5:67:VAL:HG22	1.96	0.47
7:6:299:ARG:NH1	7:6:299:ARG:HB2	2.29	0.47
11:A:1839:C:H2'	11:A:1840:C:C6	2.50	0.47
11:A:2053:U:H2'	11:A:2054:U:C6	2.49	0.47
11:A:2151:A:H2'	11:A:2152:A:C8	2.48	0.47
11:A:2694:A:C6	11:A:2985:C:H1'	2.48	0.47
13:D:130:ARG:O	13:D:138:ASP:HB3	2.14	0.47
50:q:77:PRO:O	50:q:81:GLN:HG2	2.14	0.47
7:6:184:LEU:HG	49:p:191:LYS:HE3	1.96	0.47
11:A:2349:G:O2'	11:A:2351:U:O4	2.31	0.47
11:A:2514:C:H2'	11:A:2515:U:C6	2.49	0.47
11:A:2629:A:N3	11:A:3079:G:O2'	2.47	0.47
24:P:45:ALA:O	24:P:47:GLU:N	2.47	0.47
24:P:91:GLU:HB2	24:P:106:SER:HB3	1.96	0.47
27:S:106:TRP:CE3	27:S:114:ILE:HD12	2.50	0.47
36:b:34:SER:OG	36:b:36:ASP:O	2.19	0.47
49:p:81:TYR:OH	49:p:147:LEU:HB2	2.14	0.47
49:p:137:SER:OG	49:p:149:ASP:OD1	2.32	0.47
52:s:378:ALA:HB1	52:s:383:ALA:HB1	1.96	0.47
11:A:2041:U:H2'	11:A:2042:U:C6	2.50	0.47
19:K:153:LYS:HE2	19:K:157:GLU:O	2.14	0.47
23:O:143:THR:OG1	23:O:146:ASN:ND2	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:171:ILE:HB	27:S:184:ARG:HB2	1.97	0.47
29:U:110:LEU:O	33:Y:74:TRP:HB3	2.14	0.47
37:c:75:PHE:O	37:c:79:LEU:HD12	2.15	0.47
40:f:135:LEU:HD12	40:f:145:LEU:HD21	1.96	0.47
41:g:154:ASP:OD1	41:g:154:ASP:N	2.42	0.47
46:l:68:LEU:HD12	46:l:70:THR:HG23	1.97	0.47
49:p:176:HIS:CE1	49:p:180:ILE:HD12	2.49	0.47
50:q:121:ILE:CG2	50:q:125:MET:HE3	2.44	0.47
50:q:131:MET:HE2	50:q:131:MET:HB2	1.66	0.47
52:s:165:ARG:HH21	52:s:307:ARG:NH2	2.11	0.47
11:A:2220:A:O4'	51:r:103:LYS:HB3	2.15	0.47
11:A:2296:U:O2'	26:R:40:ARG:NH1	2.47	0.47
11:A:2653:C:O2'	11:A:2654:U:H6	1.98	0.47
12:B:1633:U:H2'	12:B:1634:A:O4'	2.14	0.47
12:B:1664:G:H2'	12:B:1665:C:C6	2.50	0.47
13:D:257:ILE:O	13:D:262:ARG:NE	2.30	0.47
15:F:284:TYR:O	15:F:290:TYR:OH	2.31	0.47
17:I:42:PHE:CE2	17:I:46:LYS:HD2	2.49	0.47
20:L:94:PRO:HG2	20:L:97:THR:HG21	1.96	0.47
24:P:64:LYS:H	24:P:177:ARG:HD2	1.79	0.47
26:R:85:ALA:O	26:R:89:ASN:ND2	2.30	0.47
32:X:177:HIS:CE1	32:X:180:ASP:HB2	2.50	0.47
37:c:104:LYS:O	37:c:107:GLN:HG3	2.15	0.47
40:f:130:LYS:O	40:f:152:THR:N	2.47	0.47
43:i:93:ARG:O	43:i:97:MET:HG3	2.14	0.47
45:k:16:VAL:HG22	45:k:51:VAL:HG12	1.95	0.47
6:5:70:LEU:HD12	6:5:70:LEU:HA	1.74	0.47
6:5:252:LEU:HD11	6:5:370:LYS:HG2	1.96	0.47
6:5:323:GLN:O	6:5:327:LEU:HG	2.15	0.47
7:6:63:GLN:NE2	58:6:412:HOH:O	2.41	0.47
9:8:125:LYS:HD2	9:8:125:LYS:HA	1.71	0.47
11:A:1939:G:O2'	11:A:1973:G:H4'	2.15	0.47
11:A:2170:G:H2'	11:A:2171:U:C2	2.50	0.47
11:A:2751:G:H2'	11:A:2752:C:C6	2.50	0.47
11:A:2795:U:H2'	11:A:2796:G:C8	2.50	0.47
11:A:3041:U:H2'	11:A:3042:U:C6	2.50	0.47
11:A:3157:C:N4	23:O:14:VAL:HG21	2.30	0.47
13:D:232:ARG:NE	13:D:290:PRO:HB2	2.30	0.47
16:H:141:GLU:HA	16:H:141:GLU:OE2	2.15	0.47
17:I:160:LYS:NZ	17:I:163:GLU:HB3	2.29	0.47
18:J:30:MET:O	18:J:32:GLY:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:89:TYR:HA	18:J:92:LYS:HE3	1.97	0.47
21:M:207:PRO:O	21:M:211:VAL:HG23	2.15	0.47
21:M:254:LYS:HD3	21:M:254:LYS:HA	1.64	0.47
32:X:86:ILE:HB	32:X:105:TRP:HB2	1.95	0.47
32:X:117:GLU:OE1	32:X:191:TYR:OH	2.32	0.47
34:Z:103:ILE:HG23	44:j:84:MET:HE3	1.95	0.47
36:b:35:ARG:HB2	42:h:158:TYR:CE2	2.49	0.47
37:c:162:GLY:O	37:c:166:VAL:HG22	2.15	0.47
39:e:49:GLY:HA2	39:e:232:PHE:H	1.78	0.47
40:f:78:ARG:NH1	58:f:213:HOH:O	2.47	0.47
43:i:125:GLY:O	43:i:128:ARG:NH1	2.46	0.47
45:k:8:LEU:HD21	45:k:95:ARG:HB3	1.95	0.47
6:5:36:ARG:NE	58:5:511:HOH:O	2.46	0.47
9:8:110:GLU:O	9:8:114:ARG:HG3	2.14	0.47
11:A:1875:C:H2'	11:A:1876:U:C6	2.50	0.47
11:A:3227:U:C5	14:E:156:ARG:HD2	2.50	0.47
14:E:90:TRP:CZ3	14:E:312:LYS:HE3	2.50	0.47
16:H:95:GLU:OE1	16:H:132:ALA:HB3	2.15	0.47
17:I:100:GLN:HB3	17:I:175:PRO:HD2	1.97	0.47
52:s:91:TYR:HB3	52:s:273:LEU:HD13	1.97	0.47
7:6:50:LYS:HA	31:W:121:PRO:HA	1.96	0.47
7:6:228:PRO:HD2	7:6:229:ASP:N	2.29	0.47
8:7:159:LYS:HB3	8:7:159:LYS:HE2	1.71	0.47
9:8:108:PHE:O	9:8:112:GLU:HG2	2.15	0.47
11:A:1688:A:OP2	32:X:5:LYS:NZ	2.46	0.47
11:A:2005:C:H2'	11:A:2006:C:C6	2.50	0.47
11:A:2006:C:H2'	11:A:2007:U:C6	2.49	0.47
11:A:2803:A:H2'	11:A:2804:A:O4'	2.14	0.47
12:B:1623:G:H5''	24:P:86:THR:HG21	1.96	0.47
15:F:72:PHE:HZ	15:F:205:GLU:HB3	1.79	0.47
40:f:114:CYS:HB2	40:f:119:ILE:HD11	1.96	0.47
41:g:45:TYR:O	41:g:49:GLU:HG3	2.15	0.47
41:g:108:THR:CG2	41:g:153:PHE:H	2.27	0.47
44:j:40:TYR:CG	44:j:40:TYR:O	2.68	0.47
45:k:90:PHE:O	45:k:94:ILE:HG23	2.15	0.47
11:A:1805:A:O2'	11:A:1806:U:OP1	2.29	0.47
13:D:253:ASN:OD1	13:D:253:ASN:N	2.48	0.47
17:I:94:ARG:HG3	17:I:159:PRO:HD3	1.96	0.47
19:K:120:THR:O	19:K:124:ARG:HD3	2.14	0.47
37:c:175:VAL:O	37:c:179:THR:OG1	2.30	0.47
39:e:118:GLN:HA	39:e:121:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:152:LYS:HZ3	39:e:155:ARG:HB2	1.80	0.47
40:f:97:ALA:HB2	40:f:182:VAL:HA	1.96	0.47
7:6:116:ASN:OD1	7:6:118:GLU:N	2.48	0.46
7:6:206:TYR:OH	7:6:242:GLY:O	2.28	0.46
7:6:339:GLU:N	31:W:148:LEU:O	2.48	0.46
8:7:162:TYR:HE1	8:7:188:LYS:HD3	1.80	0.46
11:A:2027:A:O2'	11:A:2048:U:OP1	2.29	0.46
11:A:2277:U:H2'	11:A:2278:A:H8	1.81	0.46
11:A:2572:C:H2'	11:A:2573:G:H8	1.80	0.46
11:A:2682:A:H4'	26:R:41:LEU:HD13	1.97	0.46
1:0:116:LEU:HD11	8:7:98:TRP:CZ2	2.50	0.46
12:B:1628:C:H2'	12:B:1629:A:C8	2.49	0.46
19:K:178:LEU:HD21	51:r:35:PHE:CD1	2.50	0.46
30:V:126:MET:HB3	30:V:152:ARG:HH11	1.80	0.46
36:b:116:ARG:O	36:b:117:LYS:HB3	2.15	0.46
37:c:97:TYR:HB2	37:c:181:SER:HA	1.96	0.46
38:d:246:VAL:HG23	38:d:264:LYS:HG2	1.96	0.46
50:q:48:PRO:HB2	50:q:50:TRP:CD1	2.50	0.46
1:0:179:ARG:HE	1:0:179:ARG:HB3	1.55	0.46
11:A:2747:U:H2'	11:A:2748:A:C8	2.50	0.46
12:B:1607:U:O4	12:B:1664:G:O6	2.33	0.46
13:D:132:ASP:HB2	13:D:139:ILE:HG12	1.96	0.46
13:D:141:LEU:HB2	13:D:150:TRP:CZ3	2.50	0.46
18:J:49:PHE:HE1	18:J:80:ILE:HG12	1.80	0.46
19:K:177:ARG:HH21	45:k:85:GLU:HG2	1.79	0.46
21:M:169:LYS:HE3	21:M:242:TYR:HB2	1.96	0.46
32:X:107:PRO:HG2	32:X:109:LEU:HD21	1.96	0.46
34:Z:83:LYS:NZ	58:Z:205:HOH:O	2.40	0.46
36:b:35:ARG:HD2	36:b:36:ASP:OD1	2.15	0.46
38:d:164:VAL:HG11	38:d:172:MET:HE1	1.98	0.46
38:d:244:GLU:OE2	38:d:264:LYS:NZ	2.28	0.46
39:e:212:HIS:HA	39:e:231:VAL:O	2.14	0.46
46:l:136:LYS:NZ	58:l:208:HOH:O	2.48	0.46
6:5:112:LEU:HD11	6:5:314:LEU:HD11	1.98	0.46
7:6:92:LEU:HD21	7:6:274:LYS:HD3	1.97	0.46
7:6:130:VAL:HG22	24:P:115:HIS:CE1	2.50	0.46
7:6:183:ASP:CB	49:p:189:ARG:HB3	2.44	0.46
8:7:246:GLN:OE1	8:7:246:GLN:N	2.46	0.46
11:A:1809:U:C4	11:A:1810:A:H1'	2.50	0.46
11:A:2022:G:N2	11:A:2272:C:H1'	2.30	0.46
11:A:2235:C:N4	58:A:3737:HOH:O	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:191:ASP:OD2	15:F:192:SER:N	2.48	0.46
21:M:62:ARG:HB3	43:i:128:ARG:HD2	1.96	0.46
24:P:132:LEU:HA	24:P:135:ARG:CD	2.46	0.46
27:S:103:SER:OG	27:S:103:SER:O	2.32	0.46
29:U:11:ARG:HG3	30:V:211:LYS:HD2	1.98	0.46
30:V:134:GLU:OE2	30:V:148:THR:HG22	2.16	0.46
36:b:44:ARG:NH1	48:o:99:LYS:O	2.48	0.46
38:d:40:ARG:H	38:d:40:ARG:HG2	1.54	0.46
38:d:135:LYS:O	38:d:138:PRO:HD2	2.15	0.46
39:e:63:LEU:HD12	39:e:63:LEU:HA	1.69	0.46
40:f:100:MET:HG3	40:f:101:THR:N	2.30	0.46
46:l:122:ARG:O	46:l:126:ILE:HG12	2.14	0.46
8:7:163:MET:H	8:7:186:ASP:HB3	1.79	0.46
11:A:3195:A:OP2	11:A:3196:G:O2'	2.21	0.46
17:I:151:ASN:OD1	17:I:151:ASN:N	2.47	0.46
17:I:181:ILE:O	17:I:184:THR:OG1	2.28	0.46
18:J:124:LYS:NZ	58:J:221:HOH:O	2.47	0.46
19:K:154:ARG:HA	51:r:127:LEU:HG	1.98	0.46
22:N:250:ARG:O	22:N:251:VAL:HG12	2.15	0.46
39:e:155:ARG:HH21	39:e:257:LYS:H	1.64	0.46
40:f:138:GLN:HB2	40:f:141:GLY:O	2.16	0.46
52:s:162:ARG:HG3	52:s:164:HIS:CD2	2.50	0.46
52:s:164:HIS:O	52:s:168:GLU:HG3	2.16	0.46
52:s:374:LEU:HD21	52:s:377:LEU:HD13	1.97	0.46
4:3:100:ARG:NH1	11:A:1754:G:OP1	2.49	0.46
9:8:165:ASP:OD1	39:e:185:ARG:NH1	2.49	0.46
10:9:40:GLY:O	11:A:1705:A:N6	2.48	0.46
11:A:2118:U:C2	11:A:2119:U:C5	3.04	0.46
11:A:2172:A:C8	18:J:23:ILE:HG22	2.51	0.46
11:A:2190:C:OP2	46:l:123:LYS:HE2	2.15	0.46
11:A:2344:C:C5	11:A:2362:A:H1'	2.50	0.46
11:A:2508:C:H2'	11:A:2509:A:C8	2.51	0.46
11:A:2728:C:H2'	11:A:2729:U:H6	1.81	0.46
11:A:3210:C:OP1	14:E:158:ALA:HA	2.16	0.46
18:J:84:GLN:HG3	18:J:124:LYS:HA	1.97	0.46
36:b:36:ASP:OD1	48:o:100:LYS:HG2	2.16	0.46
52:s:403:GLU:HG3	52:s:404:THR:HG23	1.96	0.46
9:8:150:LEU:HD21	9:8:157:LEU:HB3	1.98	0.46
10:9:76:TYR:CE2	30:V:165:ILE:HG21	2.51	0.46
11:A:1925:A:H2'	11:A:1926:A:C8	2.50	0.46
11:A:3174:U:H2'	11:A:3175:A:H8	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:200:PRO:HA	14:E:273:VAL:HG23	1.98	0.46
15:F:164:MET:HE2	43:i:69:HIS:CE1	2.51	0.46
18:J:113:THR:HG23	18:J:115:LYS:H	1.81	0.46
24:P:68:TRP:CD1	24:P:75:ARG:HD3	2.50	0.46
32:X:133:ASP:O	32:X:137:GLU:HG3	2.15	0.46
40:f:80:ILE:HB	40:f:87:GLU:HG2	1.97	0.46
52:s:84:THR:HB	52:s:280:ASN:HB2	1.98	0.46
7:6:45:LEU:HA	7:6:48:LEU:HG	1.98	0.46
9:8:154:SER:OG	9:8:157:LEU:HB2	2.15	0.46
11:A:2674:U:H2'	11:A:2675:G:O4'	2.16	0.46
11:A:2993:U:H1'	57:A:3400:ZLD:H24A	1.97	0.46
11:A:3213:A:H2'	11:A:3214:C:C6	2.51	0.46
12:B:1607:U:HO2'	12:B:1608:G:P	2.39	0.46
15:F:128:TRP:CD1	15:F:128:TRP:O	2.68	0.46
21:M:168:GLU:OE2	21:M:220:ARG:NE	2.31	0.46
26:R:42:ALA:O	26:R:46:VAL:HG23	2.15	0.46
39:e:216:LYS:N	58:e:334:HOH:O	2.49	0.46
45:k:13:VAL:HA	45:k:68:PHE:HB2	1.98	0.46
50:q:147:GLN:O	50:q:151:GLU:HG2	2.16	0.46
7:6:193:VAL:HG13	7:6:197:GLU:HB2	1.98	0.46
7:6:325:ASP:O	7:6:328:THR:HG22	2.16	0.46
11:A:1911:C:H2'	11:A:1912:A:C8	2.51	0.46
11:A:2055:U:H2'	11:A:2056:G:C8	2.47	0.46
23:O:95:PRO:O	23:O:98:LYS:HG2	2.16	0.46
28:T:196:ALA:O	28:T:200:ILE:HG12	2.15	0.46
30:V:73:GLN:OE1	30:V:123:VAL:HG11	2.16	0.46
31:W:61:VAL:HG13	31:W:65:ASN:HB2	1.97	0.46
37:c:287:GLU:HG2	37:c:288:THR:HG23	1.98	0.46
7:6:138:GLU:HA	7:6:141:ARG:HD3	1.97	0.46
11:A:2521:A:C2	13:D:205:GLN:HG2	2.51	0.46
11:A:2552:U:C2	11:A:2553:G:C8	3.03	0.46
11:A:2875:A:H5''	24:P:180:GLU:HB3	1.98	0.46
14:E:80:LEU:HD11	14:E:320:PHE:HB3	1.98	0.46
16:H:143:GLU:HA	16:H:146:LEU:HG	1.98	0.46
19:K:107:ALA:O	19:K:111:MET:HG3	2.16	0.46
26:R:23:GLU:HA	26:R:26:LYS:NZ	2.31	0.46
30:V:214:TYR:O	33:Y:184:TRP:N	2.49	0.46
40:f:168:GLU:OE2	40:f:169:ILE:HG12	2.16	0.46
4:3:100:ARG:NH2	16:H:72:ARG:NH2	2.63	0.45
6:5:245:GLU:O	6:5:248:LYS:HD2	2.15	0.45
7:6:52:ARG:NH2	7:6:56:ARG:HH22	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:175:GLY:H	40:f:183:ARG:HE	1.63	0.45
11:A:2417:C:OP2	52:s:310:ARG:NH1	2.49	0.45
11:A:2668:A:H2'	11:A:2669:A:C8	2.51	0.45
19:K:44:LYS:NZ	19:K:55:ASP:OD1	2.48	0.45
21:M:130:GLN:HB3	21:M:132:LEU:O	2.16	0.45
22:N:199:ARG:O	22:N:203:GLU:HG3	2.16	0.45
23:O:67:ASP:OD2	52:s:44:TYR:OH	2.25	0.45
24:P:94:VAL:O	24:P:102:VAL:HG22	2.16	0.45
46:l:129:HIS:O	46:l:133:SER:OG	2.28	0.45
2:1:24:ALA:CA	50:q:124:CYS:HB3	2.46	0.45
7:6:126:ARG:NH2	24:P:122:VAL:HG21	2.30	0.45
11:A:1804:A:C6	38:d:68:PRO:HB3	2.51	0.45
11:A:2814:G:N3	11:A:2814:G:H5'	2.31	0.45
19:K:23:GLY:O	19:K:147:GLN:NE2	2.49	0.45
45:k:18:VAL:HG21	45:k:34:LEU:HD12	1.97	0.45
49:p:112:ALA:HB3	49:p:115:VAL:HG12	1.98	0.45
50:q:140:ARG:HD3	50:q:143:TRP:CE3	2.51	0.45
2:1:34:ARG:NH1	2:1:58:GLU:OE2	2.48	0.45
8:7:67:VAL:HG13	8:7:79:PHE:HB2	1.97	0.45
10:9:129:GLN:HG2	10:9:134:ASN:HB2	1.98	0.45
11:A:2588:C:H2'	11:A:2589:A:C8	2.51	0.45
15:F:238:LYS:NZ	50:q:25:TYR:OH	2.49	0.45
23:O:15:PHE:HE1	25:Q:270:MET:HG2	1.81	0.45
28:T:77:ARG:HG2	28:T:80:ILE:HG12	1.99	0.45
33:Y:91:ARG:HG3	33:Y:145:VAL:HG22	1.99	0.45
33:Y:137:ASP:OD1	33:Y:138:SER:N	2.49	0.45
37:c:259:ARG:HB2	37:c:271:PHE:HB2	1.98	0.45
41:g:143:VAL:HG12	48:o:88:ILE:HA	1.97	0.45
45:k:58:ASP:OD1	45:k:58:ASP:N	2.47	0.45
46:l:73:MET:HE1	46:l:83:ASP:OD1	2.15	0.45
52:s:63:ILE:HA	52:s:66:TRP:CD1	2.51	0.45
2:1:16:ILE:HD11	2:1:36:ARG:NH2	2.31	0.45
11:A:1808:A:H4'	11:A:1809:U:OP1	2.17	0.45
11:A:2748:A:H2'	11:A:2749:A:H8	1.81	0.45
11:A:3117:C:H2'	11:A:3118:U:H6	1.81	0.45
12:B:1639:U:H2'	12:B:1640:A:C8	2.52	0.45
22:N:104:MET:HE3	22:N:104:MET:HB3	1.79	0.45
27:S:111:GLU:HG3	36:b:19:LEU:HD21	1.98	0.45
29:U:40:VAL:HB	29:U:97:VAL:HG22	1.98	0.45
39:e:53:LEU:O	39:e:158:VAL:HA	2.15	0.45
40:f:100:MET:HB3	40:f:153:HIS:CD2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:70:VAL:HG22	50:q:71:VAL:N	2.32	0.45
8:7:178:ALA:HB2	8:7:320:SER:HB2	1.99	0.45
10:9:136:LEU:HD23	29:U:19:VAL:HB	1.99	0.45
11:A:1720:C:H4'	11:A:1909:A:H2	1.82	0.45
11:A:2235:C:H2'	11:A:2236:C:O4'	2.17	0.45
11:A:3024:U:H2'	11:A:3025:A:C8	2.51	0.45
11:A:3139:G:H2'	11:A:3140:A:C8	2.51	0.45
11:A:3198:A:H2'	11:A:3198:A:N3	2.31	0.45
18:J:58:LYS:HD2	18:J:58:LYS:HA	1.76	0.45
21:M:264:GLN:NE2	21:M:267:PHE:O	2.49	0.45
27:S:115:LEU:HB3	36:b:118:PRO:HB2	1.98	0.45
38:d:76:ILE:HD12	38:d:76:ILE:N	2.31	0.45
41:g:85:PHE:O	41:g:114:GLU:N	2.47	0.45
41:g:122:LYS:NZ	41:g:126:ASP:OD2	2.49	0.45
42:h:148:LEU:HD22	42:h:152:LEU:HD22	1.98	0.45
45:k:7:ARG:NH1	45:k:7:ARG:HA	2.31	0.45
51:r:83:TYR:OH	51:r:150:TYR:HB2	2.17	0.45
1:0:104:LYS:HE2	1:0:104:LYS:HB3	1.71	0.45
1:0:108:ASP:OD2	1:0:108:ASP:N	2.50	0.45
11:A:1745:U:H5'	32:X:55:LYS:HE2	1.99	0.45
11:A:2225:C:H2'	11:A:2226:U:C6	2.52	0.45
11:A:2315:A:H1'	11:A:2357:C:N4	2.32	0.45
11:A:2728:C:H2'	11:A:2729:U:C6	2.52	0.45
15:F:160:SER:HB3	43:i:80:LEU:HD13	1.99	0.45
16:H:95:GLU:HA	16:H:113:SER:HA	1.98	0.45
21:M:263:ARG:HD2	49:p:43:TYR:HD2	1.81	0.45
25:Q:92:PHE:O	25:Q:96:ARG:HB2	2.16	0.45
25:Q:182:ARG:HG3	25:Q:187:LEU:HD11	1.97	0.45
33:Y:236:LYS:HE3	33:Y:236:LYS:HB3	1.82	0.45
42:h:91:LEU:HD21	42:h:100:LEU:HD23	1.99	0.45
45:k:17:ARG:NH1	45:k:65:ASP:HB3	2.32	0.45
52:s:43:ARG:NH1	52:s:43:ARG:HB2	2.32	0.45
52:s:365:LYS:HB2	52:s:402:TYR:CZ	2.51	0.45
11:A:2635:G:H2'	11:A:2636:G:H8	1.82	0.45
16:H:99:THR:O	16:H:108:ARG:NH1	2.50	0.45
23:O:41:ARG:NH2	23:O:131:PRO:O	2.34	0.45
26:R:138:PRO:O	26:R:139:GLU:HG3	2.16	0.45
29:U:112:PRO:HA	29:U:113:GLU:HA	1.68	0.45
30:V:84:ASN:HB3	30:V:117:HIS:CD2	2.51	0.45
1:0:133:GLU:OE2	1:0:177:ARG:NH1	2.50	0.45
6:5:72:PRO:HG2	6:5:74:PHE:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:112:LEU:HD13	6:5:118:GLN:HB3	1.98	0.45
11:A:2072:A:H2'	11:A:2073:A:C8	2.52	0.45
12:B:1605:A:H2'	12:B:1606:G:C8	2.52	0.45
19:K:100:PRO:HB2	19:K:129:PRO:HB3	1.99	0.45
24:P:178:ILE:HG22	24:P:179:TYR:HD1	1.81	0.45
30:V:33:ARG:HG3	30:V:33:ARG:NH1	2.32	0.45
36:b:2:THR:HG22	36:b:5:GLY:H	1.81	0.45
52:s:369:PHE:HE1	52:s:421:ILE:HG12	1.82	0.45
6:5:156:VAL:HG22	6:5:182:ASN:HB3	1.98	0.45
6:5:176:CYS:O	6:5:180:VAL:HG23	2.16	0.45
7:6:360:ARG:NH1	11:A:2869:A:N7	2.58	0.45
11:A:1799:U:H2'	11:A:1800:G:O4'	2.16	0.45
11:A:1926:A:H2	11:A:1978:A:N1	2.15	0.45
11:A:2666:U:H2'	11:A:2667:U:O4'	2.17	0.45
12:B:1665:C:H2'	12:B:1666:U:C6	2.52	0.45
13:D:194:ASN:OD1	13:D:243:THR:OG1	2.33	0.45
15:F:252:SER:O	15:F:256:HIS:ND1	2.49	0.45
25:Q:170:ARG:NH2	58:Q:309:HOH:O	2.50	0.45
36:b:65:VAL:HB	42:h:154:ILE:HD13	1.98	0.45
37:c:207:GLY:O	37:c:211:THR:HG23	2.16	0.45
39:e:45:TRP:HE1	39:e:230:LYS:HB2	1.82	0.45
41:g:96:VAL:HG22	41:g:110:ILE:HG12	1.98	0.45
7:6:219:THR:HG21	7:6:298:PHE:CE2	2.52	0.45
8:7:158:PHE:N	35:a:90:GLN:HE21	2.15	0.45
11:A:1934:U:N3	11:A:1935:A:O2'	2.49	0.45
11:A:2584:C:H2'	11:A:2585:G:C8	2.52	0.45
11:A:3067:U:H5''	14:E:232:GLY:O	2.17	0.45
58:A:3547:HOH:O	16:H:72:ARG:NH2	2.50	0.45
14:E:135:LYS:NZ	14:E:141:LYS:O	2.46	0.45
20:L:138:LEU:HD23	20:L:144:PHE:CE2	2.51	0.45
22:N:172:VAL:HA	22:N:175:PHE:CE2	2.52	0.45
27:S:84:ASN:O	27:S:88:VAL:HG13	2.17	0.45
30:V:137:PHE:CE1	30:V:143:ARG:HB2	2.52	0.45
36:b:19:LEU:HA	36:b:19:LEU:HD23	1.63	0.45
37:c:60:ARG:NH1	37:c:63:LYS:HB2	2.32	0.45
39:e:79:ILE:HG23	47:m:50:ARG:NH2	2.32	0.45
6:5:124:LYS:HG2	6:5:370:LYS:HG3	1.99	0.44
7:6:171:VAL:HG12	7:6:314:ALA:HB1	1.99	0.44
11:A:1719:G:H2'	11:A:1720:C:H6	1.82	0.44
11:A:2146:A:N6	36:b:117:LYS:HB2	2.32	0.44
11:A:2807:U:H2'	11:A:2808:U:C6	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:90:TRP:HD1	14:E:316:PHE:CD1	2.35	0.44
14:E:94:SER:HB2	14:E:316:PHE:CZ	2.52	0.44
15:F:52:GLU:N	15:F:52:GLU:OE2	2.50	0.44
17:I:190:GLY:HA2	17:I:193:ASN:HD21	1.82	0.44
22:N:135:SER:O	22:N:138:HIS:HB2	2.17	0.44
31:W:108:PRO:HA	31:W:114:VAL:HG11	1.99	0.44
33:Y:228:ARG:NH1	58:Y:305:HOH:O	2.50	0.44
36:b:136:LYS:O	37:c:259:ARG:NH2	2.49	0.44
52:s:271:LEU:HD23	52:s:273:LEU:HG	2.00	0.44
1:0:160:TYR:HB3	1:0:179:ARG:O	2.18	0.44
6:5:68:PRO:HG2	6:5:69:TRP:CE2	2.52	0.44
6:5:294:ASP:HB2	6:5:347:ASP:HA	1.99	0.44
7:6:139:TRP:O	7:6:144:GLY:N	2.50	0.44
9:8:128:GLU:HA	9:8:131:MET:HE3	1.98	0.44
11:A:2186:C:O2'	11:A:2187:C:OP1	2.31	0.44
11:A:2605:C:OP2	11:A:2606:U:O2'	2.30	0.44
11:A:2669:A:H2'	11:A:2670:C:C6	2.52	0.44
13:D:73:THR:HG22	13:D:106:MET:HE3	1.99	0.44
22:N:101:HIS:NE2	22:N:184:PRO:HG3	2.32	0.44
25:Q:283:TRP:HA	25:Q:286:ILE:HG22	2.00	0.44
25:Q:288:ALA:HA	25:Q:291:ARG:HD2	1.99	0.44
27:S:164:THR:OG1	27:S:165:GLU:N	2.50	0.44
29:U:130:LEU:HD12	30:V:107:THR:HG21	1.98	0.44
30:V:80:ILE:HB	30:V:85:TRP:HB2	1.98	0.44
39:e:45:TRP:HD1	39:e:229:ALA:HA	1.80	0.44
39:e:238:LEU:HD12	39:e:238:LEU:O	2.17	0.44
52:s:110:THR:HG23	52:s:333:PHE:CD1	2.53	0.44
6:5:208:PHE:O	6:5:222:ARG:HA	2.18	0.44
11:A:2801:A:H2'	11:A:2802:A:C8	2.52	0.44
11:A:3128:A:O2'	11:A:3129:A:O5'	2.35	0.44
11:A:3204:C:H5'	14:E:298:LYS:NZ	2.32	0.44
12:B:1605:A:H2'	12:B:1606:G:H8	1.82	0.44
12:B:1612:C:H2'	12:B:1613:U:C6	2.52	0.44
13:D:202:ARG:NE	13:D:205:GLN:OE1	2.44	0.44
13:D:237:LEU:HD23	13:D:237:LEU:HA	1.88	0.44
24:P:127:SER:O	24:P:131:VAL:HG22	2.17	0.44
39:e:61:LYS:HE3	58:e:304:HOH:O	2.17	0.44
8:7:146:CYS:O	8:7:278:TYR:OH	2.34	0.44
11:A:1803:A:H4'	11:A:1804:A:H3'	1.99	0.44
11:A:2313:A:H2'	11:A:2314:C:C6	2.52	0.44
11:A:2532:U:H2'	11:A:2533:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2798:A:H2'	11:A:2799:U:C6	2.53	0.44
11:A:3151:A:N1	11:A:3152:C:N4	2.66	0.44
12:B:1623:G:H2'	12:B:1624:C:O4'	2.18	0.44
15:F:53:LEU:HG	15:F:274:LEU:HD12	2.00	0.44
16:H:108:ARG:NH2	16:H:143:GLU:OE1	2.50	0.44
17:I:108:ASP:O	17:I:112:MET:SD	2.75	0.44
18:J:89:TYR:OH	58:J:201:HOH:O	2.19	0.44
22:N:130:PRO:HB2	22:N:147:ILE:HG12	1.98	0.44
23:O:38:ARG:NH2	23:O:84:ASP:OD1	2.50	0.44
33:Y:226:LEU:O	33:Y:230:LYS:HG2	2.18	0.44
46:l:93:PRO:HG2	46:l:95:TRP:CZ2	2.53	0.44
50:q:84:GLU:HA	50:q:84:GLU:OE2	2.17	0.44
52:s:346:TRP:CH2	52:s:348:GLU:HB2	2.53	0.44
1:0:95:ARG:NH2	11:A:1818:A:OP1	2.50	0.44
6:5:81:TYR:HD1	29:U:11:ARG:NH2	2.16	0.44
6:5:211:THR:N	6:5:274:ASN:OD1	2.37	0.44
6:5:379:GLN:OE1	6:5:412:LYS:NZ	2.47	0.44
7:6:152:ALA:HB2	7:6:316:LEU:HD21	1.99	0.44
8:7:204:LYS:NZ	58:7:416:HOH:O	2.50	0.44
10:9:39:LYS:HD2	29:U:7:TYR:CG	2.52	0.44
11:A:2174:G:H22	18:J:102:ARG:CZ	2.30	0.44
12:B:1643:A:H61	24:P:88:HIS:HE1	1.65	0.44
30:V:72:LYS:HG3	30:V:91:LEU:HD13	1.99	0.44
32:X:175:GLN:H	32:X:184:ARG:HD3	1.82	0.44
34:Z:85:ILE:HG13	34:Z:112:VAL:HG11	1.99	0.44
39:e:79:ILE:HG23	47:m:50:ARG:HH22	1.82	0.44
49:p:189:ARG:NE	58:p:313:HOH:O	2.50	0.44
54:TA:74:LEU:HD23	54:TA:74:LEU:HA	1.81	0.44
6:5:212:TRP:HZ3	6:5:221:VAL:HG12	1.83	0.44
7:6:217:LEU:HD11	7:6:298:PHE:CZ	2.53	0.44
11:A:1809:U:N3	11:A:1810:A:O2'	2.51	0.44
11:A:2669:A:H2'	11:A:2670:C:H6	1.83	0.44
11:A:2905:A:H2'	11:A:2906:C:C6	2.52	0.44
11:A:2991:U:C5	57:A:3400:ZLD:H8	2.52	0.44
12:B:1604:G:H2'	12:B:1605:A:C8	2.52	0.44
14:E:147:VAL:HB	14:E:179:PHE:HE1	1.83	0.44
14:E:222:TRP:CD1	14:E:256:LYS:HB3	2.53	0.44
17:I:147:PHE:HB3	58:I:327:HOH:O	2.17	0.44
20:L:81:LYS:HE3	20:L:81:LYS:HB2	1.66	0.44
31:W:101:LYS:HD2	40:f:56:ILE:HG21	2.00	0.44
40:f:162:LEU:HB3	40:f:167:ALA:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:122:THR:HG23	49:p:123:HIS:CD2	2.52	0.44
52:s:89:MET:HE3	52:s:89:MET:HB3	1.85	0.44
52:s:316:CYS:HB3	52:s:319:GLN:HB2	2.00	0.44
7:6:262:GLY:HA3	7:6:342:PHE:O	2.17	0.44
8:7:106:ALA:O	8:7:112:PRO:HA	2.18	0.44
8:7:181:TYR:OH	8:7:262:ASP:OD2	2.36	0.44
8:7:225:VAL:HA	8:7:228:GLU:HG2	2.00	0.44
8:7:238:ASP:OD1	8:7:238:ASP:C	2.60	0.44
11:A:2056:G:H2'	11:A:2057:C:H6	1.83	0.44
11:A:2674:U:OP1	28:T:112:LYS:NZ	2.39	0.44
11:A:2748:A:H2'	11:A:2749:A:C8	2.53	0.44
14:E:148:GLY:HA3	14:E:173:LYS:HG3	1.99	0.44
18:J:180:GLU:O	18:J:183:LEU:HG	2.18	0.44
32:X:30:ARG:NH2	58:X:301:HOH:O	2.36	0.44
37:c:312:ARG:HA	37:c:312:ARG:HD3	1.79	0.44
43:i:78:ILE:HD12	43:i:78:ILE:HA	1.90	0.44
45:k:77:ARG:HD2	51:r:50:GLU:OE2	2.18	0.44
4:3:164:SER:HA	4:3:167:LYS:HG3	1.99	0.44
10:9:27:PRO:HD2	10:9:30:PHE:CG	2.53	0.44
10:9:123:GLN:HE21	10:9:130:LEU:H	1.64	0.44
12:B:1664:G:H2'	12:B:1665:C:H6	1.83	0.44
15:F:227:PRO:HG2	15:F:230:ILE:HG22	1.98	0.44
25:Q:189:TYR:CG	25:Q:243:ILE:HD11	2.52	0.44
25:Q:196:GLU:HA	25:Q:199:THR:HG22	2.00	0.44
25:Q:244:ARG:HE	25:Q:244:ARG:HB3	1.55	0.44
33:Y:95:ASN:OD1	33:Y:149:ARG:NH1	2.50	0.44
42:h:116:ARG:HG3	42:h:116:ARG:HH11	1.82	0.44
43:i:87:GLU:OE1	43:i:117:LEU:HD11	2.18	0.44
45:k:58:ASP:CG	54:TA:53:LEU:HD11	2.43	0.44
50:q:128:MET:O	50:q:129:PRO:C	2.61	0.44
54:TB:74:LEU:HD23	54:TB:79:ILE:HG12	1.99	0.44
7:6:173:LEU:HD21	7:6:175:VAL:HG13	1.99	0.44
8:7:167:VAL:HB	8:7:182:ASP:HB2	1.99	0.44
11:A:2530:A:H4'	11:A:2531:U:C5'	2.42	0.44
11:A:2967:C:H2'	11:A:2968:A:O4'	2.18	0.44
11:A:3152:C:OP1	25:Q:141:SER:OG	2.22	0.44
12:B:1632:U:H1'	12:B:1636:A:N6	2.33	0.44
15:F:130:GLN:NE2	15:F:137:ARG:HD2	2.33	0.44
23:O:141:HIS:HD2	23:O:146:ASN:HB3	1.83	0.44
25:Q:268:ASP:C	25:Q:270:MET:H	2.26	0.44
26:R:122:ARG:HH22	27:S:72:GLU:CD	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:203:PRO:C	33:Y:205:VAL:H	2.25	0.44
37:c:98:ILE:O	37:c:102:GLU:HG2	2.18	0.44
37:c:279:LYS:HE3	37:c:279:LYS:HB3	1.77	0.44
52:s:237:PRO:HB3	52:s:300:HIS:CE1	2.53	0.44
11:A:1702:A:HO2'	11:A:1704:U:H5	1.65	0.43
11:A:2131:A:OP1	48:o:23:ARG:NH2	2.32	0.43
11:A:2579:C:H2'	11:A:2580:U:C1'	2.47	0.43
11:A:3174:U:H2'	11:A:3175:A:C8	2.53	0.43
13:D:293:LYS:HE3	13:D:293:LYS:HB3	1.61	0.43
19:K:20:LEU:HB2	19:K:141:LEU:HD13	2.00	0.43
19:K:26:GLN:HE21	19:K:148:PRO:CD	2.31	0.43
21:M:236:LEU:HD23	21:M:236:LEU:HA	1.85	0.43
21:M:268:GLY:HA3	41:g:47:PHE:CG	2.53	0.43
23:O:57:GLU:HA	23:O:104:TYR:HE1	1.81	0.43
30:V:192:LYS:HG3	30:V:196:GLU:HB2	2.00	0.43
34:Z:71:ARG:HB2	34:Z:91:LEU:HB3	1.99	0.43
39:e:256:THR:O	39:e:260:LEU:HB2	2.16	0.43
42:h:143:LEU:HD12	42:h:143:LEU:HA	1.88	0.43
52:s:332:LEU:HD13	52:s:372:TYR:HB2	2.00	0.43
1:O:113:CYS:SG	1:O:115:HIS:HB2	2.58	0.43
7:6:268:LEU:HB2	7:6:319:PHE:CE1	2.53	0.43
11:A:2283:C:O2	37:c:43:LYS:NZ	2.45	0.43
11:A:2495:U:O4	11:A:2509:A:H2	2.00	0.43
11:A:2802:A:H2'	11:A:2803:A:O4'	2.18	0.43
11:A:3112:A:HO2'	11:A:3168:C:HO2'	1.57	0.43
13:D:90:ARG:NH1	58:D:504:HOH:O	2.38	0.43
13:D:124:GLU:HB3	13:D:142:VAL:CG1	2.48	0.43
15:F:268:PHE:O	15:F:272:LYS:HG2	2.17	0.43
58:F:401:HOH:O	42:h:114:ASN:O	2.21	0.43
18:J:60:ILE:HG22	18:J:62:GLU:H	1.83	0.43
24:P:86:THR:HG22	24:P:87:GLN:H	1.82	0.43
29:U:64:PRO:HB2	29:U:100:ALA:HB3	1.99	0.43
33:Y:171:ASP:HB3	33:Y:177:ILE:HD13	2.01	0.43
42:h:49:ILE:HG23	42:h:50:LEU:HG	1.99	0.43
43:i:79:TRP:O	43:i:93:ARG:NE	2.47	0.43
45:k:78:GLY:HA3	45:k:86:MET:HE1	1.99	0.43
8:7:121:LYS:HD3	8:7:121:LYS:N	2.33	0.43
11:A:1929:A:H2'	11:A:1930:C:C6	2.53	0.43
17:I:127:PRO:HG2	17:I:130:VAL:HG22	2.01	0.43
17:I:171:VAL:HB	17:I:174:LEU:HD13	2.00	0.43
21:M:109:ARG:NH2	41:g:91:MET:HE3	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:68:TRP:C	24:P:70:THR:H	2.22	0.43
27:S:94:ARG:HA	27:S:94:ARG:HD3	1.88	0.43
30:V:100:LYS:HA	30:V:105:ARG:HG3	2.00	0.43
38:d:61:ARG:HD3	38:d:61:ARG:HA	1.81	0.43
39:e:64:THR:HB	39:e:67:GLN:HB2	1.99	0.43
49:p:72:ILE:HD11	49:p:155:ARG:HG2	2.00	0.43
51:r:44:GLY:O	51:r:45:LYS:HG2	2.18	0.43
52:s:94:TYR:O	52:s:106:TYR:OH	2.34	0.43
1:0:94:ARG:HA	1:0:99:LYS:HD2	2.00	0.43
1:0:167:GLU:HA	1:0:170:GLN:NE2	2.33	0.43
6:5:47:ASP:HB2	6:5:49:VAL:HG12	2.00	0.43
8:7:225:VAL:O	8:7:228:GLU:HG3	2.18	0.43
11:A:1762:A:H62	50:q:63:ARG:NH2	2.15	0.43
13:D:74:ILE:HD13	13:D:150:TRP:CD1	2.53	0.43
13:D:220:VAL:HG12	13:D:221:ASN:N	2.29	0.43
16:H:94:LEU:CD2	16:H:116:LYS:HA	2.48	0.43
18:J:64:ILE:HG23	18:J:89:TYR:CE2	2.54	0.43
18:J:111:LEU:HD22	18:J:166:ALA:HB1	2.00	0.43
27:S:94:ARG:O	36:b:126:ILE:HG12	2.18	0.43
32:X:51:LYS:O	32:X:60:GLU:HG3	2.18	0.43
33:Y:170:ARG:NH1	33:Y:201:ALA:HB2	2.33	0.43
50:q:132:ILE:O	50:q:133:VAL:C	2.61	0.43
10:9:109:PHE:CD1	10:9:109:PHE:C	2.96	0.43
11:A:1806:U:H4'	11:A:1807:U:O5'	2.19	0.43
11:A:2003:A:OP2	11:A:2734:A:O2'	2.35	0.43
11:A:2491:C:H2'	11:A:2492:G:C8	2.52	0.43
11:A:3056:C:H2'	11:A:3057:C:C6	2.52	0.43
17:I:85:GLU:O	17:I:89:VAL:HG22	2.19	0.43
17:I:153:LEU:HD13	17:I:155:VAL:HG13	2.00	0.43
19:K:7:ALA:HB3	19:K:8:PRO:HD3	1.99	0.43
33:Y:186:ILE:HD12	33:Y:190:LEU:HD12	2.00	0.43
38:d:265:ILE:HD12	38:d:265:ILE:HA	1.84	0.43
39:e:216:LYS:HE3	39:e:216:LYS:HB3	1.68	0.43
4:3:116:ARG:HG3	4:3:122:TRP:CE2	2.54	0.43
6:5:125:THR:HG21	6:5:356:PHE:CE1	2.53	0.43
9:8:156:LYS:H	9:8:156:LYS:HD2	1.83	0.43
11:A:1851:G:H2'	11:A:2693:A:N7	2.33	0.43
11:A:1950:U:H2'	11:A:1951:C:C6	2.53	0.43
11:A:2085:A:H2'	11:A:2086:A:C8	2.53	0.43
11:A:2699:C:H2'	11:A:2700:G:H8	1.84	0.43
11:A:2894:U:H5''	11:A:2895:U:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:275:ARG:HD3	14:E:331:ASP:OD1	2.19	0.43
16:H:53:THR:N	16:H:86:THR:HB	2.32	0.43
18:J:66:LEU:HD23	18:J:67:PRO:O	2.17	0.43
24:P:54:ARG:NH1	24:P:57:GLU:OE2	2.52	0.43
29:U:60:ILE:HD13	33:Y:106:LEU:HD21	2.01	0.43
30:V:129:LYS:HD3	30:V:129:LYS:HA	1.83	0.43
31:W:120:LEU:HD23	40:f:63:ILE:HG23	2.00	0.43
38:d:186:VAL:HG21	38:d:239:PRO:HB3	1.99	0.43
58:f:201:HOH:O	53:u:104:UNK:O	2.21	0.43
11:A:2410:U:H2'	11:A:2411:U:C6	2.50	0.43
14:E:109:LEU:HD21	14:E:337:VAL:HG22	2.00	0.43
16:H:95:GLU:OE1	16:H:95:GLU:C	2.62	0.43
26:R:44:ARG:NH1	58:R:207:HOH:O	2.52	0.43
30:V:99:GLY:O	30:V:105:ARG:HG3	2.18	0.43
30:V:115:LEU:HD23	30:V:115:LEU:HA	1.91	0.43
32:X:38:PRO:HB3	32:X:151:GLU:O	2.19	0.43
42:h:55:LEU:HD12	42:h:56:ARG:H	1.83	0.43
50:q:123:GLU:HG2	50:q:127:LYS:HD2	2.01	0.43
51:r:103:LYS:HD2	51:r:104:ILE:HG12	2.00	0.43
54:TA:64:ILE:HG23	58:TB:216:HOH:O	2.19	0.43
2:1:19:ARG:HH12	11:A:2905:A:H61	1.67	0.43
7:6:52:ARG:CZ	7:6:56:ARG:HH22	2.31	0.43
9:8:169:PHE:HE2	40:f:188:GLU:HB2	1.84	0.43
11:A:1737:A:N6	11:A:1760:G:H1'	2.34	0.43
11:A:1884:G:N7	15:F:281:ARG:HD2	2.34	0.43
11:A:2315:A:HO2'	11:A:2316:U:H6	1.66	0.43
11:A:2365:U:H2'	11:A:2366:G:C8	2.54	0.43
11:A:3204:C:H5'	14:E:298:LYS:HZ3	1.83	0.43
14:E:268:GLU:HG2	14:E:271:LEU:HD11	2.01	0.43
17:I:94:ARG:HH12	17:I:181:ILE:HG22	1.83	0.43
20:L:72:GLN:NE2	20:L:134:TYR:OH	2.39	0.43
20:L:123:ILE:O	20:L:144:PHE:HA	2.19	0.43
34:Z:84:ASP:O	34:Z:88:MET:HG3	2.19	0.43
34:Z:99:VAL:HG21	44:j:77:VAL:HG22	1.99	0.43
35:a:83:ASN:HB3	35:a:95:ARG:HH11	1.84	0.43
37:c:148:MET:HE2	37:c:305:TYR:HB3	2.00	0.43
41:g:63:HIS:HB2	41:g:66:TYR:CE1	2.54	0.43
42:h:58:ARG:HB2	42:h:136:ASP:CG	2.44	0.43
7:6:45:LEU:HD21	40:f:64:LYS:HB3	2.01	0.43
7:6:141:ARG:HG3	7:6:141:ARG:NH1	2.32	0.43
11:A:1828:A:H4'	11:A:1829:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1883:G:C5'	41:g:91:MET:HE2	2.48	0.43
11:A:2585:G:H2'	11:A:2586:U:O4'	2.19	0.43
11:A:2960:U:H3'	11:A:2962:C:H41	1.84	0.43
22:N:170:GLU:O	22:N:173:GLN:HG3	2.19	0.43
28:T:203:LEU:O	28:T:206:ARG:HG2	2.19	0.43
30:V:72:LYS:HB2	38:d:256:TYR:CZ	2.54	0.43
39:e:156:ASN:HB3	58:e:445:HOH:O	2.18	0.43
41:g:121:GLN:O	41:g:125:GLU:HG3	2.18	0.43
7:6:87:LYS:HB2	7:6:166:THR:HG22	2.00	0.43
9:8:178:TYR:HB2	47:m:63:THR:HB	2.00	0.43
11:A:2032:G:N7	58:A:3647:HOH:O	2.37	0.43
11:A:3165:C:H2'	11:A:3166:U:C6	2.54	0.43
14:E:90:TRP:CH2	14:E:92:PRO:HA	2.54	0.43
18:J:135:VAL:CG1	18:J:139:SER:HB2	2.49	0.43
25:Q:205:LYS:HA	25:Q:205:LYS:HD2	1.78	0.43
27:S:67:PRO:HG2	27:S:72:GLU:OE1	2.19	0.43
39:e:147:THR:HG23	39:e:252:HIS:O	2.19	0.43
1:0:95:ARG:HG3	28:T:88:TRP:CH2	2.54	0.42
4:3:165:PHE:O	4:3:168:ARG:HG2	2.18	0.42
6:5:336:GLU:H	6:5:336:GLU:CD	2.25	0.42
11:A:2628:U:H4'	11:A:2629:A:O5'	2.16	0.42
13:D:154:THR:C	13:D:248:SER:HB3	2.44	0.42
14:E:199:ARG:HD3	14:E:199:ARG:HA	1.74	0.42
15:F:81:ASP:OD1	15:F:81:ASP:C	2.61	0.42
17:I:176:LEU:HD13	17:I:178:GLY:H	1.84	0.42
19:K:6:ARG:HH12	37:c:230:GLU:CD	2.27	0.42
24:P:175:PRO:HG3	49:p:177:ARG:HD2	2.01	0.42
33:Y:86:THR:HG22	33:Y:88:GLN:H	1.83	0.42
39:e:67:GLN:NE2	47:m:40:LEU:HD23	2.31	0.42
40:f:135:LEU:HD23	40:f:135:LEU:H	1.84	0.42
52:s:175:PRO:HA	52:s:178:ASP:OD1	2.19	0.42
7:6:178:ALA:HA	49:p:194:HIS:CD2	2.54	0.42
11:A:1749:C:OP2	11:A:2899:C:O2'	2.36	0.42
11:A:1771:C:OP1	26:R:11:ARG:HG2	2.19	0.42
11:A:2610:U:H2'	11:A:2611:C:C6	2.52	0.42
11:A:3008:C:C2	11:A:3032:G:N2	2.87	0.42
11:A:3191:A:C2	51:r:133:PRO:HB3	2.53	0.42
17:I:146:LEU:HD23	17:I:146:LEU:O	2.20	0.42
18:J:65:PRO:HD2	18:J:89:TYR:HE2	1.82	0.42
21:M:91:ARG:HG2	21:M:136:TYR:CE1	2.54	0.42
35:a:70:GLU:HA	36:b:141:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:238:VAL:HG12	38:d:240:LYS:HG2	2.01	0.42
50:q:162:GLU:HA	50:q:163:LEU:HA	1.78	0.42
52:s:162:ARG:HB2	52:s:163:VAL:C	2.44	0.42
1:0:159:LEU:HD13	1:0:163:GLU:O	2.19	0.42
7:6:139:TRP:NE1	7:6:144:GLY:HA2	2.34	0.42
7:6:225:LEU:HB3	24:P:44:VAL:HA	2.00	0.42
11:A:2167:A:N6	11:A:2211:U:H5'	2.34	0.42
11:A:2989:G:O2'	11:A:2990:A:OP2	2.33	0.42
11:A:3050:U:H1'	11:A:3053:A:N6	2.34	0.42
18:J:69:LYS:NZ	58:J:212:HOH:O	2.36	0.42
24:P:156:ASP:OD1	24:P:156:ASP:N	2.52	0.42
31:W:111:THR:HA	31:W:114:VAL:HG22	2.01	0.42
34:Z:75:THR:O	34:Z:83:LYS:HE3	2.19	0.42
39:e:269:LEU:O	39:e:272:VAL:HG22	2.19	0.42
40:f:179:PRO:O	40:f:179:PRO:HD2	2.19	0.42
41:g:79:PRO:HB3	41:g:85:PHE:HE1	1.85	0.42
42:h:62:PRO:HD3	42:h:133:PRO:HB3	2.00	0.42
44:j:88:LEU:HD12	44:j:88:LEU:HA	1.75	0.42
45:k:9:GLY:C	45:k:11:ARG:H	2.26	0.42
47:m:69:ARG:HG2	47:m:70:GLU:N	2.32	0.42
52:s:270:LYS:NZ	58:s:510:HOH:O	2.39	0.42
52:s:411:LYS:HD2	52:s:411:LYS:HA	1.71	0.42
54:TA:88:LYS:C	54:TA:88:LYS:HD3	2.44	0.42
10:9:128:PHE:HZ	30:V:199:MET:HE3	1.84	0.42
11:A:2872:C:O2'	31:W:88:CYS:SG	2.74	0.42
12:B:1638:U:H2'	12:B:1639:U:H6	1.84	0.42
14:E:94:SER:HB2	14:E:316:PHE:HZ	1.84	0.42
18:J:157:LYS:HE2	18:J:157:LYS:HB2	1.70	0.42
19:K:142:VAL:HG12	19:K:143:GLU:HB2	2.00	0.42
23:O:86:ILE:HB	23:O:87:PRO:HD3	2.01	0.42
32:X:41:VAL:HG11	32:X:83:GLU:HB3	2.01	0.42
32:X:79:LEU:HB2	32:X:125:VAL:HG11	2.00	0.42
33:Y:193:ARG:HG3	33:Y:196:ARG:NH2	2.34	0.42
39:e:160:LEU:HA	39:e:174:PRO:HD3	2.00	0.42
45:k:56:ARG:NH1	45:k:61:GLU:H	2.13	0.42
49:p:191:LYS:HB2	49:p:192:ARG:H	1.52	0.42
50:q:81:GLN:O	50:q:85:LEU:HD13	2.19	0.42
51:r:62:ASN:O	51:r:62:ASN:ND2	2.52	0.42
51:r:89:LEU:HB3	51:r:119:VAL:HG23	2.01	0.42
7:6:141:ARG:HG3	7:6:142:THR:HG23	2.02	0.42
7:6:150:ARG:O	7:6:153:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:226:LEU:HD23	7:6:226:LEU:H	1.85	0.42
10:9:17:ARG:HB2	10:9:18:MET:HE2	2.01	0.42
10:9:54:LYS:HA	10:9:54:LYS:HD2	1.95	0.42
11:A:2146:A:OP2	26:R:61:LYS:HE3	2.18	0.42
11:A:2847:C:H2'	11:A:2848:A:O4'	2.19	0.42
11:A:3113:A:H2'	11:A:3114:U:H6	1.84	0.42
11:A:3128:A:O2'	11:A:3129:A:H8	2.03	0.42
14:E:248:ILE:HG23	14:E:250:ARG:H	1.84	0.42
16:H:122:ARG:HA	16:H:122:ARG:HD3	1.74	0.42
18:J:75:ASP:OD1	18:J:75:ASP:N	2.53	0.42
28:T:94:ILE:HG23	28:T:142:ILE:HD13	2.01	0.42
32:X:51:LYS:HE2	32:X:51:LYS:HB2	1.71	0.42
39:e:47:LEU:HD23	39:e:178:TRP:CE3	2.55	0.42
41:g:62:LYS:NZ	58:g:304:HOH:O	2.52	0.42
4:3:100:ARG:HB2	11:A:1742:G:O6	2.20	0.42
7:6:259:PRO:HG3	7:6:321:CYS:SG	2.60	0.42
8:7:215:PRO:HG3	8:7:271:ARG:NH2	2.35	0.42
9:8:136:ILE:HA	9:8:139:MET:HE2	2.01	0.42
11:A:2455:U:H2'	11:A:2456:U:C6	2.54	0.42
12:B:1628:C:C2	12:B:1629:A:C8	3.07	0.42
15:F:94:ASP:OD2	15:F:94:ASP:C	2.61	0.42
18:J:81:LYS:HD3	18:J:81:LYS:HA	1.76	0.42
23:O:108:LEU:HD11	23:O:135:LEU:HD23	2.01	0.42
31:W:51:GLN:HG2	31:W:69:THR:HG22	2.00	0.42
33:Y:197:LYS:HD2	33:Y:199:PHE:CZ	2.55	0.42
38:d:117:ALA:O	38:d:120:VAL:HG12	2.20	0.42
46:l:120:ARG:O	46:l:124:GLN:HG2	2.19	0.42
6:5:108:HIS:CE1	6:5:109:ARG:HG3	2.55	0.42
6:5:172:ARG:NH2	11:A:2395:A:OP1	2.36	0.42
6:5:229:LEU:HD23	6:5:229:LEU:HA	1.93	0.42
7:6:53:SER:OG	7:6:56:ARG:HD3	2.20	0.42
7:6:92:LEU:HD12	7:6:170:ARG:HB2	2.01	0.42
8:7:315:LYS:HB3	23:O:152:LEU:HD11	2.01	0.42
11:A:2087:U:H2'	11:A:2088:U:C6	2.54	0.42
11:A:2349:G:N2	11:A:2353:A:N1	2.68	0.42
11:A:3117:C:H2'	11:A:3118:U:C6	2.55	0.42
11:A:3119:C:H2'	11:A:3120:C:C6	2.55	0.42
12:B:1666:U:H2'	12:B:1667:C:C6	2.54	0.42
13:D:184:LEU:HD21	13:D:193:ILE:HD13	2.02	0.42
14:E:324:ASP:N	14:E:324:ASP:OD1	2.53	0.42
15:F:59:ARG:O	15:F:84:PRO:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:105:LYS:HG2	19:K:122:MET:HE1	2.01	0.42
22:N:36:VAL:HG13	46:l:128:ARG:HG3	2.01	0.42
39:e:214:THR:HG23	39:e:230:LYS:HZ1	1.84	0.42
47:m:77:MET:HA	47:m:78:PRO:HD3	1.90	0.42
51:r:188:SER:C	51:r:190:THR:H	2.27	0.42
8:7:52:LYS:HE3	8:7:52:LYS:HB3	1.80	0.42
11:A:1919:C:H2'	11:A:1920:U:O4'	2.19	0.42
11:A:3148:C:O2'	11:A:3149:C:H5'	2.19	0.42
13:D:162:THR:O	13:D:163:ILE:HD13	2.20	0.42
21:M:274:VAL:HB	21:M:283:LEU:HB2	2.02	0.42
23:O:100:GLN:H	23:O:100:GLN:HG2	1.67	0.42
24:P:134:GLN:O	24:P:138:GLU:HG3	2.20	0.42
24:P:159:LYS:NZ	24:P:159:LYS:HB3	2.34	0.42
25:Q:290:LYS:HE2	25:Q:290:LYS:HB2	1.76	0.42
32:X:237:GLN:NE2	32:X:237:GLN:HA	2.33	0.42
38:d:168:CYS:HB3	38:d:262:HIS:O	2.19	0.42
38:d:189:LEU:HD23	38:d:189:LEU:HA	1.94	0.42
49:p:128:ASN:CG	49:p:129:ARG:N	2.77	0.42
6:5:207:THR:HA	6:5:223:GLY:O	2.20	0.42
11:A:1800:G:N1	11:A:1803:A:OP2	2.52	0.42
11:A:1893:A:H4'	11:A:1894:G:H5'	2.01	0.42
11:A:2037:U:H4'	11:A:2040:G:N1	2.35	0.42
11:A:2503:A:H5'	11:A:3095:G:H4'	2.02	0.42
11:A:2805:A:H2'	11:A:2806:U:C6	2.55	0.42
11:A:3127:G:C2'	11:A:3128:A:H2'	2.50	0.42
12:B:1622:A:H2'	12:B:1623:G:C8	2.55	0.42
18:J:133:GLN:HB2	18:J:135:VAL:HG23	2.01	0.42
21:M:151:LYS:HG3	21:M:151:LYS:O	2.17	0.42
22:N:172:VAL:O	22:N:176:LEU:HB2	2.18	0.42
26:R:111:LYS:HB2	36:b:127:GLN:CD	2.45	0.42
44:j:31:GLN:HB2	44:j:33:LEU:HD12	2.02	0.42
49:p:99:ALA:CB	49:p:146:ASN:HB3	2.49	0.42
7:6:183:ASP:HB2	49:p:189:ARG:CB	2.47	0.42
7:6:299:ARG:HB2	7:6:299:ARG:CZ	2.50	0.42
8:7:192:TRP:CD1	8:7:295:ARG:HH22	2.38	0.42
13:D:216:LEU:HD12	13:D:225:ILE:O	2.20	0.42
15:F:255:LYS:HE3	43:i:47:TRP:CZ3	2.55	0.42
18:J:153:ILE:HG13	18:J:154:ARG:H	1.84	0.42
25:Q:165:GLU:HB2	25:Q:168:ASN:HB2	2.02	0.42
30:V:124:ASP:HA	30:V:125:PRO:HD3	1.94	0.42
30:V:136:ARG:NH1	30:V:146:VAL:HG11	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:126:GLN:HA	39:e:129:LEU:HD23	2.02	0.42
40:f:169:ILE:O	40:f:172:GLU:HG3	2.20	0.42
47:m:54:VAL:HG22	47:m:72:ARG:O	2.19	0.42
7:6:311:MET:O	44:j:112:LYS:NZ	2.53	0.41
11:A:1713:A:H2'	11:A:1714:C:O4'	2.20	0.41
11:A:1735:A:OP2	32:X:9:TRP:NE1	2.53	0.41
11:A:1958:G:H5'	11:A:1959:C:OP2	2.19	0.41
11:A:2472:A:O2'	11:A:2478:G:N7	2.38	0.41
11:A:3044:A:H2'	11:A:3045:A:C8	2.55	0.41
17:I:97:ALA:HB1	17:I:176:LEU:HD21	2.02	0.41
19:K:101:VAL:HB	19:K:127:LEU:HD23	2.02	0.41
25:Q:74:ARG:HB3	25:Q:283:TRP:CZ2	2.55	0.41
31:W:112:GLU:HA	31:W:115:ASP:OD2	2.20	0.41
33:Y:169:ARG:HD2	33:Y:199:PHE:CD1	2.55	0.41
34:Z:38:ARG:HG2	34:Z:81:TRP:CE2	2.54	0.41
37:c:45:LEU:O	37:c:49:ARG:HG3	2.20	0.41
39:e:119:ASP:HA	39:e:122:ASP:OD2	2.20	0.41
39:e:175:GLN:O	39:e:191:THR:HG21	2.19	0.41
42:h:70:LEU:HD23	42:h:70:LEU:HA	1.77	0.41
42:h:71:GLU:HB3	42:h:75:LYS:NZ	2.35	0.41
43:i:34:ILE:HG22	43:i:35:ARG:O	2.19	0.41
49:p:147:LEU:O	49:p:151:LEU:HG	2.20	0.41
52:s:100:LEU:O	52:s:322:VAL:HG11	2.20	0.41
52:s:179:GLN:O	52:s:183:THR:HG23	2.20	0.41
7:6:189:CYS:O	24:P:139:ALA:HA	2.20	0.41
9:8:123:LEU:HD11	12:B:1643:A:H5'	2.02	0.41
9:8:157:LEU:HD21	39:e:184:LEU:CD2	2.50	0.41
11:A:1862:U:H2'	11:A:1863:A:C8	2.55	0.41
13:D:233:GLN:HB2	13:D:292:MET:SD	2.60	0.41
14:E:328:LEU:HD13	14:E:332:LEU:HD11	2.01	0.41
15:F:83:HIS:CE1	15:F:274:LEU:HD11	2.55	0.41
15:F:283:LEU:O	21:M:189:LYS:NZ	2.37	0.41
17:I:78:LEU:HG	46:l:118:TRP:CD1	2.55	0.41
18:J:87:VAL:HG23	18:J:124:LYS:HE2	2.01	0.41
24:P:54:ARG:NH1	24:P:79:HIS:HE1	2.18	0.41
24:P:118:SER:O	24:P:121:ASN:HB2	2.20	0.41
26:R:85:ALA:HB1	26:R:124:ARG:HD2	2.01	0.41
37:c:79:LEU:HD22	37:c:214:PHE:CE2	2.55	0.41
43:i:57:TYR:CE1	50:q:30:PRO:HB3	2.55	0.41
52:s:155:PHE:CD2	52:s:156:TYR:HB2	2.56	0.41
52:s:300:HIS:HB2	52:s:361:ILE:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:157:ILE:HD11	6:5:381:LEU:HG	2.02	0.41
7:6:221:LEU:HA	7:6:231:GLU:HG2	2.03	0.41
10:9:131:TYR:HB3	10:9:132:PRO:HD3	2.03	0.41
11:A:1883:G:O6	21:M:128:THR:HG21	2.20	0.41
11:A:2188:A:N1	11:A:2198:A:O2'	2.41	0.41
11:A:2314:C:H2'	11:A:2315:A:H5''	2.01	0.41
11:A:2370:A:OP2	11:A:2370:A:H8	2.04	0.41
11:A:2489:C:H2'	11:A:2490:C:H6	1.85	0.41
11:A:2950:U:H2'	11:A:2951:A:C8	2.55	0.41
11:A:3027:U:H4'	11:A:3173:G:H5'	2.02	0.41
14:E:331:ASP:HB3	14:E:333:TYR:CE1	2.56	0.41
17:I:107:GLU:H	17:I:107:GLU:CD	2.27	0.41
20:L:42:ASP:O	20:L:48:ASN:ND2	2.52	0.41
22:N:250:ARG:HD2	22:N:250:ARG:HA	1.75	0.41
29:U:11:ARG:HA	29:U:11:ARG:HD2	1.80	0.41
29:U:28:LEU:O	33:Y:114:THR:HG23	2.21	0.41
33:Y:137:ASP:OD1	33:Y:137:ASP:C	2.62	0.41
33:Y:170:ARG:CZ	33:Y:201:ALA:HB2	2.50	0.41
38:d:267:PRO:HB2	38:d:269:TRP:CD1	2.55	0.41
41:g:84:TYR:HB3	41:g:116:ASP:O	2.20	0.41
49:p:104:HIS:HA	49:p:132:GLU:HA	2.01	0.41
50:q:40:PRO:HG2	50:q:51:GLN:O	2.20	0.41
7:6:233:LEU:HD21	7:6:236:LEU:HD22	2.01	0.41
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.55	0.41
9:8:142:ALA:HB1	39:e:274:ARG:NH2	2.36	0.41
10:9:134:ASN:O	29:U:8:PRO:HB3	2.20	0.41
11:A:1993:A:H8	11:A:2498:U:O2'	2.03	0.41
11:A:2241:A:OP1	51:r:150:TYR:OH	2.31	0.41
11:A:2392:U:H2'	11:A:2394:A:H62	1.84	0.41
11:A:2661:U:H2'	11:A:2662:A:C8	2.55	0.41
11:A:2664:U:H2'	11:A:2665:U:C6	2.55	0.41
11:A:3196:G:O2'	11:A:3197:U:OP2	2.38	0.41
17:I:83:ARG:NH1	17:I:134:PHE:HB2	2.35	0.41
17:I:150:HIS:O	45:k:31:ARG:NH2	2.49	0.41
21:M:62:ARG:HB3	43:i:128:ARG:HH11	1.86	0.41
21:M:140:LEU:HD21	21:M:167:ILE:CD1	2.50	0.41
22:N:211:ASN:OD1	22:N:211:ASN:C	2.63	0.41
24:P:177:ARG:HD3	58:P:210:HOH:O	2.19	0.41
30:V:73:GLN:N	38:d:256:TYR:OH	2.53	0.41
30:V:193:THR:OG1	30:V:196:GLU:HG2	2.20	0.41
37:c:50:LEU:HD12	37:c:50:LEU:HA	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:138:ASP:N	52:s:138:ASP:OD1	2.51	0.41
52:s:259:ILE:O	52:s:259:ILE:HD12	2.21	0.41
1:0:167:GLU:O	1:0:170:GLN:HG2	2.21	0.41
7:6:232:TYR:CZ	7:6:293:LEU:HD22	2.56	0.41
9:8:165:ASP:OD1	9:8:165:ASP:N	2.53	0.41
10:9:128:PHE:CZ	30:V:199:MET:HE3	2.55	0.41
11:A:1720:C:H4'	11:A:1909:A:C2	2.55	0.41
11:A:2060:A:O2'	11:A:2061:C:H5''	2.20	0.41
14:E:271:LEU:HB3	14:E:285:VAL:HG13	2.02	0.41
17:I:151:ASN:HB2	58:I:337:HOH:O	2.20	0.41
19:K:85:GLY:O	19:K:88:ARG:NH2	2.53	0.41
30:V:161:ARG:HG3	30:V:163:ASP:HB2	2.02	0.41
38:d:240:LYS:HE3	38:d:240:LYS:HB3	1.93	0.41
39:e:187:THR:HB	58:e:404:HOH:O	2.19	0.41
39:e:265:LYS:HE3	39:e:265:LYS:HB3	1.78	0.41
1:0:150:LYS:HA	1:0:150:LYS:HD3	1.80	0.41
6:5:188:LYS:HE3	52:s:186:GLY:HA3	2.02	0.41
7:6:74:TYR:OH	24:P:65:GLU:OE1	2.33	0.41
8:7:115:MET:HE1	8:7:127:PHE:HD1	1.86	0.41
9:8:128:GLU:OE1	47:m:37:ARG:NH1	2.54	0.41
11:A:1773:A:OP2	37:c:31:VAL:N	2.53	0.41
11:A:2455:U:H2'	11:A:2456:U:H6	1.85	0.41
11:A:2476:C:H2'	11:A:2477:G:O4'	2.21	0.41
11:A:2532:U:H2'	11:A:2533:A:H8	1.85	0.41
13:D:113:ARG:HG3	13:D:113:ARG:O	2.21	0.41
17:I:114:HIS:HA	17:I:117:ARG:CG	2.48	0.41
20:L:100:PHE:CZ	20:L:124:PRO:HD3	2.55	0.41
21:M:38:ARG:HD2	21:M:45:ARG:HE	1.86	0.41
21:M:225:ASP:HB3	49:p:49:TYR:CD1	2.56	0.41
21:M:285:PRO:HB2	21:M:290:LEU:HD13	2.03	0.41
27:S:111:GLU:HG2	36:b:19:LEU:HD11	2.03	0.41
34:Z:79:PRO:HD2	34:Z:82:GLU:CD	2.45	0.41
35:a:66:ASP:OD2	35:a:66:ASP:N	2.53	0.41
37:c:160:LEU:HD21	37:c:223:MET:HG2	2.01	0.41
42:h:139:LYS:HB3	48:o:101:TRP:HE3	1.85	0.41
46:l:110:LEU:HD23	46:l:117:TYR:CA	2.46	0.41
47:m:70:GLU:O	47:m:72:ARG:HG3	2.21	0.41
50:q:134:ASN:O	50:q:137:GLN:HG3	2.21	0.41
52:s:267:LYS:HB3	52:s:267:LYS:HE2	1.74	0.41
52:s:337:GLY:O	52:s:341:MET:HG3	2.20	0.41
5:4:67:LYS:HD2	5:4:67:LYS:HA	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:163:TRP:HA	52:s:287:LYS:HD2	2.02	0.41
11:A:1952:U:H2'	11:A:1953:A:H8	1.86	0.41
11:A:2033:A:H1'	11:A:2866:A:N7	2.35	0.41
11:A:2067:C:OP2	40:f:58:LYS:HG3	2.20	0.41
11:A:2159:U:H5'	11:A:2160:A:OP1	2.21	0.41
11:A:2175:C:C4	11:A:2176:C:C4	3.09	0.41
11:A:2332:C:H2'	11:A:2333:G:O4'	2.21	0.41
11:A:2353:A:H5''	28:T:171:TYR:OH	2.20	0.41
11:A:2942:C:H2'	11:A:2943:G:H8	1.86	0.41
13:D:85:ARG:HH12	13:D:269:ARG:HH12	1.68	0.41
16:H:87:LYS:HG3	16:H:88:HIS:ND1	2.32	0.41
23:O:65:LEU:HA	23:O:65:LEU:HD23	1.86	0.41
23:O:115:LEU:HD23	23:O:115:LEU:HA	1.89	0.41
27:S:161:ILE:HD13	27:S:161:ILE:HA	1.75	0.41
33:Y:187:PRO:HG2	33:Y:190:LEU:HG	2.03	0.41
37:c:59:ARG:HB2	37:c:62:GLU:HG2	2.01	0.41
39:e:146:ARG:HA	39:e:151:ARG:HD2	2.02	0.41
39:e:268:TYR:CD1	39:e:269:LEU:HD22	2.43	0.41
40:f:163:SER:OG	40:f:164:ALA:N	2.54	0.41
42:h:62:PRO:HA	42:h:63:PRO:HD3	1.93	0.41
47:m:50:ARG:HD3	47:m:52:TYR:OH	2.20	0.41
50:q:128:MET:CB	50:q:129:PRO:CD	2.99	0.41
52:s:350:ASP:O	52:s:351:VAL:HG13	2.20	0.41
6:5:241:ARG:O	6:5:241:ARG:HD3	2.20	0.41
6:5:249:ASN:OD1	6:5:249:ASN:C	2.64	0.41
7:6:151:LEU:HA	7:6:151:LEU:HD23	1.77	0.41
11:A:2067:C:OP2	11:A:2067:C:H3'	2.20	0.41
11:A:2152:A:H2'	11:A:2153:A:O4'	2.21	0.41
11:A:2155:A:HO2'	11:A:2156:A:C4'	2.33	0.41
11:A:2553:G:H2'	11:A:2554:A:H8	1.86	0.41
11:A:2663:C:H2'	11:A:2664:U:C6	2.56	0.41
12:B:1639:U:H2'	12:B:1640:A:H8	1.85	0.41
16:H:84:GLU:OE1	32:X:44:ARG:NH2	2.53	0.41
18:J:84:GLN:CD	18:J:85:PRO:HD2	2.46	0.41
21:M:105:ILE:HG12	21:M:112:PRO:HG3	2.02	0.41
22:N:68:ASN:O	22:N:71:ASP:OD1	2.39	0.41
22:N:191:SER:H	22:N:194:THR:HB	1.86	0.41
24:P:40:GLU:C	24:P:40:GLU:OE1	2.64	0.41
24:P:90:VAL:O	24:P:107:THR:HG23	2.20	0.41
25:Q:152:ARG:HG3	25:Q:161:GLU:HG2	2.01	0.41
28:T:55:ASN:HB3	28:T:132:HIS:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:66:ALA:HB3	52:s:100:LEU:HD21	2.03	0.41
31:W:73:PHE:HZ	31:W:83:VAL:HG21	1.85	0.41
32:X:35:GLU:OE2	32:X:35:GLU:O	2.39	0.41
33:Y:154:ARG:NH1	33:Y:163:ALA:HB2	2.35	0.41
41:g:116:ASP:OD2	41:g:116:ASP:C	2.64	0.41
3:2:57:ASN:HB2	10:9:27:PRO:HD3	2.03	0.41
5:4:85:ARG:HA	51:r:158:SER:HB2	2.03	0.41
6:5:164:GLN:HE22	6:5:175:TYR:HA	1.86	0.41
7:6:60:ARG:HD2	7:6:63:GLN:NE2	2.36	0.41
7:6:193:VAL:HB	7:6:319:PHE:CE2	2.56	0.41
11:A:1898:A:H2'	11:A:1899:G:C8	2.56	0.41
11:A:2346:U:H2'	11:A:2347:C:C6	2.56	0.41
11:A:2653:C:O2'	11:A:2654:U:C6	2.71	0.41
11:A:3018:A:H61	11:A:3130:A:N6	2.19	0.41
11:A:3169:C:H1'	11:A:3198:A:O2'	2.20	0.41
11:A:3224:G:H2'	11:A:3225:G:H8	1.85	0.41
12:B:1624:C:C4	12:B:1625:A:C8	3.08	0.41
14:E:292:HIS:ND1	14:E:293:LYS:O	2.41	0.41
15:F:47:VAL:HG13	15:F:78:GLY:HA3	2.02	0.41
15:F:59:ARG:HD2	41:g:114:GLU:OE2	2.20	0.41
15:F:91:PRO:O	15:F:176:VAL:HG13	2.20	0.41
17:I:48:MET:HA	22:N:250:ARG:HH21	1.86	0.41
17:I:78:LEU:HG	46:l:118:TRP:CG	2.56	0.41
17:I:120:LYS:HD3	17:I:120:LYS:HA	1.73	0.41
18:J:61:LYS:HG3	18:J:62:GLU:OE1	2.21	0.41
19:K:159:THR:O	19:K:159:THR:OG1	2.36	0.41
19:K:175:ASP:OD1	19:K:175:ASP:O	2.38	0.41
21:M:65:LEU:HD13	43:i:128:ARG:O	2.21	0.41
21:M:280:LYS:H	21:M:280:LYS:HG3	1.56	0.41
22:N:171:GLU:HG2	22:N:172:VAL:N	2.36	0.41
24:P:122:VAL:O	24:P:126:GLU:OE1	2.39	0.41
25:Q:193:ALA:HA	25:Q:224:MET:HA	2.02	0.41
26:R:98:ASN:OD1	26:R:98:ASN:N	2.49	0.41
30:V:108:MET:HE3	30:V:108:MET:HB2	1.91	0.41
34:Z:71:ARG:HA	34:Z:117:ILE:HG22	2.03	0.41
34:Z:87:LYS:HB2	34:Z:87:LYS:HE2	1.76	0.41
36:b:40:SER:O	36:b:44:ARG:HB2	2.21	0.41
37:c:123:GLN:O	37:c:127:GLU:HG3	2.21	0.41
38:d:199:CYS:SG	38:d:200:SER:N	2.94	0.41
39:e:126:GLN:O	39:e:129:LEU:HG	2.21	0.41
39:e:260:LEU:HD13	39:e:264:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:43:ARG:HE	45:k:43:ARG:HB2	1.60	0.41
47:m:73:ARG:O	47:m:74:MET:HG3	2.21	0.41
49:p:119:ILE:HD11	49:p:158:ILE:HA	2.02	0.41
50:q:61:PHE:HE1	50:q:66:ALA:HB2	1.86	0.41
52:s:47:ILE:O	52:s:47:ILE:HG22	2.20	0.41
52:s:341:MET:HE2	52:s:341:MET:HB3	1.83	0.41
1:0:116:LEU:HD12	1:0:116:LEU:HA	1.90	0.41
6:5:392:LYS:HB2	6:5:392:LYS:HE2	1.81	0.41
9:8:121:TRP:CZ3	12:B:1629:A:H5'	2.56	0.41
11:A:1991:A:H5''	11:A:1992:C:OP1	2.21	0.41
11:A:2065:A:H2'	11:A:2066:C:H1'	2.02	0.41
11:A:2471:G:OP1	20:L:37:ARG:N	2.45	0.41
11:A:3144:A:H2'	11:A:3145:A:C8	2.55	0.41
11:A:3168:C:C2	14:E:303:LYS:NZ	2.89	0.41
16:H:99:THR:C	16:H:108:ARG:HD3	2.46	0.41
21:M:176:THR:HG21	21:M:213:TYR:HE1	1.85	0.41
30:V:132:GLU:O	30:V:148:THR:HG23	2.21	0.41
33:Y:203:PRO:C	33:Y:205:VAL:N	2.79	0.41
37:c:199:ILE:HD12	37:c:215:ILE:HG22	2.03	0.41
40:f:60:LYS:HA	40:f:63:ILE:HG13	2.02	0.41
48:o:68:ARG:O	48:o:72:GLU:HG2	2.21	0.41
49:p:102:ARG:HA	49:p:133:LEU:O	2.21	0.41
54:TA:56:ALA:HB1	54:TA:58:LYS:NZ	2.36	0.41
7:6:138:GLU:O	7:6:141:ARG:HG2	2.22	0.40
7:6:266:HIS:CD2	7:6:266:HIS:N	2.89	0.40
11:A:1814:A:H2'	11:A:1815:A:C8	2.56	0.40
11:A:2461:A:OP1	14:E:238:ARG:N	2.52	0.40
11:A:2554:A:H2'	11:A:2555:C:C6	2.56	0.40
11:A:2981:A:O2'	22:N:137:GLY:HA2	2.21	0.40
13:D:62:ASN:OD1	13:D:62:ASN:N	2.54	0.40
19:K:155:LEU:HG	51:r:86:VAL:HB	2.03	0.40
22:N:71:ASP:OD1	22:N:71:ASP:N	2.41	0.40
22:N:214:THR:HG22	22:N:216:GLU:N	2.35	0.40
23:O:26:ILE:HD13	23:O:26:ILE:HA	1.95	0.40
26:R:90:LEU:HD23	26:R:90:LEU:HA	1.92	0.40
27:S:68:ASP:O	27:S:71:GLU:HG3	2.22	0.40
35:a:70:GLU:H	35:a:70:GLU:CD	2.29	0.40
38:d:138:PRO:HG3	38:d:194:VAL:HG23	2.02	0.40
39:e:211:GLY:H	39:e:233:PHE:HB2	1.86	0.40
39:e:260:LEU:HA	58:e:468:HOH:O	2.20	0.40
50:q:132:ILE:O	50:q:134:ASN:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:229:LEU:HD23	52:s:229:LEU:HA	1.84	0.40
11:A:2506:A:O2'	11:A:2507:A:H5'	2.21	0.40
11:A:3040:G:H2'	11:A:3041:U:O4'	2.20	0.40
15:F:175:LYS:HD2	15:F:273:LEU:HB3	2.02	0.40
18:J:98:GLU:OE1	46:l:72:ALA:HB2	2.21	0.40
18:J:119:GLU:HG2	18:J:122:ARG:HE	1.86	0.40
21:M:191:VAL:HB	21:M:192:PRO:HD3	2.04	0.40
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.56	0.40
26:R:108:TYR:CE2	28:T:212:LEU:HB2	2.57	0.40
27:S:95:LEU:HB3	27:S:138:ALA:HB2	2.03	0.40
30:V:165:ILE:HD12	30:V:165:ILE:HA	1.85	0.40
32:X:228:LYS:HA	32:X:231:VAL:HG12	2.03	0.40
33:Y:131:ARG:O	33:Y:135:VAL:HG23	2.21	0.40
34:Z:121:PRO:HG3	48:o:48:TRP:CH2	2.56	0.40
35:a:45:CYS:SG	35:a:62:HIS:HB2	2.62	0.40
36:b:33:VAL:O	36:b:67:SER:HA	2.20	0.40
38:d:288:LYS:H	38:d:288:LYS:CD	2.34	0.40
42:h:122:ARG:HH21	42:h:124:ARG:NH1	2.14	0.40
52:s:169:SER:HB3	52:s:304:ASP:OD2	2.21	0.40
2:1:20:MET:HE3	2:1:20:MET:HB3	1.82	0.40
8:7:44:ARG:HG3	8:7:229:ILE:HG22	2.04	0.40
8:7:107:LEU:HA	8:7:111:GLN:O	2.22	0.40
11:A:1751:A:OP1	21:M:75:TYR:OH	2.14	0.40
11:A:1884:G:H1'	11:A:1895:C:H1'	2.03	0.40
11:A:2519:G:N7	13:D:230:SER:OG	2.52	0.40
11:A:2672:A:H4'	28:T:110:ASP:O	2.22	0.40
11:A:2899:C:H2'	11:A:2900:C:O4'	2.20	0.40
11:A:2950:U:H2'	11:A:2951:A:H8	1.87	0.40
12:B:1604:G:H2'	12:B:1605:A:H8	1.87	0.40
21:M:86:GLY:O	21:M:90:ARG:HG3	2.22	0.40
23:O:49:VAL:HG12	23:O:107:MET:SD	2.60	0.40
23:O:104:TYR:O	23:O:105:THR:OG1	2.38	0.40
29:U:126:LEU:HD21	38:d:78:LEU:HD21	2.02	0.40
31:W:120:LEU:HD11	31:W:126:LEU:HD21	2.04	0.40
32:X:149:PRO:HD2	32:X:152:ASP:HB2	2.04	0.40
33:Y:77:GLU:O	33:Y:78:LYS:HG2	2.21	0.40
37:c:211:THR:O	37:c:215:ILE:HG23	2.22	0.40
38:d:165:THR:OG1	38:d:262:HIS:HA	2.21	0.40
49:p:121:ILE:HD13	49:p:121:ILE:HA	1.94	0.40
49:p:129:ARG:HD3	49:p:129:ARG:HA	1.82	0.40
6:5:73:ILE:HD12	6:5:73:ILE:HA	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:218:LEU:HG	7:6:234:HIS:HB2	2.04	0.40
8:7:114:ASP:OD1	8:7:117:LYS:HB2	2.20	0.40
8:7:213:ASP:HB3	8:7:271:ARG:HH11	1.85	0.40
11:A:1861:U:H2'	11:A:1862:U:H6	1.87	0.40
20:L:82:LYS:HG2	20:L:107:LEU:HD22	2.04	0.40
23:O:97:TYR:OH	23:O:126:LYS:O	2.36	0.40
26:R:102:LEU:HD23	26:R:102:LEU:HA	1.95	0.40
29:U:54:ARG:O	29:U:58:GLU:HG3	2.22	0.40
30:V:19:TYR:OH	30:V:31:ASP:OD2	2.29	0.40
38:d:212:ILE:HD12	38:d:259:TRP:CH2	2.57	0.40
38:d:245:TYR:HB2	38:d:265:ILE:HG22	2.02	0.40
39:e:203:LYS:O	39:e:237:LEU:N	2.53	0.40
40:f:91:LEU:HD12	40:f:91:LEU:HA	1.87	0.40
3:2:78:VAL:HG22	3:2:81:ARG:NH2	2.36	0.40
4:3:151:ASN:O	4:3:155:SER:OG	2.31	0.40
6:5:154:LEU:HD23	6:5:154:LEU:HA	1.96	0.40
6:5:309:ARG:NE	6:5:377:SER:HB2	2.36	0.40
7:6:138:GLU:HG2	24:P:111:ALA:HA	2.04	0.40
8:7:165:ASN:HB3	8:7:184:VAL:HG23	2.03	0.40
10:9:75:SER:OG	30:V:172:ASP:OD1	2.25	0.40
11:A:2010:U:OP2	43:i:115:ARG:NH1	2.43	0.40
11:A:2346:U:H2'	11:A:2347:C:H6	1.86	0.40
14:E:107:MET:HE2	14:E:107:MET:HB3	1.93	0.40
18:J:122:ARG:HD2	18:J:123:ILE:N	2.36	0.40
18:J:149:ARG:NH1	46:l:102:GLY:O	2.55	0.40
25:Q:221:LYS:HB3	25:Q:244:ARG:HG2	2.03	0.40
26:R:111:LYS:HB2	36:b:127:GLN:OE1	2.22	0.40
29:U:114:LYS:N	58:U:208:HOH:O	2.51	0.40
31:W:144:LEU:HD12	31:W:144:LEU:HA	1.90	0.40
32:X:150:LYS:HB3	32:X:159:MET:HE2	2.04	0.40
37:c:301:LEU:HD12	37:c:301:LEU:HA	1.87	0.40
38:d:263:THR:HG22	38:d:264:LYS:H	1.86	0.40
39:e:47:LEU:HG	58:e:337:HOH:O	2.20	0.40
42:h:66:LEU:HG	58:h:205:HOH:O	2.20	0.40
51:r:146:GLN:O	51:r:146:GLN:HG2	2.19	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	0	106/188 (56%)	94 (89%)	12 (11%)	0	100	100
2	1	50/65 (77%)	47 (94%)	3 (6%)	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
6	5	391/423 (92%)	373 (95%)	16 (4%)	2 (0%)	24	44
7	6	352/380 (93%)	324 (92%)	28 (8%)	0	100	100
8	7	295/338 (87%)	279 (95%)	15 (5%)	1 (0%)	36	56
9	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
13	D	237/305 (78%)	225 (95%)	11 (5%)	1 (0%)	30	49
14	E	304/348 (87%)	283 (93%)	20 (7%)	1 (0%)	36	56
15	F	248/311 (80%)	228 (92%)	20 (8%)	0	100	100
16	H	96/267 (36%)	87 (91%)	9 (9%)	0	100	100
17	I	177/261 (68%)	164 (93%)	13 (7%)	0	100	100
18	J	173/192 (90%)	162 (94%)	10 (6%)	1 (1%)	21	39
19	K	175/178 (98%)	157 (90%)	17 (10%)	1 (1%)	21	39
20	L	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
21	M	285/296 (96%)	254 (89%)	30 (10%)	1 (0%)	30	49
22	N	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
23	O	150/175 (86%)	132 (88%)	18 (12%)	0	100	100
24	P	141/179 (79%)	130 (92%)	10 (7%)	1 (1%)	18	35
25	Q	218/292 (75%)	211 (97%)	7 (3%)	0	100	100
26	R	138/149 (93%)	128 (93%)	10 (7%)	0	100	100
27	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	T	164/212 (77%)	157 (96%)	7 (4%)	0	100	100
29	U	150/153 (98%)	144 (96%)	6 (4%)	0	100	100
30	V	204/216 (94%)	200 (98%)	4 (2%)	0	100	100
31	W	109/148 (74%)	103 (94%)	6 (6%)	0	100	100
32	X	241/256 (94%)	226 (94%)	15 (6%)	0	100	100
33	Y	174/250 (70%)	164 (94%)	10 (6%)	0	100	100
34	Z	118/161 (73%)	109 (92%)	9 (8%)	0	100	100
35	a	106/142 (75%)	103 (97%)	3 (3%)	0	100	100
36	b	146/155 (94%)	139 (95%)	7 (5%)	0	100	100
37	c	287/332 (86%)	265 (92%)	22 (8%)	0	100	100
38	d	255/306 (83%)	241 (94%)	14 (6%)	0	100	100
39	e	211/279 (76%)	194 (92%)	17 (8%)	0	100	100
40	f	144/194 (74%)	136 (94%)	8 (6%)	0	100	100
41	g	130/166 (78%)	121 (93%)	9 (7%)	0	100	100
42	h	108/158 (68%)	99 (92%)	9 (8%)	0	100	100
43	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	j	91/123 (74%)	87 (96%)	4 (4%)	0	100	100
45	k	94/112 (84%)	90 (96%)	4 (4%)	0	100	100
46	l	70/138 (51%)	62 (89%)	8 (11%)	0	100	100
47	m	43/128 (34%)	39 (91%)	4 (9%)	0	100	100
48	o	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	p	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
50	q	166/222 (75%)	154 (93%)	6 (4%)	6 (4%)	2	3
51	r	160/196 (82%)	150 (94%)	10 (6%)	0	100	100
52	s	391/439 (89%)	364 (93%)	27 (7%)	0	100	100
54	TA	43/198 (22%)	39 (91%)	4 (9%)	0	100	100
54	TB	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
54	TC	69/198 (35%)	64 (93%)	5 (7%)	0	100	100
All	All	8449/11190 (76%)	7907 (94%)	527 (6%)	15 (0%)	44	64

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	70	LEU
24	P	69	ARG
50	q	43	GLU
50	q	132	ILE
19	K	160	GLN
21	M	288	GLU
14	E	317	PRO
6	5	72	PRO
50	q	42	PRO
50	q	128	MET
50	q	133	VAL
8	7	110	GLY
50	q	79	PRO
13	D	207	ILE
18	J	31	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	0	97/164 (59%)	95 (98%)	2 (2%)	47	72
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	85 (97%)	3 (3%)	32	58
5	4	37/89 (42%)	36 (97%)	1 (3%)	39	65
6	5	353/368 (96%)	333 (94%)	20 (6%)	18	38
7	6	313/332 (94%)	299 (96%)	14 (4%)	24	48
8	7	272/303 (90%)	264 (97%)	8 (3%)	37	63
9	8	91/190 (48%)	89 (98%)	2 (2%)	45	70
10	9	104/112 (93%)	100 (96%)	4 (4%)	29	54
13	D	193/245 (79%)	184 (95%)	9 (5%)	23	46
14	E	260/290 (90%)	251 (96%)	9 (4%)	32	57
15	F	217/262 (83%)	213 (98%)	4 (2%)	51	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	H	88/228 (39%)	84 (96%)	4 (4%)	24	48
17	I	164/232 (71%)	158 (96%)	6 (4%)	30	55
18	J	138/150 (92%)	132 (96%)	6 (4%)	26	49
19	K	155/156 (99%)	151 (97%)	4 (3%)	40	66
20	L	98/124 (79%)	95 (97%)	3 (3%)	35	61
21	M	245/249 (98%)	241 (98%)	4 (2%)	55	78
22	N	189/211 (90%)	184 (97%)	5 (3%)	40	66
23	O	133/150 (89%)	131 (98%)	2 (2%)	57	79
24	P	125/154 (81%)	121 (97%)	4 (3%)	34	60
25	Q	202/256 (79%)	201 (100%)	1 (0%)	81	91
26	R	118/126 (94%)	116 (98%)	2 (2%)	53	76
27	S	141/180 (78%)	136 (96%)	5 (4%)	32	57
28	T	146/182 (80%)	138 (94%)	8 (6%)	19	39
29	U	125/135 (93%)	123 (98%)	2 (2%)	55	78
30	V	184/191 (96%)	179 (97%)	5 (3%)	39	65
31	W	91/119 (76%)	86 (94%)	5 (6%)	19	39
32	X	219/229 (96%)	210 (96%)	9 (4%)	27	52
33	Y	159/223 (71%)	155 (98%)	4 (2%)	42	68
34	Z	111/147 (76%)	108 (97%)	3 (3%)	39	65
35	a	101/133 (76%)	97 (96%)	4 (4%)	28	53
36	b	130/135 (96%)	127 (98%)	3 (2%)	44	69
37	c	253/288 (88%)	244 (96%)	9 (4%)	31	56
38	d	224/274 (82%)	214 (96%)	10 (4%)	24	48
39	e	188/236 (80%)	183 (97%)	5 (3%)	39	65
40	f	122/173 (70%)	117 (96%)	5 (4%)	27	52
41	g	122/148 (82%)	118 (97%)	4 (3%)	33	59
42	h	104/148 (70%)	96 (92%)	8 (8%)	12	25
43	i	86/110 (78%)	84 (98%)	2 (2%)	44	69
44	j	74/97 (76%)	72 (97%)	2 (3%)	39	65
45	k	81/90 (90%)	74 (91%)	7 (9%)	10	20
46	l	67/116 (58%)	67 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m	40/113 (35%)	39 (98%)	1 (2%)	42	68
48	o	80/87 (92%)	79 (99%)	1 (1%)	61	81
49	p	134/181 (74%)	127 (95%)	7 (5%)	21	42
50	q	114/178 (64%)	107 (94%)	7 (6%)	17	35
51	r	147/169 (87%)	143 (97%)	4 (3%)	39	65
52	s	336/381 (88%)	324 (96%)	12 (4%)	31	56
54	TA	39/158 (25%)	38 (97%)	1 (3%)	40	66
54	TB	26/158 (16%)	25 (96%)	1 (4%)	29	54
All	All	7413/9468 (78%)	7162 (97%)	251 (3%)	33	58

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	153	THR
1	0	179	ARG
4	3	152	LYS
4	3	173	VAL
4	3	188	VAL
5	4	73	LYS
6	5	35	VAL
6	5	69	TRP
6	5	70	LEU
6	5	100	ASP
6	5	139	VAL
6	5	156	VAL
6	5	158	SER
6	5	173	GLU
6	5	206	SER
6	5	222	ARG
6	5	233	ASP
6	5	255	PHE
6	5	261	ILE
6	5	273	LYS
6	5	293	LEU
6	5	344	VAL
6	5	346	THR
6	5	369	VAL
6	5	371	ASN
6	5	414	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	6	40	ILE
7	6	87	LYS
7	6	90	ILE
7	6	125	LEU
7	6	173	LEU
7	6	179	VAL
7	6	191	ASN
7	6	217	LEU
7	6	251	THR
7	6	284	ASP
7	6	288	SER
7	6	300	THR
7	6	312	THR
7	6	370	ARG
8	7	63	GLU
8	7	67	VAL
8	7	138	VAL
8	7	153	VAL
8	7	192	TRP
8	7	275	CYS
8	7	324	VAL
8	7	325	THR
9	8	111	THR
9	8	139	MET
10	9	28	ARG
10	9	29	SER
10	9	87	THR
10	9	129	GLN
13	D	75	THR
13	D	177	ARG
13	D	189	VAL
13	D	191	THR
13	D	196	VAL
13	D	221	ASN
13	D	235	GLN
13	D	253	ASN
13	D	294	SER
14	E	69	ASP
14	E	77	LEU
14	E	78	CYS
14	E	142	MET
14	E	159	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	E	187	ILE
14	E	248	ILE
14	E	285	VAL
14	E	322	ASP
15	F	47	VAL
15	F	133	THR
15	F	204	THR
15	F	234	THR
16	H	53	THR
16	H	83	VAL
16	H	93	ASN
16	H	101	SER
17	I	39	VAL
17	I	43	GLN
17	I	50	VAL
17	I	102	VAL
17	I	170	THR
17	I	171	VAL
18	J	68	THR
18	J	86	THR
18	J	104	THR
18	J	136	PRO
18	J	159	LEU
18	J	187	GLU
19	K	124	ARG
19	K	155	LEU
19	K	156	ASP
19	K	158	TYR
20	L	38	VAL
20	L	105	VAL
20	L	125	THR
21	M	119	THR
21	M	128	THR
21	M	146	ASP
21	M	258	THR
22	N	32	THR
22	N	62	VAL
22	N	68	ASN
22	N	132	THR
22	N	229	VAL
23	O	20	LEU
23	O	114	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	P	56	LEU
24	P	84	ILE
24	P	110	TRP
24	P	141	ILE
25	Q	120	THR
26	R	95	VAL
26	R	136	LYS
27	S	95	LEU
27	S	103	SER
27	S	110	SER
27	S	154	VAL
27	S	161	ILE
28	T	47	ILE
28	T	72	GLU
28	T	94	ILE
28	T	98	SER
28	T	118	LYS
28	T	133	ASN
28	T	191	THR
28	T	209	VAL
29	U	97	VAL
29	U	144	ARG
30	V	38	TRP
30	V	82	GLN
30	V	166	VAL
30	V	177	THR
30	V	199	MET
31	W	42	LEU
31	W	125	VAL
31	W	126	LEU
31	W	131	VAL
31	W	148	LEU
32	X	39	THR
32	X	60	GLU
32	X	99	LYS
32	X	125	VAL
32	X	127	VAL
32	X	150	LYS
32	X	176	LEU
32	X	224	VAL
32	X	237	GLN
33	Y	150	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	Y	185	VAL
33	Y	202	LEU
33	Y	235	LEU
34	Z	73	LYS
34	Z	105	SER
34	Z	148	GLN
35	a	45	CYS
35	a	54	ASP
35	a	57	THR
35	a	64	SER
36	b	23	VAL
36	b	51	VAL
36	b	147	GLU
37	c	72	ILE
37	c	79	LEU
37	c	119	LEU
37	c	126	SER
37	c	131	SER
37	c	150	THR
37	c	175	VAL
37	c	203	LEU
37	c	308	THR
38	d	81	THR
38	d	153	ASN
38	d	164	VAL
38	d	181	VAL
38	d	188	SER
38	d	203	MET
38	d	214	VAL
38	d	242	VAL
38	d	253	THR
38	d	261	MET
39	e	62	PRO
39	e	147	THR
39	e	153	LEU
39	e	256	THR
39	e	272	VAL
40	f	96	THR
40	f	119	ILE
40	f	149	VAL
40	f	160	SER
40	f	186	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	g	55	THR
41	g	68	THR
41	g	144	THR
41	g	147	LEU
42	h	50	LEU
42	h	85	ASN
42	h	94	SER
42	h	96	LEU
42	h	103	HIS
42	h	115	SER
42	h	118	HIS
42	h	126	VAL
43	i	63	LEU
43	i	98	VAL
44	j	40	TYR
44	j	81	SER
45	k	8	LEU
45	k	16	VAL
45	k	18	VAL
45	k	27	VAL
45	k	45	THR
45	k	47	LEU
45	k	92	SER
47	m	35	SER
48	o	82	PHE
49	p	42	ILE
49	p	52	SER
49	p	96	ASN
49	p	139	SER
49	p	159	THR
49	p	164	THR
49	p	180	ILE
50	q	68	SER
50	q	90	ARG
50	q	111	GLU
50	q	123	GLU
50	q	127	LYS
50	q	129	PRO
50	q	131	MET
51	r	54	THR
51	r	119	VAL
51	r	139	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	r	159	VAL
52	s	71	HIS
52	s	112	THR
52	s	118	LEU
52	s	169	SER
52	s	240	GLN
52	s	257	VAL
52	s	284	VAL
52	s	318	ASP
52	s	331	SER
52	s	351	VAL
52	s	405	ILE
52	s	410	VAL
54	TA	46	GLU
54	TB	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	106	ASN
3	2	77	GLN
4	3	170	ASN
6	5	108	HIS
6	5	149	GLN
6	5	190	GLN
6	5	250	HIS
6	5	268	ASN
6	5	337	GLN
6	5	371	ASN
7	6	108	GLN
7	6	295	GLN
7	6	307	HIS
10	9	90	GLN
10	9	123	GLN
10	9	129	GLN
13	D	168	HIS
14	E	233	GLN
14	E	286	ASN
14	E	336	ASN
15	F	83	HIS
15	F	208	HIS
16	H	148	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	I	43	GLN
17	I	100	GLN
18	J	54	ASN
19	K	26	GLN
19	K	70	ASN
20	L	52	HIS
20	L	103	ASN
21	M	58	GLN
22	N	210	GLN
23	O	112	ASN
23	O	150	GLN
25	Q	132	GLN
25	Q	172	GLN
25	Q	203	ASN
26	R	12	ASN
26	R	22	GLN
28	T	62	GLN
29	U	16	GLN
31	W	62	HIS
32	X	4	HIS
32	X	46	HIS
33	Y	88	GLN
33	Y	157	GLN
34	Z	67	HIS
35	a	44	ASN
35	a	90	GLN
36	b	27	GLN
36	b	102	GLN
37	c	128	GLN
37	c	315	ASN
38	d	161	HIS
39	e	75	GLN
39	e	207	ASN
39	e	212	HIS
39	e	248	ASN
42	h	119	GLN
44	j	89	GLN
45	k	35	GLN
48	o	58	GLN
49	p	152	GLN
50	q	120	HIS
50	q	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	q	157	GLN
51	r	79	HIS
51	r	109	GLN
52	s	101	ASN
52	s	107	GLN
54	TB	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1523/1559 (97%)	360 (23%)	24 (1%)
12	B	51/72 (70%)	12 (23%)	1 (1%)
All	All	1574/1631 (96%)	372 (23%)	25 (1%)

All (372) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1678	C
11	A	1679	U
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1710	A
11	A	1711	C
11	A	1713	A
11	A	1714	C
11	A	1715	C
11	A	1716	U
11	A	1717	U
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1733	C
11	A	1734	C
11	A	1735	A
11	A	1736	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1762	A
11	A	1763	A
11	A	1766	U
11	A	1767	G
11	A	1770	G
11	A	1781	A
11	A	1782	G
11	A	1794	A
11	A	1803	A
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1808	A
11	A	1809	U
11	A	1810	A
11	A	1811	A
11	A	1817	C
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1849	C
11	A	1854	U
11	A	1856	A
11	A	1867	A
11	A	1869	A
11	A	1872	U
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1893	A
11	A	1901	C
11	A	1903	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1918	G
11	A	1935	A
11	A	1936	A
11	A	1937	A
11	A	1938	A
11	A	1940	A
11	A	1944	C
11	A	1958	G
11	A	1968	G
11	A	1974	A
11	A	1985	G
11	A	1987	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2000	C
11	A	2001	C
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2031	A
11	A	2036	C
11	A	2037	U
11	A	2038	U
11	A	2039	A
11	A	2060	A
11	A	2065	A
11	A	2066	C
11	A	2067	C
11	A	2069	U
11	A	2072	A
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2099	U
11	A	2105	G
11	A	2113	G
11	A	2125	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2126	U
11	A	2134	A
11	A	2135	A
11	A	2141	U
11	A	2142	A
11	A	2147	G
11	A	2154	A
11	A	2158	U
11	A	2160	A
11	A	2161	A
11	A	2163	A
11	A	2166	C
11	A	2169	A
11	A	2171	U
11	A	2172	A
11	A	2173	G
11	A	2177	U
11	A	2180	A
11	A	2181	A
11	A	2182	G
11	A	2183	C
11	A	2184	A
11	A	2187	C
11	A	2189	C
11	A	2192	A
11	A	2193	U
11	A	2198	A
11	A	2200	A
11	A	2202	C
11	A	2204	U
11	A	2210	C
11	A	2211	U
11	A	2215	C
11	A	2217	C
11	A	2218	C
11	A	2219	C
11	A	2220	A
11	A	2222	U
11	A	2224	C
11	A	2227	A
11	A	2228	A
11	A	2229	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2242	U
11	A	2245	A
11	A	2246	A
11	A	2250	A
11	A	2251	A
11	A	2252	C
11	A	2260	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2324	U
11	A	2332	C
11	A	2345	G
11	A	2350	A
11	A	2351	U
11	A	2356	A
11	A	2357	C
11	A	2360	U
11	A	2361	G
11	A	2362	A
11	A	2364	C
11	A	2365	U
11	A	2370	A
11	A	2371	U
11	A	2374	A
11	A	2381	A
11	A	2389	C
11	A	2390	A
11	A	2393	C
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2414	C
11	A	2415	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2426	C
11	A	2434	A
11	A	2443	C
11	A	2444	A
11	A	2446	A
11	A	2447	A
11	A	2451	A
11	A	2458	A
11	A	2478	G
11	A	2479	C
11	A	2484	C
11	A	2493	C
11	A	2502	C
11	A	2506	A
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2522	U
11	A	2523	C
11	A	2524	A
11	A	2527	A
11	A	2531	U
11	A	2540	C
11	A	2557	C
11	A	2558	A
11	A	2559	U
11	A	2560	G
11	A	2570	C
11	A	2575	U
11	A	2576	A
11	A	2578	C
11	A	2580	U
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2601	A
11	A	2603	C
11	A	2607	U
11	A	2618	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2626	U
11	A	2627	G
11	A	2629	A
11	A	2630	U
11	A	2632	A
11	A	2633	A
11	A	2634	U
11	A	2635	G
11	A	2645	G
11	A	2656	U
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2739	U
11	A	2740	A
11	A	2745	A
11	A	2747	U
11	A	2750	U
11	A	2755	A
11	A	2756	C
11	A	2757	A
11	A	2758	G
11	A	2760	A
11	A	2792	A
11	A	2803	A
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2831	G
11	A	2832	A
11	A	2833	A
11	A	2842	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2844	G
11	A	2847	C
11	A	2854	U
11	A	2864	U
11	A	2865	C
11	A	2881	C
11	A	2893	A
11	A	2906	C
11	A	2910	A
11	A	2912	C
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2932	G
11	A	2935	A
11	A	2940	A
11	A	2956	A
11	A	2962	C
11	A	2963	A
11	A	2965	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	2994	U
11	A	3005	A
11	A	3007	C
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3042	U
11	A	3043	C
11	A	3053	A
11	A	3054	G
11	A	3059	A
11	A	3060	C
11	A	3063	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	3069	A
11	A	3072	U
11	A	3073	C
11	A	3086	U
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3098	U
11	A	3100	U
11	A	3102	U
11	A	3109	U
11	A	3113	A
11	A	3123	G
11	A	3124	U
11	A	3129	A
11	A	3141	A
11	A	3150	U
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3172	C
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3196	G
11	A	3197	U
11	A	3199	U
11	A	3200	U
11	A	3201	A
11	A	3204	C
11	A	3207	A
11	A	3208	C
11	A	3210	C
11	A	3211	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	1607	U
12	B	1608	G
12	B	1609	U
12	B	1611	G
12	B	1613	U
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1644	G
12	B	1645	A
12	B	1659	U
12	B	1669	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1703	C
11	A	1709	G
11	A	1713	A
11	A	1805	A
11	A	1806	U
11	A	1807	U
11	A	1823	A
11	A	1871	A
11	A	2186	C
11	A	2245	A
11	A	2361	G
11	A	2457	A
11	A	2507	A
11	A	2530	A
11	A	2559	U
11	A	2606	U
11	A	2628	U
11	A	2905	A
11	A	2989	G
11	A	3041	U
11	A	3072	U
11	A	3092	U
11	A	3123	G
11	A	3196	G
12	B	1607	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 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$
57	ZLD	A	3400	56	26,26,26	0.88	1 (3%)	36,36,36	1.21	2 (5%)

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
57	ZLD	A	3400	56	-	2/13/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	3400	ZLD	C7-N4	-2.31	1.34	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	3400	ZLD	C6-C8-C9	4.30	118.25	113.38
57	A	3400	ZLD	O10-C7-O15	-2.63	119.32	122.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

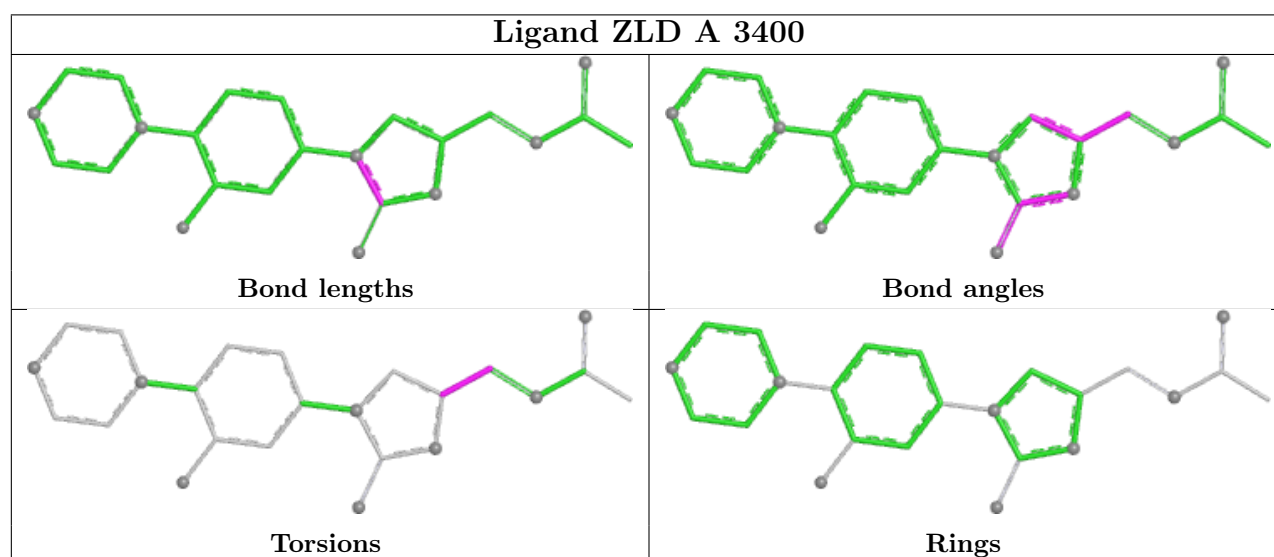
Mol	Chain	Res	Type	Atoms
57	A	3400	ZLD	C6-C8-C9-N11
57	A	3400	ZLD	O10-C8-C9-N11

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	3400	ZLD	3	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	u	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	414:UNK	C	601:UNK	N	50.73
1	u	106:UNK	C	301:UNK	N	32.84
1	u	315:UNK	C	399:UNK	N	24.40
1	u	615:UNK	C	700:UNK	N	14.68

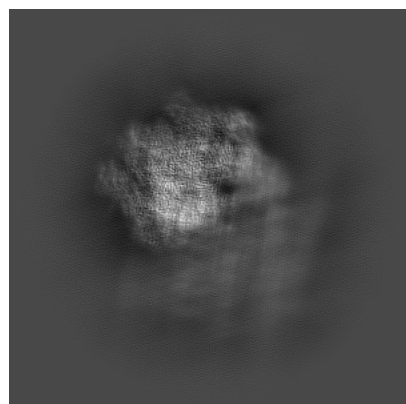
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45757. These allow visual inspection of the internal detail of the map and identification of artifacts.

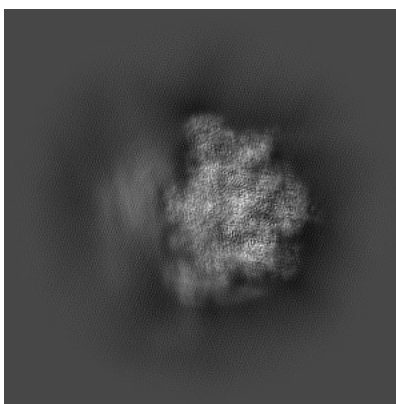
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

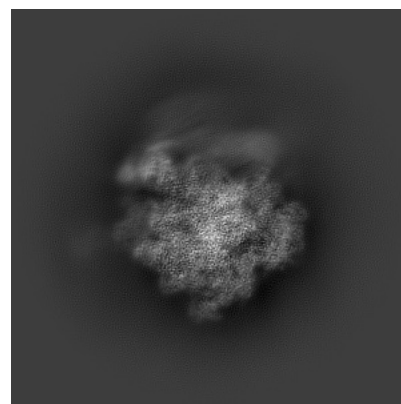
6.1.1 Primary map



X

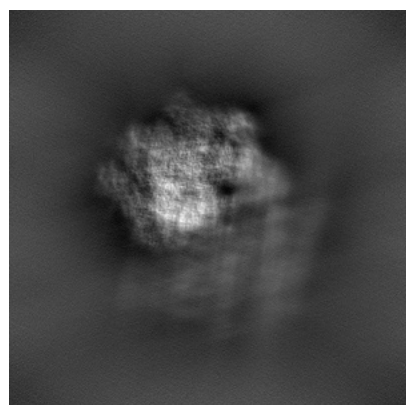


Y

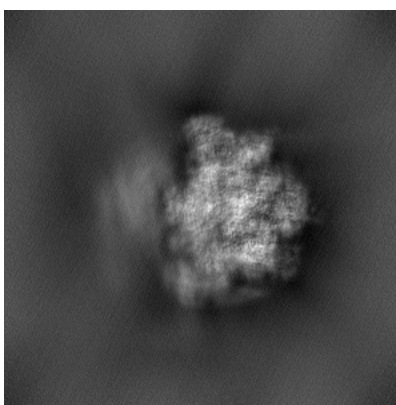


Z

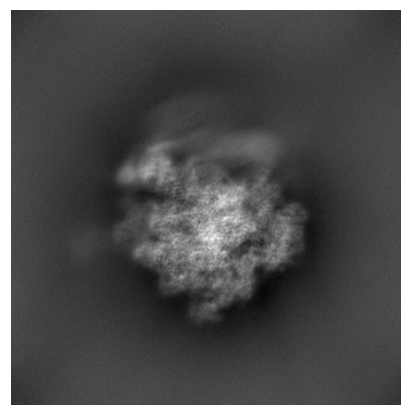
6.1.2 Raw map



X



Y

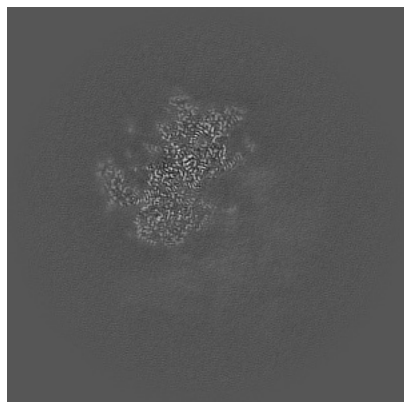


Z

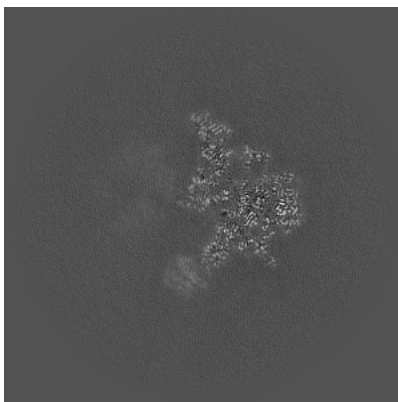
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

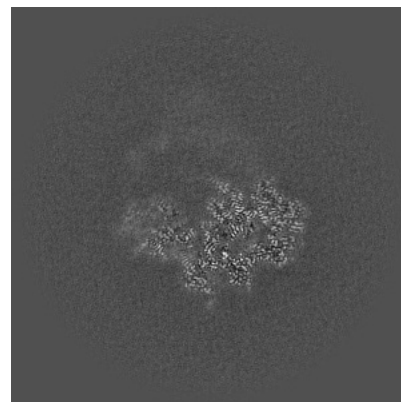
6.2.1 Primary map



X Index: 280

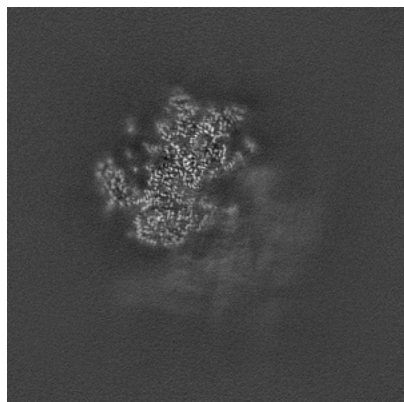


Y Index: 280

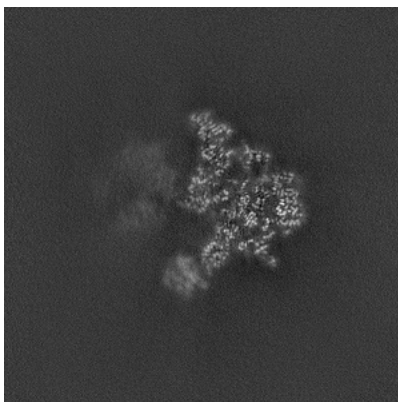


Z Index: 280

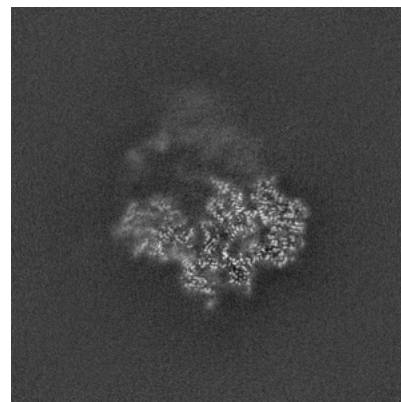
6.2.2 Raw map



X Index: 280



Y Index: 280

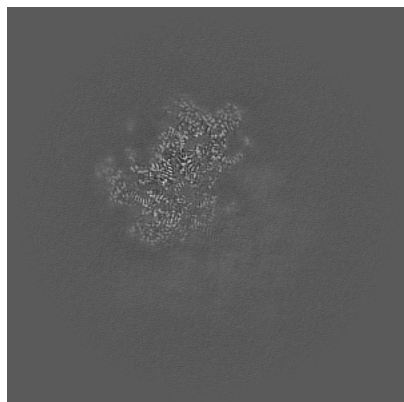


Z Index: 280

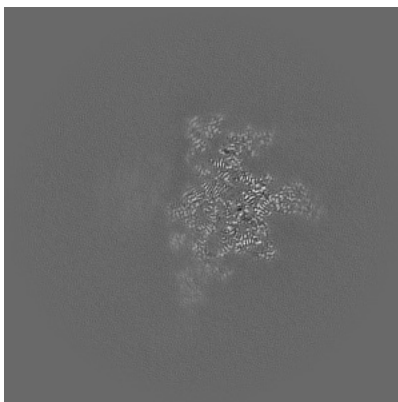
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

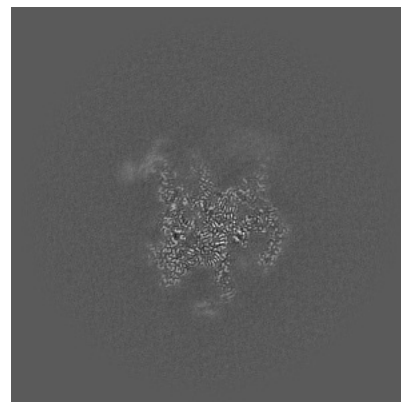
6.3.1 Primary map



X Index: 286

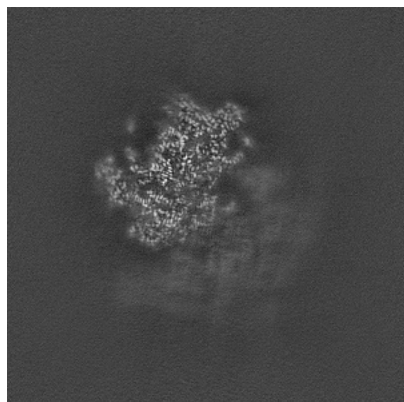


Y Index: 239

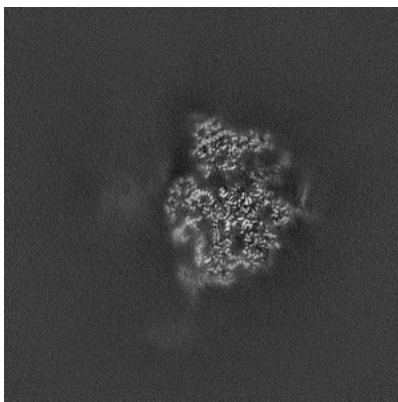


Z Index: 338

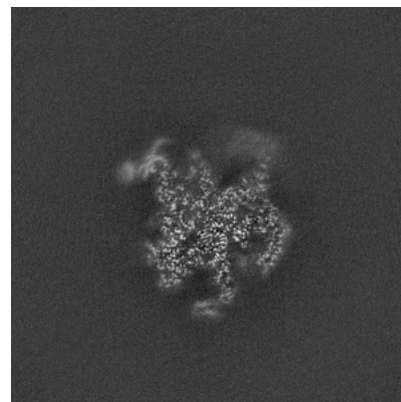
6.3.2 Raw map



X Index: 286



Y Index: 220

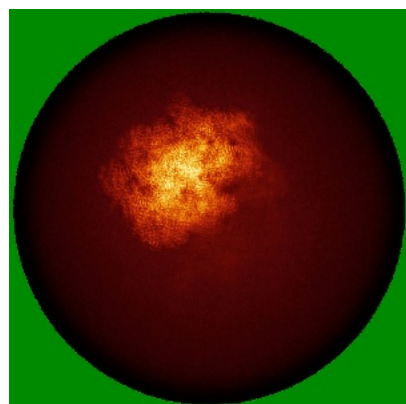


Z Index: 338

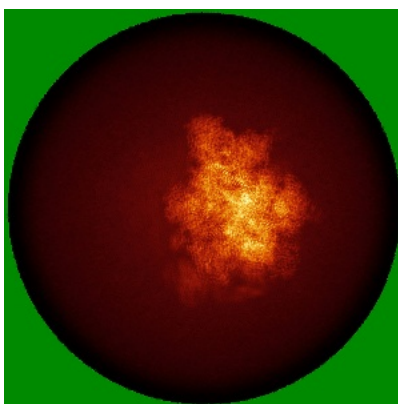
The images above show the largest variance slices of the map in three orthogonal directions.

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

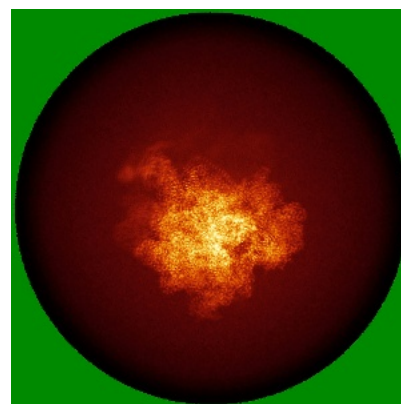
6.4.1 Primary map



X

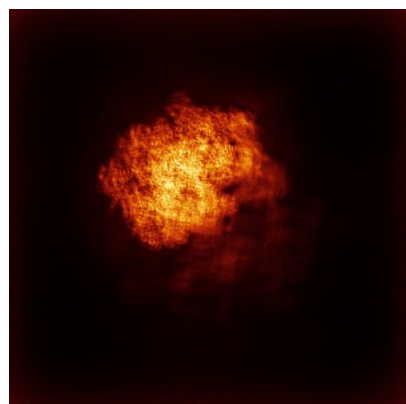


Y

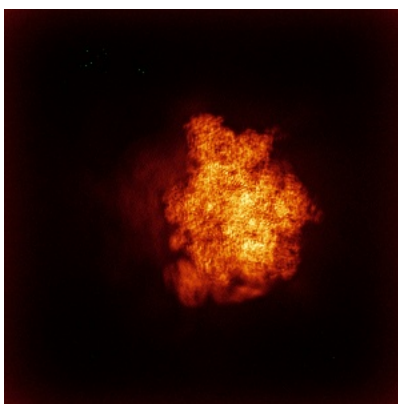


Z

6.4.2 Raw map



X



Y

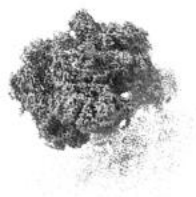


Z

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](#)

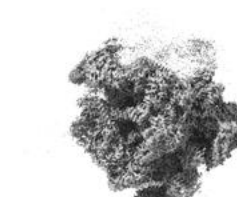
6.5.1 Primary map



X



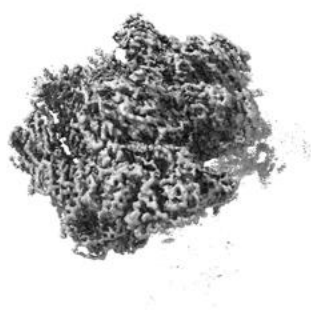
Y



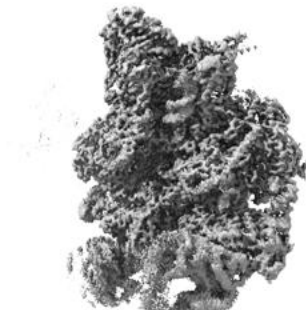
Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. 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.

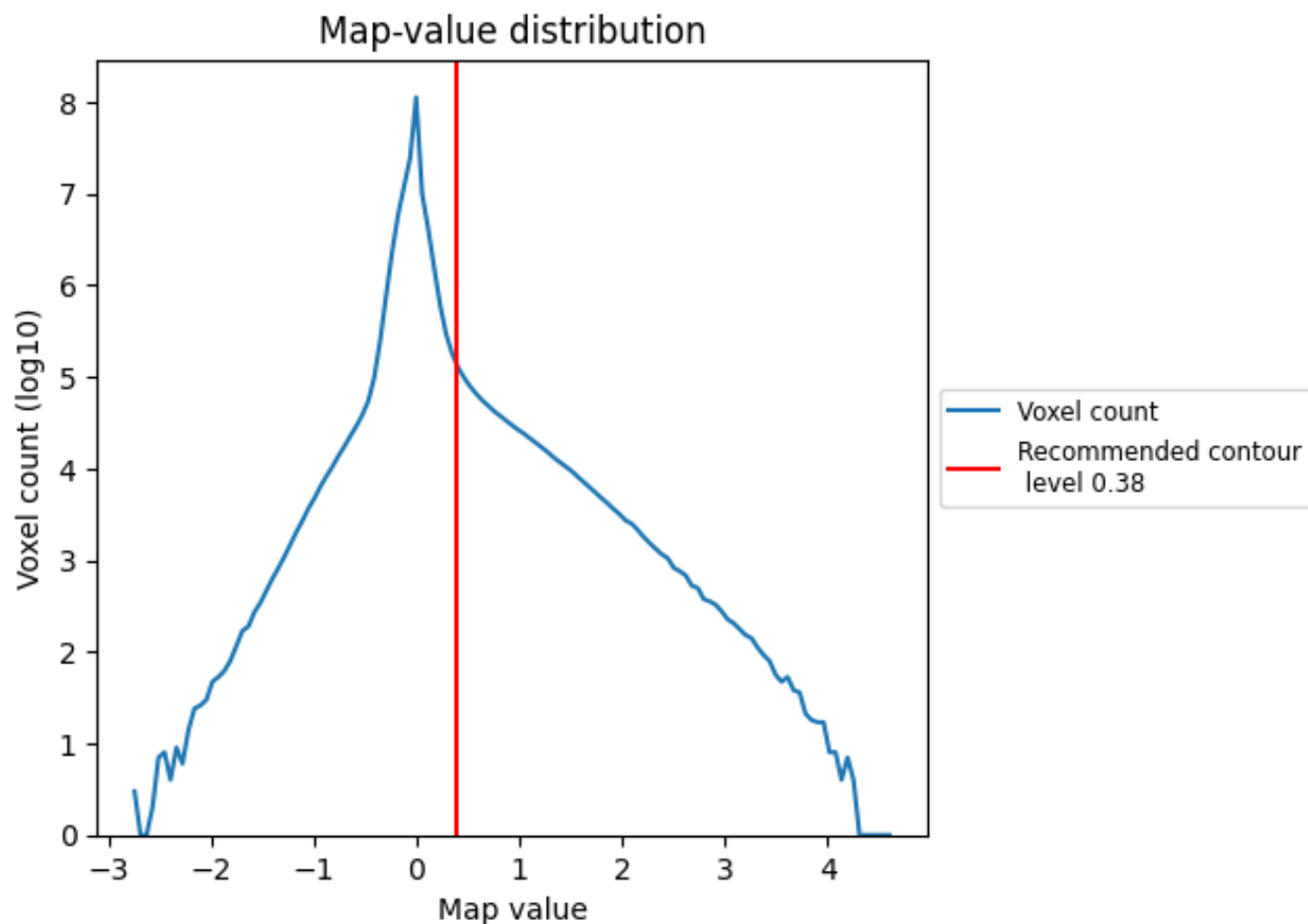
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

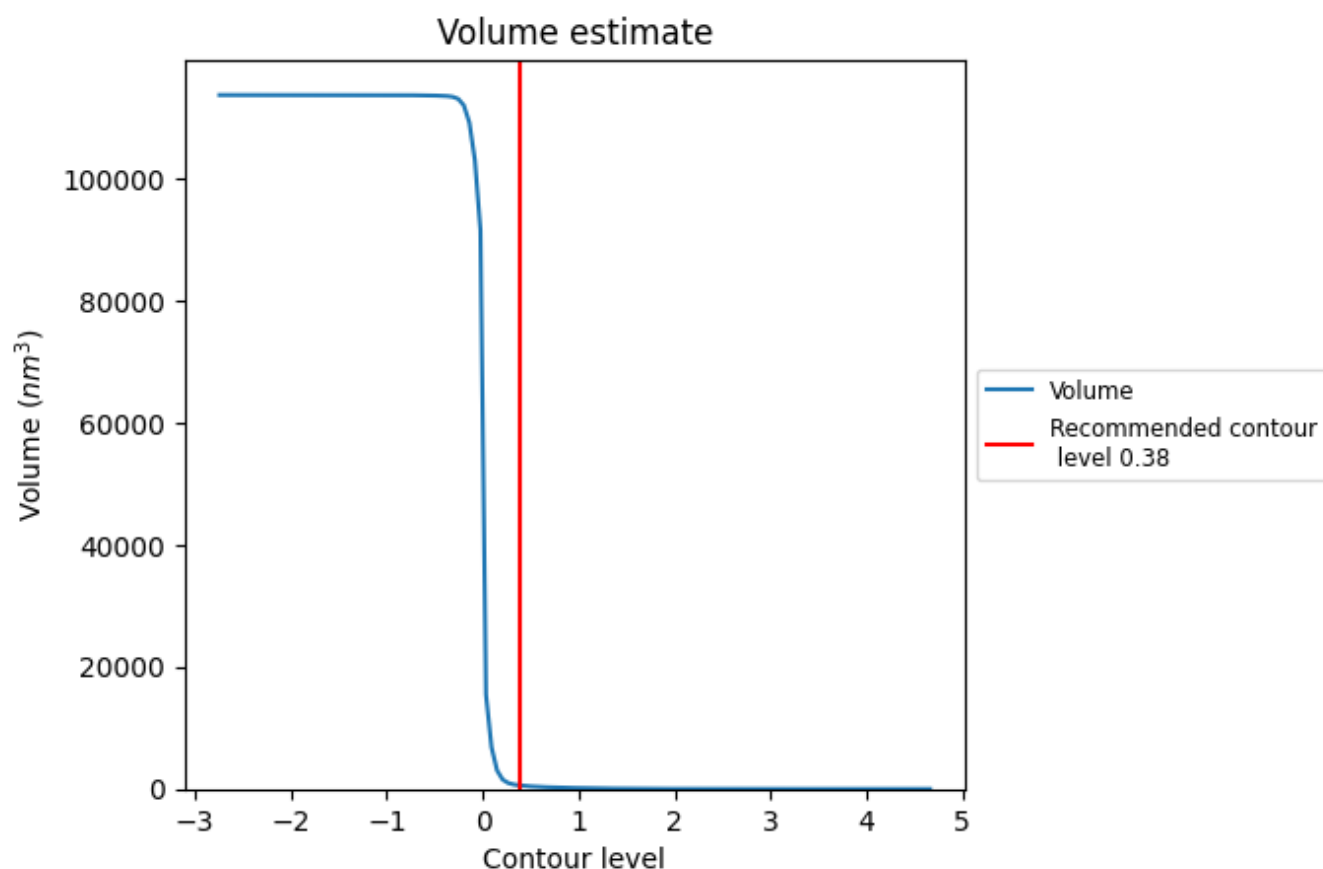
This section contains the results of statistical analysis of the map.

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.

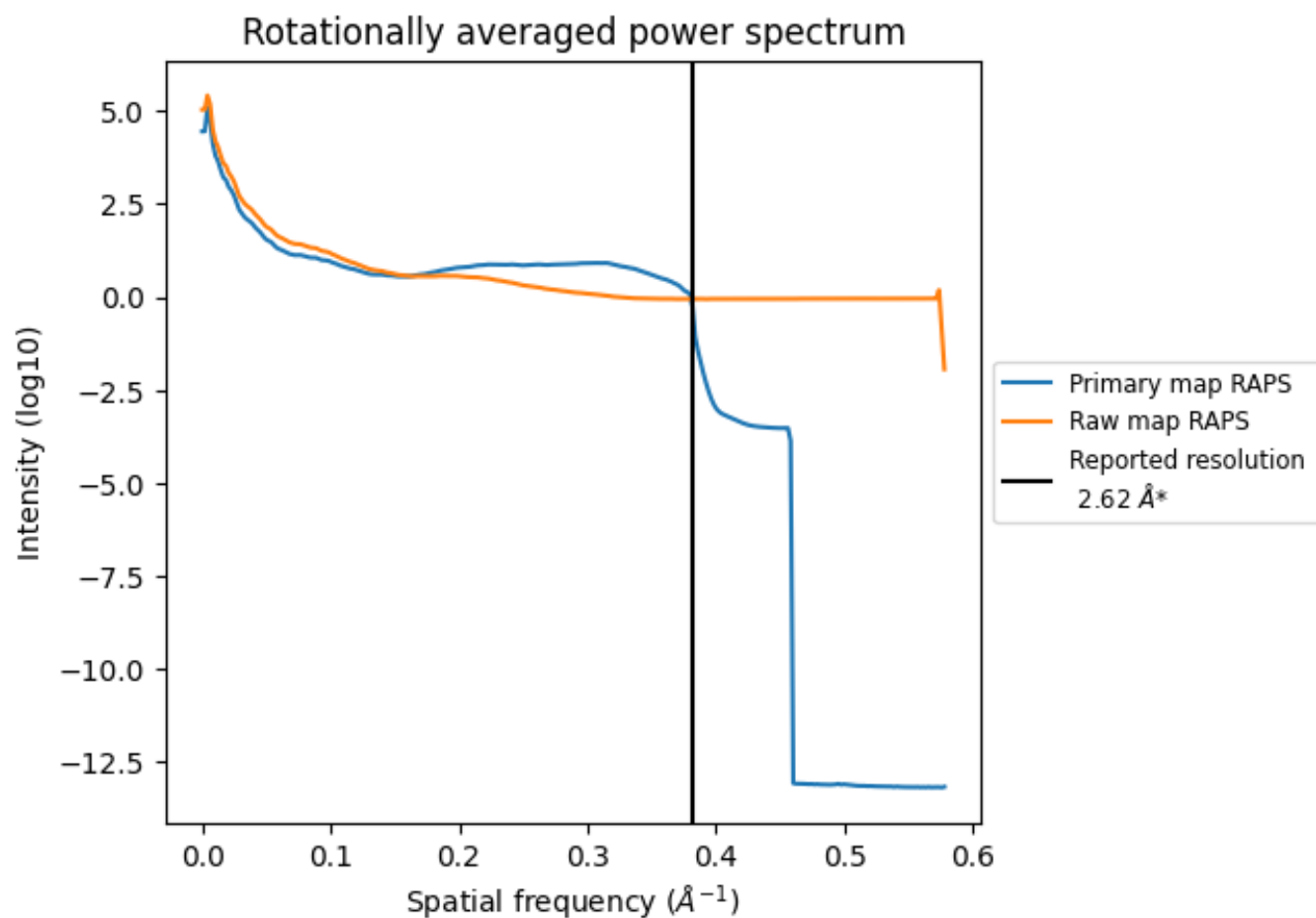
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 592 nm³; this corresponds to an approximate mass of 535 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 ⓘ

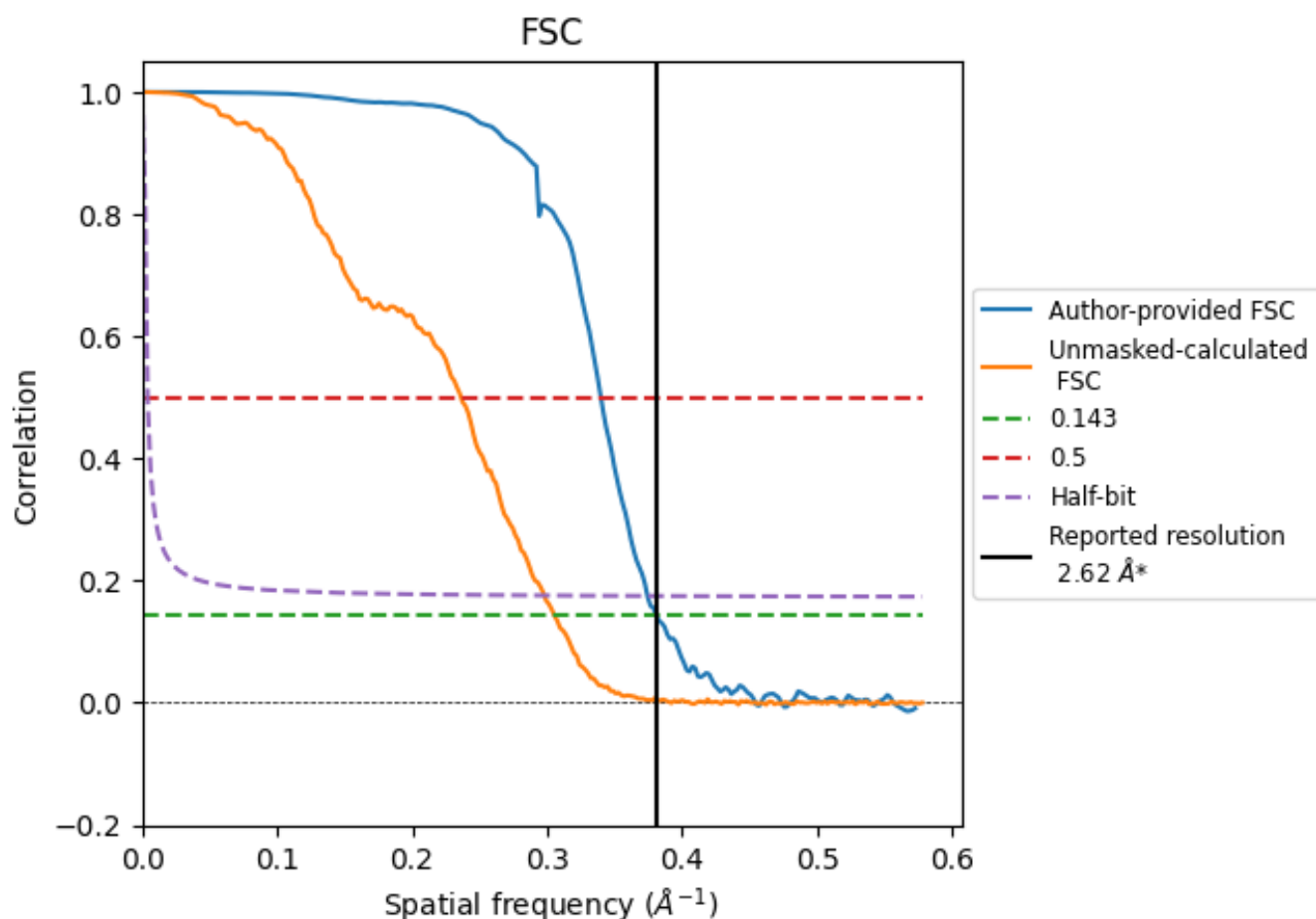


*Reported resolution corresponds to spatial frequency of 0.382 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.382 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

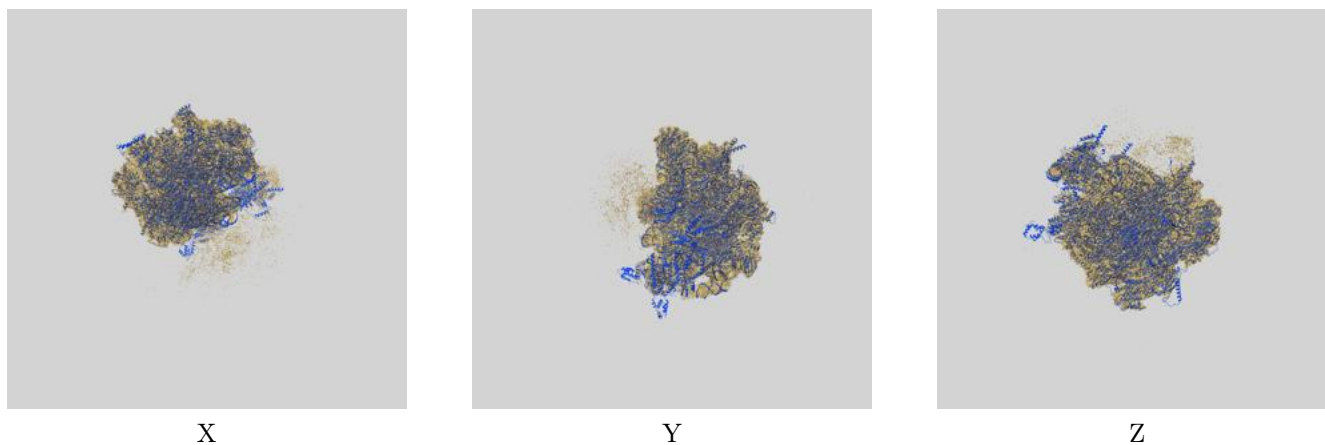
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.94	2.67
Unmasked-calculated*	3.27	4.23	3.36

*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 3.27 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

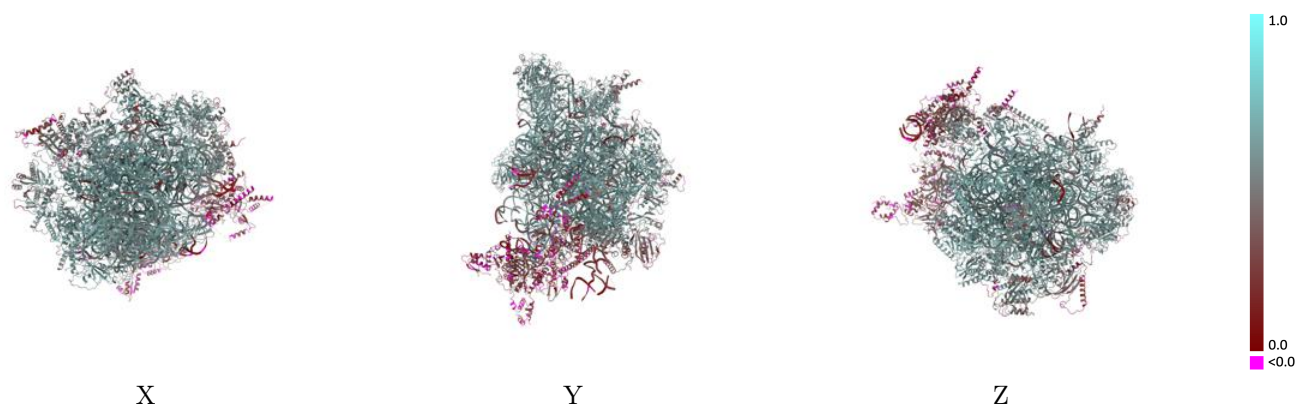
This section contains information regarding the fit between EMDB map EMD-45757 and PDB model 9CN3. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



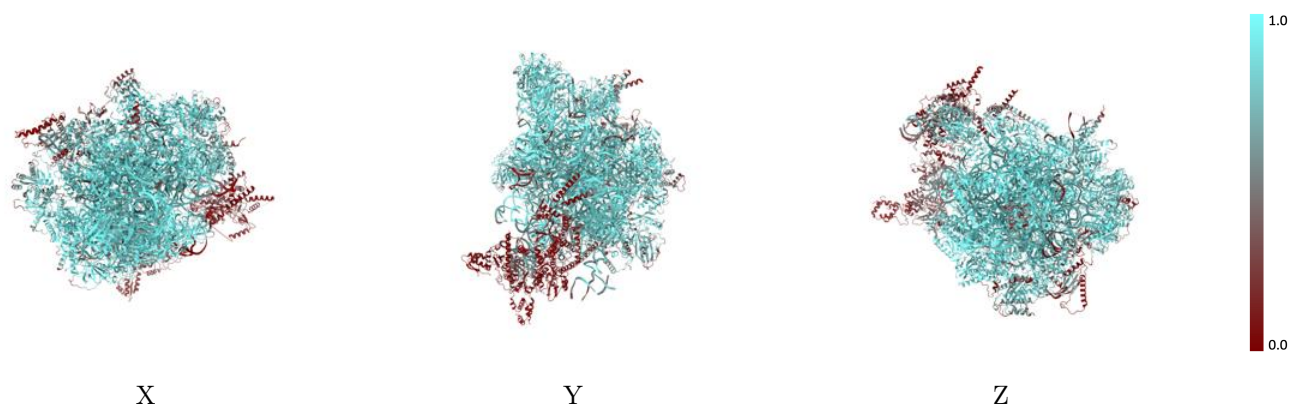
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



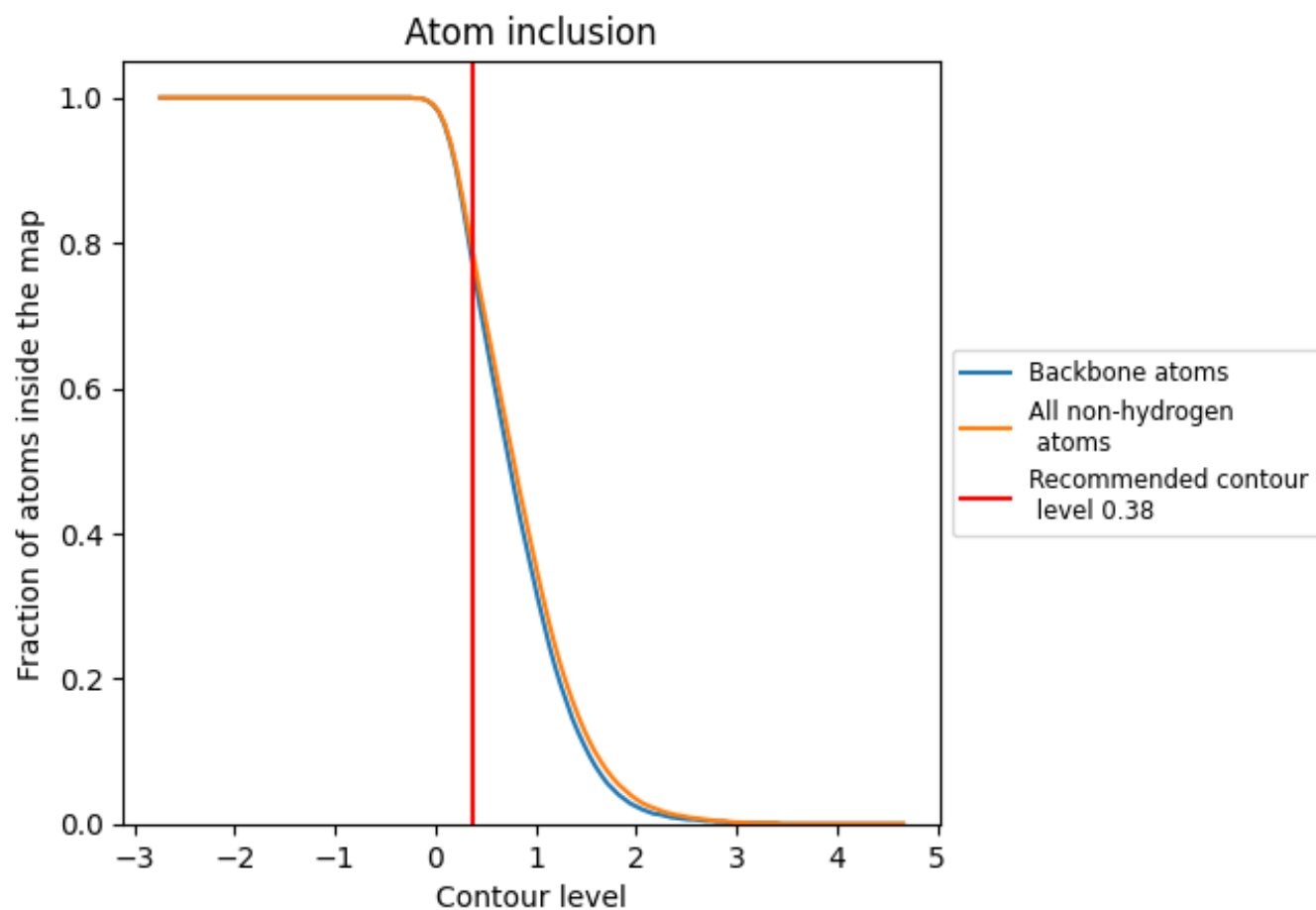
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5250
0	 0.8840	 0.5860
1	 0.8090	 0.5550
2	 0.9830	 0.6510
3	 0.9640	 0.6510
4	 0.9390	 0.6080
5	 0.8520	 0.5610
6	 0.7050	 0.4490
7	 0.7500	 0.5070
8	 0.1510	 0.1860
9	 0.7750	 0.5410
A	 0.8900	 0.5670
B	 0.6800	 0.2220
D	 0.8750	 0.5870
E	 0.8990	 0.5950
F	 0.9020	 0.6000
H	 0.7490	 0.5100
I	 0.3410	 0.2930
J	 0.1060	 0.1880
K	 0.9370	 0.6170
L	 0.8700	 0.5820
M	 0.8900	 0.5990
N	 0.8590	 0.5830
O	 0.9270	 0.6070
P	 0.8180	 0.5070
Q	 0.8540	 0.5870
R	 0.9320	 0.6180
S	 0.9500	 0.6200
T	 0.9220	 0.6250
TA	 0.0000	 0.1000
TB	 0.0000	 0.0950
TC	 0.0000	 0.0990
U	 0.7970	 0.5530
V	 0.5390	 0.4850
W	 0.9150	 0.6090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
X	 0.8270	 0.5680
Y	 0.9100	 0.5990
Z	 0.9450	 0.6270
a	 0.7170	 0.5100
b	 0.9470	 0.6200
c	 0.8330	 0.5610
d	 0.4200	 0.4060
e	 0.0830	 0.1650
f	 0.2070	 0.2670
g	 0.9000	 0.5900
h	 0.5180	 0.4440
i	 0.9430	 0.6320
j	 0.8100	 0.5520
k	 0.3390	 0.2760
l	 0.2530	 0.3000
m	 0.1440	 0.1790
o	 0.9230	 0.6150
p	 0.5740	 0.4420
q	 0.5340	 0.4170
r	 0.8410	 0.5380
s	 0.8790	 0.5800
u	 0.0090	 0.0780