



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:20 AM UTC

PDB ID : 7OID / pdb_00007oid
EMDB ID : EMD-12926
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 5A
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-05-11
Resolution : 3.70 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:

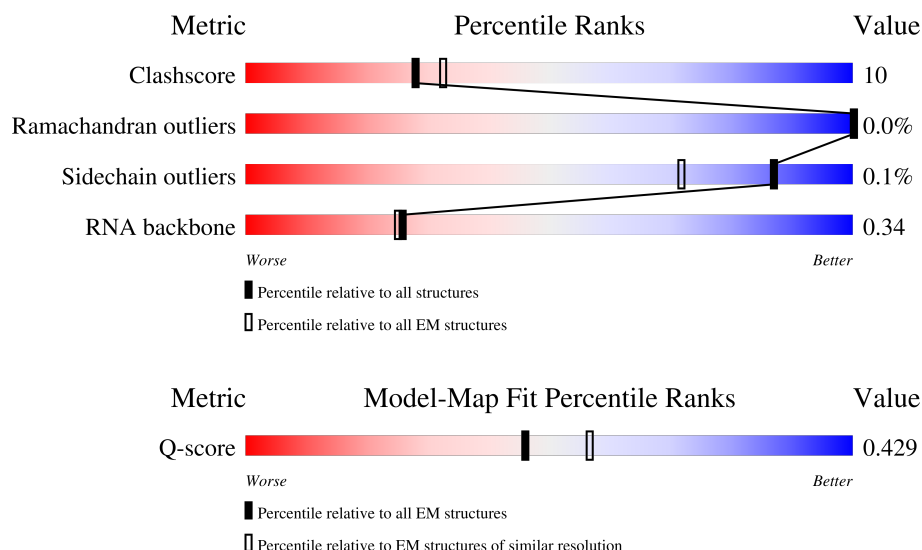
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.70 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.



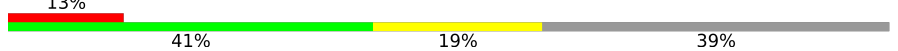
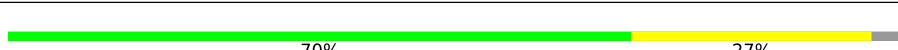
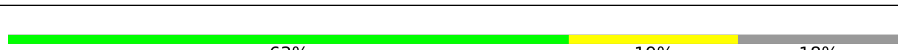
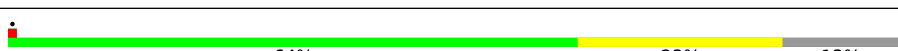
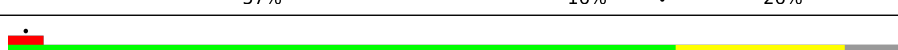
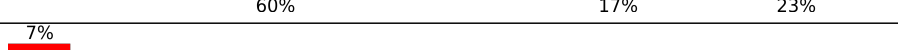
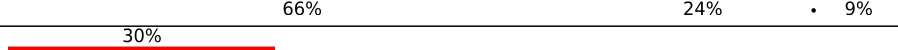
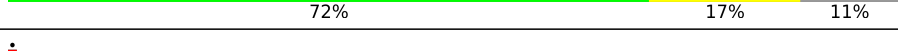
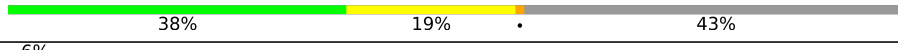
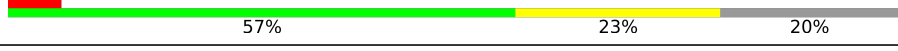
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	D	305	
2	E	348	
3	F	311	

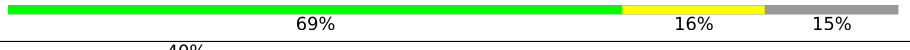
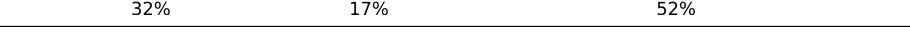
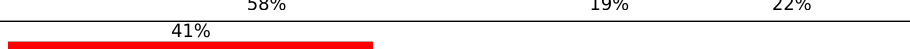
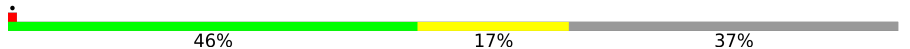
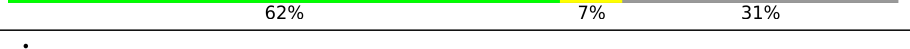
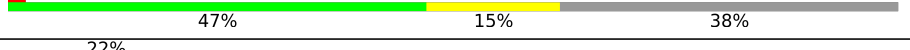
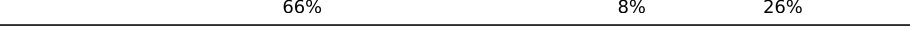
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Mol	Chain	Length	Quality of chain
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	180	
13	Q	292	
14	R	149	
15	S	205	
16	T	206	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	4	103	
28	5	423	

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Mol	Chain	Length	Quality of chain
29	6	380	
30	7	338	
31	8	206	
32	9	137	
33	a	142	
34	b	215	
35	c	332	
36	d	306	
37	e	279	
38	f	212	
39	g	166	
40	h	158	
41	i	128	
42	j	123	
43	k	112	
44	l	138	
45	m	128	
46	o	102	
47	p	206	
48	q	222	
49	r	196	
50	s	439	
51	u	234	
52	v	70	
53	w	156	

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Mol	Chain	Length	Quality of chain
54	A	1559	
55	B	69	
56	z	73	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 101125 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 L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	304	Total	C	N	O	S	0	0
			2396	1539	416	430	11		

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	95	Total	C	N	O	S	0	0
			784	498	152	134			

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	159	Total	C	N	O	S	0	0
			1305	835	239	224	7		

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	139	Total	C	N	O	S	0	0
			1154	734	220	197	3		

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	8		

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 27 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 28 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 29 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 30 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 31 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 32 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 33 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	73	Total	C	N	O	S	0	0
			611	385	115	106	5		

- Molecule 34 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 36 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 37 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 40 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 41 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 43 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 44 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 45 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	93	Total	C	N	O	S	0	0
			786	495	161	127	3		

- Molecule 47 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 48 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	164	Total	C	N	O	S	0	0
			1379	858	267	249	5		

- Molecule 49 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 50 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 51 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 52 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	69	Total	C	N	O	S	0	0
			588	372	116	100			

- Molecule 53 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 54 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	1472	Total	C	N	O	P	0	0
			31265	14027	5646	10120	1472		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1437	U	UNK	conflict	GB 1025814679

- Molecule 55 is a RNA chain called mitochondrial Val tRNA.

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

- Molecule 56 is a RNA chain called mitochondrial tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

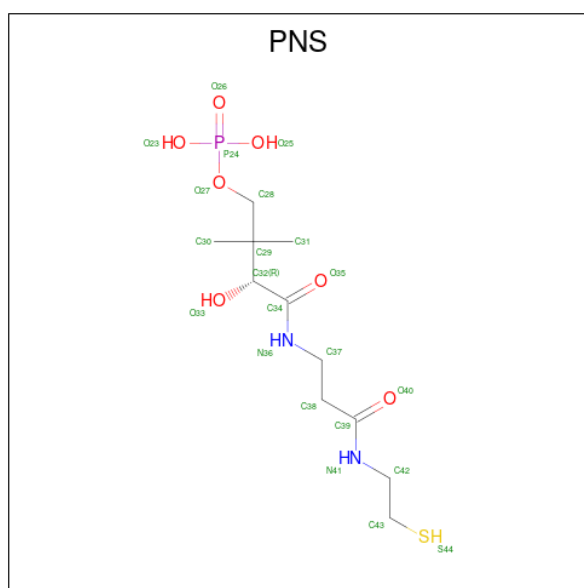
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	I	1	Total	Zn	0
			1	1	
57	0	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	g	1	Total	Mg	0
			1	1	
58	A	1	Total	Mg	0
			1	1	

- Molecule 59 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

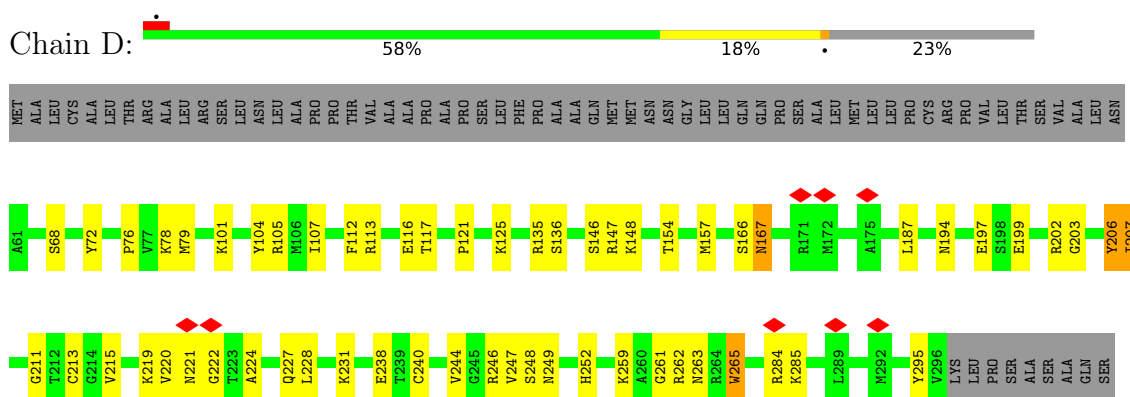


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
59	v	1	21	11	2	6	1	1	0

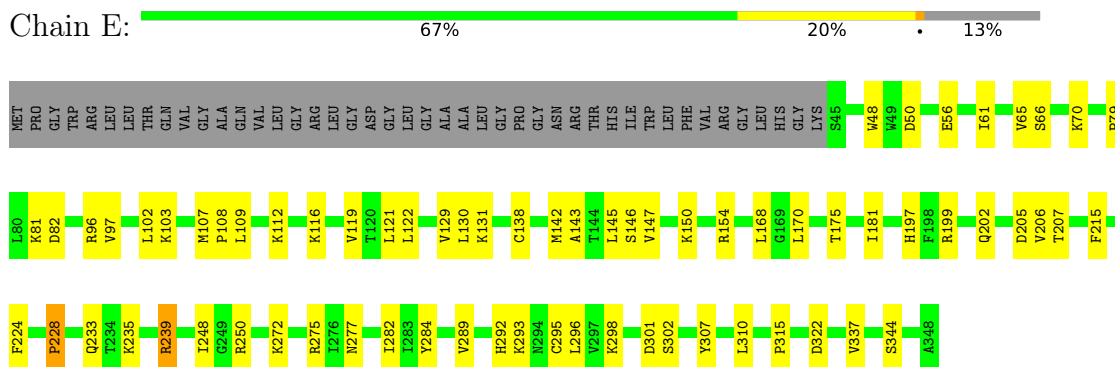
3 Residue-property plots

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

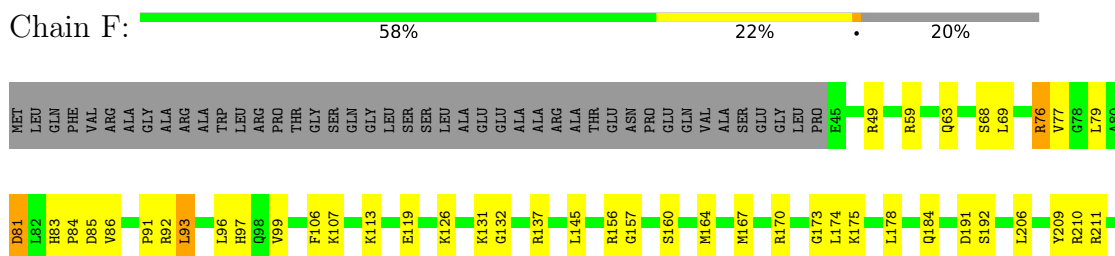
- Molecule 1: 39S ribosomal protein L2, mitochondrial



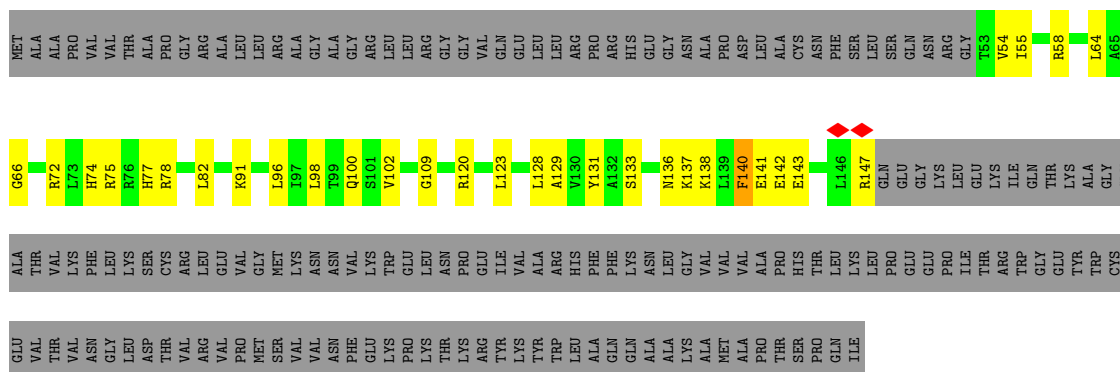
- Molecule 2: 39S ribosomal protein L3, mitochondrial



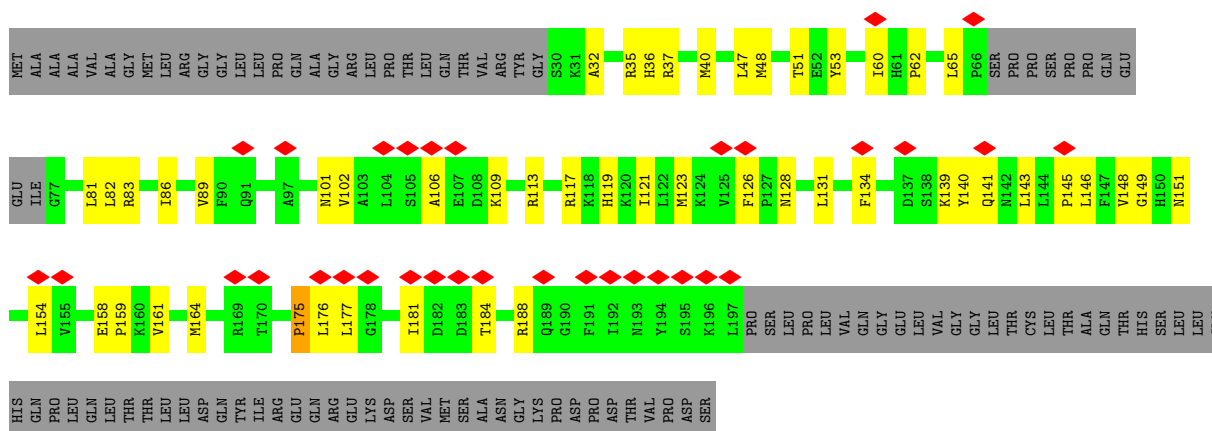
- Molecule 3: 39S ribosomal protein L4, mitochondrial



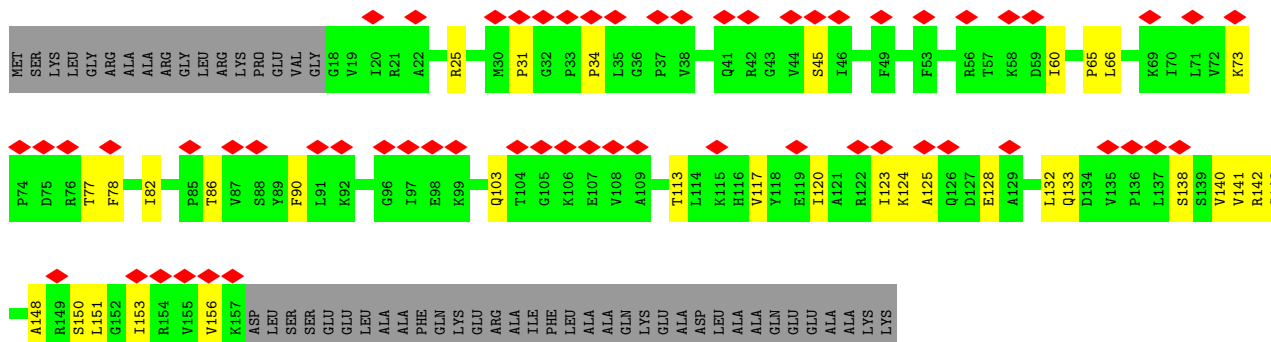
Chain H: 24% 11% 64%



Chain I:

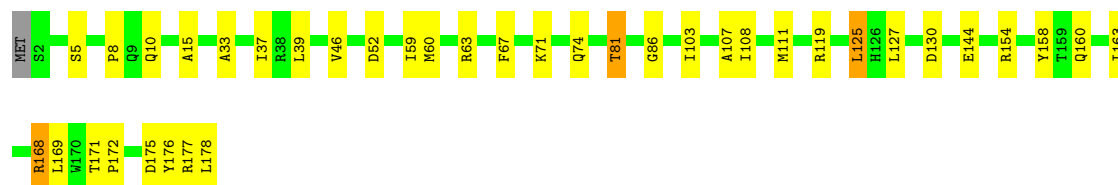


Chain J:



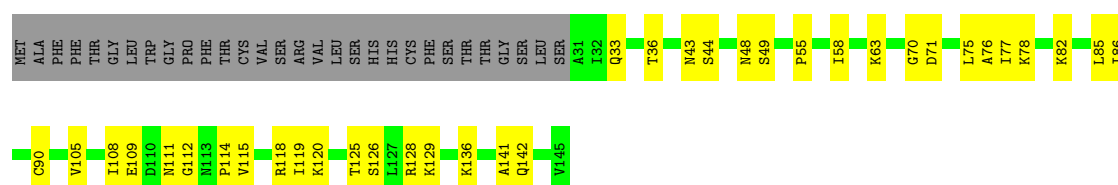
- Molecule 7: 39S ribosomal protein L13, mitochondrial

Chain K:  78% 20% ..



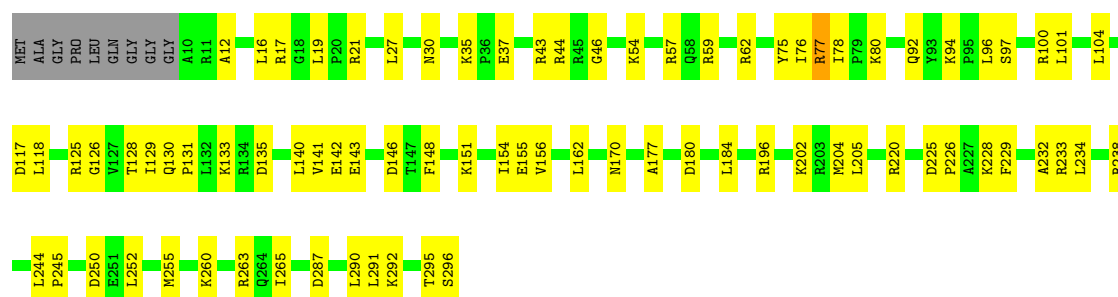
- Molecule 8: 39S ribosomal protein L14, mitochondrial

Chain L:  54% 25% 21%



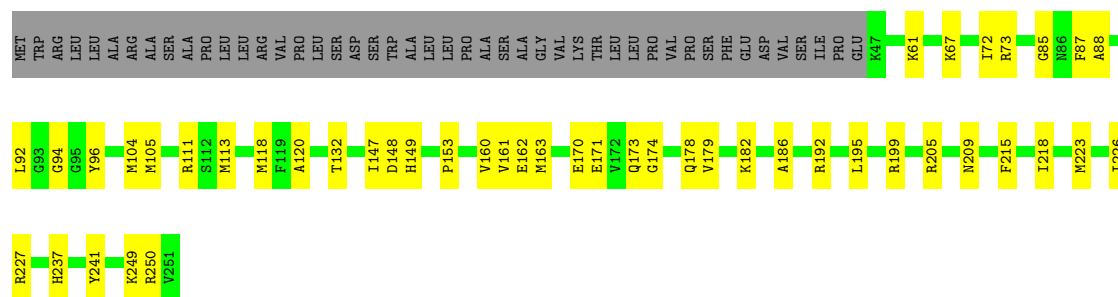
- Molecule 9: 39S ribosomal protein L15, mitochondrial

Chain M:  70% 27% .



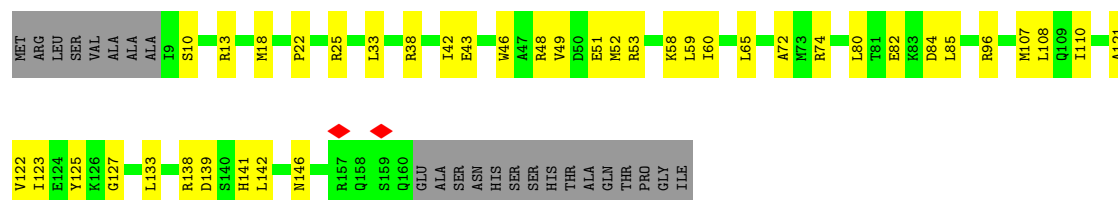
- Molecule 10: 39S ribosomal protein L16, mitochondrial

Chain N:  63% 19% 18%



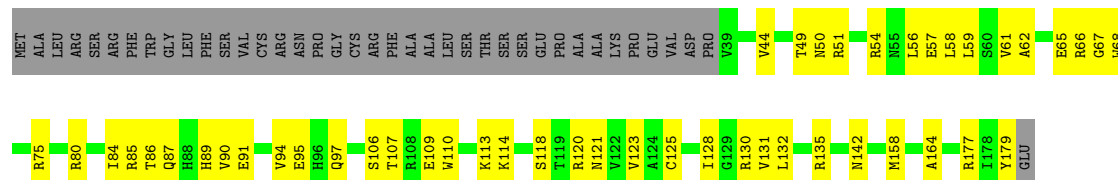
- Molecule 11: 39S ribosomal protein L17, mitochondrial

Chain O:  64% 23% 13%



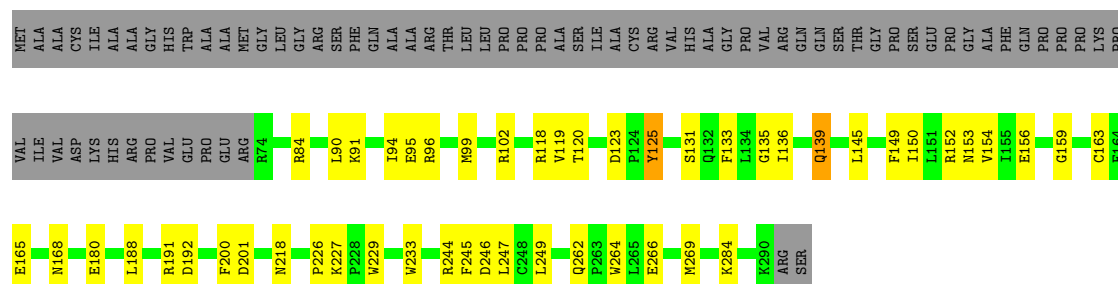
- Molecule 12: 39S ribosomal protein L18, mitochondrial

Chain P:



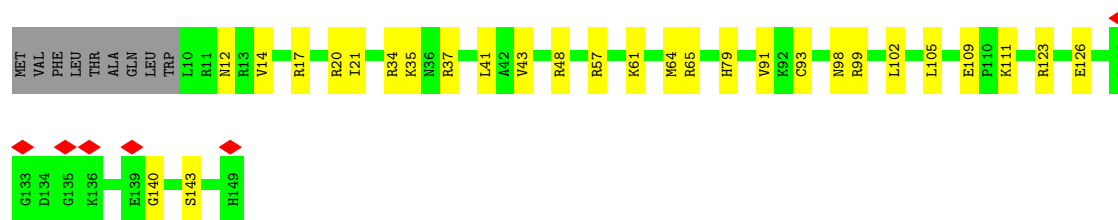
- Molecule 13: 39S ribosomal protein L19, mitochondrial

Chain Q:



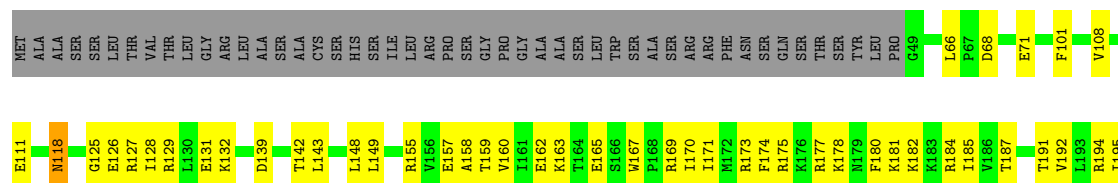
- Molecule 14: 39S ribosomal protein L20, mitochondrial

Chain R:



- Molecule 15: 39S ribosomal protein L21, mitochondrial

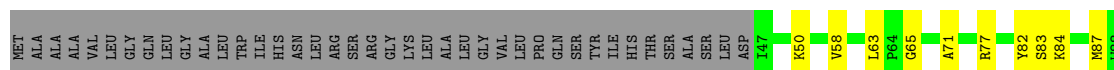
Chain S:





- Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T: 60% 17% 23%



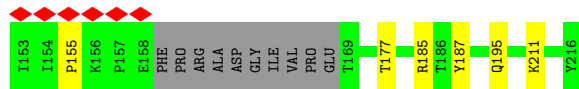
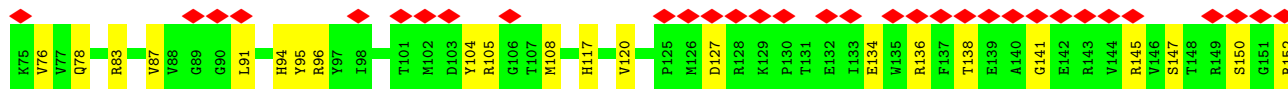
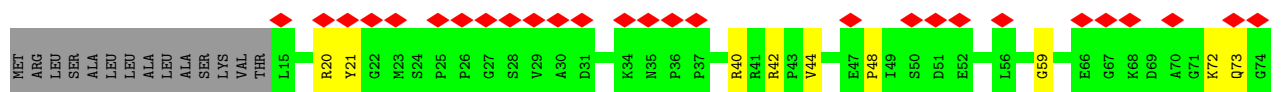
- Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U: 7% 66% 24% 9%



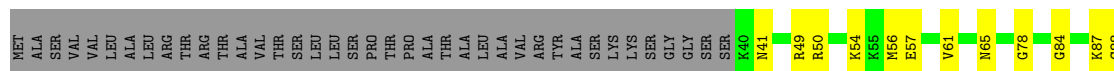
- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 30% 72% 17% 11%



- Molecule 19: 39S ribosomal protein L27, mitochondrial

Chain W: 55% 18% 26%



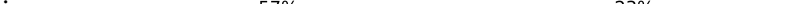
- Molecule 20: 39S ribosomal protein L28, mitochondrial

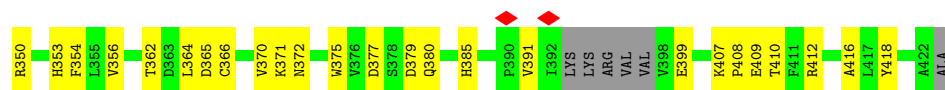
R216	E220	I235	Q236	Q237	Q240	Q241	A242	L243	S244	GLU	PRO	ALA	VAL	VAL	GLN	LYS	ARG	ALA	SER	GLY	GLN	MT	P2	K5	L14	I20	R23	H42	Y43	I52	K55	N56	R61	V62	E63	G62	I66	D95	K96	F114	L119	D120	K121	K122	D136	E151	R163	L166	L167	R168	L176	H177	D180	R184	D189	K192	I196
------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- [illegible]

- | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|
| Met | Ala | Gly | Ile | Leu | Arg | Val | Val | Gln | Trp | Pro | Pro | Gly | Arg | Leu | Gln | Thr | Val | Thr | Lys | Gly | Val | Glu | Ser | Leu | Ile | Cys | Thr | Asp | Thr | Ile | Arg | His | K35 |
| V112 | L116 | I117 | L122 | K123 | M134 | E144 | Q148 | W149 | H150 | L151 | V154 | Glu | Gln | Lys | Ala | His | Glu | Ser | | | | | | | | | | | | | | | |

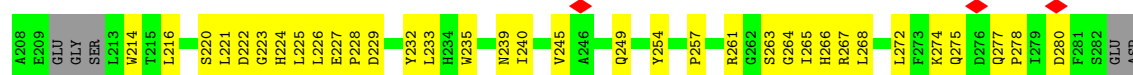
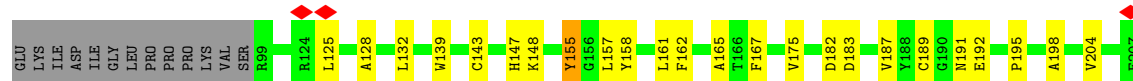
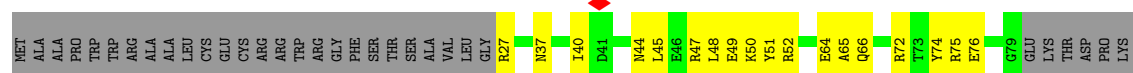
- | | | | |
|------|-----|------|-----|
| Q144 | THR | ASP | MET |
| L159 | GLY | THR | ALA |
| Y160 | SER | GLY | LEU |
| S166 | LYS | SER | ALA |
| E167 | GLU | LYS | LEU |
| R173 | ASN | ASN | VAL |
| I174 | SER | SER | VAL |
| R177 | LEU | LEU | SER |
| T186 | ASP | ASP | PRO |
| GLN | SER | TRP | TRP |
| ASN | ILE | ASP | ALA |
| | PHE | ILE | ALA |
| | TRP | PHE | ALA |
| | MET | TRP | ARG |
| A79 | LEU | MET | GLY |
| A80 | ARG | LEU | VAL |
| P81 | ASN | ARG | LEU |
| R84 | TYR | ASN | ASN |
| R85 | TRP | TYR | TRP |
| I87 | GLU | TRP | GLU |
| N90 | LEU | ARG | ARG |
| R91 | LEU | LEU | LEU |
| C92 | LYS | ARG | LEU |
| A93 | LEU | LYS | LEU |
| R94 | PRO | C92 | PRO |
| R95 | GLN | A93 | GLN |
| N96 | SER | R94 | SER |
| P97 | ARG | R95 | ARG |
| L100 | PRO | N96 | PRO |
| N106 | GLY | P97 | GLY |
| I107 | SER | L100 | PHE |
| D108 | PRO | N106 | SER |
| V109 | PRO | I107 | PRO |
| C110 | TRP | D108 | PRO |
| E112 | GLY | V109 | TRP |
| C113 | PRO | C110 | GLY |
| G114 | ALA | E112 | PRO |
| H115 | LEU | C113 | ALA |
| L116 | ALA | G114 | LEU |
| E133 | VAL | H115 | ALA |
| E136 | GLN | L116 | VAL |
| I137 | PRO | E133 | GLN |
| R138 | ALA | E136 | GLY |
| R139 | MET | I137 | ALA |
| Q140 | THR | R138 | PRO |
| I141 | PHE | R139 | THR |
| G142 | GLU | Q140 | GLU |
| Z143 | PRO | I141 | PRO |
| | ASN | G142 | ASN |
| | | Z143 | ALA |

- Chain 1:  6% 57% 23% 14%



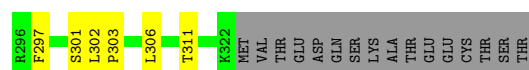
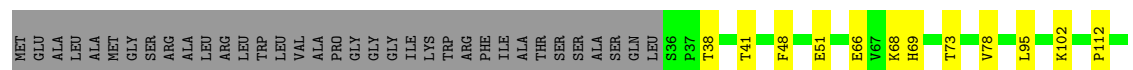
- Molecule 29: 39S ribosomal protein L38, mitochondrial

Chain 6: 58% 27% 15%



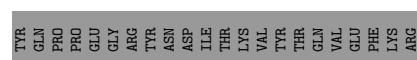
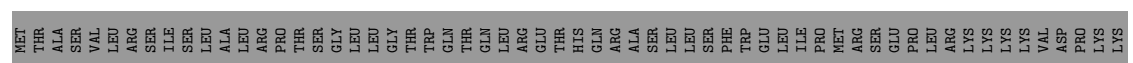
- Molecule 30: 39S ribosomal protein L39, mitochondrial

Chain 7: 69% 16% 15%



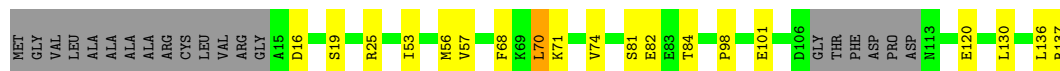
- Molecule 31: 39S ribosomal protein L40, mitochondrial

Chain 8: 40% 32% 17% 52%



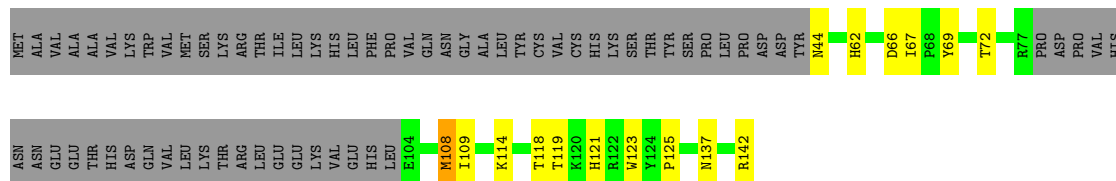
- Molecule 32: 39S ribosomal protein L41, mitochondrial

Chain 9: 



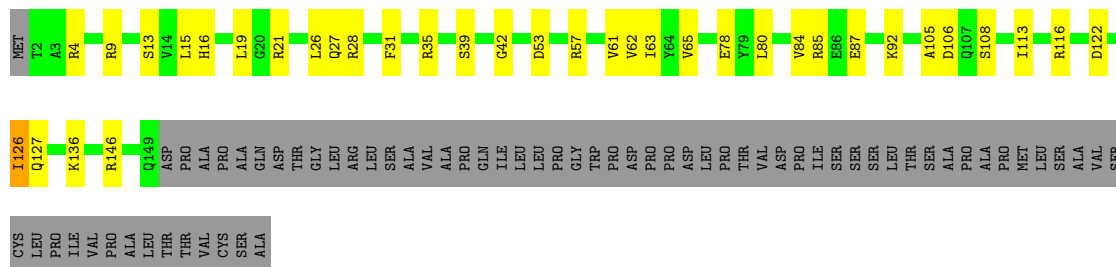
- Molecule 33: 39S ribosomal protein L42, mitochondrial

Chain a: 



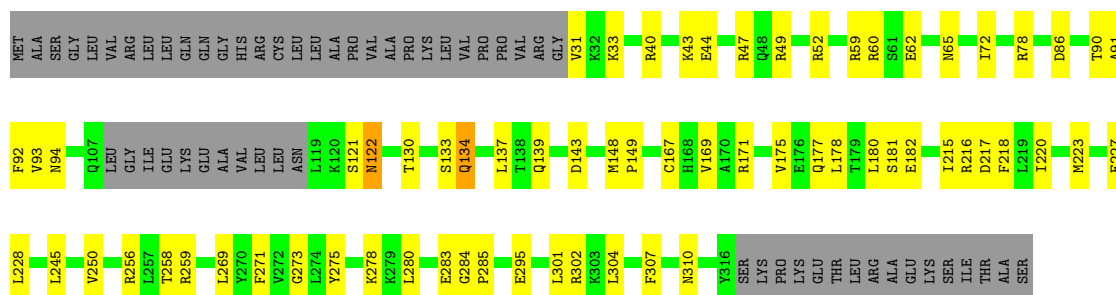
- Molecule 34: 39S ribosomal protein L43, mitochondrial

Chain b: 

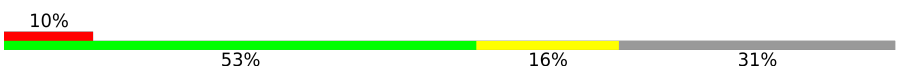


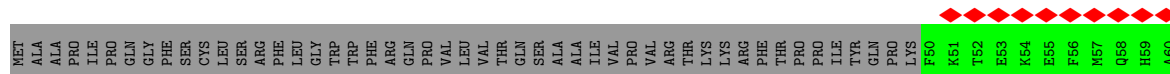
- Molecule 35: 39S ribosomal protein L44, mitochondrial

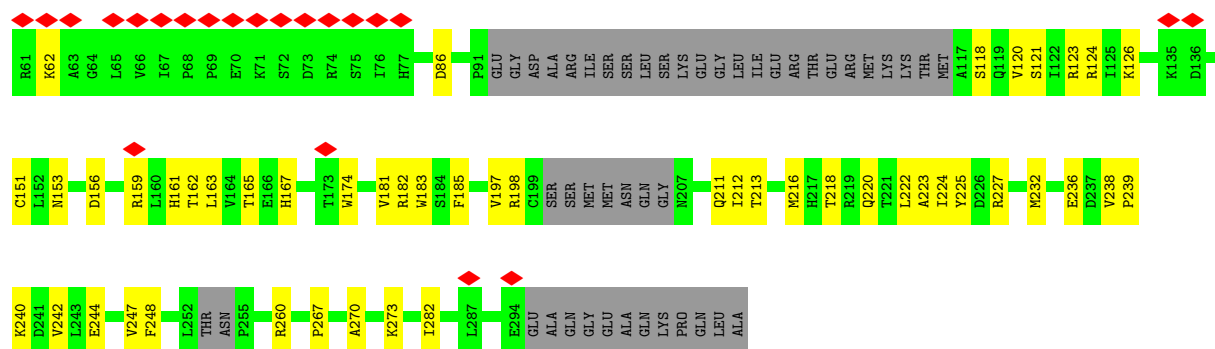
Chain c: 



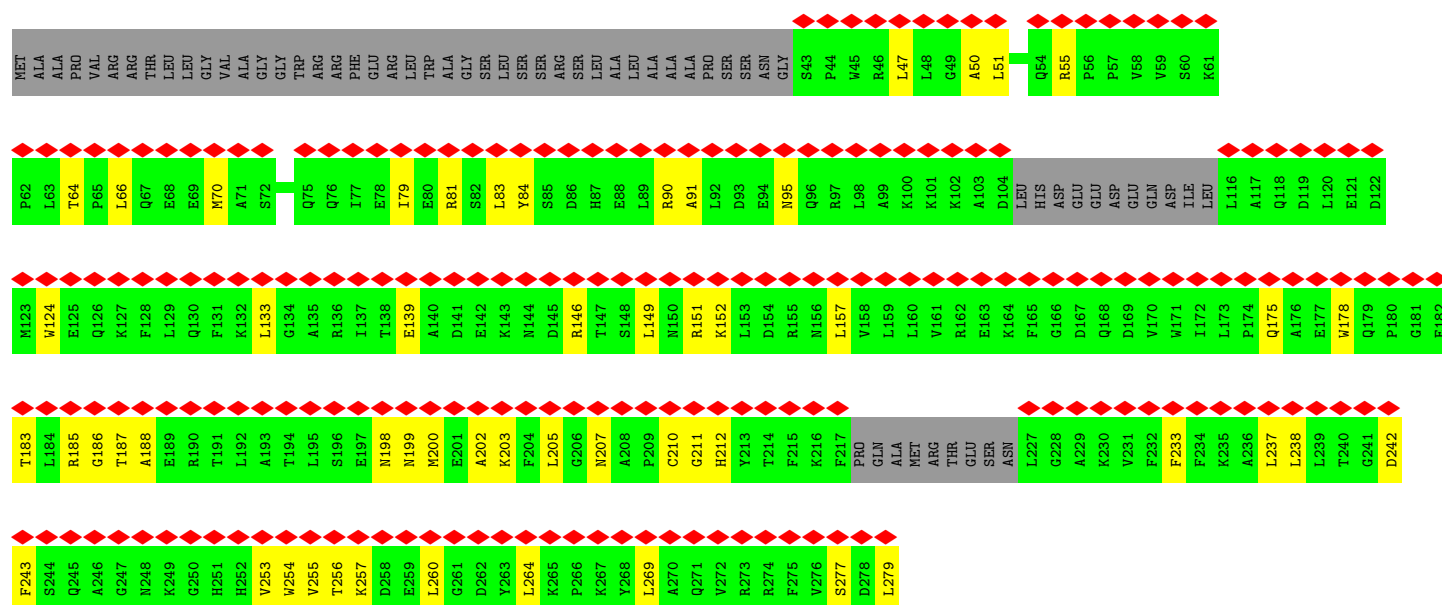
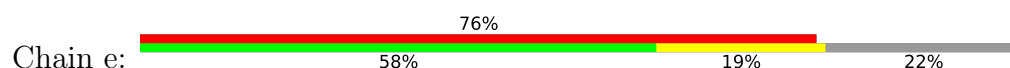
- Molecule 36: 39S ribosomal protein L45, mitochondrial

Chain d: 

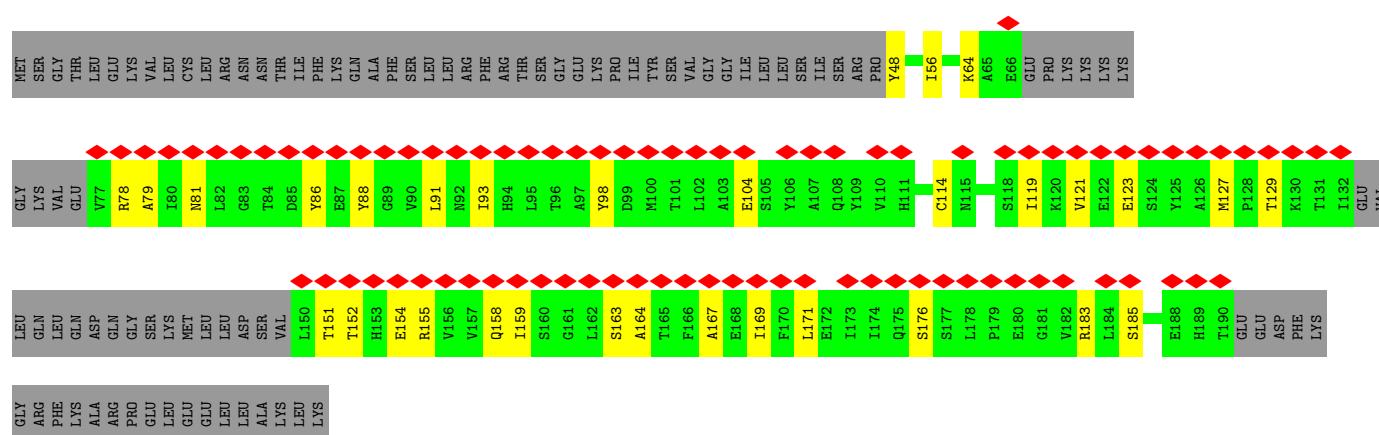
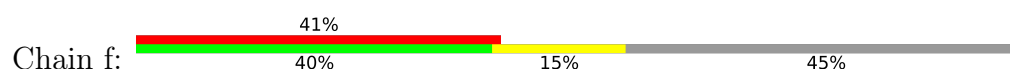




• Molecule 37: 39S ribosomal protein L46, mitochondrial

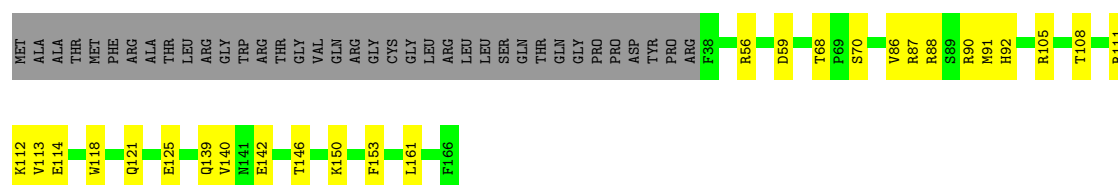


• Molecule 38: 39S ribosomal protein L48, mitochondrial

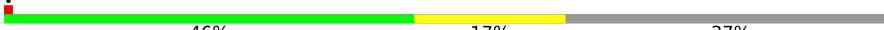


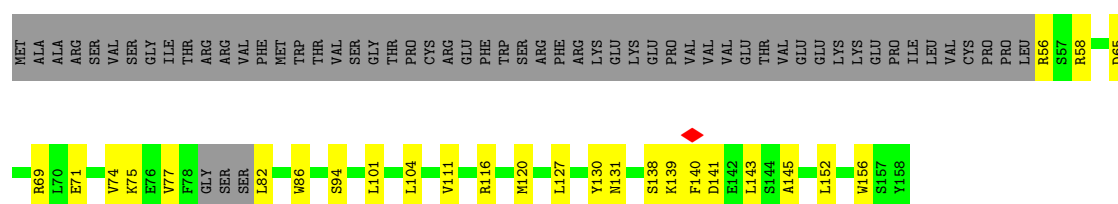
- Molecule 39: 39S ribosomal protein L49, mitochondrial

Chain g:  62% 16% 22%



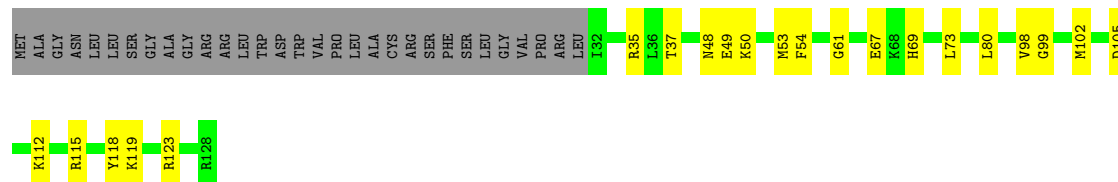
- Molecule 40: 39S ribosomal protein L50, mitochondrial

Chain h:  46% 17% 37%



- Molecule 41: 39S ribosomal protein L51, mitochondrial

Chain i:  59% 16% 24%

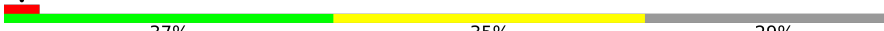


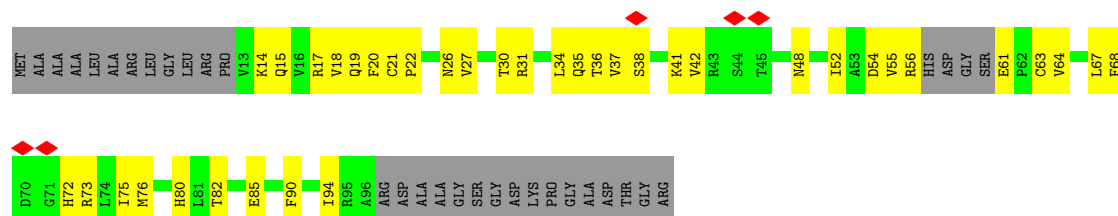
- Molecule 42: 39S ribosomal protein L52, mitochondrial

Chain j:  62% 7% 31%



- Molecule 43: 39S ribosomal protein L53, mitochondrial

Chain k:  37% 35% 29%



- Molecule 44: 39S ribosomal protein L54, mitochondrial

- Molecule 45: 39S ribosomal protein L55, mitochondrial

Chain m:

35%
26%
9%
65%

MET
ALA
ALA
VAL
GLY
SER
LEU
LEU
ARG
ARG
LEU
ARG
GLN
THR
THR
VAL
LYS
LYS
ALA
THR
THR
GLY
PRO
ALA
LEU
ARG
ARG
LEU
HIS
THR
THR
SER
SER
TRP
ARG
ALA
D34
S35
S36
R37
A38
S39
L40
T41
R42
V43
H44
R45
Q46
A47
Y48
A49
R50
L51
Y52
P53
V54
L55
L56
V57
K58
Q59
D60

G61
S62
T63
I64
H65
T66
R67
Y68
R69
E70
P71
R72
R73
W74
L75
A76
W77
P78
I79
ASP
LEU
LEU
ASP
THR
THR
LEU
SER
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PRO
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GLN
SER
ARG
ARG
LYS
GLU
TYR
GLU
GLN
GLU
LEU
SER
ASP
ASP
LEU
HIS
VAL
GLU
ARG
TYR
ARG

GLN
PHE
TRP
THR
ARG
THR
LYS
LYS

- Molecule 46: Ribosomal protein 63, mitochondrial

Chain of:

CoT Type	Category
G10	70%
I11	70%
I12	70%
P13	70%
G14	70%
I15	70%
I18	70%
R23	70%
S28	70%
L29	70%
R38	70%
M45	70%
Y53	70%
M54	70%
T55	70%
R56	70%
E57	70%
R66	70%
T79	70%
P83	70%
P84	70%
H85	70%
I88	70%
L92	70%
L95	70%
W101	70%
S102	70%

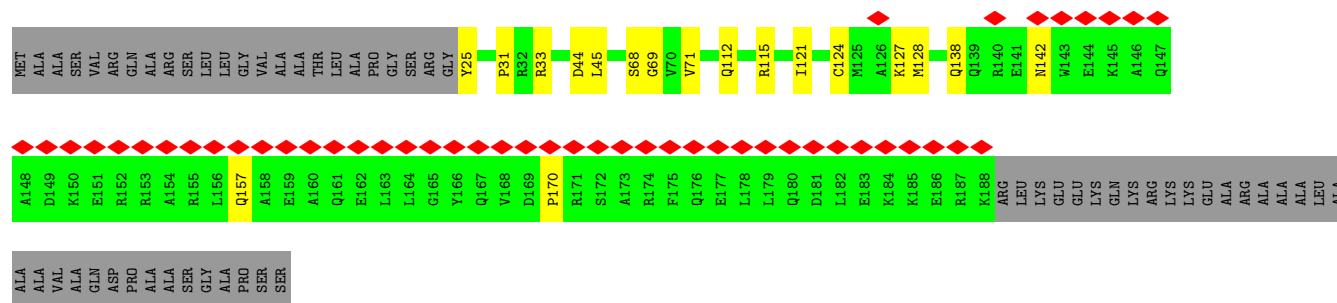
- Molecule 47: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:

Residue	Category
MET	Green
ALA	Green
ALA	Green
THR	Green
ARG	Green
CYS	Green
LEU	Green
ARG	Green
TRP	Green
GLY	Green
LEU	Green
SER	Green
ARG	Green
ALA	Green
GLY	Green
VAL	Green
TRP	Green
LEU	Green
PRO	Green
PRO	Green
PRO	Green
ALA	Green
ARG	Green
CYS	Green
PRO	Green
ARG	Green
ARG	Green
ALA	Green
LEU	Green
HIS	Green
GLN	Green
LYS	Green
LYS	Green
ASP	Green
GLY	Green
THR	Green
E38	Green
F39	Green
K40	Yellow
Y43	Yellow
G54	Yellow
S55	Yellow
D56	Yellow
T57	Yellow
R60	Grey
V61	Green
PRO	Grey
ASN	Grey
THR	Grey
GLY	Grey
ALA	Grey
LYS	Grey
GLN	Grey
ALA	Grey
ASP	Grey
SER	Grey
E76	Green

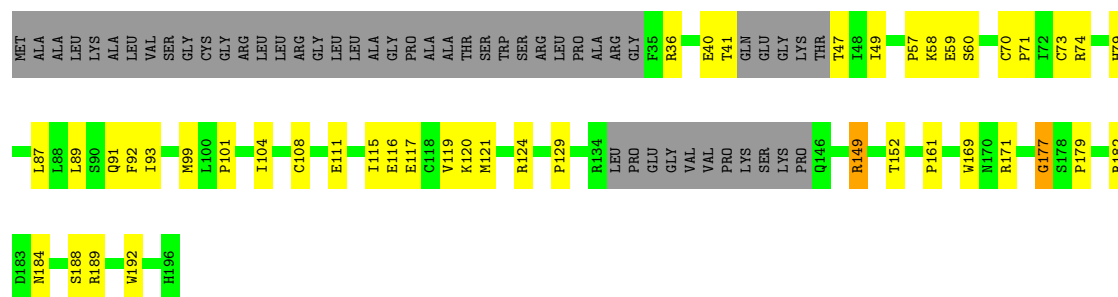
- Molecule 48: Growth arrest and DNA damage-inducible proteins-interacting protein 1





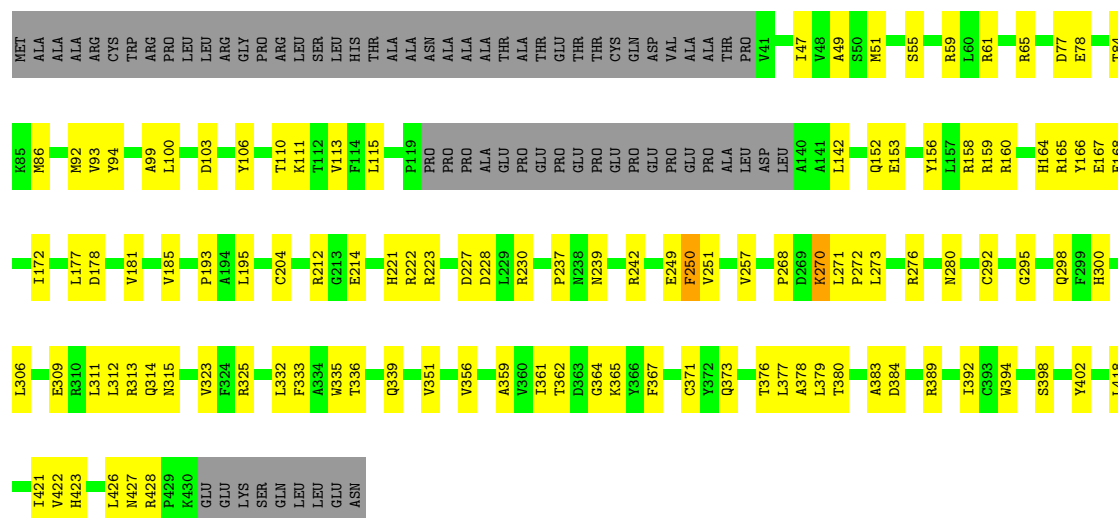
- Molecule 49: 39S ribosomal protein S18a, mitochondrial

Chain r: 52% 21% 26%



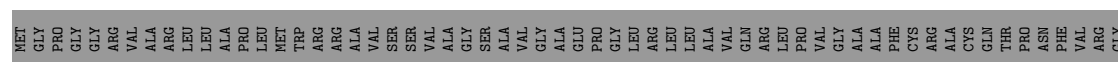
- Molecule 50: 39S ribosomal protein S30, mitochondrial

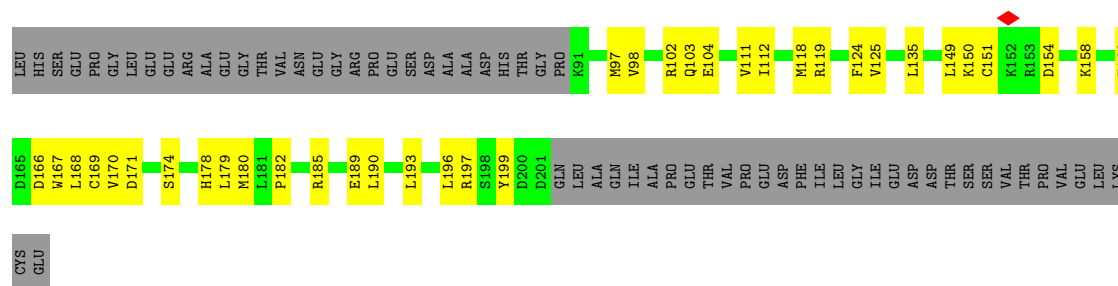
Chain s: 59% 25% 16%



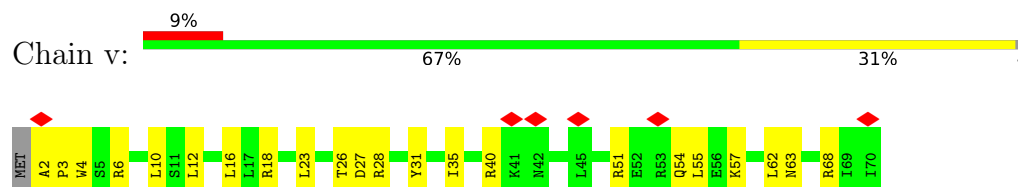
- Molecule 51: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u: 32% 15% 53%

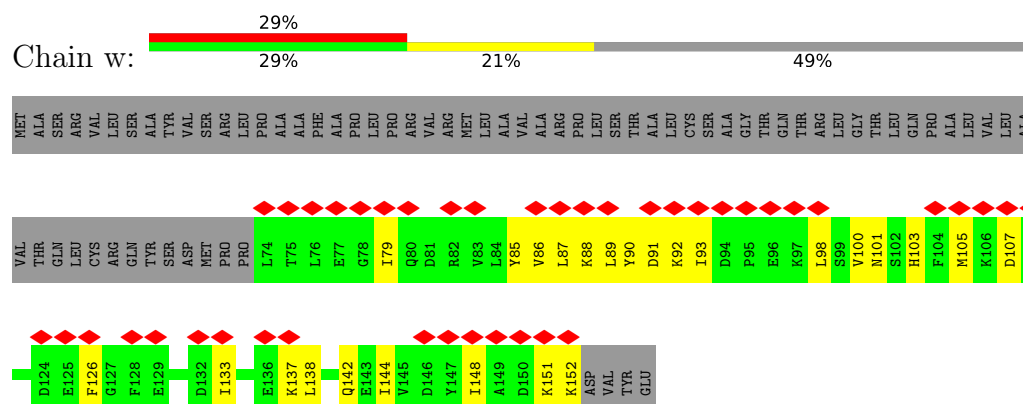




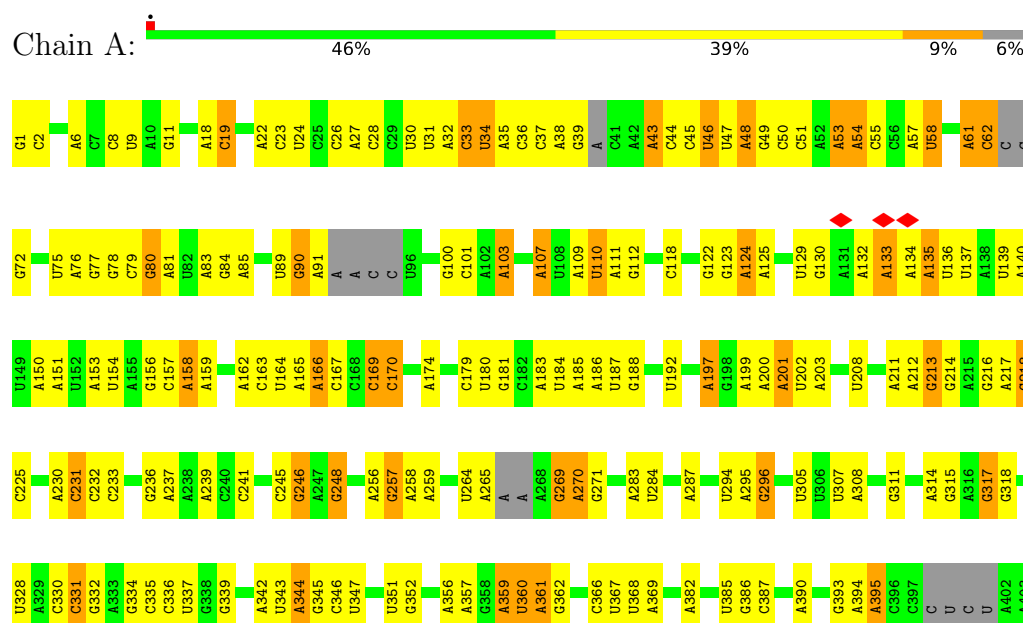
- Molecule 52: MIEF1 upstream open reading frame protein



- Molecule 53: Acyl carrier protein, mitochondrial



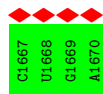
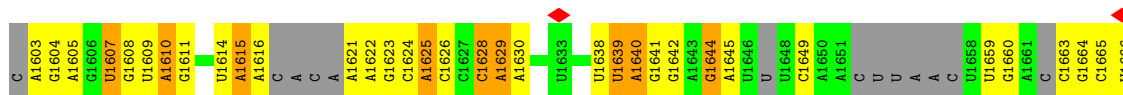
- Molecule 54: 16S rRNA



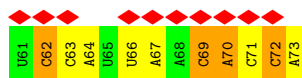
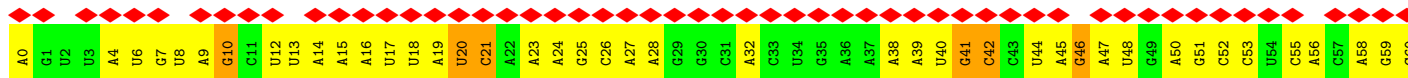
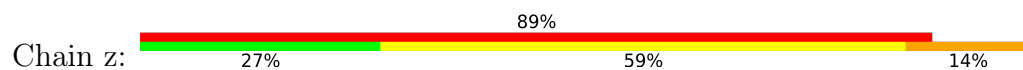
C1450	C1451	U1452	G1453	U1454	A1458	A1459	A1460	G1461	C1464	A1465	A1466	G1467	A1470	A1471	A1472	U1473	C1485	A1486	C1487	A1488	C1492	C1498	C1499	C1500	C1501	C1502	G1503	U1504	A1510	U1513	C1514	A1515	U1518	C1519	A1520	A1525	G1526	U	U	U	A	A1531	U1532	U1533	C1535	C1536	A1537	A							
U1371	U1372	C1373	A1381	A1382	A1383	G1384	A1389	C1390	A1394	U1395	C1396	U1397	G1398	A1399	U1401	U1402	C1403	C1407	C1408	G1409	G1410	A1411	G1412	A1415	U1416	C1417	C1418	A1419	G1420	G1421	U1422	C1423	U1427	U1428	C1429	U1430	A1431	U1432	U1437	U1438	U1439	C	A	A	A1443	U1444	U1445	C1446	C1447	U1448	C1449				
U1285	A1286	G1289	U1290	C1291	C1292	A1293	U1294	A1295	A1298	A1301	A1304	U1308	A1311	C1315	G1319	A1320	U1321	G1322	U1323	G1324	G1325	G1326	A1327	U1328	C1329	A1330	A1335	U1336	C1337	C1338	C1339	G1340	A1341	G1344	U1345	A1348	G1349	C1350	C1351	G1352	C1353	U1354	A1359	A1360	U1363										
C1211	U	A	C	U	A	U	A	C1219	C1220	C1221	A1222	A1223	U1224	U1225	G1226	C1229	A1232	A1233	U1234	U1235	A1236	U1237	U1238	G1239	A1240	C1241	C1242	C1245	G1246	G1247	A1248	A1251	A1252	G1253	U1254	U1255	A1256	C1257	C1258	C1259	U1260	A1261	G1262	G1263	U1264	A1265	C1269	A1270	G1271	C1274	A1281	U1282			
C	A	A	A1122	C1123	C1124	U1125	G1126	A1131	A1132	A1133	A1134	C1139	G1140	G1141	G1144	G1145	G1146	G1147	C1152	U1153	G1156	A1160	C1161	A1162	A1163	C1166	A1167	A1168	C1172	C1173	G1174	C1177	A1178	G1179	U1180	A1181	C1182	A1183	U1184	G1185	G1190	U1194	C1195	C1202	A1203	A1210									
A1053	G1054	A1055	C1056	C1057	C1058	U1059	A1060	U1061	G1062	C1066	U1069	A1070	U1073	U1074	A1075	U1076	U1077	A1078	A1079	U1080	G1081	A1085	C1086	A1087	G1088	U1089	A1090	C	C	U	U	A	A	C	C	A	A	C	G	U	C	C	U	A	A	C	C								
G965	C970	A971	C972	G975	C983	U984	G985	U988	C988	U990	C993	U996	U997	A998	G1005	A1006	A1007	A1008	U1009	A1012	C1013	C1014	U1015	G1016	C1017	C1018	C1019	A1023	A1024	G1025	A1026	G1027	G1028	G1032	U1035	A1036	A1037	C1038	A1039	G1042	C1043	A1044	C1048	G1049	A1052										
A888	U889	G890	U891	U892	A810	A811	G897	C900	G904	U905	A	C	C	U910	A911	A912	C913	U916	G917	A920	A921	G922	G923	U924	A928	U929	A930	A931	U932	G938	U939	U940	U943	U948	A949	G950	G951	G952	A953	C954	U955	U956	G957	U958	A959	U960	G961	A962	U964						
A802	A803	G808	C809	A810	A811	C814	U815	U816	C821	G822	C823	U825	U828	A911	C831	A837	C838	C841	C844	U845	C846	G849	C850	A851	U852	C853	C856	A857	G858	U859	A860	U861	U862	A863	G864	A865	G866	G867	C868	A869	C870	U875	G876	C879	A880	C887									
A724	A725	C726	C727	A728	A731	G732	G733	U734	A736	U737	U738	A739	C743	C744	C745	U746	C747	A748	C749	A755	C756	C758	A762	C763	A764	C772	C773	U774	U775	A776	A777	G778	G779	A781	A782	G783	G784	U785	A788	A789	A790	A791	A792	A793	A796	A797	G800	G801							
C644	A645	C652	A653	U654	U655	C656	U660	U661	C661	C662	G663	C664	A665	C670	C671	U672	G673	C674	G675	A678	U681	A	A	A	A	A	C	A	A604	C530	G531	C532	G533	U534	U535	C536	C540	U541	C542	A543	A544	C545	A546	C547	C548	C	A	C	U	A	U488	U489	A490	A493	C494
A559	A560	A561	A562	U563	C564	A567	A571	U572	A573	U574	A575	U578	G579	A580	A581	U586	C589	A590	C591	C592	C593	A594	A595	U596	U597	G598	A600	A601	U605	U609	C610	A611	C612	U615	A616	A624	C625	U626	A627	A628	U629	G630	A636	U637	A638	A639	C640	U641	A642	A643					
C495	C496	A497	U498	A499	G500	U501	A502	G503	G504	U507	A510	A511	G512	C513	A514	G515	C516	A518	C519	A520	A521	A522	U523	A524	A525	A526	A457	G458	A459	A460	G461	A464	A465	C466	C467	U468	U469	C470	U471	A472	A476	G477	A482	A483	A484	U487	U488	A489	A490	A493	C494				



- Molecule 55: mitochondrial Val tRNA



- Molecule 56: mitochondrial tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.973	Depositor
Minimum map value	-0.548	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, ZN, MG

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	D	0.39	0/1879	0.80	2/2527 (0.1%)
2	E	0.71	0/2465	0.90	4/3344 (0.1%)
3	F	0.80	0/2071	0.85	4/2817 (0.1%)
4	H	0.57	1/798 (0.1%)	0.97	7/1073 (0.7%)
5	I	0.44	0/1308	0.82	1/1761 (0.1%)
6	J	0.24	0/1077	0.57	0/1452
7	K	0.79	0/1495	0.84	1/2029 (0.0%)
8	L	0.65	0/904	0.86	3/1218 (0.2%)
9	M	0.81	0/2359	0.87	2/3185 (0.1%)
10	N	0.61	0/1697	0.81	1/2281 (0.0%)
11	O	0.69	0/1269	0.84	0/1708
12	P	0.47	0/1173	0.76	0/1588
13	Q	0.57	0/1846	0.83	0/2487
14	R	0.90	1/1174 (0.1%)	0.90	0/1572
15	S	0.84	1/1276 (0.1%)	0.91	0/1729
16	T	0.72	0/1335	0.80	0/1796
17	U	0.63	1/1183 (0.1%)	0.89	1/1600 (0.1%)
18	V	0.29	0/1616	0.64	0/2189
19	W	0.74	0/881	0.80	3/1188 (0.3%)
20	X	0.54	1/2090 (0.0%)	0.72	2/2825 (0.1%)
21	Y	0.58	0/1552	0.79	1/2079 (0.0%)
22	Z	0.72	0/1003	0.78	0/1354
23	0	0.68	0/895	0.86	2/1201 (0.2%)
24	1	0.26	0/438	0.74	0/583
25	2	0.90	0/357	0.80	0/475
26	3	0.91	0/852	0.92	0/1136
27	4	0.53	0/329	0.63	0/435
28	5	0.34	0/3250	0.66	4/4429 (0.1%)
29	6	0.52	1/2726 (0.0%)	0.75	1/3715 (0.0%)
30	7	0.43	0/2391	0.65	0/3234
31	8	0.26	0/855	0.69	0/1152
32	9	0.56	1/972 (0.1%)	0.79	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.61	0/630	0.86	1/852 (0.1%)
34	b	0.74	0/1202	0.87	1/1626 (0.1%)
35	c	0.52	0/2264	0.73	0/3059
36	d	0.29	0/1790	0.66	0/2423
37	e	0.19	0/1797	0.53	0/2422
38	f	0.31	0/931	0.56	0/1259
39	g	0.70	0/1102	0.79	0/1503
40	h	0.42	0/847	0.71	0/1150
41	i	0.92	0/849	0.91	1/1135 (0.1%)
42	j	0.56	0/698	0.66	0/940
43	k	0.28	0/635	0.76	0/855
44	l	0.24	0/226	0.64	0/299
45	m	0.23	0/379	0.63	0/510
46	o	0.76	0/807	0.94	0/1083
47	p	0.37	0/1071	0.67	0/1433
48	q	0.39	0/1413	0.66	1/1906 (0.1%)
49	r	0.63	0/1238	0.84	3/1676 (0.2%)
50	s	0.53	0/3114	0.73	4/4225 (0.1%)
51	u	0.37	0/949	0.81	0/1281
52	v	0.30	0/597	0.75	0/796
53	w	0.24	0/647	0.71	0/871
54	A	0.73	0/34974	0.64	4/54421 (0.0%)
55	B	0.19	0/1328	0.37	0/2056
56	z	0.16	0/1729	0.36	0/2685
All	All	0.63	7/106733 (0.0%)	0.72	54/151934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	2
3	F	0	1
5	I	0	1
7	K	0	2
9	M	0	1
13	Q	0	2
15	S	0	1
17	U	0	1
20	X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	0	0	1
29	6	0	1
35	c	0	1
49	r	0	1
50	s	0	1
All	All	0	18

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	X	52	ILE	C-N	-7.95	1.22	1.33
29	6	155	TYR	CA-C	-7.66	1.42	1.52
17	U	43	ARG	CA-CB	-6.54	1.43	1.53
4	H	75	ARG	CA-C	-5.85	1.44	1.52
32	9	70	LEU	C-N	-5.57	1.25	1.32
14	R	43	VAL	CB-CG2	-5.34	1.34	1.52
15	S	108	VAL	CB-CG1	-5.25	1.35	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	76	ARG	CG-CD-NE	-7.22	96.13	112.00
4	H	66	GLY	N-CA-C	7.07	119.43	110.38
41	i	98	VAL	N-CA-C	-6.98	105.53	112.17
28	5	85	PRO	CA-N-CD	-6.88	102.36	112.00
4	H	142	GLU	N-CA-CB	6.83	120.81	110.30
17	U	11	ARG	CG-CD-NE	6.46	126.22	112.00
2	E	239	ARG	CA-CB-CG	6.46	127.01	114.10
33	a	108	MET	CG-SD-CE	-6.45	86.72	100.90
3	F	132	GLY	N-CA-C	6.41	120.97	112.77
23	0	139	ARG	CA-CB-CG	6.40	126.90	114.10
1	D	167	ASN	N-CA-C	-6.38	106.46	114.56
5	I	175	PRO	CA-N-CD	-6.33	103.13	112.00
49	r	192	TRP	CA-CB-CG	6.25	125.47	113.60
48	q	71	VAL	CA-C-O	6.22	122.82	119.15
54	A	495	C	C2'-C3'-O3'	6.13	118.69	109.50
9	M	43	ARG	CG-CD-NE	6.01	125.23	112.00
3	F	77	VAL	N-CA-C	-5.91	106.74	112.29
29	6	368	ARG	CA-CB-CG	5.83	125.75	114.10
8	L	136	LYS	CB-CG-CD	5.78	124.60	111.30
9	M	77	ARG	CB-CA-C	-5.73	101.88	110.88
2	E	239	ARG	CB-CA-C	5.72	117.73	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	TRP	N-CA-CB	-5.71	100.84	110.49
19	W	136	ALA	CA-C-N	-5.69	112.96	121.83
19	W	136	ALA	C-N-CA	-5.69	112.96	121.83
20	X	82	GLY	N-CA-C	-5.63	106.28	115.46
54	A	704	A	P-O3'-C3'	5.61	128.61	120.20
4	H	141	GLU	CA-C-N	-5.59	111.18	120.68
4	H	141	GLU	C-N-CA	-5.59	111.18	120.68
28	5	257	TYR	CA-C-N	5.53	140.28	127.00
28	5	257	TYR	C-N-CA	5.53	140.28	127.00
54	A	495	C	P-O3'-C3'	5.52	128.48	120.20
4	H	141	GLU	N-CA-CB	5.51	119.37	110.40
23	0	139	ARG	CB-CG-CD	5.47	123.88	111.30
54	A	704	A	C2'-C3'-O3'	5.46	117.70	109.50
7	K	125	LEU	CD1-CG-CD2	-5.44	98.84	110.80
34	b	126	ILE	N-CA-C	-5.41	108.23	113.53
50	s	270	LYS	CA-C-N	-5.41	112.47	120.68
50	s	270	LYS	C-N-CA	-5.41	112.47	120.68
2	E	130	LEU	CA-C-N	-5.39	113.39	122.29
2	E	130	LEU	C-N-CA	-5.39	113.39	122.29
10	N	205	ARG	CG-CD-NE	5.38	123.83	112.00
19	W	122	LYS	CA-CB-CG	5.34	124.79	114.10
49	r	177	GLY	CA-C-N	-5.33	111.86	122.90
49	r	177	GLY	C-N-CA	-5.33	111.86	122.90
50	s	250	PHE	CA-C-N	-5.22	118.79	123.33
50	s	250	PHE	C-N-CA	-5.22	118.79	123.33
28	5	257	TYR	C-N-CD	-5.21	109.14	120.60
8	L	90	CYS	CA-C-N	-5.16	107.08	122.71
8	L	90	CYS	C-N-CA	-5.16	107.08	122.71
20	X	121	LYS	CA-CB-CG	5.15	124.41	114.10
4	H	140	PHE	CA-C-N	-5.15	112.13	121.14
4	H	140	PHE	C-N-CA	-5.15	112.13	121.14
21	Y	100	LYS	CB-CG-CD	-5.08	99.62	111.30
3	F	93	LEU	CA-CB-CG	-5.05	98.63	116.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	0	106	ASN	Peptide
29	6	49	GLU	Peptide
1	D	206	TYR	Peptide
2	E	228	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	315	PRO	Peptide
3	F	81	ASP	Peptide
5	I	101	ASN	Peptide
7	K	168	ARG	Peptide
7	K	81	THR	Peptide
9	M	46	GLY	Peptide
13	Q	125	TYR	Peptide
13	Q	226	PRO	Peptide
15	S	101	PHE	Peptide
17	U	150	TRP	Peptide
20	X	120	ASP	Peptide
35	c	122	ASN	Peptide
49	r	149	ARG	Peptide
50	s	427	ASN	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	D	1842	0	1896	46	0
2	E	2396	0	2402	48	0
3	F	2013	0	2044	61	0
4	H	784	0	832	23	0
5	I	1283	0	1369	43	0
6	J	1061	0	1141	27	0
7	K	1451	0	1448	30	0
8	L	889	0	941	26	0
9	M	2305	0	2378	69	0
10	N	1654	0	1681	33	0
11	O	1245	0	1283	29	0
12	P	1148	0	1148	40	0
13	Q	1805	0	1841	36	0
14	R	1153	0	1214	28	0
15	S	1251	0	1322	45	0
16	T	1305	0	1352	30	0
17	U	1154	0	1154	37	0
18	V	1575	0	1583	30	0
19	W	859	0	888	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	X	2035	0	2054	32	0
21	Y	1517	0	1561	29	0
22	Z	978	0	1030	20	0
23	0	880	0	902	31	0
24	1	433	0	475	11	0
25	2	351	0	375	8	0
26	3	831	0	883	24	0
27	4	322	0	346	4	0
28	5	3156	0	3138	81	0
29	6	2640	0	2464	81	0
30	7	2334	0	2343	34	0
31	8	836	0	844	33	0
32	9	947	0	949	21	0
33	a	611	0	595	16	0
34	b	1178	0	1180	34	0
35	c	2217	0	2220	51	0
36	d	1741	0	1727	38	0
37	e	1762	0	1767	44	0
38	f	915	0	917	23	0
39	g	1067	0	1056	21	0
40	h	827	0	806	22	0
41	i	827	0	857	17	0
42	j	684	0	673	9	0
43	k	627	0	636	31	0
44	l	221	0	227	8	0
45	m	372	0	387	10	0
46	o	786	0	791	20	0
47	p	1058	0	1083	20	0
48	q	1379	0	1359	13	0
49	r	1203	0	1219	35	0
50	s	3036	0	3022	83	0
51	u	927	0	921	31	0
52	v	588	0	604	16	0
53	w	638	0	636	22	0
54	A	31265	0	15878	430	0
55	B	1191	0	607	32	0
56	z	1547	0	790	37	0
57	0	1	0	0	0	0
57	I	1	0	0	0	0
58	A	1	0	0	0	0
58	g	1	0	0	0	0
59	v	21	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	101125	0	85260	1747	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 10.

All (1747) 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)
54:A:360:U:O4	54:A:454:A:C6	1.84	1.29
54:A:390:A:N6	54:A:409:C:C4	2.15	1.14
54:A:390:A:C6	54:A:409:C:N4	2.16	1.13
50:s:367:PHE:O	50:s:398:SER:HA	1.49	1.10
54:A:1446:C:H42	54:A:1470:A:N6	1.53	1.06
54:A:1446:C:N4	54:A:1470:A:H61	1.53	1.05
54:A:1450:C:N4	54:A:1466:A:H61	1.56	1.03
54:A:662:C:N4	54:A:772:U:H3	1.59	0.99
54:A:1450:C:H42	54:A:1466:A:N6	1.60	0.98
54:A:360:U:O4	54:A:454:A:N6	1.99	0.94
56:z:14:A:N6	56:z:46:G:C2	2.34	0.94
51:u:185:ARG:O	51:u:189:GLU:HB2	1.68	0.93
54:A:360:U:C4	54:A:454:A:N1	2.37	0.92
49:r:120:LYS:HB3	49:r:124:ARG:HH21	1.36	0.90
54:A:360:U:C4	54:A:454:A:C6	2.59	0.90
54:A:390:A:C6	54:A:409:C:C4	2.59	0.90
2:E:275:ARG:O	2:E:284:TYR:HB2	1.72	0.89
56:z:14:A:H62	56:z:46:G:N2	1.70	0.89
54:A:1450:C:H42	54:A:1466:A:H61	0.93	0.89
54:A:158:A:N6	54:A:1028:G:N2	2.22	0.87
54:A:390:A:N6	54:A:409:C:N3	2.24	0.86
2:E:102:LEU:HA	2:E:295:CYS:O	1.78	0.83
43:k:19:GLN:HA	43:k:54:ASP:O	1.78	0.83
54:A:360:U:O4	54:A:454:A:N1	2.12	0.83
56:z:14:A:N6	56:z:46:G:N2	2.28	0.82
54:A:447:U:HO2'	54:A:1166:C:HO2'	1.29	0.81
56:z:15:A:N6	56:z:46:G:N1	2.29	0.81
54:A:77:G:N2	54:A:80:G:O2'	2.15	0.78
3:F:184:GLN:NE2	9:M:16:LEU:O	2.15	0.78
14:R:65:ARG:NH1	54:A:579:G:OP2	2.17	0.78
18:V:177:THR:H	32:9:71:LYS:HD3	1.49	0.77
31:8:129:ARG:HE	31:8:133:ARG:HH21	1.30	0.77
12:P:54:ARG:NH1	29:6:155:TYR:OH	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:77:ARG:NH2	54:A:1246:G:N3	2.32	0.76
39:g:112:LYS:NZ	54:A:211:A:OP2	2.16	0.76
29:6:275:GLN:HG3	29:6:311:MET:HE1	1.66	0.75
10:N:88:ALA:HA	10:N:161:VAL:O	1.85	0.75
54:A:1293:A:H2	54:A:1298:A:H61	1.34	0.75
50:s:311:LEU:O	50:s:315:ASN:HB2	1.86	0.75
13:Q:120:THR:HA	13:Q:131:SER:O	1.87	0.74
10:N:92:LEU:O	10:N:186:ALA:HB3	1.87	0.74
17:U:3:ARG:HD2	17:U:24:PHE:HB3	1.67	0.74
17:U:11:ARG:NH2	18:V:211:LYS:O	2.20	0.74
14:R:99:ARG:NH2	54:A:578:U:OP1	2.17	0.74
49:r:182:ARG:NH2	54:A:488:U:OP1	2.20	0.74
29:6:175:VAL:HB	29:6:187:VAL:HB	1.68	0.74
14:R:34:ARG:NH2	54:A:1012:A:OP1	2.21	0.73
9:M:19:LEU:HD11	46:o:92:LEU:HB3	1.70	0.73
21:Y:126:MET:HG3	21:Y:128:SER:H	1.52	0.73
38:f:93:ILE:HA	38:f:185:SER:O	1.88	0.73
49:r:116:GLU:OE2	49:r:120:LYS:NZ	2.22	0.73
19:W:101:LYS:NZ	54:A:394:A:OP1	2.22	0.73
24:1:42:THR:HG22	24:1:58:GLU:H	1.52	0.73
54:A:1344:G:C2	54:A:1354:U:O2	2.41	0.73
54:A:359:A:N6	54:A:455:C:OP1	2.21	0.73
21:Y:86:THR:H	21:Y:89:GLN:HE21	1.34	0.73
51:u:178:HIS:HB3	51:u:180:MET:HE3	1.71	0.73
1:D:78:LYS:NZ	54:A:256:A:OP1	2.23	0.72
35:c:220:ILE:HG23	35:c:223:MET:HE2	1.70	0.72
19:W:49:ARG:NH2	54:A:1156:G:OP1	2.22	0.72
28:5:290:THR:HA	28:5:343:GLN:O	1.89	0.72
56:z:48:U:O2	56:z:62:C:N3	2.22	0.72
56:z:25:G:N2	56:z:42:C:O2	2.23	0.71
21:Y:154:ARG:HG3	32:9:130:LEU:HB3	1.72	0.71
56:z:14:A:N6	56:z:46:G:N1	2.38	0.71
17:U:54:ARG:HH12	50:s:314:GLN:HG3	1.55	0.71
5:I:140:TYR:HB3	5:I:143:LEU:HB2	1.72	0.71
54:A:197:A:H62	54:A:625:C:H5	1.39	0.71
4:H:123:LEU:HD21	4:H:129:ALA:HB3	1.73	0.71
25:2:85:LYS:NZ	54:A:122:G:OP2	2.24	0.71
47:p:56:ASP:HB3	47:p:60:ARG:HH12	1.55	0.71
3:F:119:GLU:OE1	3:F:156:ARG:NH1	2.24	0.71
8:L:43:ASN:HB2	8:L:118:ARG:HB2	1.71	0.71
15:S:132:LYS:NZ	42:j:48:ASP:OD1	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:51:MET:HE3	50:s:61:ARG:HH21	1.55	0.71
56:z:10:G:N1	56:z:24:A:C8	2.58	0.71
9:M:202:LYS:HD2	9:M:263:ARG:HE	1.55	0.70
31:8:139:MET:HE1	38:f:169:ILE:HG12	1.73	0.70
54:A:1446:C:N3	54:A:1470:A:N1	2.40	0.70
50:s:165:ARG:NH2	54:A:746:U:O2	2.24	0.70
56:z:15:A:N6	56:z:46:G:H1	1.89	0.70
2:E:235:LYS:NZ	54:A:791:A:O2'	2.25	0.70
54:A:360:U:C4	54:A:454:A:N6	2.57	0.70
6:J:25:ARG:HA	6:J:65:PRO:HA	1.74	0.70
31:8:133:ARG:HH12	55:B:1626:C:H4'	1.56	0.70
54:A:530:A:H2'	54:A:531:G:H8	1.56	0.69
35:c:31:VAL:N	54:A:103:A:OP2	2.25	0.69
41:i:73:LEU:HD11	48:q:31:PRO:HG3	1.75	0.69
50:s:272:PRO:O	54:A:704:A:N6	2.24	0.69
3:F:167:MET:SD	3:F:276:GLN:NE2	2.66	0.69
15:S:194:ARG:NH2	34:b:13:SER:OG	2.24	0.69
54:A:130:G:N2	54:A:133:A:C5	2.60	0.69
16:T:133:ASN:ND2	36:d:232:MET:SD	2.65	0.69
19:W:146:ALA:O	29:6:338:ARG:NH2	2.26	0.69
43:k:68:PHE:HB2	43:k:72:HIS:HB2	1.75	0.69
18:V:94:HIS:HB3	18:V:96:ARG:HH11	1.57	0.69
3:F:160:SER:HB3	41:i:80:LEU:HD13	1.73	0.69
15:S:155:ARG:NH1	15:S:157:GLU:OE2	2.22	0.69
12:P:85:ARG:NH1	12:P:125:CYS:SG	2.66	0.69
11:O:46:TRP:HD1	11:O:121:ALA:HB2	1.57	0.68
35:c:275:TYR:HA	35:c:280:LEU:HA	1.75	0.68
9:M:77:ARG:NH1	54:A:1247:G:O6	2.24	0.68
16:T:104:ALA:HB1	23:0:107:ILE:HG21	1.76	0.68
18:V:20:ARG:NH2	18:V:42:ARG:O	2.26	0.68
15:S:184:ARG:NH2	54:A:591:C:O2'	2.26	0.68
17:U:3:ARG:O	17:U:23:ASN:ND2	2.27	0.68
54:A:1078:A:H2'	54:A:1079:A:C8	2.28	0.68
1:D:285:LYS:NZ	54:A:846:C:O3'	2.27	0.68
7:K:63:ARG:NH2	7:K:130:ASP:OD1	2.27	0.68
7:K:168:ARG:NH2	49:r:58:LYS:O	2.27	0.68
20:X:96:LYS:O	54:A:58:U:O2'	2.12	0.68
46:o:38:ARG:NH2	54:A:482:A:OP1	2.26	0.68
18:V:134:GLU:HB2	18:V:136:ARG:HH21	1.59	0.67
28:5:200:ARG:HD3	28:5:233:LYS:HD3	1.76	0.67
55:B:1607:U:H3	55:B:1664:G:H1	1.36	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:58:ILE:HD11	8:L:76:ALA:HB2	1.76	0.67
54:A:801:G:N2	54:A:985:G:OP2	2.27	0.67
11:O:33:LEU:HD21	11:O:59:LEU:HD13	1.77	0.67
13:Q:118:ARG:HA	13:Q:133:PHE:O	1.95	0.67
21:Y:154:ARG:NH1	21:Y:161:GLU:O	2.28	0.67
36:d:123:ARG:HA	36:d:126:LYS:HG2	1.76	0.67
1:D:68:SER:HA	28:5:38:THR:HG21	1.76	0.67
9:M:141:VAL:HG12	9:M:143:GLU:H	1.59	0.67
3:F:93:LEU:HD23	3:F:96:LEU:HD12	1.77	0.67
17:U:71:ARG:NH1	17:U:73:GLN:OE1	2.28	0.67
5:I:121:ILE:HD11	5:I:154:LEU:HB3	1.77	0.67
51:u:158:LYS:NZ	54:A:1448:U:O3'	2.28	0.67
17:U:24:PHE:HB2	17:U:45:PRO:HG3	1.75	0.67
31:8:121:TRP:HB2	37:e:70:MET:HE1	1.77	0.67
50:s:185:VAL:HG23	50:s:195:LEU:HD23	1.77	0.67
56:z:15:A:N1	56:z:46:G:O6	2.28	0.66
54:A:360:U:C4	54:A:428:G:C6	2.83	0.66
34:b:4:ARG:NH2	54:A:167:C:OP1	2.29	0.66
4:H:140:PHE:HA	4:H:143:GLU:HG3	1.78	0.66
7:K:10:GLN:NE2	16:T:206:ARG:O	2.28	0.66
31:8:173:LYS:O	38:f:183:ARG:NH2	2.29	0.66
8:L:55:PRO:HB3	8:L:77:ILE:HG22	1.75	0.66
34:b:136:LYS:O	35:c:259:ARG:NH2	2.28	0.66
49:r:149:ARG:HD3	49:r:152:THR:HG21	1.78	0.66
54:A:1066:C:HO2'	54:A:1415:A:HO2'	1.43	0.66
5:I:148:VAL:O	43:k:31:ARG:NH2	2.28	0.65
20:X:55:LYS:NZ	54:A:76:A:OP1	2.26	0.65
9:M:54:LYS:NZ	54:A:347:U:OP1	2.26	0.65
12:P:106:SER:HB2	12:P:109:GLU:HG2	1.78	0.65
6:J:86:THR:O	6:J:90:PHE:HB2	1.95	0.65
54:A:501:U:H4'	54:A:502:A:H3'	1.78	0.65
54:A:130:G:C2	54:A:133:A:N7	2.64	0.65
3:F:145:LEU:O	54:A:630:G:N2	2.29	0.65
46:o:23:ARG:NH2	54:A:461:A:OP1	2.30	0.65
12:P:50:ASN:ND2	29:6:222:ASP:OD2	2.29	0.65
54:A:800:G:N2	54:A:803:A:N6	2.44	0.65
54:A:727:C:H3'	54:A:728:A:H8	1.61	0.64
23:0:110:CYS:HB3	23:0:115:HIS:O	1.97	0.64
54:A:523:U:C4	54:A:526:A:N1	2.65	0.64
7:K:108:ILE:HD13	7:K:125:LEU:HD11	1.78	0.64
50:s:84:THR:HB	50:s:280:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:35:LYS:HE3	54:A:230:A:H1'	1.79	0.64
11:O:141:HIS:HD2	11:O:146:ASN:HB3	1.63	0.64
35:c:167:CYS:SG	35:c:171:ARG:NH1	2.70	0.64
37:e:198:ASN:HD21	37:e:200:MET:HE2	1.62	0.64
21:Y:198:ARG:NH2	25:2:70:LEU:O	2.31	0.64
43:k:63:CYS:HA	43:k:76:MET:O	1.98	0.64
16:T:71:ALA:HB3	16:T:180:GLU:HG3	1.78	0.64
20:X:20:ILE:HD13	20:X:23:ARG:HH11	1.62	0.64
54:A:521:A:H61	54:A:527:G:H5''	1.62	0.64
36:d:211:GLN:HA	36:d:248:PHE:O	1.98	0.64
11:O:13:ARG:NH2	54:A:993:C:OP1	2.29	0.64
20:X:177:HIS:O	20:X:184:ARG:NH1	2.31	0.64
56:z:48:U:H3	56:z:62:C:H42	1.44	0.64
3:F:209:TYR:OH	40:h:56:ARG:NH2	2.31	0.64
49:r:93:ILE:HD11	49:r:119:VAL:HG21	1.80	0.64
1:D:116:GLU:HG2	1:D:117:THR:HG23	1.80	0.64
3:F:93:LEU:HD13	46:o:95:LEU:HD11	1.80	0.64
16:T:212:LEU:O	33:a:142:ARG:NH2	2.31	0.64
54:A:51:C:H4'	54:A:343:U:H5'	1.79	0.64
3:F:234:THR:O	48:q:25:TYR:N	2.31	0.63
10:N:85:GLY:O	10:N:192:ARG:NH1	2.32	0.63
23:0:110:CYS:O	23:0:114:GLY:N	2.28	0.63
37:e:183:THR:HG23	37:e:186:GLY:H	1.64	0.63
51:u:151:CYS:HB3	51:u:154:ASP:HB2	1.81	0.63
54:A:390:A:N6	54:A:409:C:N4	2.33	0.63
54:A:1048:C:H2'	54:A:1321:U:H4'	1.78	0.63
56:z:25:G:N2	56:z:42:C:C2	2.67	0.63
10:N:171:GLU:O	44:l:135:ASN:ND2	2.32	0.63
56:z:12:U:O4	56:z:21:C:N3	2.31	0.63
2:E:239:ARG:NH1	54:A:1044:A:OP1	2.30	0.63
9:M:75:TYR:O	26:3:113:ARG:NH1	2.32	0.63
50:s:103:ASP:OD1	50:s:325:ARG:NH1	2.31	0.63
54:A:850:C:O2	54:A:859:U:N3	2.32	0.63
14:R:111:LYS:NZ	15:S:139:ASP:OD2	2.32	0.63
28:5:85:PRO:HD3	54:A:743:C:H4'	1.80	0.63
22:Z:101:LYS:HE3	42:j:80:LEU:HD22	1.81	0.63
38:f:78:ARG:HE	38:f:79:ALA:H	1.47	0.63
29:6:158:TYR:HE1	29:6:167:PHE:H	1.44	0.63
39:g:105:ARG:HH12	46:o:83:PRO:HD3	1.64	0.63
2:E:107:MET:HE3	2:E:121:LEU:HD21	1.81	0.62
12:P:142:ASN:OD1	47:p:184:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:16:GLN:NE2	32:9:57:VAL:O	2.32	0.62
34:b:116:ARG:O	54:A:476:A:N6	2.32	0.62
16:T:84:LYS:HD3	16:T:149:ARG:HB3	1.80	0.62
50:s:249:GLU:HA	50:s:356:VAL:HG21	1.82	0.62
3:F:164:MET:HE2	41:i:69:HIS:CE1	2.35	0.62
6:J:148:ALA:HB1	6:J:153:ILE:HB	1.82	0.62
9:M:117:ASP:OD2	9:M:260:LYS:NZ	2.32	0.62
17:U:35:GLN:HG3	17:U:36:PRO:HD2	1.82	0.62
49:r:41:THR:O	49:r:47:THR:HA	1.99	0.62
5:I:188:ARG:HH21	43:k:22:PRO:HG3	1.63	0.62
11:O:58:LYS:NZ	13:Q:269:MET:O	2.30	0.62
14:R:48:ARG:NH1	54:A:158:A:OP2	2.33	0.62
21:Y:88:GLN:NE2	32:9:82:GLU:O	2.33	0.62
28:5:408:PRO:HG2	28:5:412:ARG:HH12	1.64	0.62
29:6:365:TYR:HA	29:6:368:ARG:HD3	1.81	0.62
31:8:99:ARG:HH12	31:8:102:PRO:HB3	1.63	0.62
7:K:15:ALA:HB3	35:c:269:LEU:HD12	1.82	0.62
6:J:128:GLU:OE1	6:J:133:GLN:NE2	2.33	0.61
12:P:61:VAL:O	12:P:177:ARG:NH2	2.33	0.61
22:Z:71:ARG:NH2	54:A:470:G:OP2	2.33	0.61
35:c:181:SER:OG	35:c:182:GLU:N	2.31	0.61
52:v:23:LEU:O	52:v:28:ARG:NH1	2.32	0.61
15:S:178:LYS:NZ	54:A:593:C:O2'	2.29	0.61
37:e:146:ARG:HA	37:e:151:ARG:HD2	1.81	0.61
53:w:100:VAL:HB	53:w:142:GLN:HB3	1.82	0.61
4:H:74:HIS:NE2	54:A:62:C:OP1	2.32	0.61
20:X:119:LEU:HD22	28:5:53:PRO:HD2	1.82	0.61
25:2:69:ARG:NH1	54:A:246:G:OP1	2.33	0.61
54:A:77:G:OP2	54:A:79:C:N4	2.33	0.61
54:A:1351:C:H2'	54:A:1352:G:H8	1.65	0.61
2:E:248:ILE:HG22	2:E:250:ARG:HG2	1.83	0.61
4:H:91:LYS:NZ	54:A:1085:A:OP1	2.33	0.61
8:L:125:THR:HG23	13:Q:125:TYR:HD2	1.63	0.61
23:0:109:VAL:HA	23:0:116:LEU:HA	1.81	0.61
26:3:151:ASN:OD1	26:3:152:LYS:N	2.34	0.61
8:L:86:ILE:HA	8:L:105:VAL:HG22	1.82	0.61
47:p:75:ARG:NH1	47:p:109:GLU:OE1	2.33	0.61
31:8:140:LEU:O	31:8:144:GLN:NE2	2.33	0.61
11:O:96:ARG:NH1	11:O:127:GLY:O	2.34	0.61
30:7:193:MET:HE1	30:7:283:VAL:HB	1.83	0.61
54:A:1289:G:H21	54:A:1295:A:H62	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:182:ARG:HB3	36:d:223:ALA:HB3	1.83	0.61
5:I:128:ASN:ND2	5:I:149:GLY:O	2.34	0.61
7:K:169:LEU:N	49:r:91:GLN:OE1	2.20	0.61
12:P:58:LEU:HD23	47:p:177:ARG:HH21	1.66	0.61
17:U:143:ARG:NH1	30:7:66:GLU:OE2	2.33	0.61
28:5:136:VAL:HA	28:5:139:LEU:HD12	1.81	0.61
50:s:49:ALA:O	50:s:61:ARG:NH1	2.34	0.61
3:F:76:ARG:NH1	40:h:111:VAL:HG11	2.16	0.61
9:M:148:PHE:O	9:M:170:ASN:ND2	2.32	0.61
18:V:21:TYR:O	18:V:83:ARG:NH1	2.34	0.61
28:5:270:ILE:O	54:A:739:A:O2'	2.19	0.61
37:e:124:TRP:HB3	45:m:73:ARG:HG3	1.83	0.61
3:F:85:ASP:OD2	39:g:87:ARG:NH2	2.33	0.60
15:S:118:ASN:C	15:S:118:ASN:HD22	2.09	0.60
35:c:92:PHE:HE1	35:c:175:VAL:HG23	1.65	0.60
6:J:113:THR:HA	6:J:156:VAL:HB	1.82	0.60
10:N:218:ILE:HG23	10:N:223:MET:HB2	1.83	0.60
22:Z:77:ARG:NH1	54:A:467:C:OP2	2.34	0.60
26:3:105:LYS:NZ	54:A:84:G:N7	2.46	0.60
48:q:68:SER:OG	48:q:69:GLY:N	2.34	0.60
19:W:84:GLY:O	19:W:87:LYS:N	2.33	0.60
34:b:126:ILE:O	35:c:310:ASN:ND2	2.34	0.60
9:M:100:ARG:NH1	9:M:126:GLY:O	2.34	0.60
28:5:165:GLN:NE2	50:s:204:CYS:SG	2.71	0.60
33:a:72:THR:O	35:c:256:ARG:NH2	2.34	0.60
11:O:38:ARG:NH2	11:O:82:GLU:OE1	2.34	0.60
36:d:267:PRO:HG2	36:d:270:ALA:HB2	1.83	0.60
38:f:129:THR:HB	38:f:151:THR:HB	1.82	0.60
31:8:119:LYS:NZ	55:B:1642:G:O2'	2.35	0.60
31:8:165:ASP:OD2	37:e:185:ARG:NH1	2.35	0.60
40:h:138:SER:O	40:h:141:ASP:N	2.34	0.60
54:A:269:G:H5'	54:A:270:A:H5''	1.83	0.60
2:E:96:ARG:NH1	2:E:301:ASP:OD2	2.33	0.60
22:Z:98:GLN:OE1	42:j:76:ARG:NH2	2.34	0.60
23:0:139:ARG:NH1	54:A:652:C:OP2	2.35	0.60
39:g:56:ARG:NH2	39:g:59:ASP:OD1	2.34	0.60
49:r:101:PRO:HG2	49:r:104:ILE:HD13	1.83	0.60
54:A:112:G:N2	54:A:124:A:OP2	2.26	0.60
17:U:3:ARG:H	17:U:23:ASN:HB3	1.67	0.60
41:i:61:GLY:HA3	54:A:216:G:H1	1.67	0.60
54:A:660:U:H3	54:A:777:A:H61	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:183:ARG:NH1	29:6:355:LYS:O	2.35	0.60
28:5:208:THR:HG21	50:s:160:ARG:HG3	1.84	0.60
36:d:118:SER:OG	36:d:197:VAL:O	2.20	0.60
37:e:211:GLY:O	37:e:233:PHE:HB2	2.02	0.60
43:k:15:GLN:HB3	43:k:67:LEU:HB2	1.82	0.60
27:4:84:ARG:NE	54:A:1518:U:OP2	2.34	0.59
37:e:199:ASN:HB2	37:e:242:ASP:HB2	1.82	0.59
12:P:107:THR:HG23	12:P:128:ILE:HD12	1.84	0.59
12:P:118:SER:OG	12:P:121:ASN:ND2	2.35	0.59
17:U:50:ARG:NH2	54:A:749:C:OP2	2.35	0.59
28:5:147:ILE:O	28:5:150:GLN:NE2	2.35	0.59
30:7:195:THR:OG1	30:7:196:LYS:N	2.35	0.59
33:a:121:HIS:NE2	54:A:1036:A:OP2	2.31	0.59
45:m:50:ARG:O	45:m:69:ARG:NH1	2.35	0.59
54:A:523:U:O4	54:A:526:A:C6	2.55	0.59
54:A:662:C:H42	54:A:772:U:H3	0.75	0.59
16:T:58:VAL:HG22	36:d:227:ARG:HG2	1.85	0.59
30:7:154:ILE:HG12	30:7:297:PHE:HE2	1.67	0.59
43:k:80:HIS:O	49:r:36:ARG:NH1	2.35	0.59
59:v:101:PNS:O27	59:v:101:PNS:O33	2.19	0.59
55:B:1625:A:N6	55:B:1644:G:C2	2.70	0.59
3:F:86:VAL:HG23	3:F:175:LYS:HG2	1.85	0.59
29:6:45:LEU:HA	29:6:48:LEU:HB3	1.83	0.59
33:a:66:ASP:HB2	35:c:280:LEU:HD21	1.84	0.59
28:5:127:LYS:HD3	28:5:248:THR:HG22	1.84	0.59
56:z:10:G:O6	56:z:23:A:C5	2.55	0.59
15:S:163:LYS:HG2	15:S:191:THR:HG22	1.85	0.59
27:4:72:LEU:HD13	27:4:90:VAL:HG23	1.84	0.59
29:6:192:GLU:HB3	29:6:320:GLN:HB2	1.85	0.59
51:u:180:MET:HB2	51:u:185:ARG:HH21	1.67	0.59
1:D:194:ASN:HD22	1:D:247:VAL:HG22	1.68	0.59
7:K:144:GLU:OE2	34:b:146:ARG:NH2	2.35	0.59
26:3:108:LYS:HD3	26:3:111:ILE:HD12	1.83	0.59
56:z:10:G:O6	56:z:23:A:C6	2.56	0.59
2:E:138:CYS:SG	54:A:1535:C:N4	2.76	0.59
7:K:154:ARG:HD3	49:r:129:PRO:HG3	1.83	0.59
9:M:140:LEU:HG	9:M:156:VAL:HG21	1.85	0.59
26:3:116:ARG:NH2	26:3:159:ASP:OD1	2.35	0.59
36:d:120:VAL:O	36:d:124:ARG:HB2	2.03	0.59
35:c:33:LYS:NZ	54:A:101:C:OP1	2.33	0.59
1:D:228:LEU:O	1:D:231:LYS:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:SER:OG	2:E:70:LYS:NZ	2.36	0.58
3:F:137:ARG:NH1	54:A:1262:G:OP1	2.36	0.58
9:M:17:ARG:HH12	40:h:116:ARG:NE	2.01	0.58
11:O:42:ILE:O	11:O:122:VAL:HA	2.03	0.58
51:u:98:VAL:HG23	51:u:102:ARG:HH21	1.68	0.58
51:u:149:LEU:HD23	51:u:150:LYS:HB2	1.84	0.58
16:T:77:ARG:NH2	16:T:119:GLU:OE2	2.35	0.58
50:s:178:ASP:OD1	50:s:239:ASN:ND2	2.35	0.58
52:v:40:ARG:HH21	53:w:113:LEU:HD23	1.68	0.58
10:N:227:ARG:NH2	22:Z:39:SER:OG	2.37	0.58
50:s:166:TYR:HB3	54:A:746:U:H3	1.68	0.58
56:z:10:G:C6	56:z:24:A:C5	2.91	0.58
11:O:49:VAL:HG12	11:O:107:MET:HE2	1.85	0.58
15:S:139:ASP:HA	34:b:127:GLN:HG2	1.86	0.58
15:S:177:ARG:NH2	54:A:183:A:OP2	2.35	0.58
30:7:185:LEU:HD12	30:7:295:ARG:HD2	1.85	0.58
50:s:214:GLU:HA	50:s:228:ASP:HA	1.86	0.58
54:A:1152:C:O2'	54:A:1245:C:OP2	2.22	0.58
54:A:1179:G:N1	54:A:1220:U:N3	2.52	0.58
54:A:1464:C:H3'	54:A:1465:A:H8	1.67	0.58
6:J:142:ARG:NH1	6:J:143:SER:OG	2.36	0.58
9:M:196:ARG:NH1	54:A:90:G:OP1	2.36	0.58
50:s:113:VAL:HG21	50:s:257:VAL:HG11	1.85	0.58
5:I:145:PRO:O	43:k:26:ASN:ND2	2.37	0.58
9:M:233:ARG:HB3	9:M:244:LEU:HD21	1.86	0.58
17:U:74:HIS:NE2	54:A:671:C:O2'	2.36	0.58
40:h:71:GLU:OE2	40:h:86:TRP:NE1	2.34	0.58
2:E:56:GLU:OE2	11:O:141:HIS:ND1	2.37	0.58
3:F:59:ARG:NH2	39:g:114:GLU:OE2	2.37	0.58
3:F:281:ARG:NH2	9:M:128:THR:OG1	2.37	0.58
15:S:181:LYS:NZ	54:A:626:U:O4	2.37	0.58
41:i:119:LYS:O	41:i:123:ARG:HB2	2.04	0.58
50:s:365:LYS:NZ	50:s:402:TYR:O	2.36	0.58
54:A:28:C:O2'	54:A:32:A:N3	2.36	0.58
5:I:51:THR:HG21	10:N:215:PHE:HB2	1.85	0.58
5:I:83:ARG:HG2	5:I:134:PHE:HE2	1.69	0.58
18:V:59:GLY:CA	18:V:76:VAL:O	2.52	0.58
54:A:1341:A:O2'	54:A:1503:G:N2	2.37	0.58
55:B:1609:U:O2	55:B:1616:A:N6	2.37	0.58
13:Q:139:GLN:HB3	13:Q:150:ILE:HG12	1.86	0.57
19:W:56:MET:SD	54:A:393:G:N2	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:277:GLN:NE2	29:6:278:PRO:O	2.37	0.57
41:i:48:ASN:OD1	41:i:49:GLU:N	2.36	0.57
50:s:313:ARG:NH1	54:A:747:C:OP1	2.37	0.57
9:M:204:MET:SD	9:M:263:ARG:NH2	2.77	0.57
36:d:216:MET:HB2	36:d:244:GLU:HB2	1.86	0.57
3:F:83:HIS:HB3	3:F:86:VAL:HG12	1.86	0.57
9:M:238:ARG:O	47:p:155:ARG:NH2	2.37	0.57
41:i:67:GLU:O	48:q:33:ARG:NH1	2.36	0.57
55:B:1607:U:O2	55:B:1664:G:N2	2.37	0.57
1:D:197:GLU:HB3	1:D:240:CYS:HB2	1.86	0.57
4:H:98:LEU:O	4:H:109:GLY:CA	2.52	0.57
35:c:121:SER:OG	35:c:122:ASN:N	2.35	0.57
50:s:93:VAL:HA	50:s:273:LEU:HD11	1.87	0.57
54:A:165:A:O2'	54:A:166:A:N7	2.35	0.57
17:U:11:ARG:HH21	18:V:211:LYS:C	2.12	0.57
53:w:105:MET:SD	53:w:115:GLN:NE2	2.77	0.57
25:2:63:LYS:NZ	54:A:248:G:OP1	2.31	0.57
29:6:239:ASN:OD1	29:6:275:GLN:NE2	2.37	0.57
18:V:72:LYS:NZ	18:V:73:GLN:O	2.35	0.57
35:c:60:ARG:NH2	35:c:65:ASN:O	2.36	0.57
50:s:165:ARG:HH22	54:A:745:C:H6	1.52	0.57
54:A:943:U:O2	54:A:949:A:N6	2.37	0.57
2:E:239:ARG:NH2	54:A:1395:U:OP2	2.37	0.57
7:K:171:THR:HG23	49:r:59:GLU:HB2	1.86	0.57
20:X:121:LYS:HZ2	28:5:53:PRO:HG3	1.70	0.57
52:v:54:GLN:HE21	52:v:57:LYS:HE2	1.69	0.57
54:A:640:G:O2'	54:A:1005:G:O6	2.18	0.57
17:U:7:TYR:HA	32:9:136:LEU:HD21	1.86	0.57
17:U:75:GLY:O	17:U:88:LYS:NZ	2.38	0.57
23:0:110:CYS:CB	23:0:115:HIS:O	2.53	0.57
28:5:68:PRO:O	54:A:43:A:N6	2.37	0.57
30:7:68:LYS:HA	30:7:78:VAL:HA	1.87	0.57
14:R:126:GLU:HA	15:S:66:LEU:HD11	1.87	0.57
50:s:152:GLN:HA	50:s:156:TYR:HB2	1.87	0.57
9:M:92:GLN:NE2	26:3:170:ASN:OD1	2.38	0.56
37:e:257:LYS:NZ	37:e:277:SER:O	2.37	0.56
54:A:850:C:N3	54:A:859:U:O2	2.38	0.56
7:K:175:ASP:OD1	49:r:36:ARG:NH1	2.39	0.56
54:A:950:G:H2'	54:A:951:G:H8	1.69	0.56
4:H:98:LEU:O	4:H:109:GLY:N	2.37	0.56
8:L:142:GLN:NE2	13:Q:156:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:142:GLU:HG3	9:M:162:LEU:HB3	1.87	0.56
10:N:182:LYS:NZ	54:A:1301:A:N3	2.42	0.56
14:R:57:ARG:NH2	15:S:170:ILE:O	2.27	0.56
16:T:137:ARG:NH2	30:7:95:LEU:O	2.39	0.56
36:d:213:THR:HG22	36:d:247:VAL:HG22	1.86	0.56
46:o:15:ARG:HB3	46:o:18:ILE:HG12	1.87	0.56
56:z:66:U:H2'	56:z:67:A:H8	1.69	0.56
12:P:54:ARG:HG2	12:P:57:GLU:HG3	1.87	0.56
15:S:178:LYS:HZ2	54:A:455:C:P	2.28	0.56
22:Z:35:LYS:HB3	54:A:449:U:H1'	1.88	0.56
28:5:173:ARG:HE	28:5:303:ARG:HH11	1.53	0.56
29:6:214:TRP:HB3	29:6:272:LEU:HD11	1.86	0.56
35:c:90:THR:HA	35:c:93:VAL:HG22	1.86	0.56
9:M:292:LYS:O	9:M:296:SER:OG	2.21	0.56
15:S:182:LYS:NZ	54:A:592:C:O5'	2.35	0.56
32:9:16:ASP:OD2	32:9:19:SER:OG	2.18	0.56
50:s:59:ARG:NE	54:A:777:A:OP1	2.27	0.56
52:v:51:ARG:HA	59:v:101:PNS:H422	1.86	0.56
54:A:49:G:H2'	54:A:50:C:H6	1.71	0.56
54:A:89:U:O2'	54:A:218:G:O6	2.21	0.56
22:Z:134:MET:HE1	42:j:78:VAL:HG21	1.87	0.56
30:7:69:HIS:NE2	30:7:73:THR:O	2.33	0.56
37:e:55:ARG:HB3	37:e:157:LEU:HB2	1.87	0.56
6:J:148:ALA:O	6:J:151:LEU:C	2.49	0.56
42:j:44:THR:O	42:j:63:GLN:NE2	2.39	0.56
54:A:844:C:H2'	54:A:845:U:H6	1.71	0.56
8:L:70:GLY:N	8:L:86:ILE:O	2.39	0.56
28:5:126:THR:HA	28:5:372:ASN:O	2.06	0.56
29:6:265:ILE:HD11	29:6:322:ARG:HE	1.71	0.56
30:7:112:PRO:HB2	30:7:267:PRO:HG2	1.87	0.56
4:H:98:LEU:O	4:H:109:GLY:HA2	2.06	0.55
6:J:142:ARG:HH21	54:A:522:A:H5'	1.71	0.55
12:P:118:SER:O	12:P:121:ASN:ND2	2.39	0.55
18:V:59:GLY:N	18:V:76:VAL:O	2.38	0.55
21:Y:171:ASP:OD2	21:Y:171:ASP:N	2.36	0.55
56:z:20:U:H5	56:z:44:U:H3	1.53	0.55
1:D:79:MET:HE3	1:D:104:TYR:HB2	1.89	0.55
1:D:197:GLU:OE2	1:D:203:GLY:N	2.36	0.55
11:O:80:LEU:HD23	11:O:85:LEU:HB2	1.89	0.55
12:P:123:VAL:HG11	29:6:128:ALA:HB3	1.89	0.55
39:g:88:ARG:NH1	39:g:92:HIS:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:165:ARG:NH1	54:A:744:C:O2'	2.38	0.55
54:A:55:C:O2	54:A:1251:A:N6	2.34	0.55
3:F:241:ASN:HD22	41:i:53:MET:HE3	1.71	0.55
12:P:65:GLU:OE1	12:P:68:TRP:NE1	2.37	0.55
14:R:35:LYS:HE2	54:A:158:A:H2'	1.89	0.55
21:Y:83:ALA:O	32:9:74:VAL:N	2.35	0.55
22:Z:35:LYS:NZ	54:A:448:U:O2'	2.27	0.55
22:Z:68:ILE:HD11	22:Z:122:LEU:HD12	1.89	0.55
36:d:212:ILE:O	36:d:247:VAL:HA	2.06	0.55
43:k:37:VAL:HA	43:k:42:VAL:HG21	1.89	0.55
54:A:156:G:H4'	54:A:158:A:H2	1.71	0.55
2:E:50:ASP:O	11:O:138:ARG:NH1	2.38	0.55
29:6:374:GLU:O	47:p:141:ARG:NH2	2.34	0.55
43:k:36:THR:HG23	43:k:37:VAL:HG13	1.89	0.55
46:o:66:ARG:NH2	54:A:412:G:OP1	2.40	0.55
56:z:14:A:H2'	56:z:15:A:H8	1.71	0.55
1:D:259:LYS:HG3	1:D:262:ARG:H	1.70	0.55
4:H:120:ARG:NH2	20:X:136:ASP:OD1	2.37	0.55
10:N:218:ILE:HA	10:N:223:MET:HG3	1.88	0.55
15:S:162:GLU:HG2	15:S:192:VAL:HB	1.88	0.55
17:U:133:GLU:OE2	36:d:167:HIS:ND1	2.38	0.55
18:V:59:GLY:HA2	18:V:76:VAL:O	2.06	0.55
29:6:162:PHE:HB3	29:6:165:ALA:HB3	1.88	0.55
37:e:90:ARG:NH2	45:m:70:GLU:OE2	2.40	0.55
54:A:72:G:O2'	54:A:84:G:O6	2.24	0.55
54:A:130:G:H22	54:A:133:A:H5''	1.71	0.55
56:z:10:G:O6	56:z:24:A:C5	2.60	0.55
25:2:59:LYS:NZ	54:A:311:G:OP2	2.38	0.55
28:5:93:LEU:HB3	28:5:270:ILE:HD11	1.89	0.55
9:M:225:ASP:OD2	9:M:228:LYS:NZ	2.40	0.55
29:6:239:ASN:ND2	29:6:249:GLN:OE1	2.36	0.55
29:6:261:ARG:HB3	29:6:341:VAL:HG12	1.88	0.55
7:K:39:LEU:HD11	7:K:125:LEU:HD12	1.87	0.55
28:5:139:LEU:O	28:5:145:ASN:ND2	2.40	0.55
29:6:182:ASP:OD2	29:6:183:ASP:N	2.40	0.55
29:6:380:TYR:OH	54:A:222:A:OP2	2.20	0.55
54:A:1025:G:N2	54:A:1389:A:OP2	2.40	0.55
8:L:71:ASP:O	8:L:85:LEU:HA	2.07	0.55
17:U:73:GLN:HE21	17:U:74:HIS:H	1.55	0.55
31:8:152:LEU:HD12	31:8:153:GLU:HG3	1.89	0.55
34:b:21:ARG:HD2	35:c:218:PHE:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:70:CYS:SG	49:r:73:CYS:CB	2.90	0.55
10:N:170:GLU:HA	10:N:173:GLN:HB2	1.88	0.55
31:8:160:GLU:OE1	37:e:207:ASN:ND2	2.40	0.55
49:r:70:CYS:SG	49:r:73:CYS:HB2	2.46	0.54
50:s:380:THR:O	50:s:384:ASP:HB2	2.06	0.54
54:A:130:G:N1	54:A:133:A:OP2	2.39	0.54
6:J:120:ILE:HA	6:J:123:ILE:HG12	1.88	0.54
8:L:119:ILE:HB	8:L:141:ALA:HA	1.90	0.54
28:5:125:LYS:NZ	28:5:364:LEU:O	2.37	0.54
54:A:693:A:H5''	54:A:694:C:H5	1.73	0.54
9:M:80:LYS:HG2	26:3:113:ARG:HE	1.71	0.54
23:0:85:ARG:NH1	54:A:638:A:OP1	2.40	0.54
5:I:36:HIS:ND1	5:I:37:ARG:O	2.40	0.54
12:P:56:LEU:HB2	12:P:62:ALA:HB2	1.88	0.54
28:5:144:ARG:O	28:5:194:LYS:NZ	2.40	0.54
54:A:294:U:H4'	54:A:764:A:H8	1.73	0.54
54:A:494:C:H42	54:A:546:A:H61	1.54	0.54
34:b:63:ILE:HB	40:h:152:LEU:HD23	1.89	0.54
54:A:1057:C:H2'	54:A:1058:C:C6	2.42	0.54
15:S:178:LYS:NZ	54:A:455:C:OP2	2.39	0.54
28:5:391:VAL:HG12	28:5:399:GLU:HB2	1.90	0.54
4:H:58:ARG:NH1	4:H:77:HIS:O	2.41	0.54
9:M:62:ARG:NH1	54:A:424:G:OP2	2.41	0.54
13:Q:84:ARG:O	54:A:1487:C:O2'	2.22	0.54
22:Z:85:ILE:HD13	22:Z:112:VAL:HG11	1.90	0.54
34:b:26:LEU:HD22	34:b:105:ALA:HA	1.88	0.54
36:d:62:LYS:HD3	54:A:678:A:H4'	1.90	0.54
43:k:14:LYS:HD3	43:k:69:GLY:H	1.72	0.54
9:M:97:SER:HA	9:M:141:VAL:HB	1.88	0.54
12:P:84:ILE:HB	12:P:91:GLU:HB2	1.89	0.54
17:U:81:ASP:OD1	17:U:82:HIS:N	2.40	0.54
28:5:288:PRO:HD2	28:5:324:GLN:NE2	2.22	0.54
29:6:267:ARG:HB3	29:6:320:GLN:HE22	1.72	0.54
30:7:186:ASP:OD2	30:7:188:LYS:NZ	2.39	0.54
43:k:82:THR:HG22	43:k:85:GLU:HG3	1.90	0.54
54:A:1344:G:N1	54:A:1354:U:C2	2.76	0.54
24:1:16:ILE:HG21	24:1:61:LYS:HB2	1.90	0.54
43:k:15:GLN:HE22	43:k:17:ARG:HB2	1.73	0.54
12:P:66:ARG:NH1	12:P:179:TYR:OH	2.41	0.54
18:V:78:GLN:HB3	18:V:87:VAL:HB	1.88	0.54
30:7:51:GLU:HG2	30:7:225:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:164:MET:HE2	41:i:69:HIS:HE1	1.72	0.53
11:O:22:PRO:HA	11:O:25:ARG:HG2	1.89	0.53
19:W:148:LEU:H	29:6:338:ARG:HH21	1.54	0.53
24:1:20:MET:O	24:1:29:CYS:HA	2.07	0.53
29:6:66:GLN:HA	29:6:75:ARG:HH22	1.72	0.53
9:M:151:LYS:NZ	9:M:250:ASP:OD2	2.41	0.53
29:6:224:HIS:HA	29:6:232:TYR:CZ	2.43	0.53
37:e:133:LEU:HD22	45:m:63:THR:HG21	1.89	0.53
54:A:1323:U:C4	54:A:1398:G:O6	2.62	0.53
54:A:1323:U:O4	54:A:1398:G:O6	2.25	0.53
8:L:109:GLU:HG3	8:L:115:VAL:HG22	1.90	0.53
23:O:133:GLU:OE2	23:O:177:ARG:NH2	2.41	0.53
28:5:112:ARG:NH2	54:A:717:U:O3'	2.41	0.53
50:s:94:TYR:O	50:s:106:TYR:OH	2.21	0.53
54:A:1085:A:H2	54:A:1122:A:H62	1.56	0.53
54:A:1412:G:N2	54:A:1415:A:OP2	2.38	0.53
1:D:136:SER:HB2	1:D:252:HIS:CE1	2.42	0.53
3:F:170:ARG:NH2	54:A:216:G:N7	2.56	0.53
5:I:40:MET:HE1	5:I:48:MET:HE2	1.90	0.53
9:M:104:LEU:HD11	9:M:126:GLY:HA3	1.88	0.53
10:N:148:ASP:OD2	10:N:149:HIS:ND1	2.35	0.53
18:V:40:ARG:NH1	54:A:103:A:N1	2.53	0.53
36:d:153:ASN:ND2	36:d:183:TRP:O	2.41	0.53
54:A:132:A:C6	54:A:135:A:C6	2.97	0.53
54:A:738:U:H2'	54:A:739:A:H8	1.72	0.53
1:D:105:ARG:NH2	54:A:733:G:OP2	2.42	0.53
1:D:154:THR:OG1	1:D:157:MET:SD	2.67	0.53
13:Q:227:LYS:O	13:Q:229:TRP:N	2.42	0.53
17:U:133:GLU:HA	17:U:136:GLN:HB2	1.89	0.53
51:u:135:LEU:HD22	51:u:179:LEU:HB3	1.91	0.53
51:u:167:TRP:CG	51:u:180:MET:HE1	2.44	0.53
6:J:128:GLU:HA	6:J:133:GLN:HE21	1.73	0.53
15:S:125:GLY:N	15:S:160:VAL:O	2.41	0.53
35:c:271:PHE:HE1	35:c:285:PRO:HB3	1.74	0.53
52:v:16:LEU:HD22	52:v:62:LEU:HD13	1.89	0.53
53:w:101:ASN:OD1	53:w:142:GLN:NE2	2.41	0.53
29:6:280:ASP:OD1	29:6:280:ASP:N	2.42	0.53
39:g:142:GLU:HB3	46:o:88:ILE:HG13	1.91	0.53
55:B:1625:A:C6	55:B:1644:G:N2	2.77	0.53
31:8:93:LYS:O	37:e:84:TYR:OH	2.23	0.53
37:e:203:LYS:N	37:e:237:LEU:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:86:VAL:HG22	39:g:113:VAL:HG22	1.90	0.53
54:A:107:A:N6	54:A:110:U:OP2	2.30	0.53
3:F:278:SER:H	39:g:90:ARG:NH2	2.07	0.53
17:U:153:LEU:HG	36:d:242:VAL:HG21	1.90	0.53
18:V:185:ARG:NH2	18:V:187:TYR:O	2.42	0.53
35:c:216:ARG:NE	35:c:217:ASP:OD1	2.40	0.53
14:R:17:ARG:NH2	54:A:625:C:OP2	2.28	0.53
15:S:165:GLU:HG2	15:S:187:THR:HG22	1.91	0.53
22:Z:102:ASN:OD1	46:o:53:TYR:N	2.42	0.53
30:7:38:THR:O	30:7:41:THR:OG1	2.24	0.53
35:c:216:ARG:HG2	35:c:220:ILE:HD12	1.90	0.53
48:q:44:ASP:OD2	48:q:45:LEU:N	2.42	0.53
4:H:64:LEU:HD12	20:X:61:ARG:HH21	1.73	0.52
16:T:190:LYS:HG3	16:T:195:HIS:CE1	2.44	0.52
19:W:148:LEU:H	29:6:338:ARG:NH2	2.06	0.52
34:b:28:ARG:NH1	34:b:78:GLU:OE1	2.32	0.52
34:b:80:LEU:HD11	35:c:78:ARG:HD3	1.91	0.52
37:e:152:LYS:HZ3	37:e:256:THR:HG21	1.74	0.52
54:A:390:A:C5	54:A:409:C:N4	2.76	0.52
22:Z:67:HIS:CE1	22:Z:102:ASN:HD22	2.27	0.52
41:i:118:TYR:OH	54:A:83:A:OP1	2.24	0.52
53:w:79:ILE:HD11	53:w:152:LYS:HD2	1.91	0.52
54:A:521:A:N6	54:A:528:A:OP1	2.42	0.52
54:A:1125:U:H2'	54:A:1126:G:H8	1.74	0.52
26:3:108:LYS:NZ	54:A:75:U:O4	2.42	0.52
28:5:111:CYS:SG	28:5:266:HIS:ND1	2.82	0.52
29:6:125:LEU:HD11	31:8:108:PHE:HE1	1.74	0.52
49:r:79:HIS:HB3	49:r:184:ASN:HA	1.91	0.52
52:v:63:ASN:O	52:v:68:ARG:NH2	2.41	0.52
54:A:530:A:H2'	54:A:531:G:C8	2.39	0.52
54:A:923:G:N2	54:A:962:A:OP2	2.37	0.52
56:z:6:U:H2'	56:z:7:G:H8	1.75	0.52
7:K:107:ALA:O	7:K:111:MET:HG2	2.10	0.52
10:N:111:ARG:NH1	54:A:1286:A:O2'	2.41	0.52
20:X:151:GLU:OE2	20:X:151:GLU:N	2.38	0.52
50:s:193:PRO:HD2	50:s:428:ARG:HH12	1.75	0.52
50:s:228:ASP:O	50:s:230:ARG:NH1	2.43	0.52
54:A:497:A:N6	54:A:542:C:OP2	2.33	0.52
9:M:205:LEU:HD23	9:M:263:ARG:HH11	1.74	0.52
21:Y:70:ASP:HB3	21:Y:73:ASN:HB2	1.92	0.52
54:A:1394:A:H2'	54:A:1431:A:N6	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:15:ASN:OD1	24:1:35:ASN:ND2	2.42	0.52
30:7:277:GLN:O	30:7:301:SER:HA	2.09	0.52
54:A:314:A:H8	54:A:317:G:H21	1.56	0.52
21:Y:98:LEU:HB3	21:Y:142:LEU:HD11	1.92	0.52
31:8:129:ARG:HA	31:8:132:GLU:HG3	1.92	0.52
34:b:85:ARG:NH1	34:b:87:GLU:OE2	2.43	0.52
36:d:225:TYR:OH	36:d:236:GLU:OE2	2.28	0.52
38:f:98:TYR:HE2	38:f:152:THR:HG22	1.75	0.52
54:A:912:A:OP2	54:A:913:C:N4	2.39	0.52
5:I:175:PRO:HB3	43:k:55:VAL:HG11	1.91	0.52
20:X:166:LEU:HD12	20:X:196:ILE:HG12	1.91	0.52
30:7:173:PRO:O	30:7:176:SER:OG	2.17	0.52
35:c:91:ALA:O	35:c:122:ASN:ND2	2.43	0.52
39:g:150:LYS:NZ	46:o:79:THR:O	2.42	0.52
41:i:35:ARG:HA	54:A:6:A:H4'	1.92	0.52
54:A:390:A:N1	54:A:409:C:N4	2.57	0.52
8:L:120:LYS:O	8:L:142:GLN:NE2	2.34	0.52
12:P:87:GLN:H	12:P:87:GLN:CD	2.17	0.52
8:L:111:ASN:OD1	8:L:112:GLY:N	2.43	0.52
20:X:56:ASN:N	20:X:56:ASN:OD1	2.41	0.52
20:X:114:PHE:O	20:X:122:LYS:HA	2.10	0.52
22:Z:99:VAL:O	42:j:76:ARG:NH2	2.43	0.52
28:5:292:TYR:HD1	28:5:345:VAL:HG22	1.75	0.52
37:e:256:THR:OG1	37:e:257:LYS:N	2.43	0.52
3:F:68:SER:O	3:F:210:ARG:NH2	2.43	0.51
16:T:50:LYS:NZ	54:A:1:G:OP1	2.35	0.51
28:5:335:VAL:HG22	28:5:370:VAL:HG21	1.90	0.51
31:8:126:GLN:NE2	55:B:1626:C:O2	2.43	0.51
40:h:139:LYS:HD2	46:o:101:TRP:CE2	2.45	0.51
50:s:168:GLU:HB2	50:s:172:ILE:HD12	1.92	0.51
2:E:292:HIS:ND1	2:E:293:LYS:O	2.43	0.51
18:V:20:ARG:HH22	18:V:44:VAL:HG13	1.75	0.51
48:q:112:GLN:OE1	48:q:115:ARG:NH2	2.36	0.51
55:B:1622:A:H2'	55:B:1623:G:H8	1.75	0.51
3:F:220:ASP:O	3:F:245:ALA:N	2.43	0.51
9:M:59:ARG:NH2	54:A:347:U:OP2	2.36	0.51
17:U:3:ARG:HB2	17:U:47:GLU:HG3	1.93	0.51
28:5:233:LYS:HA	28:5:286:PRO:HD2	1.92	0.51
44:l:119:ARG:NH2	54:A:525:A:OP2	2.34	0.51
53:w:133:ILE:O	53:w:137:LYS:NZ	2.38	0.51
54:A:1339:C:H5	54:A:1360:A:H61	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:1525:A:H3'	54:A:1526:G:H2'	1.92	0.51
6:J:142:ARG:NH2	54:A:521:A:O3'	2.44	0.51
12:P:85:ARG:HD2	12:P:158:MET:HE3	1.92	0.51
26:3:133:LEU:HD12	54:A:1237:U:H5'	1.92	0.51
34:b:27:GLN:NE2	35:c:177:GLN:OE1	2.42	0.51
54:A:158:A:H62	54:A:1028:G:N2	2.07	0.51
11:O:139:ASP:OD2	30:7:131:LYS:NZ	2.43	0.51
23:0:95:ARG:NH2	54:A:148:A:OP1	2.40	0.51
35:c:139:GLN:NE2	35:c:143:ASP:OD2	2.44	0.51
54:A:1464:C:H3'	54:A:1465:A:C8	2.45	0.51
54:A:1526:G:OP1	54:A:1526:G:N2	2.39	0.51
7:K:67:PHE:HB3	7:K:71:LYS:HB2	1.91	0.51
10:N:67:LYS:HE3	54:A:440:A:H5'	1.92	0.51
11:O:10:SER:O	11:O:10:SER:OG	2.25	0.51
13:Q:123:ASP:OD1	51:u:119:ARG:NE	2.43	0.51
42:j:66:ARG:NH1	54:A:586:U:OP1	2.43	0.51
54:A:264:U:N3	54:A:271:G:C6	2.78	0.51
3:F:223:HIS:HD2	3:F:226:MET:HE2	1.76	0.51
10:N:160:VAL:HG12	10:N:161:VAL:HG23	1.92	0.51
29:6:65:ALA:O	29:6:75:ARG:NH2	2.44	0.51
54:A:959:A:N3	54:A:1409:G:O2'	2.43	0.51
11:O:13:ARG:HH12	54:A:1488:A:H8	1.57	0.51
21:Y:95:ASN:OD1	21:Y:149:ARG:NH1	2.43	0.51
54:A:423:U:O2	54:A:596:U:O2'	2.29	0.51
9:M:287:ASP:HB3	9:M:290:LEU:HD12	1.93	0.51
17:U:134:ARG:HA	17:U:137:ARG:HG3	1.92	0.51
31:8:129:ARG:HB3	45:m:37:ARG:HH22	1.76	0.51
41:i:35:ARG:NE	41:i:37:THR:O	2.41	0.51
47:p:106:ALA:O	47:p:116:ARG:NH1	2.44	0.51
54:A:158:A:H62	54:A:1028:G:H22	1.59	0.51
7:K:160:GLN:HA	7:K:163:ILE:HG22	1.91	0.51
11:O:108:LEU:HD12	11:O:133:LEU:HD13	1.92	0.51
17:U:153:LEU:HD11	36:d:220:GLN:HB2	1.92	0.51
40:h:141:ASP:O	40:h:145:ALA:HB3	2.11	0.51
55:B:1622:A:H2'	55:B:1623:G:C8	2.46	0.51
3:F:238:LYS:HA	48:q:25:TYR:CE2	2.46	0.50
10:N:104:MET:HE1	10:N:179:VAL:HG13	1.92	0.50
17:U:137:ARG:HG2	18:V:104:TYR:CG	2.46	0.50
21:Y:164:ARG:NH1	54:A:27:A:OP2	2.32	0.50
24:1:20:MET:HB3	24:1:56:PHE:HB3	1.92	0.50
38:f:127:MET:HB2	38:f:154:GLU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:40:GLU:HA	49:r:49:ILE:HG22	1.93	0.50
54:A:893:U:O2	54:A:897:G:C6	2.64	0.50
54:A:1070:A:N3	54:A:1251:A:O2'	2.44	0.50
10:N:113:MET:HG3	10:N:118:MET:HE3	1.93	0.50
54:A:283:A:O2'	54:A:793:A:OP1	2.28	0.50
54:A:738:U:H2'	54:A:739:A:C8	2.46	0.50
54:A:789:A:N6	54:A:998:A:O2'	2.41	0.50
1:D:202:ARG:NH2	54:A:851:A:OP2	2.45	0.50
14:R:64:MET:HE1	16:T:210:HIS:CG	2.47	0.50
50:s:51:MET:SD	50:s:65:ARG:NH1	2.84	0.50
1:D:284:ARG:HB2	54:A:892:U:H4'	1.94	0.50
12:P:110:TRP:HA	12:P:113:LYS:HE3	1.94	0.50
17:U:98:GLN:HE21	50:s:100:LEU:HB3	1.76	0.50
19:W:88:CYS:SG	54:A:1202:C:O2'	2.67	0.50
20:X:177:HIS:HB3	20:X:180:ASP:HB2	1.93	0.50
31:8:110:GLU:OE1	31:8:114:ARG:NH2	2.40	0.50
35:c:86:ASP:OD2	35:c:86:ASP:N	2.42	0.50
36:d:162:THR:HG23	36:d:163:LEU:HG	1.93	0.50
54:A:144:A:N3	54:A:192:U:O2'	2.42	0.50
54:A:900:C:O5'	54:A:922:G:O2'	2.30	0.50
54:A:1074:U:O2'	54:A:1075:A:O5'	2.29	0.50
54:A:1237:U:H2'	54:A:1238:U:C6	2.47	0.50
17:U:153:LEU:HB2	36:d:222:LEU:HD12	1.93	0.50
29:6:376:THR:HG22	29:6:378:GLY:H	1.77	0.50
47:p:110:TRP:H	47:p:110:TRP:CD1	2.28	0.50
50:s:111:LYS:NZ	50:s:384:ASP:OD1	2.32	0.50
50:s:242:ARG:HG2	50:s:335:TRP:HZ2	1.76	0.50
51:u:169:CYS:SG	51:u:170:VAL:N	2.84	0.50
3:F:184:GLN:OE1	9:M:21:ARG:HA	2.11	0.50
3:F:218:LEU:HD23	3:F:260:VAL:HB	1.93	0.50
9:M:146:ASP:N	9:M:146:ASP:OD1	2.44	0.50
15:S:111:GLU:HG2	34:b:19:LEU:HD21	1.93	0.50
15:S:178:LYS:HZ1	54:A:593:C:HO2'	1.55	0.50
17:U:83:ARG:HB2	17:U:85:VAL:HG12	1.94	0.50
19:W:108:PRO:HA	19:W:114:VAL:HG21	1.94	0.50
28:5:246:GLU:HA	28:5:249:LYS:HG2	1.93	0.50
45:m:51:LEU:HB3	45:m:67:ARG:HB3	1.92	0.50
50:s:115:LEU:O	50:s:394:TRP:HA	2.11	0.50
52:v:6:ARG:HH22	52:v:10:LEU:HD21	1.77	0.50
54:A:950:G:H2'	54:A:951:G:C8	2.46	0.50
56:z:10:G:O6	56:z:24:A:N7	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:37:GLU:HB3	54:A:230:A:H5''	1.92	0.50
11:O:84:ASP:HA	50:s:47:ILE:HD12	1.94	0.50
37:e:279:LEU:HD11	38:f:176:SER:HB2	1.93	0.50
39:g:108:THR:HG21	39:g:153:PHE:H	1.76	0.50
41:i:115:ARG:HG3	54:A:61:A:N1	2.27	0.50
54:A:1472:A:H2'	54:A:1473:U:C6	2.46	0.50
56:z:6:U:H2'	56:z:7:G:C8	2.46	0.50
1:D:202:ARG:NH1	54:A:851:A:N7	2.58	0.50
3:F:131:LYS:NZ	54:A:1054:G:OP1	2.40	0.50
6:J:31:PRO:HB2	6:J:34:PRO:HG2	1.94	0.50
11:O:74:ARG:NH2	13:Q:266:GLU:OE2	2.45	0.50
28:5:356:VAL:HG12	28:5:375:TRP:HB2	1.94	0.50
50:s:212:ARG:NH2	50:s:379:LEU:O	2.44	0.50
2:E:175:THR:HG22	2:E:296:LEU:HD13	1.94	0.50
3:F:280:TYR:CD1	9:M:125:ARG:HD2	2.47	0.50
13:Q:244:ARG:HG2	13:Q:247:LEU:HB3	1.94	0.50
16:T:83:SER:HB3	16:T:170:VAL:HG21	1.94	0.50
23:0:166:SER:OG	23:0:167:GLU:N	2.43	0.50
25:2:82:ARG:NH2	25:2:89:SER:O	2.35	0.50
27:4:102:GLN:OE1	54:A:490:A:N6	2.41	0.50
30:7:153:VAL:O	30:7:157:ALA:HB2	2.12	0.50
49:r:89:LEU:O	49:r:92:PHE:N	2.45	0.50
54:A:1076:U:O4	54:A:1131:A:N6	2.45	0.50
7:K:46:VAL:HG13	16:T:208:ILE:HG12	1.94	0.49
54:A:863:A:H2'	54:A:864:G:H8	1.77	0.49
20:X:237:GLN:O	20:X:241:GLN:NE2	2.45	0.49
26:3:183:ARG:NH2	29:6:354:GLN:OE1	2.44	0.49
29:6:195:PRO:HA	29:6:198:ALA:HB3	1.93	0.49
54:A:53:A:H5''	54:A:54:A:H4'	1.94	0.49
54:A:79:C:OP2	54:A:1229:C:O2'	2.22	0.49
54:A:427:A:H5'	54:A:428:G:H5''	1.94	0.49
54:A:957:G:O2'	54:A:960:U:OP2	2.23	0.49
2:E:79:PRO:O	2:E:82:ASP:C	2.56	0.49
24:1:42:THR:HB	24:1:57:VAL:HA	1.94	0.49
31:8:150:LEU:HD12	37:e:212:HIS:HE1	1.77	0.49
34:b:9:ARG:HB3	34:b:113:ILE:HD11	1.95	0.49
53:w:93:ILE:HG22	53:w:110:LEU:HD21	1.94	0.49
54:A:112:G:O2'	54:A:123:G:O6	2.28	0.49
56:z:72:C:H3'	56:z:73:A:H8	1.76	0.49
3:F:63:GLN:HG2	3:F:81:ASP:HB3	1.94	0.49
8:L:77:ILE:HD11	8:L:82:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:127:TYR:OH	29:6:64:GLU:OE1	2.28	0.49
20:X:121:LYS:NZ	28:5:53:PRO:HG3	2.26	0.49
23:0:144:GLN:OE1	23:0:173:ARG:NH1	2.43	0.49
54:A:314:A:H8	54:A:317:G:N2	2.10	0.49
12:P:59:LEU:HD21	29:6:264:GLY:HA2	1.94	0.49
12:P:84:ILE:O	12:P:90:VAL:HA	2.12	0.49
13:Q:165:GLU:HB2	13:Q:168:ASN:HB2	1.94	0.49
30:7:163:MET:HB2	30:7:186:ASP:HB3	1.95	0.49
35:c:245:LEU:HD12	35:c:250:VAL:HB	1.94	0.49
35:c:258:THR:HG22	35:c:259:ARG:HG3	1.94	0.49
37:e:50:ALA:HB2	37:e:175:GLN:HG2	1.94	0.49
50:s:77:ASP:OD1	50:s:78:GLU:N	2.46	0.49
15:S:111:GLU:N	15:S:195:ILE:O	2.45	0.49
16:T:191:THR:C	33:a:108:MET:HE1	2.37	0.49
23:0:87:ILE:O	23:0:91:ARG:HB2	2.12	0.49
29:6:195:PRO:HG3	29:6:257:PRO:HB2	1.94	0.49
29:6:263:SER:HB2	29:6:342:PHE:HD2	1.78	0.49
30:7:48:PHE:HD1	30:7:256:ARG:HH11	1.60	0.49
3:F:79:LEU:HD22	40:h:94:SER:HB2	1.95	0.49
21:Y:94:SER:O	21:Y:98:LEU:HD12	2.12	0.49
23:0:97:PRO:HA	23:0:100:LEU:HD13	1.94	0.49
37:e:64:THR:HG22	37:e:66:LEU:H	1.76	0.49
37:e:264:LEU:HD23	37:e:269:LEU:HB3	1.95	0.49
15:S:127:ARG:NH2	15:S:157:GLU:OE1	2.35	0.49
47:p:135:LEU:HD12	47:p:153:LYS:HD2	1.94	0.49
54:A:893:U:C2	54:A:897:G:C6	3.01	0.49
5:I:161:VAL:HA	5:I:164:MET:HE2	1.95	0.49
15:S:143:LEU:HD12	15:S:200:ILE:HD11	1.95	0.49
28:5:223:ARG:HE	54:A:739:A:H5''	1.78	0.49
31:8:128:GLU:HB3	45:m:37:ARG:HH12	1.78	0.49
35:c:92:PHE:CE1	35:c:175:VAL:HG23	2.47	0.49
4:H:96:LEU:HD23	4:H:131:TYR:HA	1.94	0.48
5:I:128:ASN:HA	5:I:131:LEU:HB3	1.94	0.48
12:P:80:ARG:NH2	12:P:95:GLU:OE2	2.46	0.48
39:g:118:TRP:NE1	39:g:142:GLU:OE2	2.44	0.48
51:u:196:LEU:HD23	51:u:199:TYR:HB2	1.94	0.48
11:O:65:LEU:HD23	11:O:72:ALA:HB2	1.94	0.48
17:U:11:ARG:HD3	17:U:11:ARG:N	2.27	0.48
19:W:41:ASN:ND2	54:A:1172:C:OP2	2.41	0.48
19:W:148:LEU:HB2	29:6:338:ARG:HE	1.78	0.48
23:0:84:ARG:NH2	54:A:636:A:O2'	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:191:ASN:HD21	47:p:188:LEU:HD21	1.78	0.48
31:8:101:ARG:NH1	37:e:79:ILE:O	2.46	0.48
1:D:154:THR:HG22	1:D:194:ASN:HD21	1.79	0.48
1:D:213:CYS:HB3	1:D:246:ARG:HG3	1.94	0.48
7:K:81:THR:O	7:K:86:GLY:HA3	2.13	0.48
11:O:18:MET:HE3	11:O:48:ARG:HG2	1.95	0.48
16:T:89:TYR:OH	23:0:94:ARG:O	2.28	0.48
23:0:86:THR:OG1	54:A:1014:C:OP1	2.22	0.48
23:0:90:ASN:OD1	23:0:93:ARG:NH1	2.38	0.48
28:5:188:CYS:HB3	28:5:418:TYR:CD2	2.48	0.48
29:6:331:PHE:HD2	29:6:337:MET:HG3	1.78	0.48
37:e:139:GLU:HG2	37:e:152:LYS:HA	1.94	0.48
38:f:123:GLU:HB2	38:f:158:GLN:HB3	1.95	0.48
53:w:138:LEU:HD22	53:w:144:ILE:HA	1.96	0.48
54:A:875:U:H5''	54:A:876:G:H5'	1.94	0.48
1:D:248:SER:OG	1:D:249:ASN:N	2.45	0.48
29:6:235:TRP:CD1	29:6:254:TYR:HD2	2.30	0.48
54:A:1219:C:N4	54:A:1220:U:O4	2.46	0.48
14:R:93:CYS:HB2	14:R:123:ARG:HG2	1.95	0.48
16:T:145:SER:HG	16:T:174:TYR:HH	1.62	0.48
23:0:96:ASN:ND2	54:A:1038:C:O2'	2.33	0.48
29:6:359:HIS:CD2	29:6:360:ARG:HG2	2.49	0.48
31:8:120:LYS:HA	31:8:120:LYS:HD3	1.73	0.48
35:c:44:GLU:OE1	35:c:47:ARG:NH2	2.46	0.48
36:d:159:ARG:HA	36:d:162:THR:HG22	1.95	0.48
48:q:157:GLN:HE21	48:q:170:PRO:HD3	1.77	0.48
54:A:862:U:H2'	54:A:863:A:H8	1.78	0.48
54:A:1132:A:H2'	54:A:1133:A:C8	2.49	0.48
1:D:203:GLY:HA3	54:A:851:A:H61	1.78	0.48
2:E:145:LEU:HD13	2:E:181:ILE:HG21	1.95	0.48
3:F:97:HIS:HA	9:M:27:LEU:HD13	1.95	0.48
5:I:119:HIS:HE1	5:I:158:GLU:HG2	1.78	0.48
35:c:72:ILE:HD13	35:c:178:LEU:HD23	1.94	0.48
43:k:27:VAL:HG12	43:k:30:THR:H	1.78	0.48
50:s:250:PHE:HE1	50:s:371:CYS:HB3	1.77	0.48
12:P:110:TRP:HD1	12:P:114:LYS:HZ2	1.61	0.48
14:R:20:ARG:NH2	54:A:625:C:OP1	2.46	0.48
28:5:106:ILE:HA	28:5:221:GLN:O	2.12	0.48
28:5:211:ALA:HB1	28:5:322:LEU:HD22	1.96	0.48
34:b:16:HIS:HB3	34:b:19:LEU:HD12	1.96	0.48
43:k:90:PHE:O	43:k:94:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:228:ASP:N	50:s:228:ASP:OD1	2.47	0.48
51:u:97:MET:HE1	51:u:125:VAL:HG21	1.95	0.48
52:v:18:ARG:HH22	53:w:120:MET:HE1	1.78	0.48
54:A:48:A:N3	54:A:241:C:O2'	2.37	0.48
54:A:130:G:N2	54:A:133:A:C4	2.81	0.48
3:F:255:LYS:NZ	54:A:609:U:OP1	2.37	0.48
8:L:128:ARG:NH1	51:u:171:ASP:OD1	2.47	0.48
13:Q:192:ASP:OD2	13:Q:233:TRP:NE1	2.38	0.48
13:Q:201:ASP:OD1	13:Q:201:ASP:N	2.47	0.48
15:S:131:GLU:OE1	15:S:132:LYS:N	2.47	0.48
48:q:138:GLN:NE2	48:q:142:ASN:OD1	2.37	0.48
54:A:328:U:OP1	54:A:331:C:N4	2.38	0.48
54:A:457:A:H4'	54:A:581:A:C5	2.49	0.48
54:A:825:U:OP1	54:A:972:C:O2'	2.32	0.48
54:A:1252:A:H2'	54:A:1253:G:H8	1.79	0.48
2:E:307:TYR:HA	2:E:310:LEU:HD13	1.96	0.48
5:I:146:LEU:HA	43:k:26:ASN:HD21	1.79	0.48
7:K:33:ALA:O	7:K:37:ILE:HG12	2.14	0.48
44:l:120:ARG:HA	44:l:123:LYS:HD2	1.95	0.48
50:s:221:HIS:ND1	54:A:755:A:H5'	2.28	0.48
54:A:415:A:H2'	54:A:416:A:C8	2.49	0.48
54:A:862:U:H2'	54:A:863:A:C8	2.49	0.48
3:F:211:ARG:HH12	40:h:58:ARG:HH11	1.60	0.48
6:J:150:SER:OG	54:A:528:A:N1	2.39	0.48
37:e:55:ARG:NH1	37:e:149:LEU:O	2.47	0.48
41:i:50:LYS:O	41:i:54:PHE:HB2	2.14	0.48
49:r:99:MET:SD	49:r:116:GLU:HG2	2.53	0.48
1:D:206:TYR:OH	1:D:295:TYR:OH	2.28	0.47
2:E:129:VAL:HG22	2:E:147:VAL:HG22	1.96	0.47
9:M:291:LEU:O	9:M:295:THR:OG1	2.29	0.47
29:6:240:ILE:HD12	29:6:245:VAL:HA	1.96	0.47
31:8:164:ARG:HD3	38:f:164:ALA:HA	1.95	0.47
39:g:91:MET:HE3	54:A:213:G:H5'	1.95	0.47
50:s:55:SER:OG	54:A:656:C:OP2	2.28	0.47
54:A:789:A:C2	54:A:1042:G:H5'	2.49	0.47
54:A:1178:A:H2'	54:A:1179:G:H8	1.78	0.47
2:E:131:LYS:HG2	2:E:146:SER:HB2	1.96	0.47
10:N:96:TYR:HE1	10:N:153:PRO:HB3	1.77	0.47
54:A:158:A:N6	54:A:1028:G:H22	2.04	0.47
55:B:1607:U:O4	55:B:1664:G:O6	2.31	0.47
55:B:1625:A:C6	55:B:1644:G:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:87:PHE:O	10:N:162:GLU:HA	2.13	0.47
10:N:120:ALA:HB2	10:N:163:MET:HG2	1.95	0.47
20:X:61:ARG:NH2	20:X:63:GLU:OE1	2.47	0.47
29:6:44:ASN:O	29:6:47:ARG:NH1	2.48	0.47
2:E:207:THR:HG23	2:E:298:LYS:HB3	1.96	0.47
4:H:64:LEU:O	54:A:85:A:O2'	2.30	0.47
5:I:102:VAL:HG12	43:k:35:GLN:NE2	2.29	0.47
28:5:142:ASP:OD1	28:5:142:ASP:N	2.44	0.47
35:c:49:ARG:HG2	35:c:52:ARG:HH11	1.80	0.47
51:u:118:MET:HE3	51:u:197:ARG:HE	1.79	0.47
54:A:1274:C:H42	54:A:1311:A:H61	1.61	0.47
3:F:91:PRO:HG2	9:M:12:ALA:HB1	1.96	0.47
7:K:119:ARG:NH2	54:A:1035:U:OP2	2.48	0.47
8:L:129:LYS:HE2	8:L:129:LYS:HB2	1.73	0.47
13:Q:150:ILE:HG22	13:Q:163:CYS:HA	1.95	0.47
15:S:162:GLU:OE1	34:b:108:SER:OG	2.23	0.47
22:Z:75:THR:HG22	22:Z:116:LEU:HD13	1.96	0.47
23:0:92:CYS:SG	54:A:151:A:O2'	2.54	0.47
29:6:72:ARG:NH1	29:6:76:GLU:OE2	2.39	0.47
36:d:86:ASP:HB2	36:d:198:ARG:HG3	1.95	0.47
44:l:133:SER:O	54:A:530:A:O2'	2.32	0.47
51:u:166:ASP:OD1	51:u:167:TRP:N	2.47	0.47
51:u:193:LEU:HA	51:u:193:LEU:HD13	1.77	0.47
54:A:181:G:H2'	54:A:1023:A:N7	2.29	0.47
56:z:69:C:N3	56:z:70:A:N7	2.63	0.47
7:K:5:SER:HB2	7:K:8:PRO:HD2	1.97	0.47
7:K:39:LEU:HD11	7:K:125:LEU:HB2	1.96	0.47
7:K:74:GLN:HA	49:r:161:PRO:HA	1.96	0.47
7:K:158:TYR:HD2	49:r:87:LEU:HD21	1.80	0.47
13:Q:154:VAL:HA	13:Q:159:GLY:HA2	1.96	0.47
49:r:70:CYS:HB3	49:r:108:CYS:SG	2.55	0.47
54:A:201:A:N6	54:A:231:C:O2	2.47	0.47
54:A:693:A:H5''	54:A:694:C:C5	2.49	0.47
54:A:863:A:H2'	54:A:864:G:C8	2.50	0.47
54:A:1018:C:H2'	54:A:1019:C:C6	2.50	0.47
15:S:118:ASN:C	15:S:118:ASN:ND2	2.73	0.47
21:Y:102:TRP:HD1	21:Y:103:TYR:CD1	2.33	0.47
21:Y:218:ARG:NH2	41:i:105:ASP:OD1	2.47	0.47
23:0:166:SER:OG	23:0:167:GLU:OE1	2.32	0.47
28:5:93:LEU:HA	28:5:96:HIS:HD2	1.78	0.47
29:6:143:CYS:O	29:6:147:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:221:LEU:HB2	29:6:267:ARG:HG3	1.96	0.47
29:6:233:LEU:HB3	29:6:298:PHE:CE1	2.49	0.47
29:6:274:LYS:HE3	29:6:312:THR:HG22	1.96	0.47
37:e:146:ARG:HB3	37:e:253:VAL:HG13	1.95	0.47
43:k:48:ASN:OD1	43:k:48:ASN:N	2.46	0.47
44:l:119:ARG:HG2	44:l:123:LYS:HE3	1.96	0.47
50:s:177:LEU:O	50:s:181:VAL:HG23	2.14	0.47
50:s:221:HIS:CD2	50:s:222:ARG:HG3	2.49	0.47
54:A:517:C:H2'	54:A:518:A:C8	2.50	0.47
54:A:1007:A:H2'	54:A:1008:A:C8	2.49	0.47
54:A:1240:A:O2'	54:A:1242:C:OP1	2.24	0.47
2:E:81:LYS:NZ	2:E:322:ASP:OD1	2.48	0.47
2:E:168:LEU:HD23	2:E:170:LEU:HD13	1.97	0.47
2:E:344:SER:HG	13:Q:102:ARG:HH22	1.61	0.47
4:H:100:GLN:HE22	4:H:128:LEU:HA	1.79	0.47
6:J:66:LEU:HB3	6:J:82:ILE:HD11	1.95	0.47
8:L:44:SER:O	8:L:48:ASN:ND2	2.48	0.47
16:T:206:ARG:HA	54:A:164:U:C4	2.50	0.47
19:W:119:ARG:HA	29:6:50:LYS:HE3	1.97	0.47
28:5:142:ASP:OD1	28:5:145:ASN:ND2	2.47	0.47
37:e:55:ARG:HD3	37:e:157:LEU:HD13	1.96	0.47
37:e:157:LEU:HD23	37:e:254:TRP:HB3	1.95	0.47
43:k:64:VAL:HG22	43:k:76:MET:HB3	1.97	0.47
4:H:131:TYR:HE2	20:X:136:ASP:HA	1.79	0.47
6:J:45:SER:H	6:J:78:PHE:HZ	1.62	0.47
7:K:59:ILE:HB	7:K:127:LEU:HD23	1.96	0.47
9:M:44:ARG:NH1	54:A:598:G:N7	2.54	0.47
13:Q:135:GLY:HA3	13:Q:152:ARG:O	2.14	0.47
22:Z:117:ILE:O	46:o:45:ASN:ND2	2.41	0.47
28:5:59:THR:HG23	28:5:61:ALA:H	1.79	0.47
33:a:109:ILE:HG23	33:a:123:TRP:HB2	1.96	0.47
54:A:237:A:N3	54:A:1260:U:O2'	2.43	0.47
54:A:529:A:H2	54:A:530:A:H62	1.63	0.47
54:A:1324:U:H5'	54:A:1390:C:N4	2.30	0.47
54:A:1554:G:H2'	54:A:1555:G:H8	1.79	0.47
54:A:1554:G:H2'	54:A:1555:G:C8	2.50	0.47
3:F:191:ASP:OD1	3:F:192:SER:N	2.46	0.47
5:I:151:ASN:HB3	43:k:31:ARG:HH12	1.80	0.47
12:P:130:ARG:HH22	29:6:132:LEU:HD21	1.80	0.47
28:5:333:ALA:HA	28:5:362:THR:HG23	1.97	0.47
36:d:185:PHE:HE1	36:d:218:THR:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:73:ARG:HH12	43:k:75:ILE:HD13	1.80	0.47
54:A:132:A:C5	54:A:135:A:N6	2.83	0.47
54:A:1349:G:N2	54:A:1461:G:O2'	2.48	0.47
1:D:263:ASN:ND2	54:A:841:C:O5'	2.43	0.46
3:F:253:MET:HE3	3:F:259:LEU:HD22	1.96	0.46
13:Q:139:GLN:O	13:Q:149:PHE:HA	2.15	0.46
18:V:48:PRO:HD3	21:Y:234:LEU:HD11	1.96	0.46
23:O:109:VAL:HG22	30:7:102:LYS:HE3	1.96	0.46
23:O:110:CYS:SG	23:O:112:GLU:HB2	2.55	0.46
28:5:216:GLU:H	28:5:365:ASP:HA	1.80	0.46
28:5:385:HIS:HB2	54:A:725:A:H1'	1.97	0.46
2:E:48:TRP:HD1	2:E:50:ASP:H	1.61	0.46
11:O:60:ILE:HD11	11:O:125:TYR:CZ	2.49	0.46
15:S:174:PHE:HA	15:S:180:PHE:O	2.16	0.46
21:Y:123:ARG:NH2	54:A:697:A:H1'	2.30	0.46
22:Z:148:GLN:HB3	22:Z:150:HIS:NE2	2.30	0.46
28:5:279:PHE:O	50:s:158:ARG:NH2	2.48	0.46
30:7:303:PRO:HG2	30:7:306:LEU:HB2	1.97	0.46
39:g:111:ARG:HG3	39:g:146:THR:HG22	1.97	0.46
40:h:65:ASP:OD2	40:h:69:ARG:NH1	2.48	0.46
46:o:55:THR:HG23	46:o:57:GLU:HG2	1.97	0.46
50:s:222:ARG:NH1	50:s:227:ASP:OD2	2.40	0.46
53:w:114:ASP:HA	53:w:117:GLU:HG3	1.96	0.46
54:A:130:G:N2	54:A:133:A:C8	2.84	0.46
54:A:940:U:H3	54:A:952:G:H1	1.63	0.46
18:V:145:ARG:NH1	18:V:155:PRO:O	2.47	0.46
37:e:253:VAL:HG12	37:e:255:VAL:HG23	1.97	0.46
40:h:75:LYS:HZ1	40:h:82:LEU:HD12	1.81	0.46
46:o:12:ILE:HG13	46:o:23:ARG:HB2	1.96	0.46
54:A:1240:A:O5'	56:z:73:A:N6	2.48	0.46
54:A:1446:C:H2'	54:A:1447:C:H6	1.80	0.46
5:I:102:VAL:HG12	43:k:35:GLN:HE21	1.80	0.46
9:M:129:ILE:HD12	9:M:184:LEU:HD21	1.97	0.46
10:N:132:THR:HG22	10:N:147:ILE:HA	1.97	0.46
16:T:82:TYR:HD2	16:T:87:MET:HE2	1.81	0.46
18:V:95:TYR:HD1	36:d:161:HIS:ND1	2.14	0.46
18:V:117:HIS:HA	18:V:120:VAL:HG12	1.97	0.46
29:6:305:LYS:NZ	42:j:108:ALA:O	2.40	0.46
30:7:150:MET:HB2	30:7:278:TYR:OH	2.16	0.46
36:d:118:SER:OG	36:d:121:SER:OG	2.32	0.46
50:s:86:MET:HG3	54:A:776:A:C5	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:332:LEU:O	50:s:336:THR:OG1	2.32	0.46
54:A:495:C:O2'	54:A:496:C:O4'	2.31	0.46
2:E:205:ASP:OD1	2:E:302:SER:HA	2.16	0.46
3:F:217:LEU:HD12	3:F:217:LEU:HA	1.74	0.46
5:I:86:ILE:HA	5:I:89:VAL:HB	1.98	0.46
5:I:188:ARG:HD3	43:k:55:VAL:HG13	1.97	0.46
6:J:120:ILE:O	6:J:124:LYS:HB2	2.16	0.46
24:l:18:VAL:HG12	24:l:61:LYS:HA	1.98	0.46
29:6:192:GLU:HA	29:6:320:GLN:H	1.79	0.46
38:f:91:LEU:O	38:f:158:GLN:HA	2.15	0.46
54:A:496:C:O2'	54:A:497:A:O4'	2.24	0.46
55:B:1615:A:H2'	55:B:1616:A:C8	2.50	0.46
1:D:187:LEU:HD11	1:D:244:VAL:HG12	1.96	0.46
3:F:49:ARG:NH2	3:F:270:GLU:OE1	2.44	0.46
5:I:32:ALA:HB3	10:N:73:ARG:HH22	1.79	0.46
6:J:60:ILE:HG21	6:J:66:LEU:HD11	1.98	0.46
14:R:17:ARG:HG3	14:R:20:ARG:HH21	1.80	0.46
47:p:40:LYS:HD3	47:p:40:LYS:HA	1.67	0.46
47:p:54:GLY:O	47:p:57:THR:OG1	2.30	0.46
50:s:351:VAL:O	50:s:389:ARG:NH2	2.42	0.46
53:w:86:VAL:HA	53:w:89:LEU:HG	1.98	0.46
54:A:970:C:H2'	54:A:971:A:C8	2.51	0.46
54:A:1446:C:H2'	54:A:1447:C:C6	2.51	0.46
5:I:123:MET:N	5:I:123:MET:SD	2.88	0.46
9:M:59:ARG:NH1	54:A:346:C:OP2	2.47	0.46
9:M:260:LYS:NZ	9:M:265:ILE:O	2.46	0.46
21:Y:71:PRO:HA	21:Y:74:TRP:CE3	2.51	0.46
30:7:186:ASP:OD1	30:7:186:ASP:N	2.49	0.46
46:o:55:THR:OG1	46:o:56:ARG:N	2.45	0.46
54:A:800:G:N2	54:A:803:A:H62	2.13	0.46
1:D:113:ARG:O	1:D:147:ARG:NH1	2.38	0.46
1:D:262:ARG:HA	1:D:265:TRP:HB2	1.96	0.46
2:E:109:LEU:HD23	2:E:119:VAL:HG21	1.97	0.46
2:E:228:PRO:O	2:E:233:GLN:HG3	2.16	0.46
6:J:138:SER:HA	6:J:141:VAL:HG12	1.98	0.46
9:M:244:LEU:HD12	9:M:245:PRO:HD2	1.97	0.46
11:O:43:GLU:HG2	11:O:110:ILE:HD13	1.97	0.46
11:O:142:LEU:HB2	30:7:135:PRO:HD2	1.98	0.46
12:P:44:VAL:HG13	29:6:225:LEU:HD13	1.97	0.46
12:P:131:VAL:O	12:P:135:ARG:HG2	2.14	0.46
15:S:171:ILE:HB	15:S:184:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:136:PHE:HB2	16:T:139:ASN:HB2	1.97	0.46
51:u:190:LEU:HA	51:u:193:LEU:HD23	1.97	0.46
53:w:103:HIS:O	53:w:107:ASP:HB3	2.16	0.46
53:w:103:HIS:CE1	53:w:105:MET:HE2	2.50	0.46
54:A:411:U:H2'	54:A:412:G:C8	2.50	0.46
54:A:867:G:O2'	54:A:964:U:OP2	2.33	0.46
3:F:69:LEU:HD22	3:F:206:LEU:HD21	1.97	0.46
3:F:238:LYS:HA	48:q:25:TYR:HE2	1.80	0.46
7:K:8:PRO:HG2	35:c:295:GLU:HG3	1.96	0.46
12:P:89:HIS:HE2	55:B:1622:A:H5''	1.81	0.46
43:k:18:VAL:HG23	43:k:64:VAL:HG12	1.98	0.46
51:u:168:LEU:HB3	51:u:179:LEU:HB2	1.97	0.46
54:A:1146:G:H2'	54:A:1147:G:C8	2.51	0.46
9:M:155:GLU:OE2	9:M:177:ALA:HB2	2.15	0.46
15:S:128:ILE:HB	15:S:158:ALA:O	2.16	0.46
40:h:74:VAL:HA	40:h:77:VAL:HG12	1.97	0.46
54:A:236:G:H2'	54:A:344:A:H61	1.81	0.46
54:A:1408:C:N4	54:A:1409:G:O6	2.49	0.46
3:F:167:MET:HA	3:F:170:ARG:HE	1.81	0.45
9:M:78:ILE:HD11	26:3:114:PHE:CZ	2.51	0.45
14:R:12:ASN:OD1	14:R:12:ASN:N	2.45	0.45
21:Y:102:TRP:HD1	21:Y:103:TYR:HD1	1.64	0.45
34:b:53:ASP:O	34:b:57:ARG:HB2	2.16	0.45
47:p:96:ASN:ND2	47:p:139:SER:O	2.49	0.45
54:A:916:U:H2'	54:A:917:G:C8	2.51	0.45
11:O:52:MET:SD	11:O:123:ILE:HD11	2.56	0.45
11:O:60:ILE:HD11	11:O:125:TYR:CE1	2.52	0.45
17:U:17:LEU:HD11	32:9:136:LEU:HG	1.98	0.45
28:5:365:ASP:OD1	28:5:365:ASP:N	2.50	0.45
50:s:376:THR:HG22	50:s:389:ARG:HG3	1.97	0.45
51:u:179:LEU:O	51:u:180:MET:HE2	2.15	0.45
54:A:1252:A:H2'	54:A:1253:G:C8	2.50	0.45
56:z:15:A:N6	56:z:46:G:C6	2.84	0.45
3:F:99:VAL:HG21	3:F:173:GLY:HA3	1.98	0.45
6:J:125:ALA:HB2	6:J:140:VAL:HG21	1.98	0.45
24:1:19:ARG:NH1	54:A:1236:C:N3	2.63	0.45
28:5:133:PRO:HG3	28:5:239:ILE:HG12	1.98	0.45
28:5:230:LEU:HD21	28:5:418:TYR:HE1	1.81	0.45
28:5:251:HIS:O	28:5:371:LYS:NZ	2.34	0.45
29:6:139:TRP:HE1	29:6:147:HIS:CD2	2.34	0.45
35:c:301:LEU:HD23	35:c:301:LEU:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:51:LEU:HD12	37:e:188:ALA:HB1	1.97	0.45
49:r:121:MET:HE1	49:r:177:GLY:HA2	1.98	0.45
50:s:237:PRO:HB3	50:s:298:GLN:HE21	1.82	0.45
53:w:90:TYR:CE2	53:w:92:LYS:HG2	2.52	0.45
54:A:850:C:N3	54:A:859:U:C2	2.84	0.45
56:z:66:U:H2'	56:z:67:A:C8	2.50	0.45
2:E:295:CYS:SG	2:E:296:LEU:N	2.90	0.45
4:H:133:SER:OG	4:H:136:ASN:OD1	2.30	0.45
5:I:51:THR:HG22	10:N:250:ARG:HH12	1.82	0.45
9:M:96:LEU:HD21	9:M:101:LEU:HB2	1.99	0.45
14:R:17:ARG:O	14:R:21:ILE:HG12	2.16	0.45
16:T:149:ARG:O	54:A:2:C:O2'	2.32	0.45
24:1:45:HIS:HD2	24:1:56:PHE:HB2	1.80	0.45
30:7:158:PHE:HE2	30:7:185:LEU:HD21	1.80	0.45
36:d:198:ARG:HD3	36:d:198:ARG:HA	1.76	0.45
43:k:20:PHE:O	43:k:55:VAL:HA	2.16	0.45
54:A:360:U:C4	54:A:428:G:O6	2.68	0.45
54:A:929:U:H3	54:A:957:G:H5'	1.81	0.45
54:A:1410:G:H2'	54:A:1411:A:H8	1.82	0.45
1:D:284:ARG:NH2	54:A:845:U:H4'	2.31	0.45
3:F:92:ARG:NH2	54:A:208:U:O3'	2.49	0.45
3:F:97:HIS:HD2	9:M:27:LEU:HB3	1.82	0.45
3:F:219:VAL:HG12	3:F:265:THR:HG21	1.99	0.45
5:I:62:PRO:HA	5:I:65:LEU:HD13	1.99	0.45
14:R:64:MET:HE2	14:R:64:MET:HA	1.99	0.45
21:Y:219:ILE:HG12	21:Y:222:ARG:HH21	1.82	0.45
33:a:142:ARG:HG3	34:b:122:ASP:HA	1.99	0.45
36:d:62:LYS:HB3	54:A:678:A:H4'	1.98	0.45
36:d:238:VAL:HG13	36:d:240:LYS:HZ1	1.82	0.45
54:A:928:A:N1	54:A:957:G:C6	2.85	0.45
3:F:126:LYS:NZ	54:A:237:A:OP1	2.41	0.45
3:F:277:ASP:HA	39:g:90:ARG:HH22	1.81	0.45
7:K:52:ASP:O	16:T:206:ARG:NH1	2.47	0.45
8:L:36:THR:HG22	54:A:800:G:O2'	2.17	0.45
12:P:87:GLN:HA	12:P:120:ARG:HE	1.81	0.45
14:R:98:ASN:HD22	54:A:477:G:H4'	1.82	0.45
18:V:127:ASP:OD2	18:V:152:ARG:NH2	2.49	0.45
21:Y:88:GLN:HG3	32:9:81:SER:HB3	1.99	0.45
28:5:146:HIS:HB3	28:5:150:GLN:NE2	2.32	0.45
30:7:166:LEU:HD23	30:7:181:TYR:HE2	1.80	0.45
40:h:127:LEU:O	40:h:131:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:166:TYR:CD1	50:s:167:GLU:HG3	2.51	0.45
50:s:418:LEU:HA	50:s:421:ILE:HG22	1.99	0.45
52:v:12:LEU:HD23	52:v:16:LEU:HD23	1.98	0.45
53:w:79:ILE:HG23	53:w:126:PHE:HE2	1.82	0.45
54:A:130:G:C2	54:A:133:A:C5	3.05	0.45
2:E:277:ASN:HB3	2:E:282:ILE:HB	1.99	0.45
3:F:217:LEU:HB3	3:F:259:LEU:HD12	1.99	0.45
4:H:137:LYS:HG3	4:H:138:LYS:HD3	1.98	0.45
19:W:123:GLY:H	29:6:40:ILE:HD12	1.82	0.45
20:X:168:ARG:HH21	20:X:176:LEU:HA	1.82	0.45
20:X:216:ARG:O	20:X:220:GLU:HB2	2.17	0.45
50:s:223:ARG:NE	54:A:675:G:OP2	2.46	0.45
54:A:519:C:H5'	54:A:520:C:H5'	1.99	0.45
1:D:199:GLU:HB2	1:D:202:ARG:HB2	1.99	0.45
9:M:17:ARG:HH22	40:h:116:ARG:NH1	2.15	0.45
15:S:132:LYS:HA	15:S:148:LEU:HD22	1.98	0.45
48:q:124:CYS:HA	48:q:127:LYS:HZ3	1.81	0.45
50:s:373:GLN:HB3	50:s:392:ILE:HB	1.99	0.45
9:M:94:LYS:HG3	9:M:129:ILE:HG22	1.98	0.45
29:6:257:PRO:HB3	29:6:268:LEU:HD11	1.98	0.45
32:9:98:PRO:HA	32:9:101:GLU:HG3	1.99	0.45
33:a:67:ILE:HG21	35:c:258:THR:HG23	1.98	0.45
35:c:271:PHE:CE1	35:c:285:PRO:HB3	2.51	0.45
49:r:99:MET:HE2	49:r:99:MET:HB3	1.79	0.45
54:A:187:U:H2'	54:A:188:G:C8	2.52	0.45
54:A:214:G:N3	54:A:225:C:O2'	2.50	0.45
54:A:1146:G:H2'	54:A:1147:G:H8	1.81	0.45
2:E:215:PHE:O	54:A:788:A:O2'	2.30	0.45
3:F:178:LEU:HD11	3:F:269:LEU:HD13	1.99	0.45
5:I:181:ILE:O	5:I:184:THR:OG1	2.30	0.45
9:M:130:GLN:HA	9:M:131:PRO:HD3	1.79	0.45
14:R:111:LYS:HB3	33:a:62:HIS:ND1	2.32	0.45
17:U:11:ARG:HE	18:V:211:LYS:HB3	1.82	0.45
28:5:293:LEU:O	28:5:346:GLY:HA2	2.17	0.45
35:c:94:ASN:ND2	35:c:180:LEU:O	2.50	0.45
51:u:185:ARG:O	51:u:189:GLU:CB	2.54	0.45
54:A:801:G:O2'	54:A:984:U:O4	2.32	0.45
20:X:119:LEU:HB3	28:5:53:PRO:HG2	1.99	0.44
29:6:45:LEU:HD11	38:f:64:LYS:HB2	1.99	0.44
29:6:261:ARG:NH2	47:p:125:ASN:HD21	2.14	0.44
34:b:19:LEU:HA	34:b:19:LEU:HD23	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:164:HIS:CE1	54:A:744:C:H1'	2.52	0.44
54:A:454:A:H5''	54:A:454:A:H8	1.81	0.44
5:I:60:ILE:HG23	5:I:65:LEU:HD11	1.99	0.44
12:P:51:ARG:NH1	29:6:229:ASP:O	2.50	0.44
15:S:68:ASP:N	15:S:71:GLU:OE1	2.50	0.44
28:5:149:ASN:HB3	28:5:152:GLU:HB3	2.00	0.44
30:7:262:ASP:OD1	30:7:263:VAL:N	2.48	0.44
54:A:65:A:O2'	54:A:66:A:O4'	2.34	0.44
54:A:156:G:H4'	54:A:158:A:C2	2.51	0.44
2:E:215:PHE:N	54:A:1550:A:OP1	2.48	0.44
5:I:113:ARG:NH1	5:I:117:ARG:HH22	2.16	0.44
13:Q:246:ASP:OD2	13:Q:247:LEU:N	2.50	0.44
24:l:25:GLY:H	48:q:121:ILE:HD12	1.83	0.44
26:3:133:LEU:HD22	26:3:141:LYS:HG2	1.99	0.44
34:b:78:GLU:HG2	34:b:84:VAL:HG12	1.99	0.44
2:E:112:LYS:NZ	2:E:337:VAL:O	2.44	0.44
3:F:113:LYS:HD2	3:F:157:GLY:HA2	1.98	0.44
4:H:98:LEU:HD21	4:H:102:VAL:HB	2.00	0.44
37:e:81:ARG:NH1	45:m:43:VAL:O	2.40	0.44
54:A:1350:C:H2'	54:A:1351:C:O4'	2.17	0.44
9:M:205:LEU:HD23	9:M:263:ARG:NH1	2.32	0.44
15:S:129:ARG:HH12	15:S:155:ARG:HA	1.83	0.44
17:U:33:VAL:HG21	50:s:270:LYS:HE3	1.99	0.44
26:3:101:LYS:HE3	54:A:71:A:C2	2.53	0.44
28:5:240:ALA:HB2	28:5:375:TRP:HH2	1.83	0.44
29:6:175:VAL:HG22	29:6:204:VAL:HG12	2.00	0.44
47:p:104:HIS:CE1	47:p:107:THR:HG23	2.53	0.44
52:v:2:ALA:HB1	52:v:51:ARG:HG3	2.00	0.44
54:A:796:A:N1	54:A:797:A:C6	2.86	0.44
56:z:14:A:H2'	56:z:15:A:C8	2.52	0.44
6:J:90:PHE:HZ	6:J:123:ILE:HD11	1.83	0.44
7:K:177:ARG:H	7:K:177:ARG:HG2	1.56	0.44
9:M:180:ASP:O	9:M:184:LEU:HB2	2.17	0.44
13:Q:245:PHE:O	13:Q:249:LEU:HB3	2.18	0.44
21:Y:193:ARG:NH2	54:A:36:C:OP1	2.44	0.44
50:s:332:LEU:HD21	50:s:359:ALA:HB3	2.00	0.44
53:w:114:ASP:O	53:w:118:ILE:HG12	2.18	0.44
54:A:295:A:H2'	54:A:296:G:C8	2.53	0.44
54:A:472:A:C8	54:A:591:C:H5''	2.52	0.44
54:A:928:A:C2	54:A:957:G:C2	3.05	0.44
12:P:65:GLU:OE2	29:6:74:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:136:ILE:HD11	13:Q:200:PHE:HE2	1.83	0.44
16:T:77:ARG:HH22	16:T:119:GLU:CD	2.25	0.44
28:5:292:TYR:CD1	28:5:345:VAL:HG22	2.53	0.44
28:5:407:LYS:HZ1	28:5:409:GLU:HB2	1.83	0.44
29:6:45:LEU:HD21	38:f:64:LYS:HG2	2.00	0.44
35:c:228:LEU:HB2	35:c:307:PHE:CD2	2.53	0.44
36:d:183:TRP:CH2	36:d:185:PHE:HB2	2.52	0.44
45:m:42:ARG:NH1	55:B:1630:A:OP1	2.46	0.44
54:A:169:C:H2'	54:A:170:C:C6	2.53	0.44
54:A:920:A:H2'	54:A:921:A:C8	2.52	0.44
4:H:78:ARG:NH2	54:A:46:U:O4'	2.51	0.44
5:I:35:ARG:NH2	54:A:440:A:OP1	2.51	0.44
5:I:86:ILE:HD11	5:I:126:PHE:CD2	2.53	0.44
6:J:73:LYS:HB2	6:J:77:THR:HG22	1.99	0.44
8:L:108:ILE:HG22	8:L:109:GLU:O	2.18	0.44
10:N:105:MET:HE1	10:N:160:VAL:HG11	2.00	0.44
20:X:122:LYS:HE3	20:X:122:LYS:HB3	1.73	0.44
23:0:90:ASN:O	23:0:94:ARG:HG2	2.17	0.44
28:5:140:VAL:HB	28:5:416:ALA:HB2	1.98	0.44
32:9:25:ARG:HA	54:A:671:C:H41	1.83	0.44
37:e:91:ALA:O	37:e:95:ASN:ND2	2.50	0.44
3:F:220:ASP:OD1	3:F:221:LEU:N	2.46	0.44
6:J:90:PHE:HE2	6:J:120:ILE:HB	1.83	0.44
10:N:174:GLY:O	10:N:178:GLN:HG2	2.17	0.44
12:P:75:ARG:HD2	12:P:97:GLN:NE2	2.32	0.44
26:3:129:TYR:CZ	26:3:130:LYS:HD3	2.53	0.44
34:b:28:ARG:HG2	34:b:62:VAL:HG23	1.99	0.44
50:s:153:GLU:OE2	50:s:159:ARG:NH2	2.50	0.44
50:s:242:ARG:NH2	50:s:292:CYS:O	2.50	0.44
1:D:148:LYS:HD3	28:5:114:LEU:HD12	1.99	0.43
3:F:106:PHE:CE1	3:F:107:LYS:HG3	2.53	0.43
7:K:172:PRO:HG2	49:r:57:PRO:HD2	1.98	0.43
10:N:195:LEU:O	10:N:199:ARG:HG3	2.18	0.43
12:P:121:ASN:OD1	12:P:123:VAL:N	2.51	0.43
18:V:185:ARG:HA	21:Y:92:ASN:OD1	2.18	0.43
20:X:95:ASP:OD1	20:X:95:ASP:N	2.48	0.43
21:Y:180:LYS:NZ	54:A:26:C:OP2	2.34	0.43
22:Z:66:LEU:HD12	22:Z:122:LEU:HD22	2.00	0.43
25:2:82:ARG:CZ	25:2:87:ARG:HD2	2.47	0.43
26:3:94:LEU:HD11	26:3:104:ARG:HH11	1.82	0.43
31:8:143:GLN:HG2	37:e:210:CYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:31:PHE:HB2	34:b:65:VAL:HG12	2.00	0.43
39:g:139:GLN:NE2	46:o:84:PRO:O	2.48	0.43
54:A:472:A:N7	54:A:591:C:H5''	2.32	0.43
54:A:1487:C:OP2	54:A:1487:C:H4'	2.17	0.43
56:z:10:G:C6	56:z:24:A:N7	2.86	0.43
3:F:243:ILE:HG22	3:F:244:PRO:O	2.18	0.43
7:K:67:PHE:HE2	7:K:103:ILE:HD13	1.82	0.43
15:S:175:ARG:HB2	15:S:180:PHE:HB3	2.01	0.43
19:W:101:LYS:HD2	38:f:56:ILE:HG21	2.00	0.43
28:5:107:PHE:HB3	28:5:222:VAL:HG12	2.00	0.43
32:9:25:ARG:HA	54:A:671:C:N4	2.33	0.43
50:s:380:THR:O	50:s:384:ASP:CB	2.66	0.43
53:w:148:ILE:HA	53:w:151:LYS:HG2	1.99	0.43
55:B:1625:A:N1	55:B:1644:G:N2	2.65	0.43
55:B:1659:U:H2'	55:B:1660:G:H8	1.83	0.43
2:E:116:LYS:HB3	2:E:116:LYS:HE3	1.83	0.43
8:L:33:GLN:NE2	54:A:988:U:O2	2.51	0.43
14:R:140:GLY:HA3	14:R:143:SER:HB3	2.00	0.43
20:X:14:LEU:HD13	54:A:19:C:C4	2.53	0.43
22:Z:76:ARG:HD3	54:A:469:U:C4	2.54	0.43
23:0:81:PRO:O	54:A:1009:U:O2'	2.28	0.43
33:a:69:TYR:HD2	35:c:278:LYS:HD3	1.82	0.43
38:f:114:CYS:HA	38:f:119:ILE:HD12	1.98	0.43
39:g:88:ARG:HB3	39:g:92:HIS:HA	2.00	0.43
50:s:51:MET:HB2	50:s:61:ARG:NH2	2.34	0.43
51:u:167:TRP:CD1	51:u:180:MET:HE1	2.53	0.43
52:v:23:LEU:HD11	52:v:26:THR:HB	1.99	0.43
54:A:1178:A:H2'	54:A:1179:G:C8	2.54	0.43
54:A:1289:G:N2	54:A:1295:A:H62	2.16	0.43
55:B:1628:C:H2'	55:B:1629:A:H8	1.83	0.43
55:B:1639:U:H2'	55:B:1640:A:C8	2.53	0.43
1:D:211:GLY:H	1:D:247:VAL:HB	1.82	0.43
5:I:53:TYR:CD1	10:N:209:ASN:HB3	2.54	0.43
12:P:85:ARG:O	12:P:120:ARG:NH2	2.52	0.43
12:P:94:VAL:HG23	12:P:132:LEU:HD21	1.99	0.43
18:V:138:THR:OG1	18:V:141:GLY:O	2.26	0.43
32:9:71:LYS:HE2	32:9:74:VAL:HA	2.01	0.43
35:c:148:MET:HG2	35:c:149:PRO:HD2	1.99	0.43
44:l:132:LEU:HD23	44:l:132:LEU:HA	1.67	0.43
1:D:101:LYS:NZ	54:A:256:A:OP1	2.38	0.43
2:E:202:GLN:O	2:E:272:LYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:176:LEU:O	5:I:188:ARG:NH1	2.51	0.43
8:L:126:SER:HA	8:L:129:LYS:HZ3	1.82	0.43
9:M:252:LEU:HD13	9:M:255:MET:HE3	2.00	0.43
13:Q:262:GLN:HG2	13:Q:264:TRP:CH2	2.53	0.43
20:X:5:LYS:HD3	54:A:18:A:N7	2.33	0.43
24:1:54:VAL:HG12	48:q:128:MET:HE1	1.99	0.43
28:5:113:LEU:HD12	28:5:311:ALA:HB1	1.99	0.43
28:5:300:ARG:NH2	54:A:725:A:OP2	2.51	0.43
32:9:68:PHE:CE1	32:9:70:LEU:HB2	2.54	0.43
34:b:21:ARG:HD2	35:c:218:PHE:CE2	2.52	0.43
36:d:151:CYS:SG	36:d:156:ASP:HB2	2.58	0.43
38:f:121:VAL:HG22	38:f:159:ILE:HG12	2.01	0.43
50:s:166:TYR:HB3	54:A:746:U:N3	2.33	0.43
50:s:309:GLU:HA	50:s:312:LEU:HG	2.00	0.43
50:s:362:THR:HB	50:s:364:GLY:H	1.84	0.43
54:A:512:G:N3	54:A:529:A:O2'	2.38	0.43
15:S:126:GLU:O	15:S:159:THR:HA	2.18	0.43
17:U:142:PRO:HG2	36:d:282:ILE:HD12	2.01	0.43
18:V:147:SER:OG	18:V:150:SER:O	2.36	0.43
29:6:224:HIS:CD2	29:6:226:LEU:H	2.37	0.43
39:g:68:THR:HG23	39:g:70:SER:H	1.82	0.43
47:p:155:ARG:O	47:p:159:THR:HG23	2.17	0.43
50:s:423:HIS:HA	50:s:426:LEU:HG	2.00	0.43
54:A:496:C:H1'	54:A:544:A:N6	2.34	0.43
1:D:107:ILE:HD11	1:D:135:ARG:HH12	1.84	0.43
3:F:263:LEU:HD23	3:F:263:LEU:HA	1.85	0.43
5:I:106:ALA:HA	5:I:109:LYS:HE2	2.00	0.43
9:M:263:ARG:HD2	47:p:43:TYR:HD2	1.83	0.43
12:P:86:THR:O	12:P:120:ARG:NE	2.52	0.43
19:W:128:LYS:HB2	19:W:130:PHE:HE1	1.84	0.43
32:9:81:SER:OG	32:9:82:GLU:N	2.52	0.43
36:d:222:LEU:HD23	36:d:222:LEU:HA	1.86	0.43
46:o:28:SER:OG	46:o:29:LEU:N	2.52	0.43
49:r:111:GLU:O	49:r:115:ILE:HG12	2.19	0.43
54:A:130:G:N2	54:A:133:A:N7	2.67	0.43
54:A:258:A:H2'	54:A:259:A:H8	1.84	0.43
54:A:454:A:H5'	54:A:455:C:H5''	2.00	0.43
54:A:1466:A:H2'	54:A:1467:G:C8	2.52	0.43
1:D:121:PRO:HB3	1:D:166:SER:HA	2.01	0.43
4:H:109:GLY:HA3	4:H:147:ARG:HH22	1.83	0.43
8:L:108:ILE:HD13	8:L:114:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:111:ASN:ND2	51:u:164:THR:OG1	2.51	0.43
17:U:151:PHE:O	36:d:273:LYS:NZ	2.38	0.43
19:W:125:VAL:HG21	29:6:64:GLU:HG2	2.00	0.43
47:p:189:ARG:O	47:p:191:LYS:N	2.52	0.43
50:s:110:THR:HG23	50:s:333:PHE:CG	2.54	0.43
50:s:237:PRO:HA	50:s:300:HIS:HD2	1.84	0.43
52:v:31:TYR:O	52:v:35:ILE:HG12	2.19	0.43
53:w:110:LEU:HB3	53:w:114:ASP:HB2	2.00	0.43
54:A:390:A:N1	54:A:409:C:C4	2.85	0.43
13:Q:91:LYS:O	13:Q:95:GLU:HG2	2.19	0.43
18:V:72:LYS:HE3	18:V:91:LEU:HD21	2.01	0.43
23:0:143:LYS:HE3	23:0:143:LYS:HB2	1.79	0.43
28:5:343:GLN:HB3	28:5:356:VAL:HG23	2.01	0.43
29:6:223:GLY:HA2	29:6:266:HIS:CE1	2.54	0.43
40:h:101:LEU:HD13	40:h:101:LEU:HA	1.88	0.43
40:h:140:PHE:HB2	40:h:156:TRP:CD2	2.53	0.43
50:s:51:MET:SD	50:s:65:ARG:HD3	2.59	0.43
54:A:1184:U:C4	54:A:1219:C:C4	3.07	0.43
54:A:1319:G:H5''	54:A:1320:A:H5'	2.00	0.43
54:A:1450:C:N4	54:A:1466:A:N6	2.36	0.43
3:F:174:LEU:HA	3:F:174:LEU:HD12	1.83	0.43
11:O:53:ARG:HD2	11:O:107:MET:HE3	2.01	0.43
18:V:105:ARG:HD3	36:d:174:TRP:CD1	2.53	0.43
20:X:236:GLN:O	20:X:240:GLN:HG2	2.19	0.43
31:8:132:GLU:O	31:8:136:ILE:HG12	2.18	0.43
31:8:150:LEU:HB2	37:e:212:HIS:HE1	1.84	0.43
51:u:112:ILE:CG2	51:u:124:PHE:HB3	2.49	0.43
54:A:1372:U:H3'	54:A:1373:C:H6	1.84	0.43
2:E:108:PRO:HD2	13:Q:145:LEU:HB3	2.01	0.42
7:K:176:TYR:HD2	7:K:178:LEU:H	1.65	0.42
13:Q:284:LYS:HB3	13:Q:284:LYS:HE3	1.69	0.42
14:R:41:LEU:H	14:R:41:LEU:HG	1.64	0.42
20:X:189:ASP:HA	20:X:192:LYS:HB3	2.00	0.42
26:3:179:LYS:HB2	29:6:370:ARG:HH12	1.83	0.42
43:k:41:LYS:HE2	43:k:41:LYS:HB2	1.87	0.42
51:u:185:ARG:CZ	51:u:185:ARG:HB2	2.49	0.42
54:A:1024:A:C6	54:A:1315:C:H1'	2.53	0.42
56:z:69:C:N3	56:z:70:A:C8	2.87	0.42
2:E:142:MET:HG3	2:E:143:ALA:H	1.83	0.42
5:I:81:LEU:HD23	5:I:82:LEU:HD23	2.01	0.42
9:M:57:ARG:HE	9:M:57:ARG:HB3	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:61:LYS:HE3	10:N:61:LYS:HB2	1.82	0.42
14:R:79:HIS:ND1	33:a:44:ASN:O	2.46	0.42
19:W:122:LYS:O	29:6:51:TYR:OH	2.27	0.42
28:5:353:HIS:CE1	28:5:379:ASP:H	2.37	0.42
28:5:354:PHE:HB2	28:5:377:ASP:HB2	2.01	0.42
30:7:254:LEU:HD12	30:7:261:ILE:HG22	2.01	0.42
41:i:112:LYS:HD3	54:A:339:G:OP1	2.19	0.42
50:s:295:GLY:N	50:s:339:GLN:OE1	2.46	0.42
52:v:3:PRO:HD3	52:v:51:ARG:HH11	1.82	0.42
54:A:257:G:O6	54:A:307:U:O2	2.37	0.42
54:A:495:C:O2'	54:A:496:C:O5'	2.37	0.42
54:A:800:G:N2	54:A:803:A:C6	2.87	0.42
55:B:1638:U:H2'	55:B:1639:U:C6	2.55	0.42
55:B:1665:C:H2'	55:B:1666:U:C6	2.54	0.42
3:F:217:LEU:HD11	3:F:243:ILE:HD12	2.01	0.42
12:P:75:ARG:HB3	12:P:97:GLN:NE2	2.34	0.42
17:U:10:TYR:HD1	32:9:56:MET:HE2	1.84	0.42
20:X:121:LYS:HB2	20:X:122:LYS:H	1.49	0.42
27:4:97:ARG:HG3	27:4:98:HIS:CD2	2.53	0.42
29:6:272:LEU:O	29:6:313:PRO:HA	2.19	0.42
30:7:190:ASP:OD1	30:7:191:GLU:N	2.52	0.42
33:a:72:THR:HG21	35:c:275:TYR:CE1	2.54	0.42
39:g:140:VAL:HG22	46:o:85:HIS:ND1	2.34	0.42
49:r:188:SER:OG	49:r:189:ARG:N	2.52	0.42
50:s:377:LEU:HA	50:s:377:LEU:HD23	1.75	0.42
51:u:112:ILE:HG23	51:u:124:PHE:HB3	2.02	0.42
54:A:33:C:O2'	54:A:34:U:OP2	2.31	0.42
54:A:49:G:H2'	54:A:50:C:C6	2.53	0.42
54:A:1269:C:N3	54:A:1321:U:O4	2.52	0.42
1:D:125:LYS:HB2	28:5:258:PRO:HG2	2.01	0.42
9:M:17:ARG:HH12	40:h:116:ARG:CZ	2.32	0.42
20:X:163:ARG:HH21	20:X:163:ARG:HD3	1.72	0.42
28:5:122:TRP:HE3	28:5:123:LEU:HD23	1.82	0.42
30:7:166:LEU:HD23	30:7:181:TYR:CE2	2.54	0.42
31:8:110:GLU:HA	31:8:113:ARG:HG2	2.01	0.42
35:c:271:PHE:HA	35:c:284:GLY:O	2.20	0.42
43:k:17:ARG:NH1	43:k:52:ILE:HD12	2.34	0.42
47:p:114:PRO:O	47:p:118:LYS:HG2	2.19	0.42
50:s:251:VAL:O	50:s:373:GLN:NE2	2.52	0.42
54:A:360:U:C5	54:A:428:G:O6	2.72	0.42
54:A:662:C:N4	54:A:772:U:N3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:1074:U:H1'	54:A:1075:A:H8	1.84	0.42
54:A:1240:A:P	56:z:73:A:H61	2.42	0.42
54:A:1281:A:H2'	54:A:1282:U:H6	1.84	0.42
56:z:62:C:H2'	56:z:63:C:H6	1.84	0.42
5:I:47:LEU:HD13	10:N:226:ILE:HG12	2.00	0.42
15:S:142:THR:HG23	33:a:62:HIS:NE2	2.34	0.42
15:S:173:ARG:O	15:S:181:LYS:HA	2.19	0.42
15:S:185:ILE:HD12	15:S:185:ILE:HG23	1.84	0.42
17:U:20:PHE:CD2	18:V:195:GLN:HG3	2.55	0.42
30:7:160:ASP:N	30:7:160:ASP:OD1	2.51	0.42
33:a:125:PRO:HG2	54:A:153:A:C6	2.54	0.42
36:d:181:VAL:HG23	36:d:224:ILE:HG12	2.01	0.42
47:p:174:LYS:HB3	47:p:175:LEU:H	1.61	0.42
54:A:850:C:C2	54:A:859:U:N3	2.87	0.42
1:D:76:PRO:HG3	1:D:105:ARG:HE	1.84	0.42
1:D:215:VAL:HG12	1:D:227:GLN:HB3	2.01	0.42
2:E:224:PHE:HB2	54:A:1329:C:OP1	2.19	0.42
11:O:25:ARG:NH2	11:O:51:GLU:OE2	2.52	0.42
15:S:111:GLU:HA	15:S:195:ILE:O	2.20	0.42
15:S:149:LEU:HD23	15:S:149:LEU:HA	1.80	0.42
15:S:163:LYS:HB2	34:b:106:ASP:OD2	2.19	0.42
17:U:77:ASN:O	17:U:86:ARG:HD3	2.19	0.42
23:0:92:CYS:HA	54:A:151:A:H1'	2.02	0.42
26:3:183:ARG:HD2	26:3:183:ARG:HA	1.85	0.42
28:5:313:MET:HE1	28:5:353:HIS:HB3	2.02	0.42
29:6:326:SER:O	29:6:330:ILE:HD12	2.19	0.42
30:7:243:LYS:HA	30:7:243:LYS:HD2	1.86	0.42
34:b:39:SER:HB3	54:A:615:U:O2'	2.20	0.42
49:r:93:ILE:HA	49:r:93:ILE:HD13	1.67	0.42
1:D:72:TYR:HD1	28:5:33:TRP:CZ3	2.37	0.42
9:M:118:LEU:HD21	9:M:129:ILE:HD11	2.02	0.42
14:R:109:GLU:OE1	34:b:126:ILE:HG12	2.19	0.42
31:8:155:PRO:O	31:8:158:HIS:NE2	2.53	0.42
32:9:120:GLU:N	32:9:120:GLU:OE2	2.52	0.42
34:b:42:GLY:HA3	34:b:92:LYS:O	2.20	0.42
37:e:47:LEU:HB3	37:e:178:TRP:CE2	2.54	0.42
38:f:81:ASN:HB3	38:f:86:TYR:HD1	1.84	0.42
54:A:336:C:H2'	54:A:337:U:C6	2.55	0.42
54:A:516:C:O2'	54:A:517:C:OP1	2.36	0.42
55:B:1628:C:H42	55:B:1640:A:H61	1.68	0.42
5:I:177:LEU:HA	5:I:188:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:117:VAL:HG12	6:J:141:VAL:HG23	2.02	0.42
9:M:80:LYS:NZ	26:3:112:ASP:OD1	2.33	0.42
9:M:133:LYS:HG2	26:3:168:ARG:NH2	2.34	0.42
9:M:226:PRO:HA	9:M:229:PHE:HD2	1.84	0.42
13:Q:96:ARG:HA	13:Q:99:MET:HE3	2.01	0.42
14:R:91:VAL:HG11	42:j:24:GLY:HA3	2.00	0.42
37:e:255:VAL:HG11	37:e:260:LEU:N	2.35	0.42
40:h:86:TRP:CD1	40:h:86:TRP:H	2.38	0.42
44:l:122:ARG:NH2	54:A:526:A:H5'	2.35	0.42
51:u:111:VAL:HG23	51:u:125:VAL:HG22	2.02	0.42
53:w:112:SER:HA	53:w:115:GLN:OE1	2.19	0.42
54:A:360:U:H4'	54:A:361:A:OP1	2.20	0.42
54:A:792:A:H2'	54:A:793:A:C8	2.55	0.42
54:A:1074:U:H1'	54:A:1075:A:C8	2.54	0.42
54:A:1285:U:O2'	54:A:1286:A:H5''	2.20	0.42
54:A:1503:G:H2'	54:A:1504:U:O4'	2.20	0.42
1:D:259:LYS:NZ	54:A:269:G:OP2	2.40	0.42
5:I:117:ARG:NH1	6:J:133:GLN:OE1	2.53	0.42
9:M:140:LEU:HD11	9:M:154:ILE:HG21	2.01	0.42
10:N:227:ARG:HH11	10:N:227:ARG:HD3	1.64	0.42
16:T:125:GLN:HG3	16:T:140:LEU:HD12	2.01	0.42
16:T:141:TYR:CE2	16:T:184:PRO:HD3	2.55	0.42
23:0:133:GLU:OE2	23:0:160:TYR:OH	2.32	0.42
28:5:93:LEU:HA	28:5:96:HIS:CD2	2.54	0.42
28:5:407:LYS:NZ	28:5:409:GLU:HB2	2.35	0.42
29:6:52:ARG:H	29:6:52:ARG:HG3	1.69	0.42
34:b:26:LEU:HD23	34:b:61:VAL:HG11	2.01	0.42
36:d:165:THR:HG22	36:d:260:ARG:NH1	2.34	0.42
50:s:99:ALA:HB1	50:s:271:LEU:HD11	2.02	0.42
52:v:6:ARG:NH1	59:v:101:PNS:O23	2.52	0.42
54:A:356:A:H2'	54:A:357:A:C8	2.54	0.42
4:H:54:VAL:HG23	4:H:82:LEU:HD13	2.02	0.42
4:H:55:ILE:HG23	20:X:43:TYR:HA	2.02	0.42
5:I:82:LEU:HD22	5:I:126:PHE:CE2	2.55	0.42
5:I:86:ILE:HD11	5:I:126:PHE:HD2	1.84	0.42
8:L:118:ARG:HH22	51:u:193:LEU:HG	1.84	0.42
9:M:94:LYS:HB2	9:M:129:ILE:HG22	2.01	0.42
13:Q:150:ILE:HD13	13:Q:150:ILE:HG21	1.83	0.42
28:5:59:THR:HG21	28:5:73:PRO:HB3	2.01	0.42
29:6:148:LYS:NZ	29:6:189:CYS:SG	2.86	0.42
35:c:59:ARG:HG3	35:c:62:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:137:LEU:HD23	35:c:137:LEU:HA	1.81	0.42
44:l:122:ARG:HH12	54:A:525:A:H4'	1.84	0.42
54:A:503:G:H2'	54:A:504:G:H8	1.85	0.42
54:A:512:G:H1'	54:A:529:A:H2'	2.02	0.42
54:A:821:C:H2'	54:A:822:G:C8	2.55	0.42
2:E:61:ILE:O	2:E:65:VAL:HG22	2.20	0.41
11:O:58:LYS:HE3	13:Q:269:MET:HB2	2.01	0.41
14:R:34:ARG:HG2	14:R:37:ARG:NH2	2.35	0.41
18:V:195:GLN:NE2	32:9:137:ARG:O	2.53	0.41
19:W:50:ARG:O	19:W:54:LYS:NZ	2.47	0.41
20:X:121:LYS:NZ	28:5:51:GLU:O	2.52	0.41
28:5:350:ARG:NH1	54:A:725:A:H4'	2.35	0.41
29:6:214:TRP:HB2	29:6:240:ILE:HB	2.01	0.41
45:m:72:ARG:HH21	45:m:75:LEU:HD11	1.85	0.41
50:s:168:GLU:O	50:s:172:ILE:HB	2.20	0.41
55:B:1639:U:H2'	55:B:1640:A:H8	1.85	0.41
1:D:207:ILE:H	1:D:207:ILE:HG13	1.69	0.41
1:D:219:LYS:HA	1:D:224:ALA:HA	2.01	0.41
1:D:261:GLY:O	1:D:265:TRP:HB2	2.20	0.41
2:E:344:SER:OG	13:Q:102:ARG:NH2	2.43	0.41
3:F:107:LYS:HB2	3:F:107:LYS:HE2	1.73	0.41
4:H:98:LEU:HD11	4:H:102:VAL:HG21	2.02	0.41
6:J:132:LEU:HD11	54:A:500:G:H4'	2.02	0.41
8:L:75:LEU:HD12	8:L:75:LEU:HA	1.92	0.41
10:N:249:LYS:HD3	10:N:249:LYS:HA	1.77	0.41
16:T:92:LYS:HD2	16:T:92:LYS:O	2.20	0.41
19:W:57:GLU:HG3	19:W:98:ARG:HA	2.01	0.41
23:0:93:ARG:NH2	54:A:640:G:OP2	2.52	0.41
23:0:159:LEU:HB2	23:0:174:ILE:HD11	2.01	0.41
31:8:121:TRP:CE2	31:8:125:LYS:HD2	2.55	0.41
34:b:126:ILE:HG13	34:b:127:GLN:HG3	2.01	0.41
35:c:133:SER:HA	35:c:215:ILE:HD13	2.01	0.41
50:s:164:HIS:ND1	54:A:744:C:H1'	2.35	0.41
50:s:378:ALA:HB1	50:s:383:ALA:HB1	2.01	0.41
52:v:4:TRP:H	52:v:55:LEU:HD12	1.85	0.41
55:B:1663:C:H2'	55:B:1664:G:C8	2.55	0.41
7:K:60:MET:HE3	7:K:60:MET:HB2	1.79	0.41
8:L:49:SER:HB3	8:L:78:LYS:NZ	2.35	0.41
14:R:102:LEU:HD23	14:R:102:LEU:HA	1.85	0.41
18:V:96:ARG:O	18:V:108:MET:HA	2.21	0.41
19:W:61:VAL:HG13	19:W:65:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:124:ALA:HA	29:6:37:ASN:OD1	2.19	0.41
21:Y:91:ARG:NH1	32:9:84:THR:O	2.52	0.41
21:Y:102:TRP:CZ3	21:Y:139:MET:HG3	2.56	0.41
28:5:380:GLN:HB3	28:5:410:THR:HG22	2.01	0.41
41:i:99:GLY:HA2	41:i:102:MET:HG3	2.01	0.41
49:r:59:GLU:HG3	49:r:60:SER:O	2.20	0.41
49:r:171:ARG:HH12	54:A:567:A:P	2.43	0.41
50:s:92:MET:SD	50:s:276:ARG:NH2	2.92	0.41
53:w:87:LEU:HG	53:w:98:LEU:HD11	2.03	0.41
54:A:307:U:H2'	54:A:308:A:C8	2.55	0.41
54:A:323:A:H8	54:A:828:U:O2'	2.03	0.41
54:A:615:U:H2'	54:A:616:A:H8	1.85	0.41
54:A:868:C:H2'	54:A:869:A:C8	2.55	0.41
54:A:1345:U:O2	54:A:1353:C:N3	2.53	0.41
6:J:148:ALA:HA	6:J:151:LEU:HB2	2.01	0.41
9:M:76:ILE:HA	26:3:113:ARG:NH1	2.36	0.41
12:P:49:THR:HG21	29:6:228:PRO:HB3	2.03	0.41
20:X:42:HIS:CG	20:X:86:ILE:HD11	2.55	0.41
21:Y:83:ALA:N	32:9:74:VAL:O	2.53	0.41
29:6:224:HIS:CE1	29:6:227:GLU:H	2.38	0.41
35:c:130:THR:O	35:c:134:GLN:NE2	2.52	0.41
37:e:198:ASN:HD22	37:e:243:PHE:HD1	1.67	0.41
38:f:88:TYR:HB3	38:f:91:LEU:HD11	2.01	0.41
54:A:642:A:H2'	54:A:643:A:O4'	2.21	0.41
54:A:879:C:H4'	54:A:880:A:H5'	2.01	0.41
1:D:146:SER:HA	28:5:263:ILE:HD13	2.02	0.41
13:Q:188:LEU:O	13:Q:191:ARG:HG2	2.19	0.41
25:2:60:ARG:HD2	25:2:92:HIS:ND1	2.35	0.41
28:5:35:VAL:HG23	28:5:38:THR:H	1.85	0.41
31:8:150:LEU:HB2	37:e:212:HIS:CE1	2.56	0.41
35:c:304:LEU:HD23	35:c:304:LEU:HA	1.93	0.41
43:k:56:ARG:NH2	43:k:61:GLU:OE2	2.53	0.41
46:o:23:ARG:HD2	49:r:169:TRP:CD1	2.56	0.41
49:r:71:PRO:HA	49:r:74:ARG:HD3	2.02	0.41
49:r:117:GLU:O	49:r:121:MET:HG3	2.21	0.41
54:A:409:C:H3'	54:A:410:U:O2	2.20	0.41
54:A:782:A:O2'	54:A:784:G:OP2	2.30	0.41
54:A:1057:C:H2'	54:A:1058:C:H6	1.86	0.41
55:B:1604:G:H2'	55:B:1605:A:H8	1.86	0.41
1:D:222:GLY:C	1:D:238:GLU:HB2	2.45	0.41
2:E:103:LYS:HA	2:E:122:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:113:ARG:HH12	5:I:117:ARG:HH22	1.68	0.41
10:N:72:ILE:HG23	10:N:94:GLY:HA3	2.02	0.41
12:P:86:THR:OG1	12:P:87:GLN:NE2	2.54	0.41
13:Q:90:LEU:O	13:Q:94:ILE:HG12	2.20	0.41
13:Q:139:GLN:HB3	13:Q:139:GLN:HE21	1.54	0.41
14:R:57:ARG:O	14:R:61:LYS:NZ	2.48	0.41
22:Z:79:PRO:HD2	22:Z:82:GLU:HG3	2.03	0.41
31:8:99:ARG:HH22	31:8:102:PRO:HG3	1.84	0.41
37:e:202:ALA:HB2	37:e:238:LEU:HD23	2.02	0.41
39:g:121:GLN:O	39:g:125:GLU:HB2	2.21	0.41
43:k:21:CYS:SG	43:k:56:ARG:NE	2.93	0.41
49:r:179:PRO:HG3	54:A:488:U:H3'	2.03	0.41
54:A:411:U:H2'	54:A:412:G:H8	1.86	0.41
54:A:1410:G:H2'	54:A:1411:A:C8	2.54	0.41
54:A:1472:A:H2'	54:A:1473:U:H6	1.86	0.41
56:z:0:A:C8	56:z:4:A:H2'	2.56	0.41
56:z:26:C:C2	56:z:41:G:N2	2.89	0.41
2:E:199:ARG:O	2:E:202:GLN:HB2	2.21	0.41
4:H:72:ARG:HH11	4:H:72:ARG:HD2	1.75	0.41
6:J:103:GLN:O	54:A:517:C:O2'	2.34	0.41
10:N:237:HIS:HB3	10:N:241:TYR:HB2	2.02	0.41
12:P:130:ARG:HB2	12:P:164:ALA:HB1	2.01	0.41
15:S:158:ALA:HA	15:S:194:ARG:O	2.20	0.41
16:T:209:VAL:HG23	54:A:163:C:H4'	2.03	0.41
28:5:336:LEU:HD23	28:5:339:PRO:HA	2.03	0.41
40:h:139:LYS:HG3	40:h:143:LEU:HD23	2.03	0.41
54:A:284:U:H4'	54:A:792:A:H4'	2.03	0.41
54:A:844:C:H2'	54:A:845:U:C6	2.54	0.41
54:A:1125:U:H2'	54:A:1126:G:C8	2.55	0.41
2:E:145:LEU:HD13	2:E:181:ILE:HD13	2.03	0.41
5:I:139:LYS:HB2	5:I:141:GLN:HE22	1.86	0.41
9:M:154:ILE:HD12	9:M:154:ILE:HG23	1.79	0.41
13:Q:153:ASN:OD1	13:Q:154:VAL:N	2.54	0.41
32:9:53:ILE:HD12	32:9:56:MET:HE3	2.01	0.41
35:c:40:ARG:O	35:c:43:LYS:HG3	2.21	0.41
40:h:104:LEU:HD23	40:h:130:TYR:CE2	2.56	0.41
50:s:142:LEU:HD13	50:s:422:VAL:HG21	2.02	0.41
54:A:416:A:O5'	54:A:416:A:H8	2.04	0.41
54:A:662:C:N4	54:A:772:U:C4	2.87	0.41
54:A:663:G:H2'	54:A:664:C:C6	2.55	0.41
1:D:220:VAL:HG12	1:D:221:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:LEU:HD11	2:E:150:LYS:HD2	2.03	0.41
3:F:59:ARG:HE	3:F:84:PRO:HB2	1.85	0.41
3:F:243:ILE:HD13	3:F:243:ILE:HG21	1.87	0.41
9:M:94:LYS:HZ3	9:M:135:ASP:CG	2.28	0.41
9:M:220:ARG:HH12	9:M:232:ALA:HB1	1.86	0.41
13:Q:119:VAL:HG11	13:Q:149:PHE:HZ	1.86	0.41
15:S:167:TRP:O	15:S:169:ARG:HG3	2.20	0.41
15:S:173:ARG:NH1	54:A:592:C:OP2	2.54	0.41
17:U:86:ARG:HH11	17:U:86:ARG:HD2	1.72	0.41
20:X:235:ILE:HD13	20:X:235:ILE:HA	1.93	0.41
28:5:289:HIS:ND1	28:5:290:THR:OG1	2.46	0.41
29:6:216:LEU:HB3	29:6:272:LEU:HD13	2.02	0.41
29:6:291:TYR:N	29:6:295:GLN:OE1	2.53	0.41
31:8:110:GLU:CD	31:8:114:ARG:HH21	2.29	0.41
34:b:15:LEU:HD21	35:c:169:VAL:HG13	2.01	0.41
36:d:156:ASP:HB3	36:d:159:ARG:HH11	1.86	0.41
36:d:239:PRO:C	36:d:240:LYS:HZ2	2.29	0.41
37:e:83:LEU:HG	37:e:84:TYR:CD1	2.56	0.41
37:e:178:TRP:HB3	37:e:187:THR:HG21	2.02	0.41
37:e:205:LEU:HD22	38:f:171:LEU:HD11	2.02	0.41
50:s:250:PHE:CE1	50:s:371:CYS:HB3	2.56	0.41
50:s:300:HIS:HB2	50:s:361:ILE:HG22	2.03	0.41
51:u:182:PRO:HA	51:u:185:ARG:NH1	2.35	0.41
52:v:27:ASP:OD1	52:v:27:ASP:N	2.53	0.41
55:B:1615:A:H61	55:B:1621:A:H2	1.69	0.41
56:z:62:C:H2'	56:z:63:C:C6	2.56	0.41
1:D:259:LYS:HD2	54:A:269:G:C8	2.56	0.41
8:L:63:LYS:HA	8:L:63:LYS:HD3	1.78	0.41
15:S:194:ARG:NH1	34:b:19:LEU:HG	2.35	0.41
16:T:63:LEU:HD12	16:T:65:GLY:H	1.86	0.41
19:W:139:GLU:H	19:W:139:GLU:HG2	1.69	0.41
23:0:137:ILE:O	23:0:141:ILE:HG12	2.21	0.41
26:3:144:LEU:HD23	26:3:144:LEU:HA	1.84	0.41
28:5:194:LYS:HE3	28:5:195:HIS:NE2	2.36	0.41
33:a:118:THR:OG1	33:a:119:THR:N	2.53	0.41
54:A:405:U:H2'	54:A:406:C:H6	1.85	0.41
54:A:503:G:H2'	54:A:504:G:C8	2.56	0.41
54:A:1048:C:H5'	54:A:1049:G:OP1	2.21	0.41
54:A:1525:A:H2'	54:A:1526:G:C2	2.57	0.41
12:P:67:GLY:HA3	19:W:78:GLY:O	2.21	0.40
14:R:14:VAL:HG21	54:A:624:A:H4'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:112:LEU:HD23	21:Y:112:LEU:HA	1.84	0.40
28:5:52:ILE:HA	28:5:53:PRO:HD3	1.84	0.40
40:h:120:MET:HE2	40:h:120:MET:HB3	1.63	0.40
50:s:268:PRO:O	50:s:273:LEU:HB3	2.21	0.40
53:w:85:TYR:HD1	53:w:88:LYS:HZ3	1.68	0.40
54:A:1445:U:H2'	54:A:1446:C:C6	2.55	0.40
55:B:1659:U:H2'	55:B:1660:G:C8	2.57	0.40
9:M:234:LEU:HD22	9:M:238:ARG:NH1	2.36	0.40
13:Q:180:GLU:OE1	13:Q:218:ASN:ND2	2.34	0.40
26:3:135:LYS:NZ	54:A:1225:U:H5''	2.37	0.40
30:7:216:PHE:HE1	30:7:257:ILE:HG12	1.87	0.40
30:7:302:LEU:HD23	30:7:302:LEU:HA	1.87	0.40
34:b:35:ARG:NH1	46:o:101:TRP:O	2.52	0.40
35:c:227:GLU:OE1	35:c:302:ARG:NH2	2.53	0.40
38:f:163:SER:O	38:f:167:ALA:CB	2.69	0.40
53:w:91:ASP:OD2	53:w:92:LYS:N	2.52	0.40
54:A:712:A:H2'	54:A:713:U:C6	2.56	0.40
55:B:1603:A:H2'	55:B:1604:G:H8	1.86	0.40
2:E:97:VAL:HG23	2:E:181:ILE:HD12	2.03	0.40
2:E:129:VAL:HG11	2:E:145:LEU:HD23	2.02	0.40
5:I:47:LEU:CD1	10:N:226:ILE:HG12	2.51	0.40
5:I:119:HIS:CE1	5:I:158:GLU:HG2	2.56	0.40
16:T:50:LYS:HE3	16:T:50:LYS:HB2	1.86	0.40
22:Z:123:LYS:HB2	22:Z:144:GLU:HB3	2.04	0.40
28:5:185:ILE:HD13	28:5:185:ILE:HA	1.87	0.40
29:6:220:SER:HB3	29:6:232:TYR:HB2	2.02	0.40
37:e:198:ASN:OD1	37:e:198:ASN:N	2.54	0.40
37:e:260:LEU:O	37:e:264:LEU:HB2	2.22	0.40
55:B:1603:A:H2'	55:B:1604:G:C8	2.57	0.40
55:B:1628:C:N4	55:B:1640:A:H61	2.19	0.40
56:z:69:C:C4	56:z:70:A:N7	2.89	0.40
1:D:227:GLN:NE2	1:D:231:LYS:HG3	2.37	0.40
2:E:97:VAL:O	2:E:197:HIS:NE2	2.54	0.40
2:E:154:ARG:HD2	30:7:311:THR:OG1	2.22	0.40
2:E:206:VAL:HG11	2:E:289:VAL:HG22	2.02	0.40
5:I:158:GLU:HA	5:I:159:PRO:HD3	1.87	0.40
14:R:105:LEU:HD23	14:R:105:LEU:HA	1.89	0.40
16:T:117:ILE:HD13	16:T:117:ILE:HG21	1.83	0.40
23:0:136:GLU:O	23:0:139:ARG:HB2	2.21	0.40
26:3:106:THR:HG22	26:3:162:THR:HA	2.03	0.40
28:5:118:LYS:HB2	28:5:118:LYS:HE2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:125:LYS:NZ	28:5:366:CYS:O	2.46	0.40
29:6:27:ARG:HH21	29:6:27:ARG:HD2	1.77	0.40
29:6:157:LEU:O	29:6:161:LEU:CB	2.70	0.40
31:8:97:LYS:HD2	31:8:97:LYS:O	2.21	0.40
31:8:127:GLN:HG2	31:8:130:LYS:HZ2	1.86	0.40
36:d:232:MET:HE3	36:d:232:MET:HB3	1.94	0.40
38:f:104:GLU:HA	38:f:155:ARG:HH12	1.87	0.40
39:g:161:LEU:HD23	39:g:161:LEU:HA	1.86	0.40
50:s:306:LEU:HD12	50:s:323:VAL:HG21	2.04	0.40
54:A:109:A:O2'	54:A:110:U:H5''	2.22	0.40
54:A:386:G:H2'	54:A:387:C:C6	2.56	0.40
54:A:1445:U:H2'	54:A:1446:C:H6	1.86	0.40
55:B:1610:A:H1'	55:B:1644:G:H2'	2.03	0.40
1:D:112:PHE:CZ	1:D:167:ASN:HB2	2.57	0.40
3:F:91:PRO:HB3	9:M:16:LEU:HD11	2.03	0.40
9:M:225:ASP:HB3	9:M:228:LYS:HG2	2.04	0.40
21:Y:126:MET:HG3	21:Y:128:SER:N	2.27	0.40
28:5:42:GLU:HG3	28:5:43:PRO:HD2	2.04	0.40
29:6:306:LYS:HA	29:6:306:LYS:HD3	1.96	0.40
33:a:114:LYS:HE2	33:a:114:LYS:HB3	1.79	0.40
35:c:273:GLY:HA2	35:c:283:GLU:HA	2.03	0.40
35:c:280:LEU:H	35:c:280:LEU:HD23	1.87	0.40
38:f:48:TYR:N	54:A:395:A:OP1	2.55	0.40
38:f:183:ARG:CZ	38:f:183:ARG:HA	2.51	0.40
43:k:34:LEU:HA	43:k:38:SER:HB2	2.04	0.40
49:r:89:LEU:O	49:r:93:ILE:HG12	2.21	0.40
50:s:164:HIS:HD1	54:A:744:C:H1'	1.87	0.40
50:s:361:ILE:HG21	50:s:361:ILE:HD13	1.86	0.40
51:u:103:GLN:NE2	51:u:104:GLU:HG2	2.37	0.40
51:u:174:SER:O	51:u:174:SER:OG	2.39	0.40
54:A:335:C:H2'	54:A:336:C:C6	2.56	0.40
54:A:1202:C:H2'	54:A:1203:A:O4'	2.21	0.40
55:B:1664:G:H2'	55:B:1665:C:C6	2.56	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	D	234/305 (77%)	204 (87%)	29 (12%)	1 (0%)	30	60
2	E	302/348 (87%)	266 (88%)	36 (12%)	0	100	100
3	F	248/311 (80%)	229 (92%)	19 (8%)	0	100	100
4	H	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
5	I	154/261 (59%)	143 (93%)	11 (7%)	0	100	100
6	J	138/192 (72%)	126 (91%)	12 (9%)	0	100	100
7	K	175/178 (98%)	164 (94%)	11 (6%)	0	100	100
8	L	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
9	M	285/296 (96%)	271 (95%)	14 (5%)	0	100	100
10	N	203/251 (81%)	194 (96%)	9 (4%)	0	100	100
11	O	150/175 (86%)	138 (92%)	12 (8%)	0	100	100
12	P	139/180 (77%)	133 (96%)	6 (4%)	0	100	100
13	Q	215/292 (74%)	201 (94%)	14 (6%)	0	100	100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
15	S	154/205 (75%)	134 (87%)	20 (13%)	0	100	100
16	T	155/206 (75%)	150 (97%)	5 (3%)	0	100	100
17	U	135/153 (88%)	116 (86%)	19 (14%)	0	100	100
18	V	188/216 (87%)	178 (95%)	10 (5%)	0	100	100
19	W	107/148 (72%)	98 (92%)	9 (8%)	0	100	100
20	X	241/256 (94%)	229 (95%)	12 (5%)	0	100	100
21	Y	174/250 (70%)	168 (97%)	6 (3%)	0	100	100
22	Z	118/161 (73%)	111 (94%)	7 (6%)	0	100	100
23	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
24	1	50/65 (77%)	46 (92%)	4 (8%)	0	100	100
25	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
27	4	34/103 (33%)	33 (97%)	1 (3%)	0	100	100
28	5	383/423 (90%)	354 (92%)	29 (8%)	0	100	100
29	6	316/380 (83%)	298 (94%)	18 (6%)	0	100	100
30	7	285/338 (84%)	264 (93%)	21 (7%)	0	100	100
31	8	97/206 (47%)	87 (90%)	10 (10%)	0	100	100
32	9	113/137 (82%)	102 (90%)	11 (10%)	0	100	100
33	a	69/142 (49%)	64 (93%)	5 (7%)	0	100	100
34	b	146/215 (68%)	127 (87%)	19 (13%)	0	100	100
35	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
36	d	203/306 (66%)	193 (95%)	10 (5%)	0	100	100
37	e	211/279 (76%)	193 (92%)	18 (8%)	0	100	100
38	f	110/212 (52%)	100 (91%)	10 (9%)	0	100	100
39	g	127/166 (76%)	120 (94%)	7 (6%)	0	100	100
40	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
41	i	95/128 (74%)	88 (93%)	7 (7%)	0	100	100
42	j	83/123 (68%)	81 (98%)	2 (2%)	0	100	100
43	k	76/112 (68%)	72 (95%)	4 (5%)	0	100	100
44	l	21/138 (15%)	21 (100%)	0	0	100	100
45	m	43/128 (34%)	37 (86%)	6 (14%)	0	100	100
46	o	91/102 (89%)	85 (93%)	5 (6%)	1 (1%)	11	42
47	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
48	q	162/222 (73%)	155 (96%)	7 (4%)	0	100	100
49	r	140/196 (71%)	129 (92%)	11 (8%)	0	100	100
50	s	366/439 (83%)	343 (94%)	23 (6%)	0	100	100
51	u	109/234 (47%)	103 (94%)	6 (6%)	0	100	100
52	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
53	w	77/156 (49%)	70 (91%)	7 (9%)	0	100	100
All	All	8059/11129 (72%)	7508 (93%)	549 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	o	13	PRO
1	D	207	ILE

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	D	190/245 (78%)	190 (100%)	0	100	100
2	E	259/290 (89%)	259 (100%)	0	100	100
3	F	217/262 (83%)	217 (100%)	0	100	100
4	H	86/228 (38%)	86 (100%)	0	100	100
5	I	145/232 (62%)	145 (100%)	0	100	100
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	155 (100%)	0	100	100
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	245/249 (98%)	244 (100%)	1 (0%)	84	81
10	N	172/211 (82%)	172 (100%)	0	100	100
11	O	133/150 (89%)	133 (100%)	0	100	100
12	P	123/155 (79%)	123 (100%)	0	100	100
13	Q	199/256 (78%)	198 (100%)	1 (0%)	81	80
14	R	118/126 (94%)	118 (100%)	0	100	100
15	S	141/180 (78%)	140 (99%)	1 (1%)	76	77
16	T	141/176 (80%)	141 (100%)	0	100	100
17	U	124/135 (92%)	124 (100%)	0	100	100
18	V	172/191 (90%)	172 (100%)	0	100	100
19	W	89/119 (75%)	89 (100%)	0	100	100
20	X	219/229 (96%)	219 (100%)	0	100	100
21	Y	159/223 (71%)	159 (100%)	0	100	100
22	Z	111/147 (76%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	0	97/164 (59%)	97 (100%)	0	100	100
24	1	49/60 (82%)	49 (100%)	0	100	100
25	2	38/72 (53%)	38 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100
27	4	35/89 (39%)	35 (100%)	0	100	100
28	5	348/368 (95%)	348 (100%)	0	100	100
29	6	265/332 (80%)	265 (100%)	0	100	100
30	7	263/303 (87%)	263 (100%)	0	100	100
31	8	91/190 (48%)	91 (100%)	0	100	100
32	9	99/112 (88%)	99 (100%)	0	100	100
33	a	69/133 (52%)	68 (99%)	1 (1%)	59	70
34	b	130/186 (70%)	130 (100%)	0	100	100
35	c	241/288 (84%)	240 (100%)	1 (0%)	84	81
36	d	193/274 (70%)	193 (100%)	0	100	100
37	e	188/236 (80%)	188 (100%)	0	100	100
38	f	101/188 (54%)	101 (100%)	0	100	100
39	g	119/148 (80%)	119 (100%)	0	100	100
40	h	95/148 (64%)	95 (100%)	0	100	100
41	i	86/110 (78%)	86 (100%)	0	100	100
42	j	68/97 (70%)	68 (100%)	0	100	100
43	k	71/90 (79%)	71 (100%)	0	100	100
44	l	23/116 (20%)	23 (100%)	0	100	100
45	m	40/113 (35%)	40 (100%)	0	100	100
46	o	79/87 (91%)	79 (100%)	0	100	100
47	p	117/181 (65%)	117 (100%)	0	100	100
48	q	141/178 (79%)	141 (100%)	0	100	100
49	r	133/169 (79%)	133 (100%)	0	100	100
50	s	326/381 (86%)	326 (100%)	0	100	100
51	u	105/200 (52%)	105 (100%)	0	100	100
52	v	59/60 (98%)	59 (100%)	0	100	100
53	w	73/136 (54%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7239/9609 (75%)	7234 (100%)	5 (0%)	87 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	30	ASN
13	Q	139	GLN
15	S	118	ASN
33	a	137	ASN
35	c	134	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	194	ASN
1	D	249	ASN
1	D	252	HIS
1	D	271	ASN
2	E	72	GLN
2	E	128	HIS
3	F	201	GLN
3	F	228	GLN
3	F	241	ASN
5	I	189	GLN
5	I	193	ASN
6	J	48	GLN
6	J	103	GLN
7	K	56	HIS
8	L	43	ASN
9	M	92	GLN
10	N	138	HIS
11	O	39	HIS
11	O	100	GLN
12	P	87	GLN
12	P	97	GLN
12	P	142	ASN
13	Q	213	GLN
13	Q	258	GLN
15	S	140	ASN
16	T	55	ASN
16	T	105	GLN

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Mol	Chain	Res	Type
16	T	195	HIS
18	V	35	ASN
19	W	59	HIS
19	W	107	HIS
20	X	237	GLN
20	X	241	GLN
21	Y	89	GLN
21	Y	117	GLN
23	0	170	GLN
25	2	62	ASN
26	3	170	ASN
26	3	185	ASN
27	4	95	HIS
28	5	94	HIS
28	5	183	ASN
28	5	275	ASN
28	5	353	HIS
29	6	147	HIS
29	6	243	ASN
29	6	266	HIS
29	6	277	GLN
29	6	320	GLN
30	7	207	HIS
31	8	144	GLN
34	b	129	GLN
36	d	251	GLN
37	e	198	ASN
37	e	212	HIS
39	g	141	ASN
40	h	99	ASN
42	j	26	GLN
42	j	30	GLN
42	j	99	GLN
43	k	15	GLN
43	k	26	ASN
43	k	35	GLN
47	p	184	ASN
48	q	60	GLN
48	q	120	HIS
48	q	136	GLN
49	r	146	GLN
50	s	240	GLN

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Mol	Chain	Res	Type
50	s	298	GLN
51	u	113	GLN
53	w	101	ASN
53	w	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	A	1460/1559 (93%)	448 (30%)	26 (1%)
55	B	51/69 (73%)	16 (31%)	1 (1%)
56	z	70/73 (95%)	36 (51%)	0
All	All	1581/1701 (92%)	500 (31%)	27 (1%)

All (500) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
54	A	8	C
54	A	9	U
54	A	11	G
54	A	19	C
54	A	22	A
54	A	23	C
54	A	24	U
54	A	30	U
54	A	31	U
54	A	34	U
54	A	35	A
54	A	37	C
54	A	38	A
54	A	39	G
54	A	43	A
54	A	44	C
54	A	45	C
54	A	46	U
54	A	47	U
54	A	48	A
54	A	53	A
54	A	54	A
54	A	57	A
54	A	58	U
54	A	61	A

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Mol	Chain	Res	Type
54	A	62	C
54	A	66	A
54	A	67	A
54	A	71	A
54	A	78	G
54	A	80	G
54	A	81	A
54	A	90	G
54	A	91	A
54	A	100	G
54	A	103	A
54	A	107	A
54	A	110	U
54	A	111	A
54	A	118	C
54	A	124	A
54	A	125	A
54	A	129	U
54	A	133	A
54	A	134	A
54	A	135	A
54	A	136	U
54	A	137	U
54	A	139	U
54	A	140	A
54	A	142	C
54	A	150	A
54	A	154	U
54	A	157	C
54	A	158	A
54	A	159	A
54	A	162	A
54	A	166	A
54	A	169	C
54	A	170	C
54	A	174	A
54	A	179	C
54	A	180	U
54	A	184	U
54	A	185	A
54	A	186	A
54	A	197	A

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Mol	Chain	Res	Type
54	A	199	A
54	A	200	A
54	A	201	A
54	A	202	U
54	A	203	A
54	A	212	A
54	A	213	G
54	A	217	A
54	A	218	G
54	A	219	C
54	A	222	A
54	A	223	A
54	A	231	C
54	A	232	C
54	A	233	C
54	A	239	A
54	A	245	C
54	A	246	G
54	A	248	G
54	A	257	G
54	A	265	A
54	A	269	G
54	A	270	A
54	A	287	A
54	A	296	G
54	A	305	U
54	A	315	G
54	A	317	G
54	A	318	G
54	A	322	C
54	A	323	A
54	A	324	A
54	A	325	A
54	A	330	C
54	A	331	C
54	A	332	G
54	A	334	G
54	A	342	A
54	A	344	A
54	A	345	G
54	A	351	U
54	A	352	G

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Mol	Chain	Res	Type
54	A	359	A
54	A	361	A
54	A	362	G
54	A	366	C
54	A	367	U
54	A	368	U
54	A	369	A
54	A	382	A
54	A	385	U
54	A	395	A
54	A	404	A
54	A	407	C
54	A	409	C
54	A	410	U
54	A	413	U
54	A	415	A
54	A	421	A
54	A	423	U
54	A	426	U
54	A	427	A
54	A	428	G
54	A	439	A
54	A	440	A
54	A	443	G
54	A	454	A
54	A	455	C
54	A	456	U
54	A	459	G
54	A	464	A
54	A	465	A
54	A	466	C
54	A	471	U
54	A	472	A
54	A	477	G
54	A	484	A
54	A	487	U
54	A	488	U
54	A	489	U
54	A	493	A
54	A	496	C
54	A	498	U
54	A	501	U

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Mol	Chain	Res	Type
54	A	502	A
54	A	503	G
54	A	507	U
54	A	510	A
54	A	511	A
54	A	512	G
54	A	513	C
54	A	514	A
54	A	515	G
54	A	516	C
54	A	517	C
54	A	520	C
54	A	523	U
54	A	524	U
54	A	525	A
54	A	527	G
54	A	528	A
54	A	530	A
54	A	531	G
54	A	532	C
54	A	534	U
54	A	540	C
54	A	545	C
54	A	546	A
54	A	560	A
54	A	562	A
54	A	563	U
54	A	564	C
54	A	567	A
54	A	571	A
54	A	573	A
54	A	575	A
54	A	589	C
54	A	592	C
54	A	593	C
54	A	594	A
54	A	604	A
54	A	605	U
54	A	610	C
54	A	611	A
54	A	612	C
54	A	627	A

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Mol	Chain	Res	Type
54	A	628	A
54	A	629	U
54	A	630	G
54	A	639	A
54	A	645	A
54	A	652	C
54	A	654	U
54	A	661	C
54	A	665	A
54	A	670	C
54	A	672	U
54	A	674	C
54	A	675	G
54	A	678	A
54	A	694	C
54	A	701	U
54	A	702	U
54	A	704	A
54	A	705	C
54	A	710	C
54	A	711	A
54	A	716	C
54	A	717	U
54	A	718	A
54	A	720	A
54	A	723	C
54	A	726	C
54	A	731	A
54	A	733	G
54	A	734	U
54	A	737	U
54	A	744	C
54	A	745	C
54	A	746	U
54	A	756	C
54	A	758	C
54	A	762	A
54	A	764	A
54	A	772	U
54	A	774	A
54	A	776	A
54	A	777	A

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Mol	Chain	Res	Type
54	A	779	G
54	A	781	A
54	A	782	A
54	A	785	U
54	A	808	G
54	A	809	C
54	A	811	A
54	A	814	C
54	A	815	U
54	A	816	U
54	A	823	C
54	A	831	C
54	A	837	A
54	A	838	C
54	A	841	C
54	A	849	G
54	A	850	C
54	A	851	A
54	A	852	U
54	A	853	C
54	A	856	C
54	A	857	A
54	A	860	A
54	A	861	U
54	A	866	G
54	A	869	A
54	A	870	C
54	A	876	G
54	A	887	C
54	A	888	A
54	A	889	U
54	A	890	G
54	A	900	C
54	A	904	G
54	A	911	A
54	A	920	A
54	A	922	G
54	A	923	G
54	A	924	U
54	A	929	U
54	A	930	A
54	A	931	A

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Mol	Chain	Res	Type
54	A	932	U
54	A	938	G
54	A	948	U
54	A	949	A
54	A	954	C
54	A	956	U
54	A	957	G
54	A	958	U
54	A	959	A
54	A	960	U
54	A	962	A
54	A	963	A
54	A	964	U
54	A	965	G
54	A	975	G
54	A	984	U
54	A	990	U
54	A	996	U
54	A	1013	C
54	A	1014	C
54	A	1016	G
54	A	1024	A
54	A	1025	G
54	A	1026	A
54	A	1028	G
54	A	1032	G
54	A	1036	A
54	A	1039	A
54	A	1043	C
54	A	1048	C
54	A	1049	G
54	A	1052	A
54	A	1053	A
54	A	1054	G
54	A	1055	A
54	A	1056	C
54	A	1060	A
54	A	1061	U
54	A	1062	G
54	A	1069	U
54	A	1070	A
54	A	1073	U

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Mol	Chain	Res	Type
54	A	1075	A
54	A	1076	U
54	A	1077	U
54	A	1078	A
54	A	1080	U
54	A	1081	G
54	A	1086	C
54	A	1088	G
54	A	1124	C
54	A	1131	A
54	A	1134	A
54	A	1139	C
54	A	1140	G
54	A	1141	G
54	A	1144	G
54	A	1145	G
54	A	1153	U
54	A	1160	A
54	A	1161	G
54	A	1162	A
54	A	1163	A
54	A	1168	A
54	A	1174	G
54	A	1177	C
54	A	1181	A
54	A	1182	C
54	A	1184	U
54	A	1185	G
54	A	1190	G
54	A	1194	U
54	A	1195	C
54	A	1210	A
54	A	1222	A
54	A	1223	A
54	A	1225	U
54	A	1226	G
54	A	1232	A
54	A	1236	C
54	A	1238	U
54	A	1239	G
54	A	1240	A
54	A	1241	C

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Mol	Chain	Res	Type
54	A	1247	G
54	A	1248	A
54	A	1253	G
54	A	1254	U
54	A	1256	A
54	A	1257	C
54	A	1258	C
54	A	1259	C
54	A	1262	G
54	A	1264	G
54	A	1265	A
54	A	1271	G
54	A	1285	U
54	A	1291	C
54	A	1292	C
54	A	1293	A
54	A	1295	A
54	A	1304	A
54	A	1308	U
54	A	1315	C
54	A	1319	G
54	A	1320	A
54	A	1322	G
54	A	1324	U
54	A	1325	G
54	A	1327	A
54	A	1330	A
54	A	1335	A
54	A	1337	C
54	A	1348	A
54	A	1359	A
54	A	1363	U
54	A	1371	U
54	A	1372	U
54	A	1381	A
54	A	1383	A
54	A	1384	G
54	A	1390	C
54	A	1397	U
54	A	1399	A
54	A	1400	G
54	A	1402	U

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Mol	Chain	Res	Type
54	A	1403	C
54	A	1407	C
54	A	1416	U
54	A	1417	C
54	A	1418	C
54	A	1419	A
54	A	1420	G
54	A	1423	C
54	A	1427	U
54	A	1428	U
54	A	1430	U
54	A	1432	U
54	A	1437	U
54	A	1438	U
54	A	1439	U
54	A	1444	U
54	A	1452	U
54	A	1453	G
54	A	1454	U
54	A	1458	A
54	A	1459	A
54	A	1461	G
54	A	1465	A
54	A	1471	A
54	A	1485	C
54	A	1486	A
54	A	1487	C
54	A	1488	A
54	A	1492	C
54	A	1498	C
54	A	1499	C
54	A	1500	C
54	A	1502	C
54	A	1503	G
54	A	1510	A
54	A	1513	U
54	A	1514	C
54	A	1515	A
54	A	1519	C
54	A	1520	A
54	A	1526	G
54	A	1532	U

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Mol	Chain	Res	Type
54	A	1547	A
54	A	1548	A
54	A	1551	A
55	B	1607	U
55	B	1608	G
55	B	1610	A
55	B	1611	G
55	B	1614	U
55	B	1615	A
55	B	1624	C
55	B	1625	A
55	B	1628	C
55	B	1629	A
55	B	1639	U
55	B	1640	A
55	B	1641	G
55	B	1644	G
55	B	1645	A
55	B	1649	C
56	z	8	U
56	z	9	A
56	z	10	G
56	z	13	U
56	z	16	A
56	z	17	U
56	z	18	U
56	z	19	A
56	z	20	U
56	z	21	C
56	z	27	A
56	z	28	A
56	z	32	A
56	z	38	A
56	z	39	A
56	z	40	U
56	z	41	G
56	z	42	C
56	z	45	A
56	z	46	G
56	z	47	A
56	z	50	A
56	z	51	G

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Mol	Chain	Res	Type
56	z	52	C
56	z	53	C
56	z	55	C
56	z	56	A
56	z	58	A
56	z	59	G
56	z	60	C
56	z	62	C
56	z	64	A
56	z	69	C
56	z	70	A
56	z	71	C
56	z	72	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	A	33	C
54	A	133	A
54	A	136	U
54	A	139	U
54	A	201	A
54	A	324	A
54	A	360	U
54	A	495	C
54	A	512	G
54	A	516	C
54	A	519	C
54	A	704	A
54	A	736	A
54	A	837	A
54	A	860	A
54	A	888	A
54	A	889	U
54	A	958	U
54	A	983	C
54	A	1074	U
54	A	1235	A
54	A	1319	G
54	A	1371	U
54	A	1422	U
54	A	1443	A

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Mol	Chain	Res	Type
54	A	1531	A
55	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 5 ligands modelled in this entry, 4 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
59	PNS	v	101	-	14,20,21	2.15	4 (28%)	18,26,29	1.47	3 (16%)

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
59	PNS	v	101	-	-	12/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	v	101	PNS	C39-N41	5.04	1.45	1.33
59	v	101	PNS	C34-N36	4.82	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	v	101	PNS	O40-C39	-2.49	1.18	1.23
59	v	101	PNS	O35-C34	-2.33	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	v	101	PNS	C37-C38-C39	-3.47	106.61	112.39
59	v	101	PNS	C38-C37-N36	-2.26	107.19	112.00
59	v	101	PNS	C31-C29-C32	2.11	112.36	108.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	101	PNS	O27-C28-C29-C30
59	v	101	PNS	O27-C28-C29-C31
59	v	101	PNS	O27-C28-C29-C32
59	v	101	PNS	C28-C29-C32-O33
59	v	101	PNS	C28-C29-C32-C34
59	v	101	PNS	C30-C29-C32-C34
59	v	101	PNS	C31-C29-C32-O33
59	v	101	PNS	C31-C29-C32-C34
59	v	101	PNS	N41-C42-C43-S44
59	v	101	PNS	C37-C38-C39-O40
59	v	101	PNS	C30-C29-C32-O33
59	v	101	PNS	C37-C38-C39-N41

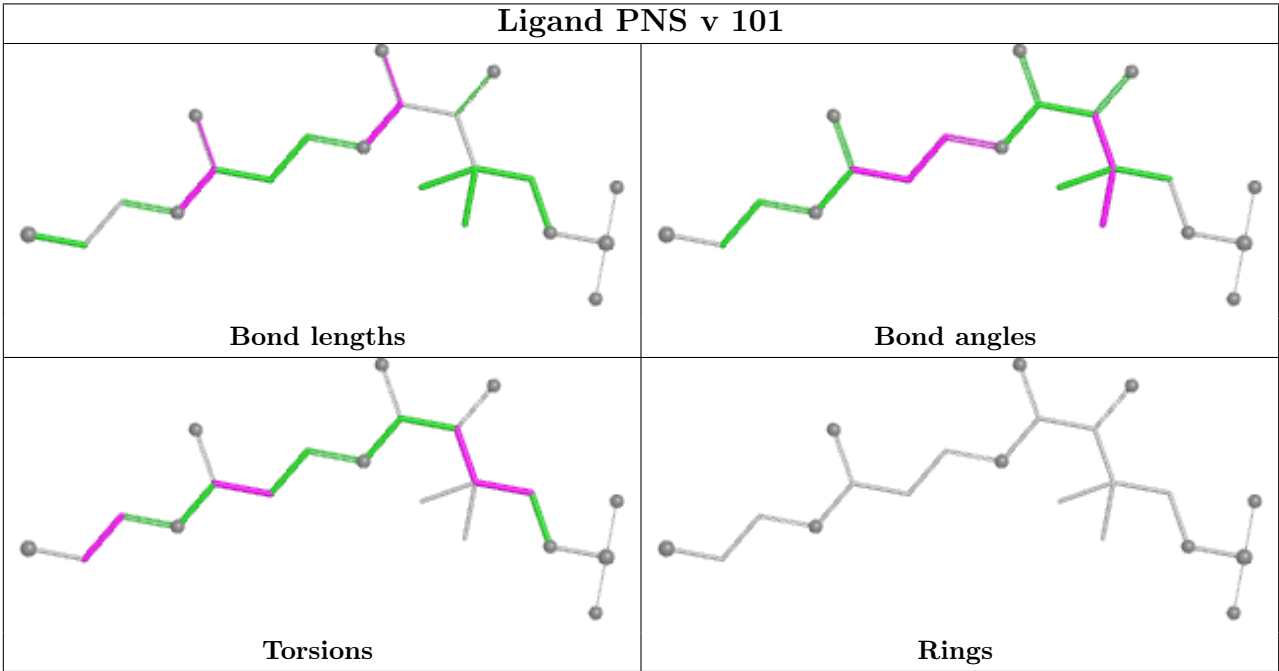
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	v	101	PNS	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
56	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	4:A	O3'	6:U	P	9.11

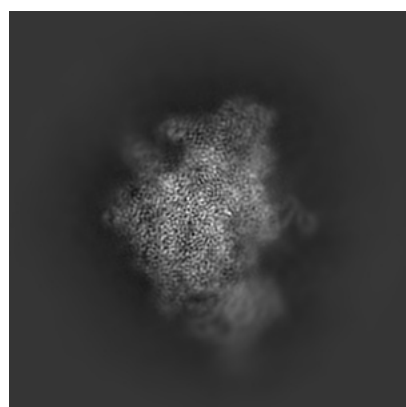
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12926. These allow visual inspection of the internal detail of the map and identification of artifacts.

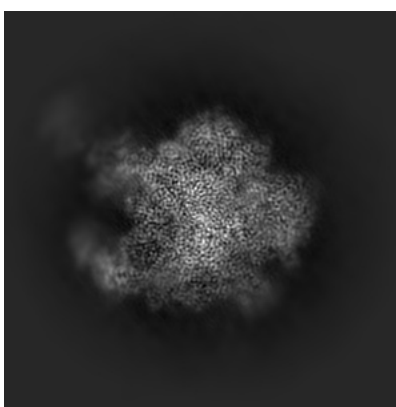
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

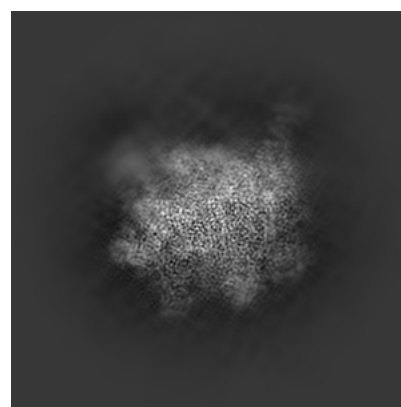
6.1.1 Primary map



X



Y

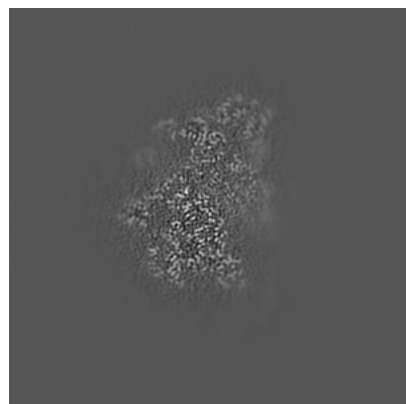


Z

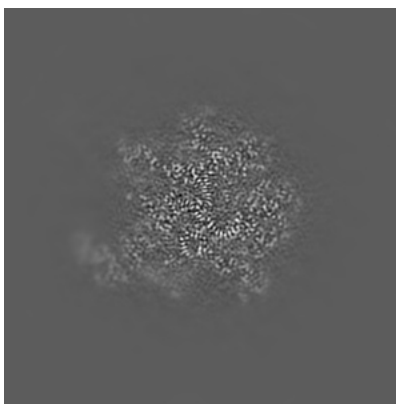
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

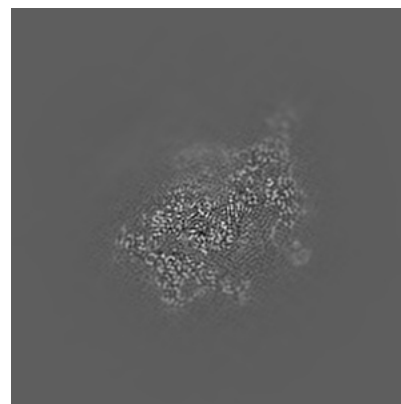
6.2.1 Primary map



X Index: 180



Y Index: 180

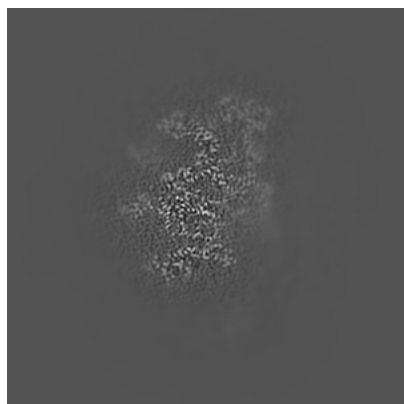


Z Index: 180

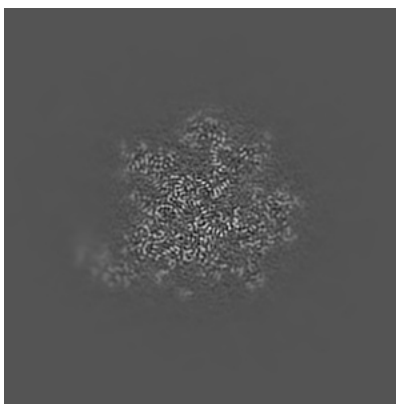
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

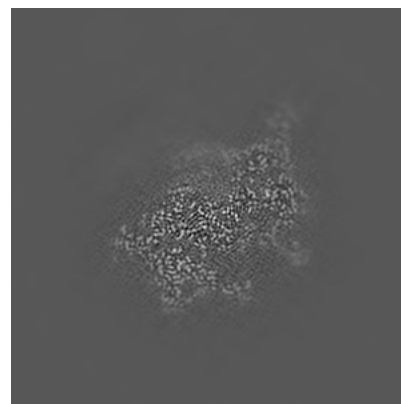
6.3.1 Primary map



X Index: 172



Y Index: 173

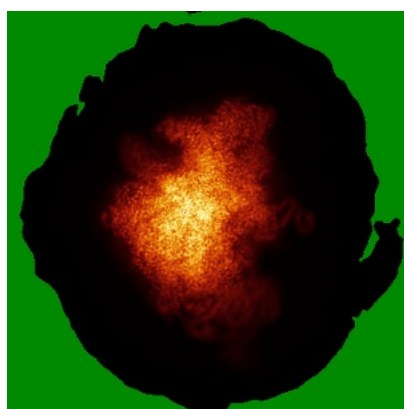


Z Index: 179

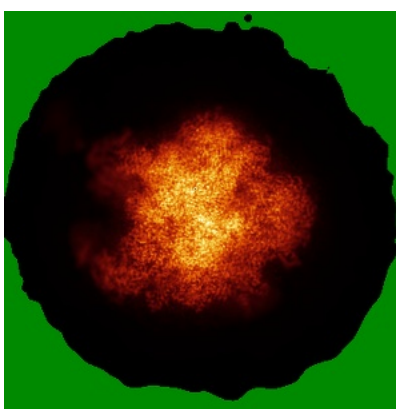
The images above show the largest variance slices of the map in three orthogonal directions.

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

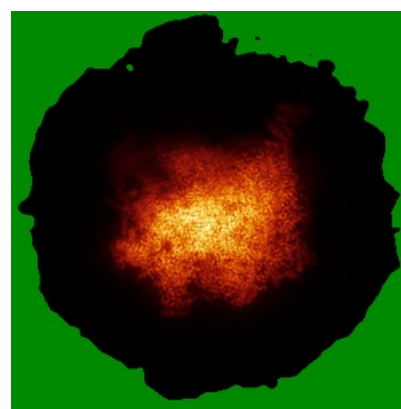
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

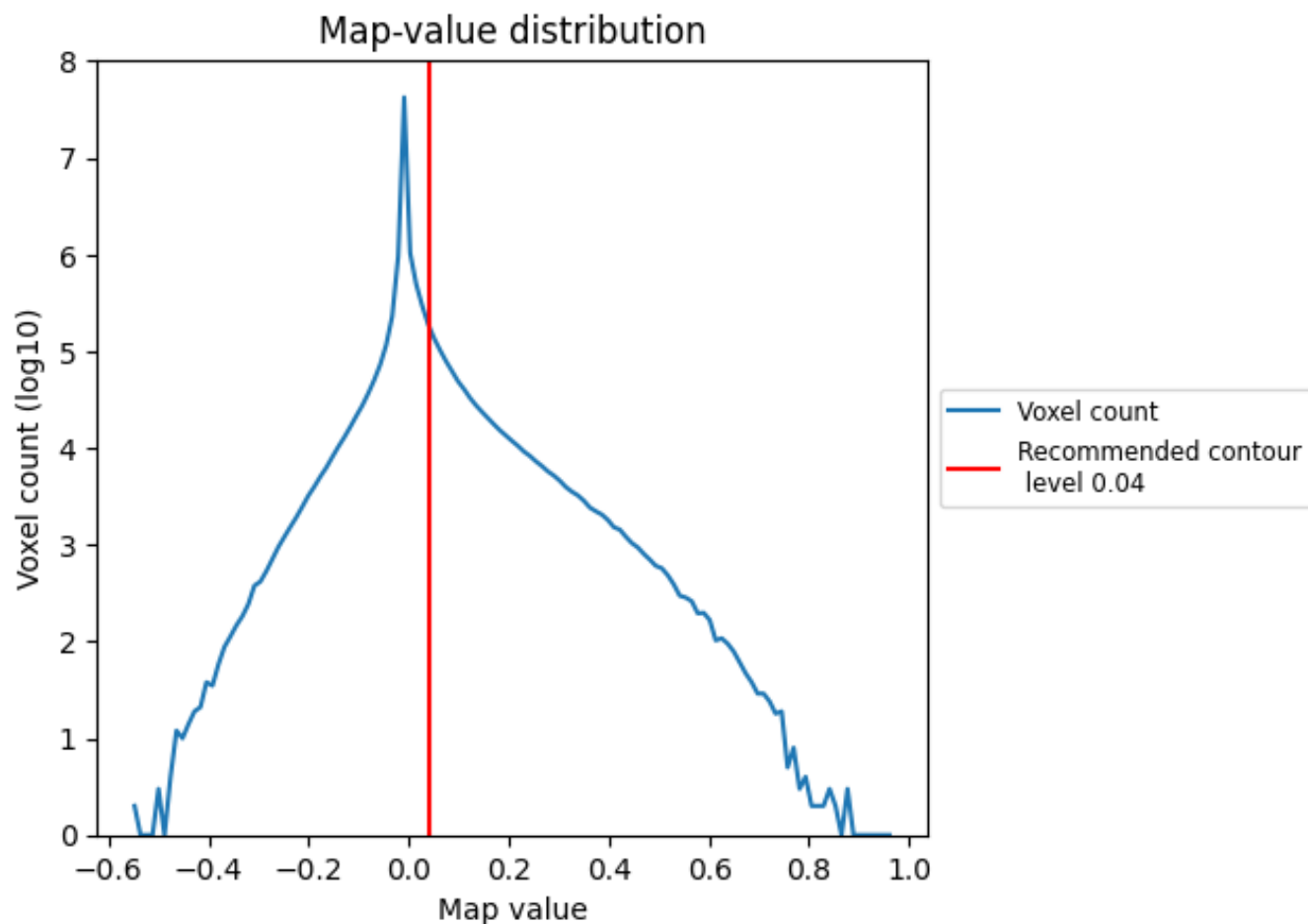
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

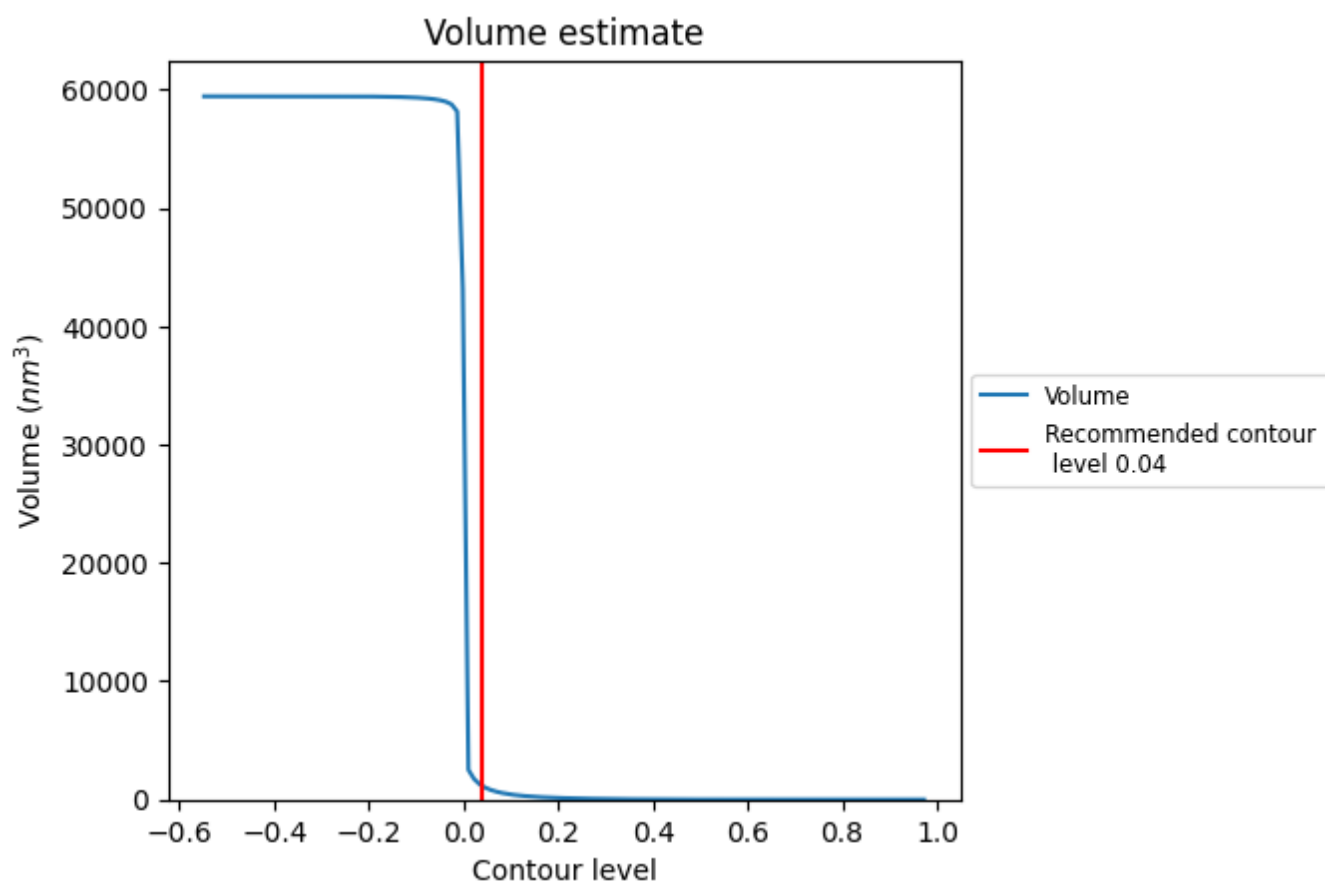
This section contains the results of statistical analysis of the map.

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.

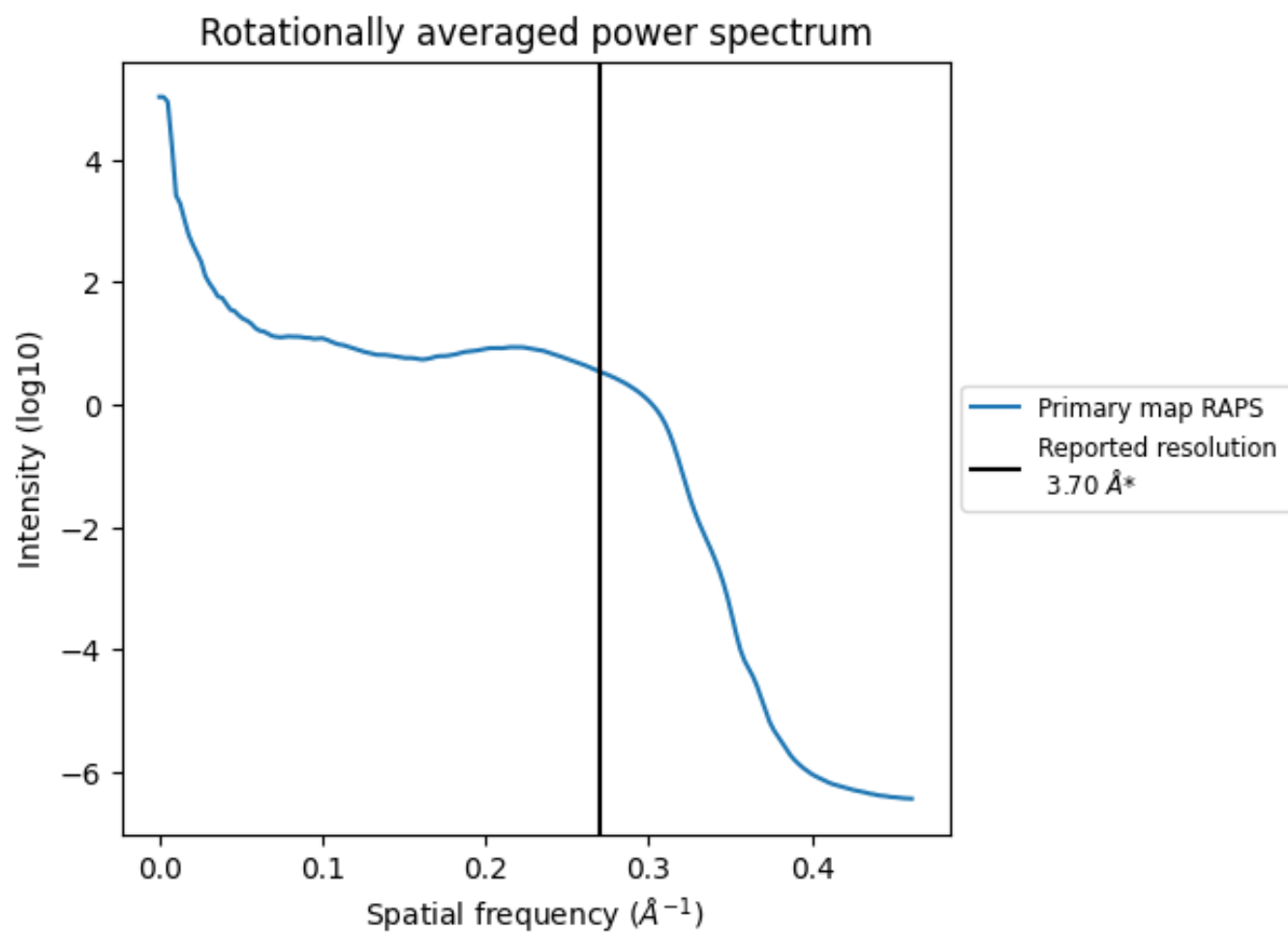
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1150 nm^3 ; this corresponds to an approximate mass of 1038 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 ⓘ

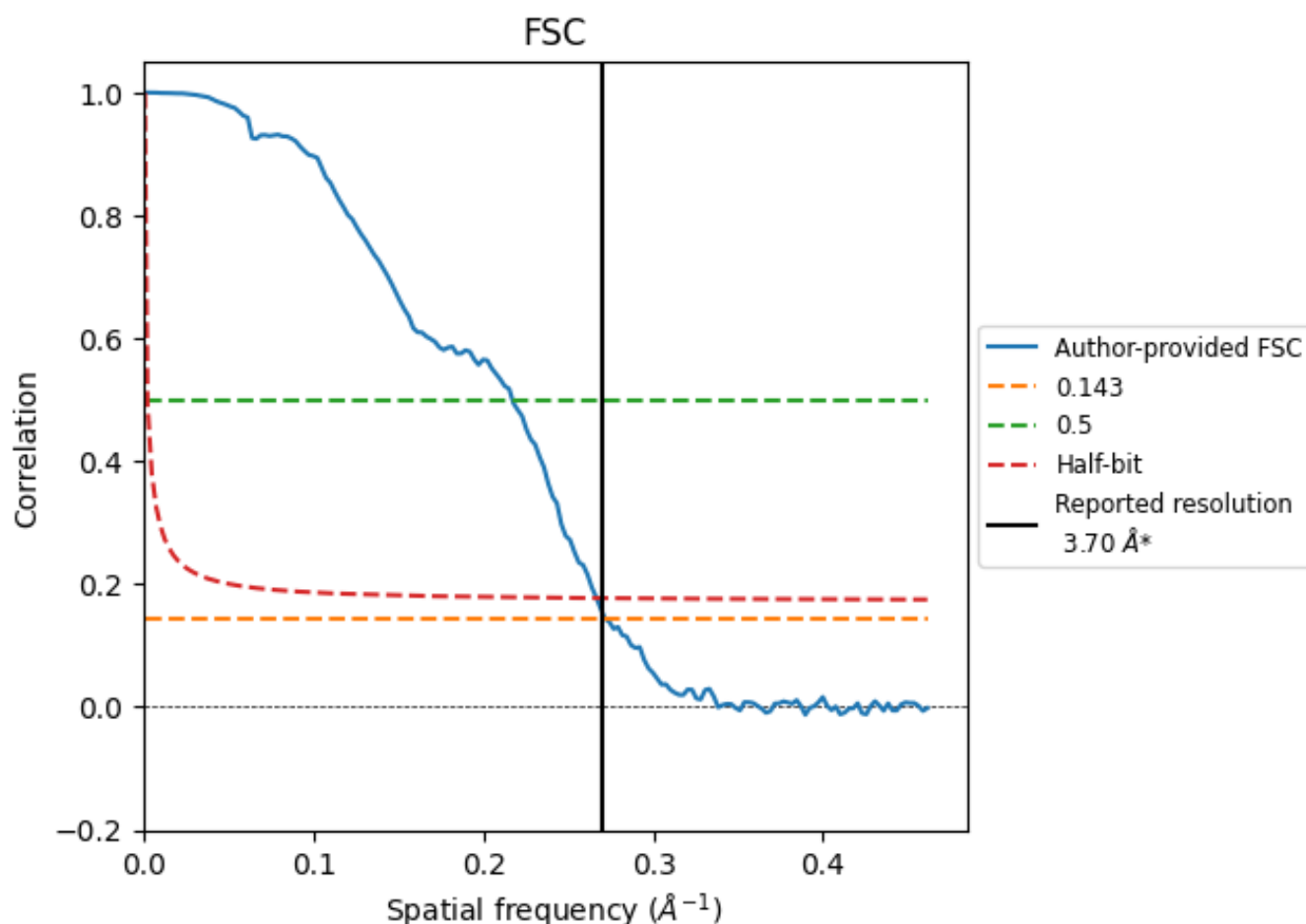


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

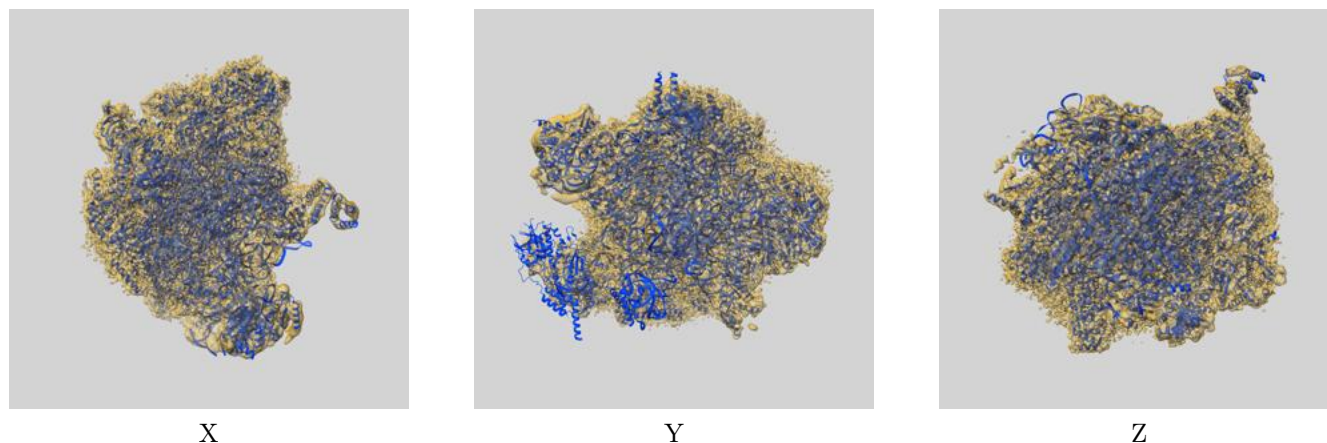
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.60	3.75
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

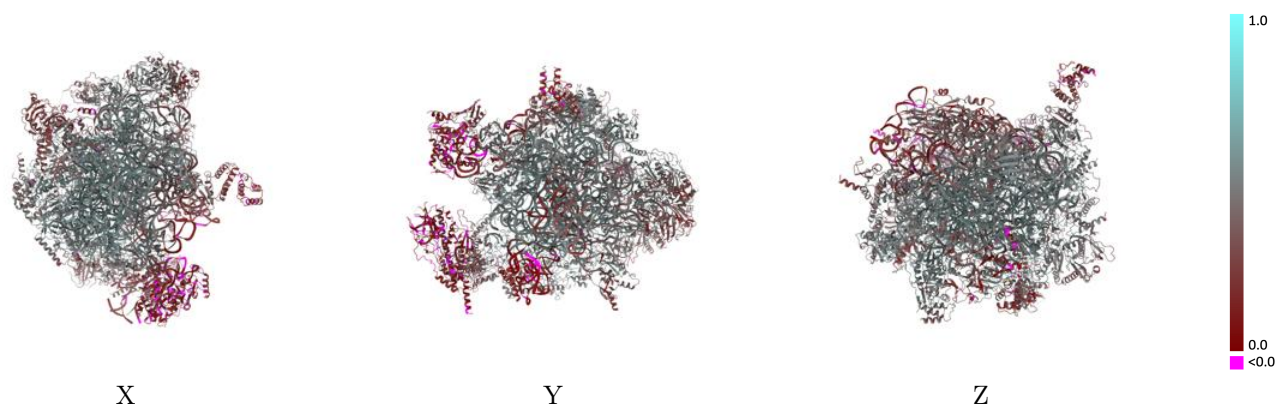
This section contains information regarding the fit between EMDB map EMD-12926 and PDB model 7OID. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



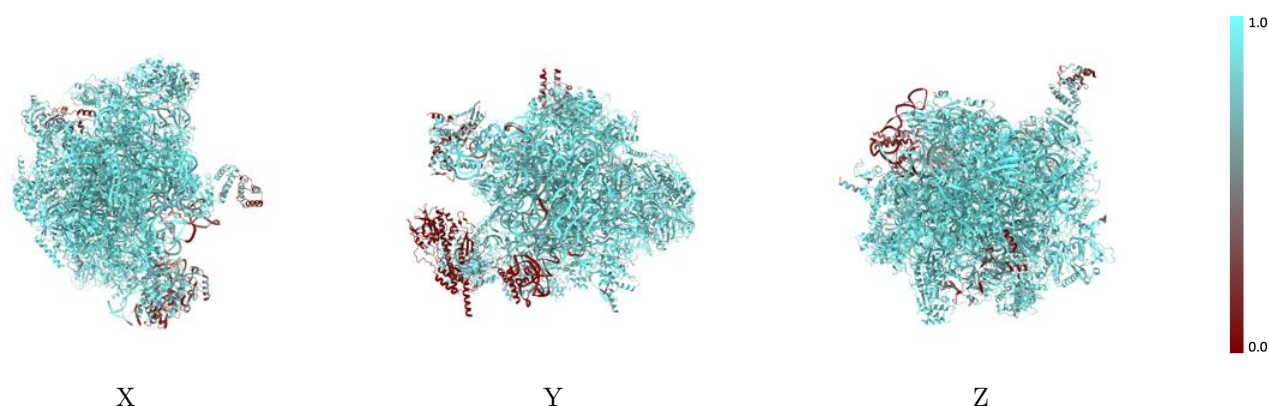
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



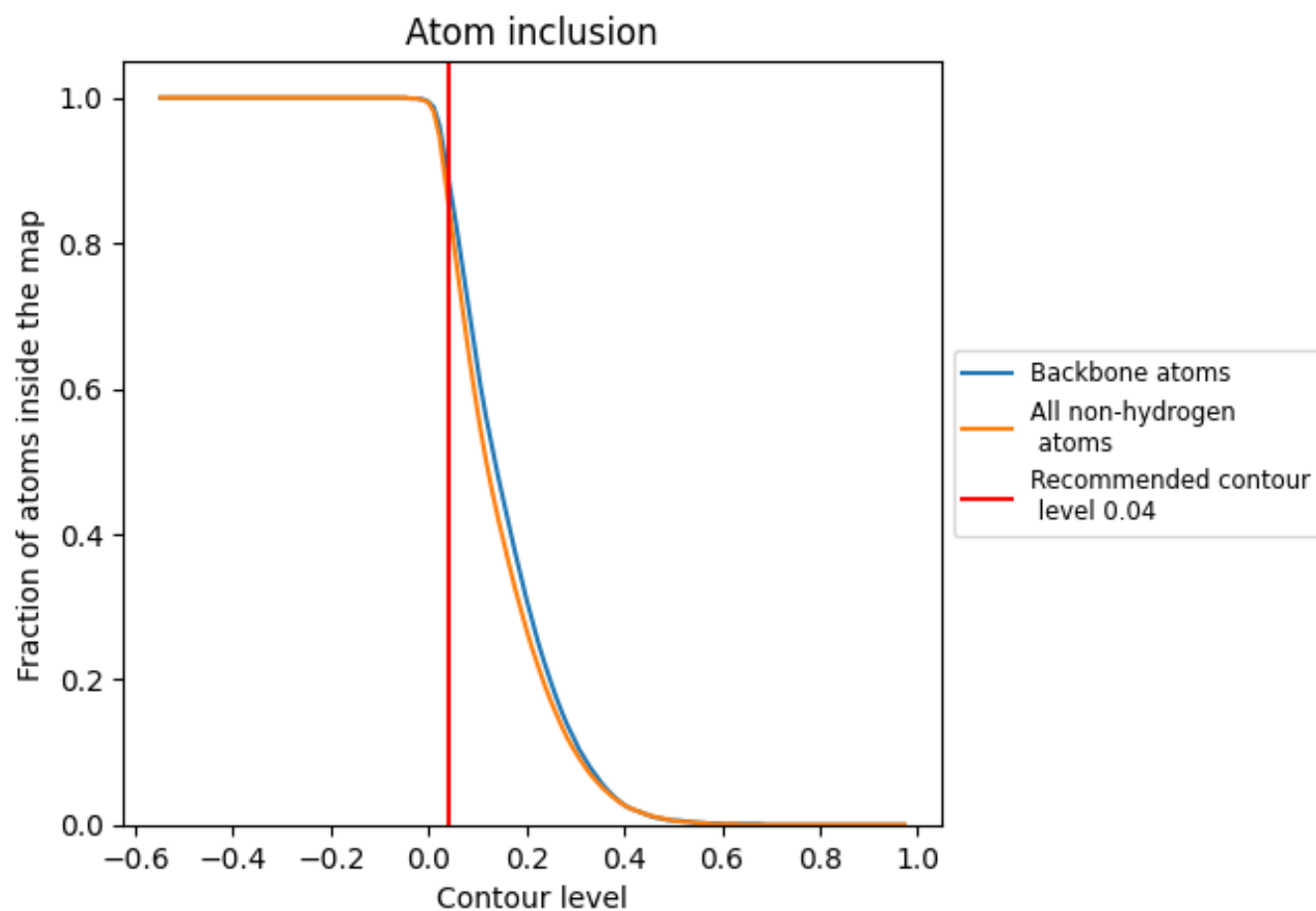
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.4290
0	 0.9320	 0.4950
1	 0.7860	 0.2170
2	 0.9700	 0.5770
3	 0.9700	 0.5670
4	 0.9740	 0.5030
5	 0.8270	 0.3580
6	 0.8840	 0.3890
7	 0.9010	 0.4220
8	 0.1400	 0.1470
9	 0.9150	 0.4500
A	 0.9440	 0.4660
B	 0.8380	 0.2300
D	 0.8710	 0.4200
E	 0.9490	 0.5060
F	 0.9560	 0.5370
H	 0.8640	 0.4200
I	 0.6800	 0.2380
J	 0.4590	 0.1140
K	 0.9500	 0.5270
L	 0.9290	 0.4890
M	 0.9610	 0.5340
N	 0.9520	 0.5040
O	 0.9420	 0.5090
P	 0.9100	 0.4240
Q	 0.9300	 0.4840
R	 0.9070	 0.5130
S	 0.9280	 0.5110
T	 0.9610	 0.5320
U	 0.8690	 0.4510
V	 0.5660	 0.2700
W	 0.9450	 0.5280
X	 0.9310	 0.4790
Y	 0.9260	 0.4760
Z	 0.9220	 0.5110



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Chain	Atom inclusion	Q-score
a	 0.9630	 0.5170
b	 0.9570	 0.5210
c	 0.9350	 0.4800
d	 0.7050	 0.2860
e	 0.0180	 0.1000
f	 0.2500	 0.2060
g	 0.9550	 0.5170
h	 0.8970	 0.4000
i	 0.9540	 0.5560
j	 0.9360	 0.4850
k	 0.7680	 0.2300
l	 0.7960	 0.1800
m	 0.0030	 0.0760
o	 0.9540	 0.5370
p	 0.9090	 0.4520
q	 0.6280	 0.3440
r	 0.9280	 0.4850
s	 0.9260	 0.4710
u	 0.8720	 0.3690
v	 0.7090	 0.2550
w	 0.3600	 0.1620
z	 0.1260	 0.0760